Tallies

An Introduction

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Fundamentals

MCNP6 Output

MCNP6 can generate a lot of output for the “outp” file.

- **Output that is always there**
- **Output that you can turn on or off via the print card**
- **User requested / defined tallies**

Automatic Output

MCNP6 automatically creates standard summary information that gives the user a better insight into the physics of the problem and the adequacy of the Monte Carlo simulation.

- a complete listing of the input
- a complete accounting of the creation and loss of all tracks and their energy
- the number of tracks entering and re-entering a cell plus the track population in the cell
- the number of collisions in a cell
- the average weight, mean free path, and energy of tracks in a cell
- the activity of each nuclide in a cell (that is, how particles interacted with each nuclide, not the radioactivity)
- a complete weight balance for each cell
- KCODE cycle summaries
- basic print tables

Print Tables

- **Much information is organized in print tables that can be turned on or off.**
  - Only limited information about fluxes, spectra, reaction rates, etc.
- **The tables are numbered.**
  - Table number appears in the upper right-hand corner of the table, providing a convenient pattern when scanning the output file with an editor.
  - The pattern is PRINT TABLE *n*, where *n* is always preceded by one space and is a two- or three-digit number.

The Print Card

PRINT *x*

x = no entry … gives the full, basic output print

x = *x1 x2* (positive entries) *...* prints basic output plus the tables specified by the table numbers *x1*, *x2*, ...

x = −*x1* −*x2* (negative entries) ... prints full, basic output except the tables specified by *x1*, *x2*, ...

Default: No PRINT card in the INP file or no PRINT option on the execution line will result in a reduced output print.

"basic" tables can't be turned off; "default" tables printed automatically can be turned off.

Use is optional but highly recommended.

Table of Print Tables (1)

Table Number	Type	Description
10		Source coefficients and distribution
20		Weight window information
30		Tally description
32		Mesh tally description
35		Coincident detectors
40		Material composition
50		Cell volumes and masses, surface areas
60	basic	Cell importances
62	basic	Forced collision and exponential transform
70		Surface coefficients
72	basic	Cell temperatures
80		ESPLT/TSPLT Importance Ratios
85		Electron range and straggling tables
86		Electron bremsstrahlung and secondary production
90		KCODE source data
98		Physical constants and compile options

Table of Print Tables (2)

Table Number	Type	Description
100	basic	Cross-section tables
102		Assignment of S(α,β) data to nuclides
110		First 50 starting histories
120		Analysis of the quality of your importance function
126	basic	Particle activity in each cell
128		Universe map
130		Neutron/photon/electron weight balance
140		Neutron/photon nuclide activity
150		DXTRAN diagnostics
160	default	TFC bin tally analysis
161	default	*f*(*x*) tally density plot (empirical history score PDF)
162	default	Cumulative *f*(*x*) and tally density plot
170		Source distribution frequency tables, surface source
175	shorten	Estimated *keff* results by cycle
178		Estimated *keff* results by batch size
190	basic	Weight window generator summary
198		Weight windows from multi-group fluxes
200	basic	Weight window generated windows

Tallies

What is a tally?

- Not explicitly defined in the MCNP manual
- Manual states that the code “provides” them

Some definitions:

- A record of a reckoning, score, or count
- A number or group of items recorded
- A tabulation of results

Getting Results from MCNP6

- **MCNP produces k-eff information in tables.**
- **In fixed-source problems, MCNP6 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.**
- **Tallies in MCNP6 are often called <u>edits</u> in many other codes**
  - Fluxes
  - Currents
  - Reaction rates
- **Edits in MCNP are associated with its unstructured mesh feature.**

Tally Types

MCNP6 tally types:

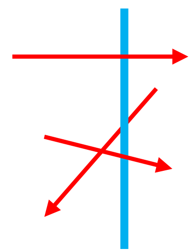
F1:	Current on a surface	
F2:	Flux on a surface	
F4:	Flux in a cell	(track-length estimate)
F5:	Flux at a point or ring detector	
F6:	Energy deposition	(track-length estimate)
F7:	Fission energy deposition	(track-length estimate)
F8:	Pulse height tally	
FMESH:	Mesh tallies	

Basic Tallies

F1:<pl> - Current across surface

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

W = total source weight



F2:<pl> – Flux on a 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

μ = Ω • [surface normal]

The concept of weight will be discussed in the variance reduction section. For now, consider wgt = 1.0

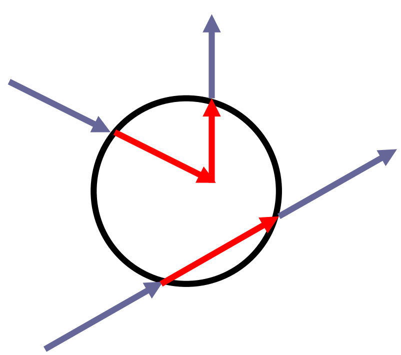
Basic Tallies

F4:<pl> - Flux in a cell

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

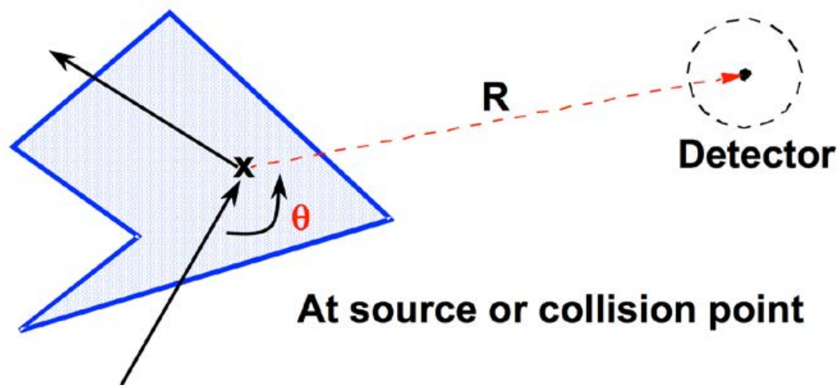
V = cell volume

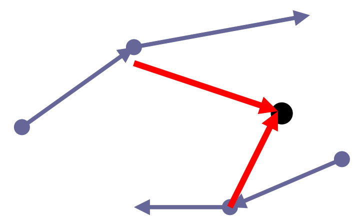
W = total source weight



F5:<pl> - Flux at a point

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





F6:<pl> – energy deposition tally

F7:<pl> – fission energy deposition tally

- Volume tallies like F4
- Units of MeV/g, unless
- *F6 or *F7 then units are jerks/g

Tally Normalization & Units

- **All MCNP6 tallies are normalized to be the response for 1 source particle**
- **If your actual source strength is 4000 particles/sec, then**
  - MCNP6 tally results should be multiplied by 4000
  - Units for tallies should be "per second"
  - Applies when the **rate** of source particle production is known
- **If your actual source strength is 4000 particles, then**
  - MCNP6 tally results should be multiplied by 4000
  - Units for tallies should **not** be "per second"
  - Applies the **total** source particle production is known (e.g., a pulse)
- **You can have MCNP6 do the multiplication:**
  - Supply the source strength on a tally multiplier card (**FMn card**)

  OR

  - Supply the source strength on the **sdef card** (include **wgt = ... ,** but not recommended when using weight windows)

Tally Quantities Scored

Type	Where	Units
F1: Surface Current . . . All particles	surface	#
F2: Surface Flux . . . All particles	surface	# / cm^2
F4: Track length estimate of cell flux . All particles	Cell	# / cm^2
F5: Flux at a point or ring detector . N or P	point or ring	# / cm^2
F6: Track length est. of energy deposition. All particles	cell	MeV / g
F7: Track length est. of fission energy dep. N	cell	MeV / g
F8: Pulse height tally . . . All particles	cell	pulses

The + Modifier

- **A preceding plus-sign can be applied to F6 for collision heating (+F6) and F8 for charge deposition (+F8)**
  - **+F6 Collision heating MeV/g**
    - **Always applies to all particles listed on the mode card**
    - **No particle designator**
  - **+F8:<pl> Charge deposition charge**
- **The +F8 tally is the negative particle weight for electrons and the positive weight for positrons.**
  - Refer to the MCNP manual for more information on the F8 tally, how it can be modified, and how it can be used.

