

Testing Nesting DXTRAN Spheres for Neutron Transport in Air

2017 ANS Annual Meeting
San Francisco, CA

M. L. Fensin, K. C. Kelley, J. S. Hendricks,
B. W. Cox, J. T. Goorley and S. S. McCready



June 11-15, 2017



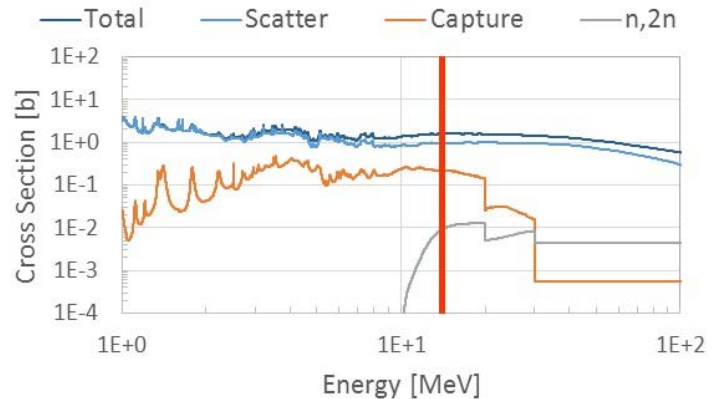
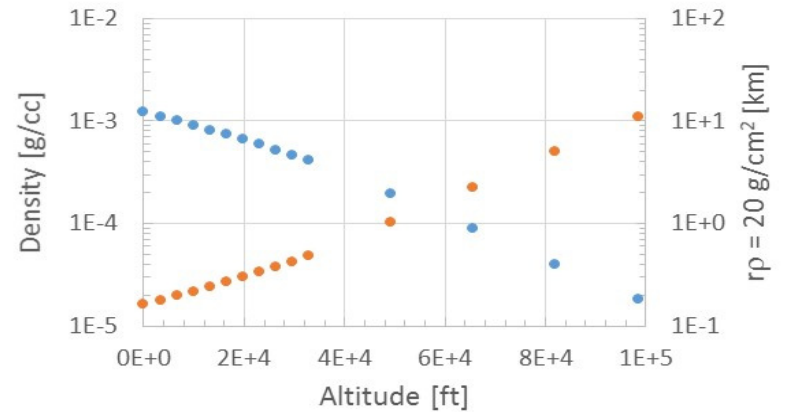
Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

Outline

- **Transport Considerations for Neutron Transport in Air**
- **Statistics**
- **VR Feature Descriptions**
- **Results**
- **Conclusions**

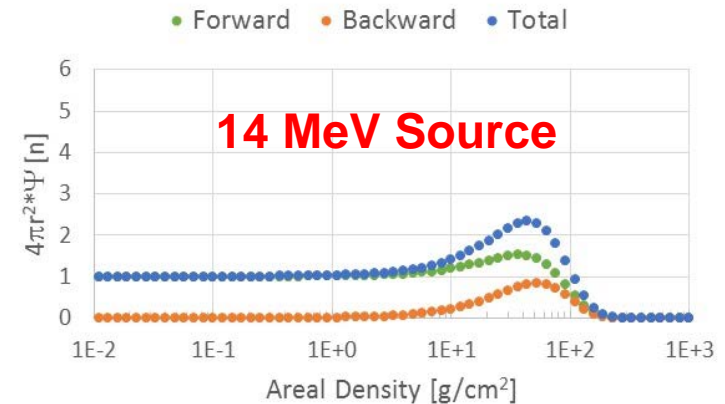
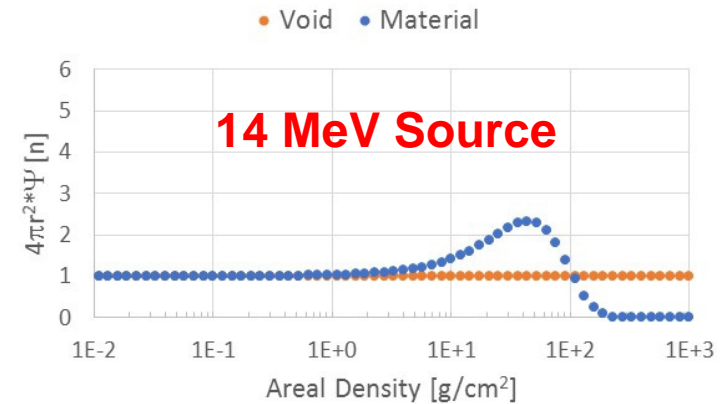
Neutron Transport in Air

- **Neutron transport in air for large standoff detection**
 - Small solid angle
 - Scatter dominates
- **Deterministic**
 - Ray effects
- **Monte Carlo**
 - Analog is extremely inefficient
 - Variance Reduction required to get particles to a detector



Transport Considerations

- **Surface fluence of isotropic point source emitted in a void $\sim 1/r^2$**
 - $4\pi r^2 \Psi(\vec{r})$ is therefore independent of r in a void
- **Departure from $1/r^2$ is related to scatter and capture**
 - Buildup peak between starts $\sim 10 \text{ g/cm}^2$



