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Title: Using MCNP for Nonproliferation Applications

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Los Alamos
NATIONAL LABORATORY
EST. 1943

Using MCNP for Nonproliferation Applications

ANTPC MCNP6 Workshop

Garrett E McMath

9/28/16

Agenda

- **Introduction to the Monte Carlo method**
- **Brief tutorial on MCNP basics**
- **Introduction to a couple Nonproliferation features**
  - Background
  - ROC curves
- **Conclusions**

Monte Carlo Method

- A statistical “game” for solving complex integration over multiple dimensions or for simulating “real-world events” in a statistically correct manner.
- An approximate answer to an exact problem vs. deterministic which is an exact answer to an approximate problem.

Monte Carlo - Simple

- **Common example:**

  Determine the value of pi by counting the number of raindrops inside a circle inscribed in a square.

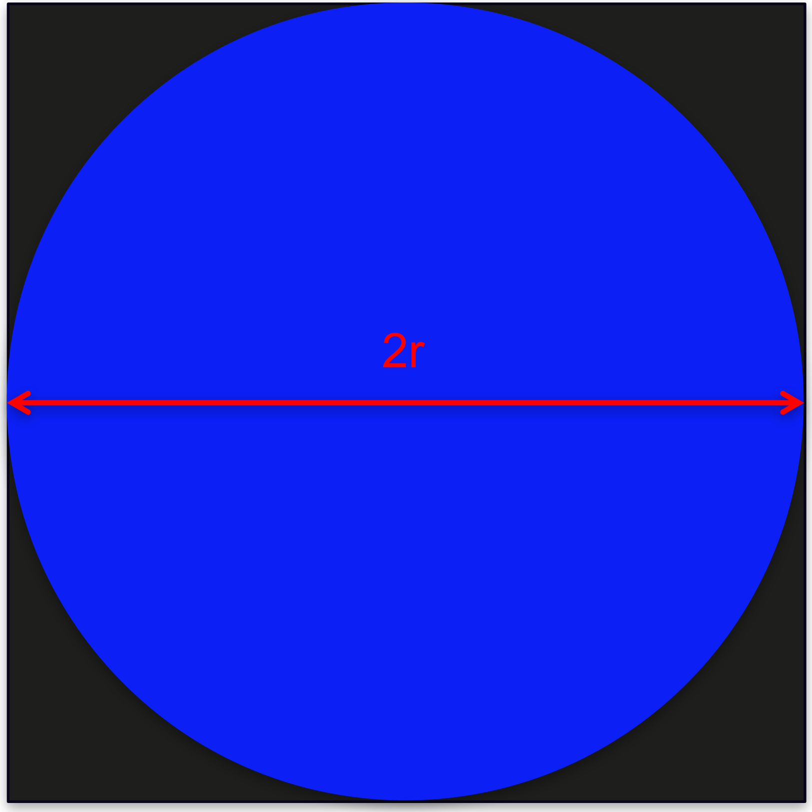
  $A_{circle} = \pi r^2$

  $A_{square} = 4r^2$

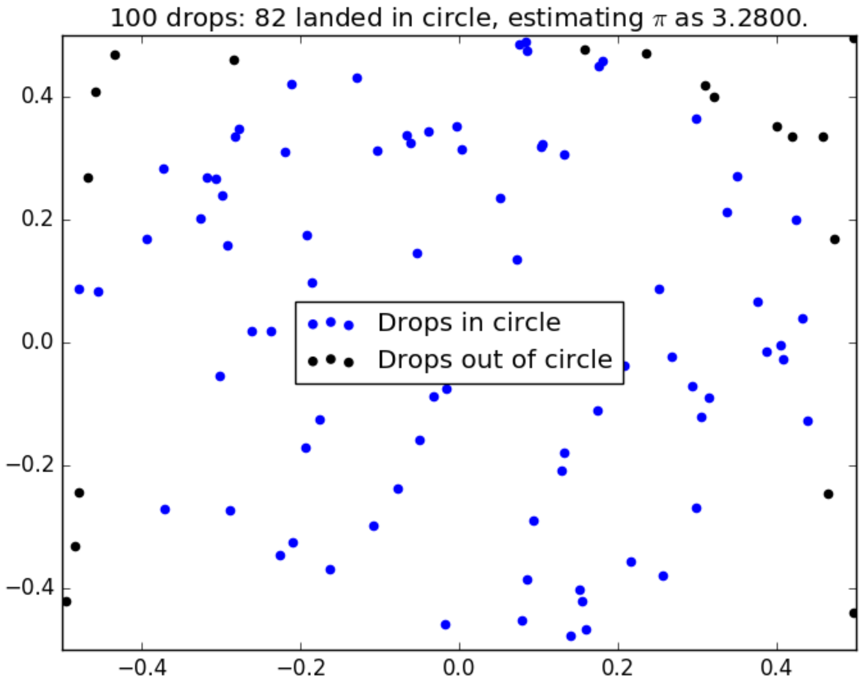
  $P(\text{raindrop in circle}) = A_{circle}/A_{total}$

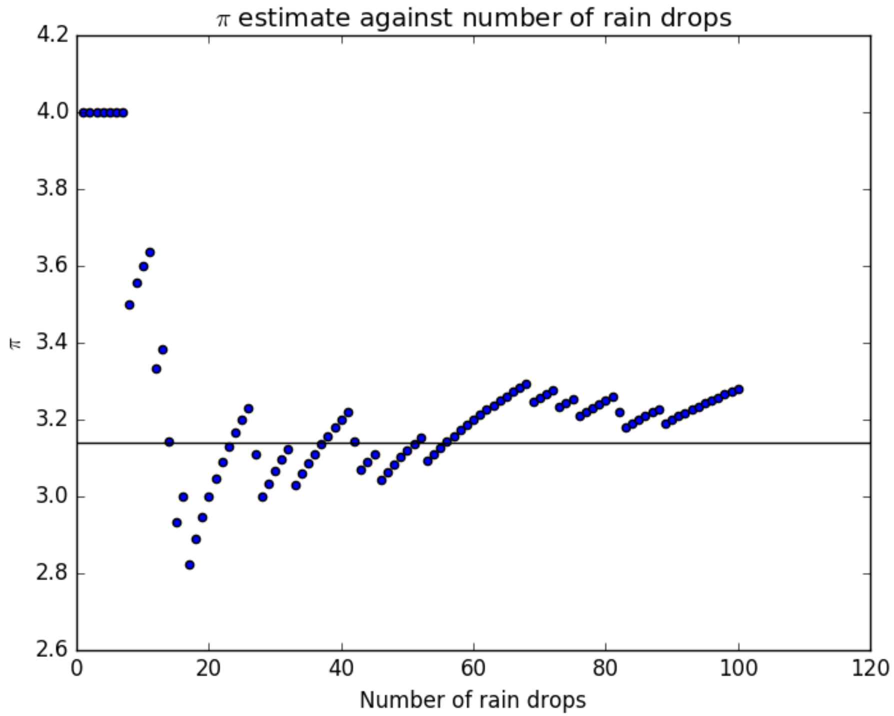
  $P(\text{raindrop in circle}) = \pi/4$

