Estimating the Mass of UO3 Powder in a Container Using MCNP-PoliMi Simulations of NMIS Measurements

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Abstract

- **The MCNP-PoliMi computer code was used to simulate NMIS measurements of a container using active interrogation with fast neutrons. Using two simulated reference measurements, three containers with unknown configurations of UO_3 powder were scanned with measurement times between 4 and 40 minutes. In every case, the estimate of the mass produced from the NMIS scan was within 3% of the true mass of UO_3 that was modeled inside of the container.**

Outline

- **Objective**
- **Fast Neutron Radiography**
- **Nuclear Materials Identification System**
- **MCNP-PoliMi**
- **Model Setup**

Outline

- **Methodology**
- **Results**
- **Uncertainty Analysis**
- **Sources of Error**
- **Conclusions**

Objective

- **Given a (simulated) stainless steel container of known geometry, determine the mass of highly enriched Uranium Trioxide (UO_3) powder inside of the container. The enrichment of the powder is assumed to be a constant 93.15 wt%.**

Fast Neutron Radiography

- **Since the geometry of the container is known, the mass of the powder can be estimated by mapping the density of the powder and multiplying it by the volume.**
- **In high Z materials, such as the Uranium Trioxide, high energy neutrons have excellent penetration power and are thus well suited for transmission measurements.**
- **By measuring the attenuation through the target at several locations, the density, and thus the mass, can be estimated.**

Fast Neutron Radiography

- **In an ideal case (narrow beam, small detector dimensions), the attenuation of neutrons is governed by:**

$$\frac{I}{I_0} = e^{-\Sigma_t x}$$

- **Unfortunately, in most real-world applications, the geometry is far from ideal.**
- **Neutrons may scatter several times before reaching the detectors, which reduces the effective attenuation.**

Enter the NMIS

- **The Nuclear Materials Identification System (NMIS) reduces the effects of scattering in two ways:**
  - **Electronically collimate the neutrons so that only the ones that are heading in the desired direction are considered.**
  - **Measure the time of flight of the neutrons to detectors, so that only those that arrive in a time window corresponding to uncollided neutrons are considered.**

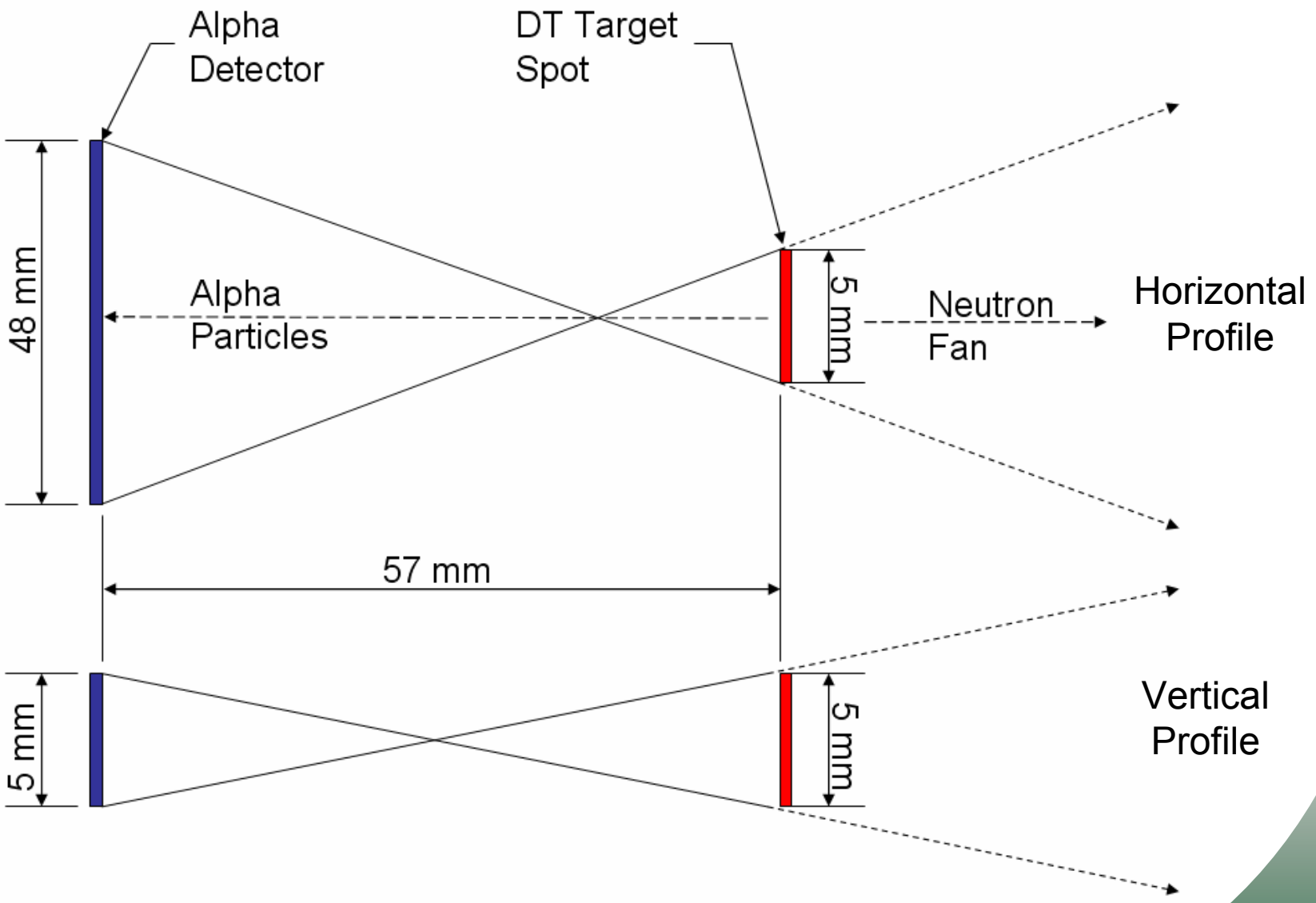
NMIS – DT Generator

- **Neutrons are generated using the reaction:**

$$^{3}\mathrm{H} + {}^{2}\mathrm{H} \rightarrow {}^{4}\mathrm{He} + \mathrm{n} + 17.6\ \mathrm{MeV}$$

- **Because there are only two products, they are monoenergetic and travel away back-to-back.**
- **The neutrons have an energy of 14.1 MeV.**
- **An alpha detector defines a fan of neutrons traveling in the opposite direction.**

NMIS – DT Generator



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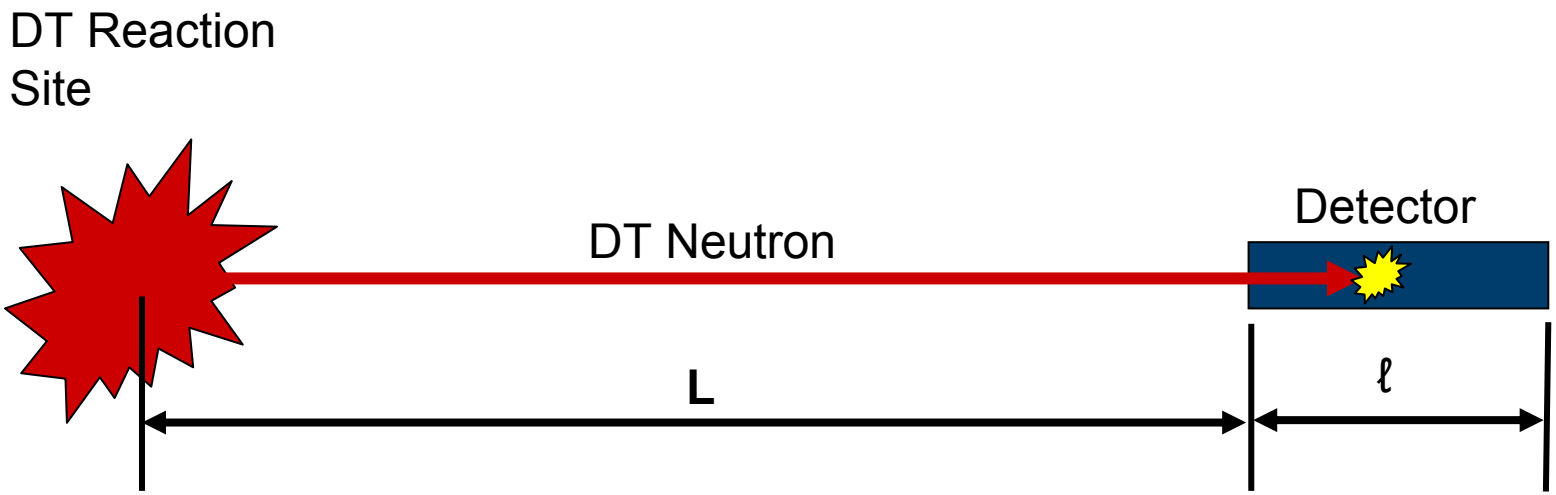
NMIS – Time of Flight measurements

- **Each time a pulse occurs in the alpha detector, the NMIS software records a start event.**
- **If a subsequent pulse is received from a neutron detector shortly thereafter, the time difference between the two pulses is recorded.**
- **Each of these correlations is recorded in a 1-ns time bin corresponding to the time difference between the two pulses.**
- **A plot of the number of correlations vs. time lag is a time correlation plot.**

