Monte Carlo Theory & Practice (MCNP)

For Radiation Transport Solutions

Lecture 5

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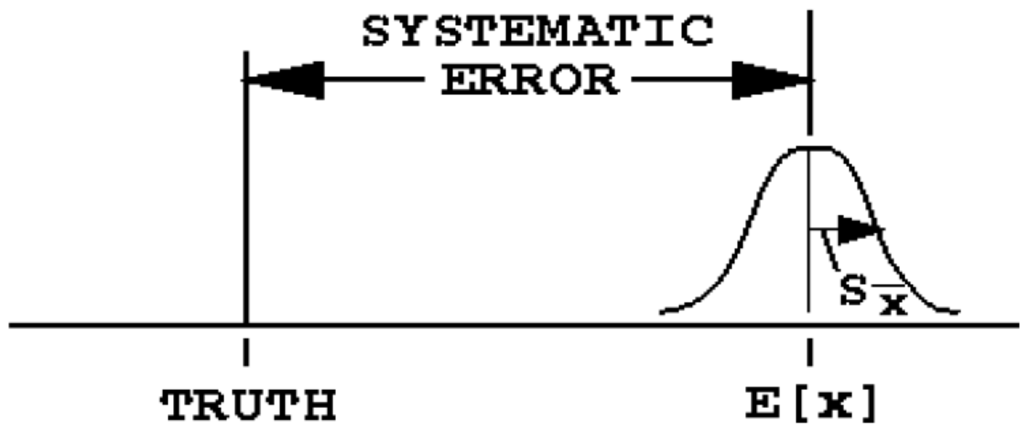
Summary

- Precision & Accuracy
- Tally Fluctuation
- Variance reduction

Precision & Accuracy

- Don’t confuse them



- $S_{\bar{x}}$ is a measure of your “stochastic uncertainty”
  - This is a random uncertainty
- There are usually many sources of systematic uncertainty too
  - How many can you think of?

Monte Carlo Precision

- Random walks are sampled and a score x_i is scored for the i^{th} random walk.
- x_i is the "history score" and depends on the particle "weight"
  - Varies for each random walk. May be zero
- $f(x)$ is history score probability density function
  - Not generally known

$$E(x) = \int x f(x) dx = \text{true mean.}$$

- In Monte Carlo sampling we don't know "true mean", we calculate the "sample mean"

$$\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$$

Monte Carlo Precision

- If $E(x)$ is finite then
  - $\bar{x}$ tends to the limit $E(x)$ at $N \rightarrow \infty$
- Variance of the population of x values
  - A measure of the spread of x

$$\sigma^2 = \int (x - E(x))^2 f(x) dx = E(x^2) - (E(x))^2$$

  - σ is the standard deviation (also not known)
  - Can be estimated from Monte Carlo sampling as S

$$S^2 = \frac{\sum_{i=1}^{N} (x_i - \bar{x})^2}{N-1} \approx \overline{x^2} - \bar{x}^2 \qquad \overline{x^2} = \frac{1}{N} \sum_{i=1}^{N} x_i^2$$

  - S is the estimated standard deviation of the population of x based on actual values of x_i that were sampled

Monte Carlo Precision

- Estimated variance of $\bar{x}$ is given by

$$S_{\bar{x}}^2 = \frac{S^2}{N}$$

- Standard deviation is $S_{\bar{x}}$
  - Proportional to 1/√N
  - aka the “error”
  - Relative error, $R = S_{\bar{x}} / \bar{x}$
- To halve the relative error on our estimate of the mean tally either
  - Count for four times longer
  - Reduce the spread of x_i by half S_x
- Reducing spread of tally results can be done using “variance reduction” techniques