Geometry

- **Atmosphere model**

- NRLMSISE-00 (**N**aval **R**esearch **L**aboratory **M**ass **S**pectrometer and **I**ncoherent **S**catter radar **E**xtends)-- Community Coordinated Modeling Center at Goddard Space Flight Center (2/2/2016)

- Extends the ground through exosphere and 00 is the year of the release

- 60 X 60 X 60 km

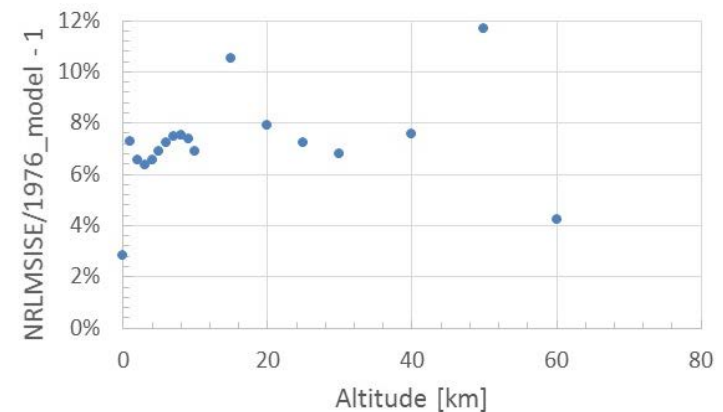
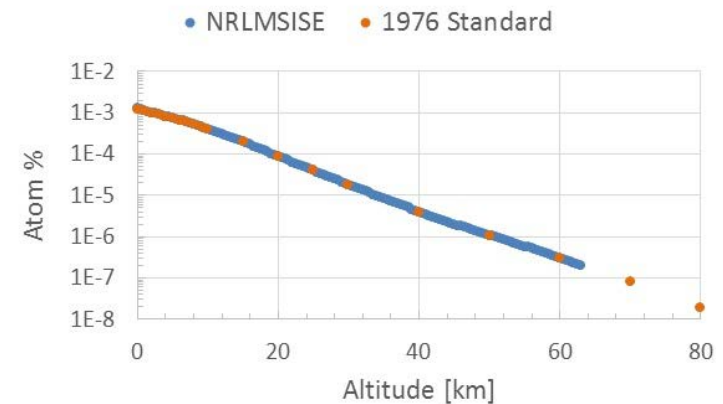
- 0.5 km altitude increments

- Nevada ground

- **N-14, O-16, Ar-40 and He-4**

- **14 MeV isotropic point source**

- 50k ft (~15.24 km) in altitude, 1 km from 3 m radius detector



Concentration Assumptions

- **Prior Analysis**

- Assuming only N-14, O-16, **He-4** and Ar-40 is reasonable

- **Assumed Concentration (at. %)**

- N-14 78.11%
- O-16 20.1%
- He-4 0.001%
- Ar-40 0.934%

Areal Density [g/cm ²]	Elastic Scatter Contribution			
	N-14	O-16	Ar-40	Total
20	81.5%	18.0%	0.3%	99.7%
40	83.9%	15.6%	0.2%	99.7%
60	85.1%	14.4%	0.2%	99.7%
80	85.8%	13.8%	0.1%	99.8%
100	86.3%	13.4%	0.1%	99.8%

Areal Density [g/cm ²]	Inelastic Scatter Contribution			
	N-14	O-16	Ar-40	Total
20	73.3%	21.8%	4.1%	99.2%
40	72.8%	22.2%	4.3%	99.2%
60	72.6%	22.5%	4.2%	99.3%
80	72.4%	22.9%	4.1%	99.4%
100	72.5%	23.0%	3.9%	99.4%

Central Limit Theorem

- **Estimated mean approaches a normal distribution with known variance as the number of random samples grows sufficiently large**

- **Mean and Variance must exist**

$$- E(x) = \mu = \int_{-\infty}^{\infty} xf(x)dx = \text{true mean}$$

$$- E(x^2) = \sigma^2 = \int_{-\infty}^{\infty} (x - E(x))^2 f(x)dx$$

- **Mean and Variance must be calculated**

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

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

- **How does one determine if the variance is finite, in order to meet the existence requirement?**