NMIS – Time of Flight measurements

- **DT neutrons are monoenergetic. They all travel at approximately 5.1 cm/ns.**
- **Thus, DT neutrons that travel directly to the neutron detector should all arrive the same amount of time after the alpha pulse.**
- **These directly transmitted neutrons create a distinctive peak on a time correlation plot.**
- **Using only the correlations in this peak greatly reduces the effect of scattering on measured attenuation.**

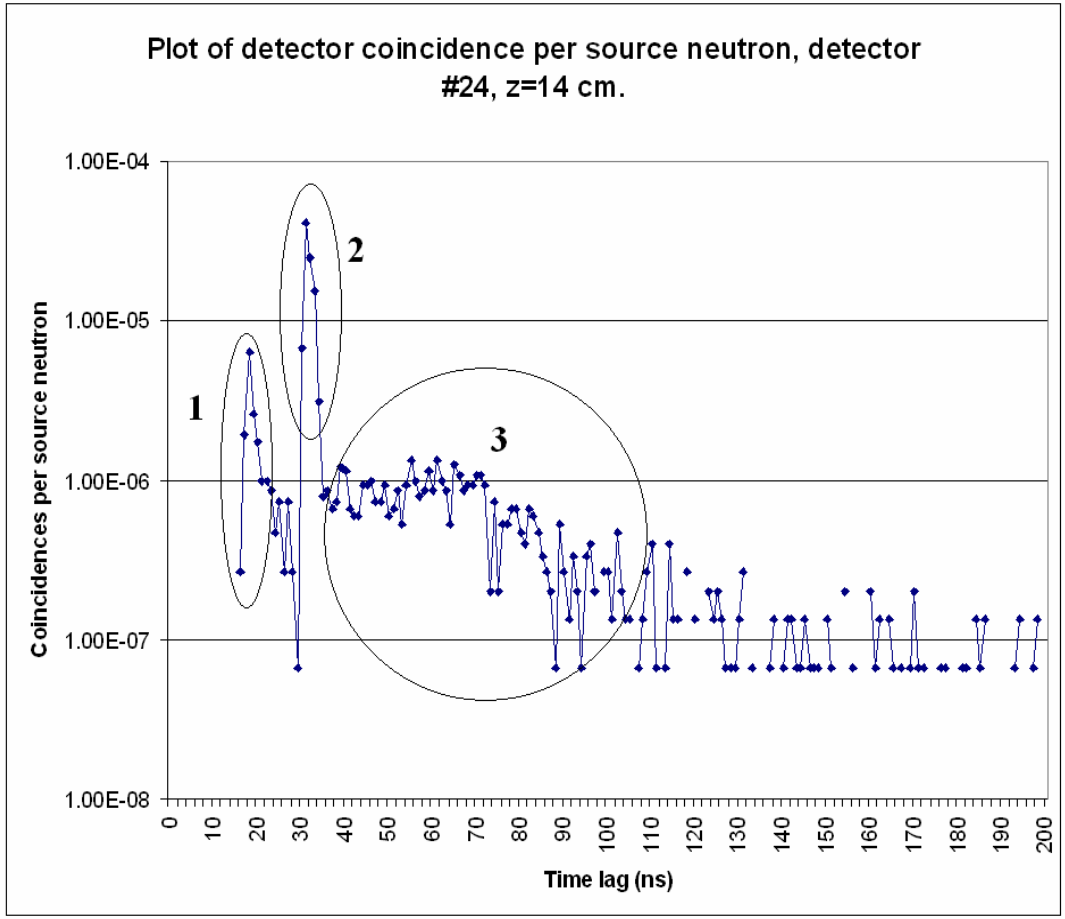
NMIS – Time of Flight measurements



$$\frac{v_n}{L} \leq t \leq \frac{v_n}{L+\ell}$$

NMIS - Correlation

- **Region 1 – Gamma rays from (n,f), (n,n'), and (n,γ) reactions in the target.**
- **Region 2 – Directly transmitted neutrons.**
- **Region 3 – Neutrons from (n,f), (n,n'), and (n,xn) reactions in the target.**



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NMIS - Correlation

- **For fast neutron radiography, the quantity of interest is the number of counts in peak 2.**
- **In order to compare the results of different measurement times, this quantity needs to be normalized:**

$$I = \frac{C}{N}$$

- **C is the total counts, and N is the number of source neutrons generated during the measurement.**

NMIS – Scanning Hardware

- **The DT generator is mounted on a mechanical scanning arm.**
- **An array of 24 fast plastic scintillators is mounted on the opposite side of the target to be scanned.**
- **Motors rotate the detectors horizontally or moves the detector array / DT generator assembly vertically.**

NMIS – Scanning Hardware

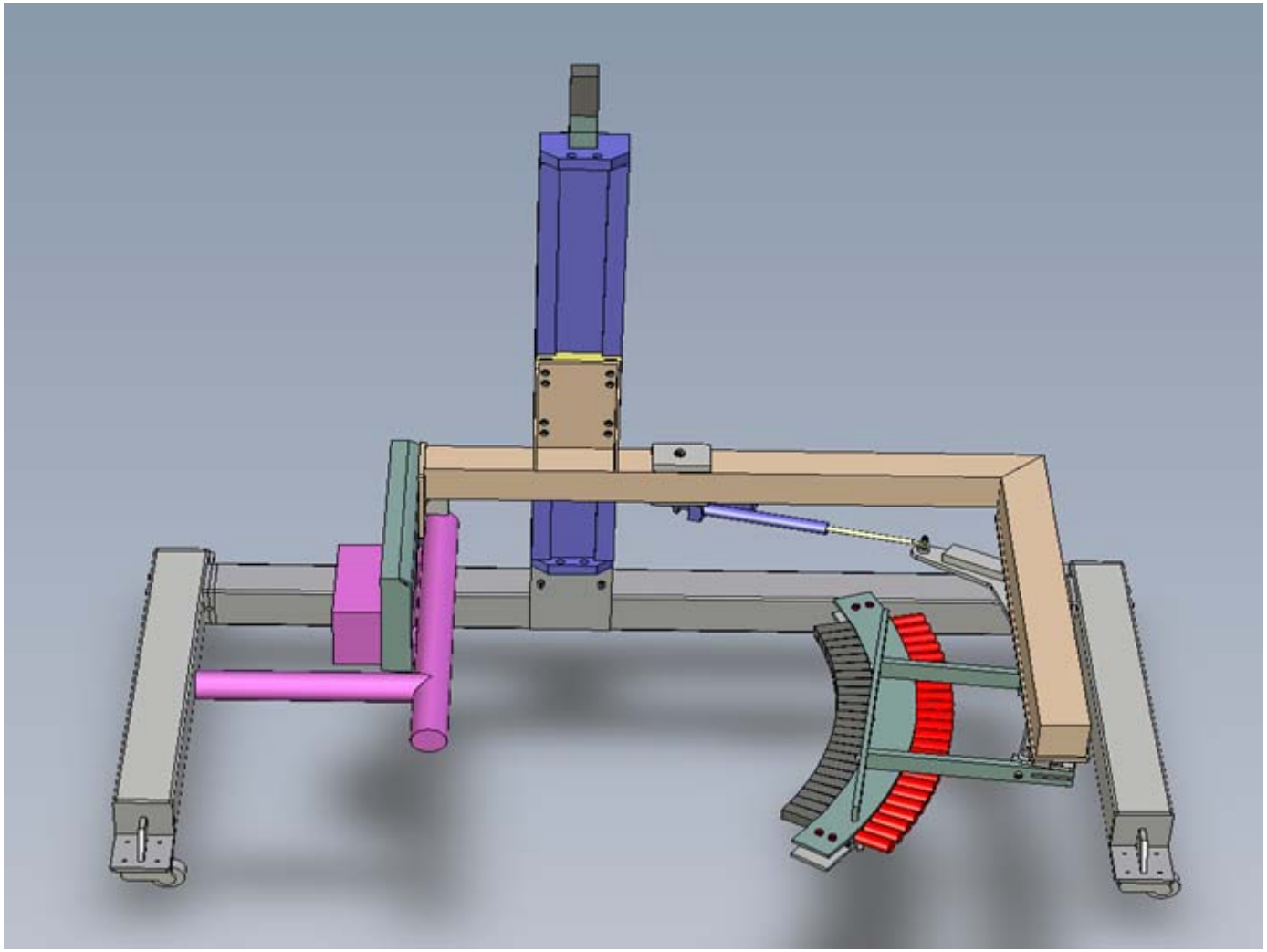


Image courtesy of J. Chesser, ORNL.