  $4P(\text{raindrop in circle}) = \pi$



Monte Carlo - Simple





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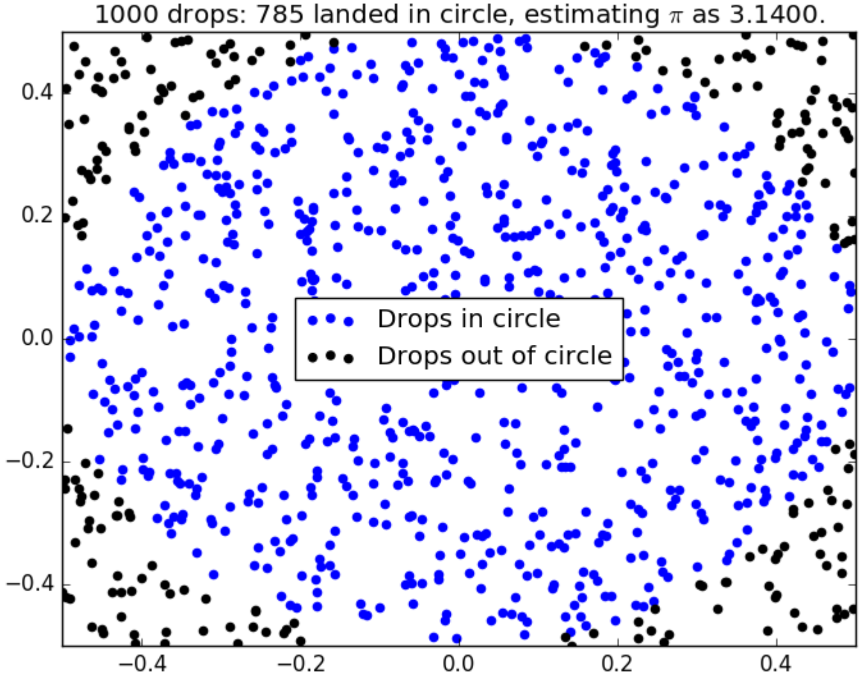
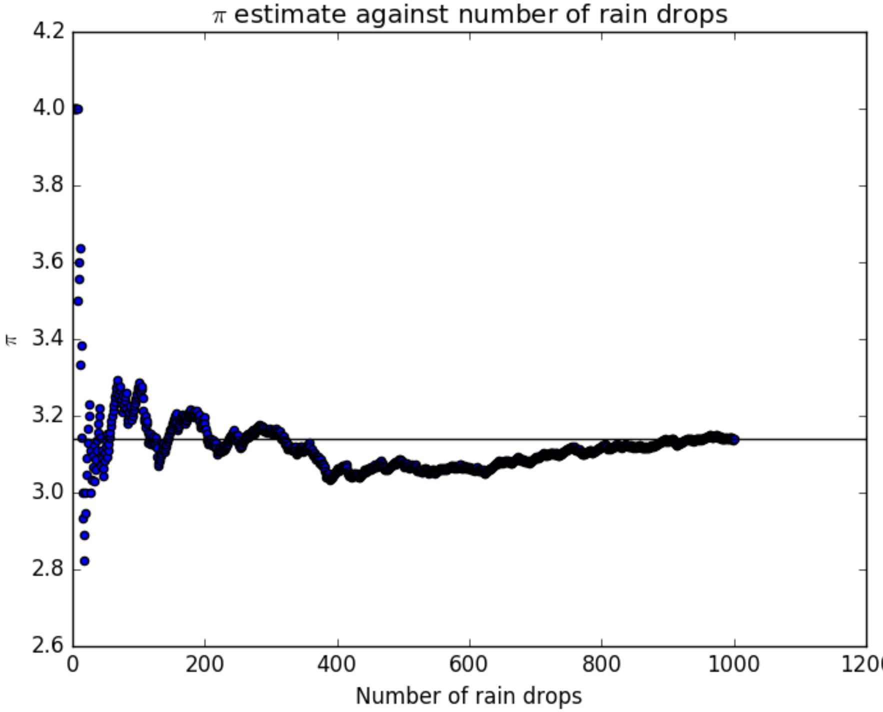
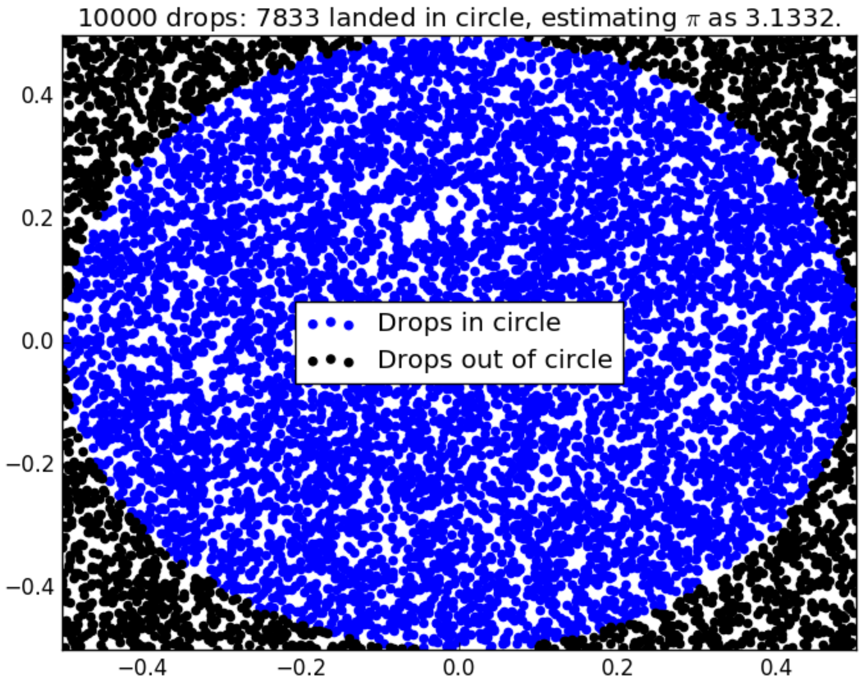
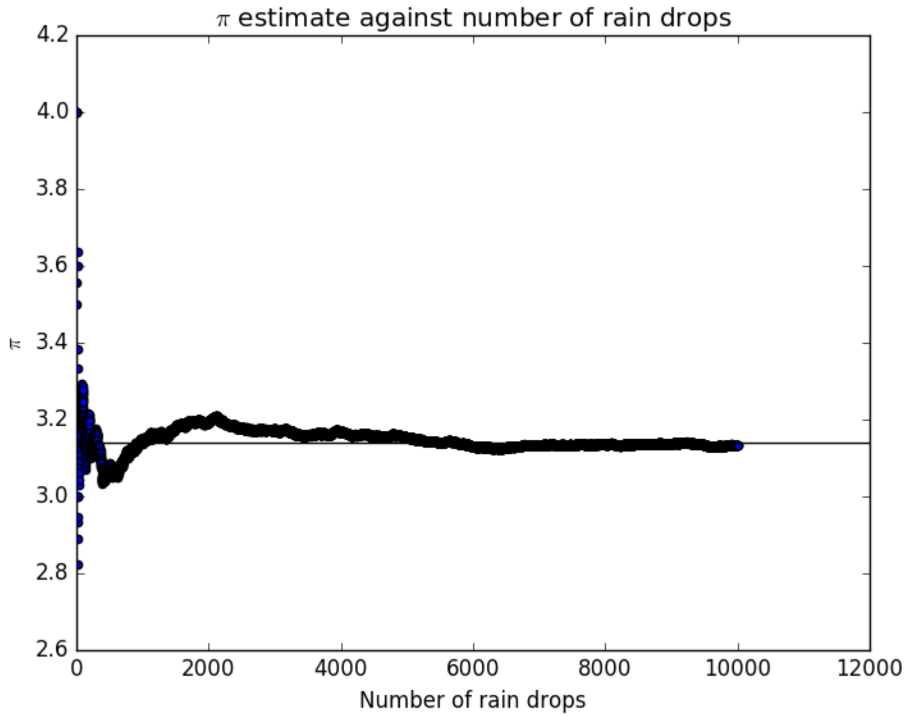