The * Modifier (1)

- **Tally types 1, 2, 4, and 5 are normally weight tallies (particles in the above table); however, if the F card is flagged with an asterisk (for example, *F1:N), energy times weight will be tallied.**
  - ***F1:<pl>   MeV**
  - ***F2:<pl>   MeV/cm2**
  - ***F4:<pl>   MeV/cm2**
  - ***F5: <pl>   MeV/cm2**
- **The asterisk flagging also can be used on tally types 6 and 7 to change the units from MeV/g to jerks/g (1 jerk = 1 GJ = 1e9 J).**

The * Modifier (2)

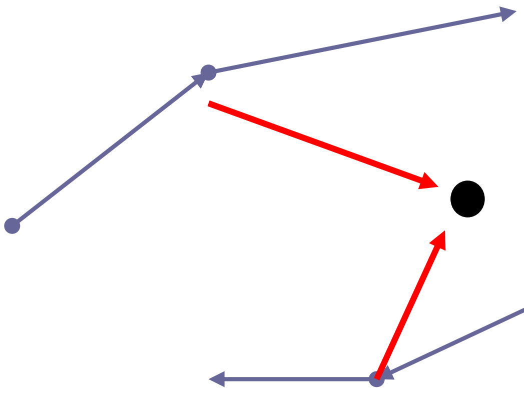
- **The asterisk on a tally type 8 converts from a pulse-height tally to an energy deposition tally.**
  - ***F8:<pl> MeV**
- **No asterisk can be used in combination with the + on the +F6 or +F8 tallies.**

Tally Card Contents

- **F1, F2, F4, F6, F7, F8:   Fn:<pl>   {list of surfaces or cells}**
  - **n = tally number = i + 10j   i = 1, 2, 4, 6, 7, 8**
    $0 \le j \le 9999$
    - **Last digit is tally type**
    - **F4:n, F14:n, F124:n   are all "F4" tallies**
  - **<pl> = particle type = particle <u>symbol</u>: n, p, e, etc.**
  - **May group entries with parentheses**
    - **Each parentheses group is a single bin**
  - **Optional entry "T" at the end to give total**

F5 Tally Card Contents (Flux at Point)

- **Form: Fn:<pl> X Y Z R**
  - **n = tally number = 5 + 10j** $0 \le j \le 999$
  - **<pl> = particle type = particle symbol: n or p (no charged particles)**
  - **At every collision, makes a deterministic estimate of flux**
  - **X, Y, 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**
    - **Use 0.0 in a void (vacuum) region**



Tally Examples

F1:p	(1 2) (3 4 5) 6	Photon surface current, 3 bins
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
F105:p	3.2 4.1 5.7 0.0	F5 photon flux at point, in a void
F35:n	100. 17. 0.0 5.0	F5 neutron flux at point, in a material
*F8:p	10 25	F8 tally of photon energy deposited in cells, MeV

Tallies Require Volumes or Areas

- **For tallies (except F1, F5, F8) to be valid, MCNP6 must know a volume or area to perform the division.**
- **Sometimes, MCNP6 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.

4) Volumes can be calculated via the stochastic volume calculation

- requires special run
- see manual

Segment Divisor Card (SD)

- **MCNP6 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 MCNP6

- **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
  - Can be used to get total absorption, rather than absorption/vol
  - Note: dividing by 1.0 instead of volume changes units, etc.

Commenting Tallies in the Output File

- **Commenting on what tallies are calculated is important, especially if others may look at your output file!**
  - Your co-workers will thank you!

- **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.
```

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**

<u>Rectangular Parallelepiped (RPP)</u>

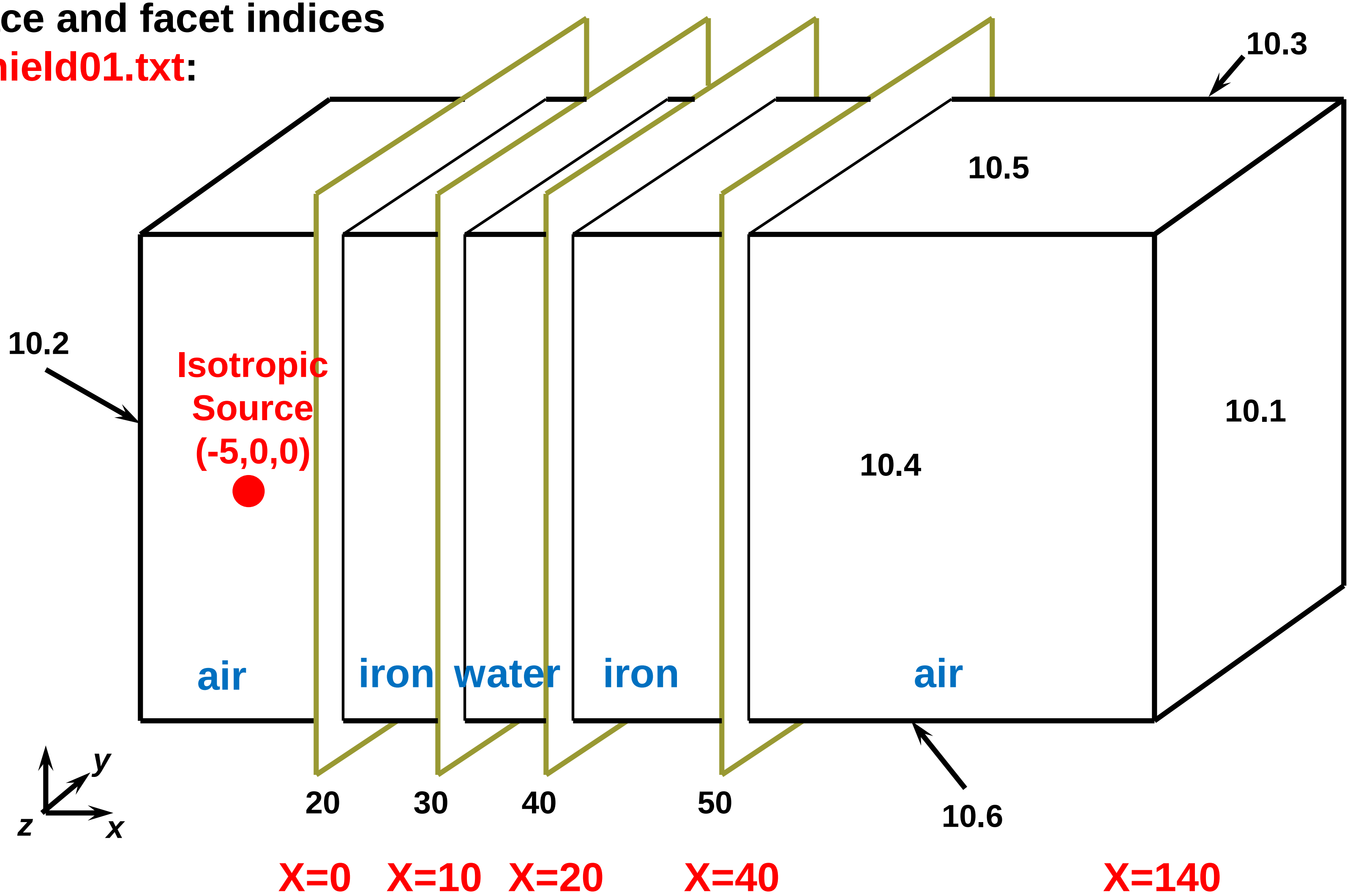
1 right side
2 left side
3 front
4 back
5 top
6 bottom

<u>Right Circular Cylinder (RCC)</u>

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

Example

Surface and facet indices for shield01.txt:



Input file for shield01.txt

```
shield01 - shielding calculation with 252-Cf neutron source
c >>>>> cell cards
100    3000   -0.0013    -10 -20          $ air left of shield
200    1000   -7.874     -10  20 -30      $ iron shield left layer
210    2000   -1.0       -10  30 -40      $ water layer
220    1000   -7.874     -10  40 -50      $ iron shield right layer
300    3000   -0.0013    -10  50          $ air right of shield
999       0               10              $ rest of the world

c >>>>> surface cards
10  rpp -10  140   -100 100   -100 100    $ problem bounding surfaces
20  px    0                               $ beginning of shield
30  px   10                               $ start of water layer
40  px   20                               $ end of water layer
50  px   40                               $ end of shield

c >>>>> data cards
nps     1e5
c --- material specification
m1000    26056    1.0                     $ shield, pure iron-56
m2000     1001    2      8016   1         $ water
mt2000    lwtr                            $ water s(a,b)
m3000     7014    0.8    8016   0.2       $ air
c --- source specification
sdef    pos=-5  0  0     erg=d1
sp1     -3   1.025   2.926                $ 252-Cf spontaneous fission
c --- importances
imp:n   1  4r  0
```

Motivation

- **Copy shield01.txt out of the SOLUTIONS directory.**
- **Analyze the input file and plot the geometry.**
  - The shield is considered to be the iron – water – iron sandwich
- **Run the problem**