NMIS - Detectors

- **Twenty-four 1x1x6 in. Plastic Scintillators (BC-420).**
- **These detectors have a time resolution of ~ 1 ns.**
- **Detectors are sensitive to both gammas and neutrons.**
- **The detector thresholds are set high enough to eliminate the 186-keV gamma from ^{235}U.**

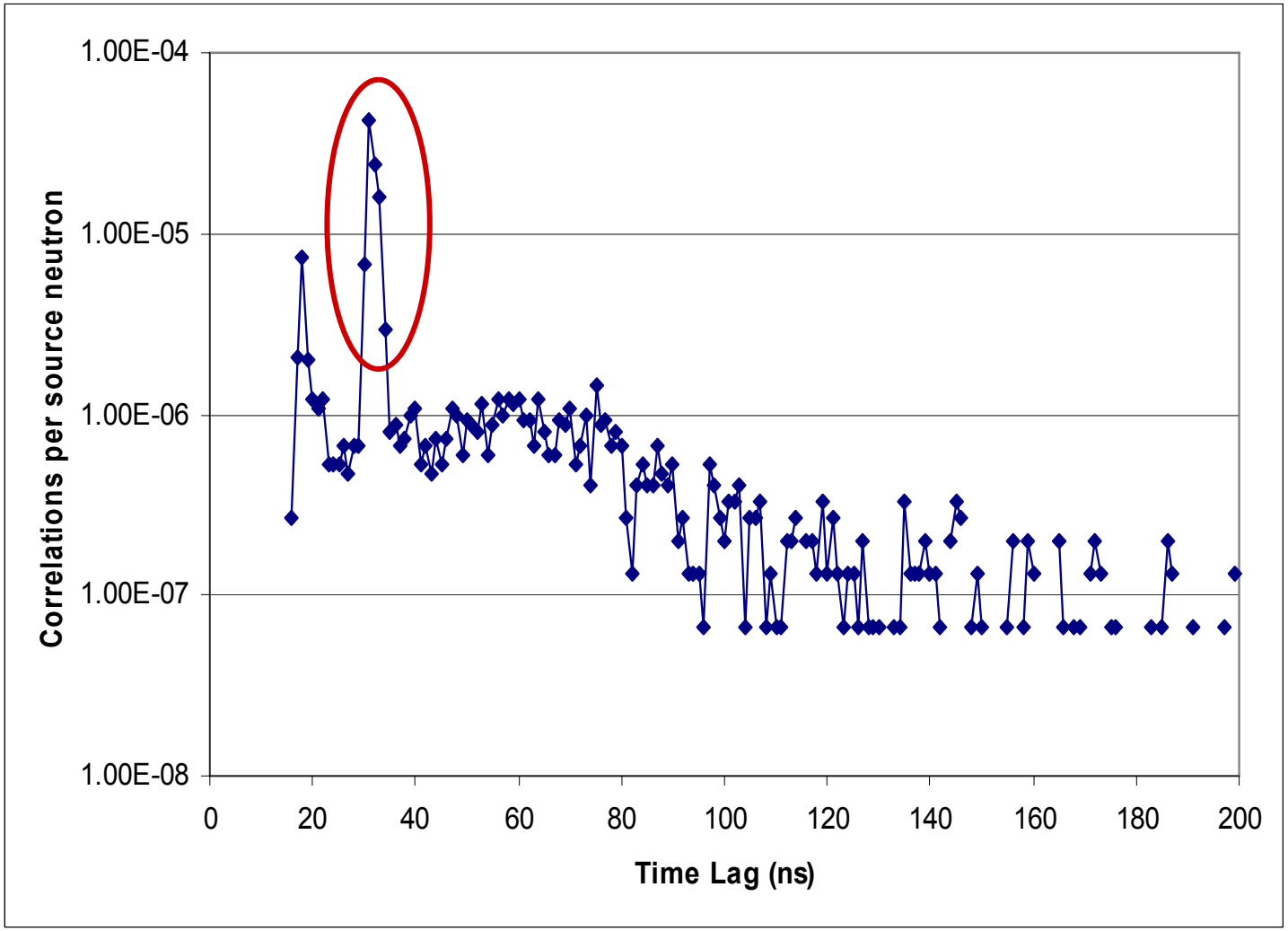
MCNP-PoliMi

- **Based on the MCNP-4c code**
- **Standard MCNP often approximates individual neutron-nucleus interactions**
  - **Produces accurate results when averaged over large numbers of collisions**
  - **Not suitable for simulating NMIS measurements, where each detector pulse is correlated back to a source event**
- **Runs in analog mode**
  - **No variance reduction techniques**

MCNP-PoliMi

- **The MCNP-PoliMi executable produces a file containing each collision in a detector cell.**
- **The output file records source particle number, type of particle, target nucleus, type of reaction, energy imparted, time of interaction, and other data.**
- **A post-processor then parses this file:**
  - **Did the collision impart enough energy to produce a pulse?**
  - **If so, a correlation is added to the time bin corresponding to the time difference between the source event and the detector pulse.**
  - **The final correlation data is output to a text file which can be imported into excel or Matlab for processing.**

MCNP-PoliMi - Output



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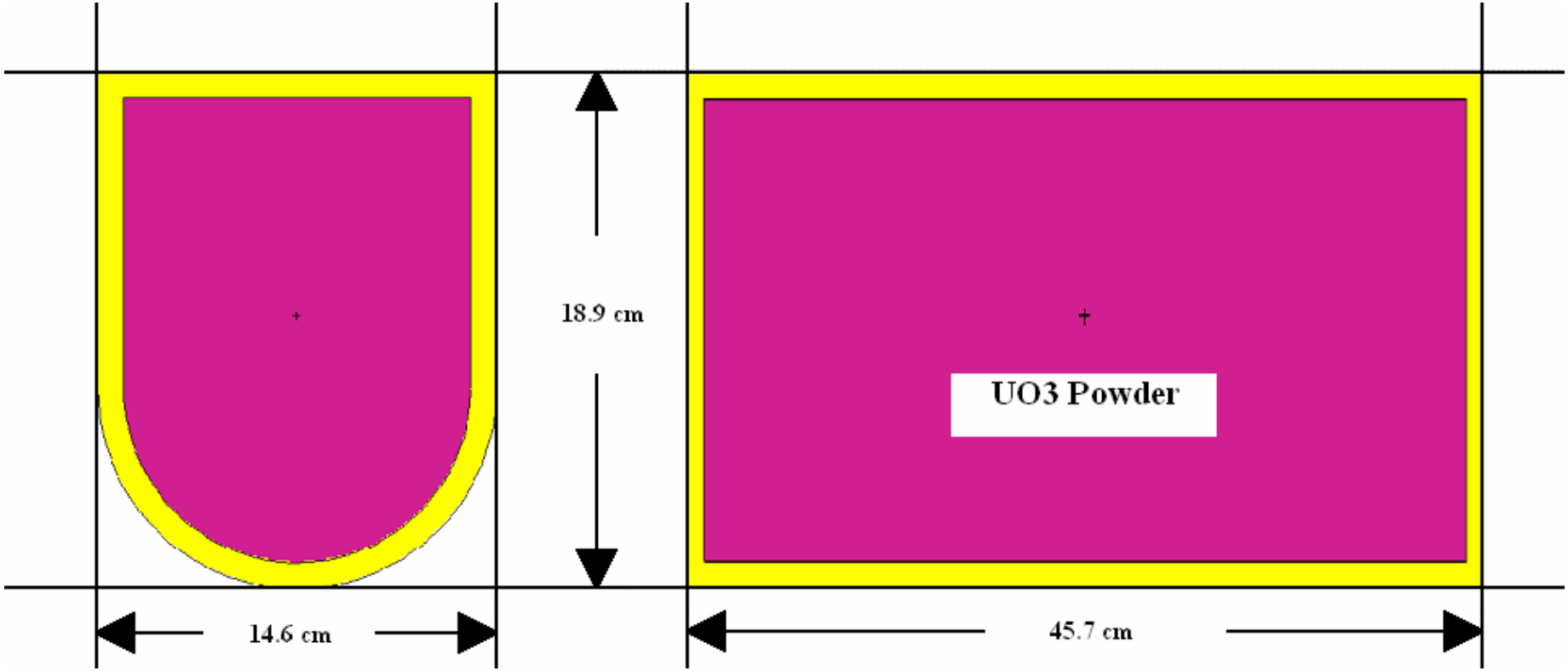
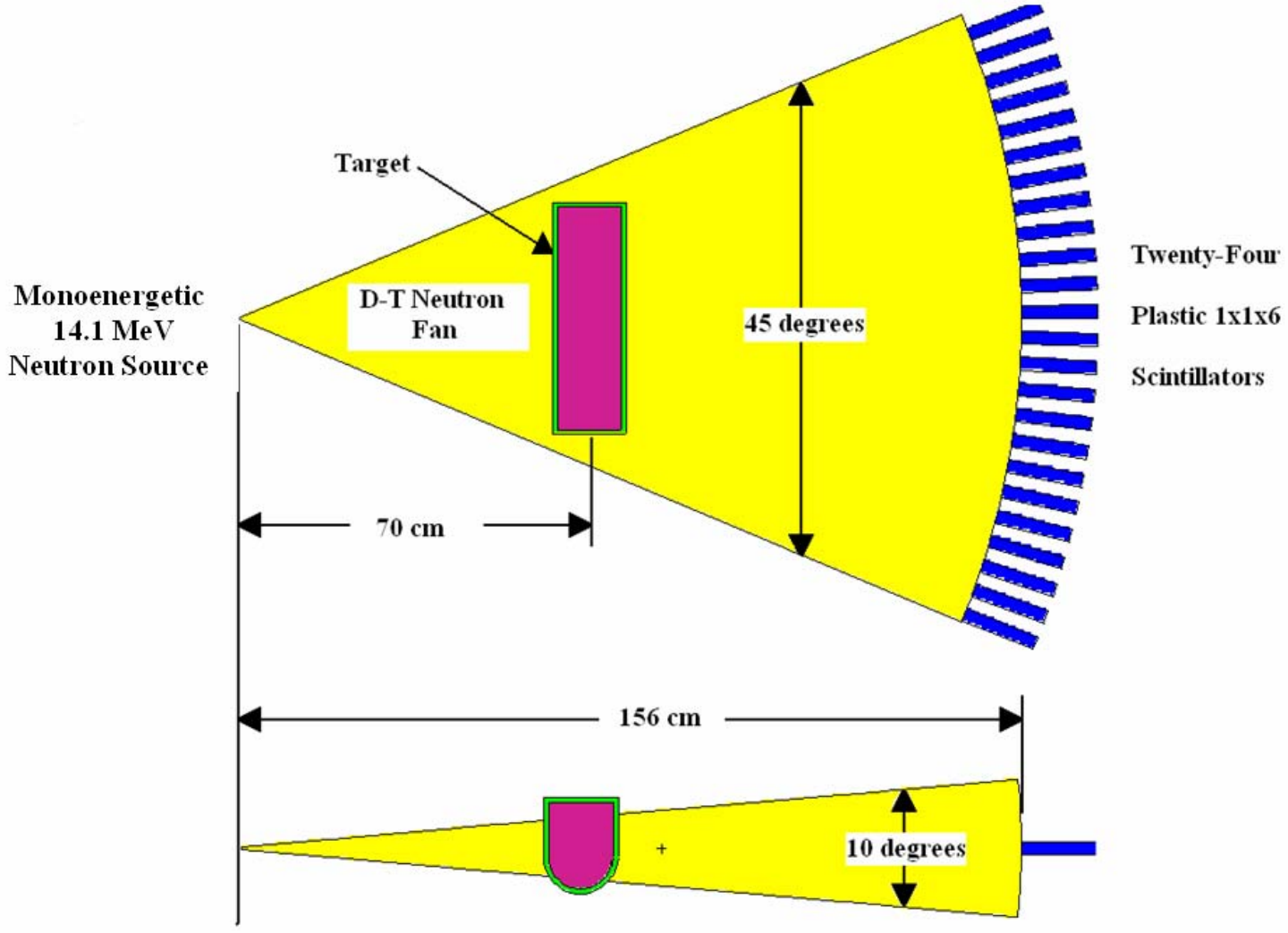
MCNP-PoliMi Model