Slope Test

- Fit $f(x)$ to a known function using “simplex” algorithm

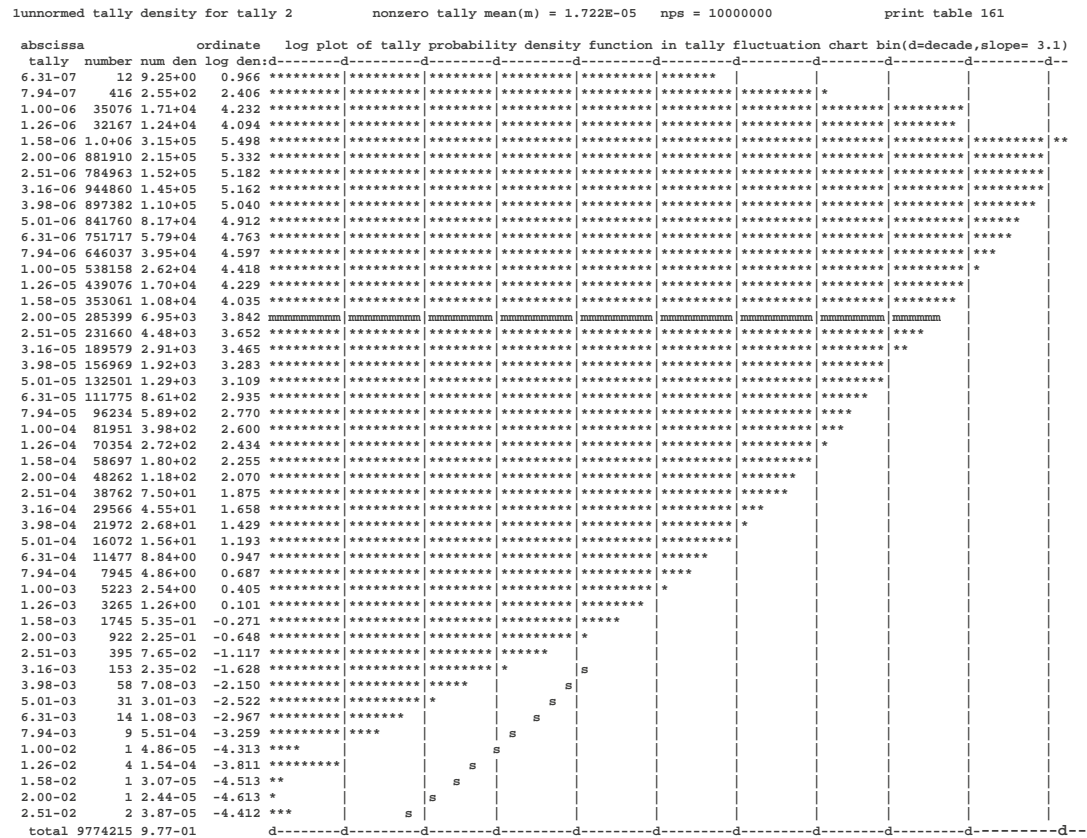
- Fit the top 201 history scores

- $$f(x) = \frac{\left(1 + \frac{kx}{a}\right)^{-\left(\frac{1}{k} + 1\right)}}{a}$$

- Slope = $(1/k) + 1$

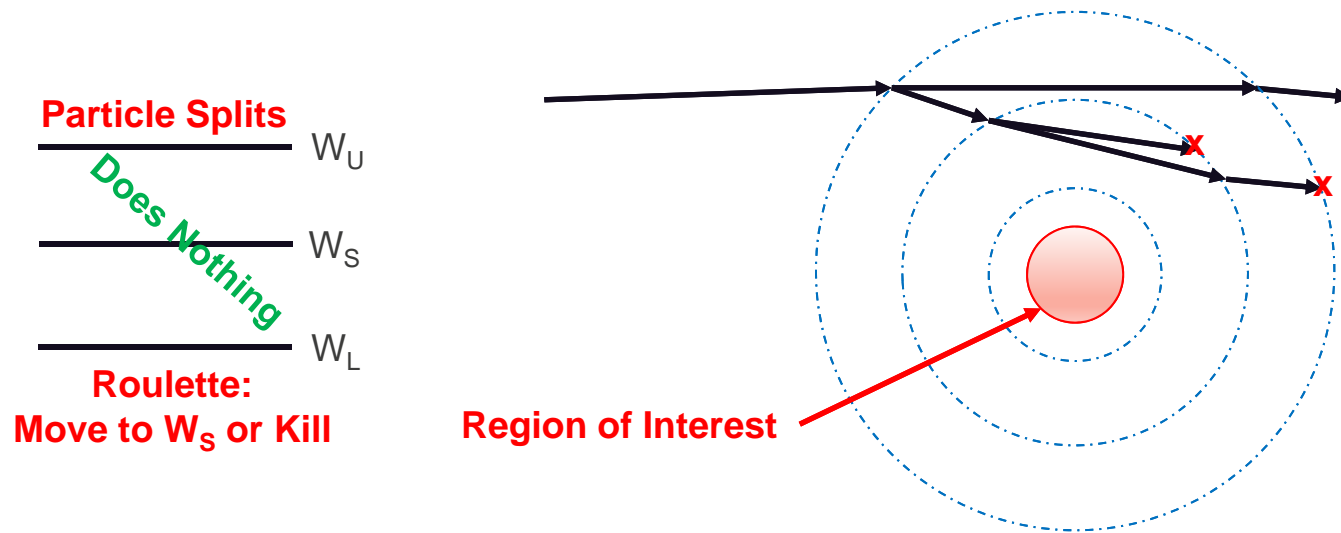
- $$E(x^2) = \int_{-\infty}^{\infty} x^2 f(x) dx$$

- If slope is not greater than 3, enough histories may not have yet been sampled



Trouble with WW's

- WWs split/roulette particles at surface crossings and collisions
- **WWs cannot focus particles towards a finite detector**