```
mcnp6   n = shield01.txt
```

- **Note the following screen output:**

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

- **Analogous to running an experiment with no detection equipment!**
- **Examine the outp file**

Example: shield02

- **Copy shield01.txt to shield02.txt**
- **Insert tallies for:**
  - Surface current at
    - Front (surface) of the shield facing source,
    - Back (surface) 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 252-Cf neutron source
c >>>>> data cards
. . .
c --- tally specification
fc1  surface current entering, exiting, and 1 m after shield
f1:n    20   50   10.1
c
fc4     average neutron flux in the shield
f4:n    (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  neutrons

 surface  20

                7.88217E-01 0.0036

 surface  50

                5.36646E-03 0.0430

 surface  10.1

                2.56677E-03 0.0613
```

Example: shield02 results

```
1tally         4        nps =      1000
                     average neutron flux in the shield

  tally type 4    track length estimate of particle flux
   tally for  neutrons

           cell  a is (200 210 220)

           volumes

                   cell:       a

                         1.60000E+06

 cell (200 210 220)

                    1.20763E-05 0.0055
```

Statistics and TFC discussion, pdf's & cdf's

Tally Fluctuation Chart

```
1tally fluctuation charts

                         tally        4
      nps        mean       error    vov  slope      fom
     8000   1.2490E-06 0.1028 0.0421  0.0     3110
    16000   1.2880E-06 0.0695 0.0178 10.0     3226
    24000   1.2224E-06 0.0564 0.0119  7.4     3228
    32000   1.2361E-06 0.0489 0.0088  7.4     3139
    40000   1.2529E-06 0.0438 0.0066 10.0     3137
    48000   1.2125E-06 0.0402 0.0057 10.0     3123
    56000   1.2178E-06 0.0368 0.0048 10.0     3289
    64000   1.2124E-06 0.0345 0.0042 10.0     3252
    72000   1.1955E-06 0.0325 0.0037 10.0     3263
    80000   1.2238E-06 0.0309 0.0033 10.0     3226
    88000   1.2256E-06 0.0293 0.0030 10.0     3240
    96000   1.2312E-06 0.0280 0.0028 10.0     3269
   100000   1.2323E-06 0.0274 0.0026 10.0     3283
```

Assessing Results

- **MCNP6 uses the Monte Carlo method.**
  - **Relies on repeated random sampling (of many cumulative distributions).**
  - **Results have statistical errors or uncertainties.**
  - **Always quote the errors when quoting the results.**
- **The influence of statistical errors or noise must be considered when assessing the reliability of Monte Carlo results.**
- **MCNP6 provides uncertainties and performs statistical checks to attempt to assess whether or not the results are reliable.**
  - **Results of tests don't prove reliability!!!**
  - **The tests look for things that seem wrong.**
  - **The tests don't prove that results are correct.**
- **Confidence intervals assume that the Central Limit Theorem is satisfied.**
  - The arithmetic mean of a sufficiently large number of samples of identically distributed, independent random variables, each with a finite mean and variance, will approach a normal distribution, regardless of the underlying distribution.

Review: Basic Statistics

- **MCNP6 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 K_{eff} 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

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

  - **Sample standard deviation** of a tally average, after N histories

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

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

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

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, i.e., 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.**

Interpreting R

For n identical scores and n << N (n out of N) $R = 1/\sqrt{n}$

Range of R	Tally Quality
0.5 – 1.0	Garbage
0.2 – 0.5	Factor of a few
0.1 – 0.2	Questionable
< 0.10	Generally reliable <u>except</u> for point detectors
< 0.05	Generally reliable for point detectors

- **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:**

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

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

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

where μ is the true mean and σ is the true standard deviation.

  - **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 1σ confidence interval.**

Relative variance of the variance (VOV) – estimated relative variance of the estimated R.

- Involves the estimated 3rd and 4th moments of the empirical history score PDF f(x).
- Much more sensitive to large history score fluctuation than is R.
- Magnitude and behavior as a function of N are indicators of tally convergence and how well S approximates σ.

Figure Of Merit

$$\mathrm{FOM} \equiv \frac{1}{R^2 T}$$

Measure of efficiency

$$R^2 \propto 1/N \qquad\qquad T \propto N$$

***R^2T* ~ constant within any one Monte Carlo run.**

If tally is well behaved, the FOM ~ constant with the exception of very early in the problem.

Empirical History Score PDF, *f(x)*

What is it?

A histogram log-log plot of *f(x)* vs *x* where

$$f(x_i) = \frac{NH_i}{N \cdot BW_i}$$

X	**=**	**history score to the tally (score from 1 complete history)**
N	**=**	**total number of histories**
$\mathbf{NH_i}$	**=**	**# of history scores in the i'th score bin**
$\mathbf{BW_i}$	**=**	**bin width for i'th score bin**
	=	$x^{i+1} - x^i = 1.2589\, x^i - x^i$

The quantity 1.2589 is $10^{0.1}$ and comes from 10 equally spaced log bins per decade.

Instructor can show where this appears in the outp file

Pareto Fit of the largest x_i's

$$\text{Pareto} \quad f(x) = a^{-1}(1 + kx/a)^{-(1/k)-1}$$

- **From this fit, the slope n in $1/x^n$ of the largest history scores *x* can be estimated to determine if and when the largest history scores decrease faster than $1/x^3$.**
- **Fits a number of extreme value distributions including:**
  - **`1/x`^{n}**
  - **`Exponential (k = 0)`**
  - **`Constant (k = -1)`**

EHS PDF -- Slope

From the Pareto fit, the slope of $f(x_{large})$ is defined as

$$\mathrm{SLOPE} \equiv (1/k) + 1$$

Where k is from the Pareto fit.

0	**-**	**not enough $f(x_{large})$ tail information exists for a slope estimate**
10	**-**	**perfect score; max value; indicates an essentially negative exponential decrease**
>3	**-**	**satisfies the 2nd moment existence requirement for CLT**
>5	**-**	**4th moment exists; VOV is believable**

Extrapolating a large score tail that decreases less steeply than $1/x^3$ to infinity would produce an infinite 2nd moment, violating the CLT.

MCNP - Ten Statistical Checks

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

1. Estimated **mean** should have random behavior for last half of problem
2. Estimated **relative error** should be < 0.05 for point detector; < 0.10 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 < 0.10
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 underlying **tally probability density** should fall off as $1/x^m$, with m>3

10 Statistical Checks Output

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

           results of 10 statistical checks for the estimated answer for the tally fluctuation chart (tfc) bin of tally        4

 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       <0.10      yes      1/sqrt(nps)       <0.10      yes        1/nps           constant    random      >3.00
 observed     random        0.03      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.


1status of the statistical checks used to form confidence intervals for the mean for each tally bin


 tally   result of statistical checks for the tfc bin (the first check not passed is listed) and error magnitude check for all bins

        4   passed the 10 statistical checks for the tally fluctuation chart bin result
         passed all bin error check:     1 tally bins all have relative errors less than 0.10 with no zero bins


 the 10 statistical checks are only for the tally fluctuation chart bin and do not apply to other tally bins.
```

The FM Card

Reaction Rates

- **Often some reaction rate, based on the flux or fluence, may be desired.**

$$R_x = N\sigma_x\phi \qquad \left(\frac{\text{nuclides}}{\text{barn}\cdot\text{cm}}\right)\circ\left(\frac{\text{barns}}{\text{nuclide}}\right)\circ\left(\frac{1}{\text{cm}^2\cdot\text{sec}}\right) = \frac{1}{\text{cm}^3\cdot\text{sec}}$$

Units = Reactions per unit volume (per unit time)

- **Need some way to <u>multiply</u> the flux tally scores by the number density and the microscopic cross section for reaction *x*.**
- **MCNP can do this with the <u>tally multiplier</u>, or FM, card.**
- **Tally multiplier card can also scale by constants and has additional uses.**

Reaction Rate Tallies

- **Fn card specifies:**
  - Type of tally - last digit of n
  - Type of particle (e.g., F4:n)
  - Location - cells or surfaces
- **FMn card specifies:**
  - Multiplier – constant, N, and/or N’s from a material
  - Type of cross-section – many options

Fn card

$$R_x = N\sigma_x\phi$$

FMn card

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 constant)**
    - **C < 0 means -- multiply tally by |*C*|, and by atom density in the tally cell**
  - **m is a material number (from an Mm card)**
    - **Which atom density to use**
  - **B_k is a reaction type identifier**
  - **B_{last} is either blank or T (T sums over previous multiplier sets)**

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 MCNP-specific to the type of library (multi-group or continuous-energy) and particle (neutron or photon) employed**

MT	Reaction Type
1	Total
2	Elastic scatter
18	Fission
101	Capture
102	(n,γ)
etc.	see Manual

	Neutrons		
Type	Continuous	Multigroup	Photons
-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)		

Note: The definitions of capture and absorption differ depending upon whether you are a physicist or a nuclear engineer. Throughout this presentation, we will use absorption = fission + capture

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              $ number densities from mat 100
                                              $ ( σF · v )
```