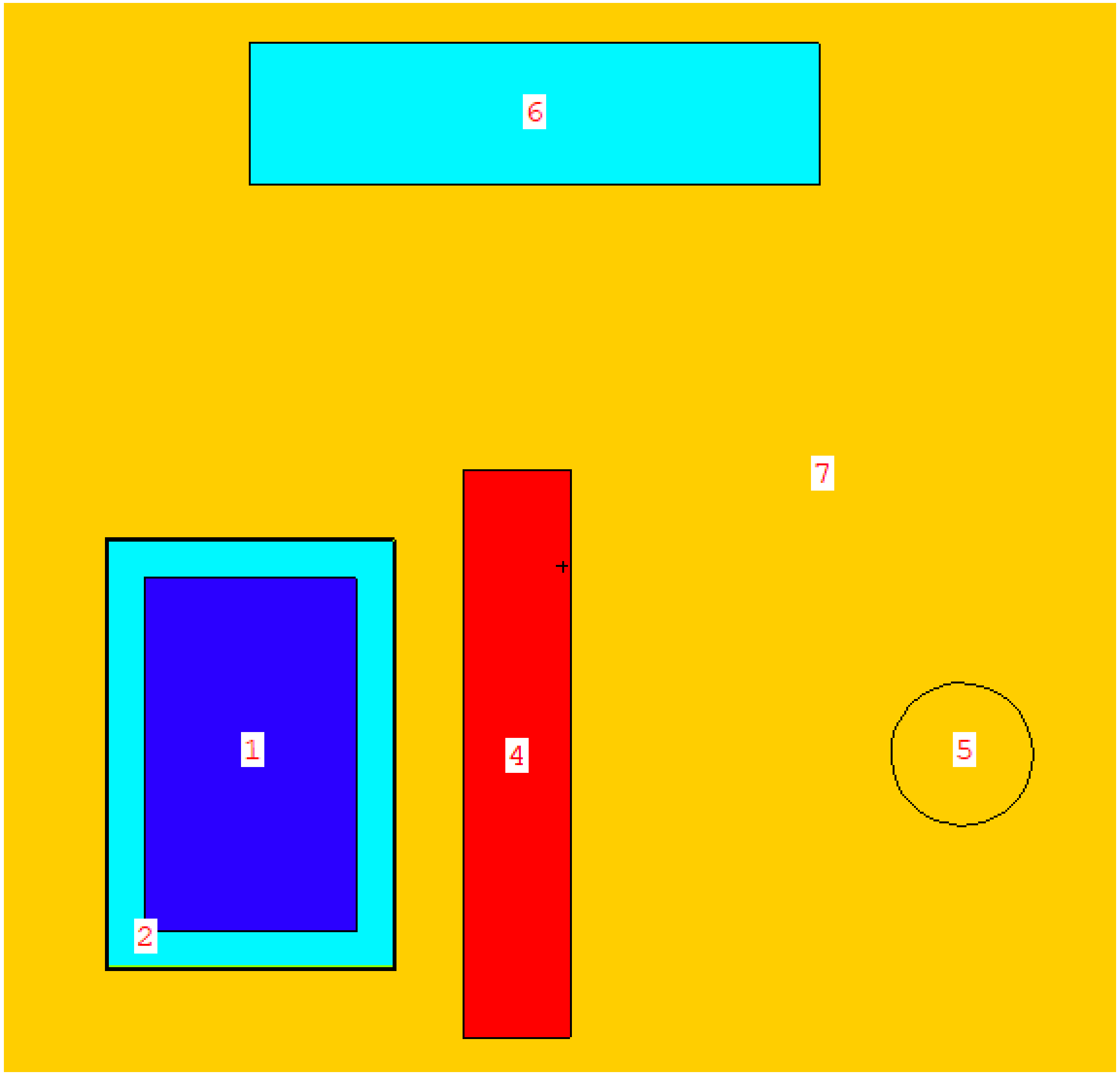
Figure of Merit & VoV

- A measure of how fast your calculation is running
  - The higher it is the more efficient your calculation is
  - $FOM = 1 / R^2T$
  - Where R is the relative “error”
  - T is the computer time (in minutes)
  - As $N \sim T$, and $R^2 \sim {}^{1}/_{N}$, FOM should be constant
  - Depends on your computer speed
- Variance of the Variance