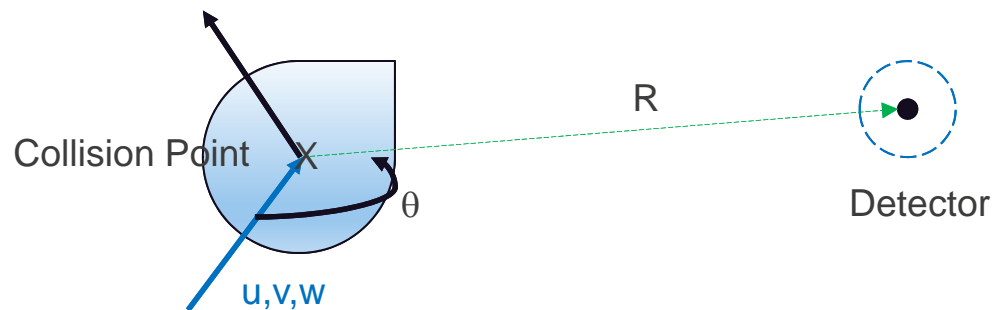


Deterministic Estimates

- Point detectors place a source or collision

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

- Large weight fluctuation can occur because of $1/R^2$,
- *The point detector estimate is assumed to be the average flux uniformly distributed within the radius of exclusion*



DXTRAN

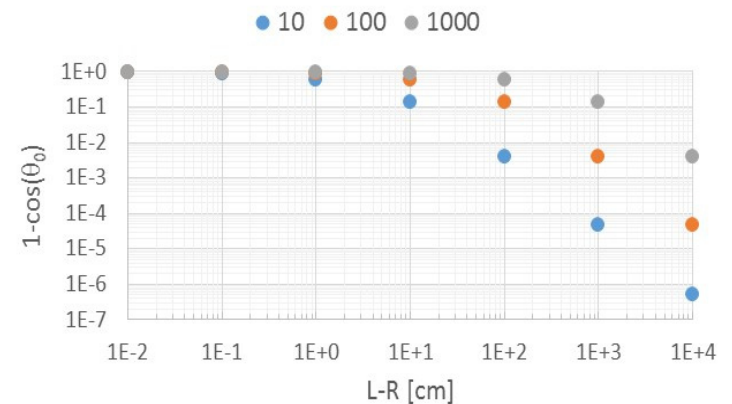
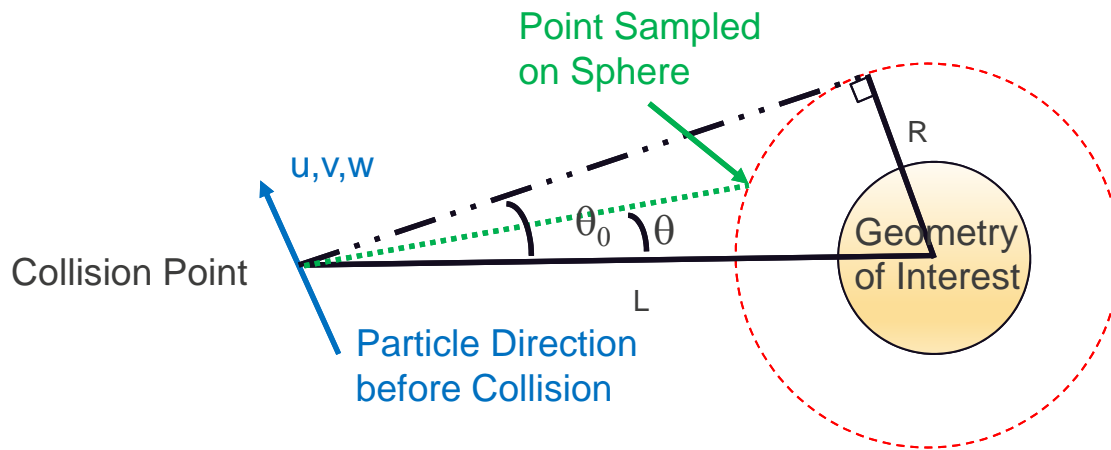
- At a collision event, a DXTRAN particle is placed on the sphere