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

```
F34:n    10
FM34     -1.0   100    -2 : -6               $ number densities from mat 100
                                              $ ( σC + σF )
```

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Exercise: shield03 -- Gamma Production

- **Copy shield01.txt to shield03.txt.**
- **Add tally to compute the total photon production rate in the iron portion of the shield.**
  - Source strength of 3.0e8 neutrons per second
  - Note the units of the tally
    (want total photon production rate in entire volume,
    not production rate density)
- **Run the problem and examine the output file.**

Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Exercise: shield03 -- Gamma Production

shield03 - shielding calculation with 252-Cf neutron source

```
c >>>>> data cards
. . .
c --- tally specification
fc4     photon production rate in iron
f4:n   (200  220)
fm4    -3.e8  1000  -5   $ source strength * γ product xs
sd4     1                $ do not divide by volume
```


Los Alamos NATIONAL LABORATORY EST. 1943
Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Exercise: Gamma Production

```
1tally        4    nps = 100
                              photon production rate in iron
  tally type 4    track length estimate of particle flux.
  tally for  neutrons

         volumes

                 cell:   (200 220)

                       1.00000E+00

 cell (200 220)

 multiplier bin:  -3.00000E+08      1000          -5

                    1.63932E+08 0.0063
```

DE / DF Cards
Dose Rates

Calculating Dose in MCNP

- **There are two methods to compute dose (energy deposited per unit mass) in MCNP6:**
  - 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 flux-to-dose conversion factors.
- **F6 tallies produce absorbed dose**
  - Units of rad or gray.
- **F2 or F4 tallies with "flux-to-dose" conversion factors produce biological dose**
  - Need "dose functions" to provide quality or tissue weighting factors.
  - Units of rem or sievert

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 is captured
  - 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 tally and a FM4 card with (-1 -4).
  - Units are MeV/g; use FM card to convert units to rad or Gy.
- **Required 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 E_1 E_2 . . . E_k

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

DFn B F_1 F_2 . . . F_k

- **F_i = 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 3.0e8 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 252-Cf neutron source

```
c >>>>> data cards
. . .
c ### tally specification
fc2     average dose rate in rem/hr, 1 m from shield from 3e8 neutrons
f2:n    10.1
fm2     3.e8         $ multiply by source strength 3.e8 n/s
c --- neutron flux to dose (rem/hr) factors
c !!! NOT RECOMMENDED FOR "OFFICIAL" CALCULATIONS !!!
de2     log   2.50e-8   1.00e-7   1.00e-6   1.00e-5   1.00e-4   1.00e-3
              1.00e-2   1.00e-1   5.00e-1   1.00e+0   2.50e+0   5.00e+0
              7.00e+0   1.00e+1   1.40e+1   2.00e+1
df2     log   3.67e-6   3.67e-6   4.46e-6   4.54e-6   4.18e-6   3.76e-6
              3.56e-6   2.17e-5   9.26e-5   1.32e-4   1.25e-4   1.56e-4
              1.47e-4   1.47e-4   2.08e-4   2.27e-4
```

Exercise: Dose Calculation

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

           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
                1.63755E-03 0.0740
```

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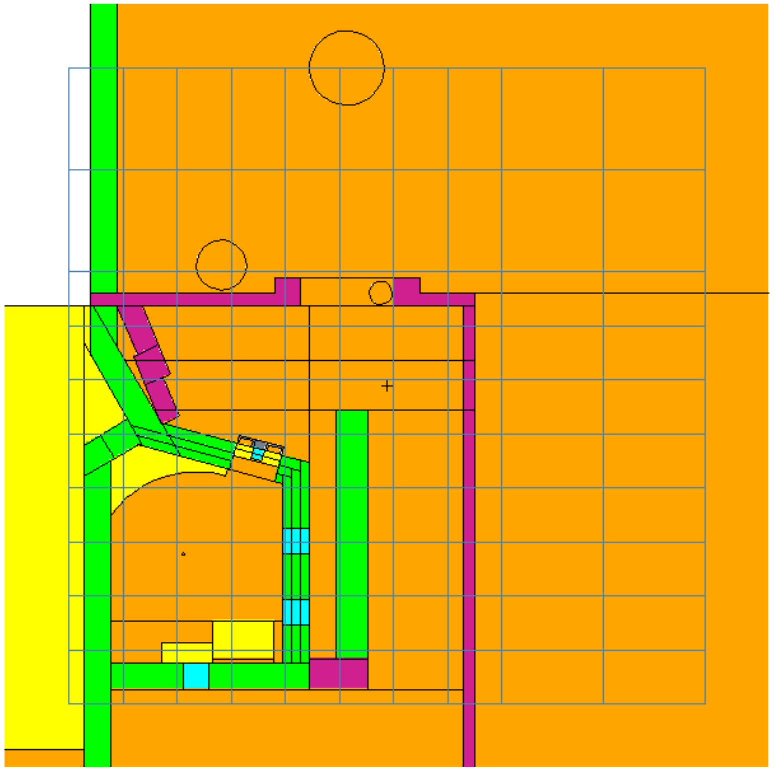
FMESH Tallies

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, fission source points, …
  - Rectangular & cylindrical meshes
  - Bin on energy & time values
  - Number & size of mesh limited only by computer parameters
  - Can be rotated and translate
  - Modified by DE/DF or FM cards
    - Can't use built in DF functions
  - Plot results in MCNP
  - Each FMESH causes MCNP to re-track on the mesh – slower performance



FMesh Tally Card (1)

```
FMESHn:p    GEOM=      ORIGIN=
            IMESH=     IINTS=
            JMESH=     JINTS=
            KMESH=     KINTS=
            AXS=       VEC=
            EMESH=     EINTS=
            FACTOR=
```

- **Can be used with DEn, DFn, and FMn cards.**
- **Caution: It is easy to create huge mesh tallies that can fill computer memory.**
- **Each mesh invokes a particle re-tracking on that mesh.**
- **Other options are available – see the manual.**

FMesh Tally Card (2)

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.
AXS	= direction vector of the cylindrical mesh axis	0, 0, 1
VEC	= direction vector along with AXS that defines the plane for $\theta = 0$	1, 0, 0
TYPE	= plots primary sdef source particle starting locations in tally plotter	source

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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.**

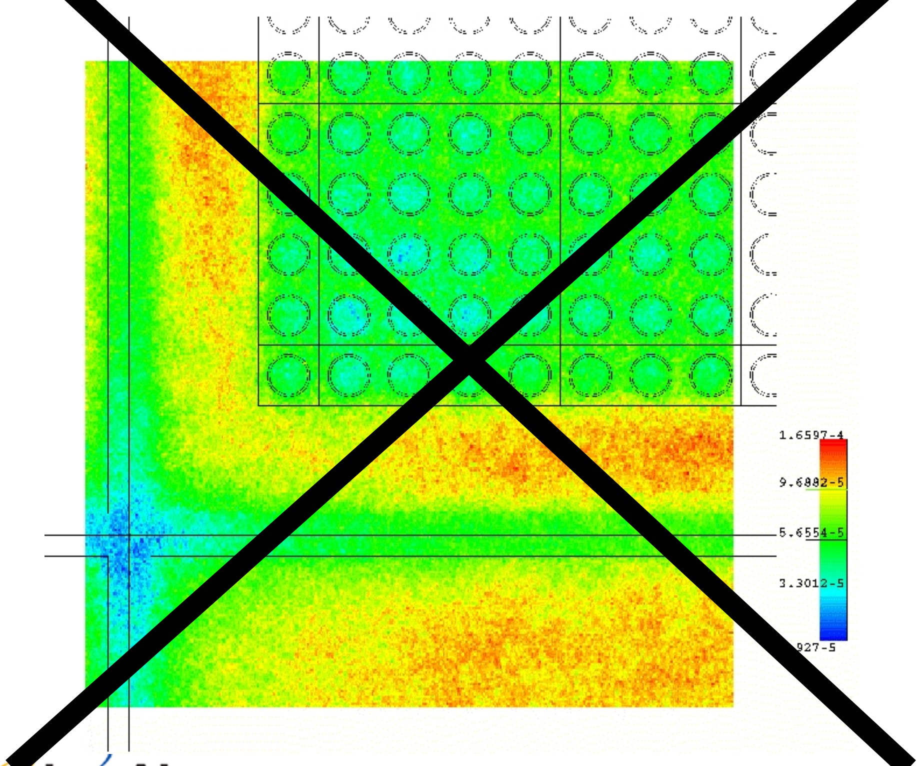
Example of the FM card for FMESH

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/cm^3) 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 Cf-252 neutron source