- **In order to conduct a proper radiograph, the entire container area must be scanned.**
- **The container is divided into regions based on detector positions.**
- **48 detector positions along a horizontal arc, multiplied by 22 vertical slices = 1,056 pixels.**
- **The total number of correlations due to fast neutron transmission is measured for each pixel.**

MCNP-PoliMi Model - Container



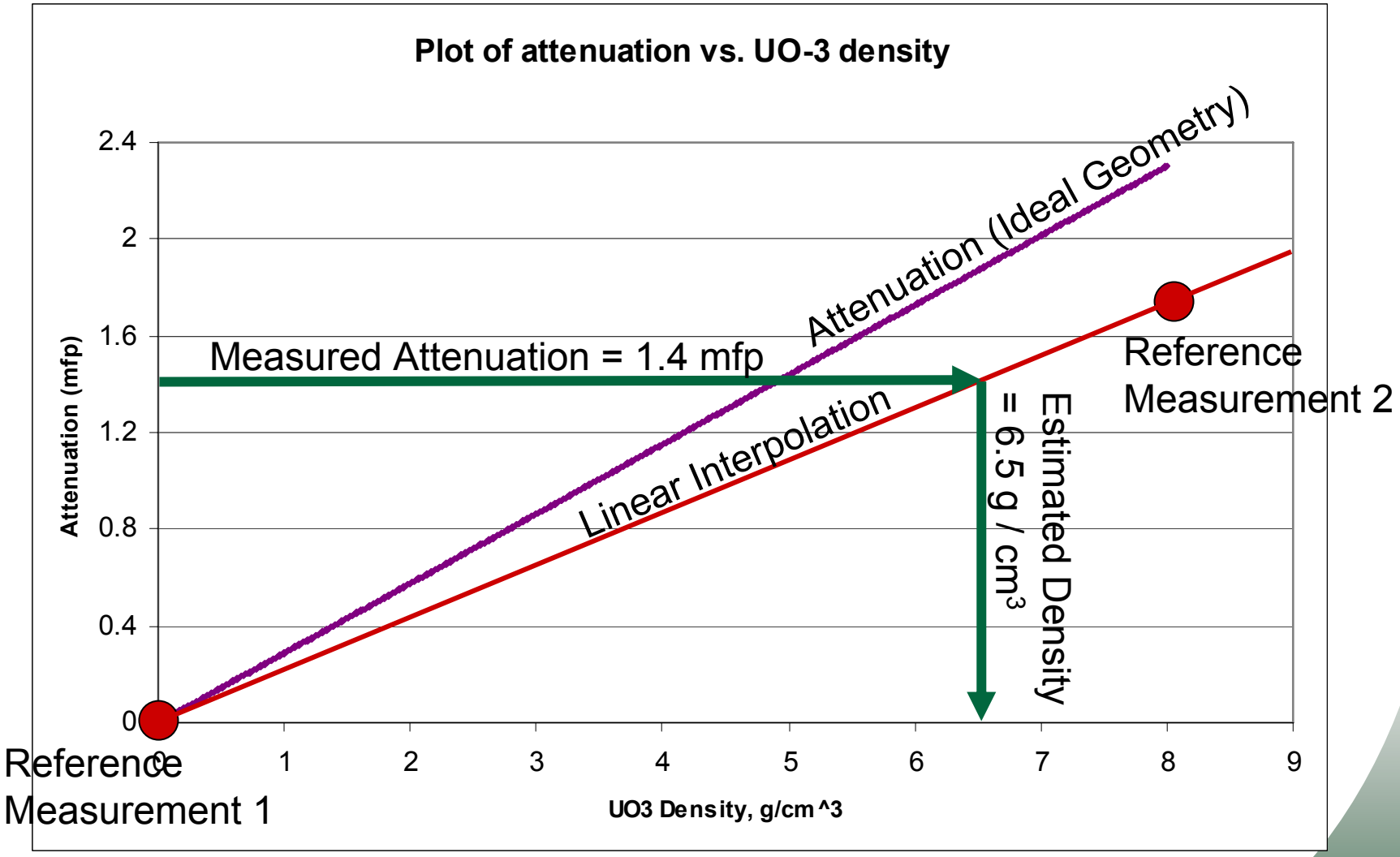
MCNP-PoliMi Model – Overall Geometry



Methodology - Assumptions

- **The geometry of the container is entirely known.**
- **The isotopic composition of the powder is entirely known.**
- **Before any unknown scans are conducted, two reference measurements are made:**
  - **Empty container 'I_0'.**
  - **Full container with known density profile 'I_8'.**
- **Measured neutron attenuation is exponential.**

Methodology



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Methodology

- **The slope of the interpolation line is computed using the formula:**

$$b_{i,j} = \frac{-\ln\left(\frac{I_8^{i,j}}{I_0^{i,j}}\right)}{\rho_8}$$

- **When an unknown 'I_U' is measured, the estimated density of that pixel is**

$$\rho_{i,j} = \frac{-\ln\left(\frac{I_U^{i,j}}{I_0^{i,j}}\right)}{-\ln\left(\frac{I_8^{i,j}}{I_0^{i,j}}\right)}\rho_8 = \frac{\ln\left(I_U^{i,j}\right)-\ln\left(I_0^{i,j}\right)}{\ln\left(I_8^{i,j}\right)-\ln\left(I_0^{i,j}\right)}\rho_8$$