$$-\cos(\theta_0) = \frac{\sqrt{L^2 - R^2}}{L}$$

- $\cos(\theta) = \cos(\theta_0) + \xi(1 - \cos(\theta_0))$

$$-w = w_0 P(\cos(\theta))(1 - \cos(\theta_0)) e^{-\int \sigma_t(s) ds}$$

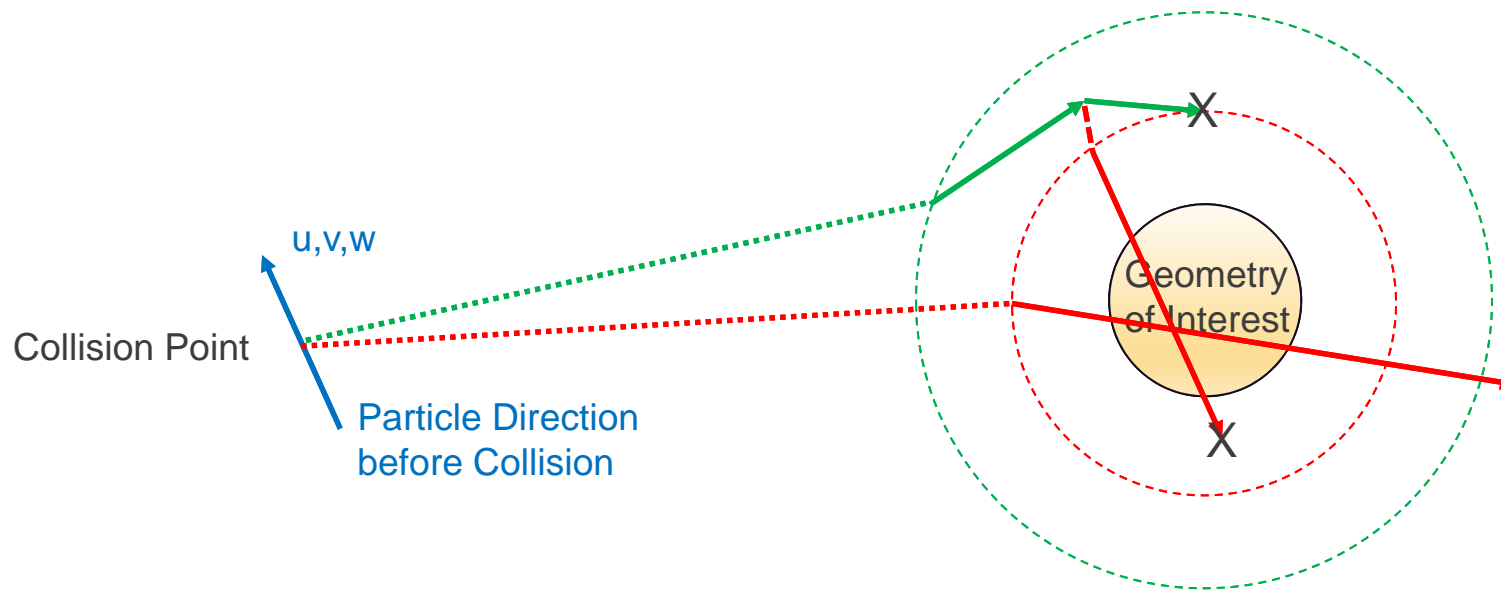
- To balance weight, NONDXTRAN particles are killed when traversing the sphere



Nested DXTRAN

- **Nested DXTRAN sphere concept was devised to control this large weight fluctuation**

– dxt $X_1 Y_1 Z_1 RI_1 RO_1 \dots X_N Y_N Z_N RI_N RO_N$ DWC₁ DWC₂ DPWT



Single DXTRAN sphere test (ex1)

```
dxt:n 0 0 1524000 310 310
```

- **A simple DXTRAN sphere 310 cm radius centered around tally**
 - dwc1 and dwc2 not set
 - 10 million histories
- **Did not pass all 10 statistical checks**

Case	Mean	Relative Error	VOV	Slope	FOM
ex1	1.4804E-11	0.0081	0.1263	2.3	163

Single DXTRAN sphere test (ex2)

```
average weight per history = 4.51829E-06      largest weight = 2.28798E-01  
largest/average = 5.06383E+04                nps of largest = 2033847
```

```
dxt:n 0 0 1524000 310 310  
4.5e-6 4.5e-7
```

**dwc's apply to particles in RI
Passed all 10 statistical checks**

Case	Mean	Relative Error	VOV	Slope	FOM
ex1	1.4804E-11	0.0081	0.1263	2.3	163
ex2	1.4589E-11	0.0049	0.0305	3.3	449

$$\text{ex2/ex1}-1 = -1.45\%$$

DD cards

- **Roulette in transmission**

- The average contribution to a DXTRAN sphere is calculated from all contributions to the sphere made by particle histories until the first TFC interval is reached → moving target. Then the average contribution is updated at each TFC rendezvous

- **DD card sets the roulette/survival weight for transmission**

- **DDn k_1 m_1 k_2 m_2 ...**

- $n = 1$ for n spheres; 2 for photon spheres

- k → If negative, if greater than $-1*k$, keep particle; else roulette

- m → print first 100 contributions greater than $-1*m*k$

Examine TFC (ex3)

```
dxt:n 0 0 1524000 310 310
      4.5e-6 4.5e-7
dd1 -4.5e-7 1e4
```

**Failed some statistical checks!!!
Examine VOV**

nps	mean	error	vov	slope	fom
512000	1.5507E-11	0.0283	0.2033	2.4	263
1024000	1.4828E-11	0.0167	0.1314	2.4	380
1536000	1.4555E-11	0.0121	0.1016	2.6	480
2048000	1.4499E-11	0.0099	0.0739	2.8	535
2560000	1.4533E-11	0.0089	0.0515	2.5	533
3072000	1.4539E-11	0.0080	0.0399	2.6	546
3584000	1.4584E-11	0.0076	0.0318	2.7	530
4096000	1.4587E-11	0.0070	0.0270	2.8	546
4608000	1.4639E-11	0.0071	0.0549	2.6	460
5120000	1.4655E-11	0.0067	0.0469	3.1	470
5632000	1.4689E-11	0.0072	0.0660	2.5	370
6144000	1.4722E-11	0.0068	0.0583	2.6	381
6656000	1.4849E-11	0.0089	0.2050	2.5	204

Case	Mean	Relative Error	VOV	Slope	FOM
ex1	1.4804E-11	0.0081	0.1263	2.3	163
ex2	1.4589E-11	0.0049	0.0305	3.3	449
ex3	1.4684E-11	0.0065	0.1527	2.7	258

ex3/ex1-1 < +/-1%

3 Nested DXTRAN spheres – ex4 and ex5

```
dxt:n 0 0 1524000 310 310
      0 0 1524000 620 620
      0 0 1524000 1240 1240
      4.5e-6 4.5e-7
```

Low FOM
Failed some statistical checks!!!

```
dxt:n 0 0 1524000 310 310
      0 0 1524000 620 620
      0 0 1524000 1240 1240
      4.5e-6 4.5e-7
dd1 -4.5e-7 1e4 -1.79e-6 1e4
     -7.2e-6 1e4
```

Failed some statistical checks!!!

