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Title: MCNP6 Class

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MCNP6 Class

Alabama Agricultural and Mechanical University

March 3 – 7, 2014

Presented by

H. Grady Hughes and Michael R. James

Los Alamos National Laboratory

Schedule

- **Monday**
  - Introduction
  - Basics
- **Tuesday**
  - Basic Tallies
  - Sources
- **Wednesday**
  - Photon & Electron Transport Physics
  - Advanced Tallies
- **Thursday**
  - Extended Electron/Photon Transport
  - Specific F8 Tally Functions
- **Friday**
  - Other topics (MPI, Variance Reduction, Compiling…)
  - 1 on 1

MCNP6

mcnp5, mcnpx, mcnp6

Monte Carlo Codes

XCP-3 & NEN-5

Los Alamos National Laboratory

MCNP Overview

Monte Carlo method for simulating radiation transport,

1940s - Von Neumann, Ulam, Fermi, Metropolis, Richtmyer

Common sense approach – simulate reality

– **Geometry:**

Ray-tracing through "exact" model of problem geometry to determine location of interactions

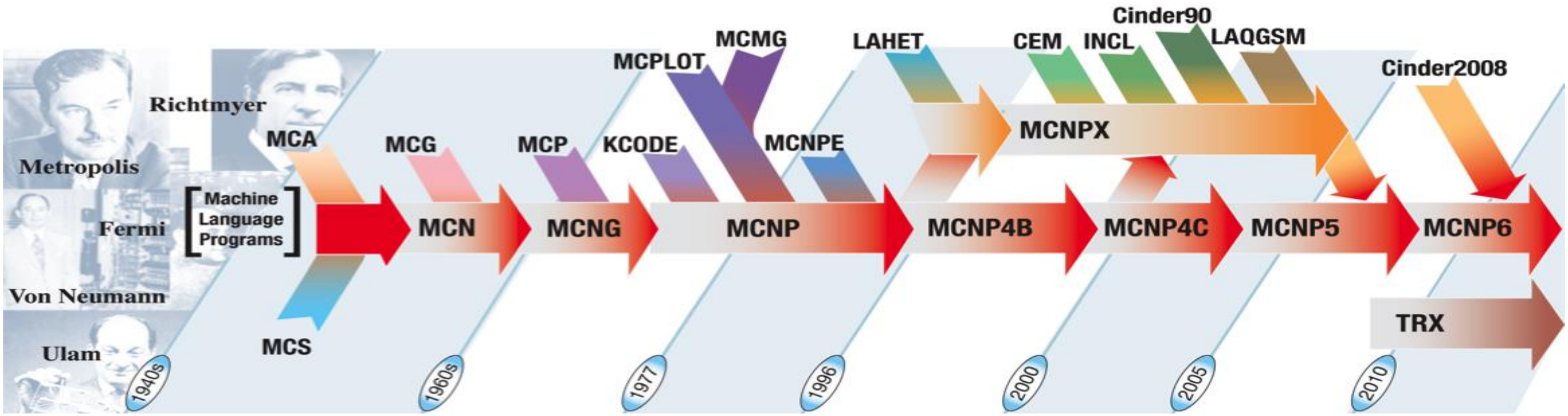
– **Physics:**

Cross-section data & physics models used as probabilities for interactions, **random sampling**

– **Tallies:**

Bookkeeping, to record how often certain events occur during the simulation.

MCNP5, MCNPX, MCNP6



- **Monte Carlo transport of particles**
  - **MCNP5 - neutrons, photons, electrons**
  - **MCNPX - neutrons, photons, electrons + more particles & ions**
  - **MCNP6 - merged code + more**

- **MCNP6 release package distributed by RSICC**

  MCNP6.1 + MCNP5-1.60 + MCNPX-2.70

  + Nuclear Data Libraries + MCNP Reference Collection

Support from DOE/NNSA, DoD,
DRTA, DHS/DNDO, NASA, & others

MCNP6

mcnp5
neutrons, photons, electrons
cross-section library physics
criticality features
shielding, dose
"low energy" physics
V&V history
documentation

mcnp6

mcnp6
protons, proton radiography
high energy physics models
magnetic fields

Partisn mesh geometry
Abaqus unstructured mesh

mcnpx
33 other particle types
heavy ions
CINDER depletion/burnup
delayed particles

High energy physics models
CEM, LAQGSM, LAHET
MARS, HETC

Sensitivity/Uncertainty Analysis
Fission Matrix
OTF Doppler Broadening

Continuous Testing System
~10,000 test problems / day

mcnp5 – 100 K lines of code
mcnp6 – 400 K lines of code

Particle Types in MCNP6:

neutrons

photons

electrons/positrons

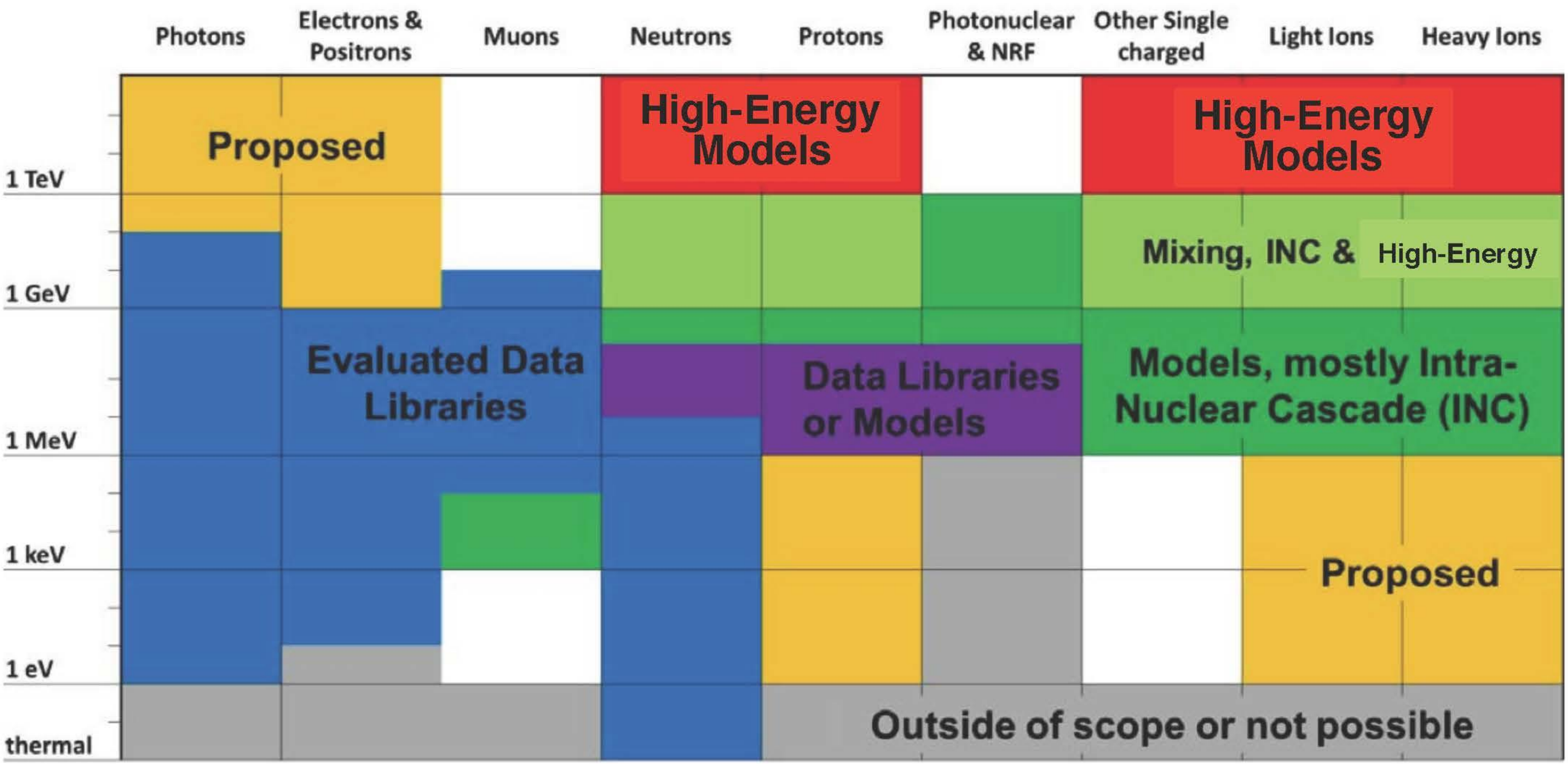
29 other fundamental particles: protons, muons, pions, sigmas, etc.

4 light ions: deuterons, tritons, helions, alphas

arbitrary heavy ions

MCNP Physics

- MCNP is physics rich – try to use best data, models, & theory



"Proposed" – future models or data libraries

What Can MCNP Do?

mcnp

Detailed models of geometry & physics

- General 3D combinatorial geometry
- Repeated structures
- Lattice geometries
- Geometry, cross section, tally plotting
- ENDF/B-VII physics interaction data

Calculate nearly any physical quantity

- Flux & current
- Energy & charge deposition
- Heating & reaction rates
- Response functions
- Detector response (pulse-height tallies)
- Mesh tallies & radiography images
- K-effective, beta-eff, lambda-eff
- Fission distributions

Unique features for criticality calc's

- Shannon entropy of the fission source for assessing convergence
- Dominance ratio, k_1 / k_0
- Stochastic geometry
- Isotopic changes with burnup

> 10,000 users around the world

- Fission and fusion reactor design
- Nuclear criticality safety
- Radiation shielding
- Waste storage/disposal
- Detector design and analysis
- Nuclear well logging
- Health physics & dosimetry
- Medical physics and radiotherapy
- Transmutation, activation, & burnup
- Aerospace applications
- Decontamination & decommissioning
- Nuclear safeguards

Portable to many computer systems

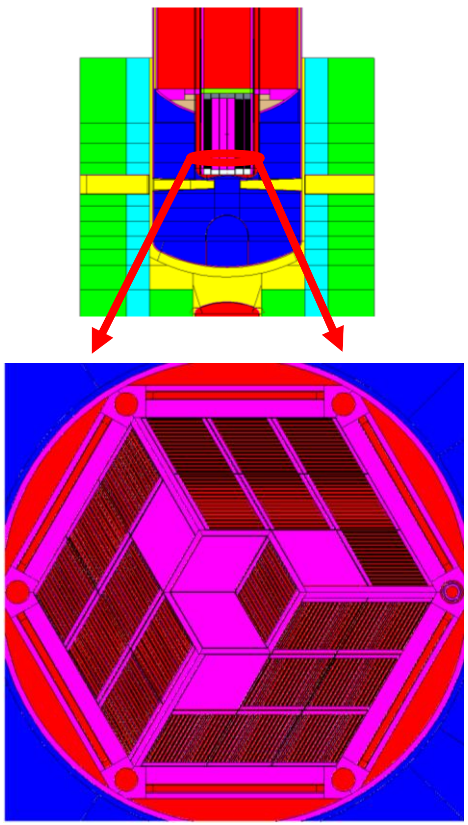
- Windows, Linux, Mac, Unix
- Multicore, clusters, netbooks, ASC, …
- Parallel, scalable - MPI + threads
- Built-in plotting

Support

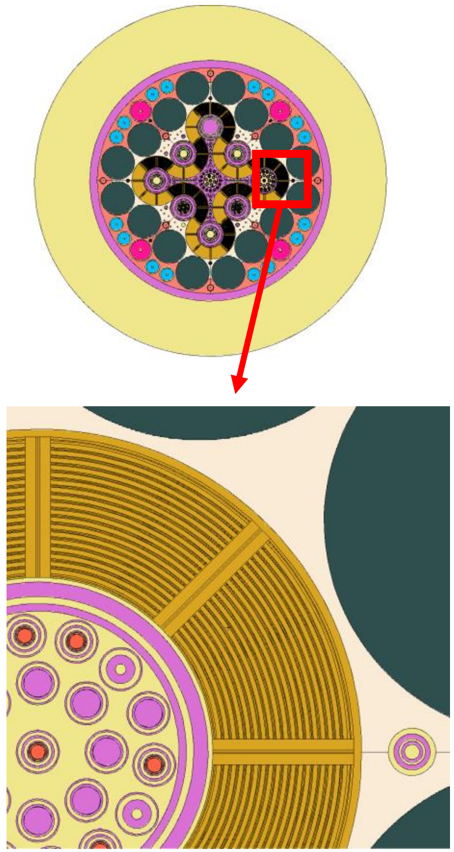
- Extensive V&V against experiments
- Web site, user groups, email forum
- Classes - 1 week, about 6 per year

Nuclear Reactors

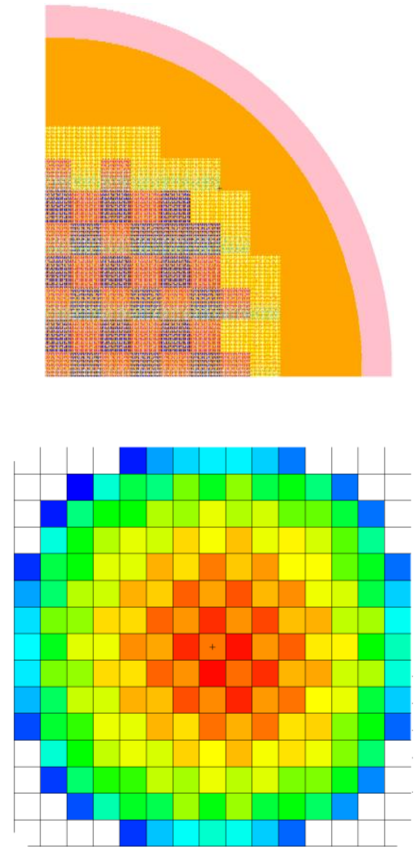
MIT
Research Reactor



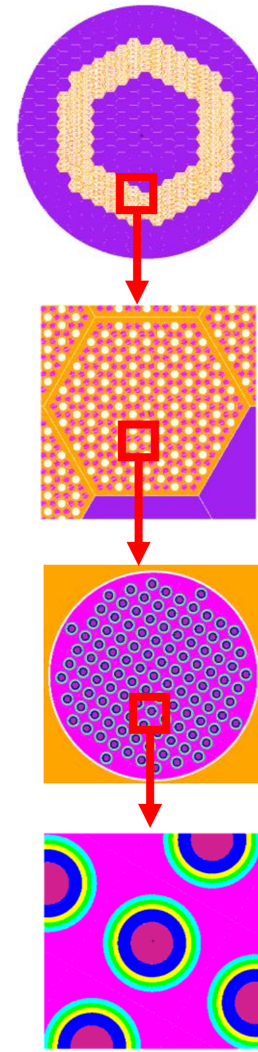
ATR
Advanced Test Reactor



PWR
Pressurized Water Reactor



VHTR
Very High Temperature Gas-Cooled Reactor

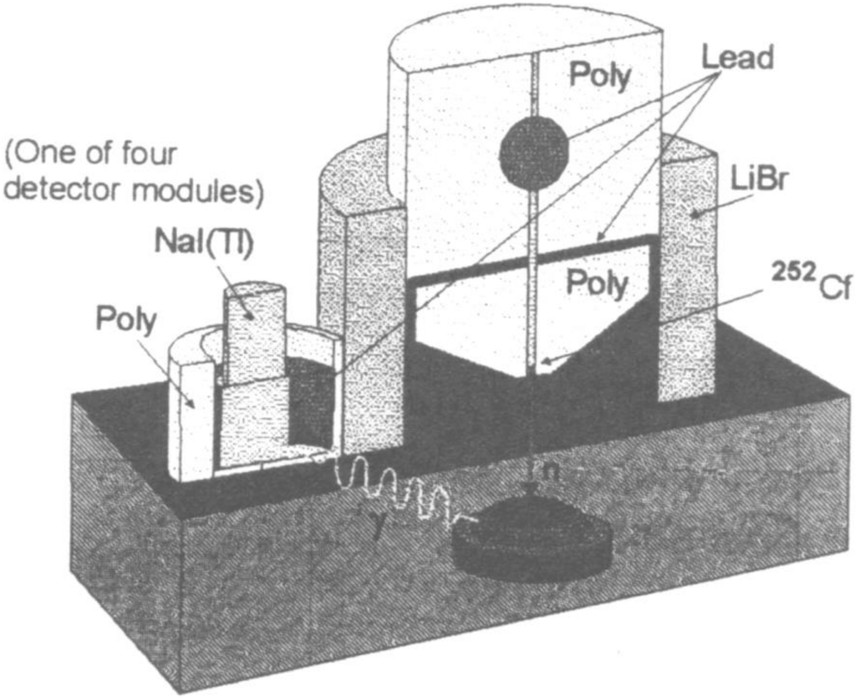


- **Accurate & explicit modeling at multiple levels**
- **Accurate continuous-energy physics & data**

• CDND designed a **landmine detector system**

• Needed to shield personnel and detector from 100 MBq ^{252}Cf source

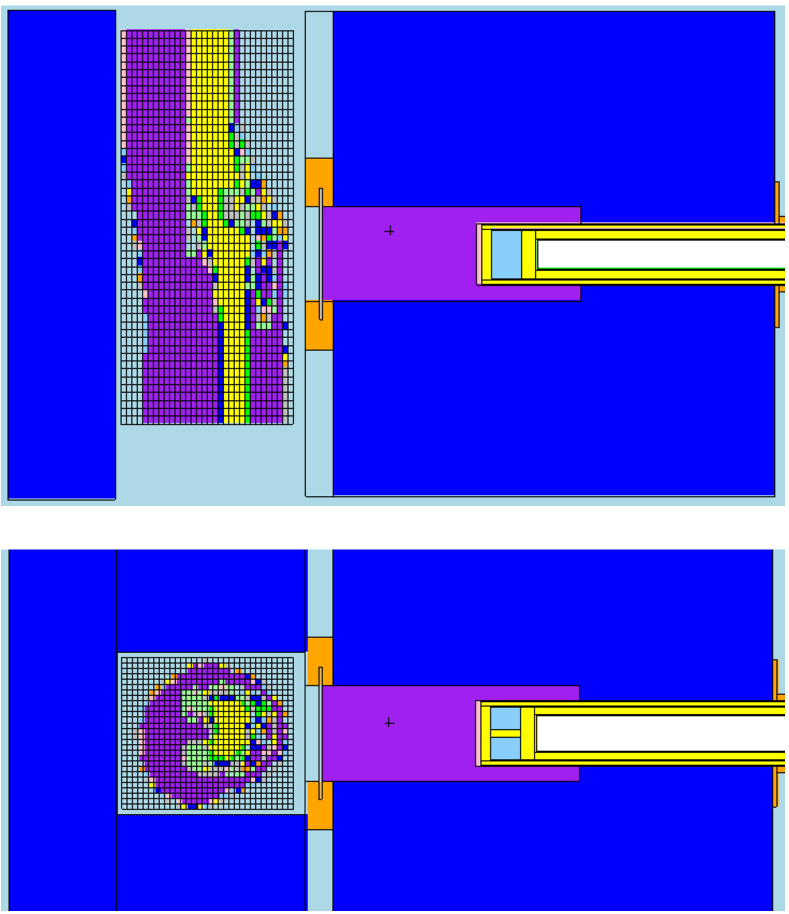
• Used MCNP to vary shielding materials and dimensions



T. Cousins, T.A. Jones, et. Al. “The development of a thermal neutron activation (TNA) system as a confirmatory non-metallic land mine detector” J. Rad. Nucl. Chem. **235** (1998) 53-58.

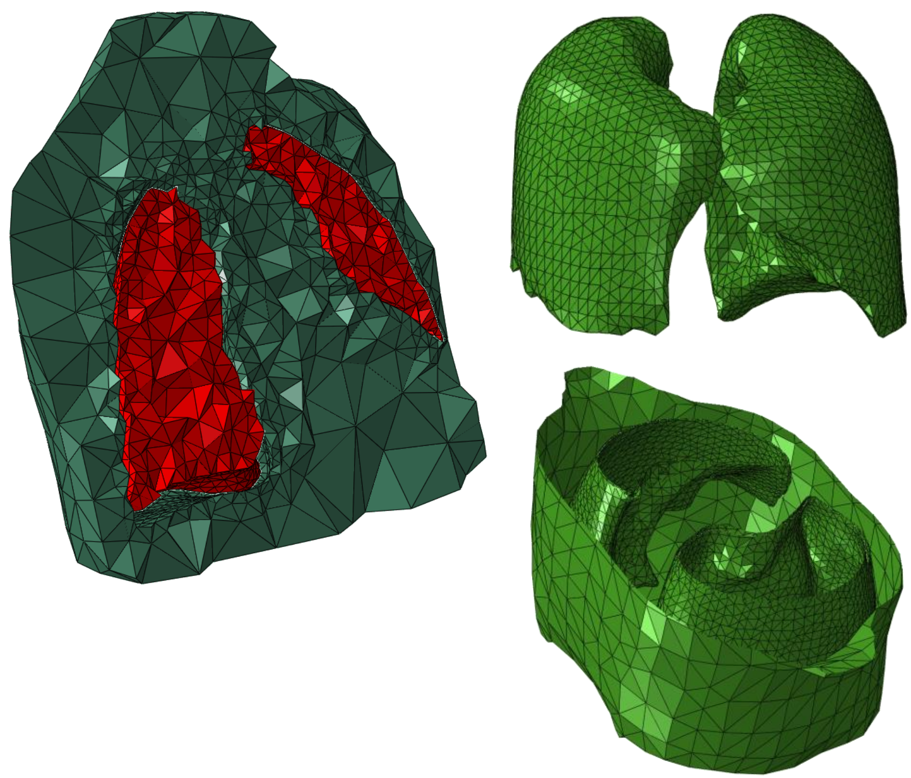
Medical Physics

- Patient-CT based model of **knee & end of accelerator**
- **Calculate dose throughout knee**



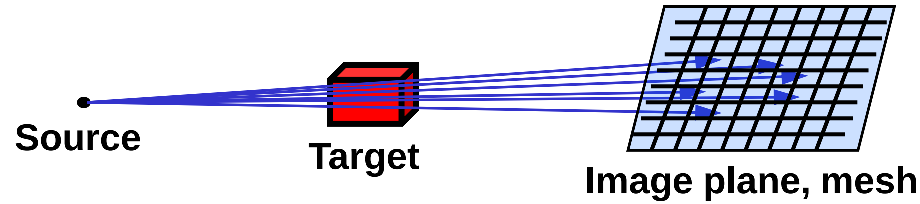
Pictures from mcnp plotter

- **MCNP6**
  - 3D unstructured mesh
  - Embedded in 3D MCNP geometry
  - Many applications
    - Radiation treatment planning
    - Linkage to Abaqus



Radiography Calculations

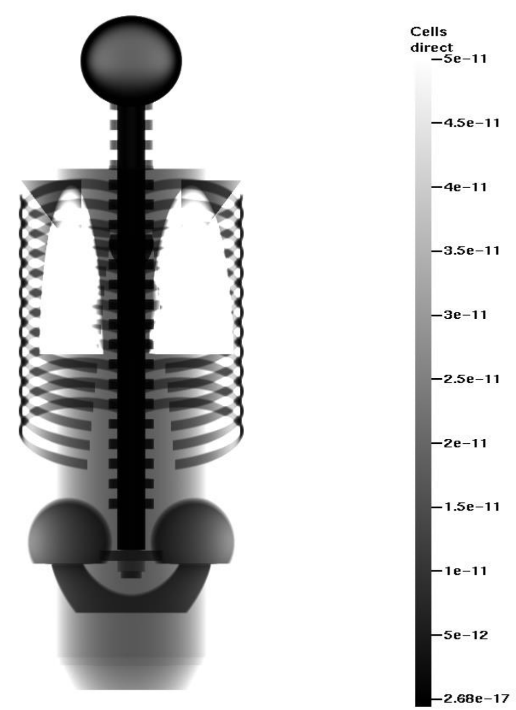
- Radiography tallies



- Neutron and photon radiography uses a grid of point detectors (pixels)
- Each source and collision event contributes to all pixels

MCNP Model of Human Torso

Simulated Radiograph - 1 M pixels



MCNP Distribution

- **Latest release from RSICC - codes, data, manuals (1 package)**
  - **MCNP5 - 1.60: Sept 2010**
  - **MCNPX - 2.7.0: May 2011**
  - **ENDF/B-VII.0 + older data libraries**
  - **MCNP6-Beta-2: Feb 2012**
  - **MCNP6-Beta-3: Jan 2013**
  - **MCNP6.1: June 2013**
- **Code distribution center:**
  - **Radiation Safety Information Computational Center, Oak Ridge, TN**

    www-rsicc.ornl.gov
- **Help:**
  - Read the manual.
  - User forum: **mcnp-forum@lanl.gov**
  - MCNP(X) home pages: **mcnp.lanl.gov** **mcnpx.lanl.gov**
  - RSICC e-notebook: **www-rsicc.ornl.gov/enote.html**
  - XCP-3 staff (limited): **mcnp6@lanl.gov**
  - NEN-5 staff (limited): **mcnpx@lanl.gov**

MCNP Development Team

Monte Carlo Development, XCP-3 & NEN-5

Forrest Brown	Jeffrey Bull	Larry Cox
Joe Durkee	Michael Fensin	Art Forster
Tim Goorley	Grady Hughes	Michael James
Russell Johns	Brian Kiedrowski	Roger Martz
Stepan Mashnik	Gregg McKinney	Richard Prael
Jeremy Sweezy	Tony Zukaitis	Jay Elson
Trevor Wilcox		

Data Team, XCP-5	Kent Parsons Jeremy Conlin	Morgan White Beth Lee
University R&D	William Martin	Anil Prinja

MCNP - Basic Concepts (1)

- **For the Monte Carlo simulation of 1 particle:**

  - Select the position, direction, & energy of a **source** particle, based on user specifications & possibly random sampling

  - Alternate between:
    - **Ray tracing** through the geometry, until a collision point is reached
    - **Collision physics** analysis, using random sampling from probability densities based on cross-section data

  - During the simulation, **tally** events of interest, such as flux in a cell, etc.
  - The simulation ends when the particle is killed by absorption or leakage

- **Repeat the above steps for all of the particles.**

- **When finished, compute the overall average results & statistics.**

MCNP - Basic Concepts (2)

- **Regions in space are called cells**. Cells may be infinite in extent.
- **All of space must be partitioned into cells, with no gaps or overlaps.** Adjacent cells must share one or more common boundary surfaces.
- **Surfaces are 1st or 2nd order analytic surfaces**, possibly infinite in extent. Surfaces divide space into 2 half-spaces, one "inside" (-) and one "outside" (+).
- **Cells are defined by intersections & unions of half-spaces** -- a list of signed surface numbers, possibly including parentheses & operators for intersection or union.
- **A collection of cells is called a universe**. A universe may be embedded inside a container cell, to produce a hierarchical geometry.
- **Properties are assigned to each cell**: material, density, temperature, universe number, ...
- **Each cell is assigned an importance**: 1 = normal transport, 0 = no transport, other = used for variance reduction
- **A material is a combination of elements (or isotopes).** The fraction by mass or by atoms is specified for each component.
- **Tallies accumulate results for flux, current, reaction rates, etc.** Tallies can be defined for cells or surfaces, for particular reactions and ranges of energy, angle, time, or other selectors.

Next:

Into the details

MCNP Basics

Basic Geometry
Cell Cards
Surface Cards
Data Cards
Execution-Line Options

MCNP Input File (1)

mcnp

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

- **Card names <u>begin in first 5 columns</u>**
- **80 columns or fewer**
- **Free field format**
- **Not case sensitive: UC, lc, MiXeD**
- **Continuation: 5 blanks or &**
- **Comment cards begin with "c "**
- **In-line comments begin with $**
- **Use spaces or <u>tabs</u>** (with mcnp5 & mcnp6)
- **For most numbers, these are the same:**

  1 1. 1.0 1e0 1e+00 1.0e+0
- **Units**

Length:	cm
Mass:	g
Energy & Temp.:	MeV
Number density:	atoms/barn-cm
Time:	shakes

(1 barn = 10^{-24} cm^2, 1 sh = 10^{-8} sec)

MCNP Input File (2)

```
Godiva critical - using ksrc & surfaces      $ Title
c   CELL CARDS                               $ Comment
10   100     -18.74      -1                  $ Cells
20    0                   1
                                             $ Blank
c   SURFACE CARDS
1  so    8.741                               $ Surfaces
                                             $ Blank
c   DATA CARDS
kcode    1000    1.0    10    50
ksrc   0.0   0.0   0.0
imp:n   1    0
m100    92235   -94.73                       $ Materials
        92238   -5.27
```

Indent 5 or more spaces
for continuation

MCNP Cells (1)

- **Cells are the basic geometry unit**
  - **Volume of space bounded by surfaces**
  - **Cartesian coordinate system**
  - **Volumes calculated for some simple cells, not for complicated ones**
- **Cells are used for:**
  - **constructing the model**
  - **specifying the materials**
  - **variance reduction methods**
  - **performing tallies**

- **All of space must be defined**
  - **Every xyz point will lie either on a surface or within a uniquely defined cell.**
  - **No gaps or overlaps for cells**
  - **At least one cell will describe the problem exterior (outside world)**
- **Repeated structure and lattice ability**
  - **Cells may contain embedded geometry - lattice or repeated structure**
- **Can take the complement of a cell**

  #100 ➜ all space **not** in cell 100

MCNP Cells (2)

Cell #	Mat #	Density	Surface List	Cell Data
30	300	0.100282	1 -2 3 -4 5 -6	

Positive Density ➜ atoms/barn-cm

Cell #	Mat #	Density	Surface List	Cell Data
10	300	-1.0	1 -2 3 -4 5 -6	imp:e=1.0

Negative Density ➜ g/cm^3

Cell #	Mat #	Density	Surface List	Cell Data
20	0		-7:8: -9	

Void ➜ Material # = 0, omit Density

Material Cards (1)

Mn ZAID$_1$ fraction$_1$ ZAID$_2$ fraction$_2$ …..

n = material number

ZAID = element or nuclide identifier: ZZZAAA

ZZZ = atomic number

AAA = atomic mass or "000"

fraction: positive = atom fraction of ZAID

negative = mass fraction of ZAID

- **MCNP normalizes the fractions for a material to sum up to 1.0**
- **Material cards know nothing of density. That comes from the <u>cell cards.</u>**
- **We will return to the "ID" part of ZAID later.**

Example for a photon/electron problem:

m200 48000 .9 30000 .1 52000 1 $ a typical CZT.

For neutrons:

m100 92238 1 8016 2 6000 .03 $ ^{238}U, ^{16}O, and natural C.

Material Cards (2)

- **Cell & material cards should be consistent**
  - The overall material density (g/cc or atoms/barn-cm) comes from the **cell card** where a material is used
  - **Fractions or number densities on a material card are normalized to sum to 1.0**

- **Examples - cell cards & corresponding material cards**

```
10   100    -1.0     1 -2 . . .            $ cell:   mat 100,  1 g/cc
. . .
m100   1000   2       8000        1        $ mat:    H2O, using atom fractions
```

```
10   100    .100282     1 -2 . . .         $ cell:   mat 100, ≈0.1 atom/barn-cm
. . .
m100   1000   2       8000        1        $ mat:    H2O
```

```
10   100   .100282     1 -2 . . .        $ cell:  mat 100, ≈0.1 atom/barn-cm
. . .
m100   1000 -.111902   8000 -.888098    $ mat card: H2O, using mass fractions
```

Importance Cards

- Each cell must have an "importance" for each type of particle
  - imp:p for photons, imp:e for electrons, imp:n for neutrons, ... etc.
- imp:p = 1
  - Track particle in the cell in the normal manner
- imp:p = 0
  - Kill particles that enter the cell
  - "Outside world" cell(s) usually 0
- imp:p = any other value
  - Invokes splitting &/or Russian roulette
  - Used for variance reduction
- Importances can be after the surfaces on all cell cards …

```
20   0           -7:8:-9   imp:p,e=1
30   100   -1.0   1 2 3    imp:p,e=1
50   0            35       imp:p,e=0
```

… or in the data card block (1 entry for each cell):

```
imp:p   1   1   0        $  three cells in this problem,
imp:e   1   1   0        $  namely 20, 30, and 50 in that order.
```

MCNP Surfaces (1)

- **Surfaces are used to define space**
- **Sign defines surface "sense"**

  +3 ➜ half-space on + side of surface 3

  -5 ➜ half-space on - side of surface 5

- **Boolean operators & parentheses**
  - **intersection** space
  - **union** :
  - **grouping** ( )
- **Cells are defined by intersections & unions of half-spaces**
  - **List of signed surfaces, spaces, colons, parentheses**
  - **Cell can also be defined as complement of another cell, using #cell**

- **1st, 2nd, 4th order equations (26):**
  - planes
  - spheres, cylinders, cones
  - ellipsoid, hyperboloid, paraboloid
  - torus (elliptical or circular)
- **Macrobodies**
  - Primitive bodies - box, finite cylinder, hex, wedge, …
  - MCNP internally translates to collections of surfaces
- **Can also specify surface by giving a few points (see manual)**
- **Special boundary surface types**
  - reflecting (mirror) *10
  - white (isotropic) +10
  - Periodic see manual
- **Some surface areas calculated**

MCNP Surfaces (2)

Surface #	Name	Data
10	px	5.0
	plane normal to x-axis, $x - D = 0$ data = D	
50	so	11.1
	sphere at origin, $x^2 + y^2 + z^2 - R^2 = 0$ data = R	
60	cz	2.54
	cylinder around Z-axis, $x^2 + y^2 - R^2 = 0$ data = R	
30	rcc	-6.0 0.0 0.0 12.0 0.0 0.0 4.0

right circular cylinder:
- center of base at (-6.0, 0, 0)
- 12.0–cm high can about x-axis
- radius 4.0

MCNP Surfaces (3)

Table 3.1: MCNP Surface Cards

Mnemonic	Type	Description	Equation	Card Entries
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

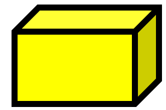
MCNP Surfaces (4)

K/X	Cone	Parallel to X-axis	$\sqrt{(y-\bar{y})^2+(z-\bar{z})^2}-t(x-\bar{x}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2\ \pm 1$
K/Y		Parallel to Y-axis	$\sqrt{(x-\bar{x})^2+(z-\bar{z})^2}-t(y-\bar{y}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2\ \pm 1$
K/Z		Parallel to Z-axis	$\sqrt{(x-\bar{x})^2+(y-\bar{y})^2}-t(z-\bar{z}) = 0$	$\bar{x}\ \bar{y}\ \bar{z}\ t^2\ \pm 1$
KX		On X-axis	$\sqrt{y^2+z^2}-t(x-\bar{x}) = 0$	$\bar{x}\ t^2\ \pm 1$
KY		On Y-axis	$\sqrt{x^2+z^2}-t(y-\bar{y}) = 0$	$\bar{y}\ t^2\ \pm 1$
KZ		On Z-axis	$\sqrt{x^2+y^2}-t(z-\bar{z}) = 0$	$\bar{z}\ t^2\ \pm 1$ ± 1 used only for 1 sheet cone
SQ	Ellipsoid Hyperboloid Paraboloid	Axis parallel to X-, Y-, or Z-axis	$A(x-\bar{x})^2+B(y-\bar{y})^2+C(z-\bar{z})^2$ $+2D(x-\bar{x})+2E(y-\bar{y})$ $+2F(z-\bar{z})+G = 0$	A B C D E F G $\bar{x}\ \bar{y}\ \bar{z}$
GQ	Cylinder Cone Ellipsoid Hyperboloid Paraboloid	Axes not parallel to X-, Y-, or Z-axis	$Ax^2+By^2+Cz^2+Dxy+Eyz$ $+Fzx+Gx+Hy+Jz+K = 0$	A B C D E F G H J K
TX	Elliptical or circular torus. Axis is parallel to X-,Y-, or Z-axis		$(x-\bar{x})^2/B^2+\left(\sqrt{(y-\bar{y})^2+(z-\bar{z})^2}-A\right)^2/C^2-1 = 0$	$\bar{x}\ \bar{y}\ \bar{z}$ A B C
TY			$(y-\bar{y})^2/B^2+\left(\sqrt{(x-\bar{x})^2+(z-\bar{z})^2}-A\right)^2/C^2-1 = 0$	$\bar{x}\ \bar{y}\ \bar{z}$ A B C
TZ			$(z-\bar{z})^2/B^2+\left(\sqrt{(x-\bar{x})^2+(y-\bar{y})^2}-A\right)^2/C^2-1 = 0$	$\bar{x}\ \bar{y}\ \bar{z}$ A B C
XYZP			Surfaces defined by points	See pages 3–15 and 3–17

MCNP Surfaces (5)

mcnp

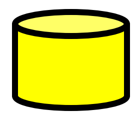
- **Rectangular Parallelepiped**



RPP xmin xmax ymin ymax zmin zmax

for infinite in a direction, use min=0 & max=0

- **Right Circular Cylinder**



RCC Vx Vy Vz Hx Hy Hz R

Vx Vy Vz = center of base

Hx Hy Hz = axis of cylinder, magnitude = height

R = radius

- **Others**

ARB, BOX, ELL, HEX (RHP), REC, TRC, WED

MCNP Surfaces (6)

$F(x,y,z) = S$

where

$F = 0$	is a surface equation
x,y,z	arbitrary 3-D coordinate
S	result of xyz point in equation

S is the "sense" of a point with respect to the surface

- **$S > 0$ - point is outside the surface**
- **$S = 0$ - point is on the surface**
- **$S < 0$ - point is inside the surface**

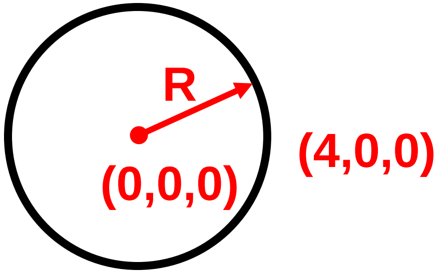
For macrobodies,

- **inside the body ➜ negative**
- **outside the body ➜ positive**

Alternate determination of sense:

- **Surface normal points in + direction**

Example



SO Surface Equation - sphere at origin

$$x^2 + y^2 + z^2 - R^2 = S \qquad \text{e.g. } R = 3.0$$

- Substitute (0,0,0), find S

  $0^2 + 0^2 + 0^2 – 3^2$ = negative

  Point (0,0,0) gives negative S.

  Inside of sphere has negative sense

- Substitute (4,0,0), find S

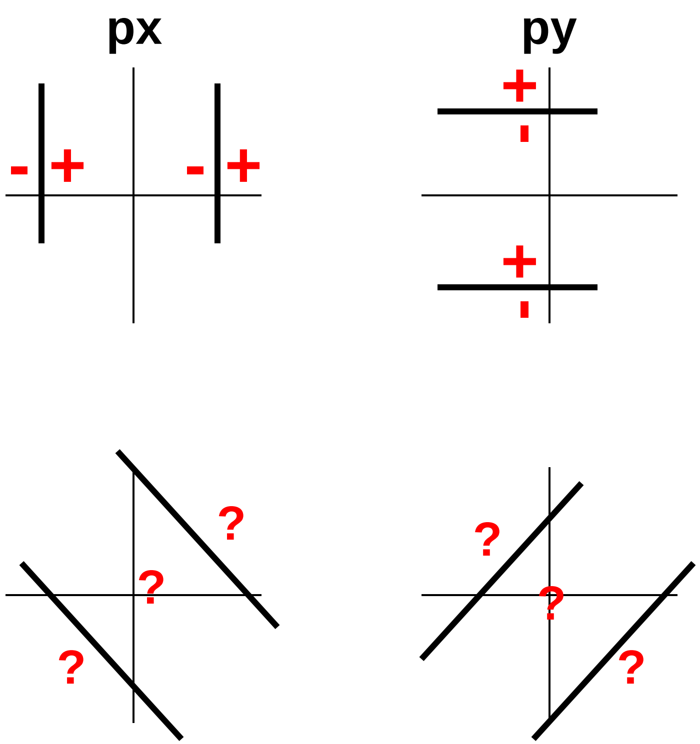
  $4^2 + 0^2 + 0^2 – 3^2$ = positive

  Point (4,0,0) gives positive S.

  Outside of sphere has positive sense

MCNP Surfaces (7)

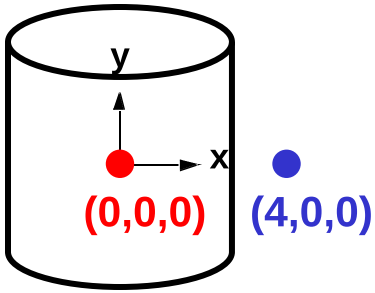
- **Planes**



Note:

The sense depends on the normalization of the surface equation. Multiplying both sides of the equation by -1 flips the sense. If in doubt, pick a convenient (x,y,z) point, substitute into surface expression to find the sense, + or -.