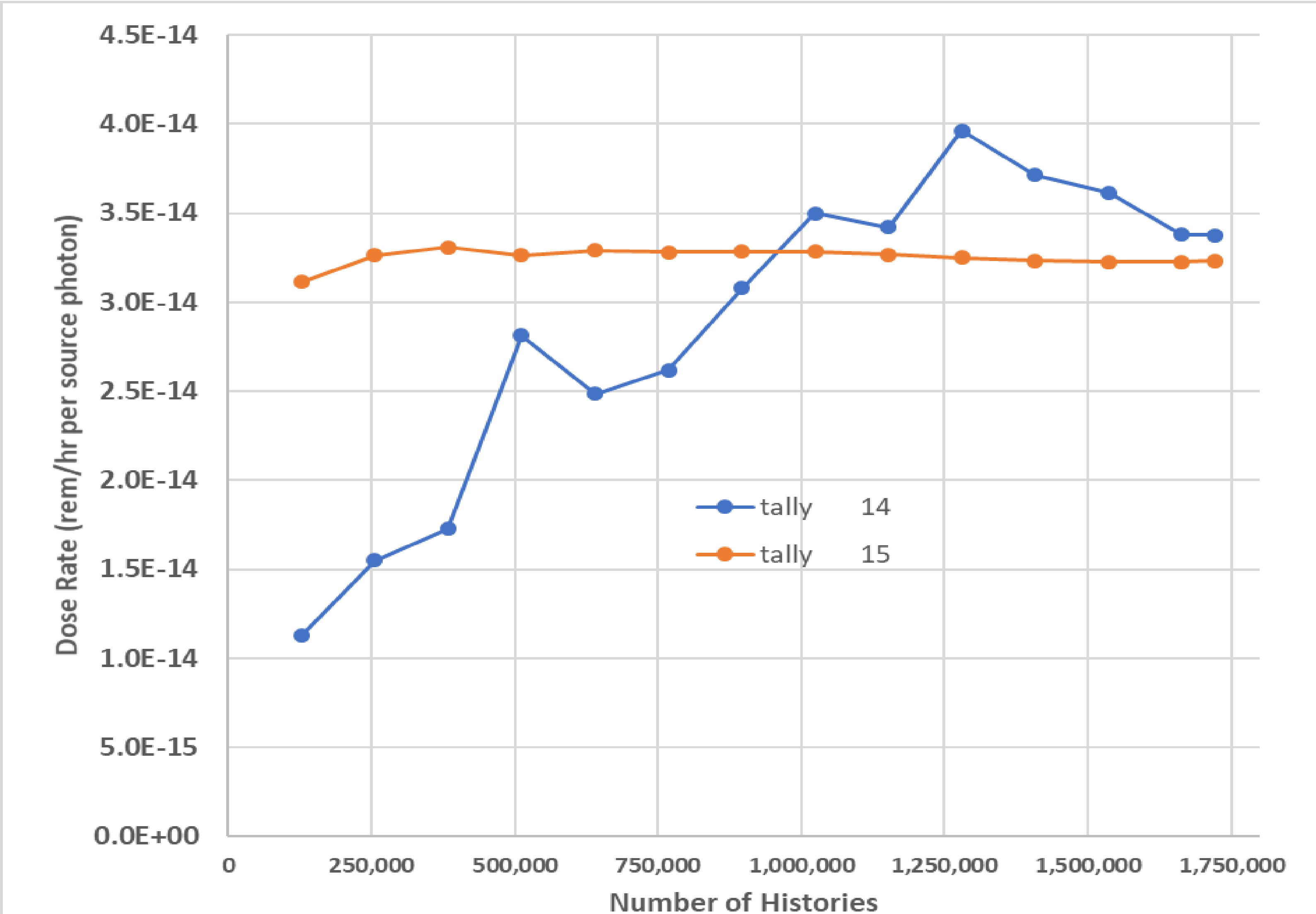
$$VOV = S^2(S_{\bar{x}}^2)/S_{\bar{x}}^4$$