```
c >>>>> data cards

. . .

c --- mesh tally specification
fmesh4:n    geom=xyz        origin=0  -100  -100
            imesh=40        iints=40
            jmesh=100       jints=40
            kmesh=100       kints=1
fm4   -3.e8   0   -1  -4         $ ( sigtot * heating )
```

Mesh Tally Plotting

- **In the command line type:**

```
mcnp6   z   r = runtpe
```

- **Where runtpe is the name of your runtpe file for shield04.**

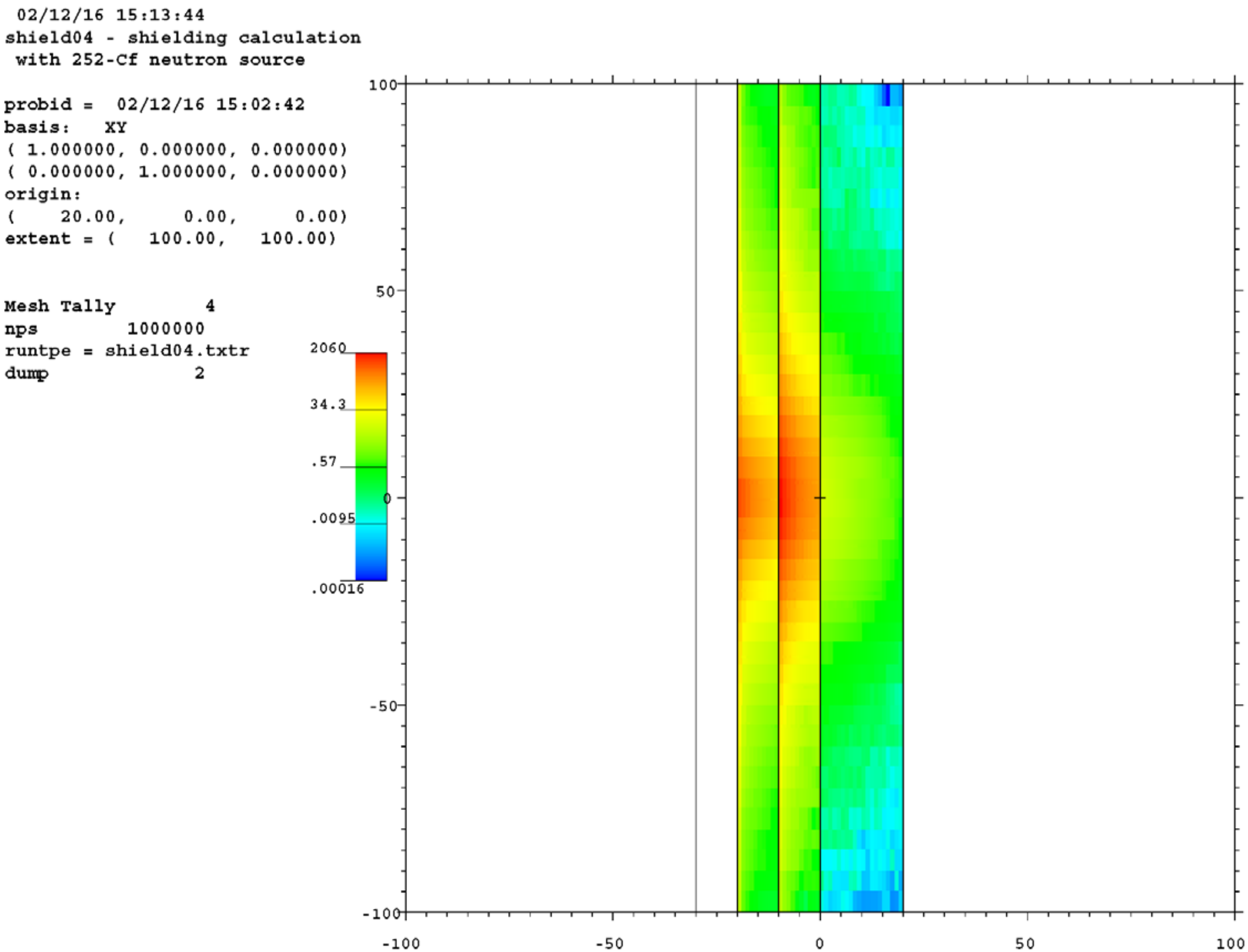
- **The following commands in `red` are useful:**

`mcplot> fmesh 4`	**Brings up the results in the geometry plotter**
`mcplot> fmrelerr`	**Plots the relative uncertainties**

fmrelerr is only recognized in the geometry plotter.

Mesh Tally Plotting

X-Y Slice



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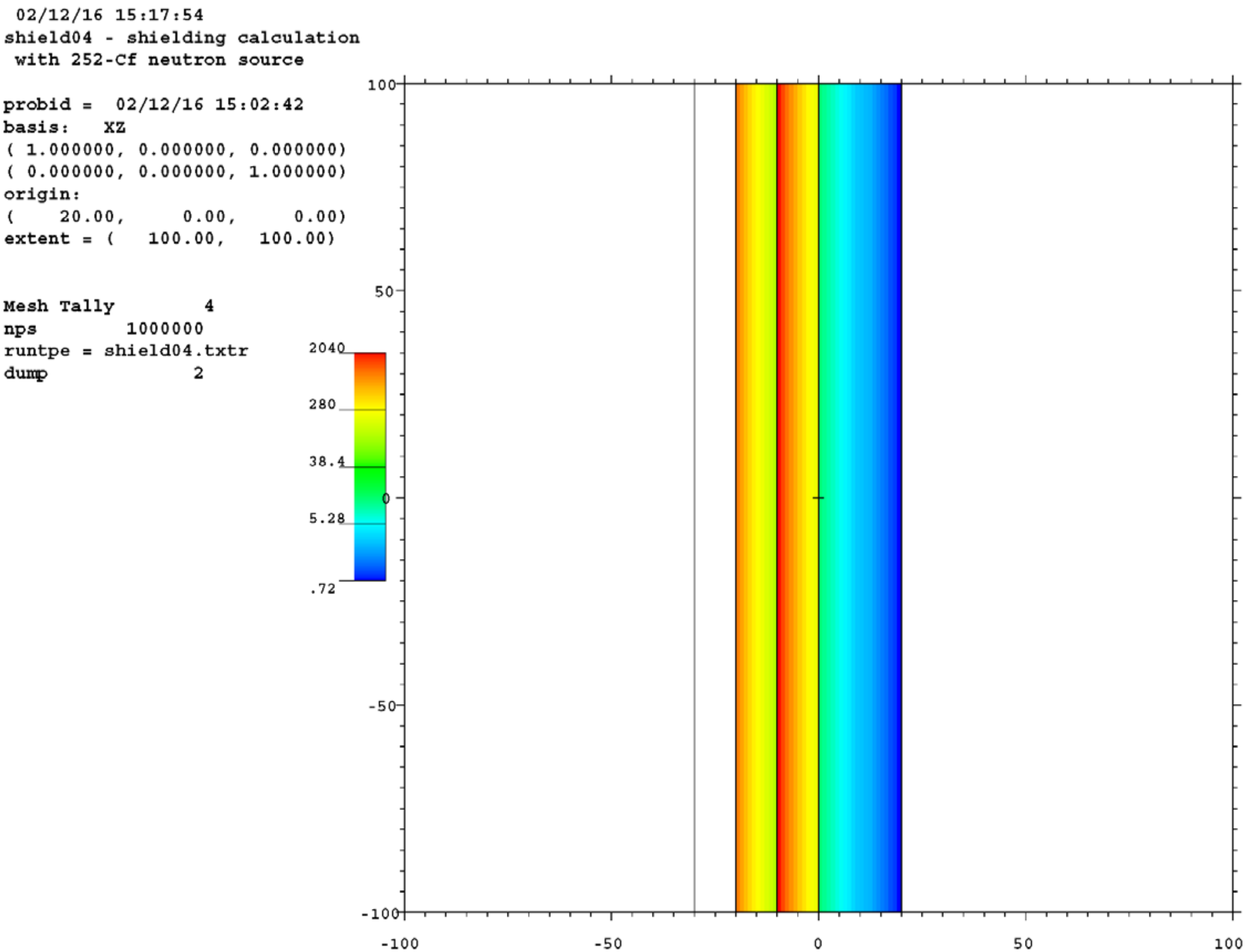
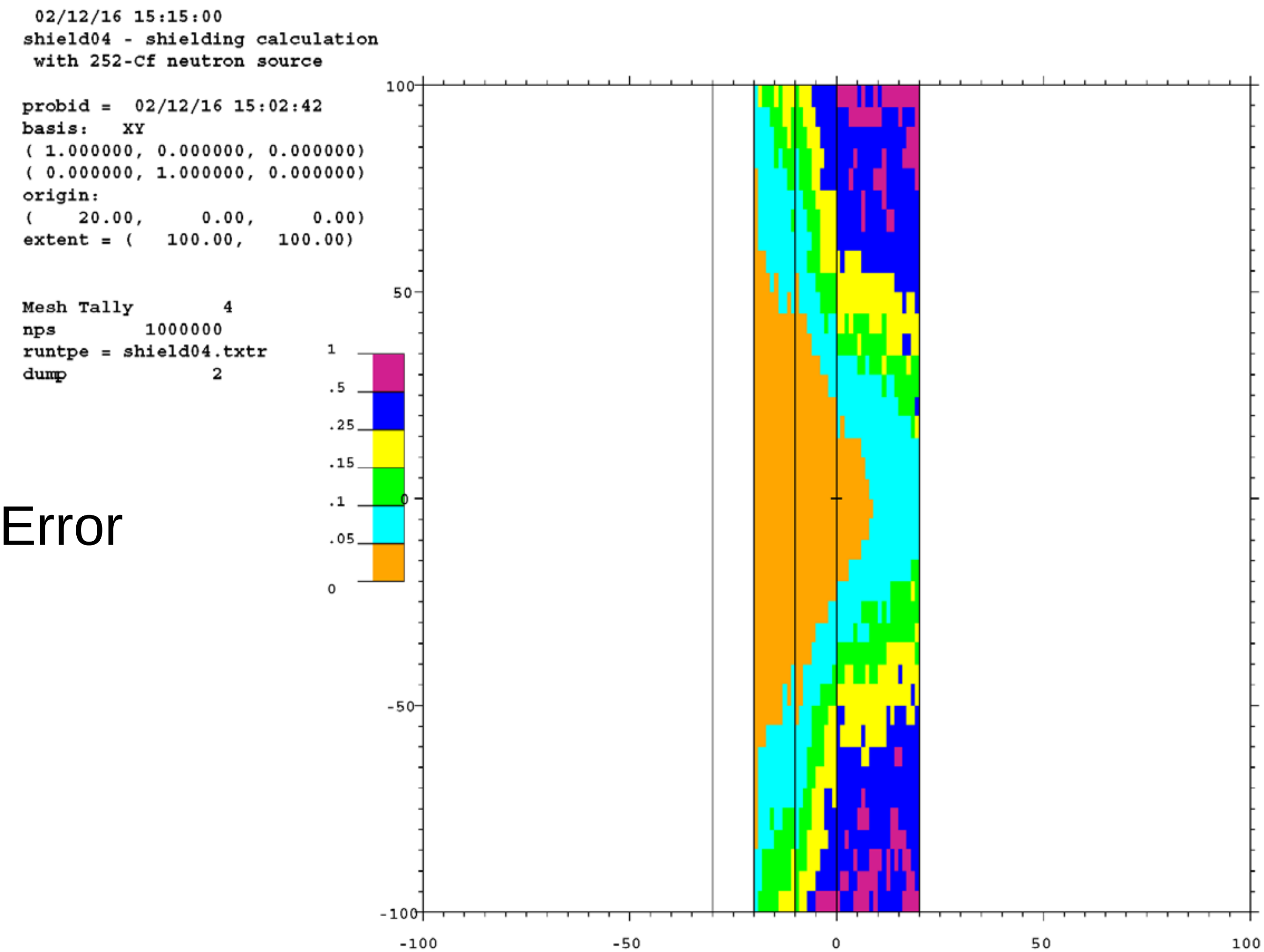
Mesh Tally Plotting



X-Z Slice

Mesh Tally Plotting

Relative Error



Spectra and Plotting

Obtaining Energy Spectra

- **Often, spectral information is useful for a lot of problems, including 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 is 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
  ```