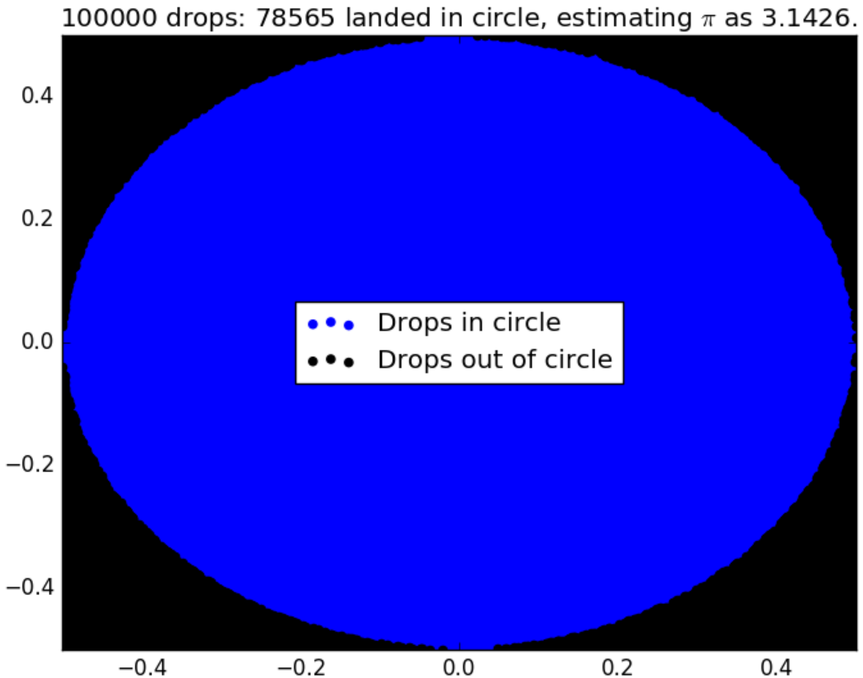


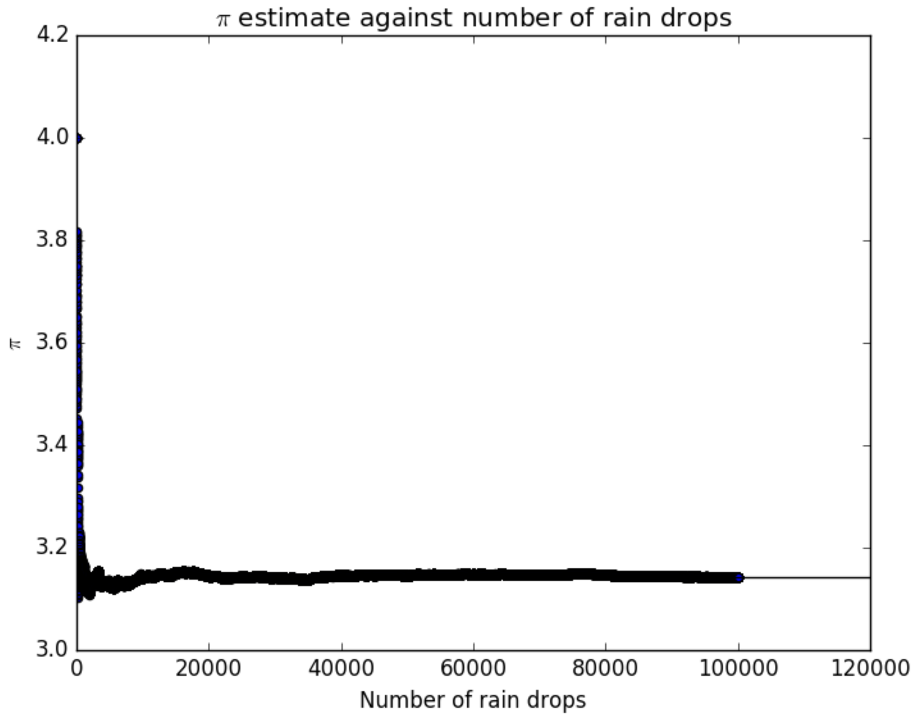
Monte Carlo - Simple



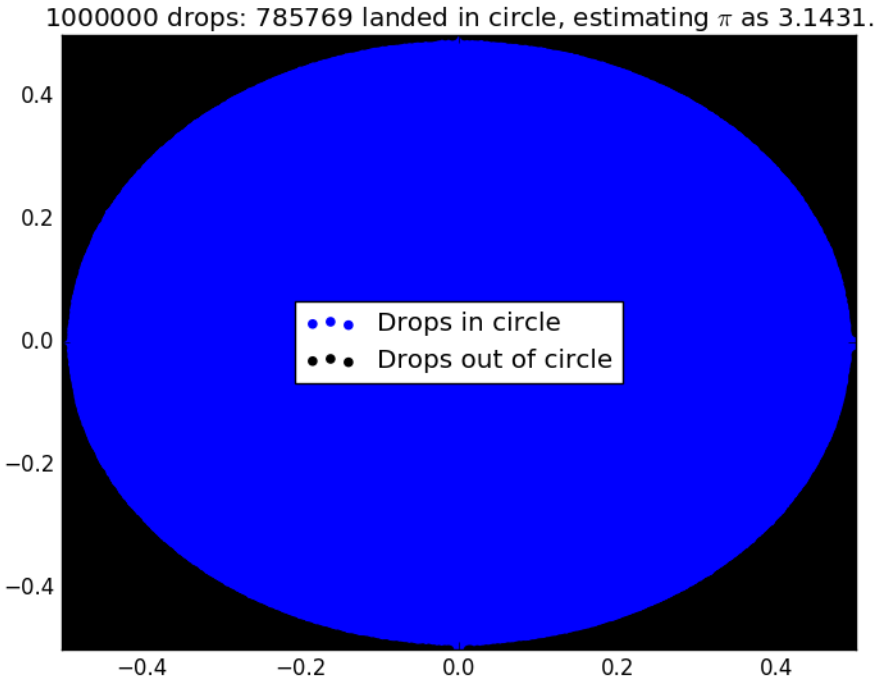


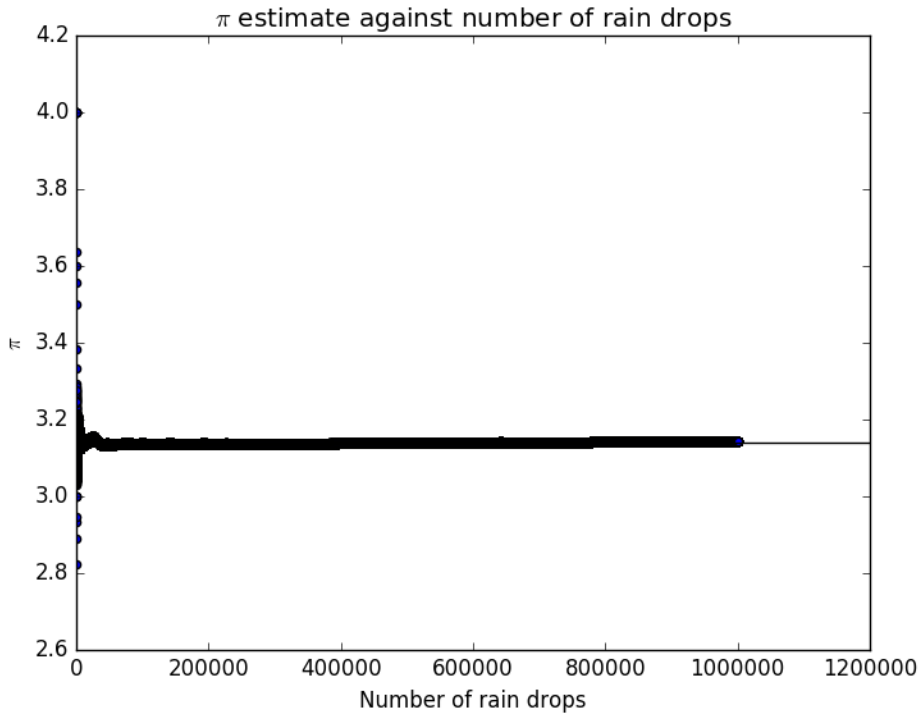
Monte Carlo - Simple





Monte Carlo - Simple





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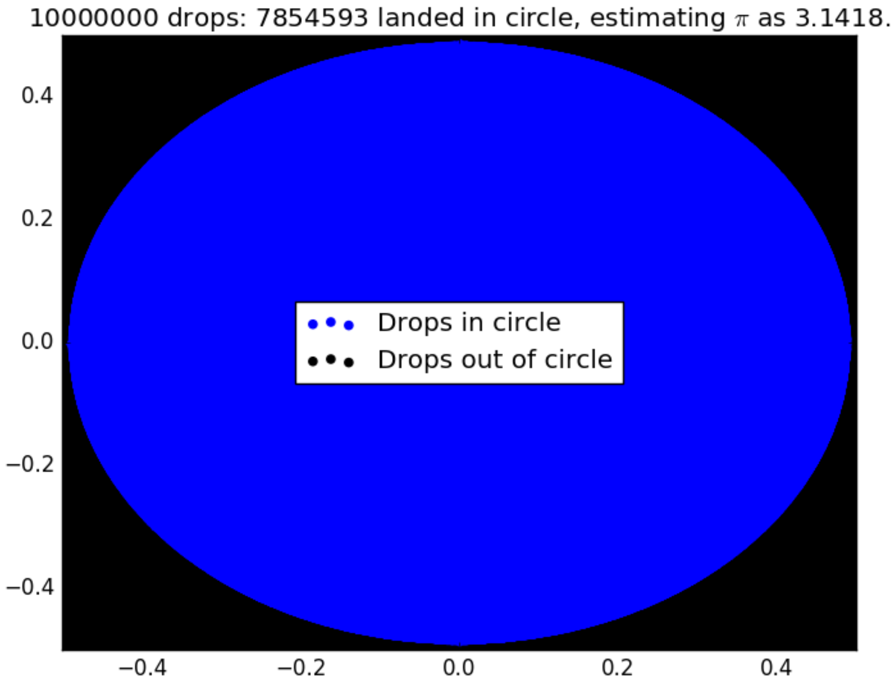