  - Should behave as ${}^{1}/_{N}$

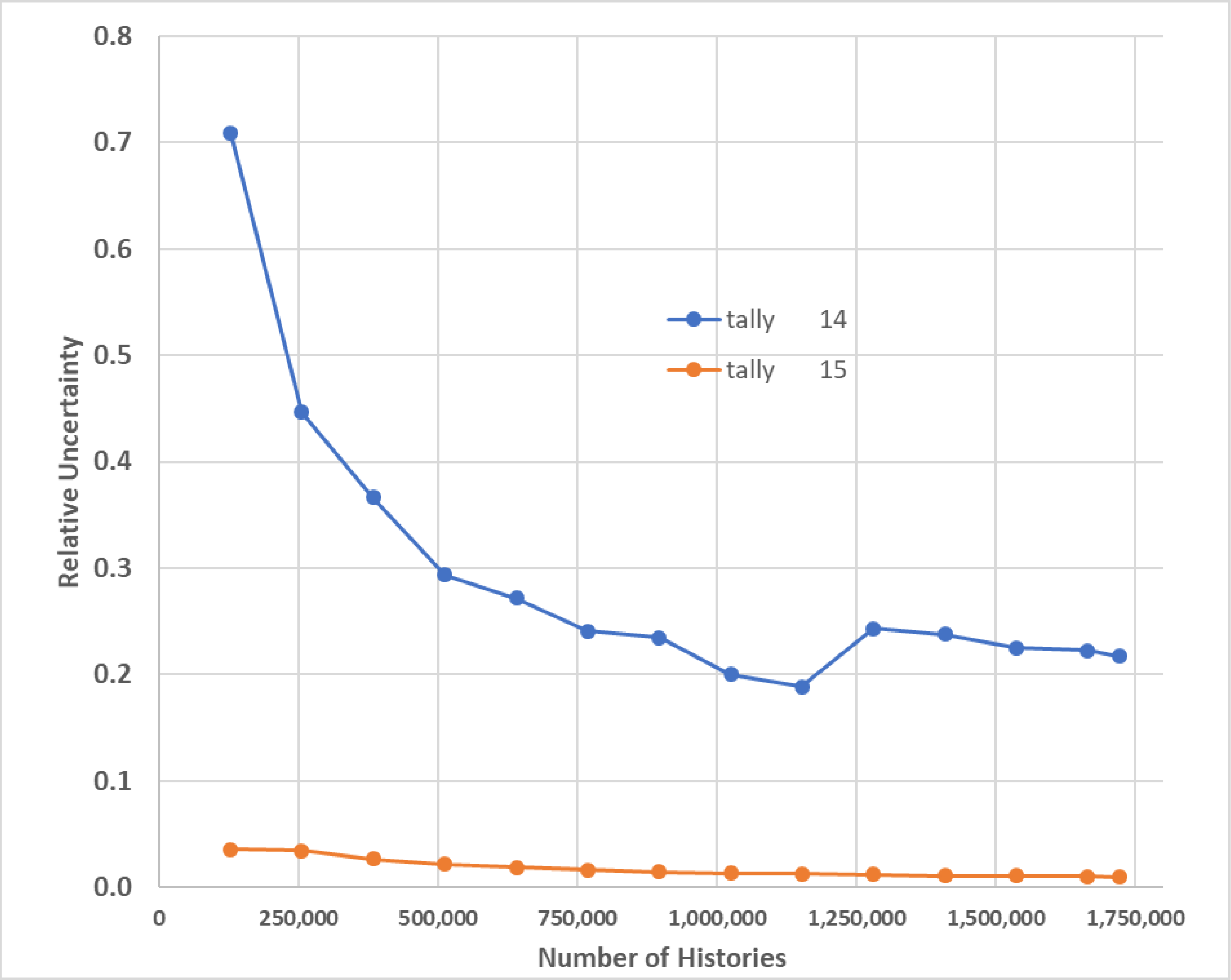
Tally Fluctuation



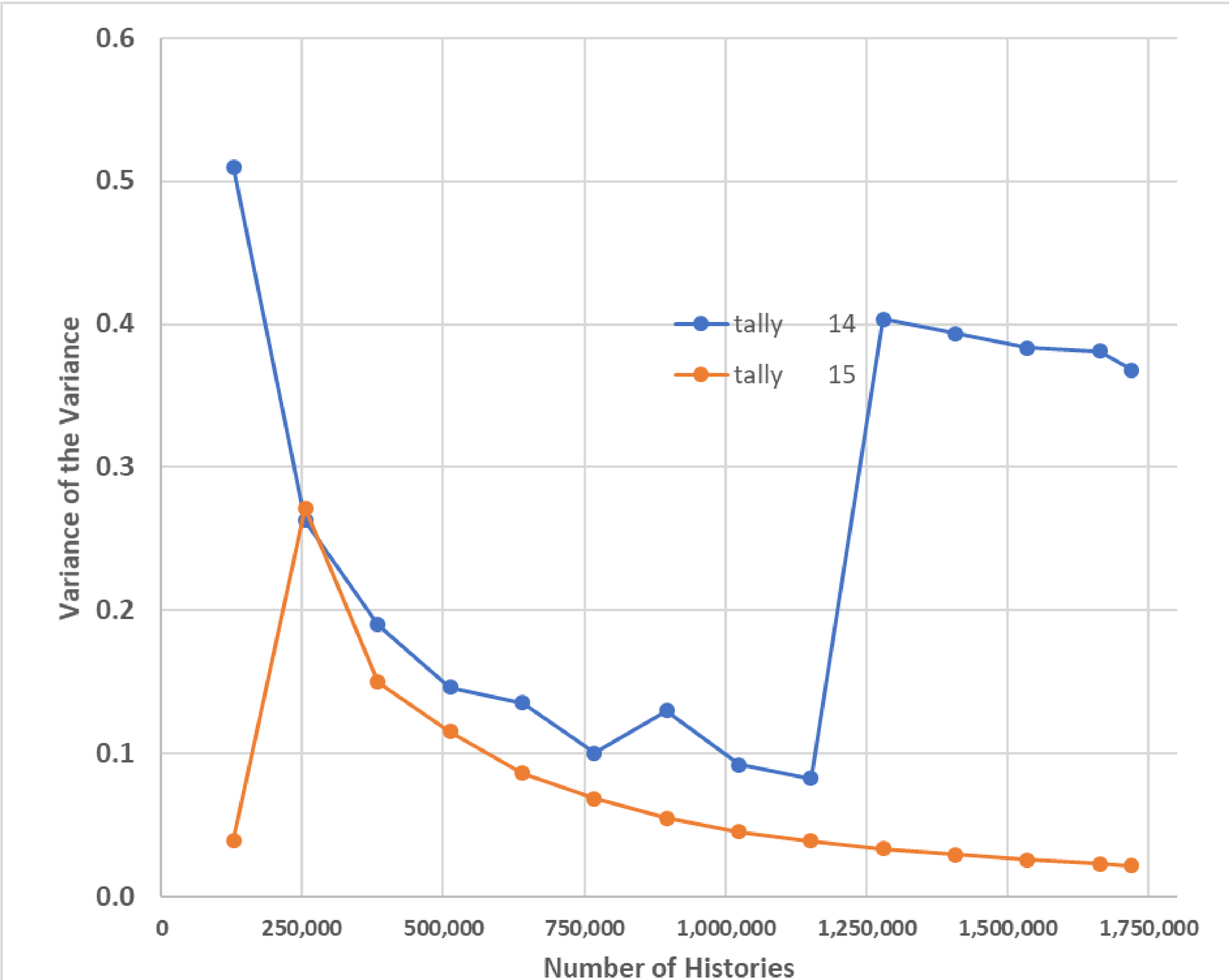
Tally Fluctuation (mean)



Tally Fluctuation (relative error)



Tally Fluctuation (variance of the variance)



Tally Fluctuation

- The quantity selected for tally analysis can be changed

TFn Tally Fluctuation Card

Form: TF*n* $I_1 \ldots I_8$

n = tally number. *n* cannot be zero.

I_i = bin number for bin type *i*. $1 \le I_i \le last$

last= IPTAL(LIPT+i,3,ITAL)

= total number of bins in one of the eight bin types.

Default: 1 1 *last* *last* 1 *last* *last* *last*

1. first cell, surface, or detector on Fn card
2. total rather than flagged or uncollided flux
3. last user bin
4. last segment bin
5. first multiplier bin on FMn card
6. last cosine bin
7. last energy bin
8. last time bin.