- **Cylinders**



Inside of cylinder has negative sense

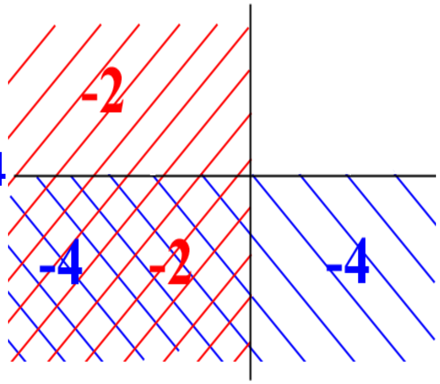
Outside of cylinder has positive sense

MCNP Geometry (1)

Intersection operator - blank between surfaces

-4 -2 means
negative sense wrt 4 AND
negative sense wrt 2

surface 4

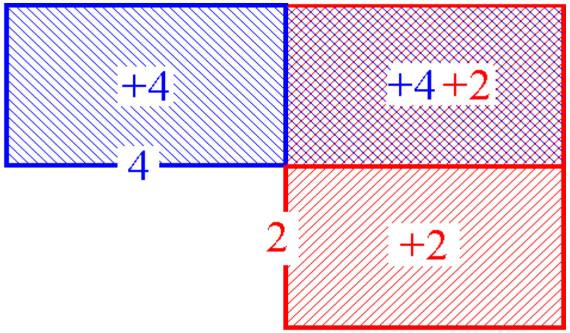


surface 2

Only the space colored BOTH red AND blue

Union operator - “:” between surfaces

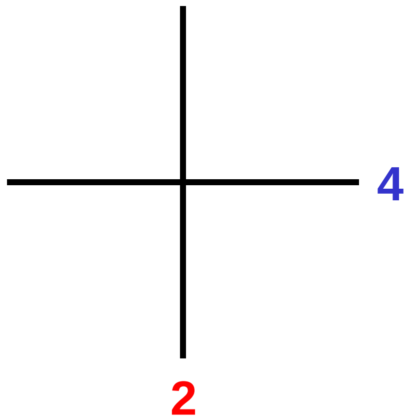
+2 : +4 means
positive sense wrt 2
OR positive sense wrt 4
OR BOTH



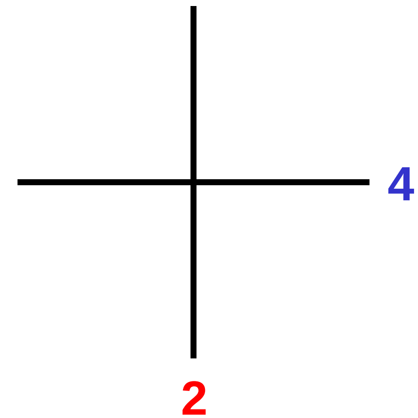
Only one sense criteria need be met for a point to be above 4 OR right of 2 OR both

MCNP Geometry (2)

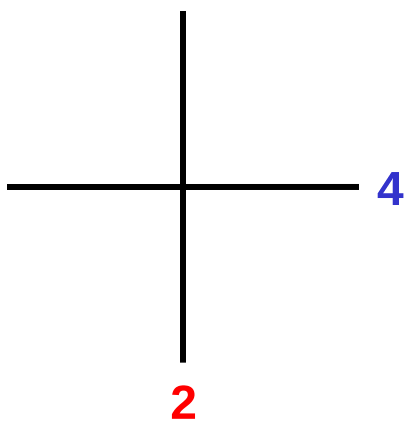
-4 -2



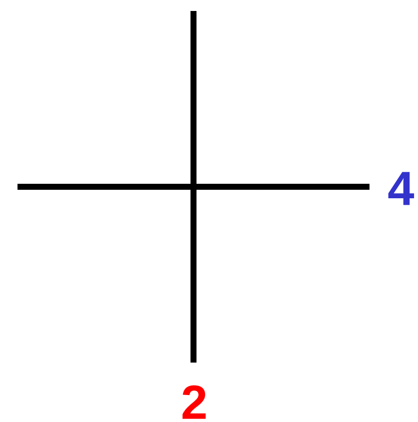
4 -2



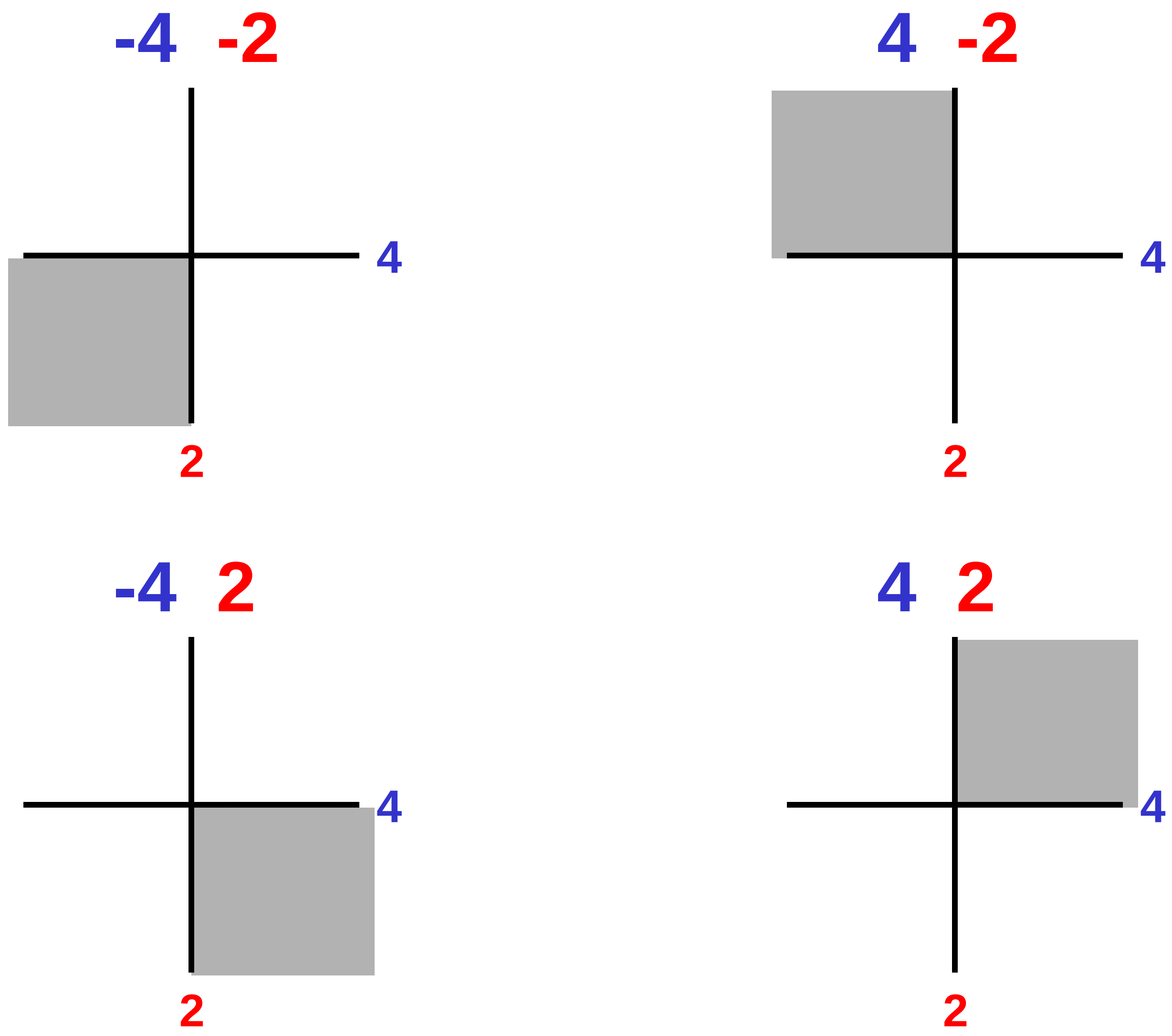
-4 2



4 2

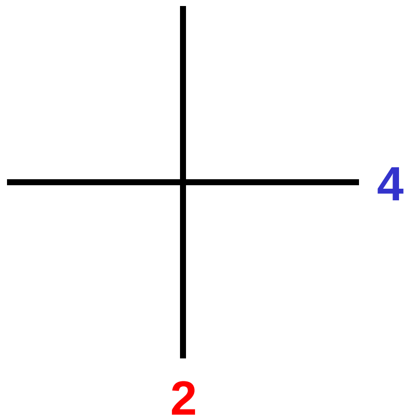


MCNP Geometry (3)

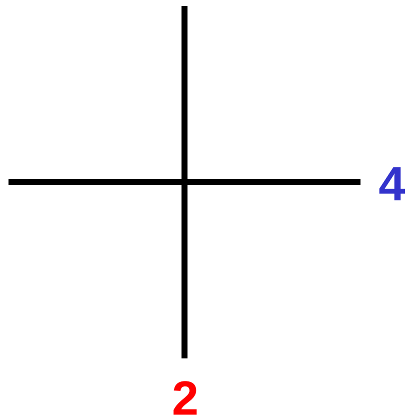


MCNP Geometry (4)

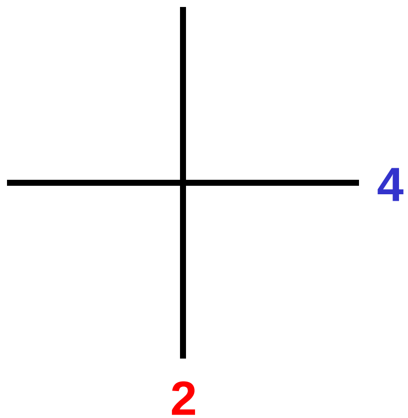
-4 : -2



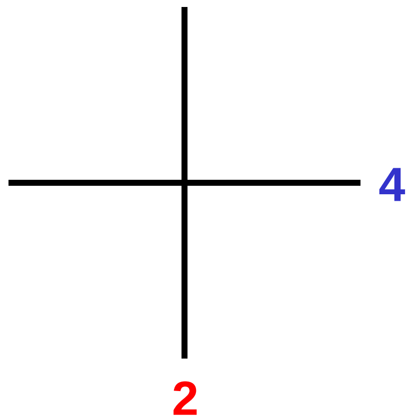
4 : -2



-4 : 2

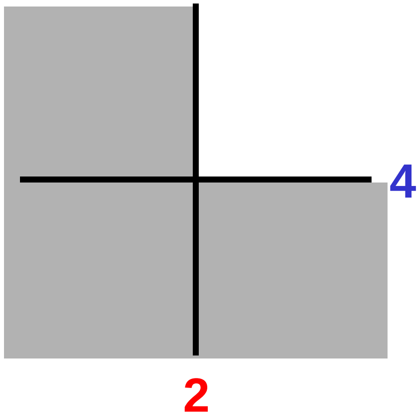


4 : 2

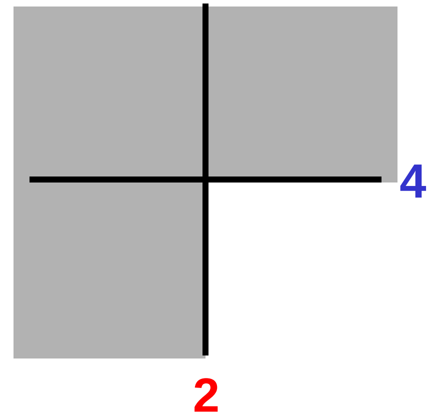


MCNP Geometry (5)

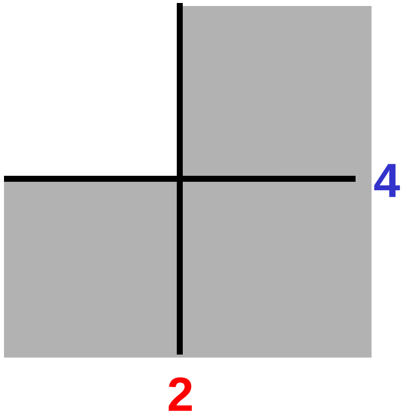
-4 : -2



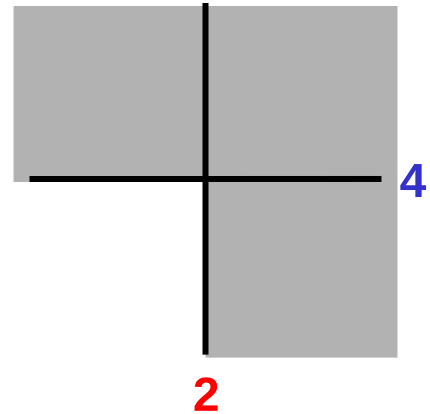
4 : -2



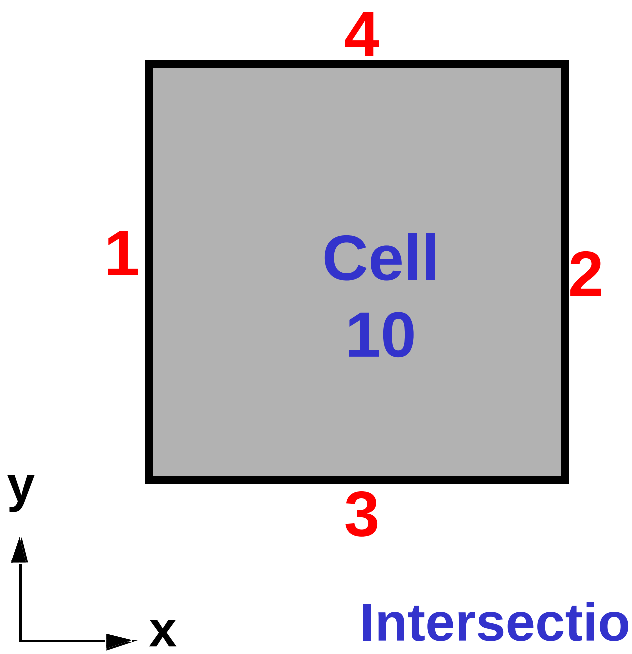
-4 : 2



4 : 2



MCNP Geometry (6)



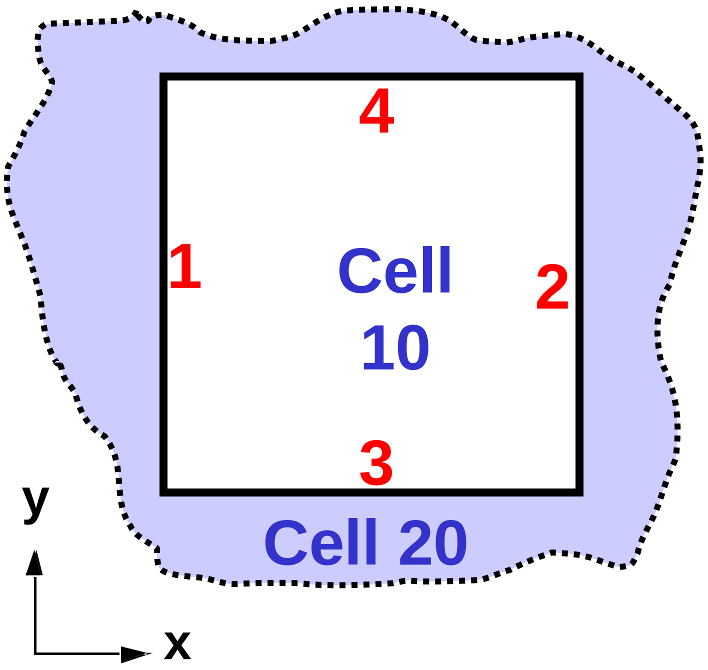
Surfaces:

1	px	-5.0
2	px	5.0
3	py	-5.0
4	py	5.0

Intersection logic for Cell 10 definition:

10 0 +1 -2 +3 -4 imp:p,e=1

All sense criteria must be true for points in Cell 10



Surfaces:

1	px	-5.0
2	px	5.0
3	py	-5.0
4	py	5.0

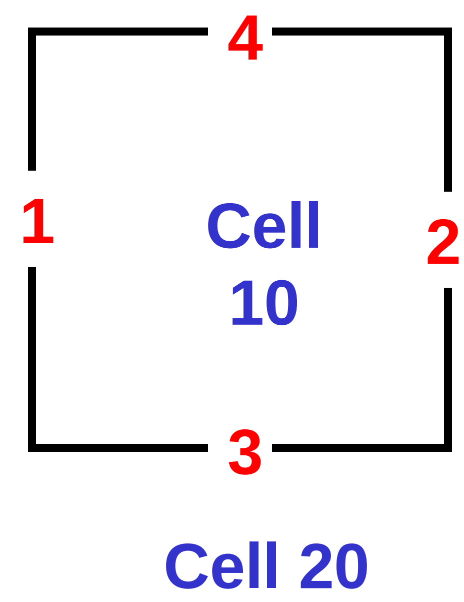
Union logic for Cell 20 definition:

20 0 -1 : 2 : -3 : 4 imp:p,e=0

Only one (or more) sense criteria need be true for points in Cell 20

MCNP Geometry (8)

Complement operator
"#" before <u>cell</u> number



Cell 10 is +1 -2 +3 -4
Cell 20 is -1 : +2 : -3 : +4

1. **Exchange each + and – ,**
2. **Exchange each " " and ":"**

Cell 20 is the *opposite* (complement) of Cell 10

Cell 20 definition using complement operator:

20 0 #10

Note:
The use of the complement operator was once discouraged on the grounds of inefficient tracking. This is no longer considered a significant problem.

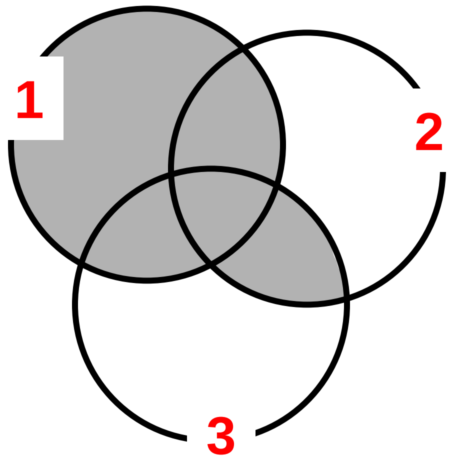
MCNP Geometry (9)

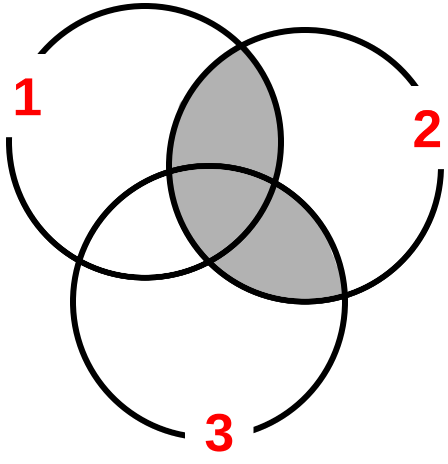
- **Intersections are done <u>before</u> unions**

-1 : -3 -2 is equivalent to -1 : (-3 -2)

- **Example**

-1 : -3 -2 is <u>not</u> the same as (-1 : -3) -2





CZT Block in a Void

--

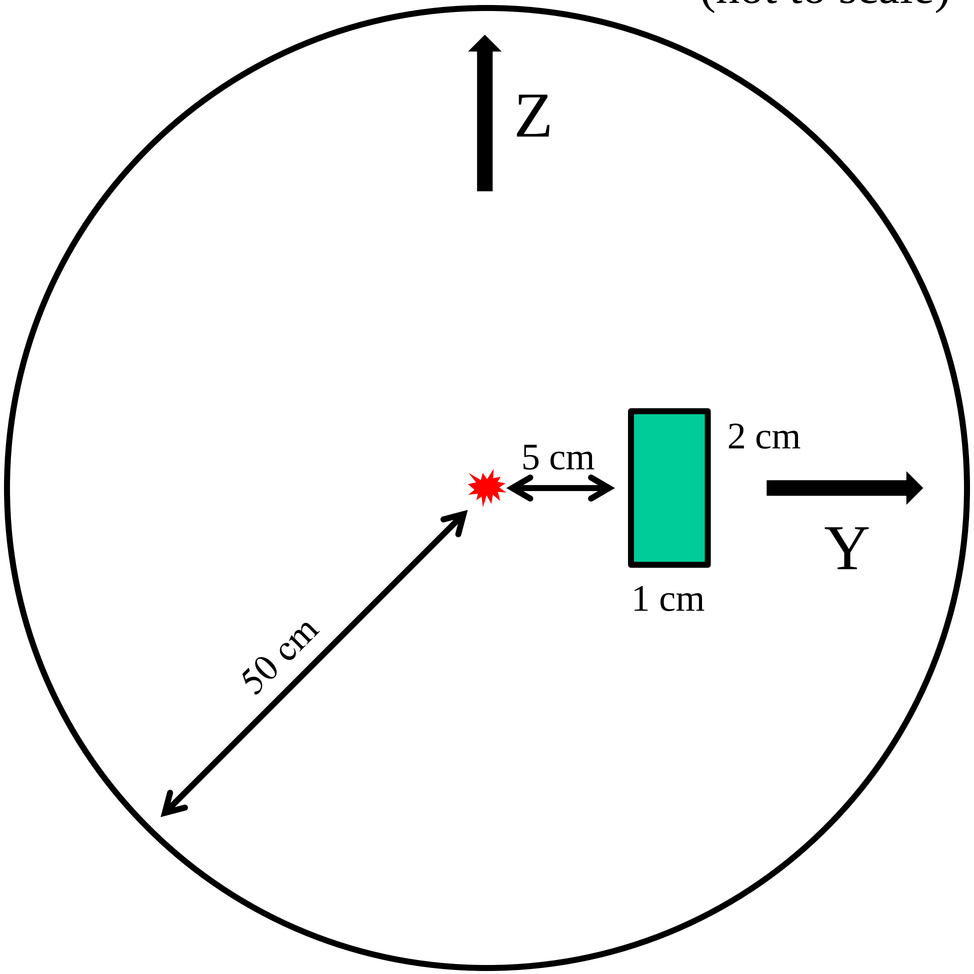
Starter input file: czt.0

Exercise 1 – Your Mission …

- **Copy MCNP6\EXAMPLES\czt.0 to MCNP6\WORK\czt.1**
- **Add two surfaces:**
  - An RPP bounding the space in
    - $-1 \le X \le 1$
    - $5 \le Y \le 6$
    - $-1 \le Z \le 1$
  - A sphere around everything.
- **Add three cells:**
  - Fill the RPP with CZT at density 6.06 gm/cm³
  - Void outside RPP inside sphere
  - Void outside sphere (imp=0).
- **Define one material, CZT as:**
  - 45% Cd, 5% Zn, 50% Te by number.
- **Run the problem:**

  mcnp6 i=czt.1

(not to scale)



Center CZT on X and Z axes.

ΔX = ΔZ = 2 cm.

Exercise 1 – Starter Input File

```
CZT block in a void.
c      Cell cards.
c      Add cell cards ....

c      Surface cards.
c      Add surface cards ....

c      Data cards.
c      Add material card ....
mode   p  e
sdef   par  p  erg 0.662  $  Cs-137
print
prdmp 2j  1
nps   10000
```

Spoiler alert!

A solution is on the next slide.

Exercise 1 – Solution

```
CZT block in a void.
c      Cell cards.
1      100  -6.06  -10          imp:p,e  1.
2        0          10  -20     imp:p,e  1.
3        0          20          imp:p,e  0.

c      Surface cards.
10       rpp      -1. 1.  5. 6.  -1. 1.
20       so       50.

c      Data cards.
m100   48000 0.9  30000 0.1  52000 1.
mode   p  e
sdef   par  p  erg 0.662  $  Cs-137
print
prdmp 2j  1
nps   10000
```

Exercise 1 – What happened?

- List the files that are now there:
  - mctal — an ASCII test record of tally results.
  - outp — the output file – a record of everything.
  - runtpe — the binary restart file – continue, plot, etc.
- First take a look at mctal:

```
mcnp   6   02/23/14   11:47:31    2      10000       1105374
CZT block in a void.
ntal      0
```

  - There is not much there: we have not yet defined any tallies.
  - But we see some information:
    - Date and time
    - Dump number
    - Number of histories
    - Number of random numbers
    - Title
    - Number of tallies
- But now look at outp.

Exercise 1 – What to see in outp

- **Information about input:**
  - an echo of the input file
  - summary of the source definition
  - material specification
  - surfaces and cells
  - information about cross sections
  - condensed-history information for charged particles
  - first 50 source particles
  - problem summary tables
  - particle activity in each cell
  - particle weight balance in each cell
  - tally results: the answers
  - statistics of the results

MCNP - Running & Plotting (1)

mcnp6 i=inp01 o=outp01 ... [options]

Default File Name	Description	Options	Operation
inp	**Input file**	**i**	**Input file reading**
outp	**ASCII output file**	**p**	**Plot the geometry**
runtpe	**Binary restart file**	**x**	**Process cross sections (XS)**
mctal	**ASCII tally results**	**r**	**Run the transport problem**
meshtal	**mesh tallies**	**z**	**Plot tally results or cross sections**
ptrac	**particle track file**		

default: ixr

Examples:

Plot problem geometry:

mcnp6 inp=test1 ip

Run problem with default file names:

mcnp6

Run problem selecting some names:

mcnp6 i=test1 o=result r=prev

Plot problem cross sections:

mcnp6 i=test1 ixz

Read restart file and plot tallies:

mcnp6 r=prev z

MCNP - Running & Plotting (2)

- **Select some file names: mcnp6 i=inp1 o=this_out r=this_run**
  - Reads inp1 and creates files:

this_out	output file
this_run	restart file
mctal	tally file (if requested on prdmp card)
srctp	fission source (for criticality)
comout	(if plotting)
ptrac	(if requested)

  - last letter changed, if file already exists: mctam, mctan, mctao, etc.

- **The "name=" option: mcnp6 i=prob.txt n=prob.**
  - Reads prob.txt and creates files:

prob.o	output file
prob.r	restart file
prob.m	tally file (if requested)
prob.s	fission source (for criticality)
prob.c	(if plotting)
prob.p	(if ptrac is requested)

  - **aborts** if any of these already exist - MCNP will **not** overwrite these files.

MCNP - Running & Plotting (3)

Plotting geometry

- **Interactive 2-dimensional slices**

- **Errors displayed as dashed (red) lines**

- **Many problem variables can be shown:**
  - cell & surface numbers
  - macrobody facets
  - importances imp:n
  - lattice variables u, lat, fill, level
  - material properties rho, den, …..
  - variance reduction parameters
  - weight windows mesh

MCNP - Running & Plotting (4)

Plotting commands

ORIGIN	**X**	**Y**	**Z**	**Position the center of the**
or	15.0	0.0	5.0	**plot window at (X,Y,Z).**
EXTENT		E_H		**Scale the plot with extent E_H**
ex	25.0			**Smaller E_H, closer view**
ex	25.0		150.0	**Choose your own aspect ratio**
PX V_X	px	3.0		**Set the view plane to $x=V_X$**
PY V_Y	py	5.0		$y=V_Y$
PZ V_Z	pz	0.01		$z=V_Z$

…. Lots of other options & commands - see MCNP manual, Appendix B

Exercise 1 – Plotting the geometry

- **mcnp6 i=czt.1   ip**
- **Explore:**
  - extent
  - origin
  - zoom
  - UP, RT, DN, LF
  - XY, YZ, ZX   basis
  - L1, L2
  - MBODY on and off
  - scales
  - cursor
  - keyboard input

A Few More Data Cards

MODE	What particles to follow
SDEF	Source specification
PRINT	How much information to print
PRDMP	Print and dump control
NPS	How long to run

The MODE Card

MODE	P	Transport only photons
MODE	P E	Transport photons and electrons
MODE	N H A	Transport neutrons, protons, alphas

… etc.

– **Available particle symbols:**

1	neutron	N	13	xi0	X	25	Alambda0	B
2	photon	P	14	xi_minus	Y	26	Asigma_plus	_
3	electron	E	15	omega_minus	O	27	Asigma_minus	~
4	mu_minus	|	16	mu_plus	!	28	Axi0	C
5	Aneutron	Q	17	Anu_e	<	29	xi_plus	W
6	nu_e	U	18	Anu_m	>	30	Aomega_minus	@
7	nu_m	V	19	Aproton	G	31	deuteron	D
8	positron	F	20	pi_plus	/	32	triton	T
9	proton	H	21	pi_zero	Z	33	helion	S
10	lambda0	L	22	k_plus	K	34	alpha	A
11	sigma_plus	+	23	k0_short	%	35	pi_minus	*
12	sigma_minus	–	24	k0_long	^	36	k_minus	?
						37	heavy_ion	#

PRINT

– PRINT card with no entries gives near-maximal output in the OUTP file.

—

– Absent PRINT card gives minimal output.

PRINT N1 N2 …

– PRINT card with positive entries gives minimal output plus additional print tables specified by the numbers N1 N2 …

PRINT –N1 –N2 …

– PRINT card with negative entries gives maximal output but without the print tables specified by the numbers N1 N2 …

The PRDMP Card

PRDMP NDP NDM MCT NDMP DMMP

- **Print tallies after every NDP histories.**
- **Dump to RUNTPE restart file after every NDM histories.**
- **MCT** **flag to write MCTAL tally file (set non-zero).**
- **NDMP** **maximum number of dumps to keep on RUNTPE file.**
- **DMMP** **control for tally fluctuation chart and rendezvous.**

Greatest routine interest: MCT and NDMP.

How Long to Run

NPS N

– Terminate the Monte Carlo calculation after **N** histories have been run.

– In a continue-run, NPS is the total number of particles - including runs before the continue run (cumulative).

– Negative entry will print output file at time of last history run.

– Applies to fixed-source problems. Criticality problems use other cards.

CTME T

– Terminate the Monte Carlo calculation at time **T** in minutes.

– Best for initial scoping of a problem.

– Easier to understand in a sequential run.

Tallies

Tally Basics
Reaction Rates
Mesh Tallies
Dose
Spectra
Plotting

Motivation

- Copy **shield01.txt** out of the SOLUTIONS directory.
- Analyze the input file and plot the geometry.
- Run the problem

```
mcnp6   i = shield01.txt
```

- Note the following screen output:

```
warning.  there are no tallies in this problem.
```

- Analogous to running an experiment with no detection equipment!

Tally Fundamentals

Getting Results from MCNP

- **MCNP produces k-eff and various information in tables.**
  - Only limited information about fluxes, spectra, reaction rates, etc.

- **In fixed-source problems, MCNP gives no physical results by default.**
  - Analogous to running an experiment without any detectors or measuring equipment!

- **Tallies are analogous to measurement devices in experiments.**

- **MCNP has several “devices” available:**

Tally Types

- **Tallies in MCNP are often called <u>edits</u> in many other codes**
  - Fluxes
  - Currents
  - Reaction rates

- **MCNP tally types:**
  - F1: Current on a surface
  - F2: Flux on a surface
  - F4: Flux in a cell (track-length estimate)
  - F5: Flux at a point or ring detector
  - F6: Energy deposition (track-length estimate)
  - F7: Fission energy deposition (track-length estimate)
  - F8: Pulse height tally
  - FMESH: Mesh tallies (MCNP5)

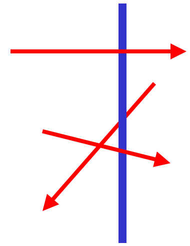
- **An energy weight can be applied to any tally by preceding it with an asterisk (e.g., `*F4`)**

- **A preceding plus-sign can be applied to F6 for collision heating (`+F6`) and F8 for charge deposition (`+F8`)**

Basic Tallies

F1 - Current across surface

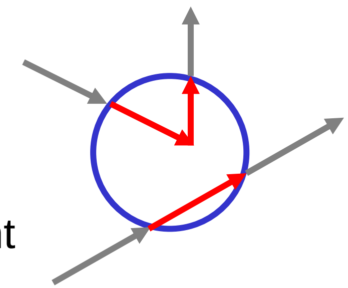
$$J = \frac{1}{W} \sum_{\substack{\text{all flights} \\ \text{crossing surface}}} wgt$$



W = total source weight

F4 - Flux in a cell

$$\phi = \frac{1}{V \cdot W} \sum_{\substack{\text{all flights} \\ \text{in cell}}} \text{wgt} \bullet \text{dist}$$

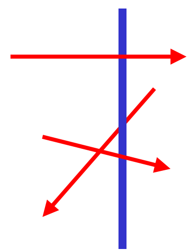


V = cell volume

W = total source weight

F2 - Flux on surface

$$\phi = \frac{1}{A \cdot W} \sum_{\substack{\text{all flights} \\ \text{crossing surface}}} \frac{\text{wgt}}{|\mu|}$$

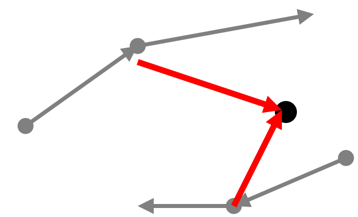


A = surface area

W = total source weight

$\mu = \Omega \bullet$ [surface normal]

F5 - Flux at a point



$$\phi = \frac{1}{W} \sum_{\substack{\text{all} \\ \text{collisions}}} \text{wgt} \cdot \frac{\text{p}(\mu)\text{e}^{-\Sigma_T R}}{2\pi R^2}$$

Tally Quantities Scored

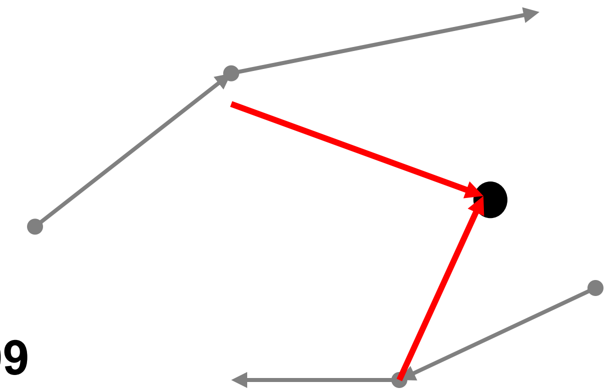
Type	Tally on surface, cell, or point
F1: Surface Current . . . All particles	surface
F2: Surface Flux . . . All particles	surface
F4: Track length estimate of cell flux . All particles	cell
F5: Flux at a point or ring detector . N or P	point or ring
F6: Trk length est. of energy deposition . All particles	cell
F7: Trk-len est. of fission energy dep. . N	cell
F8: Pulse height tally . . . All particles	cell

Tally Card Contents

- **Form (except F5): Fn:<pl> {list of surfaces or cells}**

  - **n = tally number = i + 10j** **i = 1, 2, 4, 6, 7, 8** **0 ≤ j ≤ 9999**
    - **Last digit is tally type**
    - **F4:n, F14:n, F124:n are all "F4" tallies**
  - **<pl> = particle type = particle symbol, n, p, e, etc.**
  - **May group entries by parentheses**
  - **Optional entry "T" at the end to give total**

Tally Card Contents (Flux at Point)



- **Form:** **Fn:<pl> X Y Z R**
  - **n = tally number = 5 + 10j** **0 ≤ j ≤ 99**
  - **<pl> = particle type = particle symbol, n or p (no charged particles)**
  - **At every collision, makes a deterministic estimate of flux**
  - **X, Y, and Z are position of tally where flux is desired**
  - **R is the radius of a “sphere of constant flux”**
    - **Required to keep tally variance finite**
    - **Recommended to be about one mean free path**

Tally Examples

F14:n 10 30 50	F4 neutron cell flux, 3 bins
F994:n (10 30) 50	F4 neutron cell flux, 2 bins
F44:p 10 11 12 T	F4 photon cell flux, 4 bins

Tallies Require Volumes or Areas

- **For tallies (except F5) to be valid, MCNP must know a volume or area to perform the division.**

- **Sometimes, MCNP will be unable to calculate the volume of cells or areas of surfaces. <u>You must then provide them!</u>**

- **Three methods of doing this:**

  1) Specify `vol = ####` on the respective cell card.

  2) Specify a list of volumes or areas for every cell or surface in the problem using the vol or area cards:

     VOL V_1 V_2 . . . V_m

     AREA A_1 A_2 . . . A_n

  3) Use a segment divisor (SD) card.

Segment Divisor Card (SD)

- **MCNP normalizes flux tallies by dividing by area, volume, or mass**
  - For cell flux tallies (F4), must divide by **volume**
  - For surface flux tallies (F2), must divide by **area**
  - For energy deposition (F6), must divide by **mass**
  - For fission heating (F7), must divide by **mass**
  - **Can use SD card to supply areas, volumes, or masses**
  - MUST do this if they are not calculated by MCNP

- **Form: SDn d1 d2 …**
  - n = tally number
  - d1, d2, … = divisors for each tally bin
  - Must have as many entries as there are tally bins for tally "n"
  - **Can use 1.0 to avoid dividing by volume or area or mass**

    Note: dividing by 1.0 instead of volume <u>changes units</u>, etc.

Commenting Tallies in the Output File

- **Commenting on what tallies are calculating is important, especially if others may look at your output file!**

- **Use of the FC card is recommended:**

  FCn   A String that is a Comment

- **Example**

```
F114:n    10
FC114     Cell flux tally in cell 10.
```

- **Comment your tallies**
  - Your coworkers will thank you!

Tallies With Macrobodies

- **Surfaces of most macrobodies are formed by several distinct components (referred to as "facets")**
- **Specific facet(s) must be specified for surface tallies**
- **Facet is identified as S.F, where S is the surface number for the macrobody and F is the facet number**
- **Facet numbers are fixed with respect to the orientation of the Macrobody**
- **Examples**

Rectangular Parallelepiped (RPP)

1 right side
2 left side
3 front
4 back
5 top
6 bottom

Right Circular Cylinder (RCC)

1 side of cylinder
2 top of cylinder
3 bottom of cylinder

Time Normalization - Flux vs Fluence

- **Fluence = $\int \varphi \, dt$**

- **Remember: MCNP tallies are normalized to be <u>per unit source</u>**

- **Given a tally result $X_n \pm R_n$, reactions/source-particle, then**

  - **If the real source is given as S particles/sec, then the normalized result is**

    $$X = [S \text{ src-part/sec}] * [X_n \text{ reactions/src-part}] \pm R_n$$
    $$= S*X_n \text{ reactions/sec} \pm R_n$$

    To get fluence or time-integrated result, **multiply X by Δt**

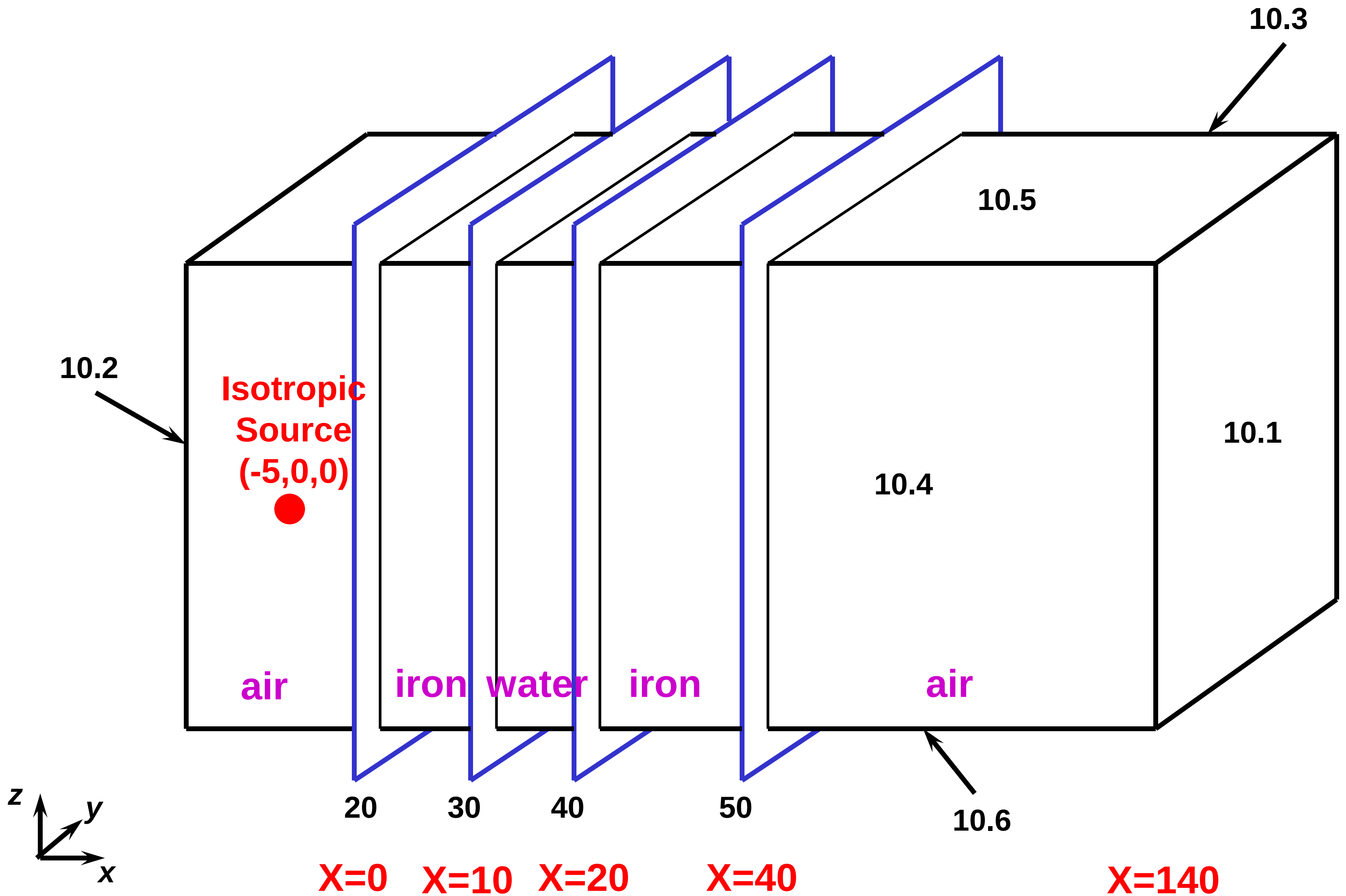
  - **If the real source is given as S particles (pulse, already time-integrated), then**

    $$X = [S \text{ src-part}] * [X_n \text{ reactions/src-part}] \pm R_n$$
    $$= S*X_n \text{ reactions} \pm R_n$$

    Don't multiply X by Δt to get fluence or time-integrated result

Example

- **Surface and facet indices for shield01.txt:**



Example: shield02

- **Copy shield01.txt to shield02.txt**

- **Insert tallies for:**
  - Surface current at
    - Front of the shield facing source,
    - Back of the shield, and
    - Rightward surface of the rpp, 1 meter away from shield
  - Cell flux averaged over the entire shield

- **Run the problem, analyze the output file**
  - Search for the string `1tally`

Example: shield02

```
shield02 - shielding calculation with a 5 MeV photon source
c >>>>> cell cards
. . .

c >>>>> surface cards
. . .

c >>>>> data cards
. . .
c ### tally specification
fc1     surface current entering, exiting, and 1 m after shield
f1:p    20   50   10.1
c
fc4     average neutron flux in the shield
f4:p    (200  210  220)
```

Example: shield02 results

```
1tally        1        nps =      100000
+                 surface current entering, exiting, and 1 m after shield
           tally type 1    number of particles crossing a surface.
           tally for  photons

 surface  20
                 6.53110E-01 0.0038

 surface  50
                 2.20000E-04 0.2132

 surface  10.1
                 1.40000E-04 0.2672
```

Example: shield02 results

```
1tally        4        nps =      100000
+                                          average photon flux in the shield
   tally type 4    track length estimate of particle flux.      units   1/cm**2
   tally for  photons

           cell  a is (200 210 220)
           volumes
                   cell:        a
                          1.60000E+06

 cell (200 210 220)
                 4.32993E-06 0.0052
```

Statistics

Assessing Results

- **The influence of <u>statistical noise</u> must be considered when assessing the reliability of Monte Carlo results.**

- **MCNP provides uncertainties and performs statistical checks to attempt to assess whether or not the results are reliable**
  - **Results of tests do not prove reliability!!!**

- **Confidence intervals assume that the <u>Central Limit Theorem</u> is satisfied.**

Review: Basic Statistics

- **MCNP tally results have the form**

  RESULT RELERR

  Where

  RESULT = average score for the tally, after N histories

  RELERR = relative error in the average score, after N histories

  All tally results are normalized to be per starting particle

- **Exception: For KCODE calculations, K-effective results are reported as**

  RESULT STD

  Where

  RESULT = average score for the tally, after N histories

  STD = standard deviation in the average score, after N histories

Review: Basic Statistics

- **Average, standard deviation, relative error**
  - Let x_k = the value of a tally for the k^{th} history
    N = number of histories run (so far)
  - **Average tally**, after N histories

$$\bar{x} = \frac{1}{N}\sum_{k=1}^{N} x_k$$

  - **Standard deviation** of average tally, after N histories

$$S_{\bar{X}} = \frac{1}{\sqrt{N-1}}\sqrt{\frac{1}{N}\sum_{k=1}^{N} x_k^2 - \bar{X}^2} \approx \frac{1}{\sqrt{N}}\sqrt{\frac{1}{N}\sum_{k=1}^{N} x_k^2 - \bar{X}^2}$$

  - **Relative error** in average tally, after N histories

$$RELERR = \frac{S_{\bar{X}}}{\bar{X}} \qquad RELERR \propto S_{\bar{x}} \propto \frac{1}{\sqrt{N}}$$

Review: Basic Statistics

- **Relative error vs number of histories (N)**

$$RELERR \propto S_{\bar{x}} \propto \frac{1}{\sqrt{N}}$$

  - To cut the relative error in **half**, must run **four times** as many histories
  - To reduce relative error by **10x**, must run **100x times** as many histories

- **Precision**

  The RELERR or STD DEV reflect the **precision** of results, ie, the uncertainty in the result caused by statistical fluctuations in the Monte Carlo simulation

- **Accuracy**

  The **accuracy** of a result is how close the average tally is to the true physical quantity being estimated.

  Accuracy depends on the geometry approximations, cross-section data realism, material definitions, physics approximations, code approximations, etc.

- **Running more histories will improve the precision of a result, not the accuracy of a result.**

Confidence Intervals

- **Confidence interval**
  - Using the computed STD DEV as an estimate of σ, we can estimate, by the Central Limit Theorem, the probability that the true mean lies with an interval:

$$\text{Prob}\left\{ \bar{x} - 1 \cdot s_{\bar{x}} \le \mu \le \bar{x} + 1 \cdot s_{\bar{x}} \right\} = 68\%$$

$$\text{Prob}\left\{ \bar{x} - 2 \cdot s_{\bar{x}} \le \mu \le \bar{x} + 2 \cdot s_{\bar{x}} \right\} = 95\%$$

$$\text{Prob}\left\{ \bar{x} - 2.6 \cdot s_{\bar{x}} \le \mu \le \bar{x} + 2.6 \cdot s_{\bar{x}} \right\} = 99\%$$

  - Think about what this means …..
    - If you repeat a calculation many times, it is likely that 1/3 of the time the true result will lie outside of the computed 1-σ confidence interval

MCNP - Ten Statistical Checks

MCNP performs 10 statistical checks on tallies to try & assess whether they are valid results

1. Estimated **mean** should have random behavior for last half of problem
2. Estimated **relative error** should be <.05 for point detector, <.10 for others
3. Estimated **RELERR** should monotonically decrease in last half of problem
4. Estimated **RELERR** should decrease as $1/N^{1/2}$ in last half of problem
5. Estimated **variance of the variance** (VOV) should be < .10
6. Estimated **VOV** should monotonically decrease in last half of problem
7. Estimated **VOV** should decrease as 1/N in last half of problem
8. Estimated **FOM** should not have obvious trends in last half of problem
9. Estimated **FOM** should show random behavior in last half of problem
10. Tail of **tally probability density** should fall off as $1/x^m$, with m>3

Reaction Rates

Reaction Rates

- Often some reaction rate may be desired rather than just flux.

$$R_x = N\sigma_x\phi$$

Units = Reactions per unit volume (per unit time)

- Need some way to multiply the flux tally scores by the number density and the microscopic cross section for reaction *x*.

- MCNP can do this with the tally multiplier, or FM, card.

- Tally multiplier card can also scale by constants and has additional uses.