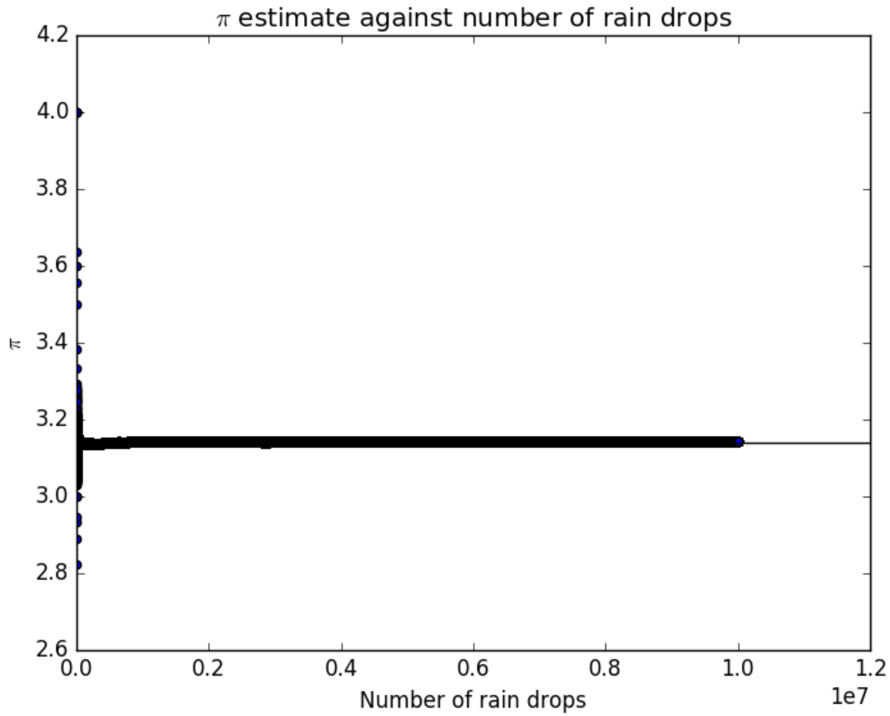
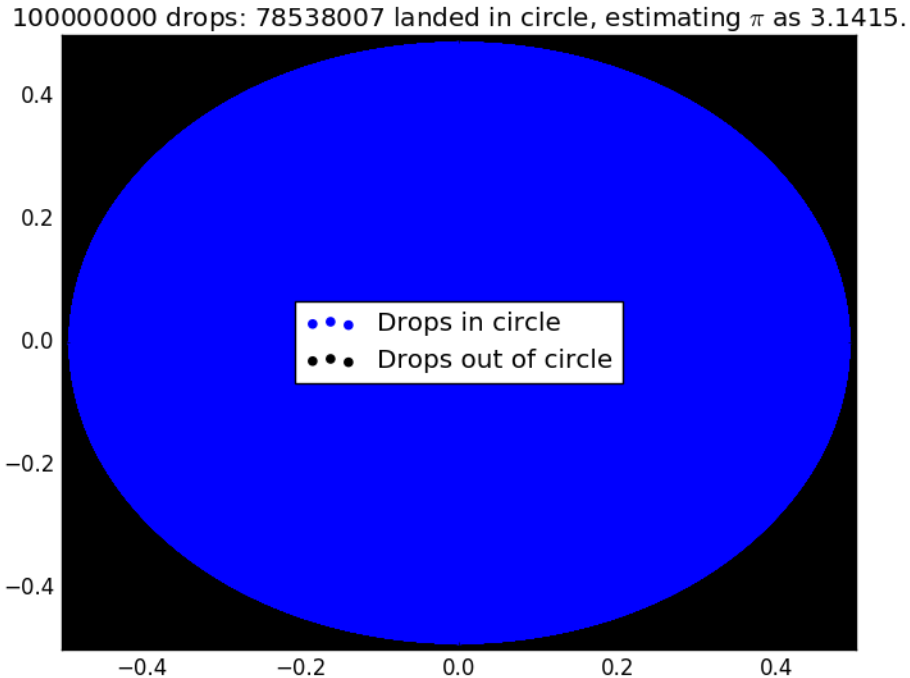
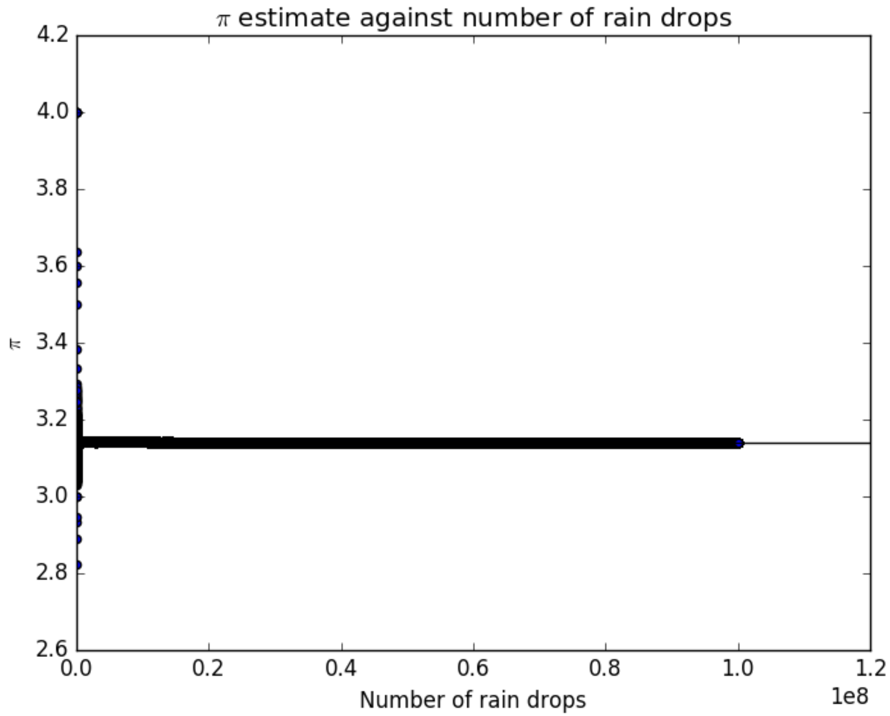


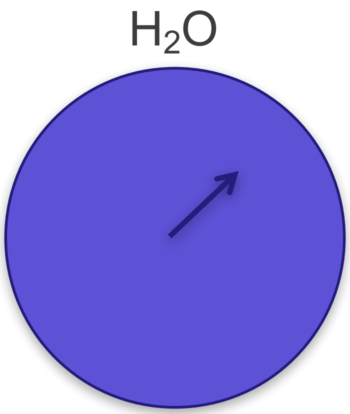


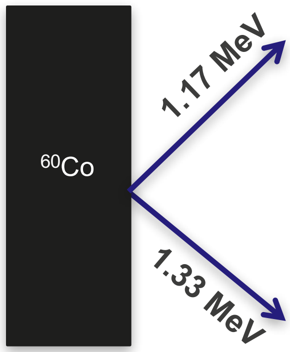
Monte Carlo - Simple

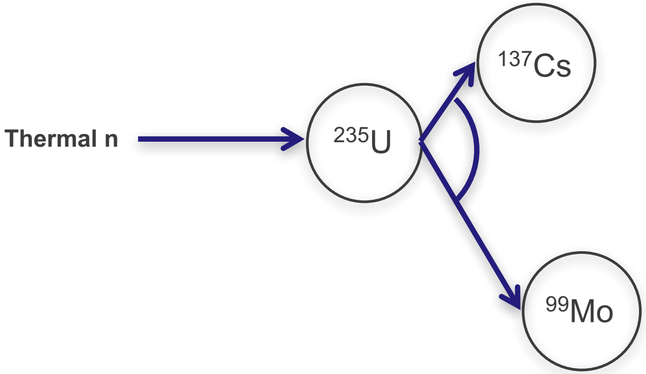




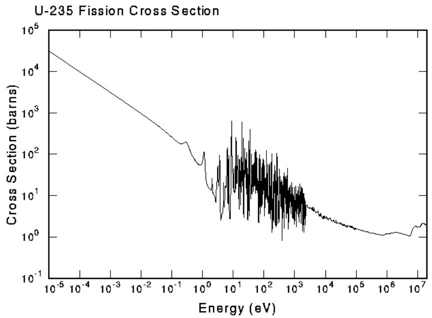
Monte Carlo – Radiation Transport Simulations