Use:Whenever one or more tally bins are more important than the default bin

The Ten Statistical Tests

- Estimated mean
  1. Must behave randomly (tested over 2nd half of run)
- Estimated relative error
  2. Should be <0.1, <0.05 for point detectors (Type 5)
  3. Should decrease monotonically (2nd half)
  4. Should decrease as ~$1/\sqrt{N}$ (2nd half)
- Estimated variance of the variance (VoV)
  5. Should be < 0.1
  6. Should decrease monotonically (2nd half)
  7. Decrease as ~$1/N$ (2nd half)
- Estimated Figure of Merit
  8. Be ~ constant (2nd half)
  9. Behave randomly with N (2nd half)
- History tally PDF, $f(x)$
  10. SLOPE must be > 3.0

Variance Reduction

- Aim to reduce R by reducing S
  - Not by just increasing T
  - Aim to increase the number of non-zero histories
  - Aim to improve sampling of important parts of phase space
- Various types
  - Implicit capture – allows absorbed particles to carry on but with an appropriately reduced weight. Default
  - Weight cutoff – why chase particles whose weight is very low? They will never add any significant score
  - Geometry splitting/Russian roulette
  - Source biasing
  - Point (and ring) detectors. These take a non-zero score from particles which don't actually pass through a tally cell or surface.

Variance Reduction

- More types
  - Energy cutoff (also time). Useful if you are not interested in low energies (esp. neutrons).
  - Forced collisions. Useful for sampling scattering event in a low Σ medium. e.g. skyshine problems. Compensate with reduced weight.
  - Exponential transform. Artificially reduces Σ in preferred direction. Must adjust weight accordingly to avoid bias.
  - Deterministic translation. Moves particles to a chosen region of interest with weight reduced by likelihood of getting there.
  - Weight Windows

Cutoffs

CUT:n *T E WC1 WC2 SWTM*

n = N or P or E for neutrons, photons, electrons

T = time cutoff (in units of 10^{-8} seconds) [very large]

E = energy cutoff (MeV) [0 for N, 0.001 for P & E]

WC1, WC2 & SWTN

are parameters to adjust weight cutoffs relative to ratio of cell important to source cell importance. The default values are adequate.

- Energy cutoff is a very simple and effective VR technique if you are definitely not interested in particles below a defined energy
- Can apply energy cutoff without affecting time cutoff

CUT:N J 0.001 $ Use of the J (jump) parameter

Sets energy cutoff to 1keV, leaves all other parameters unchanged

J means jump over a parameter. Can have 2J, 3J etc.

Energy cutoff can be defined for each cell (use the ELPT card)

Cell Importances

- Used for playing splitting/Russian roulette

IMP:n $I_1\ I_2\ I_3\ .....\ I_m$

n = particle type (N,P or E)

I_i = importance of cell i, m cells in total

If $I_i = 0$ then particles are killed in that cell.

External boundary of model is usually of zero importance. Can also have internal 100% absorbing cells.

- Must define an importance for every cell in the problem. Can use IMP:n = x on each cell card instead

IMP:P 1.0 24R 0.5 0.25 0 $ Use of R (repeat)

Sets importances of 1.0 for the first 25 cells, then 0.5, 0.25 then 0

Energy Splitting

- Similar to geometry splitting but with energy

ESPLT:n $R_1\,E_1\;\;R_2\,E_2\;....\;R_m\,E_m$

n = particle type (N,P,E)

R_i = splitting ratio when particle crosses energy boundary

E_i = the energy boundaries. Can have up to 20. Must decrease monotonically

ESPLT:N 2.0 0.1 4.0 0.001 2.0 1.0E-6

Defines splitting of 2:1 at 0.1MeV, 4:1 at 1keV and another 2:1 at 1eV. For energy increase (e.g. thermal upscatter or fission neutron produced) Russian roulette would be played.