Tally Multiplier Card

Note: Discussion here will be limited to the multiplier form of the tally multiplication card

- **Form:** **FMn C m B_1 (B_2 . . . B_i) . . . (B_j . . . B_m) B_{last}**
  - **n is tally number (e.g., FM24)**
  - **C is a multiplicative constant**
    - **C > 0 means multiply tally by C (e.g., source intensity)**
    - **C < 0 means multiply tally by |C|, and by atom density in the tally cell**
  - **m is a material number (from an Mm card)**
  - **B_k is a reaction type identifier**
  - **B_{last} is either blank or T (T sums over previous tallies)**

Combinations of Reaction Type Identifiers

- Reaction identifiers can be combined, either additively or multiplicatively, to form a single tally
- All component identifiers must be enclosed in a single set of parentheses
- Colon between two reaction type identifiers means they are to be added ($B_i : B_j : B_k$)
- Blank space between two reaction type identifiers means they are to be multiplied ($B_i \ B_j$)
- If no ( ), precedence of operations is multiply first, then add

Reaction Type Identifiers

- **Reaction type identifiers can be either positive or negative**
  - **Positive values correspond to ENDF reaction types (MT numbers)**
  - **Negative values are specific to the type of library (multipgroup or continuous-energy) and particle (neutron or photon) employed**

MT	Reaction Type
1	Total
2	Elastic scattering
18	Fission
101	Capture
102	(n,γ)

Note: The MCNP manual sometimes reverses the usual definitions of capture and absorption (physicists versus nuclear engineers). Throughout this presentation, we will use absorption = fission + capture

Other MCNP Reaction Type Identifiers

Type	Neutrons		Photons
	Continuous	Multigroup	
-1	total*	total	incoherent scatt
-2	capture	fission	coherent scatt
-3	elastic scattering*	ν (neutrons/fission)	photoelectric
-4	heating (MeV/coll)	χ (fission spectrum)	pair production
-5	γ production	capture	total
-6	fission	stopping power	photon heating
-7	ν (neutrons/fission)	momentum transfer	
-8	Q (MeV/fission)		

FM Card Examples

- **Fission rate in cell 10, which contains material 100, with continuous-energy neutron data**

```
F14:n    10
FM14     -1.0   100    -6
```

- **Nu-fission rate in cell 10, which contains material 100, with continuous-energy neutron data**

```
F24:n    10
FM24     -1.0   100    ( -6   -7 )
```

Exercise: shield03 -- Gamma Production

- **Copy shield01.txt to shield03.txt.**
- **Add tally to compute the pair production rate in the iron portion of the shield.**
  - Source strength of 3.e8 photons per second
  - Note the units of the tally (do **not** want photon production rate density)
- **Run the problem and examine the output file.**

Exercise: shield03 -- Pair Production

```
shield03 - shielding calculation a 5 Mev photon source
c >>>>> cell cards
. . .

c >>>>> surface cards
. . .

c >>>>> data cards
. . .
c ### tally specification
fc4     photon production rate in iron
f4:n    (200  220)
fm4     -3.e8  1000   -4          $ source strength * gamma production xs
sd4     1                         $ do not divide by volume
```

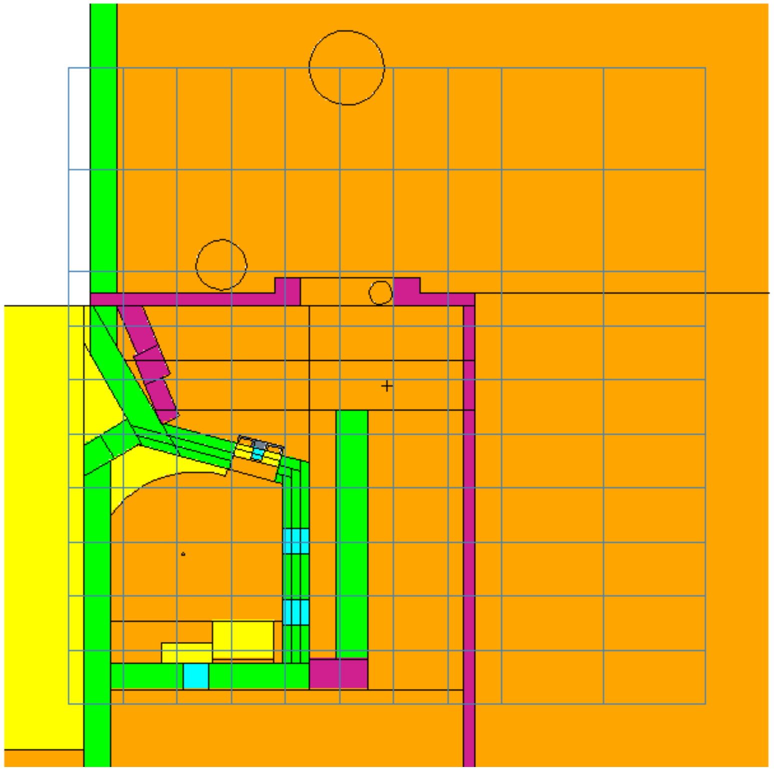
Exercise: Pair Production

```
1tally        4        nps =      100000
+                                        pair production rate in iron
           tally type 4    track length estimate of particle flux.
           tally for  photons

           volumes
                   cell:   (200 220)
                         1.00000E+00

 cell (200 220)
 multiplier bin:  -3.00000E+08      1000          -5
                 4.37228E+07 0.0053
```

Mesh Tallies
(MCNP5)

Mesh Tallies

- **Mesh tallies cover 3D regions of space independent of the problem geometry**
  - Can be used to tally flux, reaction rates, heating, particle birth, …
  - Rectangular & cylindrical meshes
  - Bin on energy values
  - Unlimited number of meshes
  - Size of mesh limited by computer parameters
  - Rotated by using a TR card
  - Modified by DE/DF or FM cards
  - Plot results in MCNP5



Mesh Tally Card

```
FMESHn:p   GEOM=      ORIGIN=      IMESH=        IINTS=        JMESH=
           JINTS=      KMESH=    KINTS=
```

- **Can be used with DEn, DFn, and FMn cards.**
- **Caution: It is easy to create huge mesh tallies that can overflow computer memory.**

GEOM	**= mesh geometry: Cartesian (xyz or rec) or cylindrical (rzt or cyl)**	**xyz**
ORIGIN	**= x,y,z coordinates in MCNP cell geometry superimposed mesh origin**	**0. 0. 0.**
IMESH	**= coarse mesh locations in x (rectangular) or r (cylindrical) direction**	**---**
IINTS	**= number of fine meshes within corresponding coarse meshes**	**1**
JMESH	**= coarse mesh locations in y (rectangular) or z (cylindrical) direction**	**---**
JINTS	**= number of fine meshes within corresponding coarse meshes**	**1**
KMESH	**= coarse mesh locations in z (rectangular) or theta (cylindrical) direction**	**---**
KINTS	**= number of fine meshes within corresponding coarse meshes**	**1**
EMESH	**= values of coarse meshes in energy**	**all energies**
EINTS	**= number of fine meshes within corresponding coarse energy meshes**	**1**
FACTOR	**= multiplicative factor for each mesh**	**1.**

Example

- **<u>Example</u>: 5 x 10 x 20 fission rate mesh tally in 5x5x5 cm box centered about the origin.**

```
fmesh4:n  geom=xyz    origin=-2.5 -2.5 -2.5
          imesh=2.5   iints=5
          jmesh=2.5   jints=10
          kmesh=2.5   kints=20
fm4    -1.0     0      -6
```

- **Material index of zero is a wildcard, uses material in the current cell.**

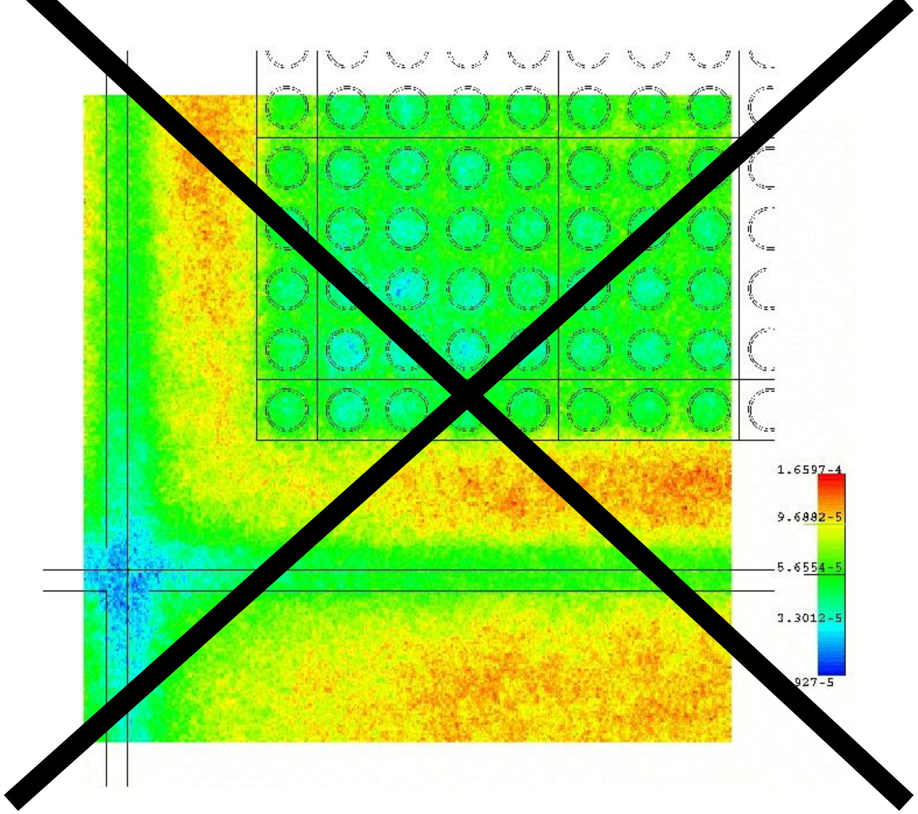
Example of the FM card (MCNP5 only)

Calculate the average fission energy deposition

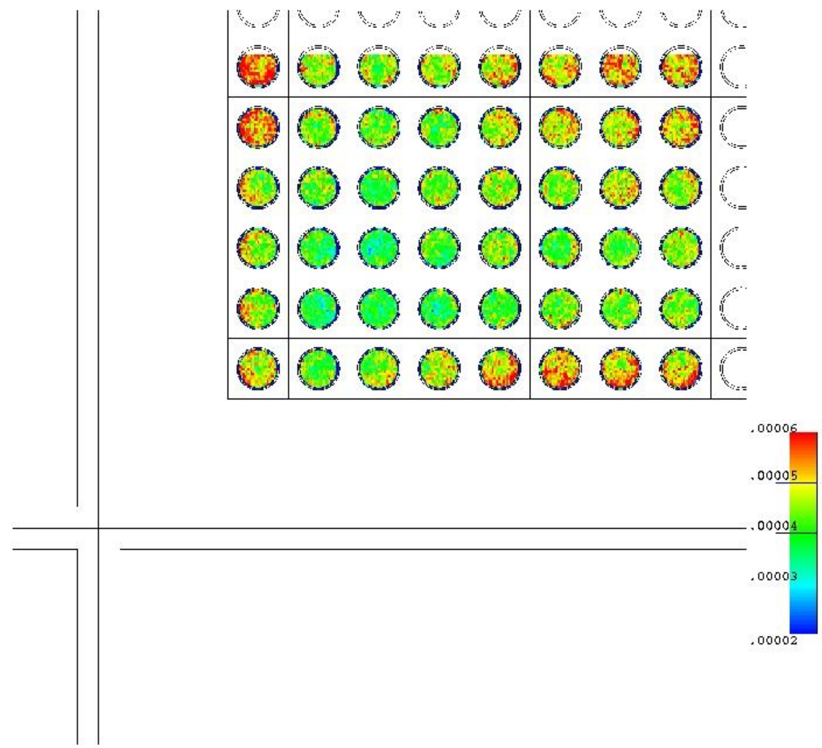
FM card format: FMn C m R1 R2

Put '0' as the material number

FM124 0.06925613 1 -6 -8



FM134 -1.0 0 -6 -8



Exercise: Mesh Tallies

- **Copy shield01.txt to shield04.txt**

- **Insert a mesh tally to compute the energy deposition (in MeV/cc) for a source of 3e8 neutrons/sec as a function of space.**
  - Mesh should cover the entire shield (do not include air)
  - Use 40 elements in x, 40 in y, and 1 in z
  - Revisit the table of special reaction numbers for the FM card
  - Remember the “0” wildcard

- **Run the problem and wait for instructions on plotting**

Exercise: Mesh Tallies

```
shield04 - shielding calculation with a 5 MeV photon source
c >>>>> cell cards
. . .

c >>>>> surface cards
. . .

c >>>>> data cards
. . .
c ### mesh tally specification
fmesh4:p    geom=xyz    origin=0  -100  -100
           imesh=40      iints=40
           jmesh=100     jints=40
           kmesh=100     kints=1
fm4   -3.e8   0   -5  -6
```

Mesh Tally Plotting

- **In the command line type:**

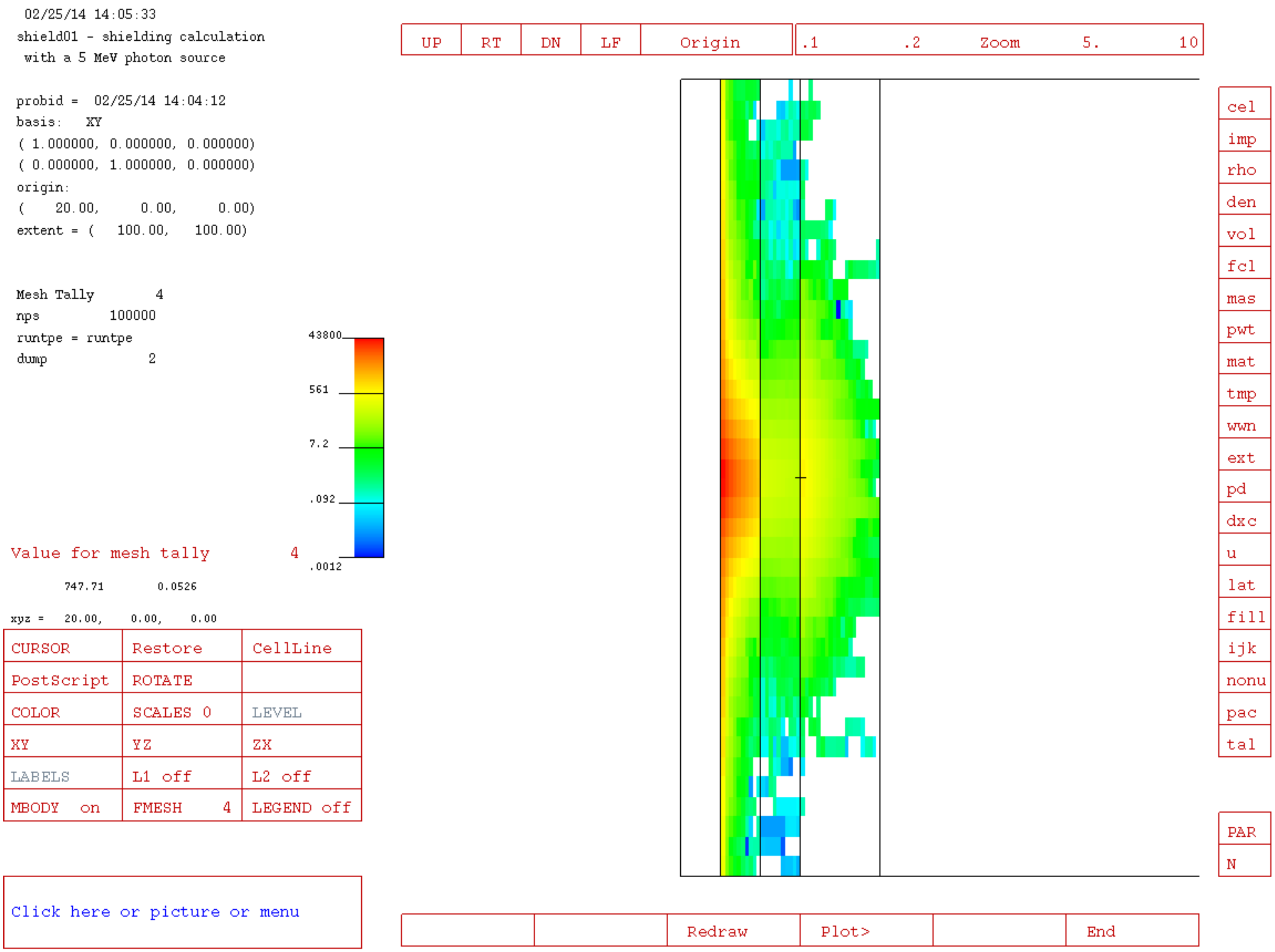
```
mcnp6   z   r = runtpe
```

- **Where runtpe is the name of your runtpe file**

- **The following commands in `red` are useful:**

`fmesh 4`	**Brings up the results**
`fmrelerr`	**Plots the relative uncertainties**

Mesh Tally Plotting



OPTIONAL

Dose Rates

Calculating Dose in MCNP

- **There are two methods to compute dose (energy deposited by unit mass) in MCNP:**
  - Explicit modeling of exposed targets (e.g., detectors, phantoms, etc.) and use of energy deposition (F6) tallies
  - Flux tallies (F2, F4, or F5) with appropriate dose functions

- **F6 tallies produce absorbed dose, not biological dose**
  - Need “dose functions” to provide quality or tissue weighting factors

Using the F6 Tally

- **If possible, model the target explicitly in the geometry and use an F6 tally to compute dose**
  - Advantage: most exact as effects of target on radiation field capture
  - Disadvantage: not always practical to model everything (e.g., locations of individuals standing in a room)

- **F6 tally is an F4 tally modified by the total cross section and heating number**
  - Equivalent to an F4 with an FM4 card with (-1 -4)
  - Units are MeV/g, use FM card to convert units to rad or Gy

- **Require to use DE and DF cards (next slide) with quality factors if biological dose required**

Dose/Response Function Cards (DE, DF)

- **Function to modify a tally response with some interpolated function (e.g. particle flux to human biological dose equivalent rate)**

$$\text{Dose} = \int_E D(E)\phi(E)dE$$

DEn A E1 E2 . . . Ek

- Ei = energy points (MeV)
- A = LOG or LIN energy interpolation method

DFn B F1 F2 . . . Fk

- Fi = corresponding value of the dose function at each energy on DEn
- B = LOG or LIN dose interpolation method

- **Appropriate for dosimetry when effect of “target” on the radiation field is small (e.g., a small detector)**

Exercise: shield04 – Dose Calculation

- **Copy shield01.txt to shield05.txt.**
- **Add tally to compute the biological dose rate (rem/hr) from neutrons to a worker standing 1 meter from the back of the shield**
  - Source strength of 3.e8 neutrons per second
  - Copy the DE and DF cards from the file: **shield_dedf.txt**
- **Run the problem and examine the output file.**

Exercise: shield05 – Dose Calculation

```
shield05 - shielding calculation with a 5 MeV photon source
c >>>>> cell cards
. . .

c >>>>> surface cards
. . .

c >>>>> data cards
. . .
c ### tally specification
fc2     average dose rate in rem/hr, 1 m from shield from 3e8 photons
f2:p    10.1
fm2     3.e8         $ multiply by source strength 3.e8 p/s
c ### photon flux to dose (rem/hr) factors
c !!! NOT RECOMMENDED FOR "OFFICIAL" CALCULATIONS !!!
de2 log 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 1.0 1.5 2. 3. 4. 5. 6. 8. 10.
df2 log 2.78e-6 1.11e-6 5.88e-7 2.56e-7 1.56e-7 1.20e-7
        1.11e-7 1.20e-7 1.47e-7 2.38e-7 3.45e-7 5.56e-7 7.69e-7
        9.09e-7 1.14e-6 1.47e-6 1.79e-6 2.44e-6 3.03e-6 4.00e-6
        4.76e-6 5.56e-6 6.25e-6 7.69e-6 9.09e-6
```

Exercise: Dose Calculation

```
1tally        2        nps =      100000
+          average dose rate in rem/hr, 1 m from shield from 3e8 photons
           tally type 2    particle flux averaged over a surface.
           tally for  photons

           this tally is modified by a dose function.

           this tally is all multiplied by  3.00000E+08

           areas
                surface:     10.1
                         4.00000E+04
 surface  10.1
                 3.59618E-06 0.3188
```

<u>OPTIONAL</u>
Spectra and Plotting

Obtaining Energy Spectra

- **Often, spectral information is useful for shield design**

- **An energy binning can be added to tallies with an E card:**

```
En      e1   e2    . . .   ei    . . .   eK
```

  - The index `n` corresponds to a tally index defined on the `F` card
    - If `n = 0`, then it is the default for all tallies
  - Each `ei` are energy bin boundaries in MeV
  - Implied lower bound always 0 MeV
  - Tallies are integrated over the entire energy bin (<u>not</u> in per MeV)

- **Also can bin in time with T card, or, for F1 tallies, in direction cosine with the C card**

Tally Plotting

- Copy **shield06.txt** out of SOLUTIONS directory, examine, run

- Read in the runtpe file to plot energy spectrum (tally 1) of current leaving shield

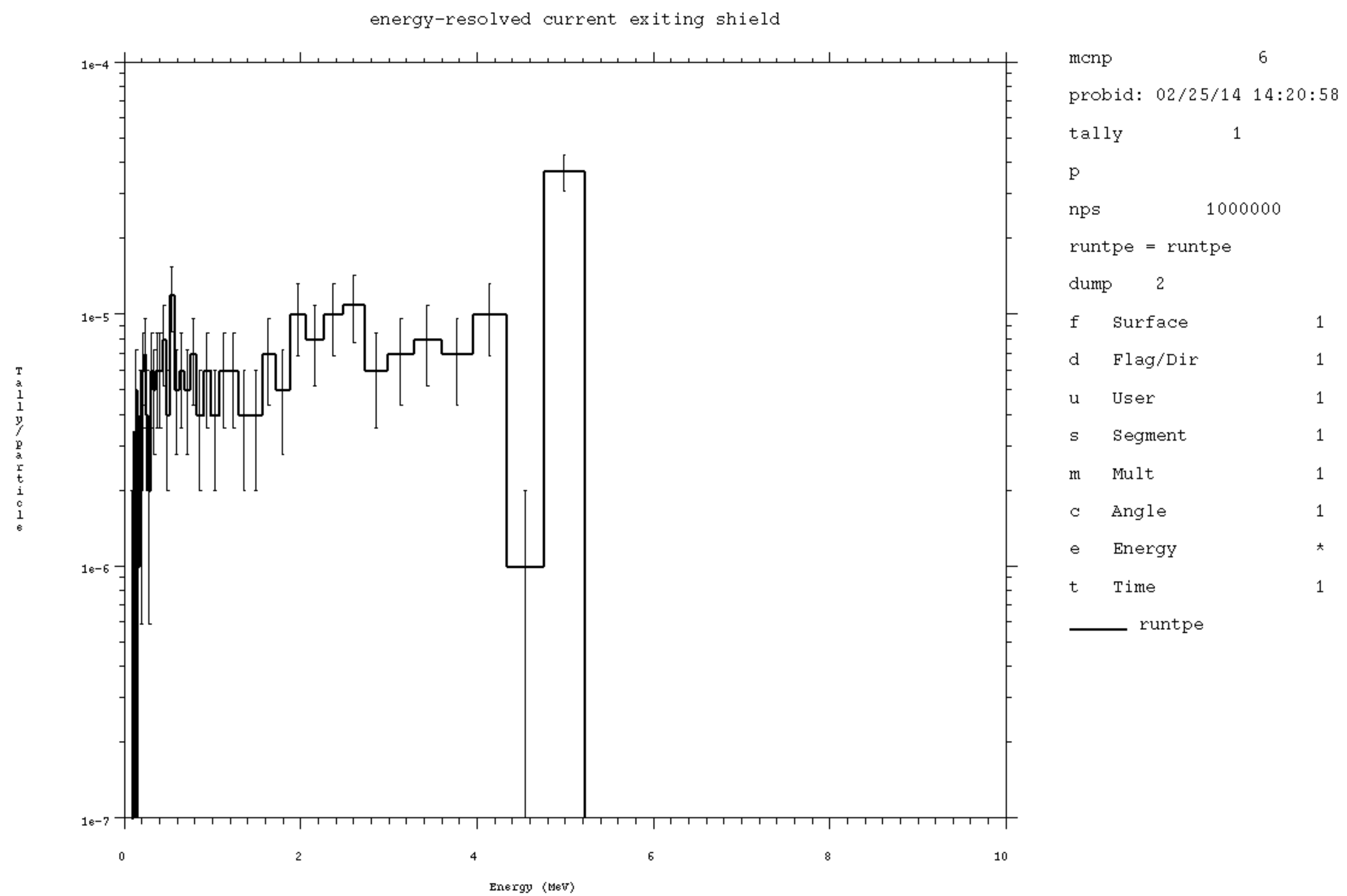
```
mcnp6  z   r = runtpe
```

  - Replace “runtpe” with the name of your runtpe file

- In the plotting command window, type text in `red`:

`tal 1`	specifies the tally to plot
`linlog`	has plot on lin-log scale
`nonorm`	removes per MeV normalization
`xlims 0 10`	sets the x-range of the plot window

Tally Plotting



Cross Section Plotting

- **Explain this behavior by plotting the cross section**

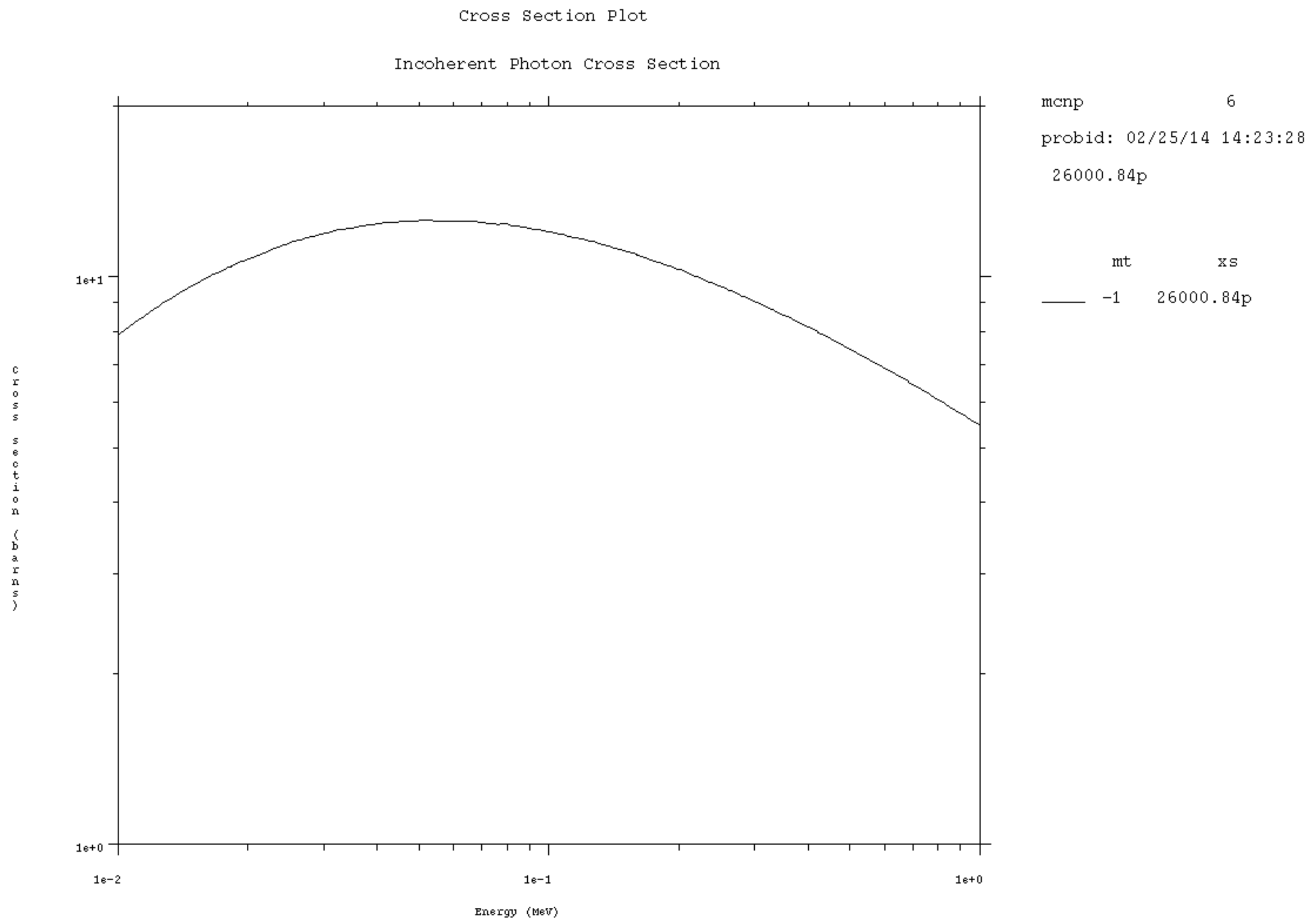
- **On the command line, type:**

```
mcnp6  ixz   i = shield06.txt
```

- **In the plotter, type the text in `red`:**

`xs    26000.84p`	**Brings up Iron-56 total xs**
`xlim  0.01  1`	**Sets energy view from 10 keV to 1MeV**
`ylim  1  20`	**Sets range of cross section**

Cross Section Plotting



Mesh Tallies (MCNPX)

FORM: (R,C,S)MESHn:<*pl*> keyword = value

n = 1, 11, 21, 31,...

(note, number must not duplicate one used for an ‘F1’ tally)

<*pl*> is a particle type. There is no default.

Example:

```
tmesh
    rmesh1:n    flux
    cora1  -15.0 100i 15.0
    corb1  -15.0 15.0
    corc1  -30.5 100i 30.5
endmd
```

Mesh Tally Keywords (MCNPX Type 1)

Keyword	Description
TRAKS	Tally the number of tracks through each mesh volume. No values accompany the keyword.
FLUX	Tally the average fluence (particle weight times track length divided by volume) in units of number/cm^2. If the source is considered to be steady state in particles per second, then the value becomes flux in number/cm^2-s.
TRANS	Translate and/or rotate the mesh, according to the specified TR card. Must be followed by a single TR card number.

Additonal keywords:

DOSE, POPUL, PEDEP, MFACT

Source Mesh Tally:

Form: **(R,C,S)MESH*n* <*pl*$_1$> <*pl*$_2$>...<*pl*$_n$> trans = #**

n = 2, 12, 22, 32, ...
(note, number must not duplicate one used for an ‘F2’ tally)

<pl> = particle type(s) (Up to 10 allowed)

Energy Deposition Mesh Tally:

General Form: **(R,C,S)MESHn** ***keyword***

n = 3, 13, 23, 33, ...

Example: ***Mesh tally of total energy deposited, all sources***

```
tmesh
     RMesh3 total
     cora3  -15.0 100i 15.0
     corb3  -15.0 15.0
     corc3  -30.5 100i 30.5
endmd
```

Keyword	Description
TOTAL	If TOTAL appears on the input line, score energy deposited from any source. (DEFAULT)
DE/DX	If DE/DX appears on the input line, score ionization from charged particles.
RECOL	If RECOL appears on the input line, score energy transferred to recoil nuclei above tabular limits.

Additional keywords

TLEST, DELCT, MFACT, NTERG, TRANS (see the manual)

General Form: **(R,C,S)MESHn:<*pl*>** **trans = #**

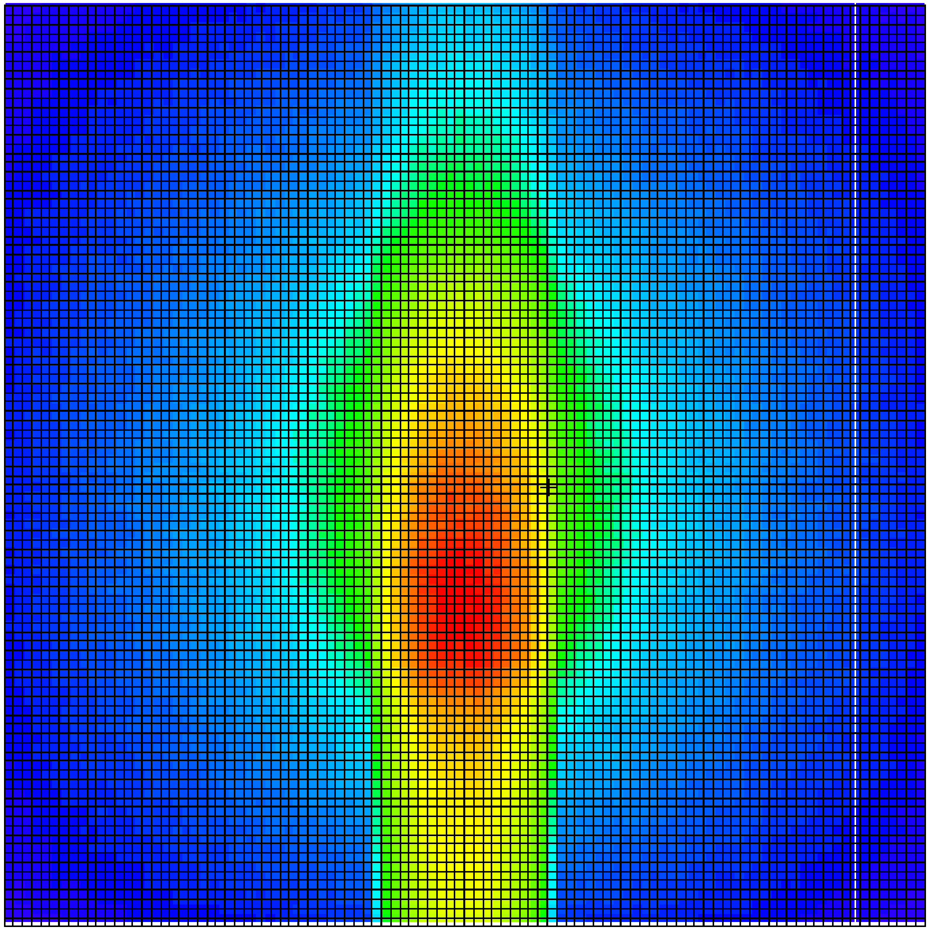
n = 4, 14, 24, 34, ...

(note, number must not duplicate one used for an 'F4' tally)

<*pl*> is a particle type. There is no default.

trans must be followed by a single reference to a TR card that can be used to translate and/or rotate the entire mesh. Only one TR card is permitted with a mesh card.

- **Instructions on MCNPX mesh tally plotting:**
  - **Command prompt:** `mcnpx z run = <runtpe filename>`
  - `mcplot> plot` **$brings up the geometry plotter**
  - `[buttons] tal, N, color`



FORM: CONTOUR [cmin cmax cstep] [commands]

All command entries are optional

cmin	minimum contour value
cmax	maximum contour value
cstep	number of contour steps
% or pct	interpret step values as percentages
log	step values logarithmic with cstep interpolates
All	contours normalized to min and max values of entire tally
noall	contours normalized to min and max values of contour slice (FIXED command)
line/noline	do/don’t draw lines around contours
color	make color contour plot
nocolor	contour lines only

EXAMPLES

```
CONTOUR  5 95 10 & line color
```

There will be 10 contour lines at 5%, 15%,…95% of the maximum value.

Lines will be drawn around the colored contours as in Figure 1.

Note: this is the default setting

```
CONTOUR 1e-4  1e-2  12 log
```

There will be 12 contour lines logarithmically spaced between 1e-4 and 1e-2

Modeling Radiation Sources in MCNP

Modeling Radiation Source in MCNP

Every Radiation Source has:

- **Location**
  - Point, surface, or volume
- **Direction**
  - Isotropic, beam-like, or angular distribution
- **Energy**
  - Single energy, multiple discrete lines, distribution
- **Particle type**
  - Photons, electrons/positrons, neutrons
  - 33 other particle types
  - Heavy ions
- **Time distribution**
  - Constant, radioactive decay, pulse

mcnp

MCNP can model physical descriptions of radiation sources in one of four ways:

- General SDEF [This Lecture]
- Criticality KSRC
- Surface SSW / SSR
- User-Supplied (Fortran Routine)

For SDEF source types, we can use source distribution functions to provide details:

- **SIn** <u>information</u> about the variable
- **SPn** <u>probability</u> of choosing a particular value
- **SBn** probability <u>biasing</u>
- **DSn** <u>dependent</u> source distribution

(More on these later.)

General Source: SDEF Data Card

Form: **SDEF** **source_variable=specification .....**

source_variable **is an abbreviation for a physical description:**

erg	**energy (MeV)**
pos	**position (location)**
dir	**cosine of angle**
vec	**reference vector (direction) for DIR**
rad	**radial distance of the position**
ext	**extents (distance or angle)**
axs	**reference vector for EXT and RAD**
cel	**cell**

… and others

Recall Exercise 1

```
CZT block in a void.
c      Cell cards.
1      100   -6.06  -10             imp:p,e  1.
2        0            10   -20      imp:p,e  1.
3        0            20            imp:p,e  0.

c      Surface cards.
10       rpp      -1. 1.   5. 6.   -1. 1.
20        so      50.

c      Data cards.
m100  48000 0.9  30000 0.1  52000 1.
mode  p  e
sdef  par  p  erg 0.662  $  Cs-137
print
prdmp 2j  1
nps   10000
```

Specification is a value or distribution, in one of three forms:

1. **Explicit value:** **SDEF ERG=0.14**

   [default values + source energy = 2.0 MeV]

2. **Distribution number:** **SDEF ERG=D1**

   [default values + source energy is a distribution ("D1" notation is explained later)]

3. **As a function of another variable:**

   SDEF POS=D1 ERG=FPOS=D2

   [default values + src position is a distribution + src energy depends on which position]

When a physical description is omitted from the SDEF card, a default is assumed

Defaults:

Energy	[erg]	14.0 MeV
Position	[pos]	0.0 0.0 0.0
Direction and	[dir]	
Direction Vector	[vec]	Isotropic
Time	[tme]	0.0
Particle Type	[par]	Lowest numbered particle found on MODE card.

But it is better to be specific: e.g. PAR=P

SDEF Source Scalar Variables

Explicit Value Only:

WGT EFF NRM

Explicit Value or Distribution:

SUR TME CCC ARA TR X Y Z

CEL ERG DIR RAD EXT PAR

DIR	**cosine of angle between reference vector VEC and u,v,w.** **azimuthal angle always sampled uniformly from 0 to 360.**
NRM	**sign of surface normal**
RAD	**radial distance of the position from POS or AXS vector**
EXT	**cell case: distance from POS along AXS** **surface case: cosine of angle from AXS**

Each vector variable has 3 entries: the x,y,z component.

VEC	reference vector for DIR
POS	reference point for sampling position
AXS	reference vector for EXT and RAD

SI, SP, SB, and DS Cards

Often, source variables are not single values.

The following cards are used in conjunction with the SDEF card to describe **distributions** in location, direction, energy, etc.

SI **information about the variable**
bins, discrete values, distribution numbers

SP **probability of choosing particular value**
true probabilities, built-in functions

SB **biased probabilities** **(see manual)**

DS **dependent distribution**
values, distribution numbers

SI (source information) Card

SDEF variable=Dn

FORM: `SIn option entries`

Option:

blank

or H entries are <u>histogram</u> bin boundaries (default)

entries are UPPER bounds of bins.

L entries are <u>discrete</u> <u>values</u>

A entries are <u>points</u> where probability density distribution is defined

S entries are <u>distribution numbers</u>

SI Card Examples

```
SDEF   ERG=D1
SI1   H  .01   .1   1.0   3.0   14.0     $  bins


SDEF   POS=D1
SI1   L   0.   0.   0.    10.   0.   0.     $  xyz values


SDEF   ERG=D1
SI1   S   3   4   5               $  other distribution #s
•
•
•
```

SP (source probability) Card

FORM: SPn option entries

OR SPn –m a b

Option:

blank	
or D	entries are bin probabilities (default)
C	entries are cumulative bin probabilities
V	entries are probability proportional to volume
–m	built-in function
a, b	parameters for function

SP Card Examples

mcnp

```
SDEF   ERG=D1
SI1    .01   0.1   1.0   3.0    14.0
SP1     0     2.    1.    1.     6.      (bin probabilities)
   OR
SP1 C   0     .2    .3     .4     1.0     (cumulative)


SDEF   POS=0 1 0   RAD=D2   CEL=D1
SI2    H    0    3
SP2    -21   2
SI1    L    30    40           (proportional to volume)
SP1    V                       (special case for CEL)
```

Cartesian Volume

point:	SDEF	X=5	Y=3	Z=6	
line:	SDEF	X=D1	Y=3	Z=6	
	si1 H	-50	50		
	sp1	0	1		
area:	SDEF	X=D1	Y=D2	Z=6	
	si1 H	-50	50		
	sp1	0	1		
	si2 H	0	10		
	sp2	0	1		
volume:	SDEF	X=D1	Y=D2	Z=D3	CEL=5
	si1 H	-50	50		
	sp1	0	1		
	si2 H	0	10		
	sp2	0	1		
	si3 H	-100	100		
	sp3	0	1		

Cell Rejection: if x,y,z are not in cell 5,
then reject and sample x,y,z again

ERG as a distribution

--

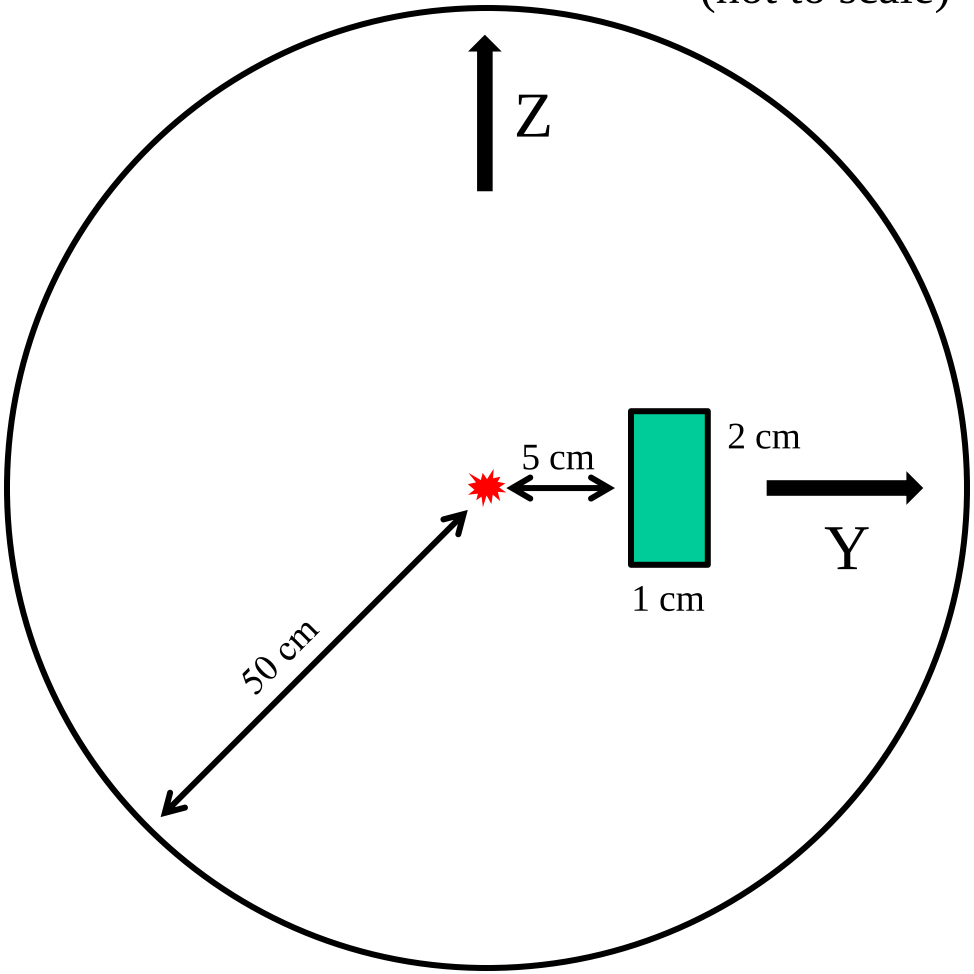
Starter input file: Tc_Cs.0

Exercise 1 – Your Mission …

- **Copy MCNP6\EXAMPLES\Tc_Cs.0 to MCNP6\WORK\Tc_Cs.1**
- **Change erg on SDEF card:**
  - 0.662 MeV from Cs-137
  - 0.14 MeV from Tc-99
  - Equal strengths: 50% / 50%.
  - Hint: Use the “L” option
- **Add tally on surface 20:**
  - Tally escaping photons.
  - Ask for 51 logarithmic energy bins from 0.001 to 0.7 MeV.
- **Run the problem:**

  mcnp6 i=Tc_Cs.1

(not to scale)



Center CZT on X and Z axes.

ΔX = ΔZ = 2 cm.

Exercise 1 – Starter Input File

```
CZT block in a void.
c      Cell cards.
1      100  -6.06  -10         imp:p,e  1.
2        0           10   -20  imp:p,e  1.
3        0                 20  imp:p,e  0.

c      Surface cards.
10     rpp  -1. 1.  5. 6.  -1. 1.
20     so   50.

c      Data cards.
m100   48000 0.9  30000 0.1  52000 1.
mode   p  e
c      CHANGE the SDEF to equal strength Cs-137 + Tc-99.
sdef   par  p  erg 0.662  $  Cs-137
c      ADD a tally for photons escaping through surface 20.
print
prdmp 2j  1
nps   10000
```

Exercise 1 – Solution

```
CZT block in a void.
1      100   -6.06   -10         imp:p,e   1.
2        0             10   -20  imp:p,e   1.
3        0                   20  imp:p,e   0.

10     rpp   -1. 1.   5. 6.   -1. 1.
20     so    50.

m100   48000 0.9   30000 0.1   52000 1.
mode   p   e
sdef   par   p   erg   d1
si1    L   0.662   0.14   $  Cs-137 + Tc-99
sp1        1.      1.     $  50% strength each.
f1:p   20
e1      0.001   50log   0.7
print
prdmp 2j   1
nps    10000
```

Checking the Results

1) Examine Print Tables in the output file.

Table 10	**source input information**
Table 110	**info about 1st 50 source particles** **x y z cell surface u v w time wgt erg**
Table 170	**source distribution frequency after run**

2) Examine the summary tables in the output file.

Weight started should be ~total source strength.

Energy started should be ~average source energy.

3) Examine the tally.

Does the spectrum make sense physically?

4) Plot the tally.

mcnp6 z

- **So far, each distribution has been independent and fully defined by the user.**
- **SDEF Distributions can also be built in functions.**
- **SDEF Distribution can also depend on previous distributions on the SDEF card.**

Some distributions already built into MCNP, mostly used for energy distributions of neutron sources

Example:

```
SDEF     ERG=D1
SP1   -3          $  Watt fission spectrum for neutron emission
                  $  default parameters, approx. U235 fission
```

Example:

```
SDEF     ERG=D1
SP1   -4          $ Gaussian fusion spectrum; default a and b
```

Built-in Functions for Source Probability and Bias Specification

Source Variable	Function No. and Input Parameters	Description
ERG	-2 *a*	Maxwell fission spectrum
ERG	-3 *a b*	Watt fission spectrum
ERG	-4 *a b*	Gaussion fusion spectrum
ERG	-5 *a*	Evaporation spectrum
ERG	-6 *a b*	Muir velocity Gaussian fusion spectrum
ERG	-7 *a b*	Spare
DIR, RAD, or EXT	-21 *a*	Power law: $p(x)=c\|x\|^a$
DIR or EXT	-31 *a*	Exponential: $p(\mu)=ce^{a\mu}$
TME, X, Y, Z	-41 *a b*	Gaussian distribution of time or position

CAUTION: Some defaults depend on which Source Variable.