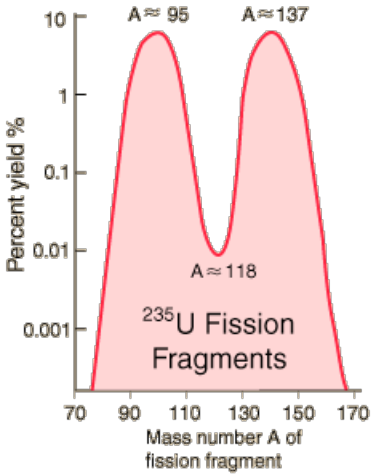




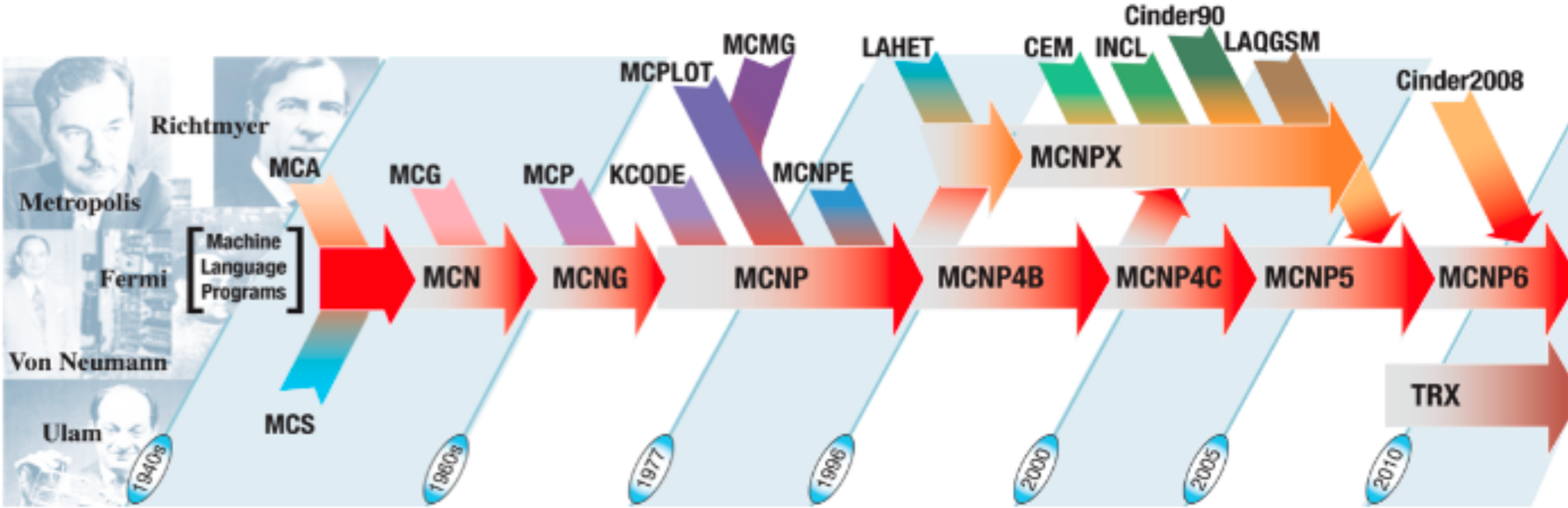


Mat	Atom %	RN
H	0.6666	[0,.666]
O	0.3333	(.666,1]





MCNP®6



A general-purpose, continuous-energy, generalized-geometry, time-dependent, Monte Carlo radiation-transport code

Repository of nuclear physics knowledge compiled since 1947

Estimated $500M invested

Used worldwide in numerous fields

MCNP®6 Basics

- **Input deck: 3 major sections**
  - Cell cards
    - 3-D volumes
  - Surface cards
    - 2-D areas (inf. and finite)
  - Data cards
    - Physics

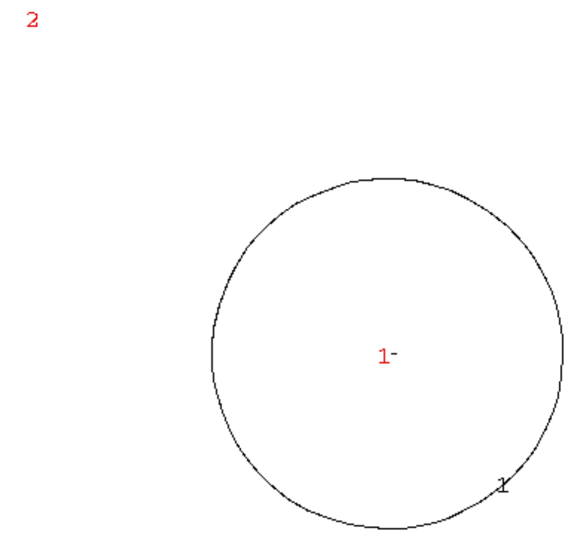
```
Message Block                       } Optional
Blank Line Delimiter
One Line Problem Title Card
Cell Cards
.
.
.
Blank Line Delimiter
Surface Cards
.
.
.
Blank Line Delimiter
Data Cards
.
.
.
Blank Line Terminator Optional, but
recommended
Anything Else Optional
```

MCNP®6 Basics: Simple input deck

```
Simple input deck
1 0 -1 imp:n=1
2 0  1 imp:n=0

1 so 1.0

sdef
nps 100
```

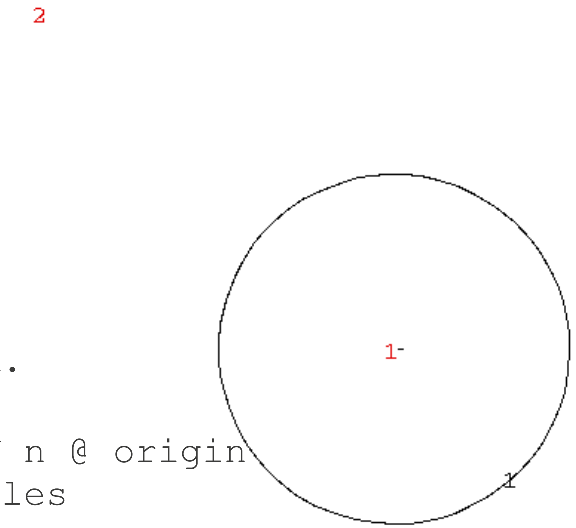


MCNP®6 Basics: Simplest input deck

```
Simple input deck $ title card (inline comment)
c This is a comment line
c
c
1 0 -1 imp:n=1     $ cell card, inside sphere
2 0  1 imp:n=0     $ cell card, outside sphere

1 so 1.0  $ surf. card, sphere @ origin, 1 cm rad.

sdef    $ data card, defaults to isotropic 14 MeV n @ origin
nps 100 $ data card, run 100 histories/src particles
```

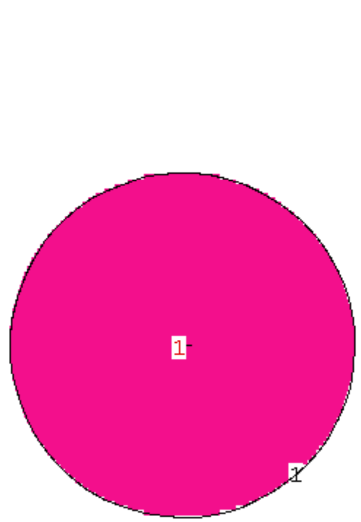


MCNP®6 Basics: Simplest input deck

```
Simple input deck $ title card (inline comment)
c This is a comment line
c
c m# Den. Surf. #s   importances/RR
1 1  -1.0   -1       imp:n=1 $ cell card, inside sphere
2 0          1       imp:n=0 $ cell card, outside sphere

1 so 1.0  $ surf. card, sphere @ origin, 1 cm rad.

m1   1001.80c 0.6666
     8016.80c 0.3333
sdef    $ data card, defaults to isotropic 14 MeV n @ origin
nps 100 $ data card, run 100 histories/src particles
```