Forced Collision

- Used to
  - increase scatter in low scattering cells
  - Increase contributions to point detectors

FCL:n $x_1 \;\; x_2 \;\; x_3 \;\; \ldots \;\; x_m$

n = particle type (N or P, not E)

x_i are used to select forced collision in cell i

If -1< x_i <0, then forced collision occurs only for particles entering the cell

If 0< x_i <1, then forced collisions also apply after subsequent collisions within the cell

If x_i = 0 then no forced collision occurs

Source Biasing

- A very useful VR method
  - Improves selection of source by energy, position, direction, cell
  - User must have some idea what energies, positions and directions are important to the tally(ies) in question

Source Biasing Example 1

```
SDEF PAR=P ERG=D1 POS=1.0 1.0 0.0
```

C *Isotropic photon point source at (1,1,0), Energy distribution defined by D1*

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SI1   L 0.667   1.33   $ Discreet energy lines (MeV)
SP1   D 0.6     0.333  $ Probability of line selection
SB1     0.1     1.0    $ Biased selection probabilities
```

- Particle weight = ratio of true probability to biased probability
  - In this case 0.667 MeV selected with weight of 0.6/1.1 = 0.545
  - 1.33 MeV selected with weight of 0.333/1.1 = 0.303

Source Biasing Example 2

SDEF PAR=N ERG=1.0 POS=0.0 0.0 0.0 VEC=1 0 0 DIR=D10

C *Isotropic neutron point source at origin.*

C Energy=1.0 MeV, direction distribution defined by D1, symmetric about x axis

SI10 -1 -0.5 0 0.5 0.75 1 $ Direction cosines – equally spaced

SP10 0 1 1 1 0.5 0.5 $ Prob of bin selection (isotropic, total=4)

SB10 0 0.1 0.2 0.5 1.0 2.0 $ Biased selection probabilities (total=3.8)

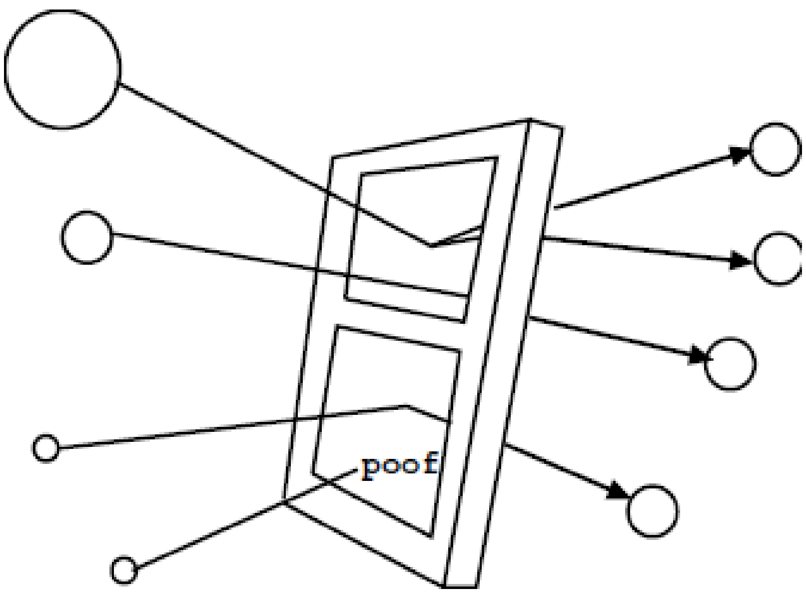
- VEC = a reference direction vector about which the source distribution DIR is defined
- DIR = source distribution.