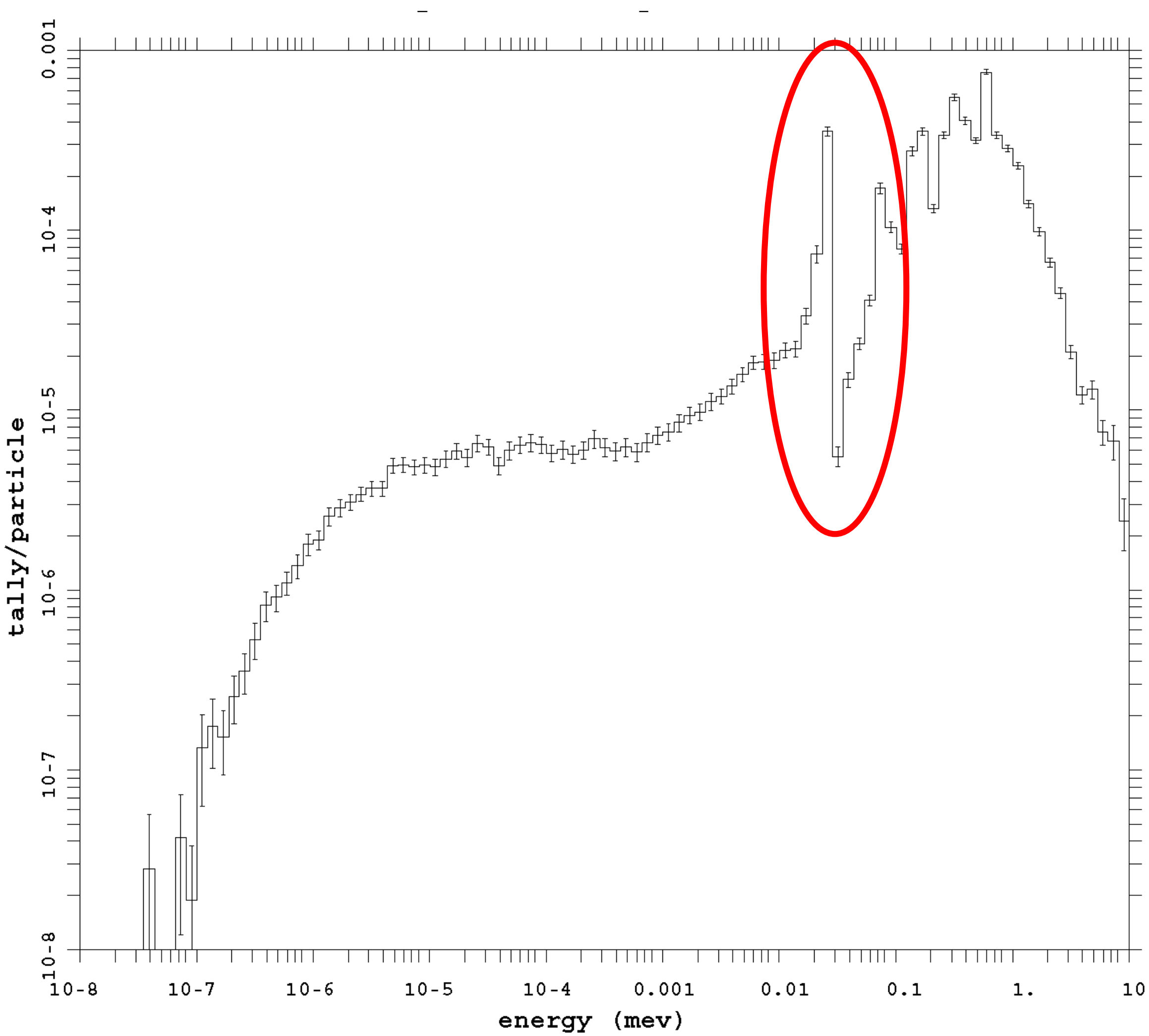
  - Replace "runtpe" with the name of your runtpe file