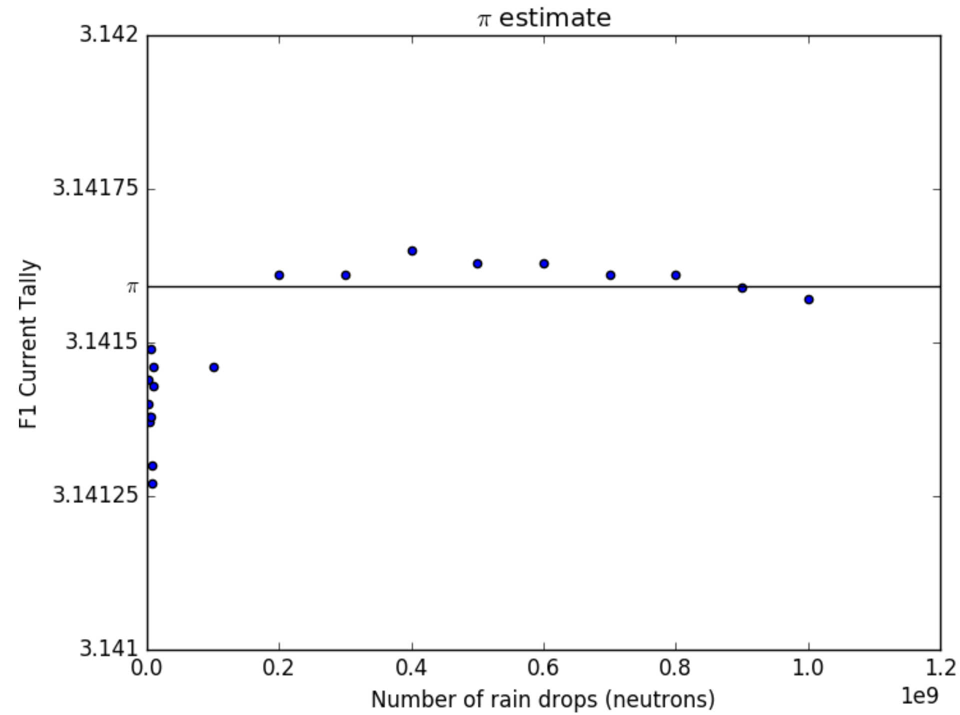


Monte Carlo – Pi Example

```
Simple raindrop approximation of pi
1 0 -1    imp:n=1
2 0  1 -2 imp:n=1
3 0  2    imp:n=0

1 rcc  0 0 -0.5 0 0 1 0.5
2 so 2

sdef x=d1 y=d2 z=0 axs=0 0 1 vec=0 0 1 dir=1
si1 -0.5 0.5
sp1    0   1
si2 -0.5 0.5
sp2    0   1
f1:n 1.2
fm1 4.0
nps 1e9
print
prdmp 1e8 1e8 1 j 1e8
```



MCNP®6 Basics: Terminology

- **MCNP is a complex Plinko game**
  - sdef (ISC)
  - geometry/materials/xs
  - physics
- **Transport**
  - In general this is correct on average
  - New features are being developed to be correct event-by-event (CGMF, FREYA)
- **Two ways of counting what happens**
  - Tallies are the bins at the bottom (8 types)
    - F, D, U, S, M, C, E, T
  - PTRAC is a large complex file containing ~all the information available about
    - Contains a wealth of information (DRiFT)
    - Can be very complicated to parse (MCNPtools)

MCNP®6: Simple ROC ex. (input deck)

Cell Cards

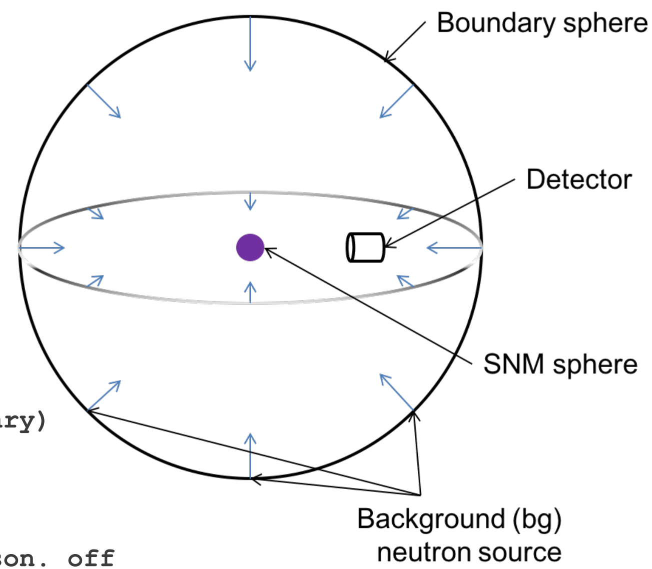
```
Simple ROC curve             $ Title
1 1 -19.0  -1      imp:n=1   $ Pure U-235 cell
2 0        -2      imp:n=0   $ Voided Detector cell
3 2 -1e-3  -3 1 2  imp:n=1   $ Air cell
4 0         3      imp:n=0   $ Outside system cell
```

Surf. Cards

```
1 so 3.9754                  $ U-235 sphere surface (5 kg)
2 rcc 50 0 0 10 0 0 5.0      $ Detector cylinder surface
3 so 100.0                   $ Model boundary sphere surface
```

Data Cards

```
mode n                       $ Track only neutrons
mphys on                     $ Turn on model physics
m1    92235  1.00            $ 100 atom% U-235 (default n library)
m2     7014  0.79
       8016  0.20            $ Air composition in atom%
      18040  0.01
phys:n 5000 5000 1           $ emax, analog capture, unres. reson. off
cut:n  2j 0 0                $ Turn on analog capture
sdef par=-bn sur=3 nrm=-1    $ bg n, surf src, dir inward w/ cos dist.
     loc=37.7 -122.7 -1      $ LLNL lat long, no elev. Scaling
f1:n 2.3                     $ Surf. current tally for detector
ft1  FFT                     $ First fission tally, see fu1
     ROC 1.494704e6 1000     $ n/s*time, max # of batches
fu1  18 0                    $ Score fission n, all other scores
tf1  1 1 3 1 1 1 1 1         $ user bin 3 is total signal + noise
     1 1 2 1 1 1 1 1         $ user bin 2 is noise
nps 1.494704e9               $ (n/batch time)*(# of batches)
prdmp j 1.494704e6           $ Rendezvous after every batch
print                        $ Print all tables in output
```



MCNP®6: Simple ROC ex. (normalization)

$$N = \frac{(A_s)\, I_{flux}\, T}{4} = \pi(100\ cm)^2 \left(0.0475779\ \frac{n}{cm^2 s}\right)(1000\ s)$$

Surf. Cards

```
1 so 3.9754                    $ U-235 sphere surface (5 kg)
2 rcc 50 0 0 10 0 0 5.0        $ Detector cylinder surface
3 so 100.0                     $ Model boundary sphere surface
```

Data Cards

```
sdef par=-bn sur=3 nrm=-1  $ bg n, surf src, dir. inward
     loc=37.7 -121.7 -1    $ LLNL lat & long, no elev. scaling
```

background.dat

location comment line
38.0 -120.0 1.69514 330
flux (n/cm2/s) 4.75779E-02 flux (p/cm2/s) 5.17399E+00 cosp (p/cm2/s) 8.19548E-02

F4 tally result with voided cells and FM

cell 1
multiplier bin: 1.00000E+00
3.17886E-05 0.0269

cell 1
multiplier bin: 3.14159E+04
9.98667E-01 0.0269

$$N = \frac{(A_s)\, I_{flux}\, T}{4} = 31415.9\ I_{flux}\ T$$

MCNP®6: Simple ROC ex. (normalization)

$$\text{NHB} = \frac{(A_s)\, I_{flux}\, \text{T}}{4} = \pi(\mathbf{100}\ cm)^2 \left(\mathbf{0.0475779}\ \frac{n}{cm^2 s}\right)(1000\ s)$$

$$\text{NHB} = 1.494704\text{e}6\ \frac{n}{batch}$$

Assuming you run more than the default max number of batches of 100 then the ROC keyword would have the following:

FTn ROC 1.494704e6 1000

Memory allocation only

and nps would be set to:

$$\text{NPS} = 1.494704\text{e}6\ \frac{n}{batch}\ 1000\ batch = 1.494704\text{e}9\ \text{n}$$

It is always safer to increase the max number of batches in case a continue run is needed to get better statistics (nps = NHB * batches).