Case	Mean	Relative Error	VOV	Slope	FOM
ex1	1.4804E-11	0.0081	0.1263	2.3	163
ex2	1.4589E-11	0.0049	0.0305	3.3	449
ex3	1.4684E-11	0.0065	0.1527	2.7	258
ex4	1.4942E-11	0.0080	0.5386	2.8	67
ex5	1.4807E-11	0.0039	0.0162	2.7	274

ex4/ex1-1 < +/-1%
ex5/ex1-1 < +/-1%

Try WWs (ex6-6c)

```
dxt:n 0 0 1524000 310 310
      0 0 1524000 620 620
      0 0 1524000 1240 1240
dd1 -4.5e-7 1e4 -1.79e-6 1e4
     -7.2e-6 1e4
C wwp:n 4j -1
wwg 2 0
mesh geom=sph ref=-100000 0 1524000
     origin 0 0 1524000
     axs=1 0 0 vec=0 1 0
     imesh 310 620 1240 1600000
     iints 2 2 2 14
     jmesh 0.5
     jints 1
     kmesh 1
     kints 1
```

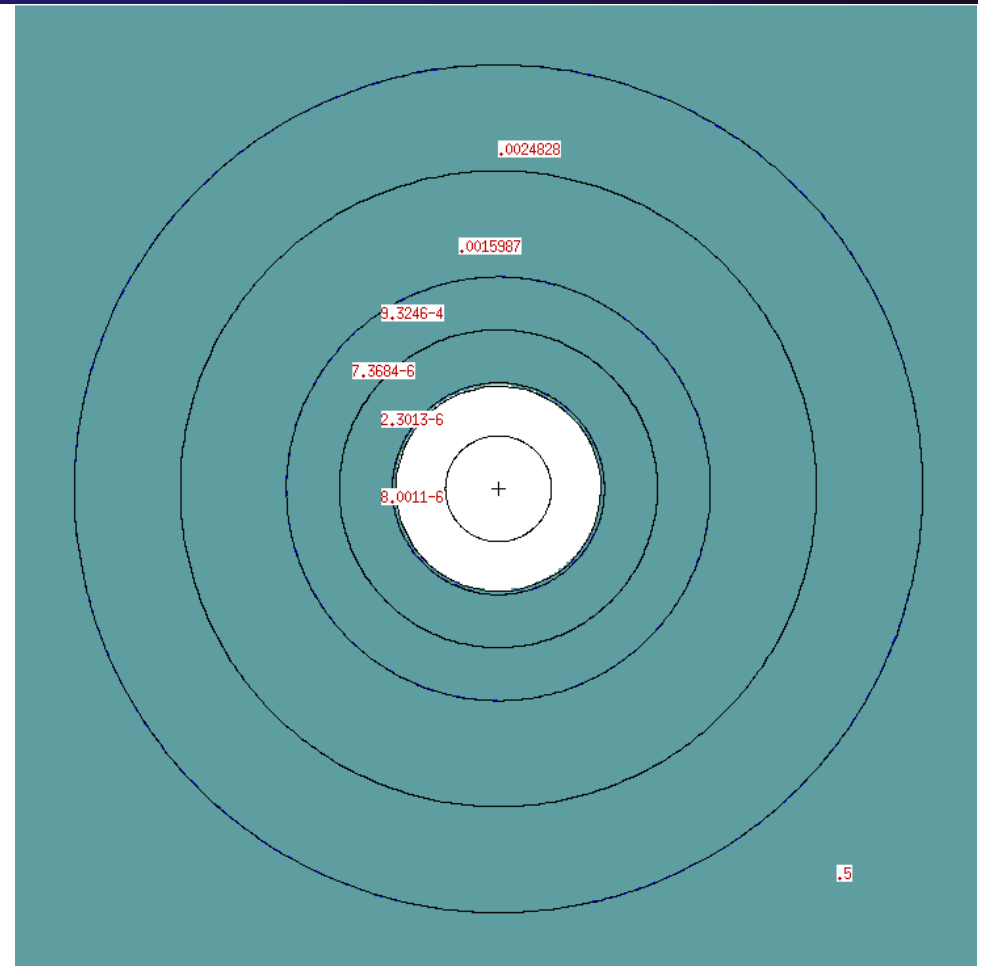
**0th and 1st 1e5, 2nd 1e6, 3rd 1e7
0th passed? 3rd passed – mean is higher!!!**

Case	Mean	Relative Error	VOV	Slope	FOM
ex2	1.4589E-11	0.0049	0.0305	3.3	449
ex6	1.4111E-11	0.0219	0.0413	3.2	840
ex6a	1.4732E-11	0.0328	0.0785	2.7	1112
ex6b	1.5344E-11	0.0248	0.2609	2.6	180
ex6c	1.4877E-11	0.0052	0.0116	4.3	416

ex6/ex1-1 = -4.68%
ex6a/ex1-1 < +/-1%
ex6b/ex1-1 = 3.65%
ex6c/ex1-1 < +/-1%

Examine WWs

- WW's varied by 2 orders of magnitude in certain regions
 - Inefficient?