  - Defined in cosine bins DIR=1 would be monodirectional in direction of VEC
  - 1st entry must = -1, last must = 1
  - Bin weights in this case are (only 5 real bins here):

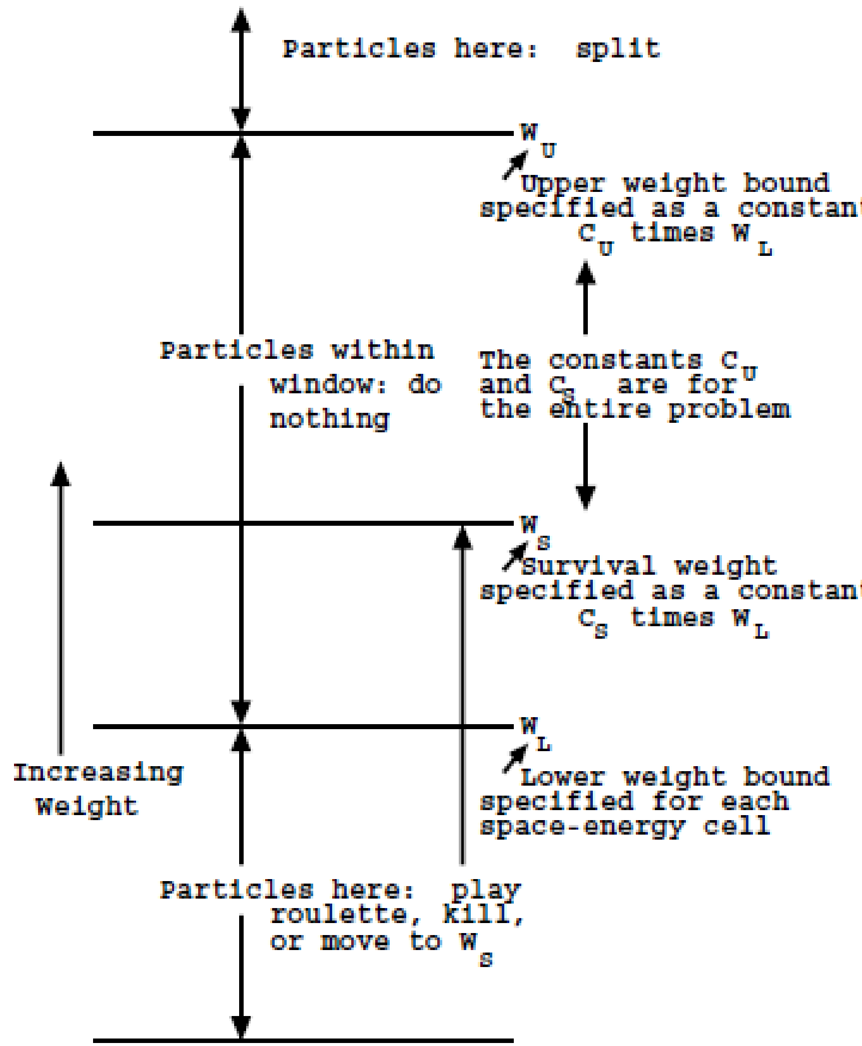
  (1/4)/(0.1/3.8)=9.5, (1/4)/(0.2/3.8)=4.75, (1/4)/(0.5/3.8)=1.9

  (0.5/4)/(1/3.8)=0.475 & (0.5/4)/(2/3.8)=0.2375

  Range of weights from the source is 9.5/0.2375 = 40. Forward direction 40x more likely to be selected than reverse direction, even though it is half as likely.

Weight Windows





VR General Comments

- Monte Carlo radiation transport collects information about you system – phase space (energy, position, direction, time)
- Splitting increases number of particle within a region
  - Improve sampling in that region and you gather more information about it – reduced variance
  - No point in splitting into a "void" – there is no more information to gather, it just wastes computer time.
- If you split particles too much this is at the expense of fewer histories in the same computer time
  - Therefore less information collected – increased variance
- Russian roulette aims to prevent time-wasting in unimportant regions of phase space
  - Thereby increasing number of histories run
  - Better sampling of more important regions and the source
- If you bias too harshly you may fail to sample an important regions of phase space
  - Systematic error

VR General Comment

- Ask yourself "which regions of phase space do I think are not important?"
  - Don't waste too much computer time sampling them
  - But can I ignore them completely?
- Best to be gentle in the application of splitting/Russian roulette and other biasing options
  - Computer time is cheap, correcting systematic errors is not

Help!

- Links MCNP web pages, manual …
- MCNP Web Pages
  - https://mcnp.lanl.gov/
- MCNP Users Forum
  - https://laws.lanl.gov/vhosts/mcnp.lanl.gov/mcnp_forum.shtml