MCNP®6: Simple ROC ex. (output)

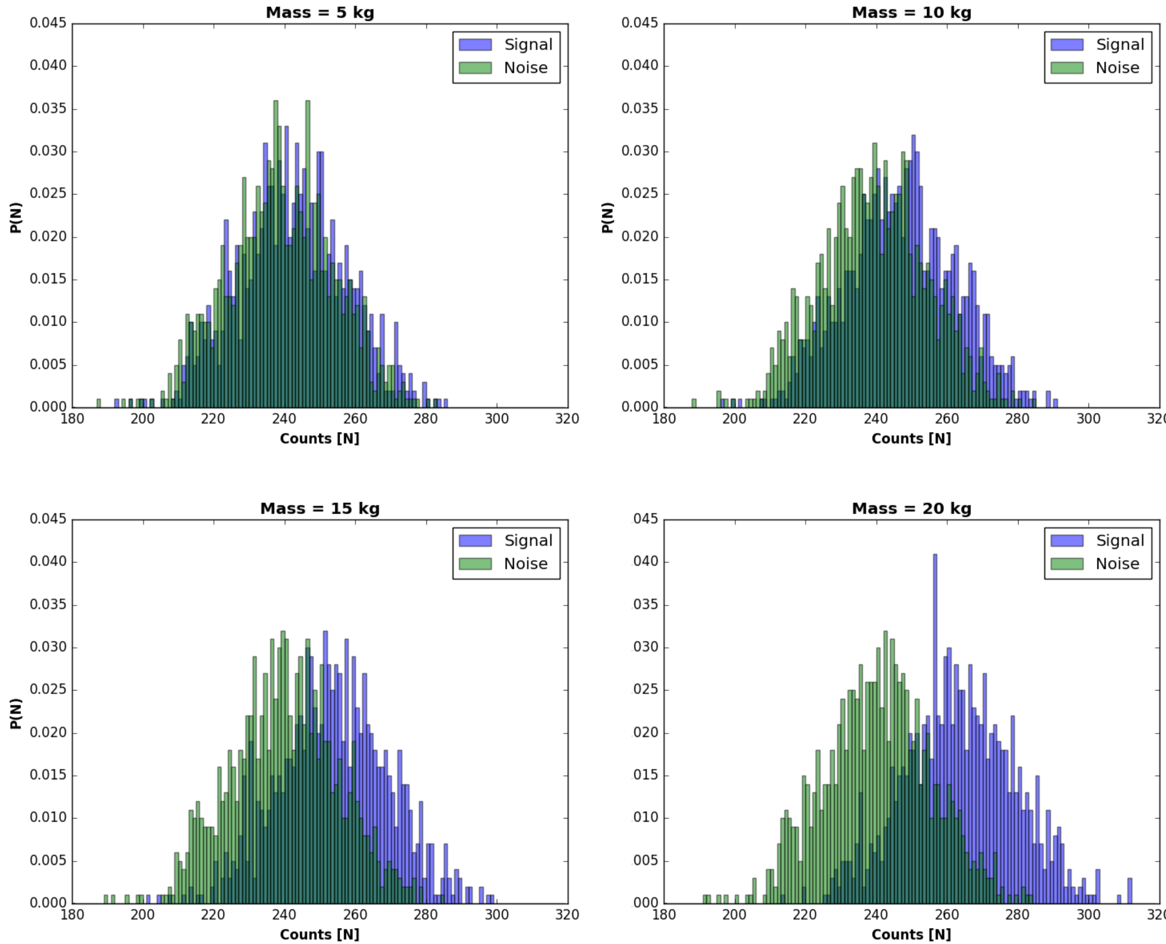
```
1roc curve for tally   1  1000 batches, signal mean= 2.629E+02 noise mean= 2.399E+02 nps =   380133000  print table
163  abscissa        ordinate          plot of probability of detection versus probability of false alarm - 0 to 100 percent
  noise          signal:-----10-----20------30-----40-----50-----60-----70-----80-----90---100
  1.000          25.550|    |    |  x |    |    |    |    |    |    |    |
  2.000          30.433|    |    |    |x   |    |    |    |    |    |    |
  3.000          35.850|    |    |    |  x |    |    |    |    |    |    |
  4.000          40.300|    |    |    |    |x   |    |    |    |    |    |
  5.000          44.900|    |    |    |    |  x |    |    |    |    |    |
  6.000          47.905|    |    |    |    |   x|    |    |    |    |    |
  7.000          50.429|    |    |    |    |    |x   |    |    |    |    |
  8.000          52.875|    |    |    |    |    | x  |    |    |    |    |
  9.000          54.625|    |    |    |    |    |  x |    |    |    |    |
 10.000          56.729|    |    |    |    |    |   x|    |    |    |    |
 11.000          59.250|    |    |    |    |    |    x    |    |    |    |
 12.000          61.750|    |    |    |    |    |    |x   |    |    |    |
 13.000          63.925|    |    |    |    |    |    | x  |    |    |    |
 14.000          66.175|    |    |    |    |    |    |   x|    |    |    |
 15.000          68.425|    |    |    |    |    |    |    x    |    |    |
 16.000          70.290|    |    |    |    |    |    |    |x   |    |    |
 17.000          71.570|    |    |    |    |    |    |    |x   |    |    |
 18.000          72.670|    |    |    |    |    |    |    | x  |    |    |
 19.000          73.817|    |    |    |    |    |    |    | x  |    |    |
 20.000          74.983|    |    |    |    |    |    |    |  x |    |    |
 21.000          76.000|    |    |    |    |    |    |    |  x |    |    |
 22.000          76.942|    |    |    |    |    |    |    |   x|    |    |
 23.000          77.826|    |    |    |    |    |    |    |   x|    |    |
 24.000          78.709|    |    |    |    |    |    |    |    x    |    |
 25.000          79.593|    |    |    |    |    |    |    |    x    |    |
 26.000          80.522|    |    |    |    |    |    |    |    |x   |    |
 27.000          81.633|    |    |    |    |    |    |    |    |x   |    |
 28.000          82.540|    |    |    |    |    |    |    |    | x  |    |
 29.000          83.140|    |    |    |    |    |    |    |    | x  |    |
 30.000          83.740|    |    |    |    |    |    |    |    | x  |    |
 31.000          84.333|    |    |    |    |    |    |    |    |  x |    |
 32.000          84.926|    |    |    |    |    |    |    |    |  x |    |
 33.000          85.515|    |    |    |    |    |    |    |    |  x |    |
 34.000          86.092|    |    |    |    |    |    |    |    |   x|    |
 35.000          86.669|    |    |    |    |    |    |    |    |   x|    |
```

tally	signal		noise	
upper bin	pdf	cum.	pdf	cum.
1.922E+02	0.000E+00	1.000E+00	2.000E-03	1.000E+00
1.934E+02	0.000E+00	1.000E+00	0.000E+00	9.980E-01
1.946E+02	0.000E+00	1.000E+00	0.000E+00	9.980E-01
1.958E+02	0.000E+00	1.000E+00	1.000E-03	9.980E-01
1.970E+02	0.000E+00	1.000E+00	1.000E-03	9.970E-01
1.982E+02	0.000E+00	1.000E+00	0.000E+00	9.960E-01
1.994E+02	0.000E+00	1.000E+00	0.000E+00	9.960E-01
2.006E+02	0.000E+00	1.000E+00	1.000E-03	9.960E-01
2.018E+02	0.000E+00	1.000E+00	0.000E+00	9.950E-01
2.030E+02	0.000E+00	1.000E+00	1.000E-03	9.950E-01
2.042E+02	0.000E+00	1.000E+00	1.000E-03	9.940E-01
2.054E+02	0.000E+00	1.000E+00	3.000E-03	9.930E-01
2.066E+02	0.000E+00	1.000E+00	0.000E+00	9.900E-01
2.078E+02	0.000E+00	1.000E+00	0.000E+00	9.900E-01
2.090E+02	0.000E+00	1.000E+00	5.000E-03	9.900E-01
2.102E+02	0.000E+00	1.000E+00	4.000E-03	9.850E-01
2.114E+02	0.000E+00	1.000E+00	2.000E-03	9.810E-01
2.126E+02	0.000E+00	1.000E+00	7.000E-03	9.790E-01
2.138E+02	1.000E-03	1.000E+00	1.000E-02	9.720E-01
2.150E+02	0.000E+00	9.990E-01	2.100E-02	9.620E-01
2.162E+02	0.000E+00	9.990E-01	9.000E-03	9.410E-01
2.174E+02	0.000E+00	9.990E-01	9.000E-03	9.320E-01
2.186E+02	0.000E+00	9.990E-01	5.000E-03	9.230E-01
2.198E+02	2.000E-03	9.990E-01	1.500E-02	9.180E-01
2.210E+02	0.000E+00	9.970E-01	2.300E-02	9.030E-01
2.222E+02	0.000E+00	9.970E-01	1.300E-02	8.800E-01
2.234E+02	0.000E+00	9.970E-01	1.800E-02	8.670E-01
2.246E+02	0.000E+00	9.970E-01	1.100E-02	8.490E-01
2.258E+02	1.000E-03	9.970E-01	1.400E-02	8.380E-01
2.270E+02	4.000E-03	9.960E-01	3.200E-02	8.240E-01
2.282E+02	4.000E-03	9.920E-01	1.400E-02	7.920E-01
2.294E+02	2.000E-03	9.880E-01	2.100E-02	7.780E-01
.	.	.	.	.
.	.	.	.	.