Want to make the energy emitted a function of location?

1) Use FUNCTION of preceding Source Variable on SDEF card.
   - Example: SDEF Z=D20 ERG = FZ = D45

2) Change its source information card (SI) to dependent source card (DS).
   - Example: DS45 L 0.662 0.14

3) Remove SP card for the dependent source, since the probability of something is now correlated to the preceding source variable.

4) Must match number of selections on SI and DS cards.

FORM: **DSn** **option** **entries**

Option:

blank	
or H	**continuous distribution values (default)**
L	**discrete values**
S	**distribution numbers**

Other choices for option exist. See the MCNP manual for more detail.

More Dependent Source Examples

```
SDEF   POS=D1        ERG=FPOS=D2
SI1  L   0.0   0.0   0.0     10.0   0.0   0.0
SP1             1                  1
DS2  S   3      4            $ other distributions
SI3  H  2.0   10.0   14.0    $ below 2, 2-10, 10-14
SP3  D   0     0.5    0.5    $ prob: 0,  1/2,   1/2
SP4  -5                      $ evaporative spectrum
```

```
SDEF   RAD=D1     POS     FRAD     D4
SI1    S     2    3
•
•
•
DS4    L    0.0   0.0   0.0     10.0   0.0   0.0
```

Separate sources
and

Starter input file: Tc_Cs.1

Exercise 2 – Your Mission …

- **Copy MCNP6\EXAMPLES\pulse.0 to MCNP6\WORK\pulse.1**

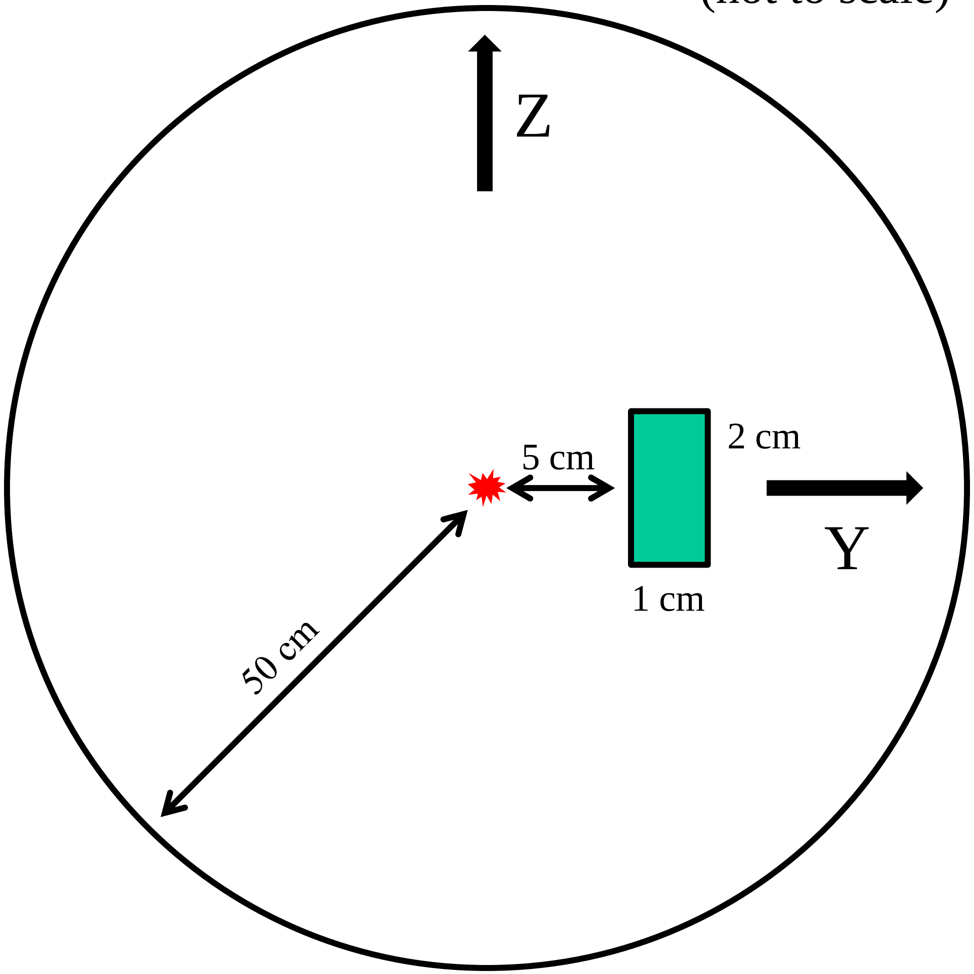
- **Change the source:**
  - Put Cs-137 at 0 0 0.5
  - Put Tc-99 at 0 0 -0.5
  - Hint: Set up “pos ... erg fpos”

- **Add pulse-height tally:**
  - F8 tally in cell 1
  - Use the energy bins from F1.

- **Run the problem:**

  mcnp6 i=pulse.1

(not to scale)



Center CZT on X and Z axes.

ΔX = ΔZ = 2 cm.

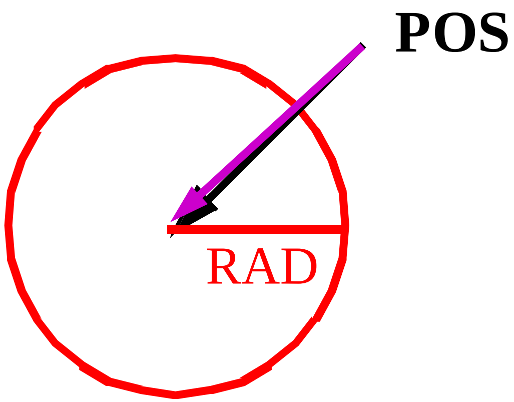
Exercise 2 – Starter Input File

```
CZT block in a void.
1      100   -6.06  -10        imp:p,e  1.
2        0            10   -20 imp:p,e  1.
3        0                  20 imp:p,e  0.

10     rpp  -1. 1.  5. 6.  -1. 1.
20     so   50.

m100  48000 0.9  30000 0.1  52000 1.
mode  p  e

sdef  par  p  erg  d1
si1   L  0.662  0.14  $  Cs-137 + Tc-99
sp1      1.     1.    $  50% strength each.
f1:p  20
e1     0.001  60log  1.0
print
prdmp 2j  1
nps   1000000
```

Exercise 2 – Solution

```
CZT block in a void.
1      100   -6.06  -10        imp:p,e  1.
2        0           10   -20  imp:p,e  1.
3        0                 20  imp:p,e  0.

10     rpp  -1. 1.  5. 6.  -1. 1.
20     so   50.

m100  48000 0.9  30000 0.1  52000 1.
mode  p  e
sdef  par  p   pos d10  erg  fpos  d1
si10  L  0 0 .5  0 0 -.5
sp10     1       1
ds1   L  0.662  0.14  $  Cs-137 + Tc-99
f8:p,e  1
e8      0.001  60log  1.0
f1:p  20
e1      0.001  60log  1.0
print
prdmp 2j  1
nps   1000000
```

uniform in volume:



SDEF RAD=D1 POS = 2 0 5
SI1 H 0 3
SP1 -21 2 $ density proportional to R^2 (default)

Uniform Spherical Volume

SP -21 2

WHY R^2 ???

Want p(r) 〈 incremental volume

$$\frac{dV}{dr} = \frac{d(4/3\,\pi\, r^3)}{dr} = 4\pi r^2$$

Prob of choosing radius r

$$p(r) \propto r^2$$

Uniform in a spherical shell:

```
SDEF  RAD=D1     POS    0    0    0
SI1       2       3
SP1    -21        2         $ default
```

Clipped Sphere and Shell Example

```
10      100   -11.4    -1 -2   imp:p=1
20      200   -1.12    +1 -2   imp:p=1
99      0              +2      imp:n=0   $ exterior

1  PX  2.0
2  So  999.


SDEF    RAD=D1    POS FRAD D5    CEL FRAD D6
SI1     S      2      4                 $  dist #2 & #4
SP1     D      1      1
SI2    H      0      3                  $  solid
SI4     H      2             3          $  shell
DS5     L   0   0   0    4   0   0
DS6     L     10            30          $  cell acceptance
```

CAUTION:

If the source starting location is always going to be on an MCNP defined surface, must add SUR to SDEF card. Otherwise particles could get lost.

Alternatively, change particle starting locations (rad, pos, or x y z) to start them in a cell, not on a surface.

Example:

```
SDEF   RAD=1.0   SUR=1
```

or

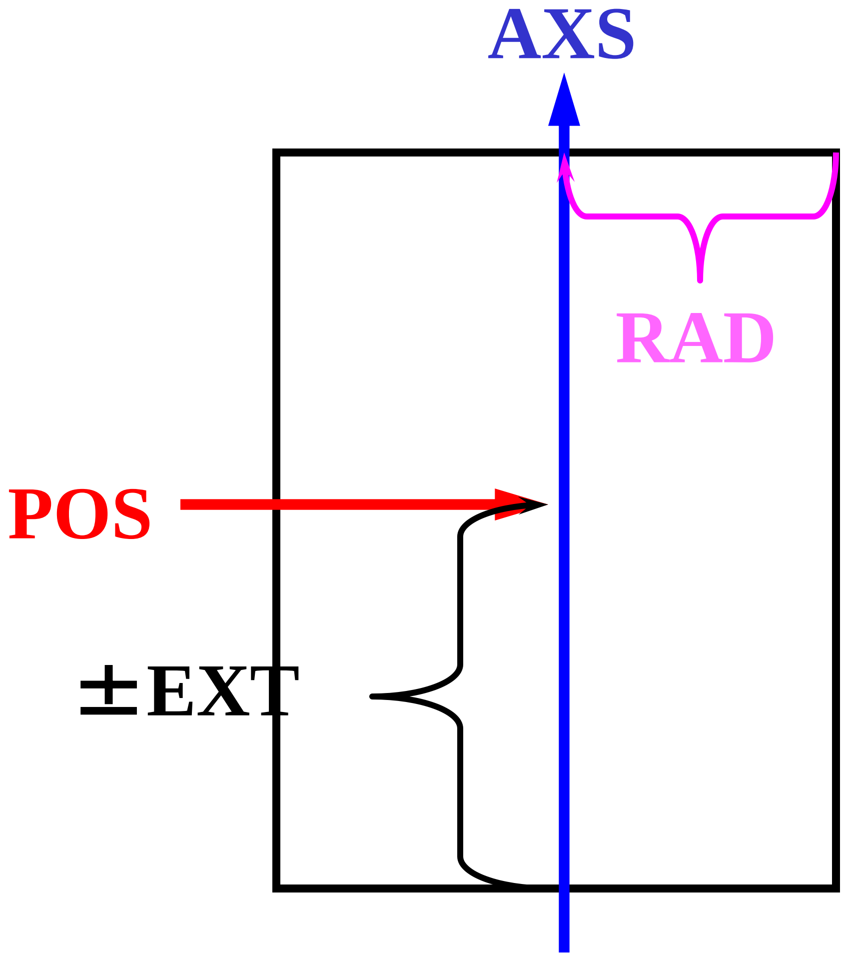
```
SDEF   RAD=0.999
```

For previous example with two spheres, SUR must be a distribution.

- For better efficiency, use a dependent distribution
- SUR can NOT depend on POS
- SDEF changed so both POS and SUR depend on energy (see file source5c)

- **A cylindrical volume source is created by adding the AXS (Axis) vector variable to the SDEF card**
- **The RAD keyword now only applies orthogonally to the AXS vector**
- **The EXT (Extent) keyword applies along the AXS vector, and defines how far along the axis from POS will be sampled.**

Cylindrical Volume Sources



AXS vector u v w

POS vector x y z

RAD distribution Dn

EXT distribution Dn

Cylindrical Volume (cont)

```
SDEF   POS   0   0   0   RAD=D1   EXT=D2   AXS   0   1   0
SI1   H    0        5.6      $  inner and outer radii
SP1       -21       1        $  default density proportional to R
SI2 H     -7        7        $  height
SP2       -21       0        $  default density constant with Y
```

Add cell acceptance/rejection:

```
SDEF   POS   0   0   0   RAD=D1   EXT=D2   AXS   0   1   0    CEL 5
```

If the cell acceptance rate is too low, the problem is terminated for inefficiency.   (EFF   Default < 1 in 100)

Source Efficiency = 0.6149 in Cell 5

Uniform Cylindrical Volume

SP -21 1

WHY R^1 ???

p(r) 〈 incremental volume

$$\frac{dV}{dr} = \frac{d(\pi r^2 h)}{dr} = 2\pi rh$$

Prob of choosing radius r

$$p(r) \propto r^1$$

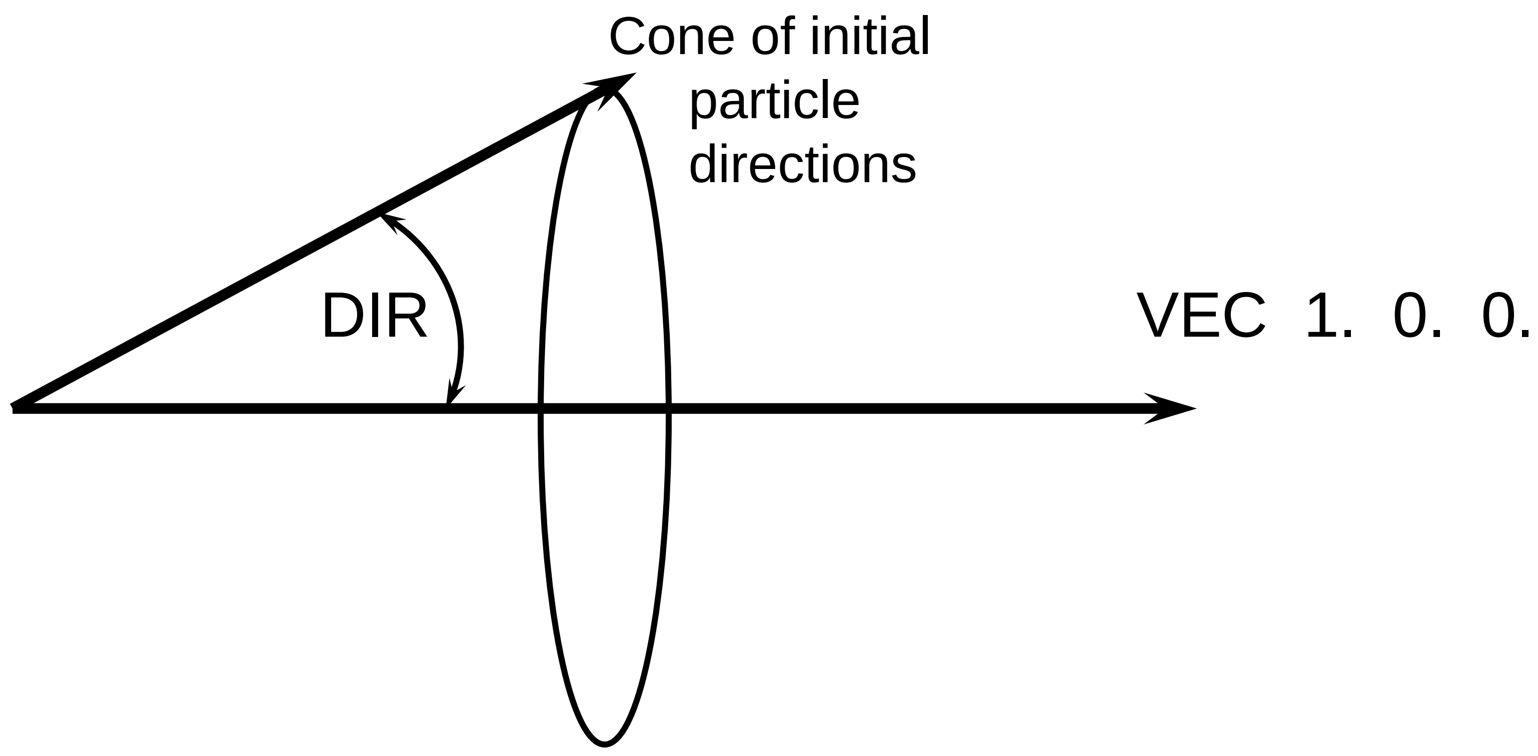
Non-Isotropic Sources

- **A non-isotropic source is created by adding the VEC vector variable to the SDEF card, and the distribution from this vector with the variable DIR**
- **DIR is the cosine of the angle, 1=forward, along direction of VEC, -1 is opposite direction of VEC.**
- **The default for DIR is equiprobable in cosine, which results in an isotropic source.**
- **Setting DIR = value results in particles being emitted in a cone.**
- **Remember, particle starting location and direction are separate (independent) variables**

Non-Isotropic Sources

- **A non-isotropic source is created by adding the VEC vector variable to the SDEF card, and the distribution from this vector with the variable DIR**

- **DIR is the cosine of the angle, 1.0=foreward, along direction of VEC.**



Photon Transport
In MCNP6

Photon Transport

- **Transporting photons in MCNP is similar to transporting neutrons in many ways.**
  - Neutral particles: straight mono-energetic paths to interaction or boundary.
  - Data tables are primarily libraries of interaction cross sections.
  - Sampling of distance to interaction, target species, choice of reaction, posting of tallies, etc., are all similar to corresponding neutron code.

- **However –**
  - Photoatomic reactions are with **atoms**, not nuclei. Use photoatomic tables.
    - No models for photoatomic reactions above the tables – no mix-and-match.
  - Photonuclear reactions are with **nuclei**. Use isotope-specific tables.
    - Models can be used above the tables – mix-and-match possible.
  - Photons are closely coupled with electrons (and positrons).
    - The cascade can introduce interesting complexities.

Photon Interactions – part 1

- **Coherent scattering (like Thomson scattering)**
  - Photon elastically scatters from atom as a whole.
    - Change of photon direction only.
    - No energy change.
    - No secondary particle produced.
- **Incoherent scattering (like Compton scattering)**
  - Photon scatters from electron within the atom.
    - Photon direction changes.
    - Photon energy changes.
    - Compton electron is produced.
    - A subshell vacancy is left. Fluorescence and/or Auger emission may follow.
- **Photoelectric interaction**
  - Incident photon is absorbed.
  - An atomic electron is ejected.
  - A subshell vacancy is left.
    - Fluorescence and/or Auger emission may follow.

Photon Interactions – part 2

- **Pair production**
  - Photon interacts with the electric field of the nucleus.
    - Incident photon disappears.
    - Electron-positron pair is created..
  - Pair and triplet production are combined and treated as pair production.

- **Photonuclear interaction**
  - Photon interacts with the nucleus itself.
    - Incident photon disappears.
    - Secondary nuclear particles are produced.
  - Best physics from isotope-specific tabular data.
  - Models available for energies above the tabular range.

Photons

When transporting photons (P on MODE card) the user has to decide:

- Should electrons be transported also?
- MCNP has two photon physics treatments:
  - Simple
  - Detailed
- There is a thick-target bremsstrahlung (TTB) option available
- Electron transport is turned on with the MODE card
- The other two options (TTB & simple/detailed) are set on the PHYS:p card

Photon Physics Treatments

- **Simple Physics Treatment**
  - Appropriate for high-energy photons and free electrons.
  - Ignores coherent scatter. Only Compton scattering with free electrons
  - Absorption by photoelectric effect is done with implicit capture. No fluorescent photons are produced.
  - Used above the energy EMCPF on the PHYS:p card.
    By default, this energy is 100 MeV.

- **Detailed Physics Treatment**
  - Appropriate for most problems. Essential for high-Z materials and deep penetration problems.
  - Includes coherent scatter with Form Factors
  - The incoherent scattering cross-section (Klein-Nishina) is modified by a form-factor specific to the atom the photon is interacting with.
  - Absorption by photoelectric effect is done with analog (explicit) capture. Zero, one or two fluorescent photons, or an Auger electron may be produced
  - Used below the energy EMCPF on the PHYS:p card.

PHYS:p Card - Preview

PHYS:p EMCPF IDES NOCOH PNINT NODOP DGB

EMCPF	sets energy cutoff for simple/detailed treatment.
IDES	turns Thick-Target Bremsstrahlung (TTB) approximation off or on, and controls secondary electron production.
NOCOH	turns off & on coherent scattering (in detailed physics).
PNINT	turns photonuclear interactions on & off and biases them.
NODOP	turns Doppler energy broadening off or on.
DGB	turns on & off delayed gammas

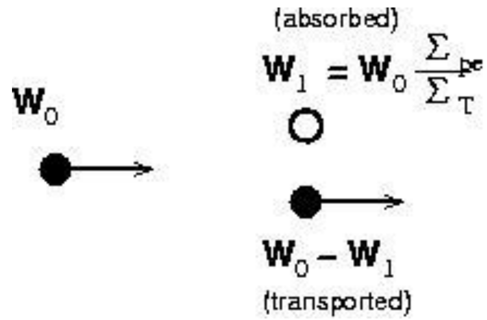
(The following slides describe what these things do.)

Photoelectric Absorption

mcnp

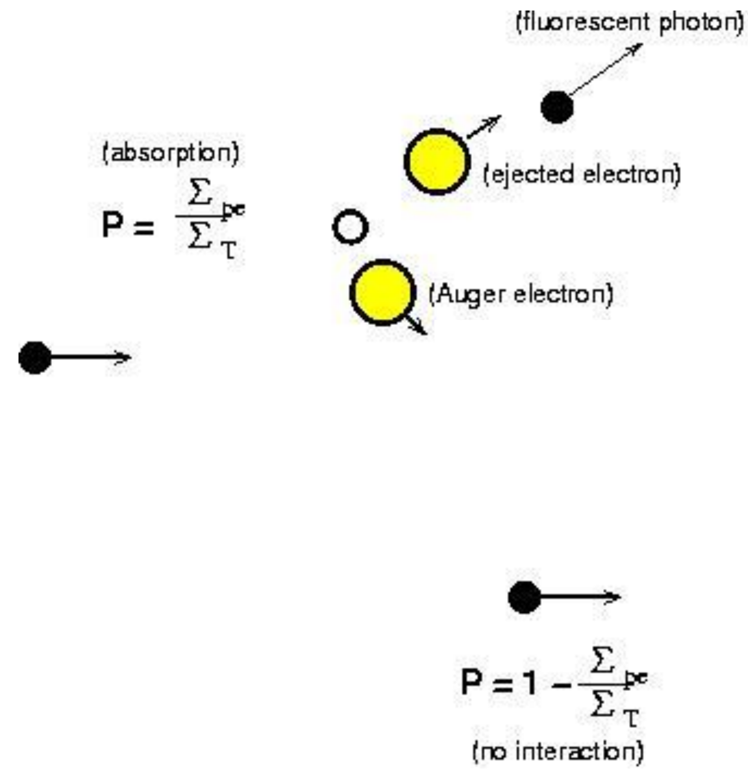
Simple physics treatment:

- Photoelectric absorption is accounted for by weight reduction
- The (reduced-weight) photon then experiences either Compton scatter or pair production



Detailed physics treatment:

- If a photoelectric event is selected, the incident photon is absorbed, and secondary particles can be produced for transport
- Otherwise, Thomson or Compton scattering or pair production occurs



Secondary Electrons

- Coherent scattering involves no energy loss and thus can't produce electrons.

- All other reactions can produce electrons.

- The user has three options for what to do with the electrons:

  1. Transport the electrons.
  2. Ignore the electrons.
  3. Thick-Target Bremsstrahlung Approximation

Thick-Target Bremsstrahlung

- **In the thick target bremsstrahlung approximation, when an electron is generated, the electron's bremsstrahlung photons are generated but the electron is terminated.**

- **If there is an E on the MODE card, MCNP transports the electrons. If there is not an E on the MODE card, TTB is the default, but it can be turned off on the PHYS:p card.**

- **Results for demo Problem, Chapter 5, MCNP Manual, running on SGI 2000 with 104,000 particles:**

MODE p, TTB off	**0.10 cpu minutes**
MODE p, TTB on	**0.14 cpu minutes**
MODE p e	**27.28 cpu minutes**

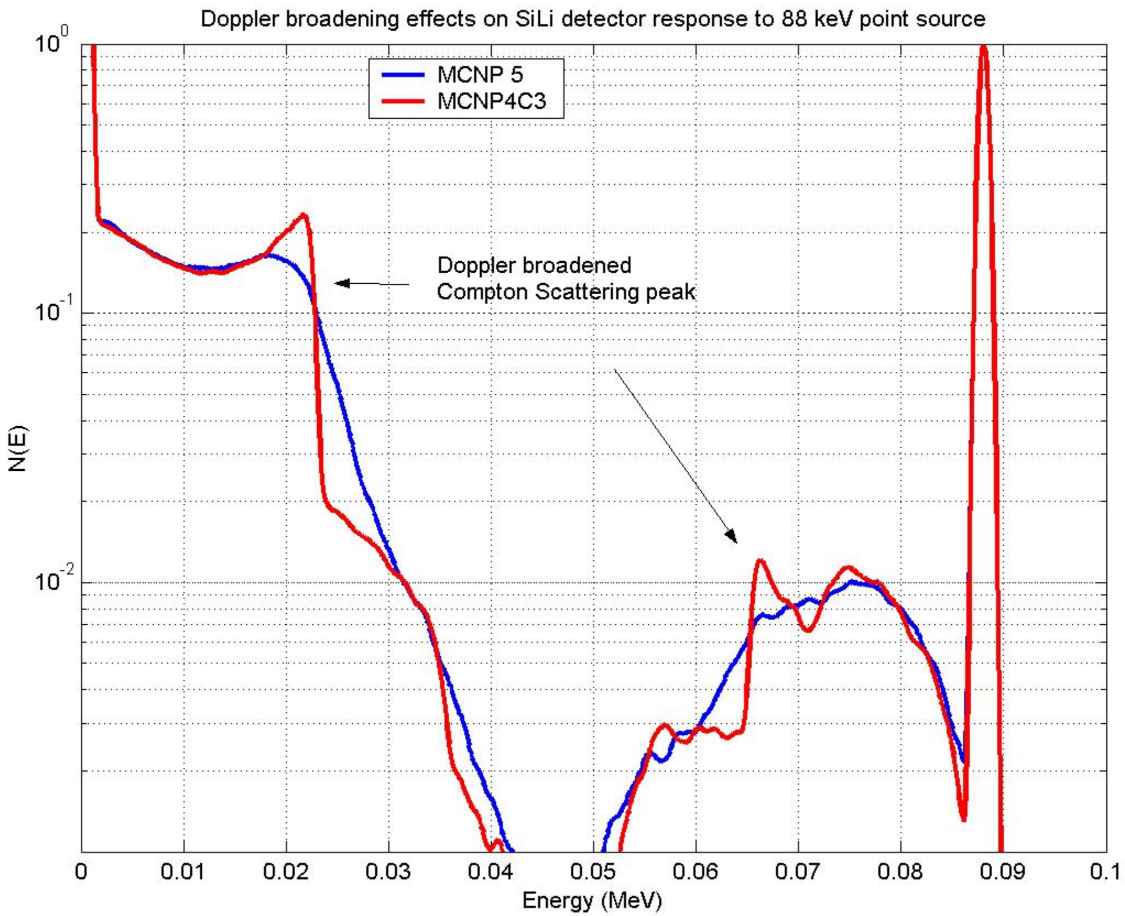
Photon Doppler Broadening

- **Incoherent photon scattering can occur with a bound electron and generate a Compton electron and a scattered photon.**
  - The electron binding effect becomes increasingly important for incident photon energies less than 1 MeV.

- **The bound electron effect on the angular distribution of the scattered photon appears as a reduction of the total scattering cross section in the forward direction.**
  - This effect has been accounted for in MCNP by modifying the Klein-Nishina cross section with a form factor.

- **The bound-electron effect on the energy distribution of the scattered photon appears as a broadening of the exit energy spectrum due to the pre-collision momentum of the electron.**
  - This second effect is the definition of Doppler energy broadening for incoherent photon scattering and is new in MCNP5.

Doppler Energy Broadening for Photons



PHYS:p Card

PHYS:p EMCPF IDES NOCOH PNINT NODOP DGB

EMCPF simple physics above EMCPF (default: 100 MeV)

IDES = 0 = TTB on or electron transport (default)
= 1 = turn off secondary electron production altogether

NOCOH = 0/1 = turn coherent scattering on/off (default: 0)

PNINT = -1 = analog photonuclear interactions on
= 0 = photonuclear physics off (default)
≤ 1 = biased photonuclear interactions on

NODOP = 0/1 = Doppler broadening on/off (default: 0 for MCNP5, 1 for MCNPX)

DGB = -102 = analog delayed gammas using line+MG models
= -101 = analog delayed gammas using MG models
= 0 = turn off delayed gamma production (default)

MCNP Photoatomic Data Libraries

- **Older Libraries:**
  - MCPLIB (e.g. 6000.01p) **–** Based largely on ENDF/B-IV. 94 elements, most 1 keV to 100 MeV.
  - MCPLIB02 (e.g. 6000.02p) **–** Enhanced using EPDL. 100 elements, all 1 keV to 100 GeV.
  - MCPLIB03 (eg. 6000.03p) – MCPLIB02, updated to include Doppler energy broadening data.
- **MCPLIB04 (e.g. 6000.04p)**
  - Based on ENDF/B-VI Release 8 (EPDL97)
  - Data provided for Z=1 to Z=100, energies from 1 keV to 100 GeV.
  - Includes Compton Doppler energy broadening data
  - Updated fluorescence data
- **MCPLIB84 (e.g. 6000.84p)**
  - Identical to MCPLIB04, but avoids a bug in the use of Compton Doppler energy broadening data.
  - **Current default in MCNP6 distribution.**
  - Similar MCPLIB63 (from MCPLIB03) also available to support backward compatibility.
- **EPRDATA12 (e.g. 6000.12p)**
  - Contains electron/photon/relaxation data supporting new enhanced electron-photon transport.
  - Changed format (not usable by MCNP5 or MCNPX).
  - Extends photon transport down to 1 eV and electron transport down to 10 eV.
  - Enables correlated sampling of subshell processes.
  - Greatly extends atomic relaxation model.
  - Testing and V&V still in progress.

Interpretation of M Cards

For photoatomic data, MCNP converts isotopic ZAIDs on M cards to elemental ZAIDs before searching for cross-section tables. Similar conversions are done for electron ZAIDs.

For example,

```
MODE    n     p
M13     6000.70c  2    92235.70c  1   92238.70c  1   plib  84p
```

is converted internally to

Neutron tables:

```
6000.70c  2          92235.70c  1          92238.70c  1
```

Photon tables:

```
6000.84p  0.5        92000.84p  0.25       92000.84p  0.25
```

Photon reaction identifiers

MT	FM	Description
501	-5	Total
504	-1	Incoherent (Compton)
502	-2	Coherent (Thomson)
522	-3	Photoelectric
516	-4	Pair production
301	-6	Heating

Electron plot quantities

MT	Description	
1	Collisional de/dx	(MeV·cm^2/g)
2	Radiative de/dx	(MeV·cm^2/g)
3	Total de/dx	(MeV·cm^2/g)
4	Total range	(g/cm^2)
5	Radiation yield, frac. energy to brems	(ratio)
6	β^2	(v^2/c^2)
7	Density correction	(MeV·cm^2/g)
8	Radiative to collisional de/dx	(ratio)
9	Major step size	(g/cm^2)
10	Energy step ave. rad. E-loss	(MeV)
11	Range for current calculation	(g/cm^2)
12	Average collisional stopping power	(MeV·cm^2/g)
13	Expected mean sampled value of λ	(dimensionless)

Cross Sections and Plotting

What is a cross section?

- **A particle travels through space in the presence of potential targets (atoms) for interaction.**

- **How likely is the particle to interact with the target?**
- **How “big” does the target look to the particle?**

- **The measure of this is the “cross section” given in units of surface area, thought of as a probability per target.**

- **Unit:** **1 barn = 10^{-24} cm²** **Symbol:** σ

Macroscopic Cross Sections

- **If σ is a cross section in barns (per atom) and N is the material density in atoms per (barn · cm) then the quantity**

$$N\left(\frac{atoms}{barn \cdot cm}\right) \cdot \sigma\left(\frac{barn}{atom}\right)$$

has the units "per cm" and so can be thought of as probability per unit length. Monte Carlo codes use this quantity together with random number generators to sample for the occurrence of interactions and for the outcome of interactions.

- **In general these cross sections depend on the composition of the target material, and on the energy of the transporting particle.**

Cross Section Data

- **For a given target element, and a given transporting particle type, cross sections for various reactions are tabulated as functions of particle energy.**

Photoelectric XS for Tungsten

Energy (MeV)	Cross Section
1.000000000002E-03	1.120554674313E+06
1.011578999997E-03	1.096187000028E+06
1.035141999998E-03	1.048971999964E+06
1.047129000005E-03	1.025979999953E+06
1.059253999998E-03	1.003533000019E+06
1.069999999998E-03	9.841321000084E+05
⋮	⋮
6.309569999956E+04	1.456286678213E-05
6.309600000140E+04	1.456279751547E-05
7.943299999851E+04	1.156666476834E-05
8.000000000352E+04	1.148465537849E-05
1.000000000030E+05	9.186955000117E-06

Pair-production XS for Tungsten

Energy (MeV)	Cross Section
1.023293000000E+00	1.896375134780E-07
1.025120000000E+00	4.575940000251E-07
1.026100000000E+00	1.034660000032E-06
1.026600000000E+00	1.458630000059E-06
1.027100000000E+00	1.984500000046E-06
1.027500000000E+00	2.485560000226E-06
⋮	⋮
6.309569999956E+04	3.449574907678E+01
6.309600000140E+04	3.449574941208E+01
7.943299999851E+04	3.451199795286E+01
8.000000000352E+04	3.451250000013E+01
1.000000000030E+05	3.451279999996E+01

- **A collection of such tabulations for a particle type and a target element, written in a standard format (known to MCNP) is a cross section data table.**

Data Libraries

- A collection of data tables is a data library.
- Typically, a library will support a single particle type, but contain a collection of different target elements or isotopes.
- MCNP is distributed together with an large set of data libraries.
- For example, the current distribution identifies
  - 8108 tables of isotopes, elements, or materials, contained in
  - 3138 libraries
- The table of contents to the available libraries is the file

  xsdir_mcnp6.1

  contained in the $DATAPATH directory.

ENDF/B & Other Libraries

- **ENDF/B**
  - **In the early 1960s, the Cross Section Evaluation Working Group (CSEWG) was founded to generate reliable nuclear data.**
  - **CSEWG continues to produce and maintain the Evaluated Nuclear Data File (ENDF).**
  - **ENDF/B-VI.0 was released in 1990, ENDF/B-VI.8 in 2000.**
  - **ENDF/B-VII.0 was released in December 2006.
ENDF/B-VII.1 was released in December 2011.**
- **Other Libraries**
  - **JEF - Joint European File**
  - **JENDL - Japanese Evaluated Nuclear Data Library**
  - **CENDL - Chinese Evaluated Nuclear Data Library**
  - **BROND - Russian**
  - **ENDL - Livermore National Laboratory**
  - **EFF - European File - Fusion**
  - **FENDL - Fusion Evaluated Nuclear Data Library**
  - **UK Nuclear Data Library**

Data Libraries for MCNP

- **Data in the ENDF/B data libraries must be processed into formats that MCNP can use -- called ACE libraries (A Compact ENDF/B).**
  - Type 1 ACE libraries - ASCII text
  - Type 2 ACE libraries - binary
  - MAKXSF code can convert & manipulate ACE libraries

- **The NJOY code is used to process ENDF/B data & produce ACE libraries for MCNP.**

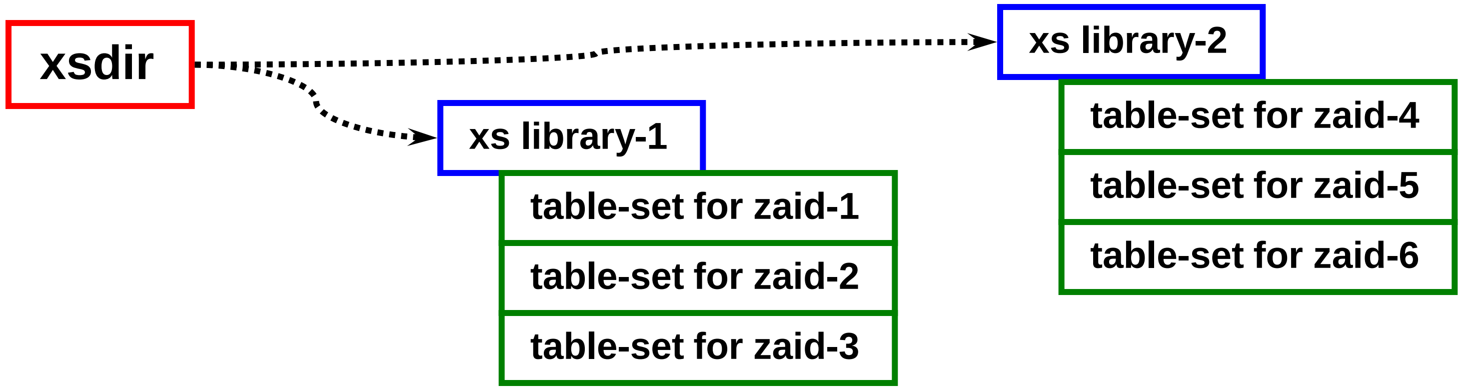
  R. E. MacFarlane and D. W. Muir, “The NJOY Nuclear Data Processing System, Version 91,” Los Alamos National Laboratory report LA-12740-M (October 1994)

- **Listing of Available ACE Data Tables, LA-UR-13-21822 on MCNP web & MCNP6 release has a listing of all the currently available ACE libraries & nuclides.**

- **In earlier releases, the xsdir file provided MCNP link between data identifiers and contents of data library.**

- **In the new release, MCNP6.1, it is the xsdir_mcnp6.1 file.**

MCNP Data



- xsdir = table of contents for cross-section libraries

- Default xsdir file: mcnp5: $DATAPATH/xsdir
  mcnp6: $DATAPATH/xsdir_mcnp6.1

- See Listing of Available ACE Data Tables, LA-UR-13-21822 for a table of available nuclide datasets

- If a nuclide is specified as just "ZZAAA" (no library identifier), the first match found in the xsdir file is used

What is in xsdir_mcnp6.1

atomic weight ratios

```
 0001  1.000000   0001  1.000000
 1000  0.99931697 1001   0.99916733   1002   1.99679968   1003   2.99013997
                        1004   3.99320563   1005   4.99205575   1006   5.99301364
⋮
118000  290.695815 118293 290.69581525
```

03/04/2013

directory

```
1001.70c 0.999167 xdata/endf70a 0 1 1 8177 0 0 2.5301E-08
1001.71c 0.999167 xdata/endf70a 0 1 2058 8177 0 0 5.1704E-08
⋮
 96242.50m 239.980599 xdata/mgxsnp 0 1 72213 1970
 96244.50m 241.967311 xdata/mgxsnp 0 1 72718 1950
 1000.84p     0.999242  xdata/mcplib84 0 1       1     1898 0 0 0.00000E+00
 2000.84p     3.968220  xdata/mcplib84 0 1     488     1970 0 0 0.00000E+00
 3000.84p     6.881380  xdata/mcplib84 0 1     993     2339 0 0 0.00000E+00
⋮
 1000.12p     0.999242 xmc/eprdata12 0 1       1    12025 0 0 0.00000E+00
 2000.12p     3.968220 xmc/eprdata12 0 1    3020    11828 0 0 0.00000E+00
 3000.12p     6.881380 xmc/eprdata12 0 1    5989    15854 0 0 0.00000E+00
⋮
 1000.03e  0.999317 xdata/el03 0 1      1    2329 0 0  .0
 2000.03e  3.968217 xdata/el03 0 1    596    2329 0 0  .0
 3000.03e  6.881312 xdata/el03 0 1   1191    2331 0 0  .0
⋮
 99000.03e  249.917466 xdata/el03 0 1   58971    2379 0 0  .0
100000.03e  254.88641 xdata/el03 0 1   59578    2379 0 0  .0
```

Back to the M Card

- **General form is ZZZAAA.nnK**

ZZZ = Atomic number, e.g. 3 (Lithium), 26 (Iron), 100 (Fermium)

AAA = Mass number: electron/photon: always 000,
neutron, e.g. 92235 — 000 means elemental.

nn = Library identifier
70-74 = ENDF/B-VII.0

K = Type of data:
- **e = condensed-history electron**
- **p = photon (may include relaxation, electron)**
- **c = continuous-energy neutron**
- **m = multigroup neutron**
- **t = thermal neutron scattering law S(α,β)**
- **… etc.**

Examples: 26000.84p 92000.03e 6000.12p

Libraries Relevant to Electrons and Photons

- **mcplib84**
  - Latest version of traditional photon transport library
  - Tables identified as ZZZAAA.84p

- **el03**
  - Current version of condensed-history electron library
  - Consistent with Integrated TIGER Series, version 3.
  - Tables identified as ZZZAAA.03e

- **eprdata12**
  - Developmental electron/photon/relaxation library
  - Allows lower-energy electron/photon transport
  - Includes improved atomic relaxation data
  - Tables identified as ZZZAAA.12p

Setting M Card Defaults

- **Recall CZT:**

  m100 48000 0.9 30000 0.1 52000 1.

- **This could be made explicit:**

  m100 48000.84p 0.9 30000.84p 0.1 52000.84p 1.

- **But the defaults can also be overridden:**

  m100 48000 0.9 30000 0.1 52000 1. plib=84p elib=03e

- **This is more important with more particle types:**

  mode n p e h

  m120 92235 1 nlib=70c plib=12p elib=03e hlib=70h

Exercise 2 — Plot some cross sections

- **Go back to MCNP6\WORK**
- **Run MCNP in cross-section plotting mode:**
  - **mcnp6 i=czt.1 ixz**
- **Type commands at the prompt.**

```
?
xs  ?
xs  30000.84p
mt  -5
xlim  .001  .1
res  xlim
mt  -5  cop  mt  -1  cop  mt  -2  cop  mt  -3  cop  mt  -4
xs  30000.84p  mt  -3  cop  xs 52000.84p
xs  m100  par e
end
```

Photon reaction identifiers

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504	-1	Incoherent (Compton)
502	-2	Coherent (Thomson)
522	-3	Photoelectric
516	-4	Pair production
301	-6	Heating

Electron plot quantities

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3	Total de/dx	(MeV·cm^2/g)
4	Total range	(g/cm^2)
5	Radiation yield, frac. energy to brems	(ratio)
6	β^2	(v^2/c^2)
7	Density correction	(MeV·cm^2/g)
8	Radiative to collisional de/dx	(ratio)
9	Major step size	(g/cm^2)
10	Energy step average rad. E-loss	(MeV)
11	Range for current calculation	(g/cm^2)
12	Average collisional stopping power	(MeV·cm^2/g)
13	Expected mean sampled value of λ	(dimensionless)

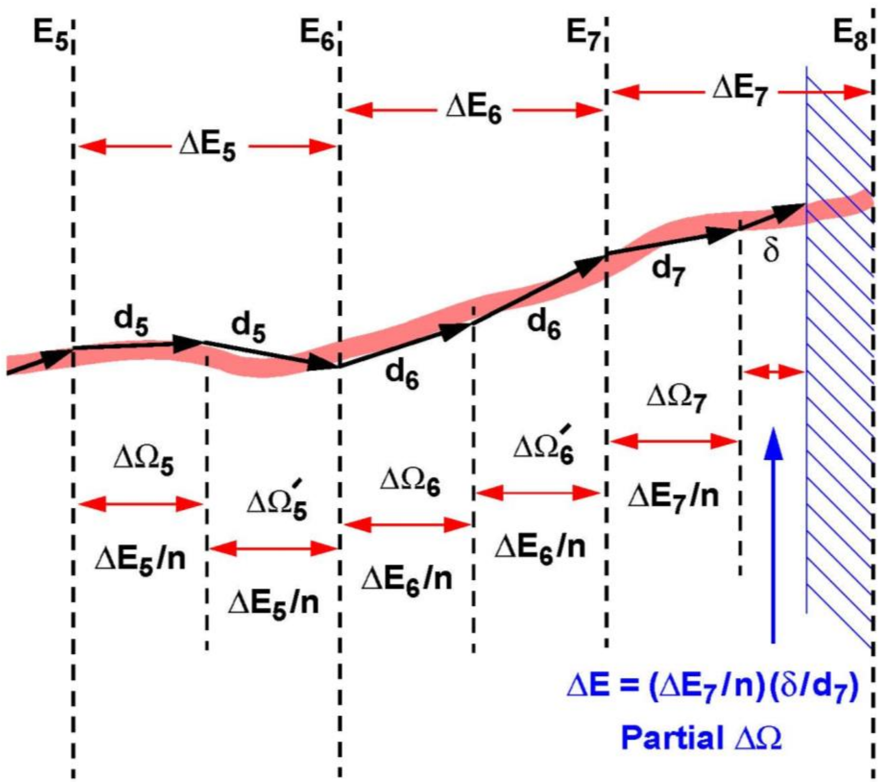
Electron Transport

In MCNP

Why are electrons different?