Better WVs? (ex7-7c)

```
dxt:n 0 0 1524000 310 310
      0 0 1524000 620 620
      0 0 1524000 1240 1240
dd1 -4.5e-7 1e4 -1.79e-6 1e4 -7.2e-6 1e4
wwp:n 4j -1
wwg 2 0
mesh geom=sph ref=-100000 0 1524000
      origin 0 0 1524000
      axs=1 0 0 vec=0 1 0
      imesh 311 621 1241 1e4 1e5 1e6
      1600000
      iints 1 6 5 9 9 9 15
      jmesh 0.5 jint 1 kmesh 1 kints 1
```

Case	Mean	Relative Error	VOV	Slope	FOM
ex6c	1.4877E-11	0.0052	0.0116	4.3	416
ex7	1.4111E-11	0.0219	0.0413	3.2	862
ex7a	1.4691E-11	0.0178	0.0309	3	2597
ex7b	1.5004E-11	0.0085	0.1455	2.8	1100
ex7c	1.4914E-11	0.0023	0.0097	3.3	1502

FOM went up!

$$\text{ex7/ex1-1} = -4.68\%$$

$$\text{ex7a/ex1-1} < +/-1\%$$

$$\text{ex7b/ex1-1} = 1.35\%$$

$$\text{ex7c/ex1-1} < +/-1\%$$

What about 6 spheres? (ex8-8d)

```

dxt:n 0 0 1524000 310 310
      0 0 1524000 700 700
      0 0 1524000 1560 1560
      0 0 1524000 3400 3400
      0 0 1524000 7500 7500
      0 0 1524000 16000 16000 1e-2 1e-7
dd1   -4.50E-07 1e4 -2.30E-06 1e4
      -1.14E-05 1e4 -5.40E-05 1e4
      -2.60E-04 1e4 -1.23E-03 1e4
wwp:n 4j -1
wwg 2 0
mesh  geom=sph ref=-100000 0 1524000
      origin 0 0 1524000
      axs=1 0 0 vec=0 1 0
      imesh 311 621 1241 1e4 1e5 1e6
      1600000
      iints 1 6 5 9 9 9 15
      jmesh 0.5 jints 1
      kmesh 1 kints 1

```

Is this a bad idea?

Case	Mean	Relative Error	VOV	Slope	FOM
ex7c	1.4914E-11	0.0023	0.0097	3.3	1502
ex8	1.4781E-11	0.0208	0.3914	3.2	500
ex8a	1.4659E-11	0.0200	0.4735	4.7	1015
ex8b	1.4857E-11	0.0200	0.4501	4.1	1035
ex8c	1.4849E-11	0.0066	0.1137	2.2	910
ex8d	1.4860E-11	0.0023	0.0236	1.7	785

**0th, 1st and 2nd 1e5 histories,
3rd 1e6 histories, 4th 1e7 histories**

ex8/ex1-1 < +/-1%
ex8a/ex1-1 < +/-1%
ex8b/ex1-1 < +/-1%
ex8c/ex1-1 < +/-1%
ex8d/ex1-1 < +/-1%

Use a point detector to generate WWs? (ex9-9d)

```

dxt:n 0 0 1524000 310 310
      0 0 1524000 700 700
      0 0 1524000 1560 1560
      0 0 1524000 3400 3400
      0 0 1524000 7500 7500
      0 0 1524000 16000 16000 1e-2 1e-7
dd1   -4.50E-07 1e4 -2.30E-06 1e4
      -1.14E-05 1e4 -5.40E-05 1e4
      -2.60E-04 1e4 -1.23E-03 1e4
f5:n 0 0 1524000 1
wwp:n 4j -1
wwg 5 0
mesh  geom=sph ref=-100000 0 1524000
      origin 0 0 1524000
      axs=1 0 0 vec=0 1 0
      imesh 311 621 1241 1e4 1e5 1e6
      1600000
      iints 1 6 5 9 9 9 15
      jmesh 0.5 jint 1
      kmesh 1 kints 1
    
```

Case	Mean	Relative Error	VOV	Slope	FOM
ex7c	1.4914E-11	0.0023	0.0097	3.3	1502
ex9	1.4410E-11	0.0122	0.0061	5.7	1178
ex9a	1.4699E-11	0.0157	0.1940	4.7	1412
ex9b	1.4256E-11	0.0186	0.4387	3.4	1021
ex9c	1.4824E-11	0.0061	0.1463	2.3	967
ex9d	1.4997E-11	0.0044	0.1327	1.7	182

Hmmmm?