MCNP®6: Simple ROC ex. (PDF)

Tally results by batch

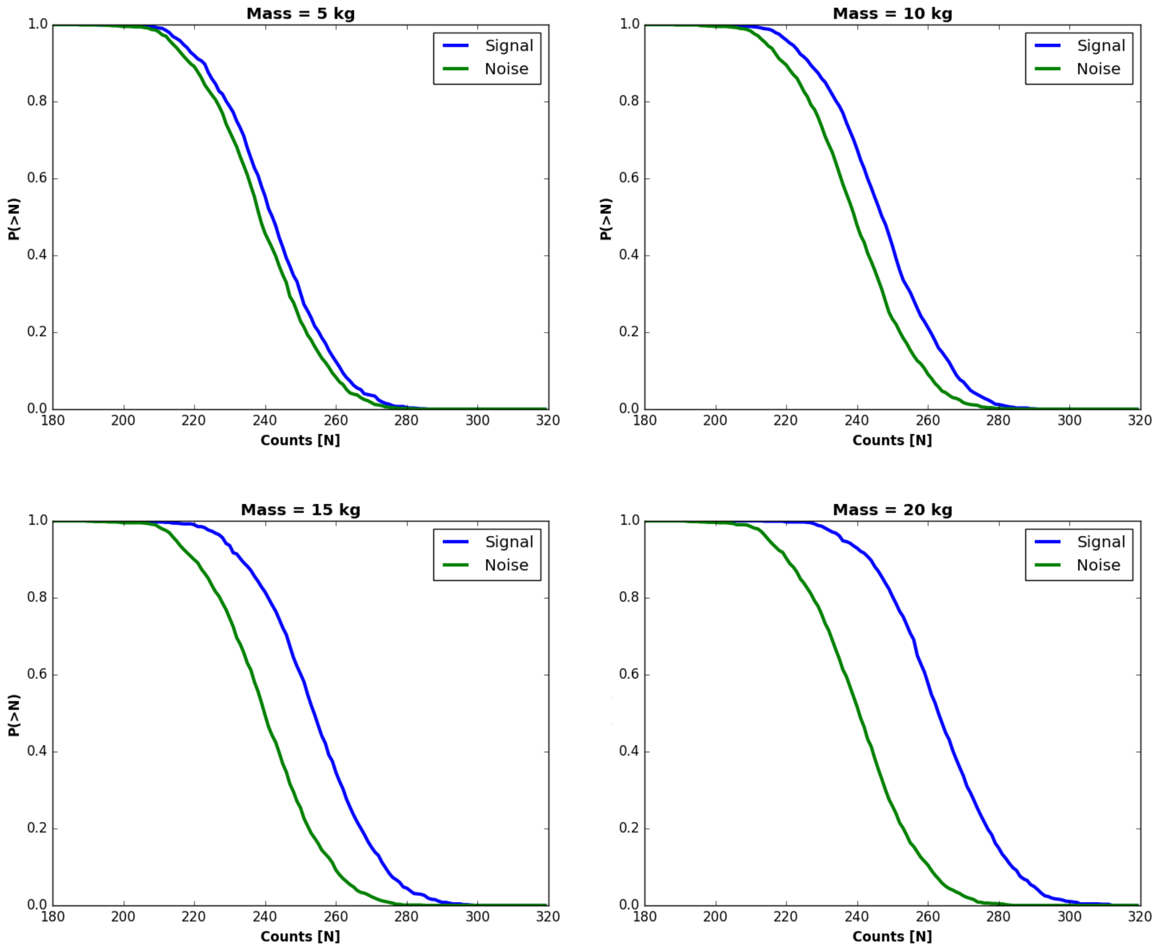
Batch	Signal	Noise
1	2.66000E+02	2.47000E+02
2	2.44000E+02	2.18000E+02
3	2.85000E+02	2.61000E+02
4	2.66000E+02	2.31000E+02
5	2.41000E+02	2.15000E+02
6	2.82000E+02	2.61000E+02
7	2.88000E+02	2.69000E+02
8	2.70000E+02	2.45000E+02
9	2.66000E+02	2.44000E+02
10	2.38000E+02	2.17000E+02
	.	
	.	
990	2.56000E+02	2.35000E+02
991	2.44000E+02	2.20000E+02
992	2.59000E+02	2.39000E+02
993	2.95000E+02	2.69000E+02
994	2.58000E+02	2.34000E+02
995	2.43000E+02	2.18000E+02
996	2.53000E+02	2.23000E+02
997	2.34000E+02	2.13000E+02
998	2.51000E+02	2.25000E+02
999	2.42000E+02	2.21000E+02
1000	2.56000E+02	2.41000E+02



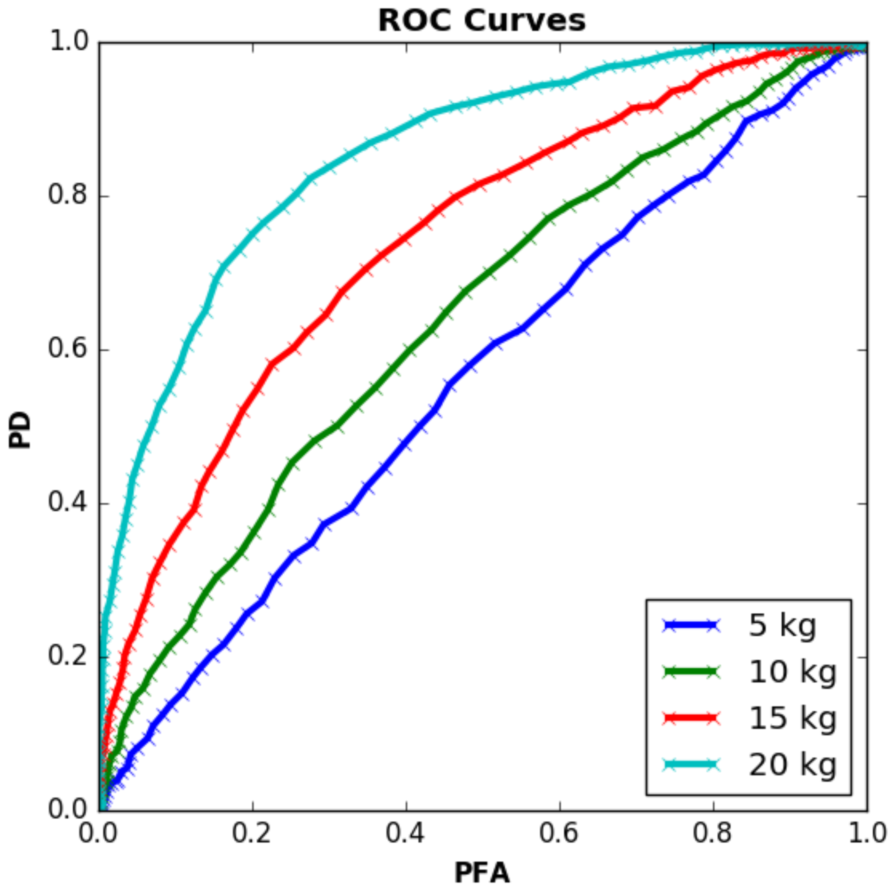
MCNP®6: Simple ROC ex. (CCDF)

Tally results by batch

Batch	Signal	Noise
1	2.66000E+02	2.47000E+02
2	2.44000E+02	2.18000E+02
3	2.85000E+02	2.61000E+02
4	2.66000E+02	2.31000E+02
5	2.41000E+02	2.15000E+02
6	2.82000E+02	2.61000E+02
7	2.88000E+02	2.69000E+02
8	2.70000E+02	2.45000E+02
9	2.66000E+02	2.44000E+02
10	2.38000E+02	2.17000E+02
	.	
	.	
990	2.56000E+02	2.35000E+02
991	2.44000E+02	2.20000E+02
992	2.59000E+02	2.39000E+02
993	2.95000E+02	2.69000E+02
994	2.58000E+02	2.34000E+02
995	2.43000E+02	2.18000E+02
996	2.53000E+02	2.23000E+02
997	2.34000E+02	2.13000E+02
998	2.51000E+02	2.25000E+02
999	2.42000E+02	2.21000E+02
1000	2.56000E+02	2.41000E+02



MCNP®6: Simplest input ex. (ROC Curve)



Conclusions

- **Monte Carlo is a powerful method for solving complex problems**
- **It can be extremely computationally expensive**
  - Use cluster computing
  - Consider variance reduction methods
- **MCNP®6 is very easy to learn (time consuming to master)**
- **Always start with simple geometries**
- **Understand the physics you are using and the normalization of your answer**
- **Use the MCNP forum**
- **Be lazy!**
  - Use scripting to create input decks
  - Use modular geometries