- **Long-range electromagnetic (Coulomb) interaction.**
- **For example, consider particles transporting in gold and slowing down from 0.5 MeV to 0.125 MeV.**
  - **Neutrons experience about 30 collisions.**
  - **Photons experience about 20 collisions.**
  - **Electrons experience about 3×10^5 Rutherford scatterings.**
- **Therefore, historically, direct analog Monte Carlo simulation of electron transport was considered impractical.**
- **The condensed-history method was developed to provide an affordable way of using Monte Carlo for charged particles.**

CLASS I CONDENSED HISTORY



d_i = standard substep distance (a function of energy).

δ = partial substep distance. $\delta < d$.

n angular substeps per energy step (here $n = 2$).

ΔE_i from CSDA plus Landau straggling, for distance $n \times d_i$.

$\Delta\Omega_i$ from Goudsmit-Saunderson theory, for distance d_i.

Multiple scattering theories

- **Continuous-Slowing-Down energy loss:**
  - **Bethe-Bloch theory for small energy exchanges.**
  - **Møller cross section for larger energy exchanges.**
  - **Density-effect corrections from Sternheimer and Peierls, or from Sternheimer, Berger, and Seltzer.**
- **Energy-loss straggling:**
  - **Landau theory with enhancements by Börsch-Supan, Blunck, Leisegang, Westphal, Chechin, Ermilova, and Seltzer.**
- **Angular deflections:**
  - **Goudsmit-Saunderson theory applied to cross sections from Riley, Rutherford, and Mott.**

Essential electron Monte Carlo references

- **Most important paper in the field:**
  - **M. J. Berger, "Monte Carlo Calculation of the Penetration and Diffusion of Fast Charged Particles," in** *Methods in Computational Physics, Vol. 1*, **edited by B. Adler, S. Fernbach, and M. Rotenberg (Academic Press, New York, 1963).**
- **Best (orange) book in the field:**
  - *Monte Carlo Transport of Electrons and Photons*, **edited by Theodore M. Jenkins, Walter R. Nelson, and Alessandro Rindi (Plenum Press, New York and London). The proceedings of the 1987 Erice, Sicily meeting.**
- **Most MCNP-specific information:**
  - **MCNP manual, chapters 2 and 3.**

Energy steps and angular substeps

- **Pre-select energy boundaries:**

  $E1 \geq E_{max}$

  $E_2 = (1/2)^{1/8} E_1$

  $E_3 = (1/2)^{1/8} E_2$

  etc…

- **Calculate energy steps:**

  D_i = average distance for $E_i \rightarrow E_{i+1}$

- **Calculate angular substeps:**

  $d_i = D_i / M(Z)$

  for a material-dependent integer M(Z).

M(Z) by element

- **Z is an average the of atomic number in a mixture:**

M(Z=1…5) = 2	**M(Z=6…9) = 3**	**M(Z=10…12) = 4**
M(Z=13…21) = 5	**M(Z=22…28) = 6**	**M(Z=29…39) = 7**
M(Z=40…49) = 8	**M(Z=50…54) = 9**	**M(Z=55…64) = 10**
M(Z=65…69) = 11	**M(Z=70…78) = 12**	**M(Z=79…84) = 13**
M(Z=85…91) = 14	**M(Z=92…100) = 15**	

- **M(Z) can be increased, if desired:**

```
m13     1000.   2.     8000.   1.     estep = 10
```

Two electron libraries

m13 1000.01e 2. 8000.01e 1.

- Essentially equivalent to ITS version 1.0

m13 1000.03e 2. 8000.03e 1.

- Essentially equivalent to ITS version 3.0
- Improved radiative stopping powers
- Improved density-effect corrections
- Eliminates some atomic relaxation inconsistencies
- More detailed sampling of bremsstrahlung production
- Allows NumB bremsstrahlung biasing
- Default data library in all recent MCNP releases

A calculation must use all .01e or all .03e

Input cards that work with electrons

mode p e
… or mode n p e

imp:e
cell importances

wwp:e
weight window parameters

wwn:e
weight window bounds

wwe:e
weight window energies or times

wwge:e
weight window generator energies or times

F6:e
electron heating

f1:e
surface current tally

f2:e
surface flux tally

f4:e
volume flux tally

f8:p,e
pulse-height tally

∗f8:p,e
energy deposition

+f8:e
charge deposition

sdef …par = e
electron source

phys:e
physics (and options) card

cut:e
time, energy, weight cutoffs

elpt:e
energy cutoffs by cell

esplt:e
energy splitting

tsplt:e
time splitting

fmesh:e, {r,c,s}mesh:e
mesh tallies

sdef …par=f (or -e)
positron source

Input cards that do not work with electrons

f5:e
No uncollided flux
∴ no point detectors

f5x:e
No uncollided flux
∴ no ring detectors

f5y:e
No ring detectors

f5z:e
No ring detectors

f7:e
No fission heating

fip:e
No pinhole radiograph
(based on detectors)

fir:e
No standard radiograph

fic:e
No cylindrical radiograph

dxt:e
No uncollided flux
∴ no DXTRAN

dxc:e
No DXTRAN probabilities

ext:e
No exponential transform

fcl:e
No forced collisions

pert:e
No perturbation theory

Special treatment for electron current tallies

F1:E tallies can distinguish between electrons and positrons:

f1:e	7	
ft1	elc	n
fq1	e	u

There are three forms:

n = 1 prints	($e^+ - e^-$)		
	8.303E-01 0.0046		
n = 2 prints	(e^+)	(e^-)	($e^+ + e^-$)
	8.473E-01 0.0042	1.700E-02 0.0774	8.643E-01 0.0044
n = 3 prints	(e^+)	($-e^-$)	($e^+ - e^-$)
	8.473E-01 0.0042	–1.700E-02 0.0774	8.303E-01 0.0046

Pulse-height and related tallies

f8:e	**7**				
e8	**0.**	**1.e-6**	**1.**	**8i**	**10.**

Fraction of source weight of particles that deposit energy in cell 7 within energy bins.

E < 0.	**identify (non-correlated) negative contributions;**
E < 1.e-6	**distinguish photons entering the cell, but not contributing;**
E < 1. etc.	**standard pulse-height energy bins.**

No variance reduction (except source biasing) allowed.

∗f8:e 7

Energy deposition in cell 7 **Units: MeV**
Variance reduction allowed.

+f8:e 7

Charge deposition in cell 7 **Units: net electron charge, with positron > 0.**
Variance reduction allowed. **(one electron charge ≅ 4.8032e-19 Coulomb.)**

Energy deposition

```
mode    p    e
*f8:p,e 7    13   …
```

This is the traditional standard method for mode p e problems.

```
mode    p    e
+f6     7    13   …
```

Consistent with *F8, with additional binning capabilities.

```
mode    p
f6:p    7    13   …
```

Only track-length estimation is available for mode p problems. It is valid only when electrons are mostly trapped in the cells where they are created.

```
mode    p    e
sdef    …    par=p
f6:p    7    13   …
```

This is allowed, but valid only when electrons are mostly trapped.

```
mode    p    e
sdef    …    par=e
f6:p    7    13   …
```

Allowed, but wrong!

Physics (and options) card

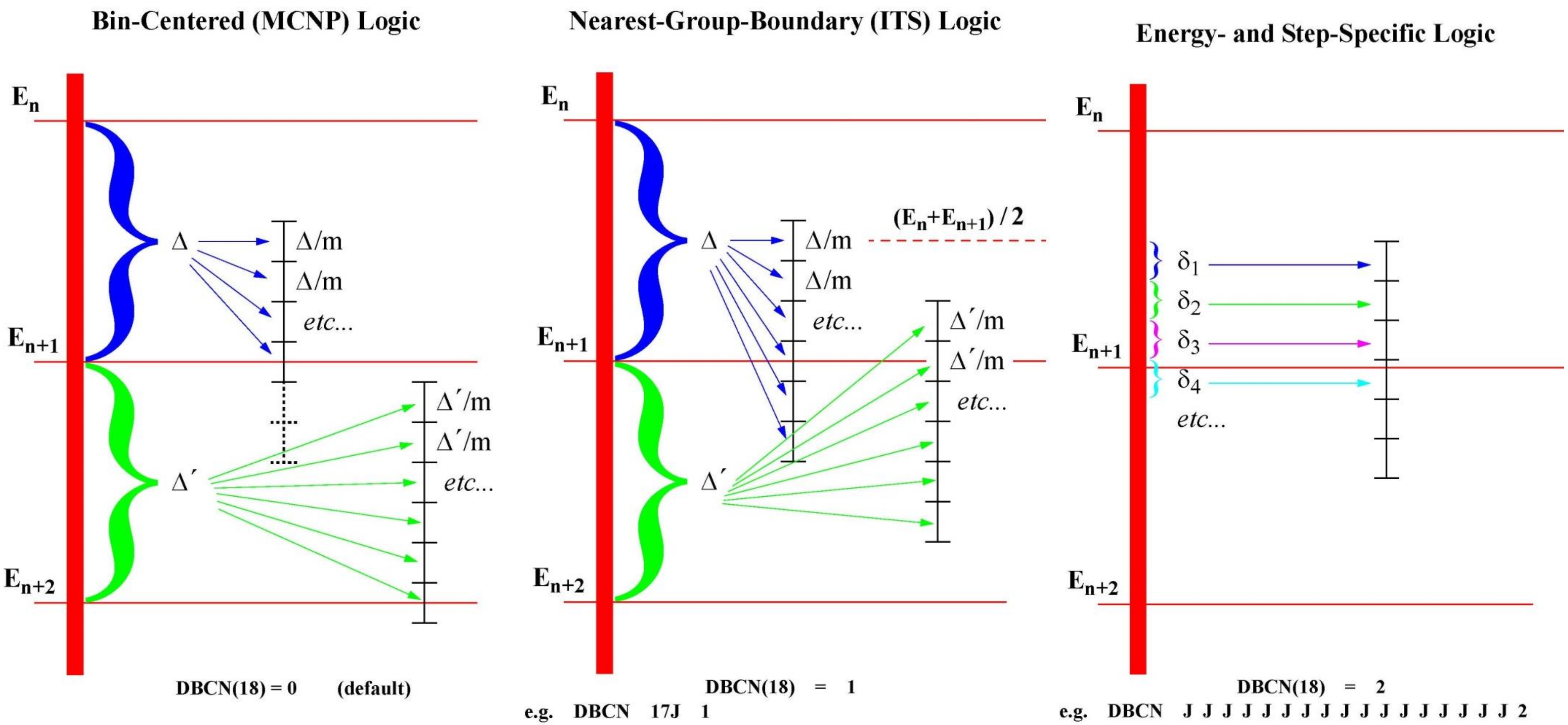
PHYS:E E_{max} I_{des} I_{phot} I_{bad} I_{strg} B_{num} X_{num} R_{nok} E_{num} Num_B

E_{max}		upper limit for electron energy	(100 MeV)
I_{des}	= 0/1 =	on/off electron production from photons	0
I_{phot}	= 0/1 =	on/off photon production from electrons	0
I_{bad}	= 0/1 =	detailed/simple bremsstrahlung angular distribution	0
I_{strg}	= 0/1 =	straggling/CSDA electron energy loss	0
B_{num}	$\geq$ 0.	scaling of bremsstrahlung photons	1
X_{num}	$\geq$ 0.	scaling of electron-induced X-rays	1
R_{nok}	$\geq$ 0.	scaling of knock-on electrons	1
E_{num}	$\geq$ 0.	scaling of photon-induced electrons	1
Num_B	= 0/1 =	off/on one-per-substep bremsstrahlung biasing	0

Three forms of the straggling logic

- **Energy- and step-specific logic:**
  - **Default option in MCNP6.**
  - **Available in MCNP5 but not in MCNPX.**
  - **Necessary for new enhanced electron/photon transport in MCNP6.**
  - **DBCN 17J 2.**
- **Nearest-group-boundary (ITS) logic:**
  - **More accurate than DBCN(18) = 0.**
  - **DBCN 17J 1.**
- **Bin-centered (MCNP) logic:**
  - **The original MCNP method. Was the default in MCNP5 and MCNPX.**
  - **DBCN 17J 0.**

Straggling Logic



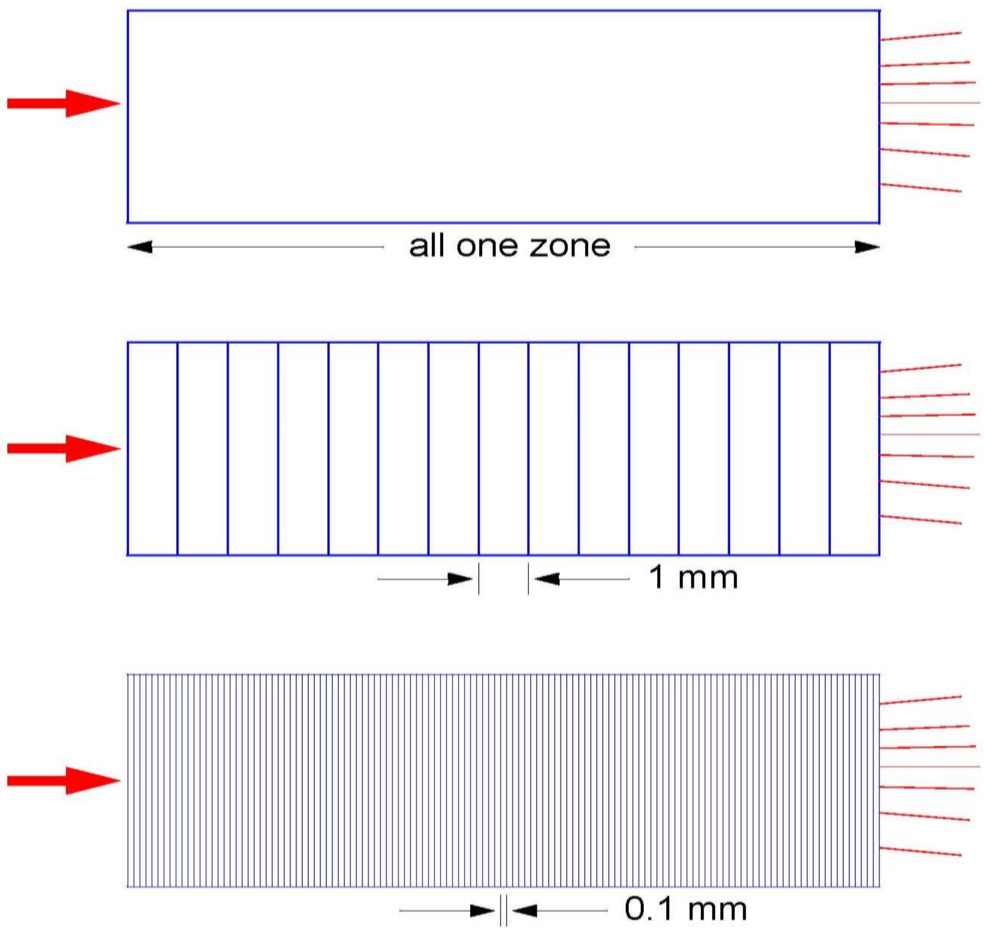
Test Problem for new algorithm…

mcnp

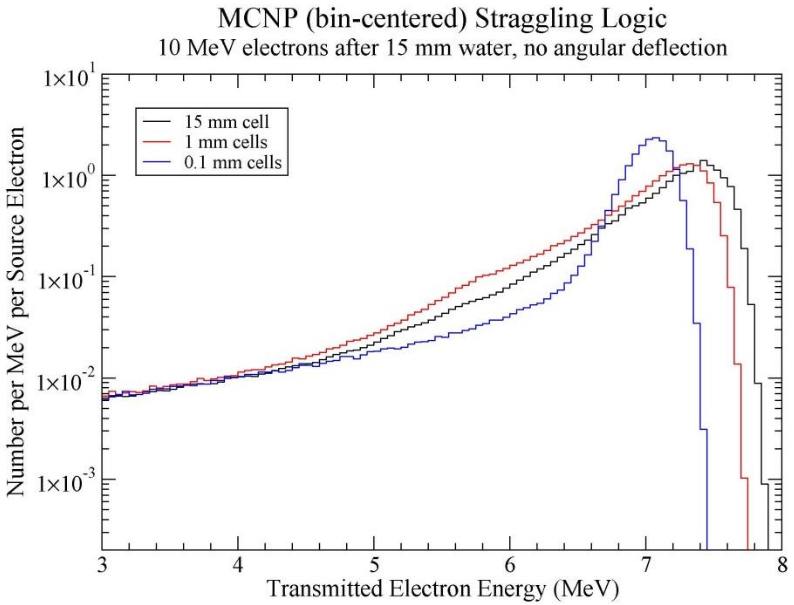
Three Equivalent Test Cases

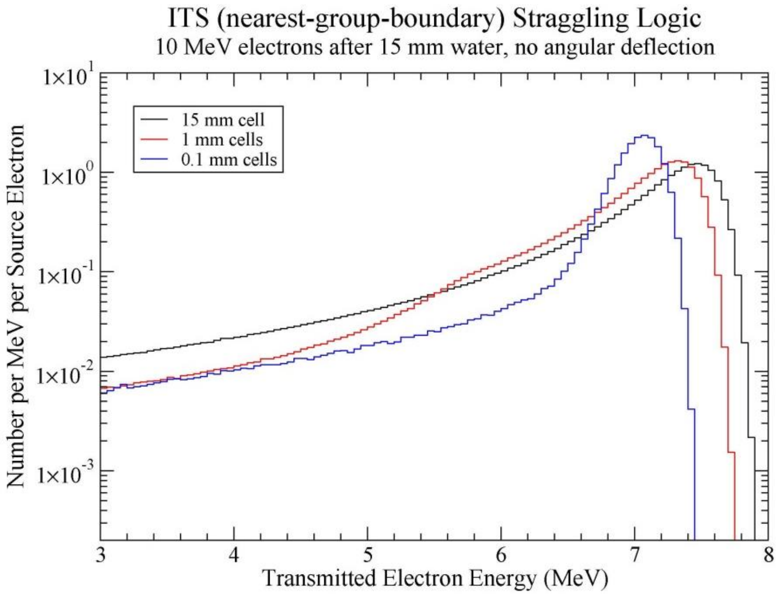
10-MeV electrons on a 15-mm slab of water

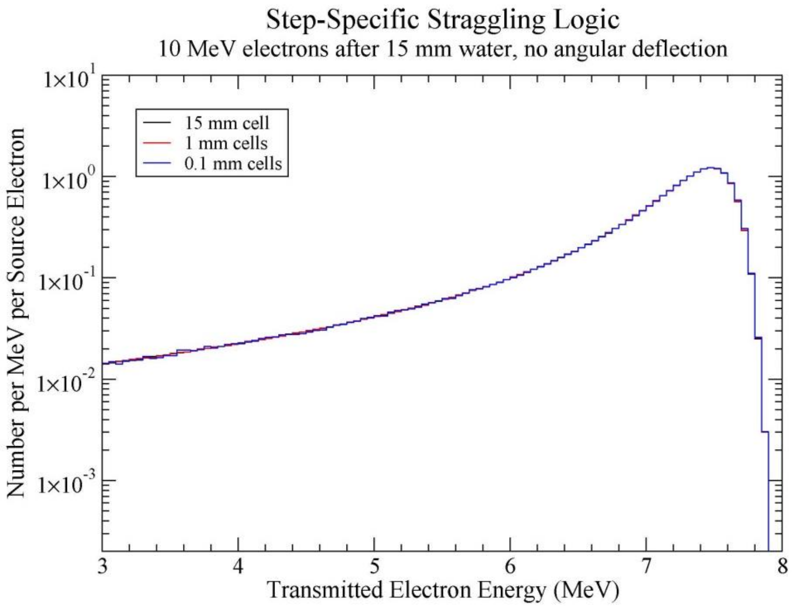
No angular deflection. Substep = 1.364 mm



Compare Results for Each Straggling Logic







MCNP5, version 1.40 and later

Electron/positron exercise - inp_w.txt

```
Simple electron/positron problem in tungsten
1     1 -19.66 -1   imp:e,p=1
2     0          1   imp:p,e 0

1     so  0.008     $ Radius is about 1/5 of an electron range.

mode     p e
sdef     erg 1.  par e
m1       74000  1
f21:p    1
e21      .1 .3 .51 .52 1.
f1:e     1
print
nps      1000
dbcn  17j   2
```

Convert to positron source

Add ELC special treatment (type 3) to electron surface current tally

Add *F8 and +F18 energy and charge deposition tallies for cell 1

Exercise solution = inp_w.txt

```
Simple electron/positron problem in tungsten
1     1 -19.66 -1   imp:e,p=1
2     0          1   imp:p,e 0

1     so   0.008     $ Radius is about 1/5 of an electron range.

mode     p e
sdef     erg 1.   par f
m1       74000  1
f21:p    1
e21      .1 .3 .51 .52 1.
f1:e     1
ft1      elc  3
fq1      e u
*f8:p,e 1
+f18:e   1
print
nps      1000
dbcn  17j   2
```

Advanced Tallies

Additional Tally Capabilities

- Particle Tracks (PTRAC)
- Reaction Multipliers (FM)
- Pulse Height (F8)
- Special Treatments (FTn)
  - Neutron Capture (CAP)
  - Pulse-Height Light (PHL)
  - Tally Tagging (TAG)
- Next Event: Point (F5), Ring (FY5)
- Special Tallies
  - Mesh Tallies
  - Radiography

PTRAC – Particle Tracks

PTRAC enables writing particles to a file for post-processing

- **Useful for particle track plotting in MORITZ**
- **Useful for post-processing using various filters**

PTRAC differs from SSW / SSR:

- **Filters events**
- **Can be ascii**

PTRAC format:

PTRAC KEYWORD=*value(s)* …

Example:

PTRAC* FILE=*asc* WRITE=*all* EVENT=*sur* MAX=*50000

PTRAC – Particle Tracks

PTRAC Options:

FILE = asc or bin	**(default=bin)**
MAX = maximum number of events	**(default=10000)**
WRITE = pos or all	**pos=x,y,z (default)**
	all=x,y,z,u,v,w,E,W,T
EVENT = src, bnk, col, sur, ter, cap	**(default=all)**
TYPE = p, p, p, …	**particle types n, p, …**
FILTER = values,parameter …	
= 2,ICL	**(cell 2)**
= .001,14.0,E	**(.001 < E < 14.0)**

History Filter Keywords:

NPS, CELL, SURFACE, TALLY, VALUE

… only write PTRAC events to particles in NPS range, passing through cells in CELL list, crossing surfaces in SURFACE list, contributing to tallies in TALLY list, etc.

Exercise 1

copy c:\MCNP6\EXAMPLES\atal1

Check that the following line is present

PTRAC **FILE=*asc*** **WRITE=*all***

Run the problem and examine output.

mcnp6 i=tal1

Exercise 1 - PTRAC output

See Appendix F in MCNP6 Manual

```
 -1
mcnp     6                        01/15/14 02/03/14 11:50:33
tal3 - PTRAC Example
   1.4000E+01  1.0000E+00  1.0000E+02  0.0000E+00  0.0000E+00  1.0000E+00  1.0000E+00  0.0000E+00  1.0000E+00  1.0000E+04
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.0000E+00  2.0000E+00  0.0000E+00  0.0000E+00
     2    7    9    8    9    8    9    8    9    8    9    0    4    0    0    0    0    0    0    0
    1    2    7    8    9   16   17   18   19   20   21   22   23   24   25   26   27   28    7    8   10   11   16   17   18   19   20   21   22   23
   24   25   26   27   28    7    8   12   13   16   17   18   19   20   21   22   23   24   25   26   27   28    7    8   10   11   16   17   18   19
   20   21   22   23   24   25   26   27   28    7    8   14   15   16   17   18   19   20   21   22   23   24   25   26   27   28
          1       1000
       3000          1         40          2          3          0          0
  -0.20000E+01  0.00000E+00  0.00000E+00  0.10000E+01  0.00000E+00  0.00000E+00  0.20000E+01  0.10000E+01  0.00000E+00
       3000          2        2.2        179          2          2          2          0
  -0.11000E+01  0.00000E+00  0.00000E+00  0.10000E+01  0.00000E+00  0.00000E+00  0.20000E+01  0.10000E+01  0.30021E-02
       4000          3        1.2        179          2          1          1          0
  -0.10000E+01  0.00000E+00  0.00000E+00  0.10000E+01  0.00000E+00  0.00000E+00  0.20000E+01  0.10000E+01  0.33356E-02
       4000          3       3000         -1          2          1          1          1
  -0.31983E+00  0.00000E+00  0.00000E+00 -0.92576E-01  0.94706E+00 -0.30743E+00  0.37435E+00  0.10000E+01  0.56044E-02
       4000          3       3000         -1          2          1          1          2
  -0.34593E+00  0.26700E+00 -0.86672E-01 -0.48678E+00 -0.51751E+00  0.70372E+00  0.17852E+00  0.10000E+01  0.65448E-02
       5000          3       3000         -3          2          1          1          3
  -0.47352E+00  0.13135E+00  0.97781E-01 -0.48678E+00 -0.51751E+00  0.70372E+00  0.17852E+00  0.10000E+01  0.74191E-02
       2011          3         12          1          2          1          1          3
  -0.47352E+00  0.13135E+00  0.97781E-01 -0.48678E+00 -0.51751E+00  0.70372E+00  0.17852E+00  0.10000E+01  0.74191E-02
. . .
```

Header

Particle track information

Los Alamos NATIONAL LABORATORY EST. 1943

Exercise 1 - PTRAC output

```
 -1
mcnp    6                      01/15/14 02/03/14 11:50:33
tal3 - PTRAC Example
```

Code Version, Run ID and Title

BUFFER=100 **FILE=ASC** **MAX=10000**

```
 1.4000E+01  1.0000E+00  1.0000E+02  0.0000E+00  0.0000E+00  1.0000E+00  1.0000E+00  0.0000E+00  1.0000E+00  1.0000E+04
 0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.0000E+00  2.0000E+00  0.0000E+00  0.0000E+00
```

WRITE=ALL

PTRAC settings echoed

Number of variables listed on given lines

```
   2    7    9    8    9    8    9    8    9    8    9    0    4    0    0    0    0    0    0    0
```

Types of variables listed on given lines

nps: 1 2

src: 7 8 9 16 17 18 19 20 21 22 23 24 25 26 27 28

bnk: 7 8 10 11 16 17 18 19 20 21 22 23 24 25 26 27 28

sur: 7 8 12 13 16 17 18 19 20 21 22 23 24 25 26 27 28

col: 7 8 10 11 16 17 18 19 20 21 22 23 24 25 26 27 28

ter: 7 8 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28

Exercise 1 - PTRAC output

See Appendix F in MCNP6 Manual

```
1      Event  node   nsr  particle  cell  material  ncp
   x        y        z        u        v        w      energy   weight   time
-0                                                  0000E+01  0.10000E+01  0.00000E+00
       Event  node surface angle particle  cell material  ncp
       3000         2       2.2       179         2         2         2         0
-0.11000E+01  0.00000E+00  0.00000E+00  0.10000E+01  0.00000E+00  0.00000E+00  0.20000E+01  0.10000E+01  0.30021E-02
       4000         3       1.2       179         2         1         1         0
-0                                                                  01  0.10000E+01  0.33356E-02
       Event  node   ZA    MTP   particle cell material  ncp
       4000         3      3000        -1         2         1         1         1
-0.31983E+00  0.00000E+00  0.00000E+00 -0.92576E-01  0.94706E+00 -0.30743E+00  0.37435E+00  0.10000E+01  0.56044E-02
.
.
.
       Event  node   nter   branch  particle cell material  ncp
-      Event  node   ZA     NTYN   particle  cell material  ncp   +00  0.10000E+01  0.74191E-02
       5000         4     32000         3         3         1         1         3
-0.47352E+00  0.13135E+00  0.97781E-01 -0.18214E+00  0.77149E-01  0.98024E+00  0.17852E+00  0.10000E+01  0.74191E-02
```

sur Line (7 8 12 13 16 17 18 19) (20 21 22 23 24 25 26 27 28)

col Line (7 8 10 11 16 17 18 19) (20 21 22 23 24 25 26 27 28)

ter Line (7 8 14 15 16 17 18 19) (20 12 22 23 24 25 26 27 28)

bnk Line (7 8 10 11 16 17 18 19) (20 21 22 23 24 25 26 27 28)

Reaction Multipliers (FM)

Form: **FMn (C_1 m_1 R_1) (C_2 m_2 R_2) . . . T**

- n = tally number
- C_i = multiplicative constant (if -1 for n=4, use cell ρ_a)
- m_i = material number identified on an Mm card
- R_i = a combination of ENDF reaction numbers

What It Does:

$$C \cdot \int \Phi(E) R_m(E) dE$$

Common Neutron R Values

- -1 = total cross section
- -2 = absorption
- -4 = heating (MeV/collision)
- -6 = fission cross-section
- -7 = fission ν
- -8 = fission Q (MeV/fission)

FM Reaction Values

NEUTRONS		PHOTONS		PROTONS	
1	Total	-1	incoherent	1	total
-2	Absorption	-2	coherent	2	non-elastic
-4	Heating	-3	photoelectric	3	elastic
-5	gamma prod'n	-4	pair production	4	heating
-6	total fission	-5	total	>4	other rxns.
-7	fission v	-6	heating	I00R	particle I from rxn. R
-8	fission Q	1	PN total		
16	(n,2n)	2	PN non-elastic		
17	(n,3n)	3	PN elastic		
18	(n,fx)	4	PN heating		
		> 4	PN other rxns.		
		I00R	PN particle I from rxn. R		

Examples of FM

F2:N	1 2	$ 36 tally bins
FM2	(1.0) (2.0) (3.0)	$ Constant multipliers
E2	.5 1 2 4 10 T	$ Energy bins
F4:N	(1 2) 3 T	$ 6 tally bins
FM4	(-1 1 -6 -7)	$ Track-length estimate of k_{eff}
	(-1 2 1 -4)	$ Neutron Heating (MeV/cm3)

Pulse Height Tally

F8:<*pl*> $C_1 \ldots C_n$

- **Different from all other tallies**
  - Surface estimator of cell energy deposition
  - Can use variance reduction with F8
  - Energy is accumulated from all tracks of a particle's history
- **Mimics pulse-height detectors: energy bins contain pulses**
  - Energy <0: non-analog negative score balance
  - Energy ~ 0: particles pass through without energy loss
  - Energy > 0: pulse of W put into appropriate energy bin

Exercise 2: Pulse Height Tallies

copy c:\MCNP6\EXAMPLES\atal2

- **Use energy bins 0 1.e-6 0.1 199i 2.0**
- **Do a pulse-height tally (F8) in H2O**
- **Run the problem.**

mcnp6 i=tal2 n=tal2a.

- **Examine output file summary table.**
- **Plot tally 8 results.**

Exercise 2: Pulse Height Tallies

- Change radius from 10000 to 10 cm
- Run the problem.

  mcnp6 i=tal2 n=tal2b.

- Examine output file summary table and Plot tally 8.
- What is different and why?

- Repeat the last two steps with "mode p e" and F8:e instead of F8:p.

Exercise 2: Pulse Height Tallies

copy c:\MCNP6\EXAMPLES\atal2

- Use energy bins 0 1.e-6 0.1 199i 2.0
- Do a pulse-height tally (F8) in H2O
- Do an energy-deposition pulse-height tally (*F8)
- Do energy deposition (F6) and equivalent FM4 energy deposition
- Do +F6 energy deposition
- Plot the tallies

Exercise 3: Pulse Height Tallies

copy c:\MCNP6\EXAMPLES\atal3

- **Use energy bins 0 1.e-6 .001 .01 .1 100ilog 101**
- **Do a pulse-height tally (F8) in H2O**
- **Do an energy-deposition pulse-height tally (*F8)**
- **Do energy deposition (F6) and equivalent FM4 energy deposition**
- **Do +F6 energy deposition**
- **Plot the tallies**

Tally Treatments (FT)

Form: **FTn id$_1$ p$_{1,1}$ p$_{1,2}$ … id$_2$ p$_{2,1}$ p$_{2,2}$… …**

n = tally number
Id = Special tally treatments given below
$p_{i,j}$ = parameter j for the i^{th} tally treatment.

Special tally treatments:

FRV Fixed arbitrary reference direction for tally 1 cosine binning.
GEB Gaussian energy broadening.
TMC Time convolution.
INC Identify the number of collisions.
ICD Identify the cell from which each detector score is made.
SCX Identify the sampled index of a specified source distribution.
SCD Identify which of the specified source distributions was used.
ELC Electron current tally.
PTT Put different multigroup particle types in different user bins.
PHL Pulse-height light tally with anticoincidence (f8 only). (MCNP6)
CAP Coincidence capture (f8 only). (MCNP6)
RES Residual nuclei. (MCNP6)
TAG Tally tagging. (MCNP6)
LET Tally stopping powers instead of energy. (MCNP6)
ROC Receiver-operator characterization (MCNP6)

FTn TAG : Tally Tagging

Tally tagging separates a tally into bins by how and where the scoring particle was produced:

1) a cell of interest where particles are produced;

2) a target nuclide from which the particle is emitted; and

3) a reaction or, in the case of spallation, a residual nuclide of interest.

not for F8 tallies!

FT*n* TAG *a*

a=1 : collided particles lose their tag; bremsstrahlung and annihilation photons included in the bin of collided particles;

a=2 : collided particles lose their tag; bremsstrahlung and annihilation photons given special tags for segregation;

a=3 : all collided particles retain their production tag.

FTn TAG : Tally Tagging

FUn card required:

FU*n bin*$_1$ *bin*$_2$ ... *bin*$_N$

bin$_J$ **= CCCCCZZAAA.RRRRR**

CCCCC ***= cell number or 00000***

ZZAAA ***= target nuclide identifier***

RRRRR ***= reaction identifier (e.g. 00102 for n,γ) or residual nuclide ZAID for model reactions***

FTn TAG : Tally Tagging

bin_J = CCCCCZZAAA.RRRRR special cases:

-0000000001 or -1 source particle tag for all cells
-CCCCC00001 source (i.e., uncollided) particle tag for cell CCCCC
0000000000 or 0 scattered particle tag
10000000000 or 1e10 everything else tag

<u>Photon tally special designations for ZZAAA.RRRRR:</u>

00000.00001	***bremsstrahlung from electrons***
ZZ000.00003	***fluorescence from nuclide ZZ***
00000.00003	***K x-rays from electrons***
00000.00004	***annihilation photons from e-***
ZZ000.00005	***Compton photons from nuclide ZZ***
ZZAAA.00006	***muonic x-rays from nuclide ZZAAA***

FTn TAG : Tally Tagging

binJ* = CCCCCZZAAA.RRRRR *special cases:

<u>Electron special designations for ZZAAA.RRRRR:</u>

ZZ000.00001 ***photoelectric from nuclide ZZ***

ZZ000.00003 ***Compton recoil from nuclide ZZ***

ZZ000.00004 ***pair production from nuclide ZZ***

ZZ000.00005 ***Auger electron from nuclide ZZ***

00000.00005 ***Auger electron from electrons***

00000.00006 ***knock-on electrons***

<u>Neutron/photon special designations for ZZAAA.RRRRR:</u>

ZZAAA.99999 ***delayed particles from fission or residuals of ZZAAA***

FTn TAG : Tally Tagging

Examples:

F5:P 0 0 0 1

FT5 TAG 3

FU5 -1.0 0000106012.00005 0000106012.00000 0000026056.00102 0000026056.00000 0000000000.00051 10000000000.00000

-1.0 ***Source photons***

0000106012.00005	***Compton from 12C cell 1***
0000106012.00000	***Remaining photons from 12C in cell 1***
0000126056.00102	***Capture gammas from 56Fe in cell 1***
0000026056.00000	***Remaining photons/gammas from 56Fe***
0000000000.00051	***Remaining 1st inelastic level [n,n'] gammas***
10000000000.00000	***Remaining gammas***

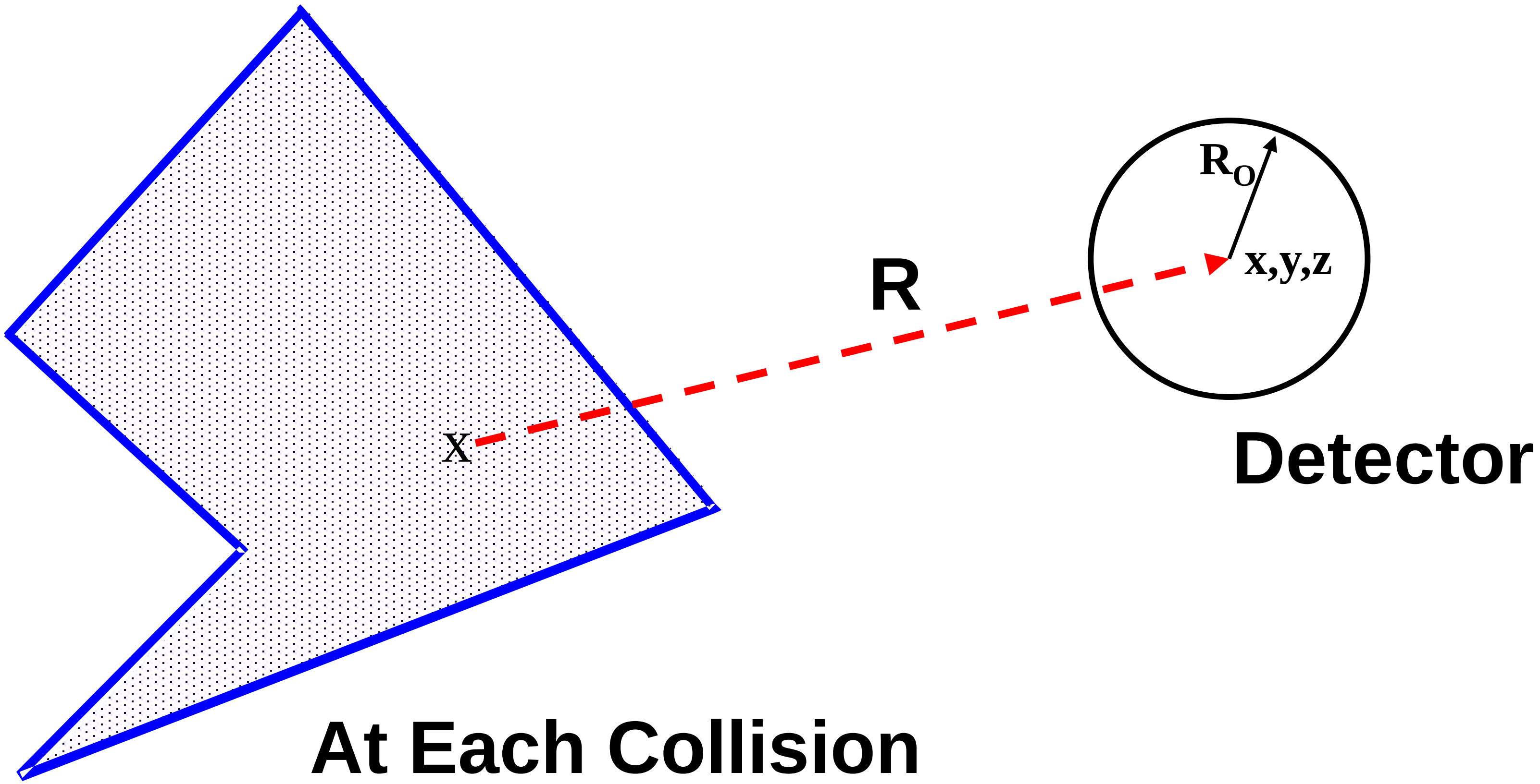
Physics muon example will use tagging

Exercise 7: Tally Tagging

copy c:\MCNP6\EXAMPLES\atal7

- **Add photon type 1 tally to back plane of water block.**
- **FT TAG option to tally 1.**
  - **Source**
  - **Bremstrahlung**
  - **Fluorescence from both**
  - **Compton from Oxygen**
  - **Annihilation photons**
  - **Everything else (1e10)**

Point Detectors



At Each Collision

$$\Phi = Wp(\mu)e^{-\lambda}/(2\pi R^2)$$

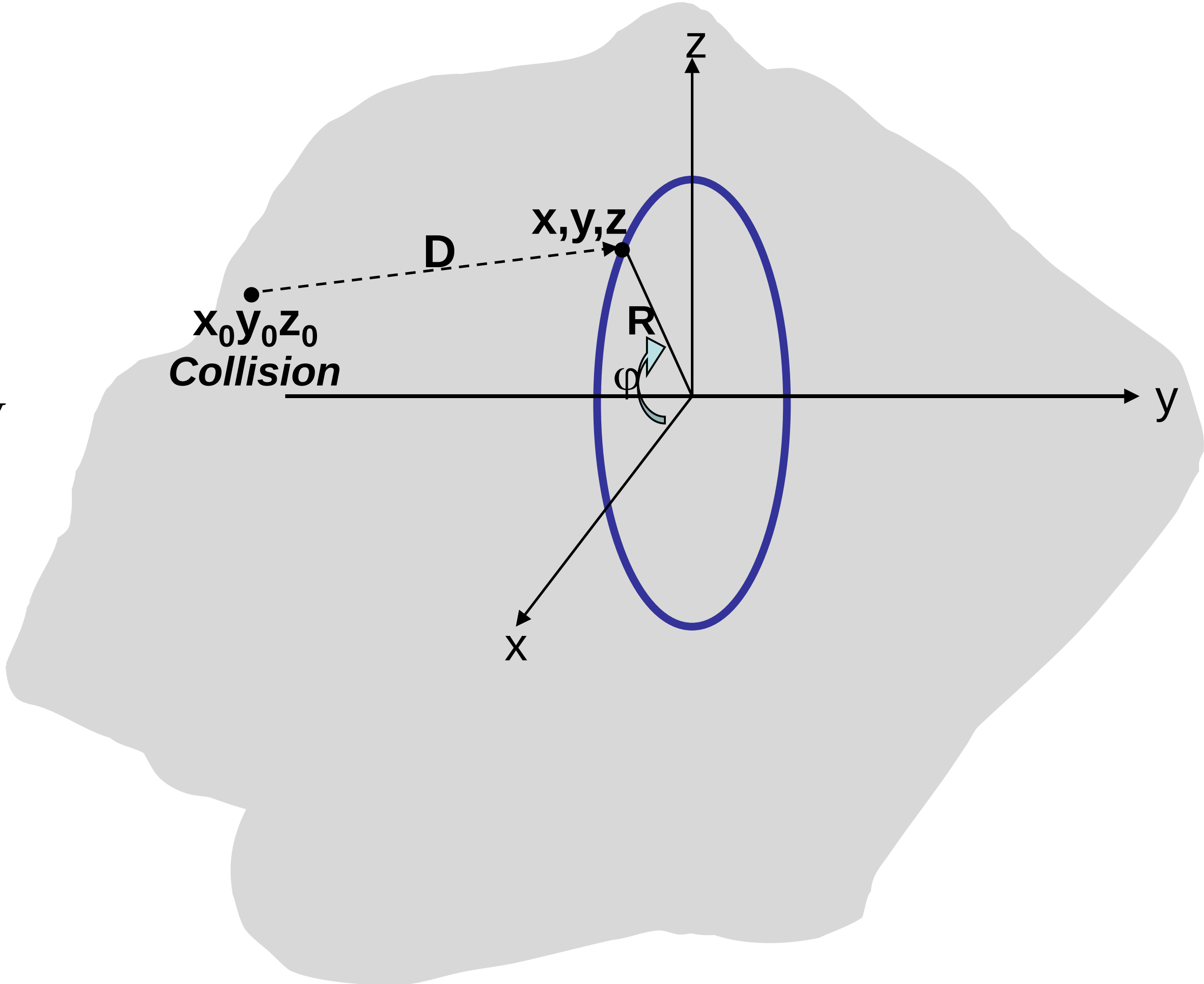
Ring Detector

Sample from:

$$\xi = \frac{C}{2\pi}\int_{-\pi}^{\varphi}\frac{d\varphi'}{R^2}$$

Adjust weight:

$$W' = \frac{D^2(\varphi)}{A}W$$



Detector Cards

Point Detectors

F5:<pl> X Y Z R_O

Ring Detectors

F5x:<pl> X R R_O
F5y:<pl> Y R R_O
F5z:<pl> Z R R_O

Radiography Tallies

FI5:<pl> X_1 Y_1 Z_1 R_O X_2 Y_2 Z_2 F_1 F_2 F_3

Exercise 8: Point Detectors

copy c:\MCNP6\EXAMPLES\atal3

- Add a point detector on axis at y=99.9

- Run the Problem, look at the output

```
1tally   5        nps =   100000
           tally type 5    particle flux at a point detector.          units   1/cm**2
           particle(s): photon

 detector located at x,y,z = 0.00000E+00 9.99000E+01 0.00000E+00
                 2.27358E-05 0.0121

 detector located at x,y,z = 0.00000E+00 9.99000E+01 0.00000E+00
 uncollided photon flux
                 0.00000E+00 0.0000

 detector score diagnostics                   cumulative          tally          cumulative
                                              fraction of         per            fraction of
   times average score      transmissions     transmissions       history        total tally
        1.00000E-01           30490             0.33210        6.85395E-07         0.03015
        1.00000E+00           53640             0.91636        3.56283E-06         0.18685
        2.00000E+00             500             0.92181        1.37010E-07         0.19288
        5.00000E+00             181             0.92378        1.52987E-07         0.19961
        1.00000E+01            2116             0.94682        3.68268E-06         0.36158
        1.00000E+02            3498             0.98493        1.42777E-05         0.98957
        1.00000E+03               0             0.98493        0.00000E+00         0.98957
        1.00000E+38               0             0.98493        0.00000E+00         0.98957
  before dd roulette           1384             1.00000        2.37164E-07         1.00000

 average tally per history = 2.27358E-05       largest score = 1.21288E-03
 (largest score)/(average tally) = 5.33468E+01      nps of largest score =    57279
```

```
score contributions by cell
       cell    misses      hits    tally per history    weight per hit
    3    13     55294     91809       2.27358E-05         2.47642E-05
    4    14    100000         0       0.00000E+00         0.00000E+00
      total    155294     91809       2.27358E-05         2.47642E-05

score misses
  russian roulette on pd                       0
  psc=0.                                  100564
  russian roulette in transmission         54730
  underflow in transmission                    0
  hit a zero-importance cell                   0
  energy cutoff                                0
```

```
1analysis of the results in the tally fluctuation chart bin (tfc) for tally   5 with nps =    100000    print table
160


 normed average tally per history  = 2.27358E-05          unnormed average tally per history  = 2.27358E-05
 estimated tally relative error    = 0.0121               estimated variance of the variance  = 0.0004
 relative error from zero tallies  = 0.0044               relative error from nonzero scores  = 0.0113

 number of nonzero history tallies =       34012          efficiency for the nonzero tallies  = 0.3401
 history number of largest  tally  =       46298          largest  unnormalized history tally = 1.29479E-03
 (largest  tally)/(average tally)  = 5.69493E+01          (largest  tally)/(avg nonzero tally)= 1.93696E+01

 (confidence interval shift)/mean  = 0.0001               shifted confidence interval center  = 2.27384E-05


 if the largest  history score sampled so far were to occur on the next history, the tfc bin quantities would change
as follows:

      estimated quantities           value at nps           value at nps+1           value(nps+1)/value(nps)-1.

      mean                            2.27358E-05             2.27485E-05                     0.000559
      relative error                  1.21135E-02             1.21195E-02                     0.000496
      variance of the variance        4.39517E-04             4.42102E-04                     0.005882
      shifted center                  2.27384E-05             2.27384E-05                     0.000000
      figure of merit                 2.00086E+05             1.99888E+05                    -0.000992

 the estimated slope of the 200 largest  tallies starting at  7.70242E-04 appears to be decreasing at least
exponentially.
 the large score tail of the empirical history score probability density function appears to have no unsampled
regions.
```

```
===========================================================================================================================

          results of 10 statistical checks for the estimated answer for the tally fluctuation chart (tfc) bin of tally   5

tfc bin     --mean--      ---------relative error---------      ----variance of the variance----      --figure of merit--     -pdf-
behavior    behavior      value   decrease   decrease rate      value   decrease   decrease rate       value     behavior     slope

desired      random       <0.05      yes      1/sqrt(nps)       <0.10      yes         1/nps          constant    random      >3.00
observed     random        0.01      yes          yes            0.00      yes          yes           constant    random      10.00
passed?       yes           yes      yes          yes             yes      yes          yes              yes        yes         yes

===========================================================================================================================



this tally meets the statistical criteria used to form confidence intervals: check the tally fluctuation chart to verify.
the results in other bins associated with this tally may not meet these statistical criteria.

estimated asymmetric confidence interval(1,2,3 sigma): 2.2463E-05 to 2.3014E-05; 2.2187E-05 to 2.3289E-05; 2.1912E-05 to 2.3565E-05
estimated  symmetric confidence interval(1,2,3 sigma): 2.2460E-05 to 2.3011E-05; 2.2185E-05 to 2.3287E-05; 2.1910E-05 to 2.3562E-05

fom = (histories/minute)*(f(x) signal-to-noise ratio)**2 = (2.936E+06)*( 2.611E-01)**2 = (2.936E+06)*(6.815E-02) = 2.001E+05
```