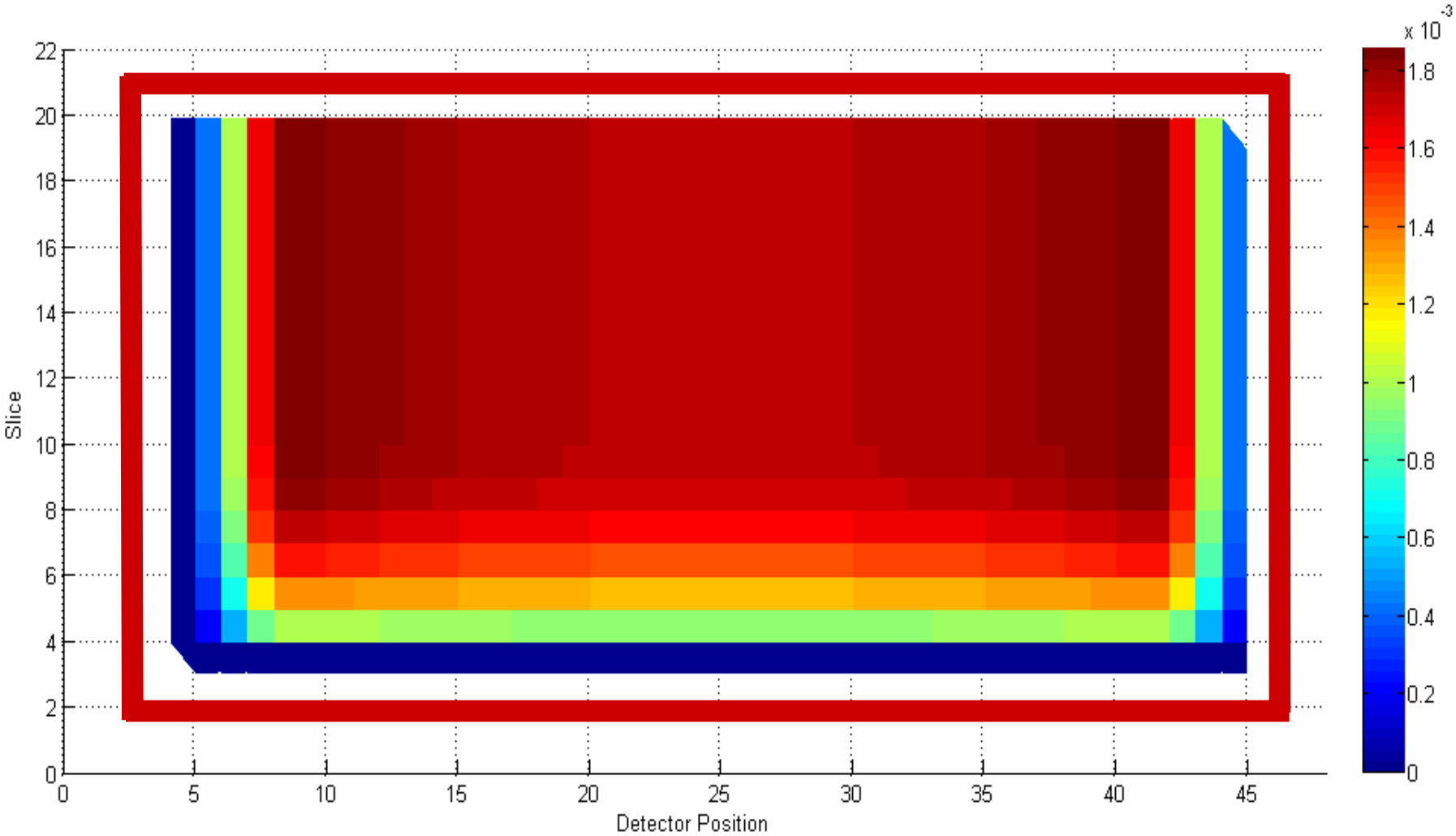
Methodology

- **The total mass of UO3 powder is then:**

$$M = \rho_8 \cdot V \sum_{i=1}^{22} \sum_{j=1}^{48} f_{i,j} \cdot \frac{\ln\left(I_U^{i,j}\right) - \ln\left(I_0^{i,j}\right)}{\ln\left(I_8^{i,j}\right) - \ln\left(I_0^{i,j}\right)}$$

- **$f_{i,j}$ is the normalized volume fraction of the container's interior belonging to pixel i,j.**

Pixel Map – Weighting ($f_{i,j}$)



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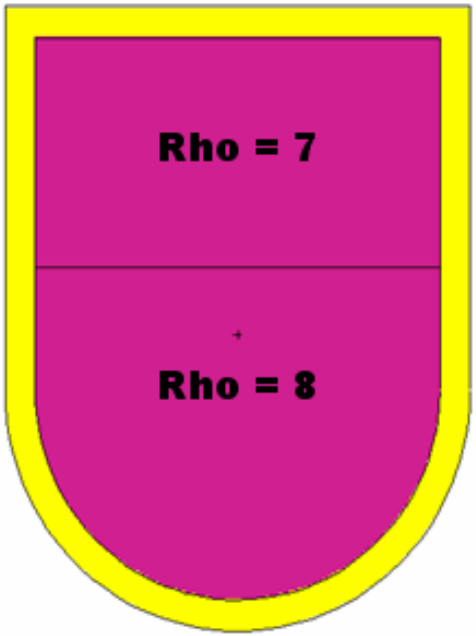
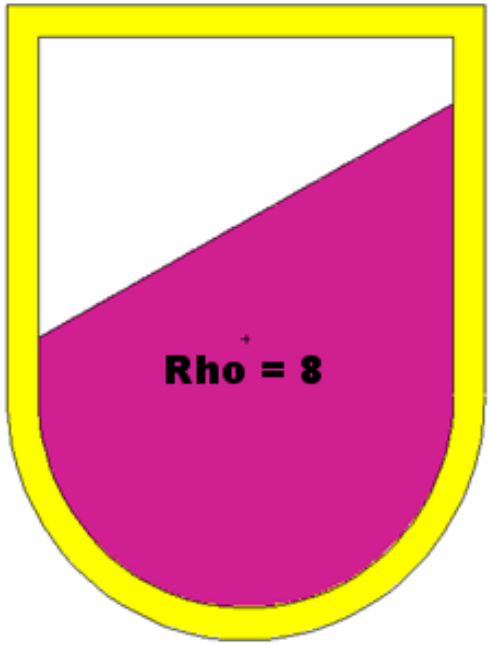
Unknowns

Test #1



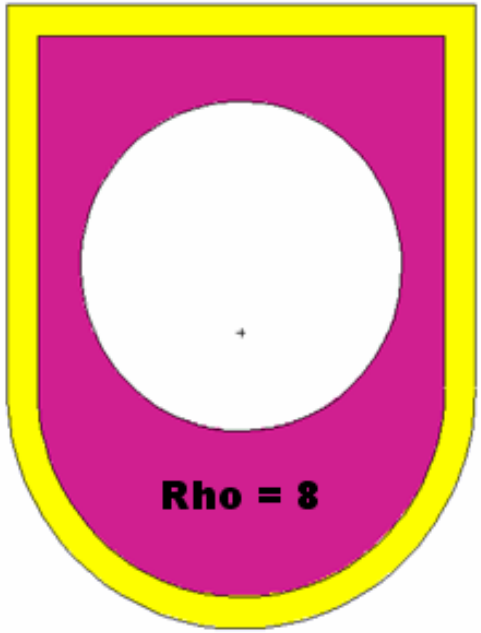
Layered

Test #2



Sloped

Test #3

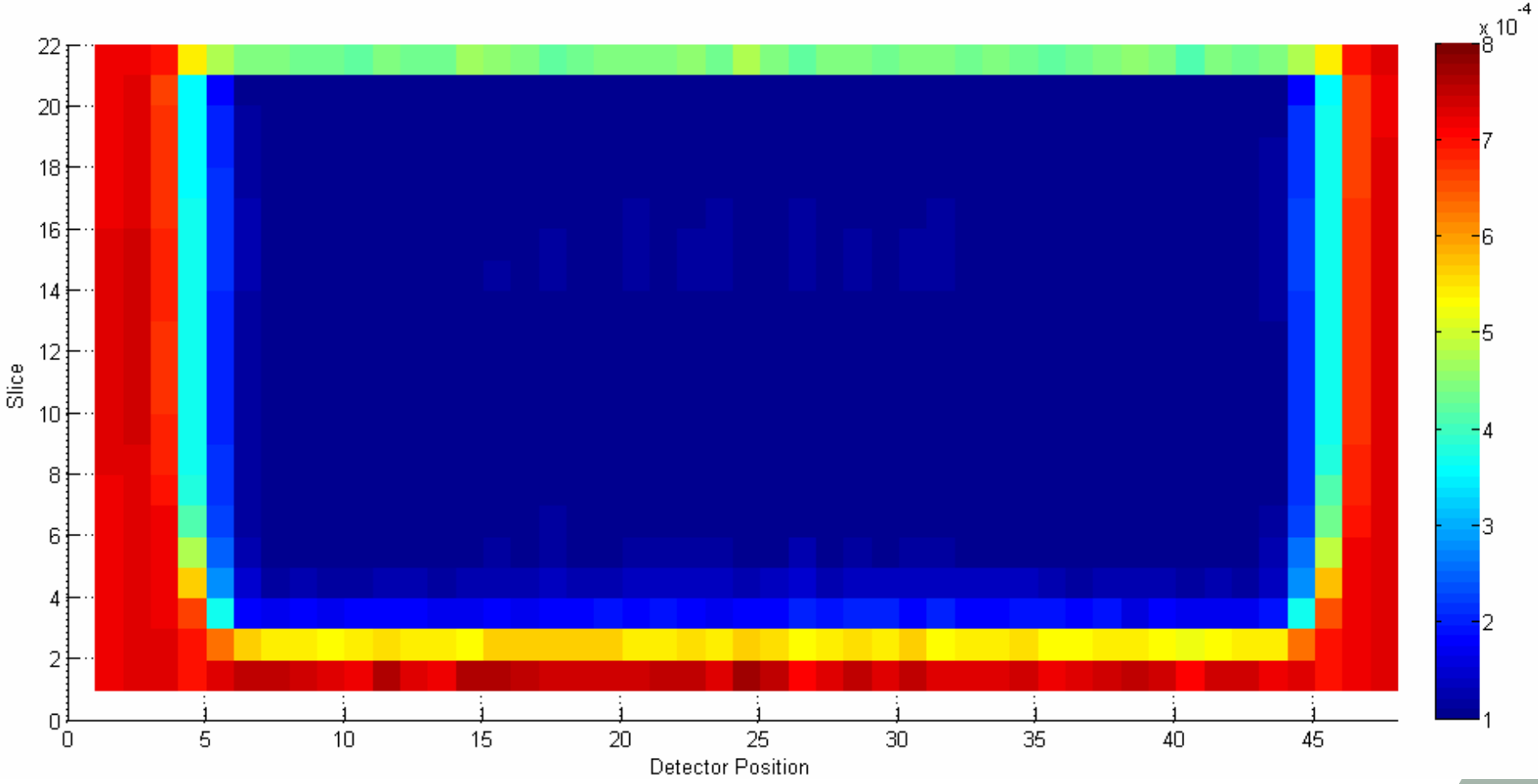


Bubble

Measurement Times

- **Assume the DT Generator produces $3x10^7$ neutrons per second isotropically, and the DT arc covers 0.35% of the total solid angle.**
- **Each NMIS sample is, by default, a multiple of 5.12 seconds.**
- **5.12 seconds x 44 samples = 3.75 minutes**
- **Three simulated measurement times:**
  - **'a' series: 1 loop per sample, time = 3.75 minutes**
  - **'b' series: 4 loops per sample, time = 15.0 minutes**
  - **'c' series: 10 loops per sample, time = 37.5 minutes**
- **Each simulation is designated by Unknown (number) and measurement time (letter), e.g., Case 1b**