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

`tal 1`	**specifies the tally to plot**
`loglog`	**has plot on log-log scale**
`nonorm`	**removes per MeV normalization**
`xlim 1.e-8  1.e+1`	**sets the x-range of the plot window**

- **Should see an interesting feature around 20 keV**

Tally Plotting



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Cross Section Plotting

- **Explain this behavior by plotting the cross section**
- **On the command line, type:**

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

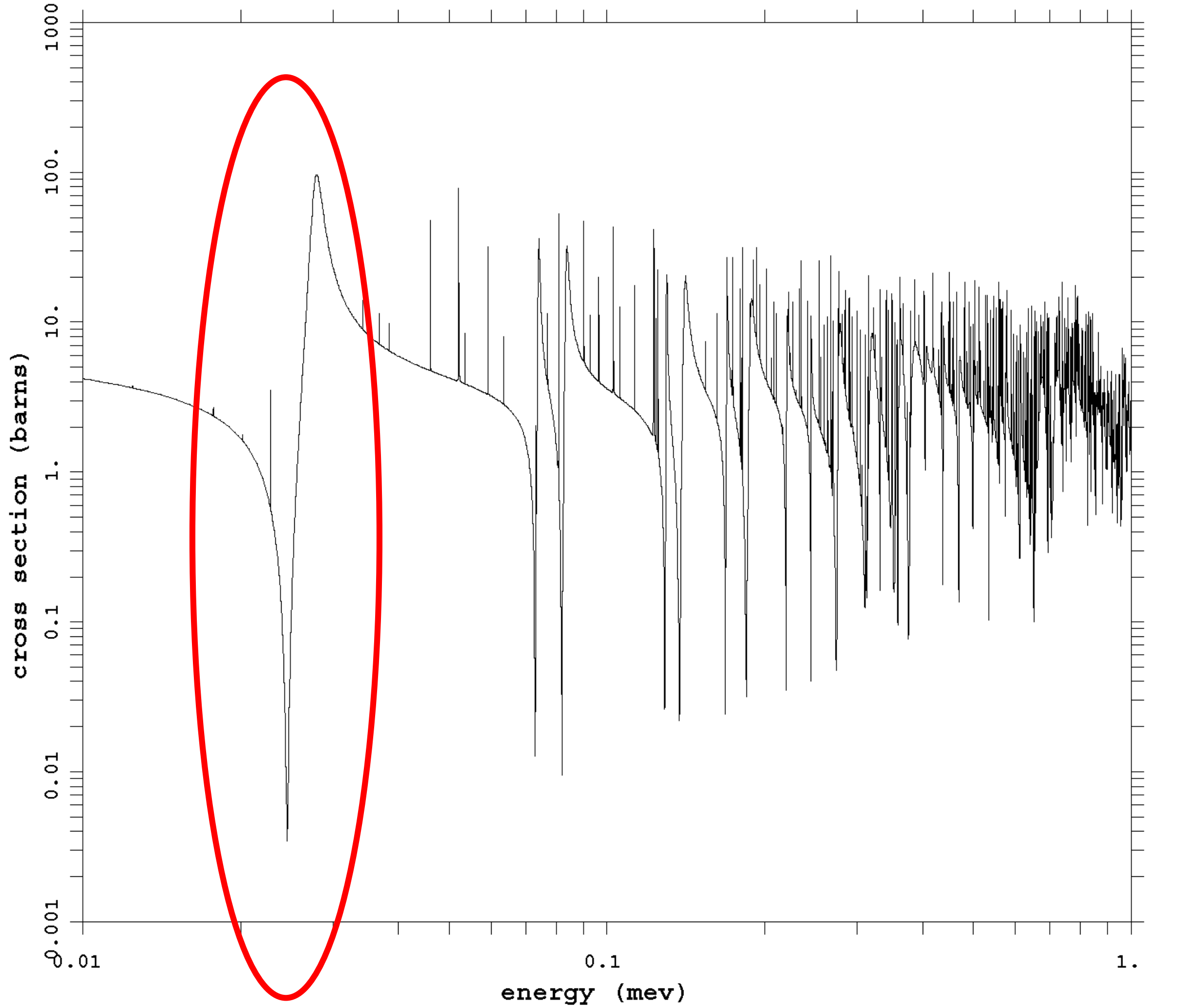
- **In the plotter, type the text in red:**

xs	26056.80c	**Brings up Iron-56 total xs**
xlim	0.01 1	**Sets energy view from 10 keV to 1MeV**
ylim	1.e-3 1.e+3	**Sets range of cross section**

- **Look at the graph of the total cross section in the resonance range**
  - Notice the wide anti-resonance (cross section window) at about 20-30 keV

Cross Section Plotting

The infamous "iron window"



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TMESH Tallies

(optional)

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 100i 15.0
    corb1  -15.0 15.0
    corc1  -30.5 100i 30.5
endmd
```

Mesh Tally Keywords (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 Tallies (Type 2)

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)

trans = TRn card number used to translate and/or rotate the mesh

Energy Deposition Mesh Tally:

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

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

Allowed keywords: see next slide

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
```

Energy Deposition TMESH Keywords

Keyword Description

Keyword	Description
TOTAL	score energy deposited from any source
DE/DF	score ionization from charged particles
RECOL	Score energy transferred to recoil nuclei above table limits

Additional keywords

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

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.

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.

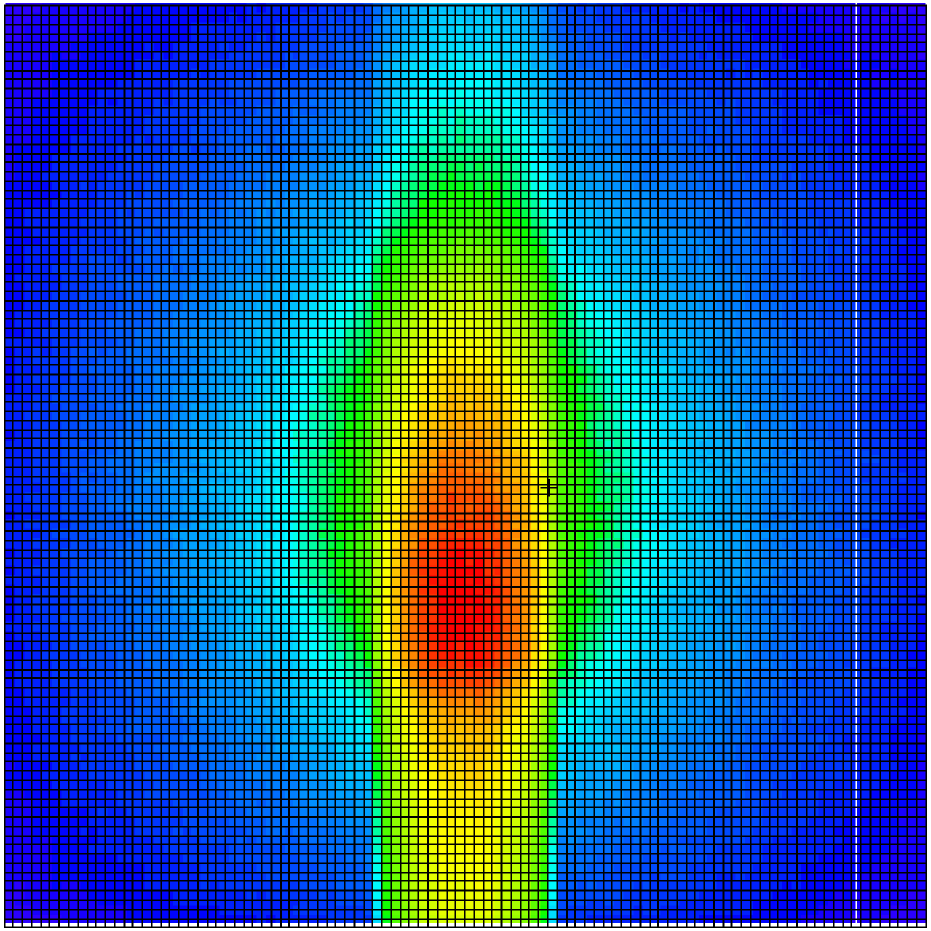
TMESH Tally Plotting

From the **command prompt:**

```
mcnp6 z run = runtpe
```

`mcplot> plot` $brings up the geometry plotter

`[buttons] tal, N, color`



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TMESH Tally Plotting

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

TMESH Plot Contour Command Examples

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 the figure.