Recommendations

- **Read output file carefully:**
  - **Understand all warning messages;**
  - **Ensure cross section tables are the ones you wanted;**
  - **Check source with 1st 50 histories;**
  - **Check summary to ensure problem is reasonable;**
  - **Check convergence.**
- **Use PRINT card;**
- **Use FC, FQ, TF;**
- **Cross compare with multiple estimators and summary table.**

Special Tallies

- Mesh Tallies

- Radiography

MCNP6 TMESH Tallies

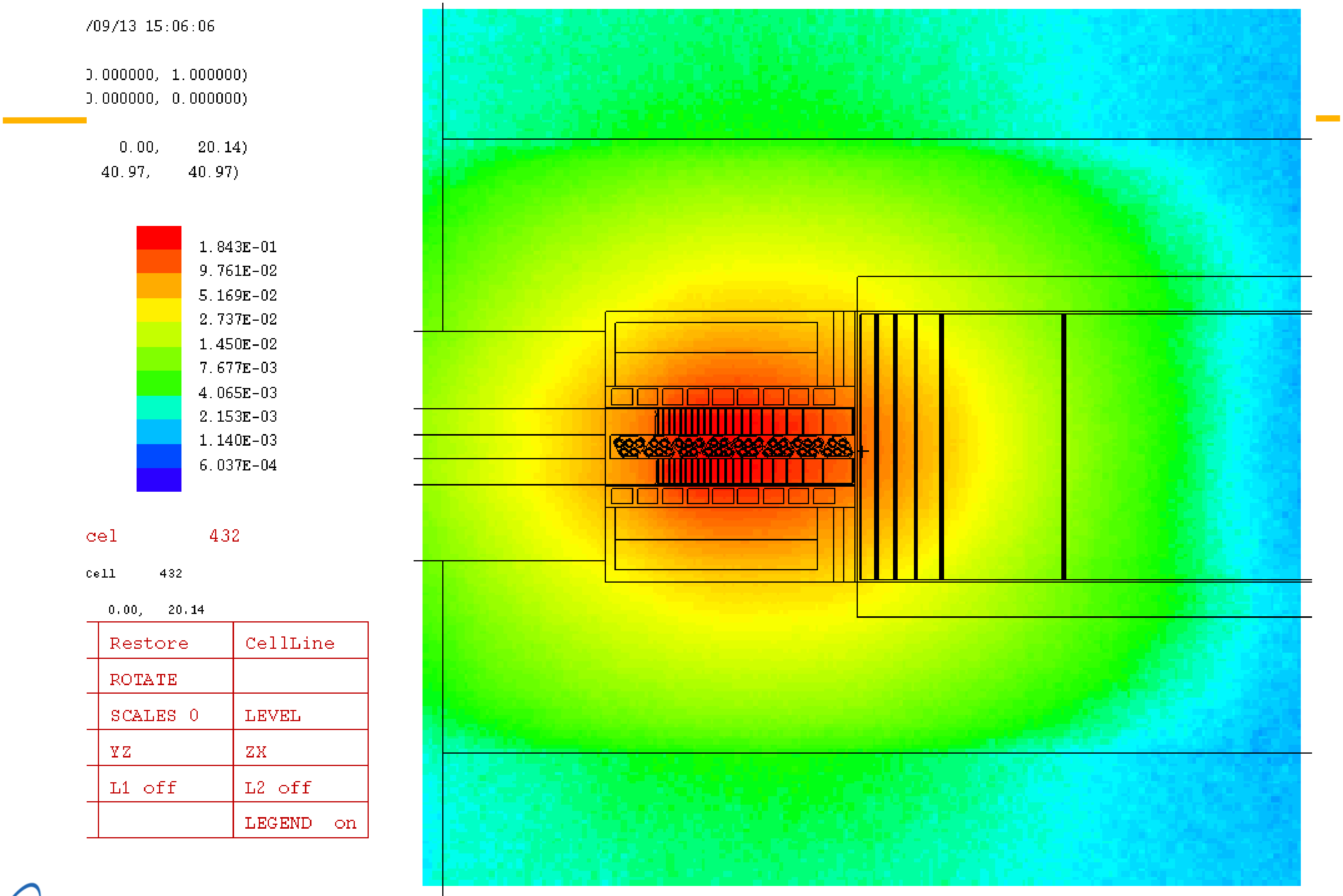
There are 4 types of MCNP6 mesh tallies :

Type 1: Track Averaged Mesh Tally

Type 2: Source Mesh Tally

Type 3: Energy Deposition Mesh Tally

Type 4: DXTRAN Mesh Tally


/09/13 15:06:06
).000000, 1.000000)
).000000, 0.000000)
0.00, 20.14)
40.97, 40.97)
1.843E-01
9.761E-02
5.169E-02
2.737E-02
1.450E-02
7.677E-03
4.065E-03
2.153E-03
1.140E-03
6.037E-04
cel 432
cell 432
0.00, 20.14
Restore
CellLine
ROTATE
SCALES 0
LEVEL
YZ
ZX
L1 off
L2 off
LEGEND on

Track Averaged Mesh Tally (type 1)

FORM: (R,C,S)MESHn:<*pl*>   keyword = value

n = 1, 11, 21, 31,... **(note, number must not duplicate one used for an 'F1' tally)**

<*pl*> is a particle type. There is no default.

Example:

```
tmesh
  rmesh1:n    flux
    cora1  -15.0 99i 15.0
    corb1  -15.0 15.0
    corc1  -30.5 99i 30.5
endmd
```

Track-Averaged Mesh Tally

Keyword	Description
TRAKS	Tally the number of tracks through each mesh volume. No values accompany the keyword
FLUX	Tally the average fluence (particle weight times track length divided by volume) in units of number/cm^2. If the source is considered to be steady state in particles per second, then the value becomes flux in number/cm^2-s
TRANS	Translate or rotate the mesh according to a specified TR card. This keyword must be followed by a single reference to a TR card.

Additional keywords:

DOSE, POPUL, PEDEP, MFACT

Source Mesh Tally (type 2)

Form: **(R,C,S)MESH*n* <*pl*$_1$> <*pl*$_2$>...<*pl*$_n$> trans = #**

n = 2, 12, 22, 32, ...(note, number must not duplicate one used for an 'F2' tally)

<*pl*> = particle type(s) (Up to 10 allowed)

Example: Source Mesh tally

```
tmesh
      RMesh2 n h
       cora2  -15.0 99i 15.0
       corb2  -15.0 15.0
       corc2  -30.5 99i 30.5
endmd
```

MCNP6 Mesh Tally Plotting

- **From MDATA files**
  - **Use gridconv and postprocessor (e.g Moritz, Tecplot, PAW, etc.)**

OR,

- **From MCTAL files make a contour plot**
  - **MCNP6 z**
  - **rmc = <mctal filename>**
  - **tal n free ik contour 5 95 10 %**
  - **this tells MCNP to plot tally "n", set the plot indices to your mesh tally coordinates (ik=xz), contour colors where blue=5<95=red, with 10 percent interpolates in between.**

OR,

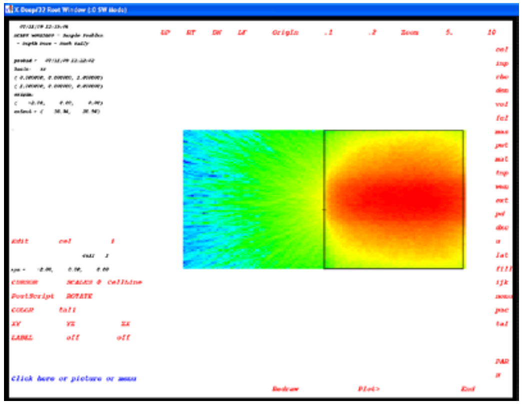
  -

Mesh Tally Plots

Superimposed on problem geometry!

- **From INP file during run:**
  - mplot freq 5000 PLOT ex 40 py 4 la 0 1 tal color on la 0 0
    (see manual for mplot command detail)

OR,



- **From runtpe:**
  - mcnp6 z run = <runtpe filename>
  - <mcplot> plot $brings up the geometry plotter
  - [buttons] tal, N, color

Mesh Tally Exercise

Copy C:\MCNP6\EXAMPLES\atal9

1. **Plot and understand the geometry.**
2. **Add a rectangular flux mesh tally for protons and neutrons within the water. Use one bin in the "y" direction.**
3. **Add a rectangular source mesh tally for protons and neutrons within the water.**
4. **Plot your results with the MCNP plotter.**

Plotting the Mesh Tally

MCNP6 Z

MCPLOT> runtpe talmhr

MCPLOT> plot

Click on tal

Click on color twice

Click on ZX

Turn surf labels off

Zoom in

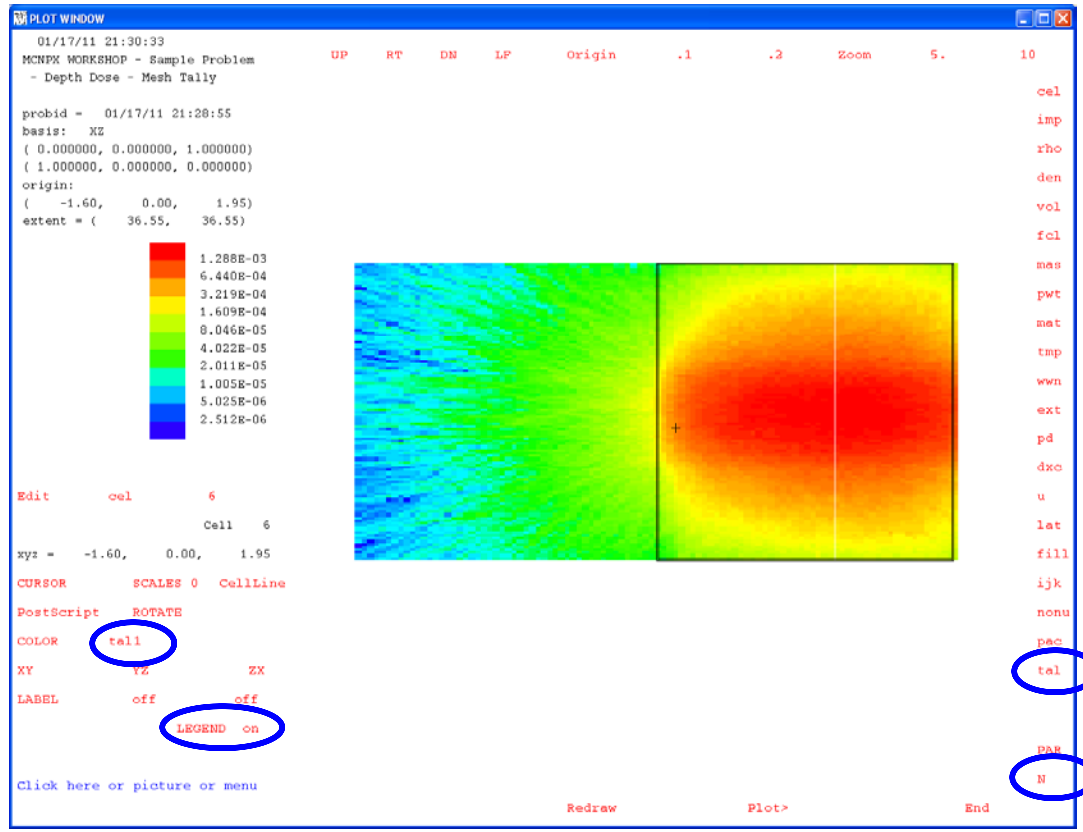
Click on Legend

To plot other tallies:

Click on tal

Click on N to cycle through tallies

Click redraw



Energy Deposition Mesh Tally (type 3)

General Form:

(R,C,S)MESHn ***keyword***

n = 3, 13, 23, 33, ...

Example: ***Mesh tally of total energy deposited, all sources***

```
tmesh
        RMesh3 total
         cora3  -15.0 99i 15.0
         corb3  -15.0 15.0
         corc3  -30.5 99i 30.5
endmd
```

Some type 3 Mesh Tally keywords

Keyword	Description
TOTAL	If TOTAL appears on the input line, score energy deposited from any source. (DEFAULT)
DE/DX	If DE/DX appears on the input line, score ionization from charged particles.
RECOL	If RECOL appears on the input line, score energy transferred to recoil nuclei above tabular limits.

Additional keywords TLEST, DELCT, MFACT, NTERG, TRANS

(see the manual)

Los Alamos
NATIONAL LABORATORY
EST. 1943

Mesh Plot Contour Command

FORM: CONTOUR [cmin cmax cstep] [commands]

All command entries are optional

cmin	minimum contour value
cmax	maximum contour value
cstep	number of contour steps
% or pct	interpret step values as percentages
log	step values logarithmic with cstep interpolates
All	contours normalized to min and max values of entire tally
noall	contours normalized to min and max values of contour slice (FIXED command)
line/noline	do/don’t draw lines around contours
color	make color contour plot
nocolor	contour lines only

Mesh Plot Contour Command

FORM: Contour [cmin cmax cstep] [commands]

EXAMPLES

CONTOUR 5 95 10 & line color

There will be 10 contour lines at 5%, 15%,…95% of the maximum value.
Lines will be drawn around the oclored contours as in Figure 1.
Note: this is the default setting

CONTOUR 1e-4 1e-2 12 log

There will be 12 contour lines logarithmically spaced between 1e-4 and 1e-2

DXTRAN Mesh Tally (type 4)

General Form: **(R,C,S)MESHn:<*pl*> trans = #**

n = 4, 14, 24, 34, ... (note, number must not duplicate one used for an 'F4' tally)

<*pl*> **is a particle type. There is no default.**

***** **use * for DXTRAN; omit * for F5**

trans **must be followed by a single reference to a TR card that can be used to translate and/or rotate the entire mesh. Only one TR card is permitted with a mesh card.**

MCNP6 FMESH Tally

FMESH4:n GEOM=cyl ORIGIN= –100 0 0

IMESH=5 10	IINTS=5 2
JMESH= 100 200	JINTS 10 5
KMESH .5 1	KINTS=1 2
AXS= 1 0 0 VEC=0 1 0	OUT=ij

Out = cf, ij, jk, ik ; GEOM = rec, cyl, xyz, rzt

- *MCNP6 has many more options and GEOM = sph, rpt*
- *MCNP6 allows E, T, FM, etc.*

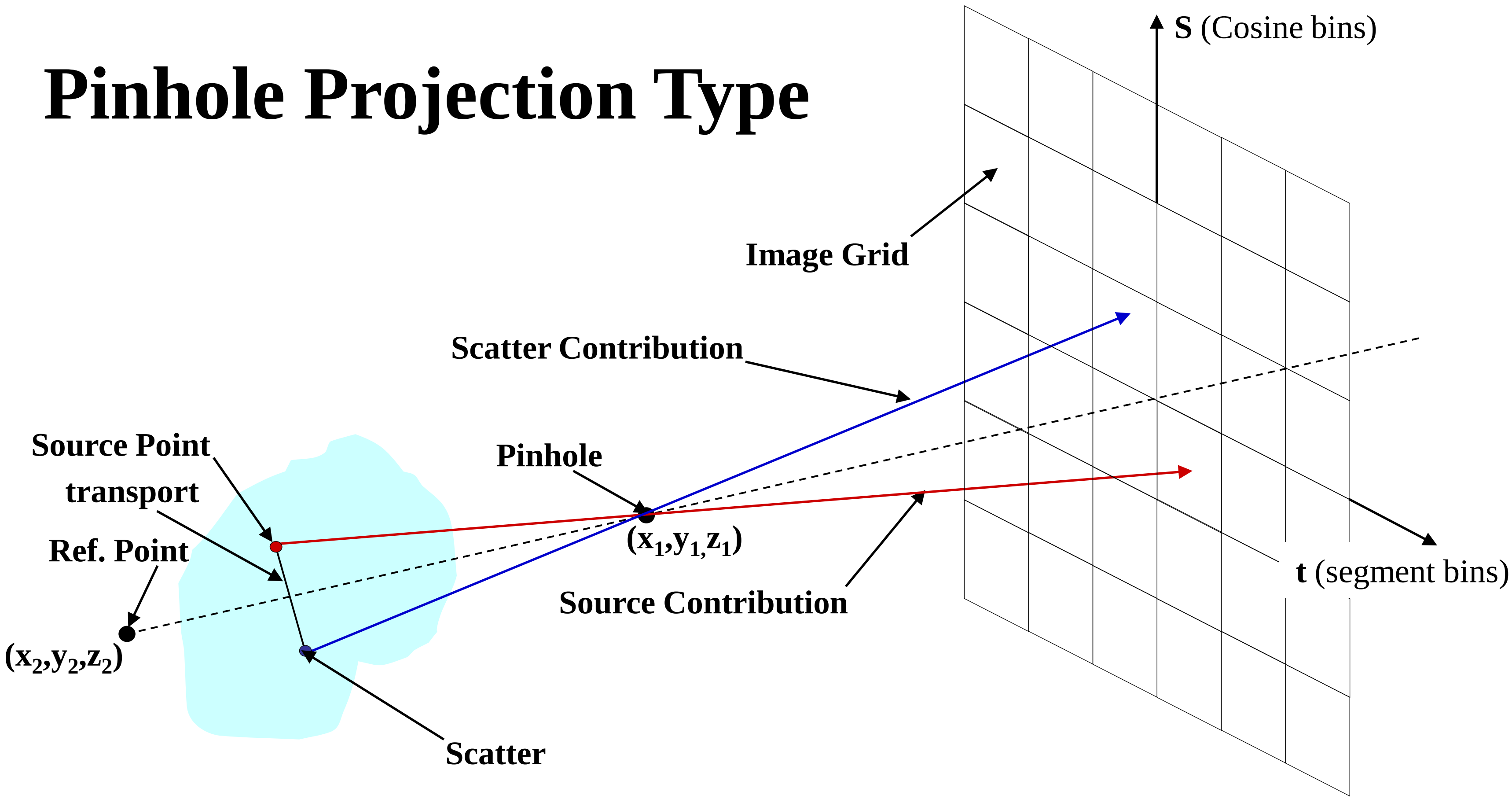
MCNP6 FMESH Tally

```
fmesh504:n geom=rec origin -400 -400 0
               imesh 400  iints 99
               jmesh 400  jints 99
               kmesh 400  kints  1

mplot    freq  5000   fmesh 504
```

In geometry plot: click fmesh

The Radiography Tally



RADIOGRAPHY TALLY
(Pinhole Projection type)

General Form:

FIPn:<*pl*> X_1 Y_1 Z_1 R_0 X_2 Y_2 Z_2 F_1 F_2 F_3

FS*n* -20. 99i 20. ***$ establishes an image grid with***

C*n* -20. 99i 20. ***$ 100 Seg. x 100 Cos. bins***

n is the tally number and must end with a 5 since this is a detector-type tally.

<*pl*> is the particle type for the tally. ***Neutrons or photons only!***

(see next slide for explanation of Argument elements)

Pinhole Radiography Arguments

X_1, Y_1, Z_1 The coordinates of the pinhole.

R_0 Pinhole Radius.

Note, neither the pinhole nor the grid should be located within a highly scattering media.

X_2, Y_2, Z_2 The reference coordinates that establish the reference direction cosines for the normal to the detector grid. This direction is defined as being from X_2, Y_2, Z_2 to the pinhole at X_1, Y_1, Z_1 .

F_1 If F1>0, the radius of a cylindrical collimator, centered on and parallel to the reference direction, which establishes a radial field of view through the object.

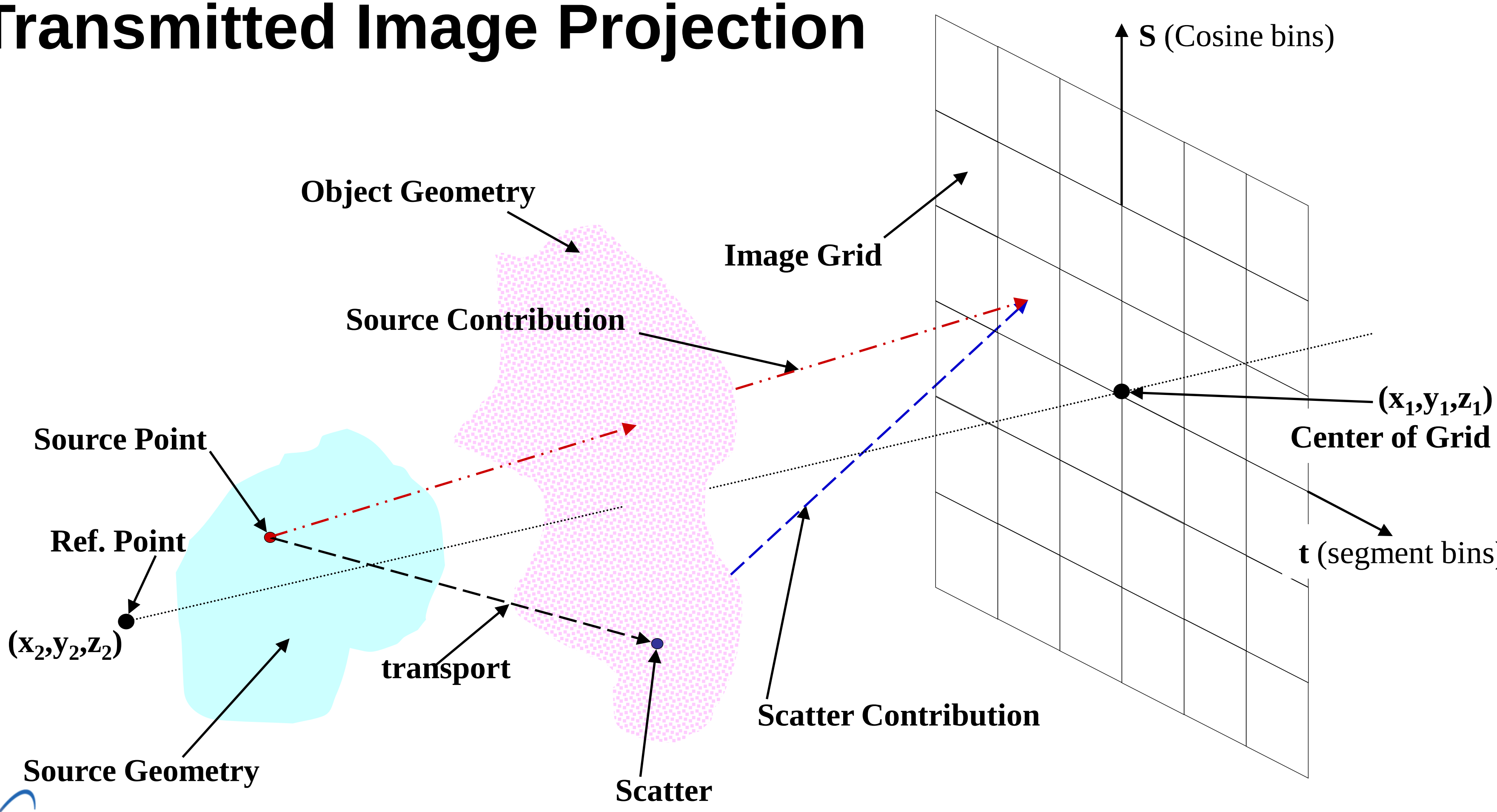
F_2 The radius of the pinhole perpendicular to the reference direction.

- F2=0 represents a perfect pinhole
- F2>0 the point through which the particle contribution will pass is picked randomly. This simulates a less-than-perfect pinhole.

F_3 The distance from the pinhole at X_1, Y_1, Z_1 to the detector grid along the direction established from X_2, Y_2, Z_2 to X_1, Y_1, Z_1 , and perpendicular to this reference vector.

Radiography Tally

Transmitted Image Projection



Radiography Tally

Transmitted Image Projection Type

General Form: FI(R/C)n:<pl> X_1 Y_1 Z_1 R_0 X_2 Y_2 Z_2 F_1 F_2 F_3

FI*R* is used to establish a grid on a *plane surface*
FI*C* is used to establish a grid on a *cylindrical surface*.

n	=	the tally number and must end with a 5 since this is a detector type tally.
<*pl*>	=	the particle type for the tally. (N or P only)
X_1 Y_1 Z_1	=	Center of rect. or cyl. grid defined with FSn and Cn
R_0	=	0.00
X_2 Y_2 Z_2	=	reference point defining rectangular grid outward normal or of cylindrical grid axis. May be thought of as the eye of the observer.
F_1	=	-1/0 Scattered contribution only/Source + scattered contributions
F_2	=	radial field of view. Cylinder along the axis.
F_3	=	0 /1 Contributions to grid bin centers/random positions

Transmitted Image Projection

NPSMG on the NPS card

NPS NPP NPSMG

NPP = number of histories requested

NPSMG = number of *direct source contributions* requested

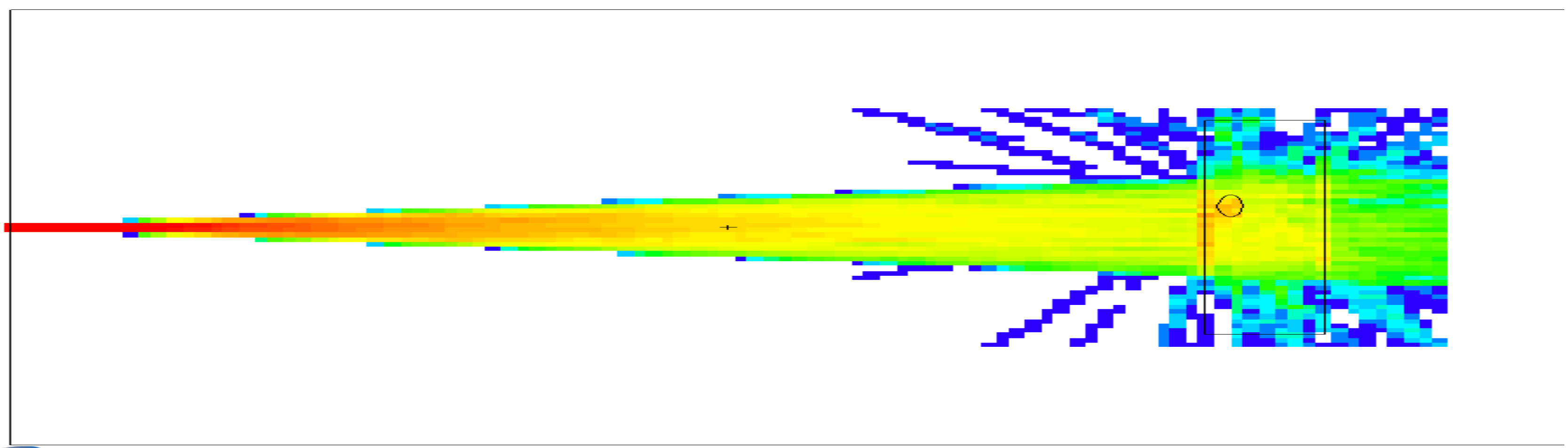
Example: NPS 100000 60000

Exercise Rad 10

Transmitted Image Projection: ^{235}U sphere in water

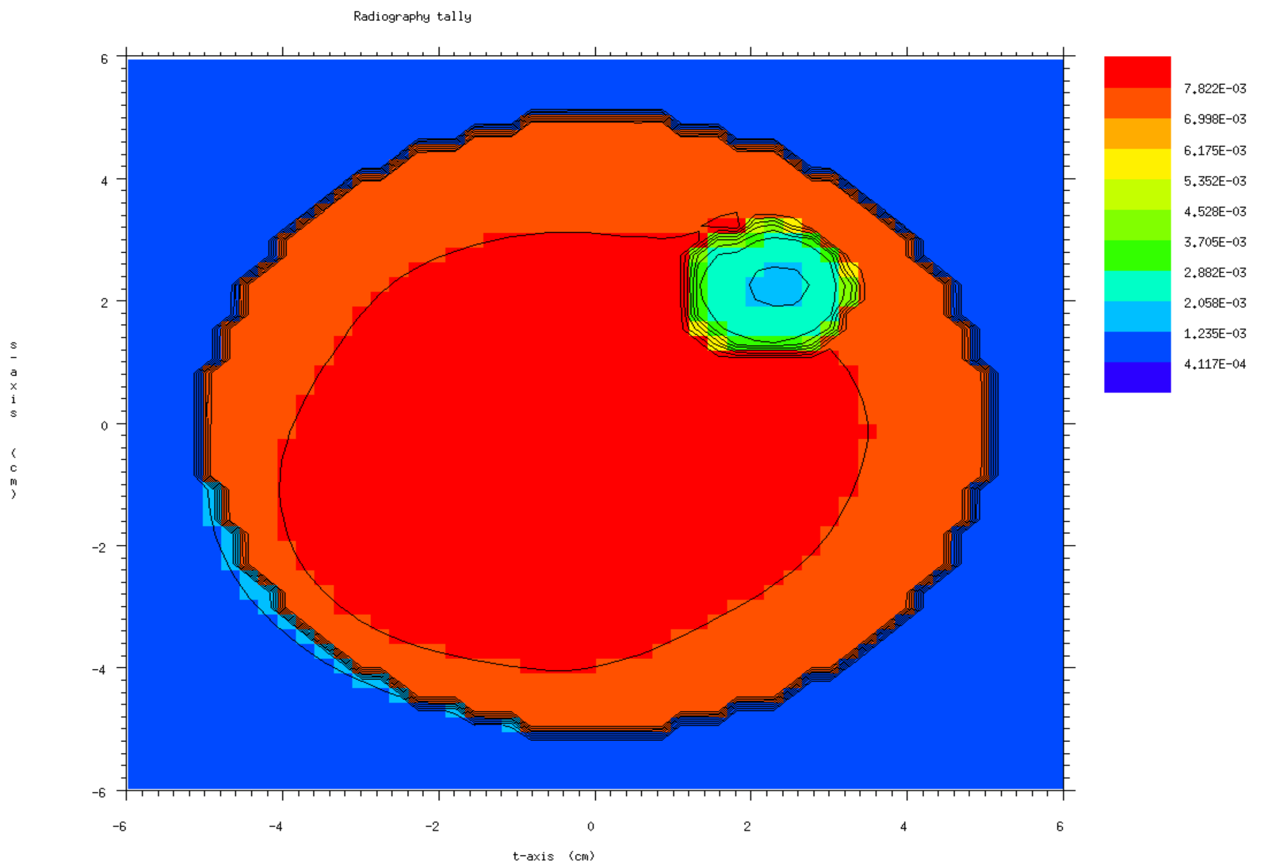
Copy %inputs%\tally\rad10

- **10-cm radius, 10-cm tall water tank**
- **2-cm radius 235U off-center sphere**
- **1-MeV photon source 100-cm away .999 < μ < 1.0 cone**
- **Radiography tally behind tank**



Exercise Rad 10

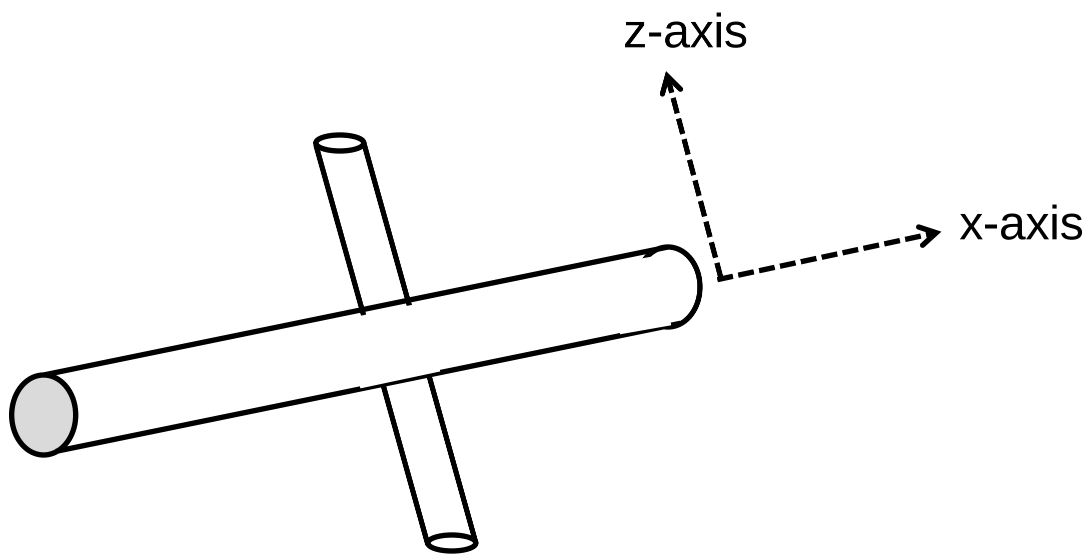
Transmitted Image Projection: ^{235}U sphere in water



Exercise Rad 11
Safeguards Radiography

Larger pipe contains 50% (atom) UO_2 and 50% H_2O. UO_2 is 10% (atom) enriched. Use a gram density of 10.0. Inner pipe radius is1.0 cm and overall length is 40 cm. Place origin at the center of this pipe. Pipe is made of ^{208}Pb with a thickness of 1.0 mm. Use a gram density of 11.4.

Enclose this geometry in a large sphere. This requires 5 cells and 4 surfaces.



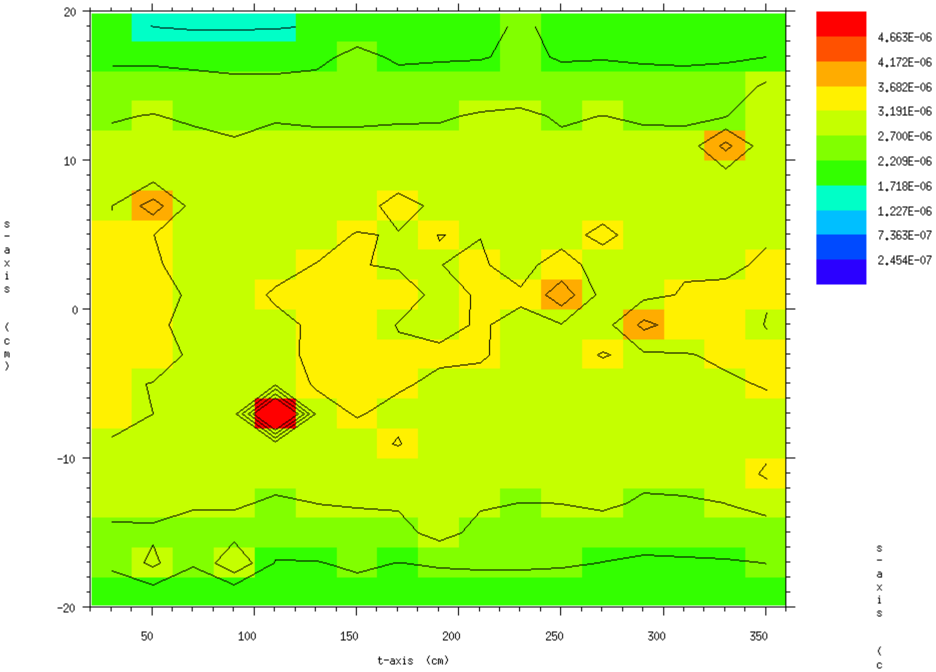
Void pipe through center of larger pipe (R=0.5 cm). Length large enough to pass through larger pipe.

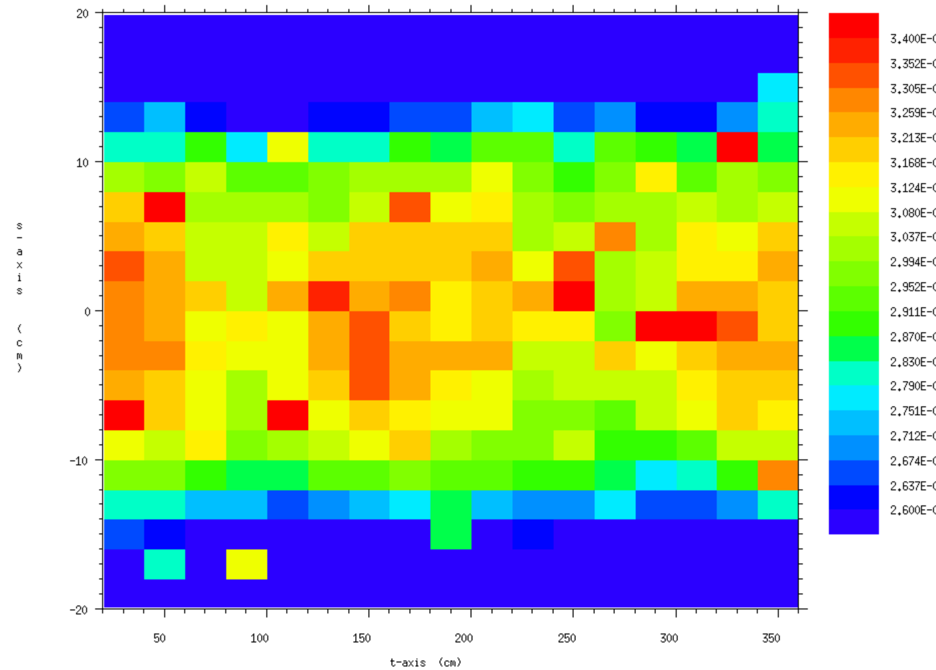
Exercise Rad 2
Safeguards Radiography

Copy %inputs%\tally\rad11

- Specify a spontaneous photon (sp) source spread uniformly throughout the HEU solution.
- Run MODE "p" only and turn on delayed gammas (PHYS:P 6th entry).
- Use a cylindrical TI tally around the larger pipe, with the image grid centered at the origin (use 0.001,0,0 due to a bug). Use a cylindrical radius of 10 cm for the image surface. Use 20 segments along the axis of the pipe and 18 angular segments around the outside surface of the pipe (i.e., every 20 degrees).
- Run 500,000 histories. You may encounter a "bad trouble" – think about this for awhile (hint: look at the volumes calculated for each cell).
- Modify the input to increase 235U component to 20% (atom). Generate contour plots of both cases that clearly show the effect of the higher enrichment.
- Can you see the void cross pipe? Why or why not?
- Note the TIC s-axis is always along the cylinder axis. What t-axis was chosen (i.e., what corresponds to q=0)? Does the cross pipe image help with this?

Exercise Rad 2
Safeguards Radiography





Recent Developments in Low-Energy Electron/Photon Transport for MCNP6

Plan of the Presentation

- Sources.
- Photon Enhancements.
- Atomic Relaxation.
- Electron Enhancements.
- Future Work.

Sources of Data

- mcplib:
  - coherent/incoherent, photoelectric, pair production, form factors
    - Storm and Israel, Los Alamos document LA-3753 (1967).
    - ENDF/B IV: Hubbell et al. *J. Phys. Chem. Ref. Data* **4**, 471 (1975).
  - fluorescence
    - Everett and Cashwell, Los Alamos document LA-5240-MS (1973).
- mcplib02:
  - coherent/incoherent, photoelectric, pair production
    - EPDL89: Cullen *et al*. LLNL document UCRL-50400, **6** (1989).
    - Implementation: Los Alamos document X-6:HGH-93-77 (1993).
- mcplib03:
  - Compton Doppler broadening data
    - Biggs *et al*. *Atomic Data and Nuclear Data Tables* **16** #3, 201 (1975).

Sources of Data

- mcplib04:
  - New data, same coverage and format
    - EPDL97: Cullen *et al*. LLNL document UCRL-50400 **6**,Rev. 5 (1997).
    - ENDF/B VI.8: Members of CSEWG, National Nuclear Data Center, Brookhaven document BNL-NCS-44945-01/04-Rev. (1990).
- eprdata12:
  - Extensions, additions, relaxation, and electrons
    - ENDF/B VI.8: Members of CSEWG, National Nuclear Data Center, Brookhaven document BNL-NCS-44945-01/04-Rev. (1990).
    - Los Alamos documentation: LA-UR-12-24213 (2012)
      LA-UR-13-27377 (2013), LA-UR-13-27632 (2013).
    - Quick-Start Guide: LA-UR-12-21068 (2012).
    - For MCNP6 only.