Results – Case 1c Correlations



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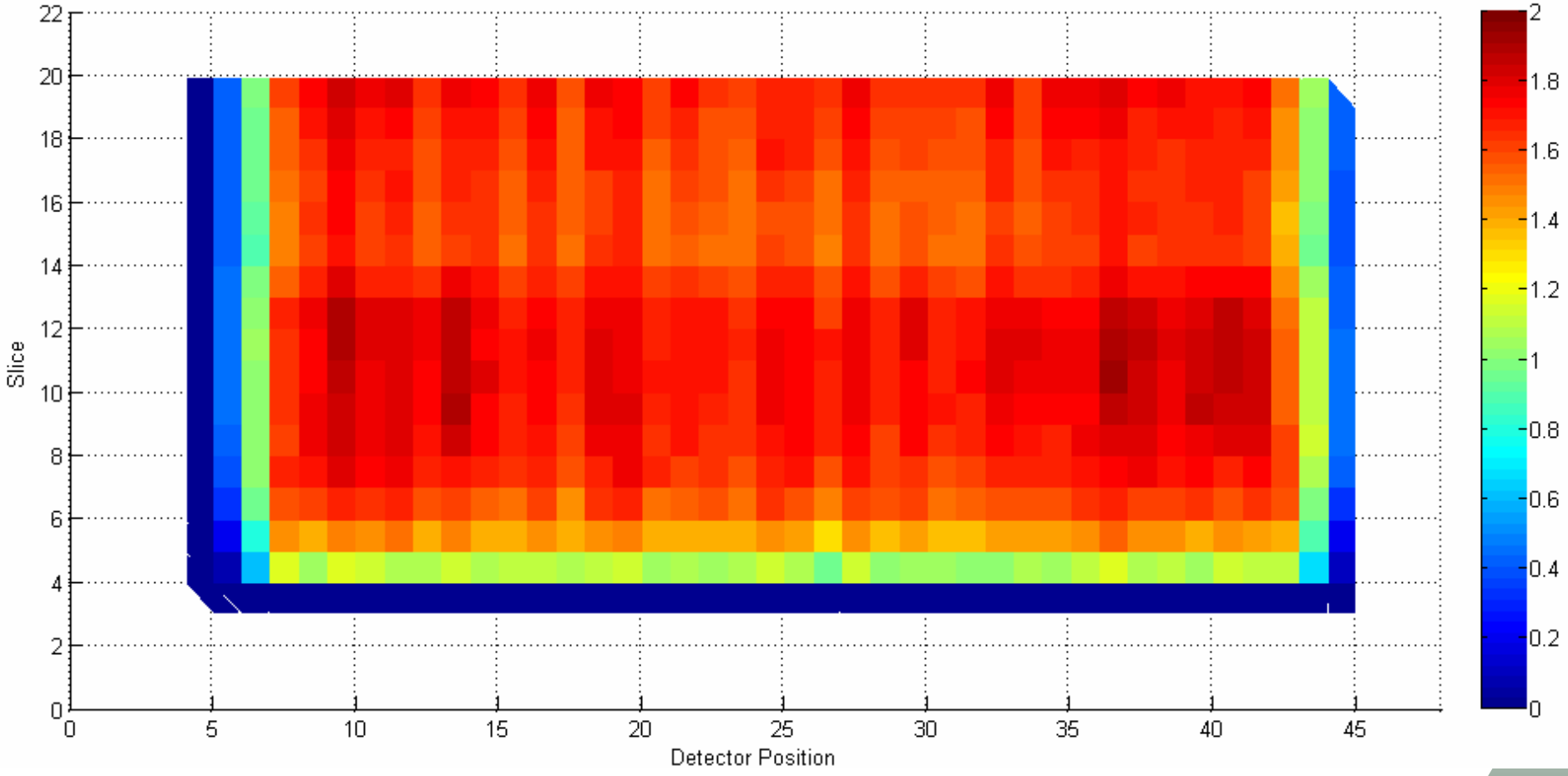
Results – Case 1c Attenuation



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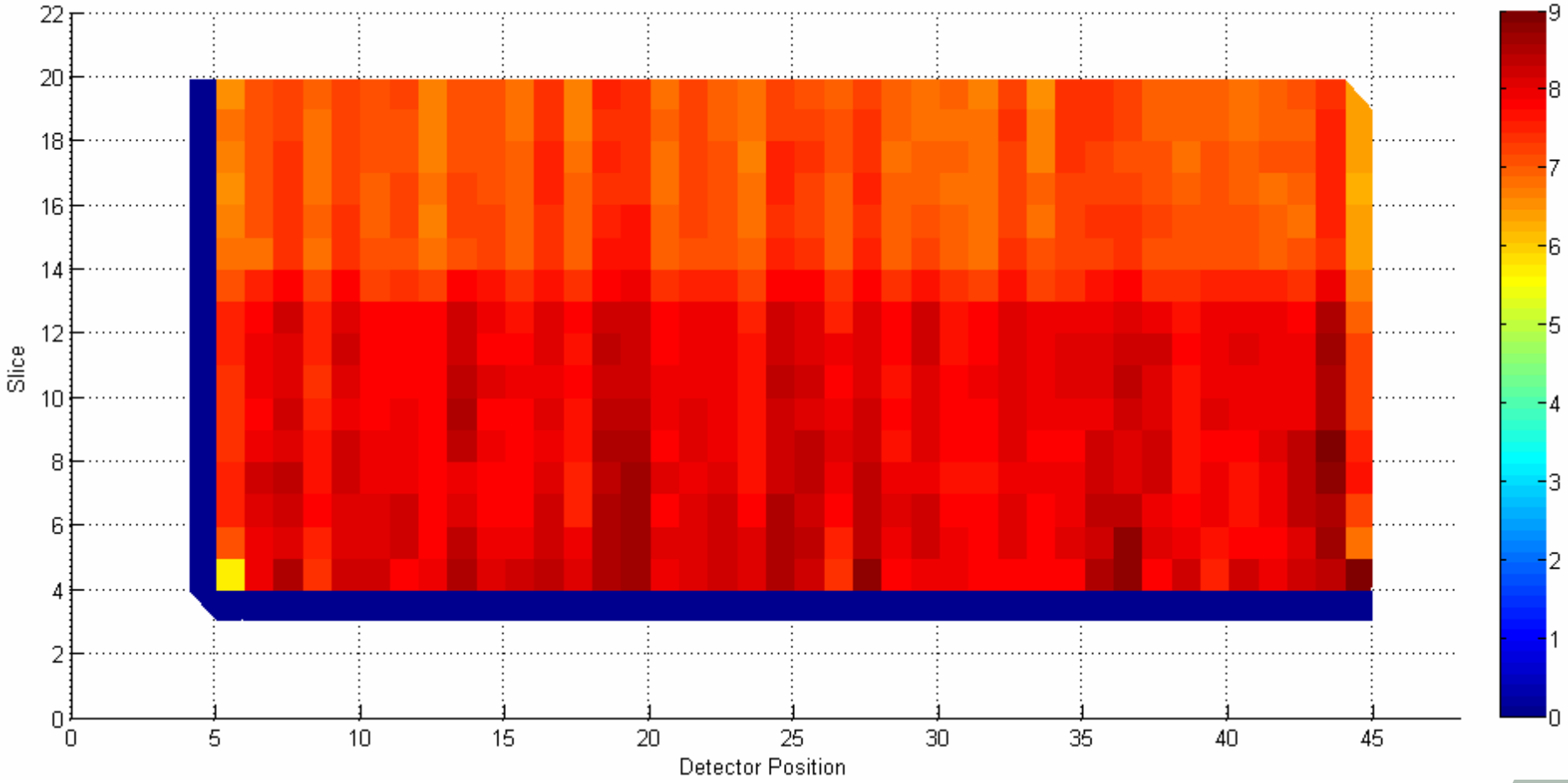
Results – Case 1c Density