Note: this is the default setting

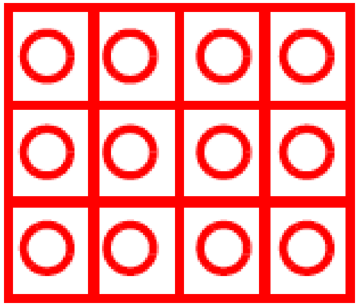
```
CONTOUR 1e-4  1e-2  12 log
```

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

Tallies & Sources in Repeated Structures (optional)

Tallies in Repeated Structures

- **What's special about a tally or source in a repeated structure?**
  - Must provide the path to tally or source cell
  - Which pin cell ??

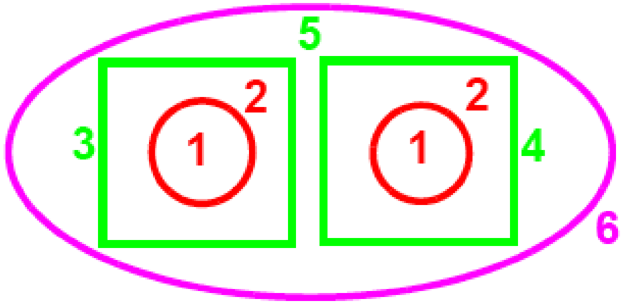


- **Enables tallies or sources in specific cells of repeated structures.**

Purpose and Definitions

- **Example - levels**

```
c cell cards
 1  0      -11  u=1
 2  0       11  u=1
 3  0      -22   fill=1               u=2
 4  0      -33   fill=1  trcl(1 0 0)  u=2
 5  0       22 33                     u=2
 6  0      -44   fill=2
```



- **Cell 6 is in the "real world", not a universe - called "Level 0"**
  Cells 3,4,5 are in Universe 2, which fills Cell 6 - called "Level 1"
  Cells 1,2 are in Universe 1, which fills Cell 3 and Cell 4 - called "Level 2"

- **The left pin (Cell 1) is contained in Cell 3, that is contained in Cell 6.**

- **Use the symbol "<" to mean "is contained in":**

1 < 3 < 6 <-- This uniquely identifies the left pin
1 < 4 < 6 <-- This uniquely identifies the right pin

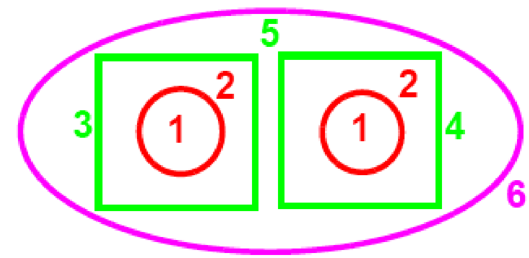
Geometric Paths & Tally Paths

Geometric chain

- A list of cells, one in each level of geometry, that uniquely specifies a particular cell in a repeated structure
- Start at the deepest level of geometry, finish in the real world

Tally path

- A subset of a geometric chain



Example

C1 < C2 == "Cell C1 is contained in Cell C2"

- All geometric paths: 1<3<6 2<3<6 1<4<6 2<4<6
  3<6 4<6 5<6 6

- Possible tally paths:

1<3<6	<-- the left pin
1<4<6	<-- the right pin
1<6	<-- BOTH pins

Tally Paths

FORM: Fn:p (E1 < C1 < C2) ...

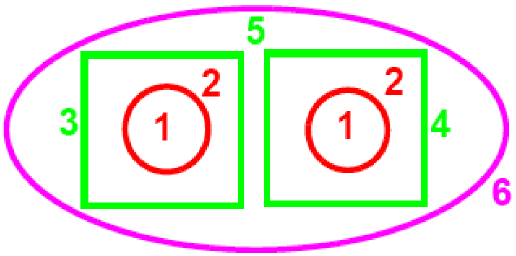
- Left arrow (<) identifies levels within a tally chain, translate it to: **"is contained in"**
- <u>Requires</u> an outer set of parentheses.
- First level entries (Ei) are either:
  - **Tally <u>surfaces</u>** **if tally type 1 or 2.**
  - **Tally <u>cells</u>** **if tally type 4, 6, 7, or 8**
- Upper level entries (Ci) must be:
  - **<u>Cells</u> with a FILL entry that is nonzero.**
  - **Produces a tally only when a particle is in a geometric chain that corresponds to an input tally chain.**

Tally Paths

```
c cell cards
 1  0      -11  u=1
 2  0       11  u=1
c
 3  0      -22   fill=1                u=2
 4  0      -33   fill=1  trcl(1 0 0)   u=2
 5  0       22 33                      u=2
 6  0      -44   fill=2

C surface cards
. . .

C data cards -- flux tallies
F4:n (1<3<6)          <-- the left pin
     (1<4<6)          <-- the right pin
     (1<6)            <-- BOTH pins
```



Tally Paths - Lattices

Form: **Fn:p ((E2 E3) < (C3 C4 [I1 ... I2]) < (C5 C6)) ...**

- **Brackets, [ ], identify one or more elements of a lattice:**
  - Must follow a filled lattice cell (C4).
  - A lattice cell listed without brackets gives the union
- **Three possible formats: over all lattice elements.**

[I]

Indicating the I-th lattice element in fully specified FILL array.

[I1:I2 J1:J2 K1:K2]

Indicating one or more lattice elements (see FILL card).

[I1 J1 K1, I2 J2 K2, ...]

Indicating lattice element (I1, J1, K1), (I2, J2, K2), etc.

Tallies - Multiple Bin Format

- **Automatically invoked for levels with multiple entries.**
- **Can be disabled at any level by ( ) around all entries.**
- **Number of total bins generated is given by the product of the number of bins at each level.**
- **The order of generated tally bins can be important,**
  - (E4 E5 < (C1 C2) < C3 C4) becomes:

    (E4 < (C1 C2) < C3) **(E5 < (C1 C2) < C3)**
    (E4 < (C1 C2) < C4) **(E5 < (C1 C2) < C4)**

  - A segment divisor entry (SD card) may be input for each generated tally bin.

Sources in Repeated Structures

- **KSRC Format**
- **SDEF CEL Format**

KSRC Format

- **No special format for repeated structures**
- **Enter x,y,z locations in the coordinate system of the highest level (the real world)**
- **All source points are absolute coordinates, i.e., "real world" coordinates**

Ksrc   1. 1. 1.   2. 3. 4.   5. 6. 7.   . . .

SDEF CEL Format

From the manual:

- The coordinate system for position and direction sampling (pds) is the coordinate system of the first negative or zero Ci in the geometric path starting from the right and proceeding left.
- Each entry in the source path represents a geometry level, where level zero is the last source path entry, level one the second to the left, etc., and level zero is above level one, level two is below level one.
- The pds level is the level associated with the pds cell or pds coordinate system. All levels above the pds level must be included in the source path. Levels below the pds level need not be specified, and when given, may include one or more zero entries.
- The default pds level is the first entry in the source path when the path has no negative or zero entry.
- Position rejection is done in cells at all levels where Ci≠0, but if any Ci has a negative universe number on its cell card and is at or above the pds level, higher level cells are not checked.

SDEF CEL Format

- **To use the SDEF card to select a particular cell inside a lattice,**

```
SDEF   x=d1   y=d2   z=d3   cel=d4
… (xyz position disributions) …
SI4   L   ( geometric-path-to-cell )
SP4      1
```

- **Example - center cell in Problem tal08**

```
SDEF      x=d1  y=d2  z=d3   cel=d4
SI1       -.7   .7
SP1        0    1
SI2       -.7   .7
SP2        0    1
SI3       -180. 180.
SP3        0    1
SI4   L   ( -10 < 40[ 0 0 0 ] < 50 )         <-- xyz coordinates in "Level 2"
SP4         1
```

SDEF CEL Format

- **Example - all fuel pins in Problem fv5**

```
SDEF     x=d1  y=d2  z=d3   cel=d4
SI1      -.7   .7
SP1       0    1
SI2      -.7   .7
SP2       0    1
SI3      -180. 180.
SP3       0    1
SI4   L  ( -10 < 40[-7:7  -7:7  0:0]< 50 )       $  xyz coordinates in "Level 2"
SP4        1   224r
```

Notes:

(1) 15 x 15 x 1 = 225 lattice elements listed on SI4

(2) Must give (relative) probability for each on SP4

(3) The minus sign in SI4 indicates which coordinate system the x,y,z sampling is done in (Level 2)

(3) Despite the order on the SDEF card, **the CEL parameter is chosen first, then x, then y, then z**