Previous Photon Libraries

- mcplib: Z = 1 – 94 (e.g. 26000.01p)
  - coherent/incoherent, photoelectric, pair production, heating,
  - form factors, fluorescence
  - E = 1 keV – 100 MeV for 87 elements
  - E = 1 keV – 15 MeV for Po, At, Fr, Ra, Ac, Pa, Np
- mcplib02: Z = 1 – 94 (e.g. 26000.02p)
  - E = 1 keV – 100 GeV for 94 elements
- mcplib03: Z = 1 – 94 (e.g. 26000.03p)
  - Includes Compton Doppler broadening data.
  - E = 1 keV – 100 GeV for 94 elements
- mcplib04: Z = 1 – 100 (e.g. 26000.04p)
  - Changes existing data for consistency with ENDF/B VI.8 release.
  - E = 1 keV – 100 GeV for 100 elements

Photon Enhancements

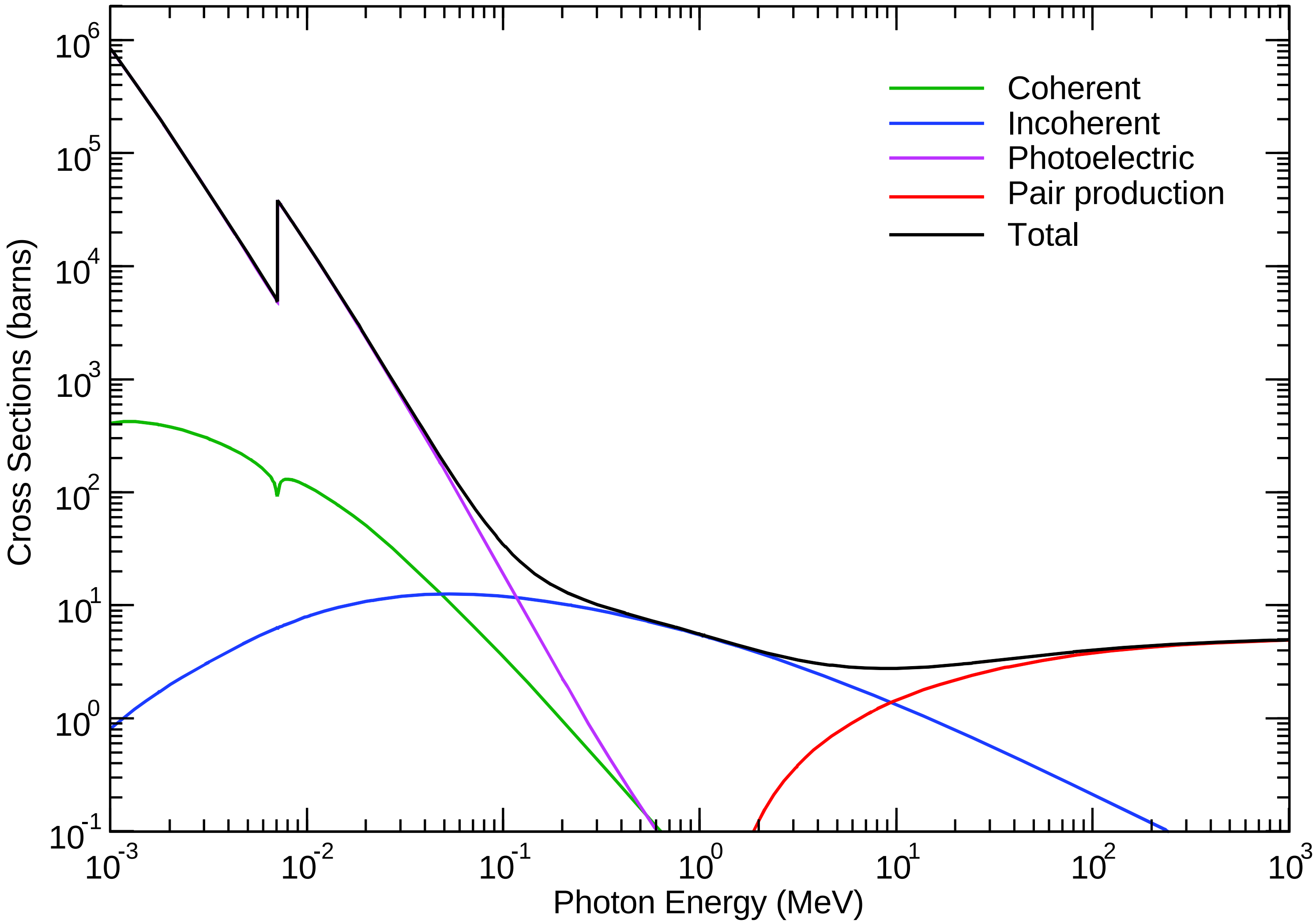
- Extension of existing data: from ≥ 1 keV down to ≥ 1 eV
  - Coherent scattering
  - Incoherent scattering
  - Photoelectric absorption

- New kinds of photoatomic data
  - Subshell-wise photoelectric cross sections
    - Detailed sampling of initial vacancy now possible
  - Complete information for electron subshells
    - Binding energies, electron populations, transitions, etc.
    - Accurate kinematics for photoelectron

- Extended scattering form factors
  - Coherent and incoherent scattering
  - Complete range of energy and angle
  - Accurate interpolation (especially for coherent scattering)

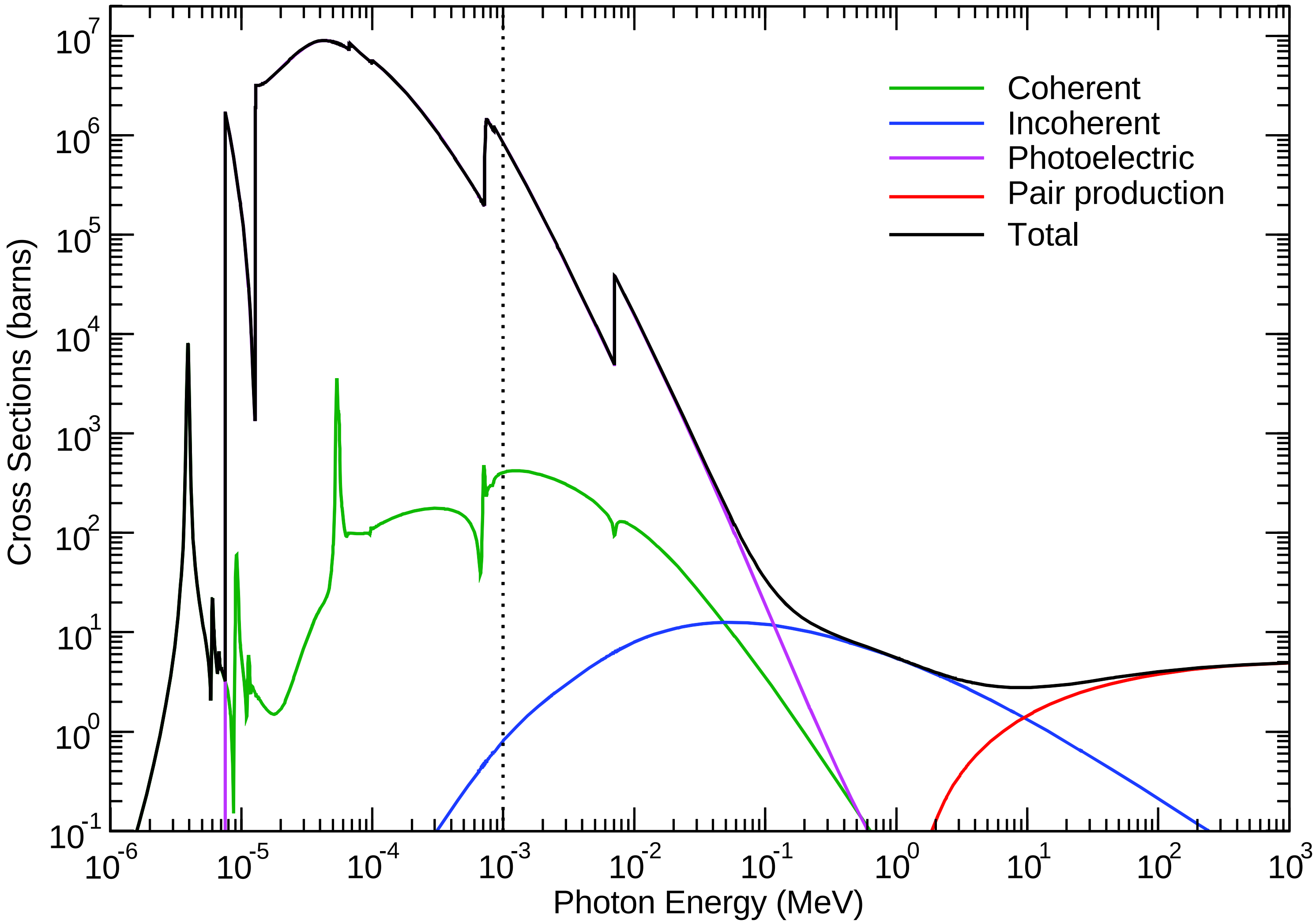
Photon Cross Sections in Iron

Data as in MCPLIB04



Photon Cross Sections in Iron

Data from ENDF/B VI.8

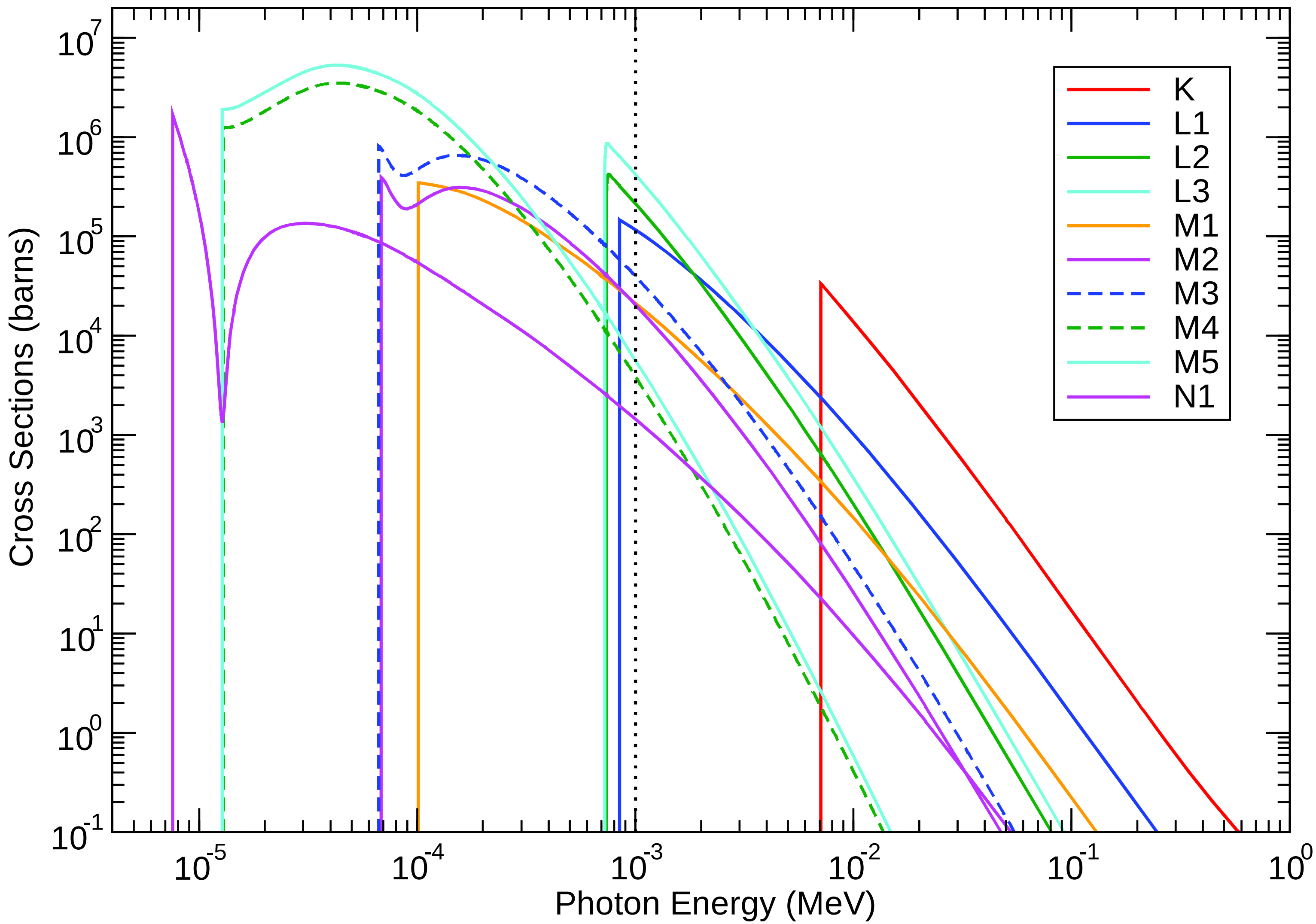


Plausible Uncertainties of Photoelectric XS (%)

Energy Range	Solid	Gas
10 – 100 eV	1000	20
100 – 500 eV	100 – 200	10 – 20
0.5 – 1.0 keV	10 – 20	5
1.0 – 5.0 keV	5	5
5 – 100 keV	2	2
0.1 – 10 MeV	1 – 2	1 – 2
10 – 100 GeV	2 – 5	2 – 5

Subshell Photoelectric Cross Sections in Iron

Data from ENDF/B VI.8

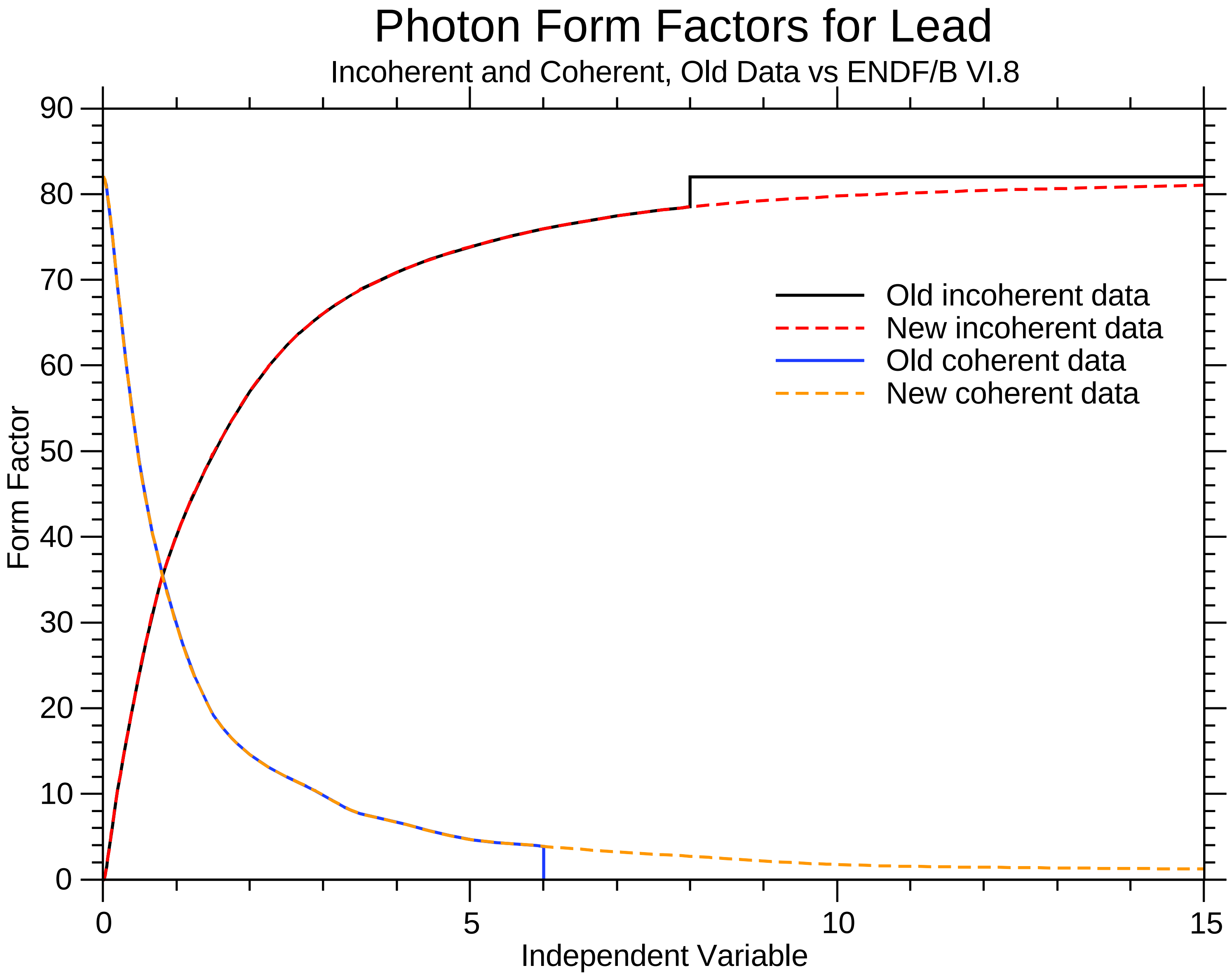


Photon Scattering Form Factors

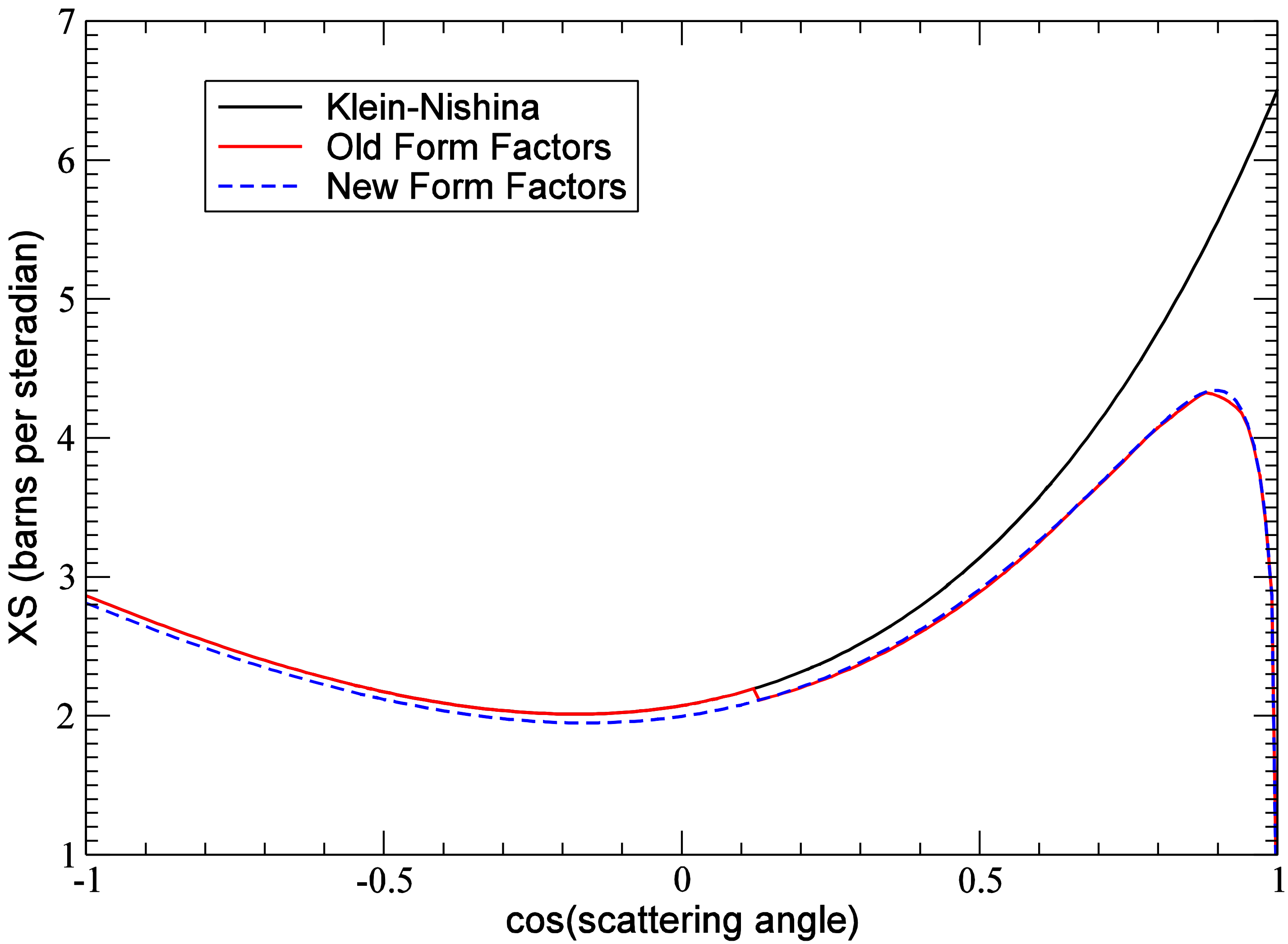
- Incoherent: $\sigma(Z,\alpha,\mu) \sim I(Z,v)\,(\alpha'/\alpha)^2\,(\alpha'/\alpha + \alpha/\alpha' + \mu^2 - 1)$
- Coherent: $\sigma(Z,\alpha,\mu) \sim C^2(Z,v)\,(1 + \mu^2)$
- …where $\alpha = E/m_ec^2$; $\alpha' = E'/m_ec^2$

  $\mu = \cos(\theta)$; $v = \kappa\ \alpha\,(1-\mu)^{1/2}$

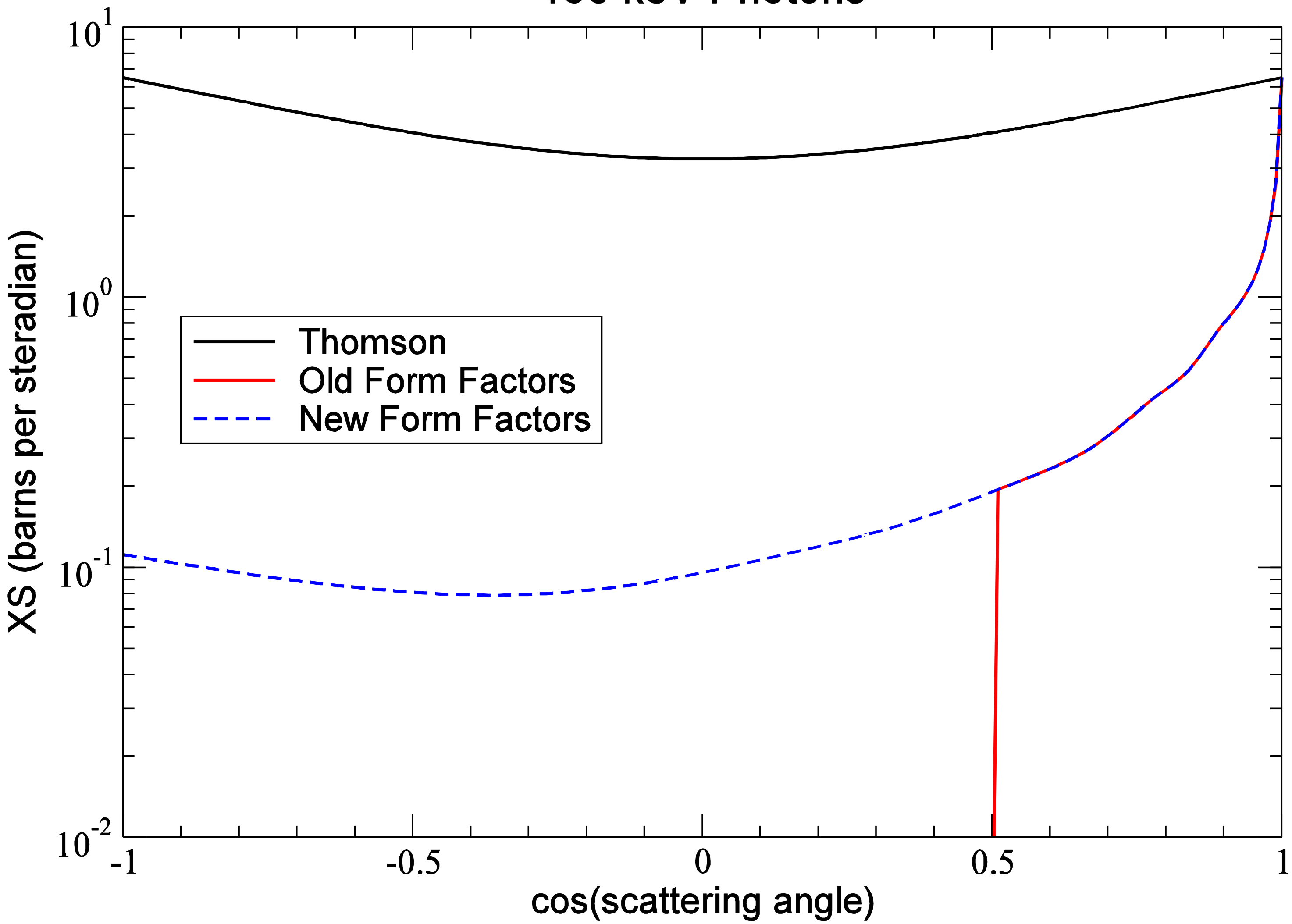
  $\kappa = 10^{-8}\,m_ec/(2^{1/2}\,h) \approx 29.1445$
- Old incoherent data: tabulated for $v = 0 \ldots 8$
  - Full tabular angular coverage for E ≤ ~99 keV
- Old coherent data: tabulated for $v = 0 \ldots 6$
  - Full angular coverage for E ≤ ~74 keV
    - e.g. at 250 keV, no coherent scattering beyond ~ 35°
- First extension: LA-UR-10-00213 (Hendricks and Kahler) 2010.


Photon Form Factors for Lead
Incoherent and Coherent, Old Data vs ENDF/B VI.8
Form Factor
0
10
20
30
40
50
60
70
80
90
0
5
10
15
Independent Variable
Old incoherent data
New incoherent data
Old coherent data
New coherent data

Incoherent Cross Section for Lead
150 keV Photons



Coherent Cross Section for Lead
150 keV Photons

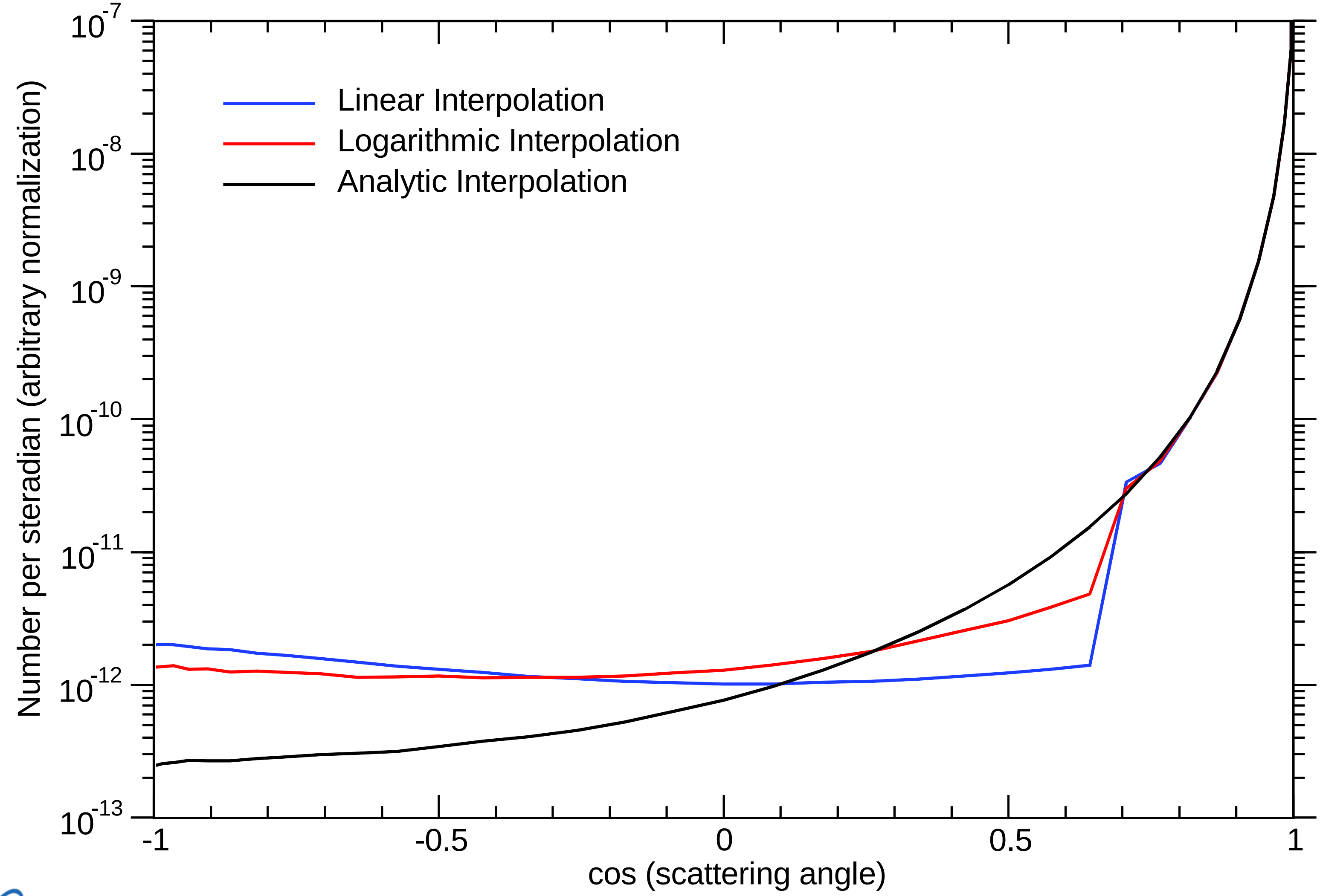


Interpolation Matters

- Incoherent scattering for transport: $I(Z,v)\ K(\alpha, \alpha', \mu)$
  - Sample from $K(\alpha, \alpha', \mu)$
  - Reject on normalized $I(Z,v)$ Log/log interpolation
- Incoherent scattering for detectors: $I(Z,v)\ K(\alpha, \alpha', \mu)$
  - Evaluate normalized $K(\alpha, \alpha', \mu)$
  - Evaluate normalized $I(Z,v)$ Log/log interpolation
- Coherent scattering for transport: $C^2(Z,v)\ T(\mu)$
  - Sample from $C^2(Z,v)$ Analytic interpolation
  - Reject on normalized $T(\mu)$
- Coherent scattering for detectors: $C^2(Z,v)\ T(\mu)$
  - Evaluate normalized $C^2(Z,v)$ Log/log interpolation
  - Evaluate normalized $T(\mu)$

Coherent Angular Distribution

3 MeV Photons on Lead



Atomic Relaxation

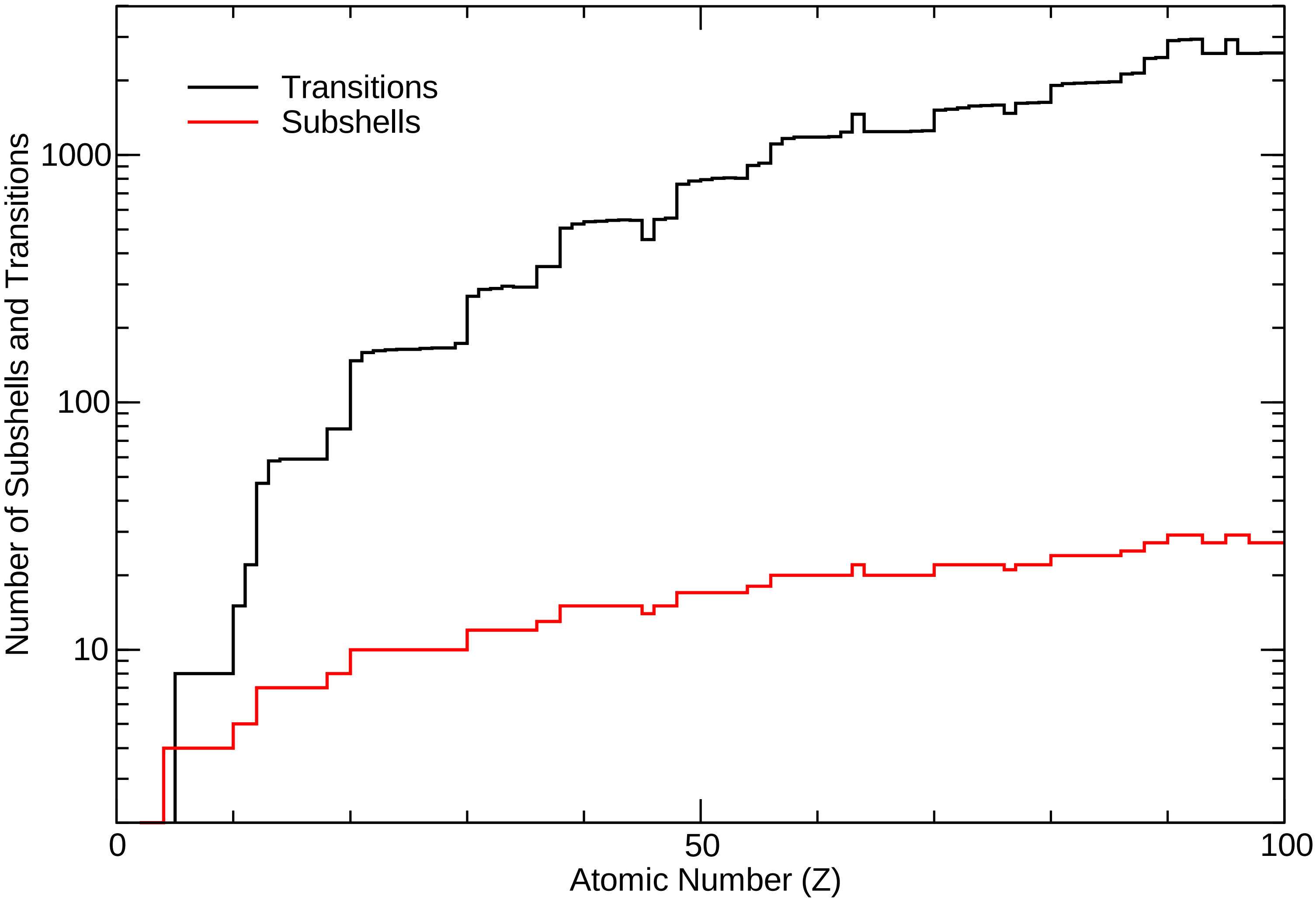
- Consistent data for electron subshells
  - Binding energies
  - Electron populations
  - Number of transitions
  - Photoelectric subshell cross sections down to 1 eV
- Consistent data for transitions
  - Transitions with photon fluorescence (radiative)
  - Auger and Coster-Kronig transitions (non-radiative)
- Full analog sampling of the relaxation cascade
- New process: Compton-induced atomic relaxation

Old MCNP Fluorescence Model

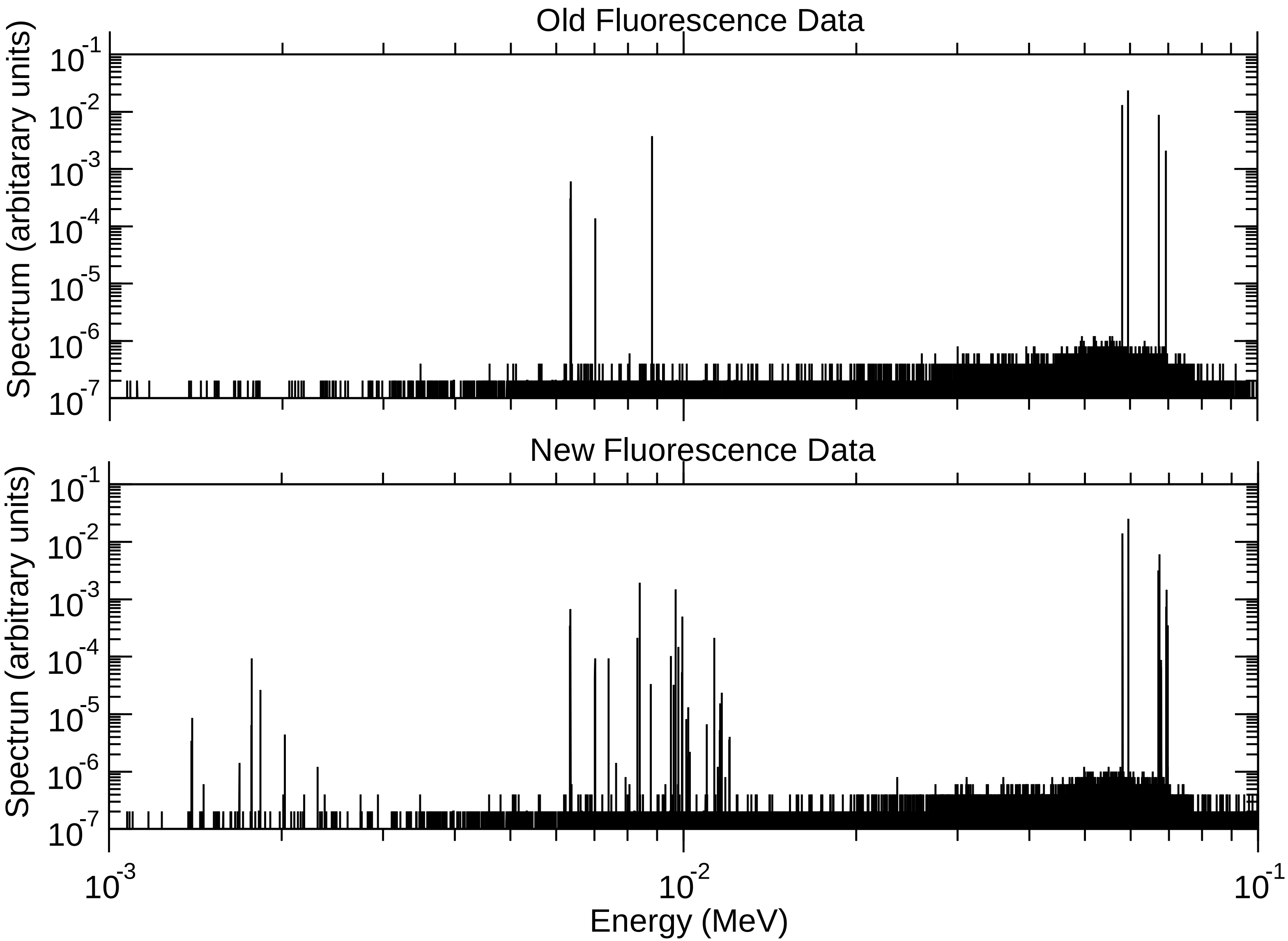
$Z = 1 – 11$:	no fluorescence	
$Z = 12 – 19$:	1 line	$< \; K \leftarrow L2, \; K \leftarrow L3 \; >$
$Z = 20 – 30$:	3 lines	$K \leftarrow L2, \quad K \leftarrow L3$
		$< \; K \leftarrow M2, \; K \leftarrow M3, \; K \leftarrow M4 \; >$
$Z = 31 – 36$:	4 lines	$K \leftarrow L2, \quad K \leftarrow L3$
		$< \; K \leftarrow M2, \; K \leftarrow M3, \; K \leftarrow M4 \; >$
		$< \; L1, L2, L3 \; > \; \leftarrow \; < \; \text{higher lines} \; >$
$Z = 37 – 100$:	5 lines	$K \leftarrow L2, \quad K \leftarrow L3$
		$< \; K \leftarrow M2, \; K \leftarrow M3, \; K \leftarrow M4 \; >$
		$< \; K \leftarrow N2, \; K \leftarrow N3 \; >$
		$< \; L1, L2, L3 \; > \; \leftarrow \; < \; \text{higher lines} \; >$

Electron Subshells and Relaxation Transitions

From ENDF/B VI.8 Data



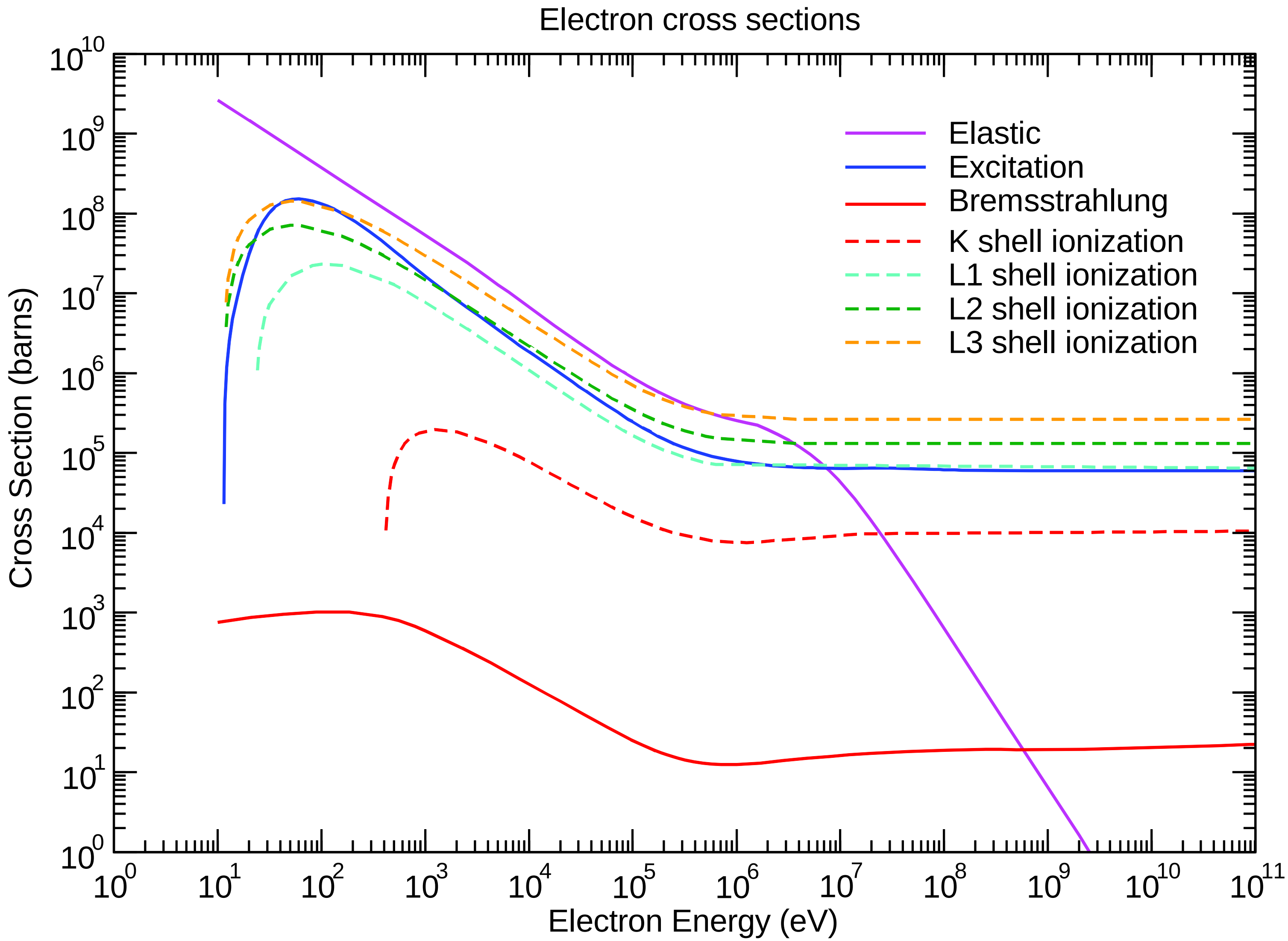
Iron / Tungsten Target, 100 keV photons



Electron Enhancements

- Microscopic electron cross sections down to 10 eV
- Electron elastic scattering
  - Electron angular distribution as function of electron energy
- Atomic excitation
  - Electron mean energy loss as function of electron energy
- Subshell-wise electroionization
  - Knock-on energy distribution as function of electron energy
  - Knock-on direction and primary energy loss from conservation
- Bremsstrahlung
  - Photon energy distribution as function of electron energy
  - Electron mean energy loss as function of electron energy
  - No photon angular distribution given

Atomic Nitrogen



Single-Event Electron Transport

- Get total cross section and distance to collision

  $\Sigma(i) = N(i) \cdot (\sigma_{elas}(i) + \sigma_{brem}(i) + \sigma_{exc}(i) + \sigma_{ion}(i))$

  $D = -\ln (random()) / (\Sigma(1) + \ldots + \Sigma(m))$

- Select target

  $R = random() \cdot (\Sigma(1) + \ldots + \Sigma(m))$

  $m = 1 \parallel R < \Sigma(1) \quad \longrightarrow \quad t = 1$

  otherwise find $\Sigma(1) + \ldots + \Sigma(t\text{-}1) \leq R < \Sigma(1) + \ldots + \Sigma(t)$

- Select process

  $R = random() \cdot (\sigma_{elas}(t) + \sigma_{brem}(t) + \sigma_{exc}(t) + \sigma_{ion}(t))$

if $R < \sigma_{elas}$	process elastic collision
else if $R < \sigma_{elas} + \sigma_{brem}$	process bremsstrahlung
else if $R < \sigma_{elas} + \sigma_{brem} + \sigma_{exc}$	process excitation
else	process electro-ionization

Process Collisions

- Excitation
  - No angular deflection
  - No secondary particles
  - Apply energy loss as unique function of energy: $F_{exc}(E)$
  - (No sampling for this process)
- Electro-ionization
  - Sample for individual subshell
  - Sample knock-on energy from tabulation: $F_{knock}(E,\mu)$
  - Reduce incident energy by $E_{knock} + E_{binding}$
  - Get incident and knock-on directions from conservation
  - "Recursively" fill vacancy using new relaxation data

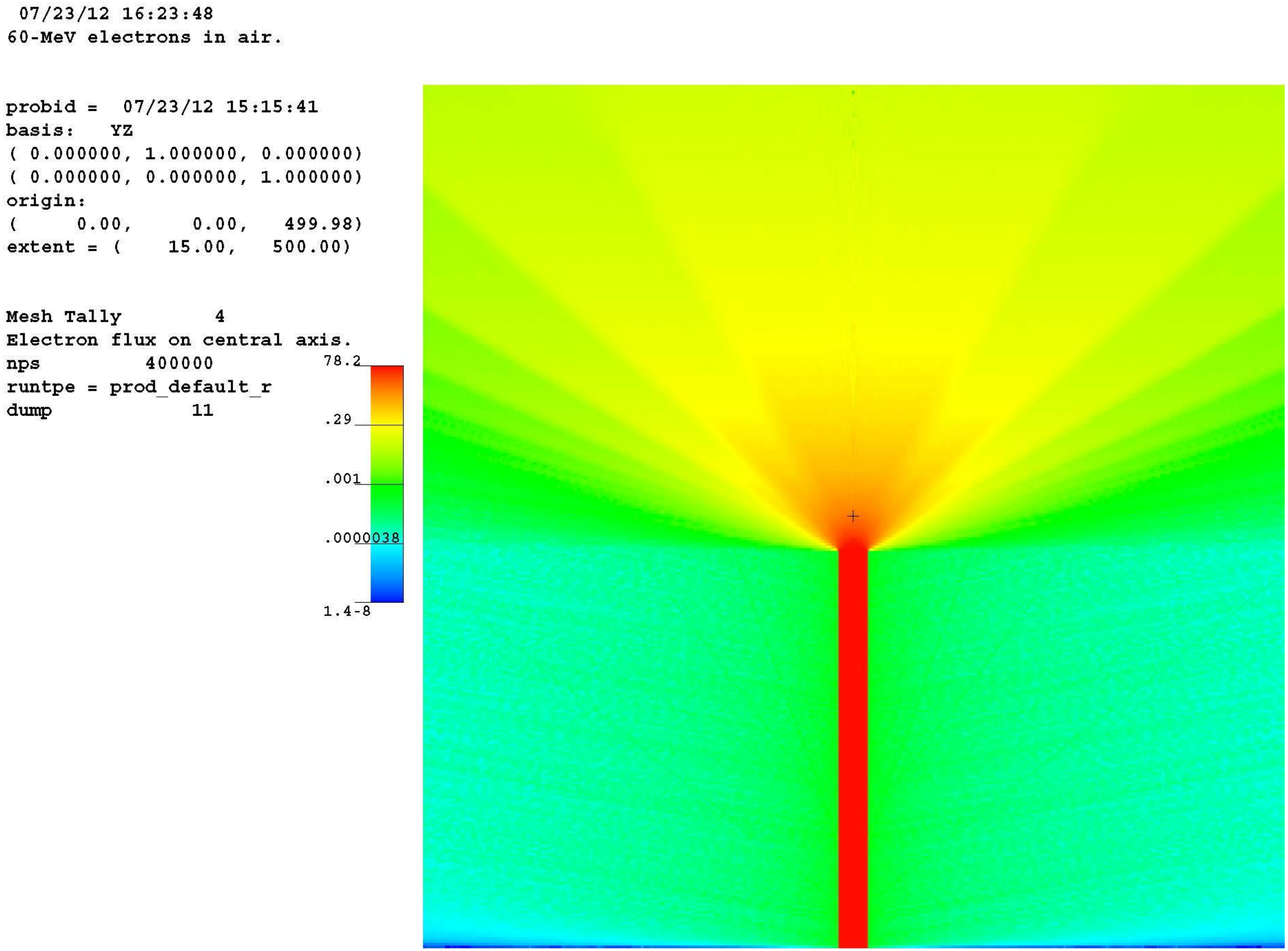
Process Collisions

- Elastic collision
  - No energy loss
  - No secondary particles
  - Sample deflection from tabulation: $F_{elas}(E,\mu)$
- Bremsstrahlung
  - No change in electron direction
  - Sample photon energy from tabulation: $F_{brems}(E)$
  - Reduce incident energy by E_{brems}
  - Sample photon direction in three energy ranges:
    - $E > 1$ GeV: $p(\mu) = \frac{1}{2} (1 - \beta^2) / (1 - \beta\mu)^2$
    - $1 \text{ keV} \le E \le 1$ GeV: tabular distribution from condensed history
    - $E < 1$ keV: Currently $p(\mu)$
      Planned: dipole distribution

Brief User Guide

- Use the new data tables:
  - **`M1   1000.12p  2   8000.12p  1`**
  - **`M1   1000  2   8000  1   plib  12p   elib  03e`**
- Use the right problem modes:
  - **`MODE   P  E`**
  - **`DBCN   17J  2  $  now the default`**
- The default energy cutoff is still 1 keV:
  - **`CUT:P  J  1.0e-06  $  1 eV`**
  - **`CUT:E  J  1.5e-05  $ 15 eV avoid the Sargasso Sea`**
- Single-event starting point is adjustable:
  - **`PHYS:E  10. 13J  2.0e-03  $  start at 2 keV`**

60-MeV electrons in air, default condensed history.