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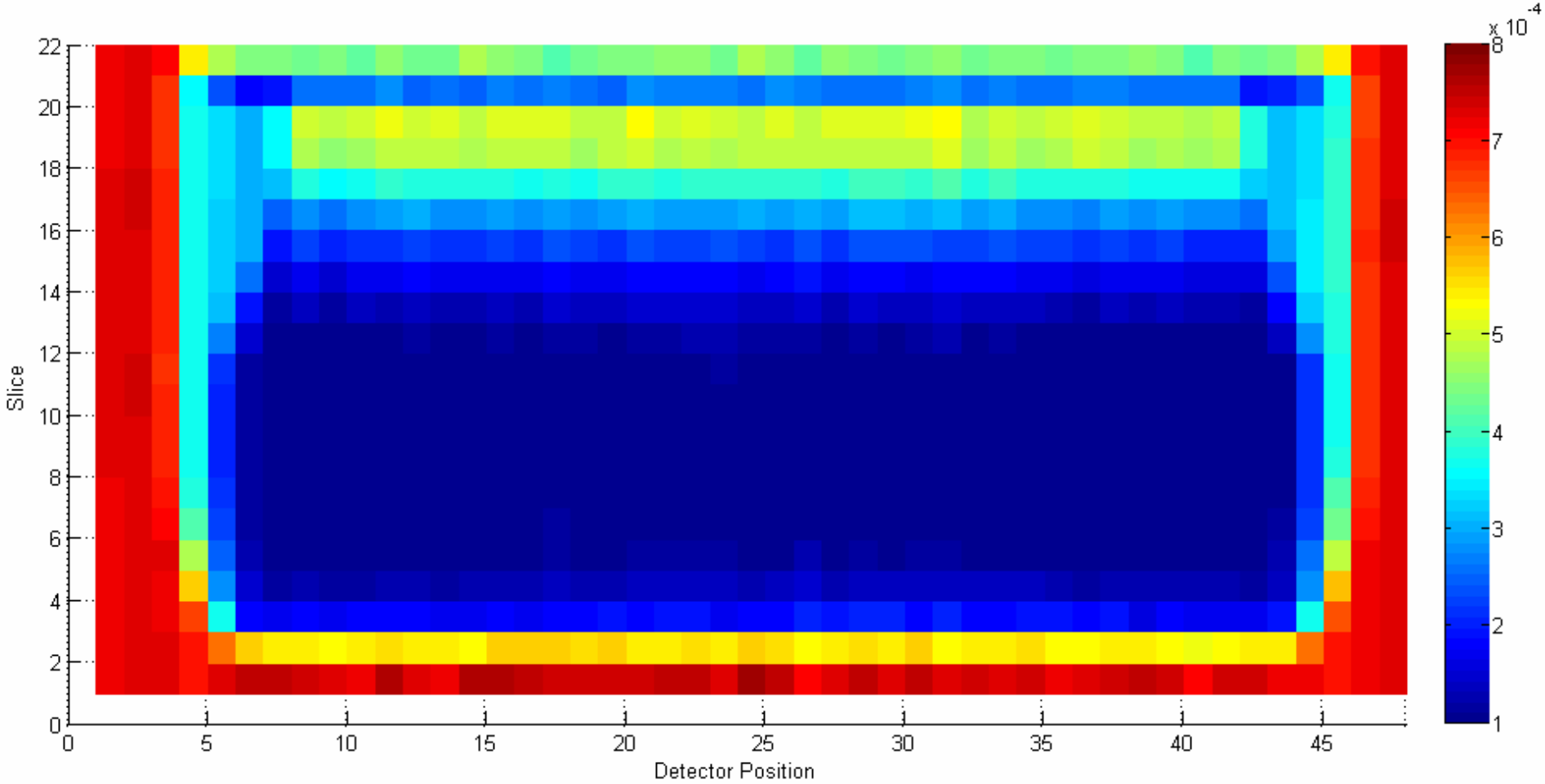
Results – Case 2c Correlations



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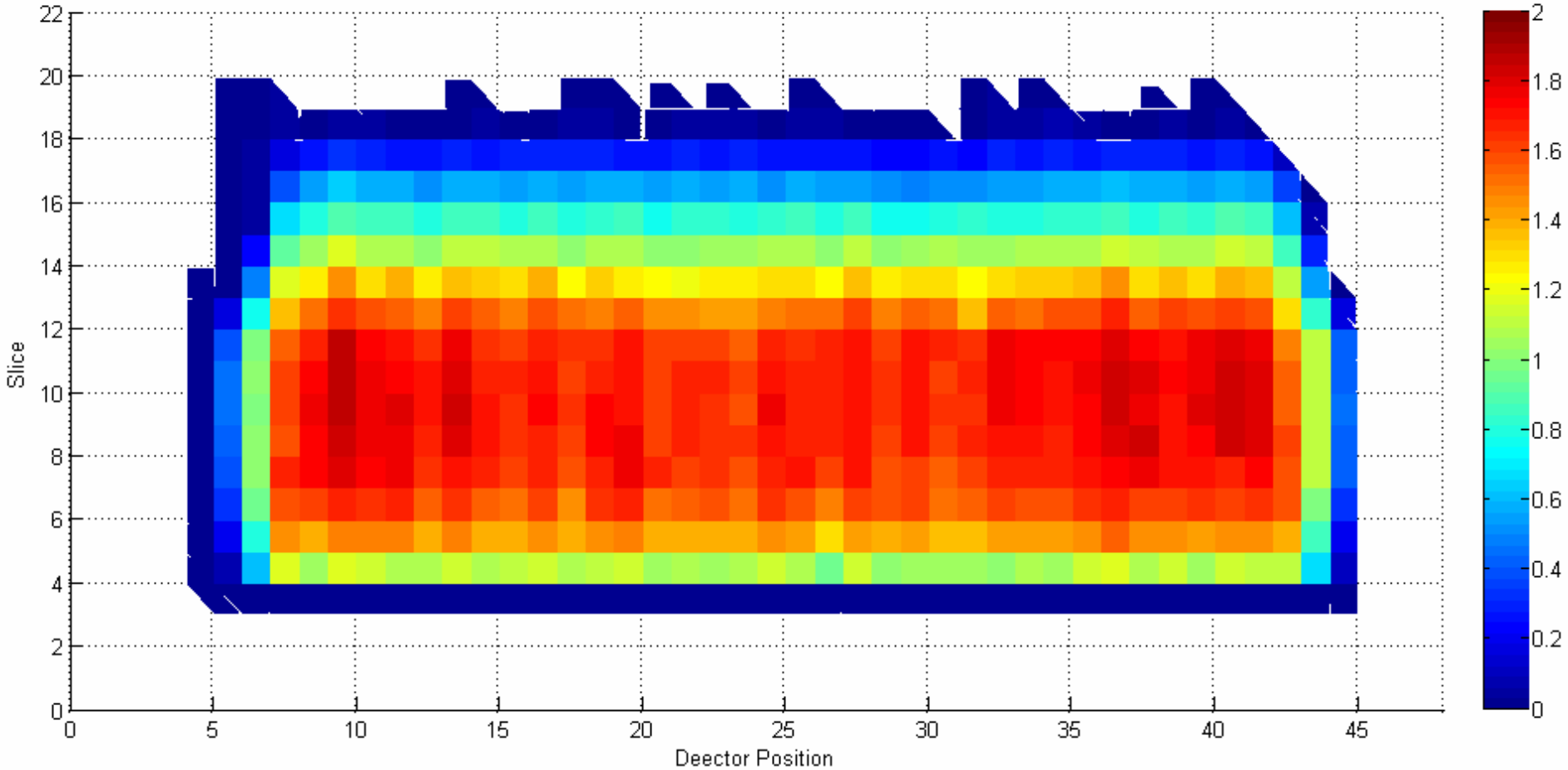
Results – Case 2c Attenuation



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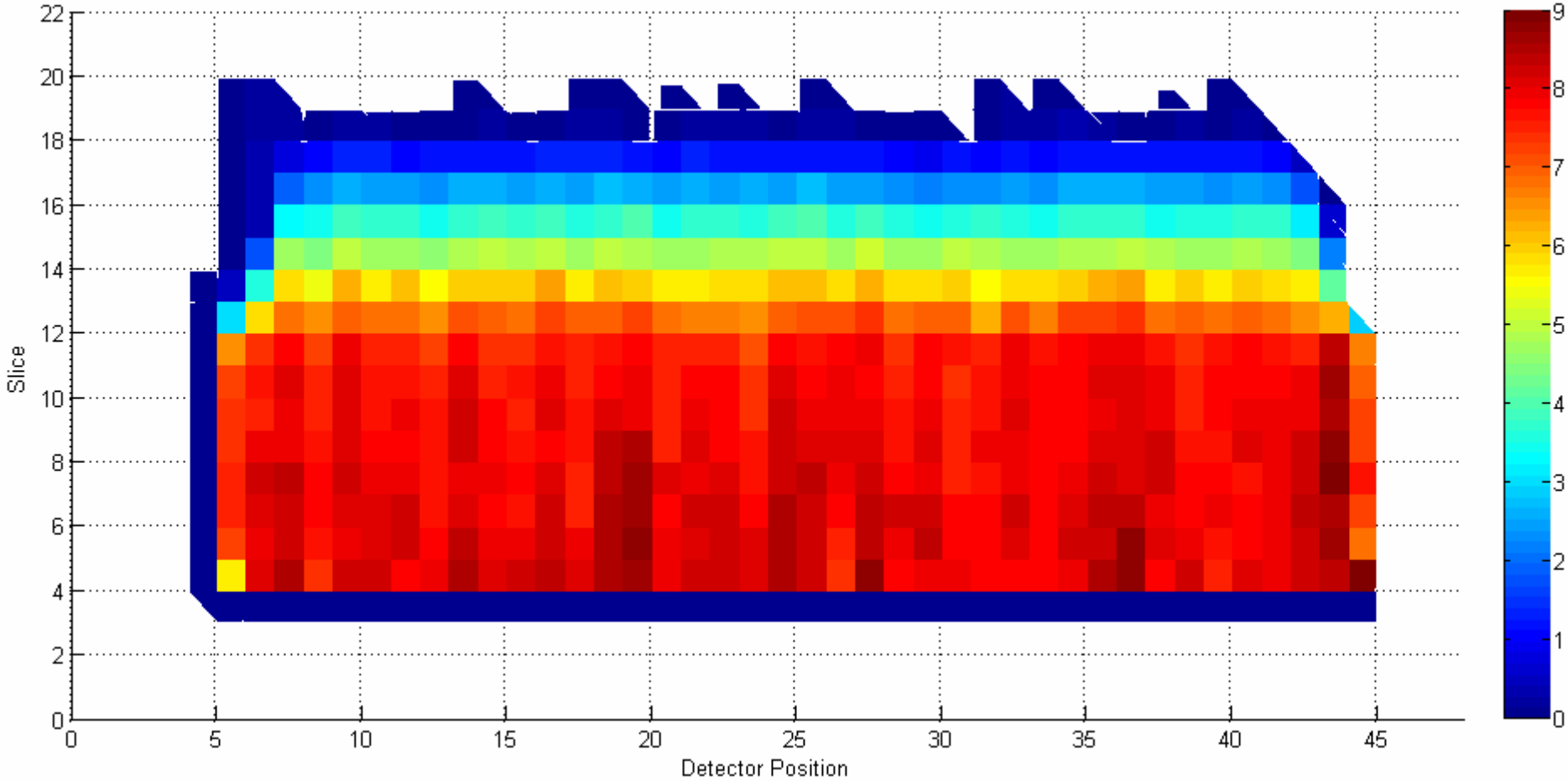
Results – Case 2c Density