$ex9/ex1-1 < -2.66\%$
 $ex9a/ex1-1 < +/-1\%$
 $ex9b/ex1-1 < 3.70\%$
 $ex9c/ex1-1 < 0.14\%$
 $ex9d/ex1-1 < 1.3\%$

What is going on

- **A 14 MeV neutron has a MFP of ~770 m at 50,000 ft; therefore the source placement was less than 2 MFP's from the tally**
 - As a result of distance, solid angle from source to tally was still really small
- **Sampling enough histories eventually resulted in sampling a collision in the vicinity of the DXTRAN sphere, which caused a larger weight score (view factor close to 1) that spiked the VOV and reduced the slope**
- **In cases ex6 and ex7, particles were pushed closer to the DXTRAN sphere as a result of splitting through the weight window**
 - Collisions cannot be guaranteed as a result of WW splitting; and therefore due to large MFP of the air in the vicinity of the DXTRAN sphere, a particle will only rarely collide and contribute to the surface tally

Use fcl? (ex10-10d)

```

dxt:n 0 0 1524000 310 310
      0 0 1524000 700 700
      0 0 1524000 1560 1560
      0 0 1524000 3400 3400
      0 0 1524000 7500 7500
      1e-2 1e-7
ddl   -4.50E-07 1e4 -2.30E-06 1e4
      -1.14E-05 1e4 -5.40E-05 1e4
      -2.60E-04 1e4
wwp:n j j j j -1 J J
wwg 1 0 j J J J J j
mesh  geom=sph ref=-100000 0 1524000
      origin 0 0 1524000
      axs=1 0 0 vec=0 1 0
      imesh 311 701 1561 3401 7501 16001
      1e5 1e6 1600000
      iints 1 6 6 6 6 9 9 9 15
      jmesh 0.5 jint 1
      kmesh 1 kints 1
  
```

Case	Mean	Relative Error	VOV	Slope	FOM
ex7c	1.4914E-11	0.0023	0.0097	3.3	1502
ex10	1.4742E-11	0.0144	0.0114	5.5	828
ex10a	1.4763E-11	0.0120	0.0045	5.7	1403
ex10b	1.4838E-11	0.0119	0.0032	10	1420
ex10c	1.4889E-11	0.0038	0.0006	4.6	1384
ex10d	1.4878E-11	0.0012	0.0004	3.1	1344

ex10n/ex1-1 < +/-1%

902 32 -1.991E-04 901 -902 imp:n=1 fcl:n=0.7
 903 32 -1.991E-04 902 -903 imp:n=1 fcl:n=0.8
 904 32 -1.991E-04 903 -904 imp:n=1 fcl:n=0.9
 905 32 -1.991E-04 904 -905 imp:n=1 fcl:n=1

VOV not decreasing by 1/N for ex10a and ex10d; however, this may be to small VOV.

Conclusions

- **At 50,000 ft, the areal density is ~20 g/cm²**
 - Within buildup region → $1.48E-11 * 4 * \pi * r^2 = \sim 1.86 \text{ n}$ → 1-D model had **~1.86 n** at ~20 g/cm²
- **DXTRAN requires weight window bounds**
 - Setting dwc1 to the mean and dwc2 to 10% of mean sped up by a factor of 2.75
 - DD cards roulette in transmission
 - Called before dwc's or WW's
 - May help set different weight bounds for different spheres, but may not help so significantly if few MFP's away
- **1 DXTRAN resulted in “false” convergence – but was within <2%**
- **Nested spheres benefit from WW's if spheres are spaced far enough**
 - If chosen strategically WW's can speed calculation by a factor of 3-4
- **Forced collision biasing in the vicinity of the DXTRAN sphere **may** be useful**
 - But running 3 spheres without fcl still outperformed 6 spheres with fcl
 - For many of the calculations that did not pass all 10 statistical checks the 1 std. confidence interval bounded the correctly converged result
- **What about $RI \neq R0$, or what about high survival weight?**

Future Work

```

dxt:n 0 0 1524000 310 1e3
      0 0 1524000 5e3 1e4 1.0e-2 1e-6
dd1
  -4.7e-6 1e4
  -4.7e-4 1e4
mesh geom=sph ref=-100000 0 1524000
  origin 0 0 1524000
  axs=1 0 0 vec=0 1 0
  imesh 311 1001 10001 1e5 1e6 1.6e7
  iints 1 6 9 9 9 15
  jmesh 0.5 jints 1
  kmesh 1 kints 1
  
```

Case	Mean	Relative Error	VOV	Slope	FOM
ex40	1.4786E-11	0.0039	0.0191	6.9	855
ex43	1.4816E-11	0.0109	0.0649	2.6	1000
ex43a	1.4958E-11	0.0121	0.1188	2.4	1849
ex43b	1.4914E-11	0.0042	0.0295	5.6	1461

ex40/ex1-1 < +/-1%

ex43b/ex1-1 < +/-1%

ex40, ex43, and ex43a used 1e6 histories
ex43b used 1e7 histories

If I choose dwc1=1e-5, performance increases by a factor of 4 but slope drops to 3.1 (f(x) seems like a good fit)... In ex40 and ex43, reported slope seems to be a bad fit when comparing to f(x).