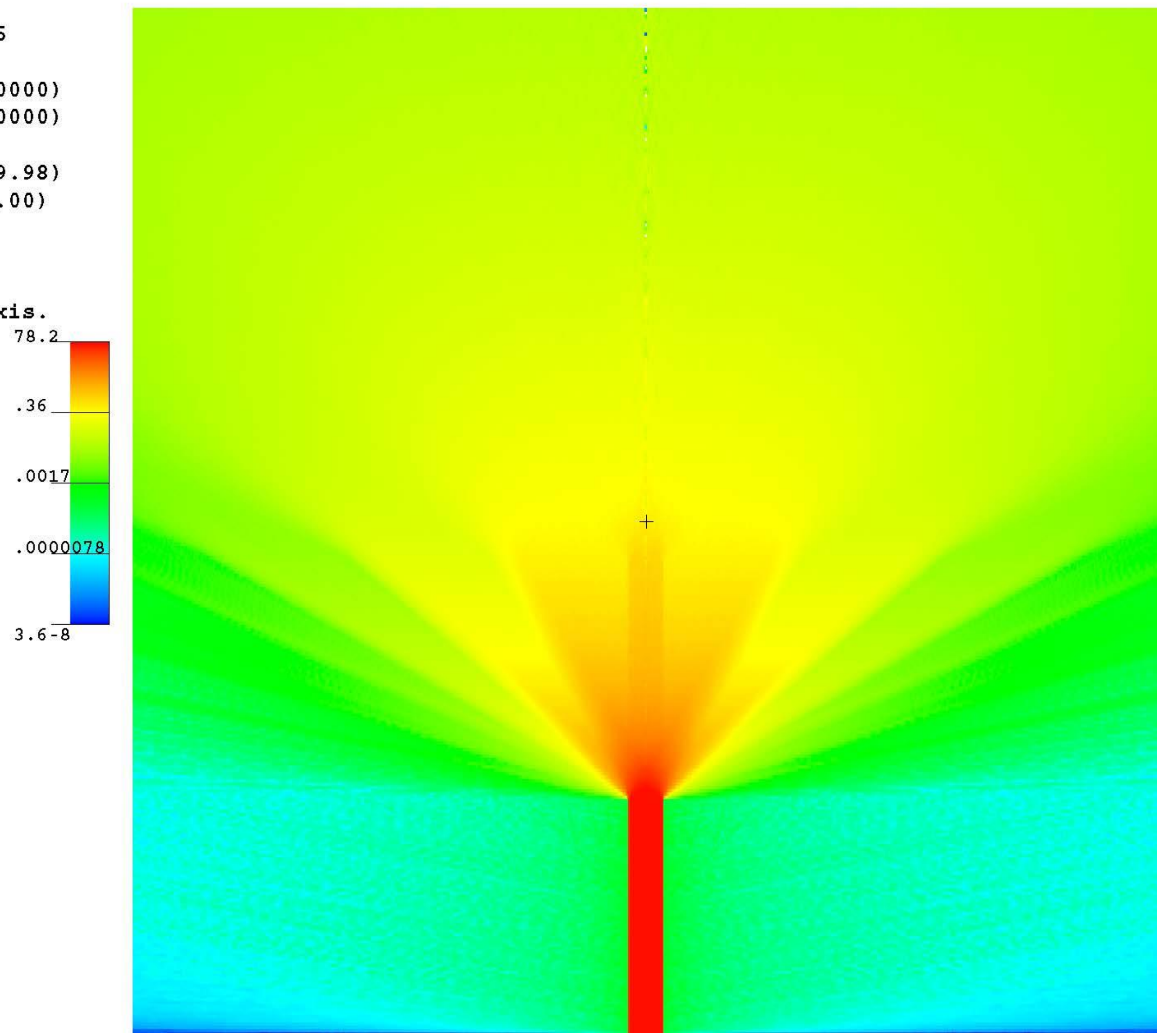


60-MeV electrons in air, more angular substeps.

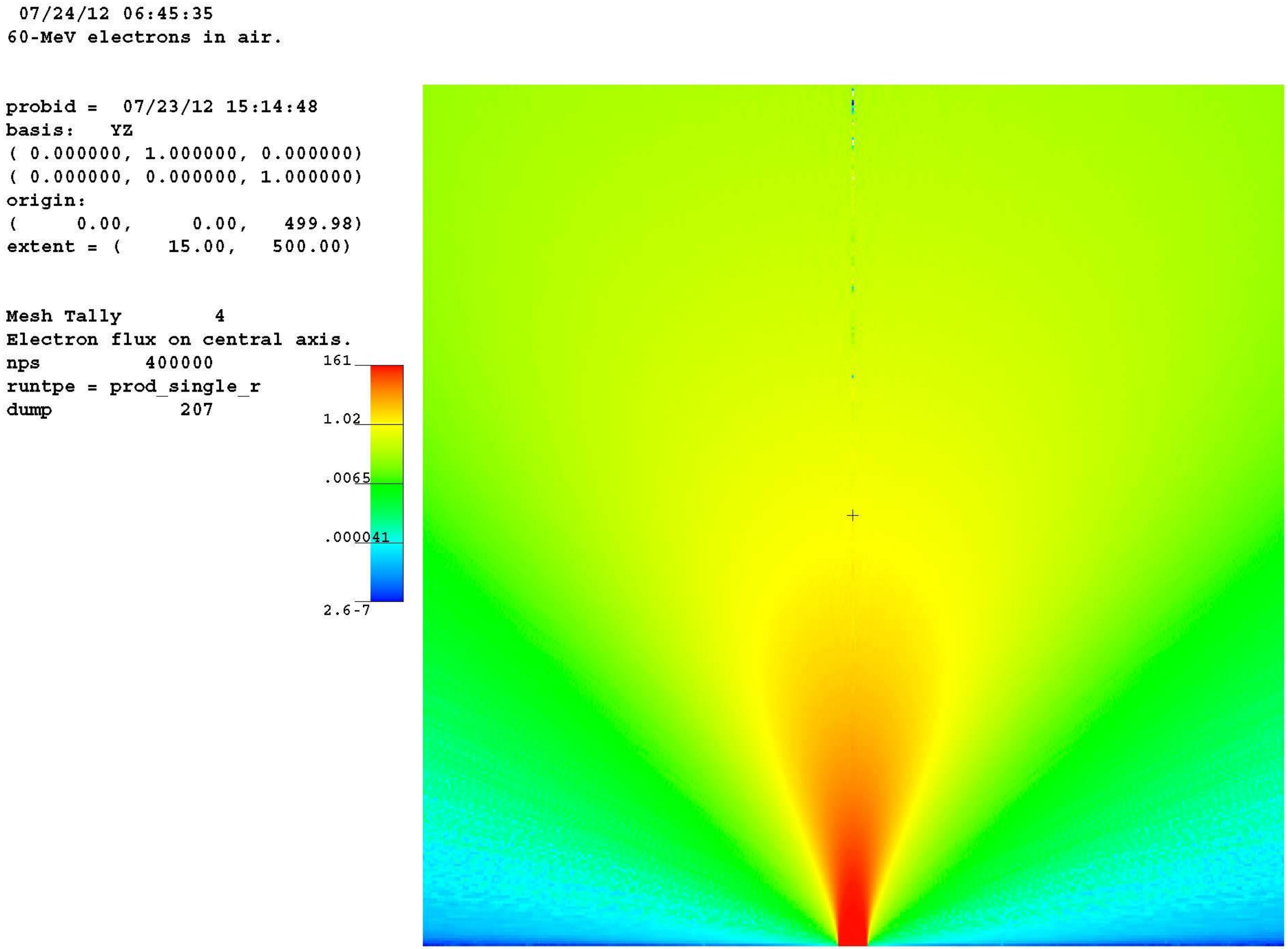
07/23/12 16:37:22
60-MeV electrons in air.

probid = 07/23/12 15:15:25
basis: YZ
(0.000000, 1.000000, 0.000000)
(0.000000, 0.000000, 1.000000)
origin:
(0.00, 0.00, 499.98)
extent = (15.00, 500.00)

Mesh Tally 4
Electron flux on central axis.
nps 400000
runtpe = prod_double_r
dump 19



60-MeV electrons in air, single-event transport.



Future Work — Finishing Touches

- Photon heating numbers
- Bremsstrahlung angular distribution at low energies
- Resolve electron elastic scattering peak
- New relaxation data with condensed-history electrons
- Molecular cross sections and relaxation
- Full integration of other MCNP features
- Formalities of ACE format libraries
- Electromagnetic fields (with single-event electrons)
- Single-event electrons at high energies

Future Work — Speculation

- Photon polarization
- Anomalous scattering factors
- Reflection/refraction
- Cerenkov and synchrotron radiation
- Impact electrons from heavy charged particles
- Variance reduction (computer speed)
- Finite temperatures, condensed matter, etc.
- Collective effects
- Transport in plasmas

Photon Detector Modeling in MCNP6

- F8 PHT & Gaussian Energy Broadening (GEB).
- Coupled F8 PHL tally with F6
- DE/DF for response functions
  - Custom
  - Pre-defined
- Coincidence/Anti-coincidence
- Time Dependent F8
- Triggered detector
- Other ?

- Describe the detection process in CZT
- Compare to physics available in MCNP6
- How can we approximate true physics?
- Find an example of CZT spectrum

CZT is a Semiconductor Diode (Solid State) Detector

- Gamma interacts with semiconducter and created secondary electrons.
- Electrons created electron-hole pairs as they slow down.
- The electron hole pairs migrate under applied electric field and counted.
- Can suffer from hole trapping which leads to asymmetric broadening of peaks (“tails”).
- Overcome with “coplanar grid” to gather electrons only.

MCNP6 Physics Representation

- Coupled p-e transport in MCNP6 can simulate the photon transport and secondary electron production.
- The energy loss as the electrons slow down is simulated along with knock-on electron production.
- But MCNP6 does not calculate the complete electron-hole production cascade.

Example 1: F8 Tally

- 15x15x7.5 mm $Cd_{0.8}Zn_{0.2}Te$ crystal.
- Start with Cs-137 gamma source and use an F8 tally.
- F8 can only register a pulse based on cell accounting and account for statistical variation of charge collection with Gaussian Energy Broadening (GEB).
- GEB parameters based on specific crystal response.
- GEB a b c which defines FWHM.

$$FWHM = a + b\sqrt{E + cE^2}$$

```
F8:p 1
FT8 GEB 3.6e-3 1.5e-1 0.1 $ Values for CZT
```

Example 1: F8 Tally

- Copy C:\MCNP6\EXAMPLES\phl_ex1
- Run the example:

```
mcnp6 i=phl_ex1 n=ex1.
```

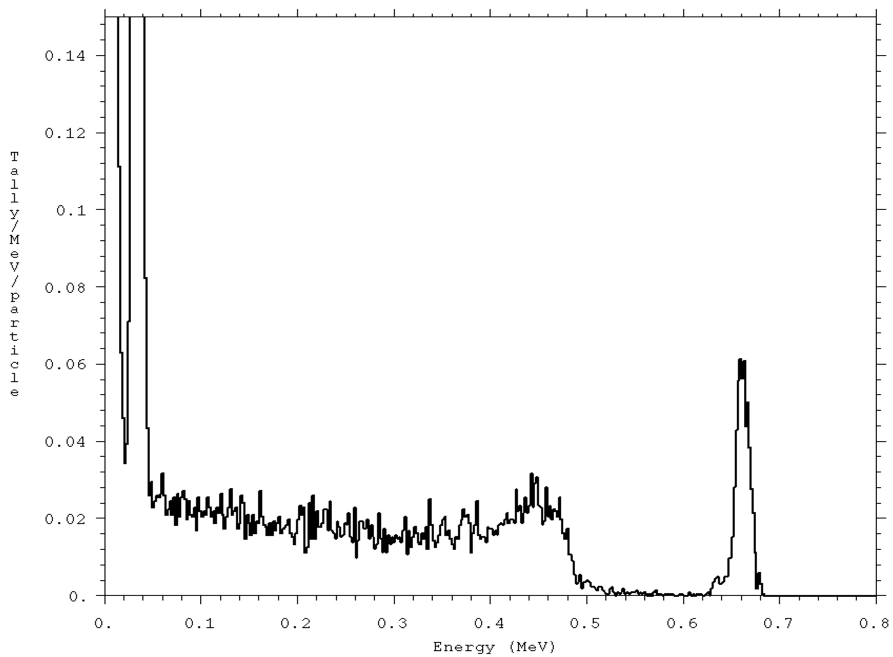
- Display results in plotter:

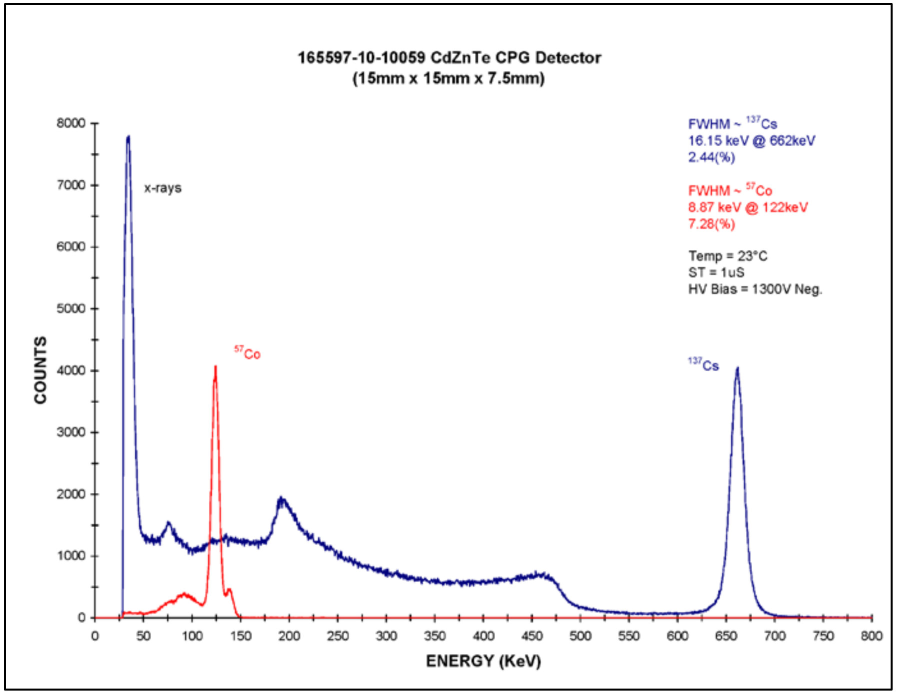
```
mcnp6 z run=ex1.r

mcplot> tal 8 ylims 0 0.15 linlin
```

Example 1: F8 Tally

- Results compared with published vendor spectrum.





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FT PHL Tally

- Uses F6 energy deposition tallies to create pulses.
- Allows more physics detail to be incorporated into pulses.
  - DE/DF
  - Time
  - Triggering
- Better able to deal with nuclear reactions.

FT PHL Tally - Syntax

$$
\begin{array}{l}
\mathrm{PHL}\ \underbrace{[n}_{\text{\# of F6 tallies}}\ \underbrace{t_{a1}\ b_{a1}\ t_{a2}\ b_{a2}\ \ldots\ t_{an}\ b_{an}]}\ [det_1] \\
\quad [m\ t_{b1}\ b_{b1}\ t_{b2}\ b_{b2}\ \ldots\ t_{bm}\ b_{bm}]\ [det_2] \\
\quad [j\ t_{c1}\ b_{c1}\ t_{c2}\ b_{c2}\ \ldots\ t_{cj}\ b_{cj}]\ [det_3] \\
\quad [k\ t_{d1}\ b_{d1}\ t_{d2}\ b_{d2}\ \ldots\ t_{dk}\ b_{dk}]\ [det_4]\ [TDEP\ tg\ tt]
\end{array}
$$

# of F6 tallies for each detector region

Optional detector description

Pairings of tally number and F-bin number for the n F6 tallies of each detector region

Optional trigger keyword, The first entry (tg) specifies the trigger tally number, the second (tt) specifies an energy threshold (MeV).

Very complicated!!

FT PHL Tally - Syntax

PHL [n t_{a1} b_{a1}] 0

Let's start simple with one region and one tally.

```
PHL 1 6 1 0
```

n=1 means one tally. The 6 means tally F6 will be used.
The next '1' means the first F-bin (cell bin) of that tally.
'0' ends the input.

```
F6:e 1   $ Here's the F6 tally we'll use
F8:p 1   $ F8 tally, particle, cell designators are placeholders only
FT8 PHL 1 6 1 0  $ PHL definition
E8   0 1023i 8  $ energy bins for pulses
```

Now we have defined an F8 tally which is fed by and F6.
This case duplicates the function of a normal F8 PHT.

Example 2: Simple F8 PHL

- Copy file phl_ex2 and note added electron tally and added F8 PHL to gather electron energy. GEB is included as before:

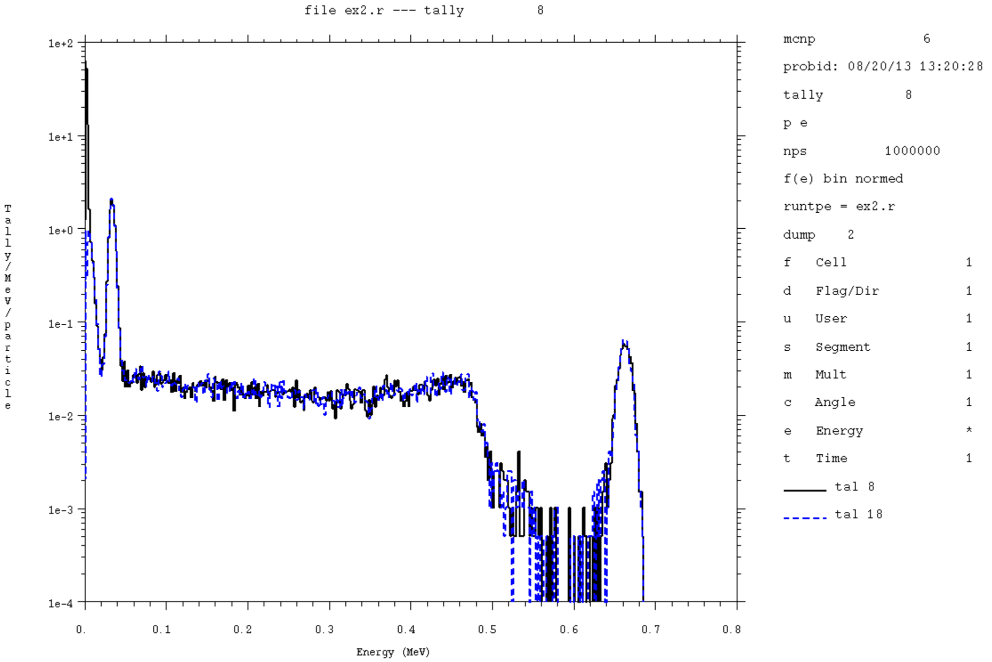
```
F6:e 1
F18:p 1
FT18 PHL 1 6 1 0 GEB  3.6e-3   1.5e-1   0.1
E18  0 1e-6 400i 0.8
```

- Run the problem:

```
mcnp6 i=example2 n=ex2.
```

Example 2: F8 PHL (cont.)

- If no response function is used, results of F8 and F8 PHL should match almost exactly.




```
mcplot>  tal 8 la “tal 8” cop tal 18 la “tal 18”
```

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MCNP6 Physics Representation

- To simulate the creation, migration and collection of the electron hole pairs, we can tally the energy deposition of electrons.
- If electron-hole production is non-linear with energy, we can assign an energy-dependent modifier to energy deposition tally (DE/DF).

DE/DF Response for F8 PHL

- A DE/DF card can be added to F6 tally to adjust the magnitude of energy deposited to allow for larger/smaller scores (pulses) based on energy of electron.
- Example:
  - `DE6   0.1 0.5 0.80 1.0`
  - `DF6   0.8 0.9 0.95 1.0`
- Creates lower-energy pulses from energy deposited by electrons at lower energies.
- Reflects (in)efficiencies in scintillation light, ionization pair, electron hole pair production, etc.

Photon Material Response for PHL

- Some material response functions have been included in MCNP6.
- These adjust the DE/DF responses automatically.
- Can be added as specification on PHL line.
- See Section 3.3.5.18 of MCNP6 manual.
- No function for CZT available.

Table 3-99. Detector Descriptors for the FT PHL Option

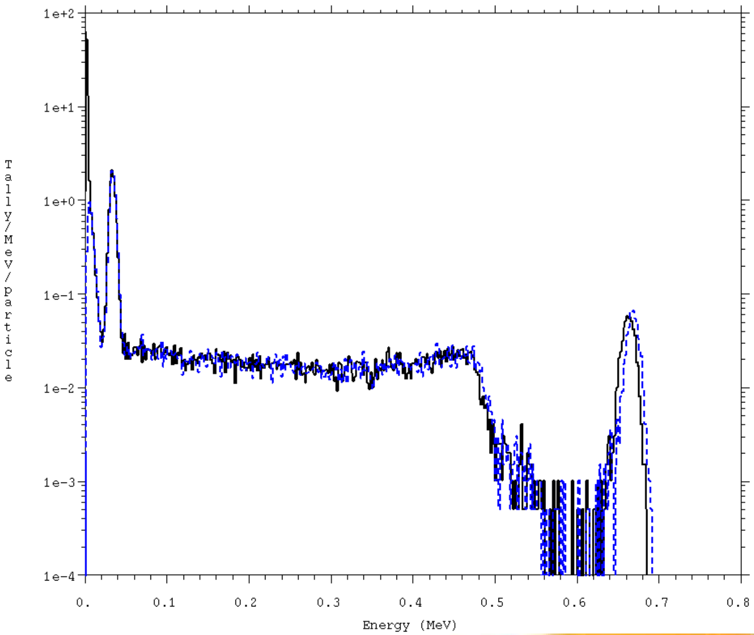
Descriptor	Description
HE3-1	He-3 neutron detector, option 1
BF3-1	BF3 neutron detector, option 1
LIG-1	Li glass neutron detector, option 1
LII-1	LiI neutron detector, option 1
ZNS-1	ZnS neutron detector, option 1
NAI-1	NaI photon detector, option 1
BGO-1	BGO photon detector, option 1
CSI-1	CsI photon detector, option 1
BC4-1	BC400 photon detector, option 1
HPG-1	HPGe photon detector, option 1

Example 3: Photon Material Response for PHL

- Add CSI-1 response keyword to detector in Example 2.

```
ft18 phl 1 6 1 0 csi-1 geb 3.6e-3 1.5e-2 0.1
```

- Small shift in pulse is introduced.



Coincidence/Anti-coincidence

- It is possible to use multiple F6 tallies/tally regions to build F8 tallies.
- Multiple F6 tallies can be added together.
- Or multiple F6 tallies can used in combination to create a matrix of results.

FT PHL Tally - Syntax

PHL [n t_{a1} b_{a1}]
[m t_{b1} b_{b1}] 0

Now we'll use two regions, 1 tally per region.

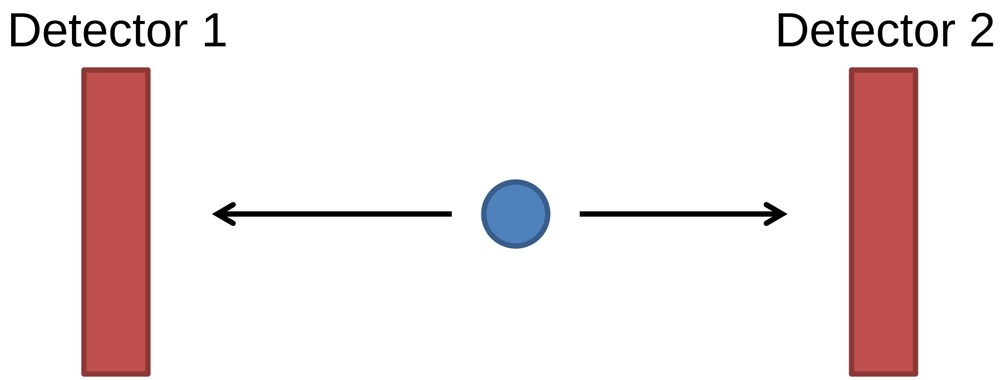
```
PHL 1 6 1
    1 16 1 0
```

As before, but now a second region is defined with using tally F16.

```
F6:e 1
F16:e 1  $ Two F6 tallies
F8:p 1
FT8 PHL 1 6 1
        1 16 1 0  $ two region PHL definition
E8   0 1023i 8  $ energy bins for 1st region
U8   0 1023i 8  $ energy bins for 2nd region
```

Coincidence Detection

- FT8 PHL Tally can be used to create pulses which register two simultaneous (within same history) events.



- This is more useful for neutrons and less useful for photon events given limitation in MCNP6 correlated photon emissions.

Example 4 – Coincidence Detection

- Copy C:\MCNP6\EXAMPLES\phl_ex4
- Example 4 creates two CZT detectors around spontaneous photons (SP) Co-60 source (illustration on previous slide).
- This source simulates decay of Co-60 but samples energy of each photon independently.
- F8 Energy bins are simplified to two bins (zero and non-zero)
- Examine and run Example 4.

```
mcnp6 i=phl_ex4 n=ex4.
```

Example 4 – Coincidence Detection

- Each region has only two energy bins.
- Results are shown in matrix form (score/not-score):

Detector 1

Detector 2

```
cell  1
     user bin:      0.0000E+00            2.0000E+00             total
      energy
    0.0000E+00   2.00000E-05 0.7071   4.56900E-02 0.0145   4.57600E-02 0.0144
    2.0000E+00   4.59200E-02 0.0144   2.41000E-03 0.0643   4.82800E-02 0.0140
      total      4.59400E-02 0.0144   4.81000E-02 0.0141   9.40400E-02 0.0098
```

Example 5 – Coincidence Detection

- Extra Credit:
- Design F8 PHL tally to test emission of specific energies from Co-60 SP source.
- Hint: Refine energy bin structure in Example 4.

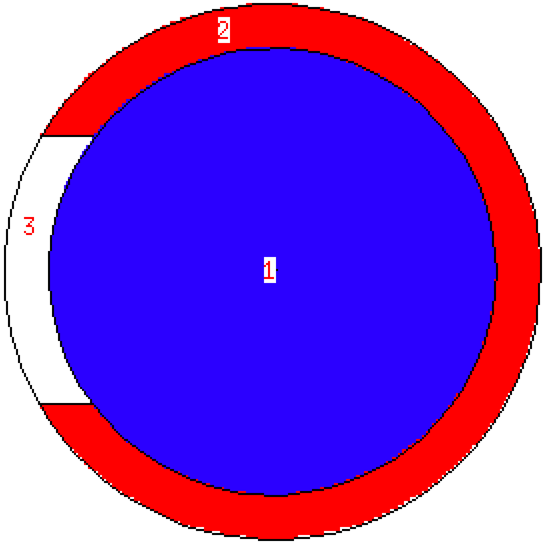
cell 1

user bin: energy	0.0000E+00		1.1000E+00		1.2000E+00		1.3000E+00		1.4000E+00	
0.0000E+00	3.372E-05	0.2582	2.760E-02	0.0089	2.965E-03	0.0275	5.395E-05	0.2041	1.965E-03	0.0338
1.1000E+00	2.781E-02	0.0089	8.610E-04	0.0511	1.326E-04	0.1302	4.496E-06	0.7071	2.922E-05	0.2773
1.2000E+00	3.181E-03	0.0265	1.169E-04	0.1387	**4.496E-06**	0.7071	0.000E+00	0.0000	**2.248E-06**	1.0000
1.3000E+00	5.845E-05	0.1961	2.248E-06	1.0000	0.000E+00	0.0000	0.000E+00	0.0000	0.000E+00	0.0000
1.4000E+00	1.980E-03	0.0337	1.573E-05	0.3780	**2.248E-06**	1.0000	0.000E+00	0.0000	**2.248E-06**	1.0000
2.0000E+00	7.419E-05	0.1741	2.248E-06	1.0000	0.000E+00	0.0000	0.000E+00	0.0000	0.000E+00	0.0000
total	3.314E-02	0.0081	2.860E-02	0.0087	3.104E-03	0.0269	5.845E-05	0.1961	1.998E-03	0.0335

Two 1.33 gammas
One 1.17 and one 1.33
Two 1.17 gammas

Example 6: Anti-Coincidence

- Copy C:\MCNP6\EXAMPLES\phl_ex6
- Multiple F6 tallies can be combined to do anti-coincidence.
- Sphere of BGO surrounded by plastic scintillator.
- Source inward-directed 1 MeV photons.
- Two energy bins for plastic, detailed energy bins for BGO.




```
mcnp6 i=phl_ex6 n=ex6.
```

Example 6: Anti-Coincidence

```
1tally       18         nps =       500000
           tally type 8    pulse height distribution.                         units    number
           particle(s): photons   electrons
           this tally is modified by    ft   geb   phl

 cell  1
     user bin:       0.0000E+00           1.2000E+00            total
      energy
    0.0000E+00   7.20000E-05 0.1667   8.93340E-02 0.0045   8.95240E-02 0.0045
    6.0000E-03   3.72000E-04 0.0733   1.90000E-04 0.1026   5.46000E-04 0.0605
    1.2000E-02   4.14000E-04 0.0695   2.08000E-04 0.0980   6.64000E-04 0.0549
    1.8000E-02   4.42000E-04 0.0673   2.40000E-04 0.0913   7.50000E-04 0.0516
    2.4000E-02   4.94000E-04 0.0636   2.20000E-04 0.0953   7.14000E-04 0.0529
    3.0000E-02   5.26000E-04 0.0616   2.34000E-04 0.0924   6.70000E-04 0.0546
    3.6000E-02   4.32000E-04 0.0680   2.50000E-04 0.0894   7.12000E-04 0.0530
    4.2000E-02   4.48000E-04 0.0668   2.24000E-04 0.0945   6.96000E-04 0.0536
    4.8000E-02   5.68000E-04 0.0593   1.88000E-04 0.1031   7.32000E-04 0.0523
    5.4000E-02   5.64000E-04 0.0595   2.02000E-04 0.0995   7.20000E-04 0.0527
    6.0000E-02   4.82000E-04 0.0644   2.00000E-04 0.1000   6.86000E-04 0.0540
    6.6000E-02   4.46000E-04 0.0670   2.06000E-04 0.0985   6.50000E-04 0.0555
    7.2000E-02   5.28000E-04 0.0615   1.60000E-04 0.1118   7.34000E-04 0.0522
    7.8000E-02   5.46000E-04 0.0605   2.04000E-04 0.0990   7.06000E-04 0.0532
    8.4000E-02   5.32000E-04 0.0613   2.16000E-04 0.0962   7.36000E-04 0.0521
    9.0000E-02   5.16000E-04 0.0622   1.54000E-04 0.1140   6.82000E-04 0.0541
    9.6000E-02   5.22000E-04 0.0619   1.74000E-04 0.1072   6.78000E-04 0.0543
    1.0200E-01   5.32000E-04 0.0613   1.66000E-04 0.1098   7.24000E-04 0.0525
    …            …                    …                    …
```

Plastic

B
G
O

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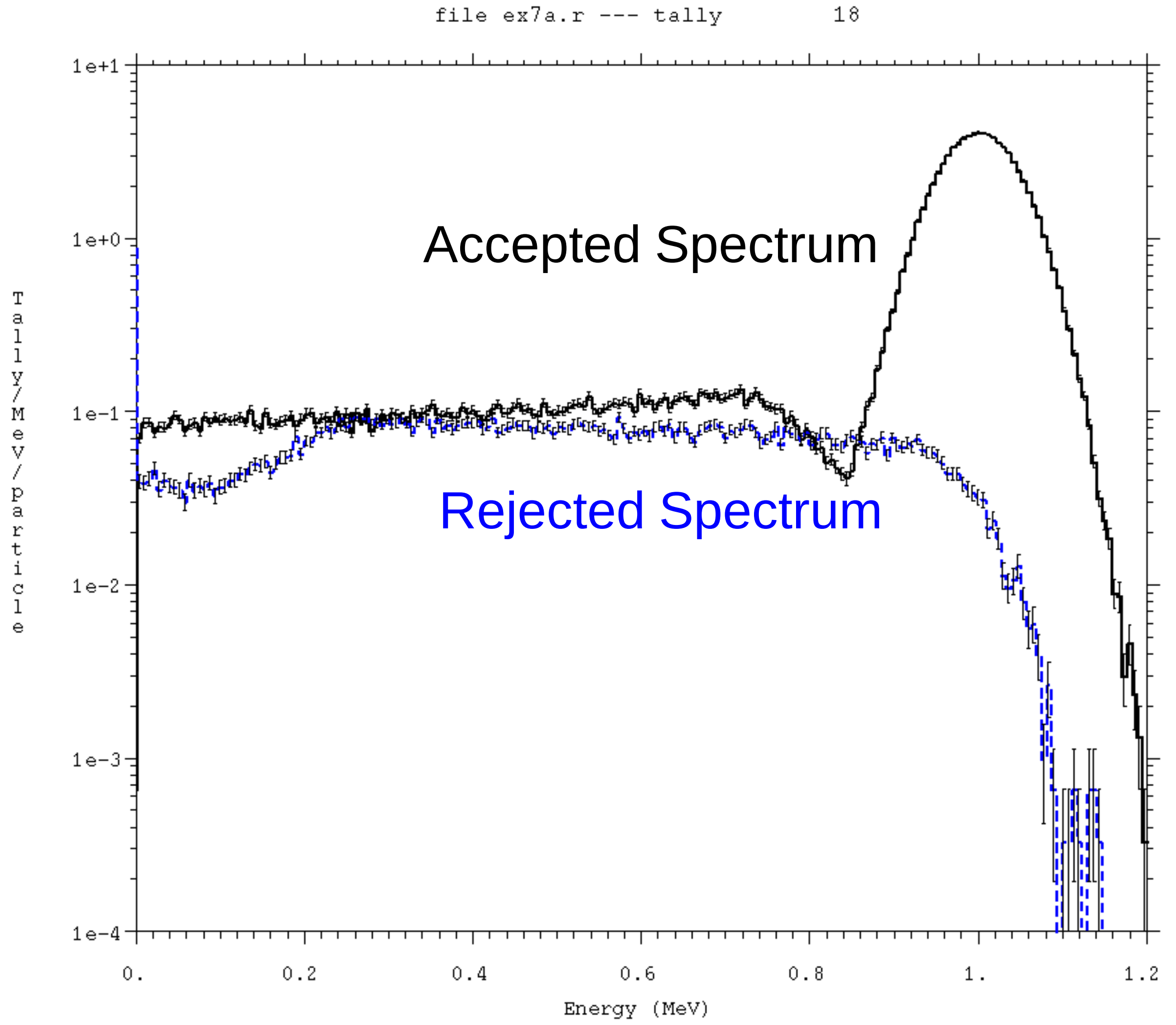
Example 6: Anti-Coincidence



FT PHL Tally - Syntax

PHL [n t_{a1} b_{a1} t_{a2} b_{a2} ... t_{an} b_{an}]

What if we used two tallies per region?

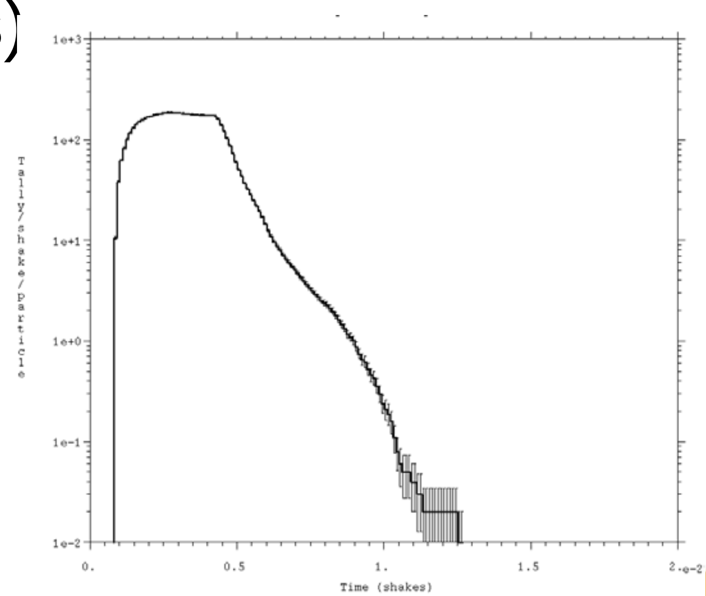
```
PHL 2 6 1  16 1  0
```

Now the response of the two F6 tallies are summed.

```
F6:e 1
F16:e 1  $ Two F6 tallies
F8:p 1
FT8 PHL 2 6 1 16 1 0  $ two tally region PHL definition
E8   0 1023i 8  $ energy bins for 1st region
```

Example 7: Time Binning on F8

- It is possible to subdivide F8 PHL into time bins since F6 records the time structure of energy deposition.
- The file phl_ex7 is the same as phl_ex2 but with time bins added.
  - `T18 0 199i 2e-2` (shakes)
- 1 pulse is distributed over time by ratio of energy in those time bins.
- Time structure of electron pulses.



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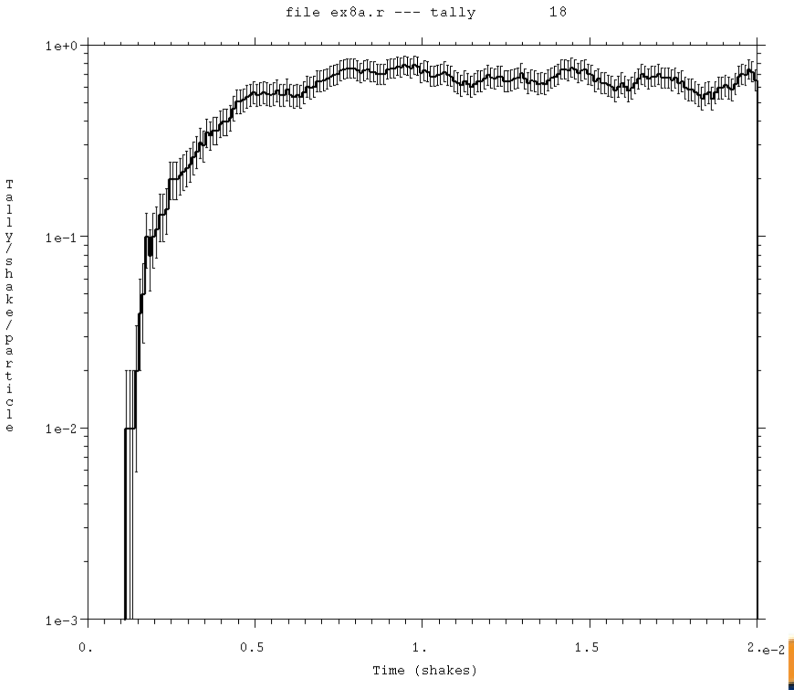
Time Trigger Option

PHL [n t_{a1} b_{a1} t_{a2} b_{a2} ... t_{an} b_{an}] [det_1] [TDEP tg tt]

- A ‘tdep’ keyword can be used on the F8 PHL to set a trigger region and energy threshold.
- Usually more useful for neutron tallies.
- By default, the F8 tally with the tdep is used with zero energy threshold.

Example 8: Time Trigger (Step 1)

- Starting with example 7 and create time-dependent source from 0 to 1 shake.
- Run this and note results
- Result: flat distribution out to 2e-2 shakes (and beyond).



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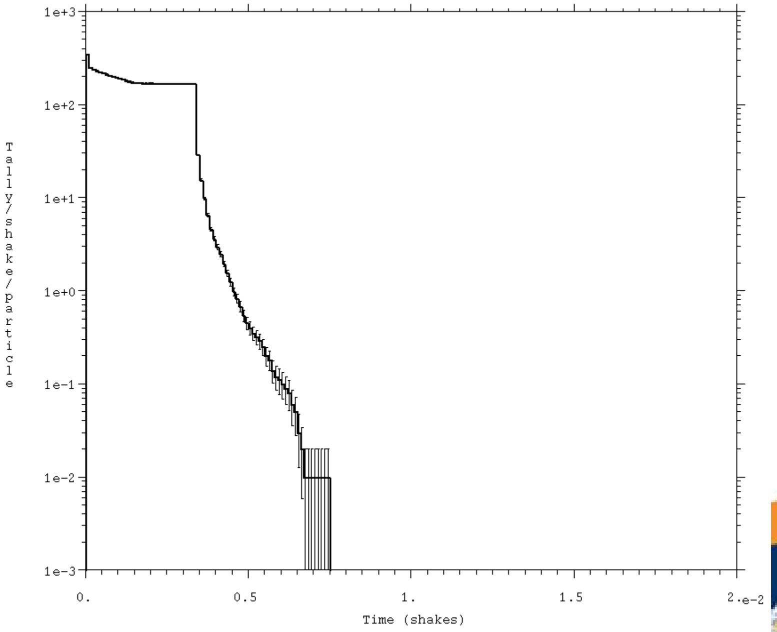
Example 8: Time Trigger (Step 2)

- Add tdep card to F8 PHL tally to make time bins relative to when first energy score is recorded.
- `ft18 phl 1 6 1 0 tdep 18 0 geb 3.6e-3 1.5e-2 0.1`
- Tdep 18 0 will cause tally to trigger on itself (i.e all time-dependent results will be reset to the same relative point in time.
- Results: Similar to Example 7 but the early time bins are all non-zero.



TF Card

- The TF card can be used to indicate which F6 bins should contribute to the F8 PHL.
- Multiple F-bins can be used on the F6 tallies and can be referred to on the PHL interface.