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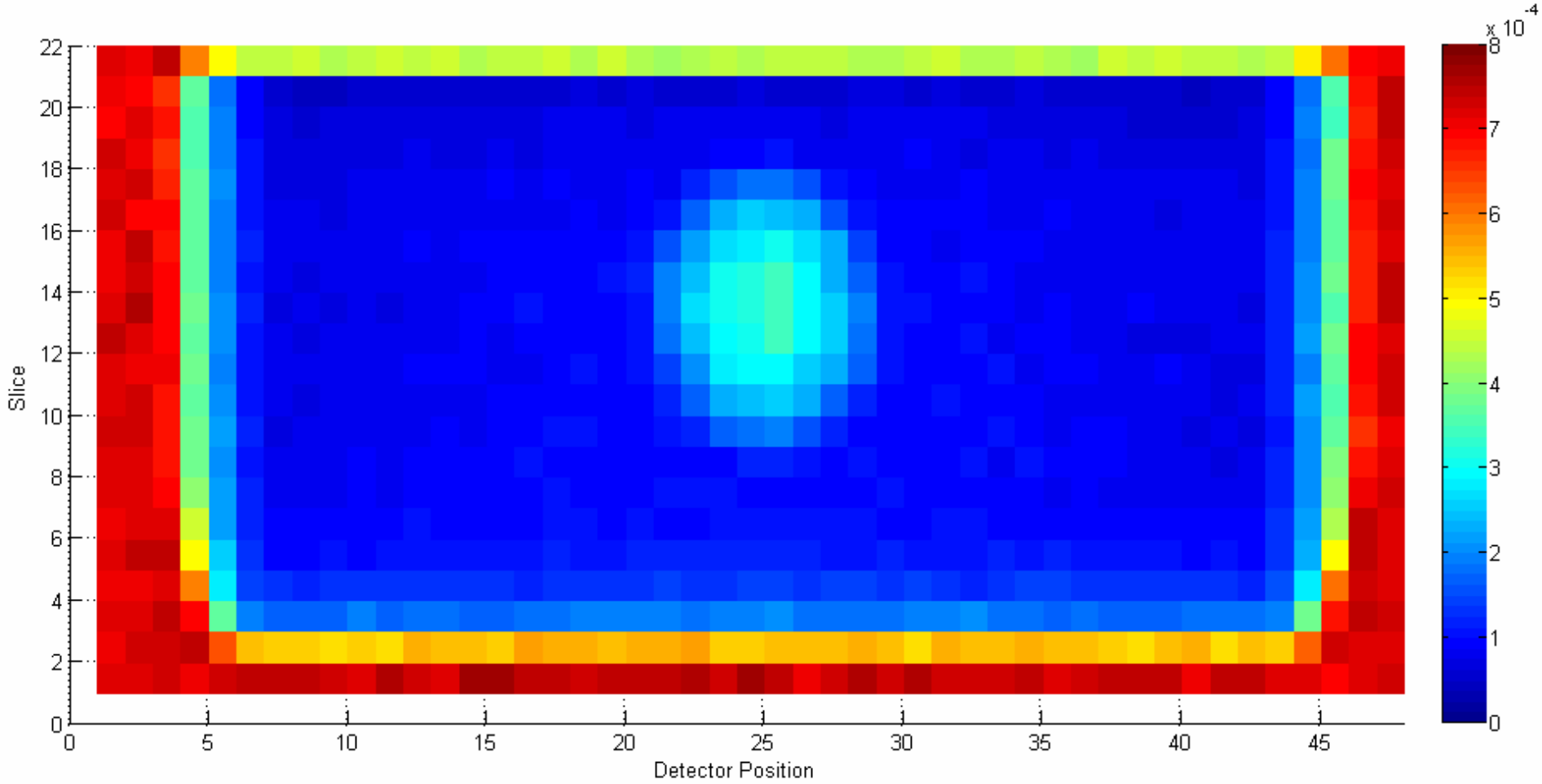
Results – Case 3c Correlations



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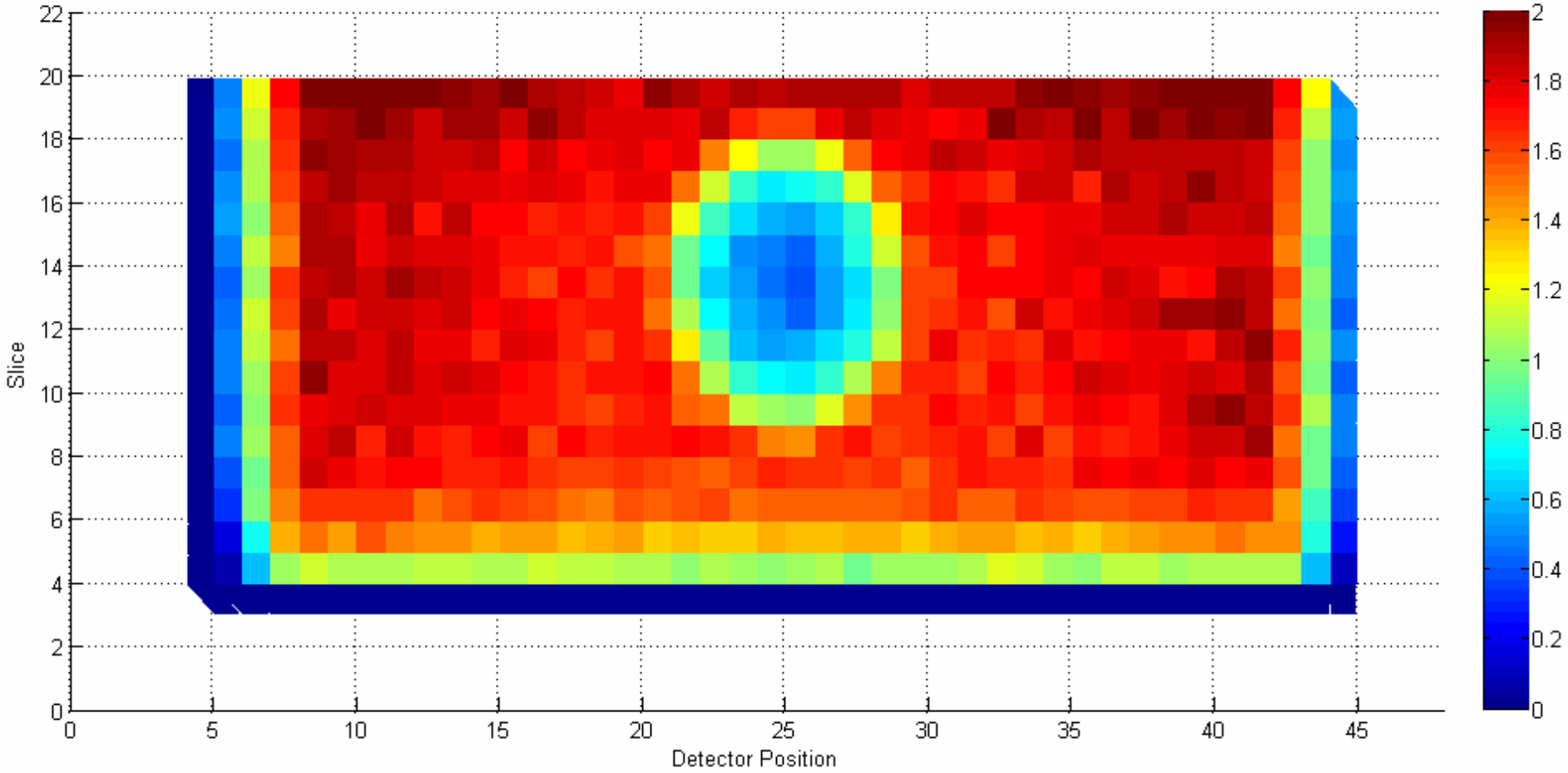
Results – Case 3c Attenuation



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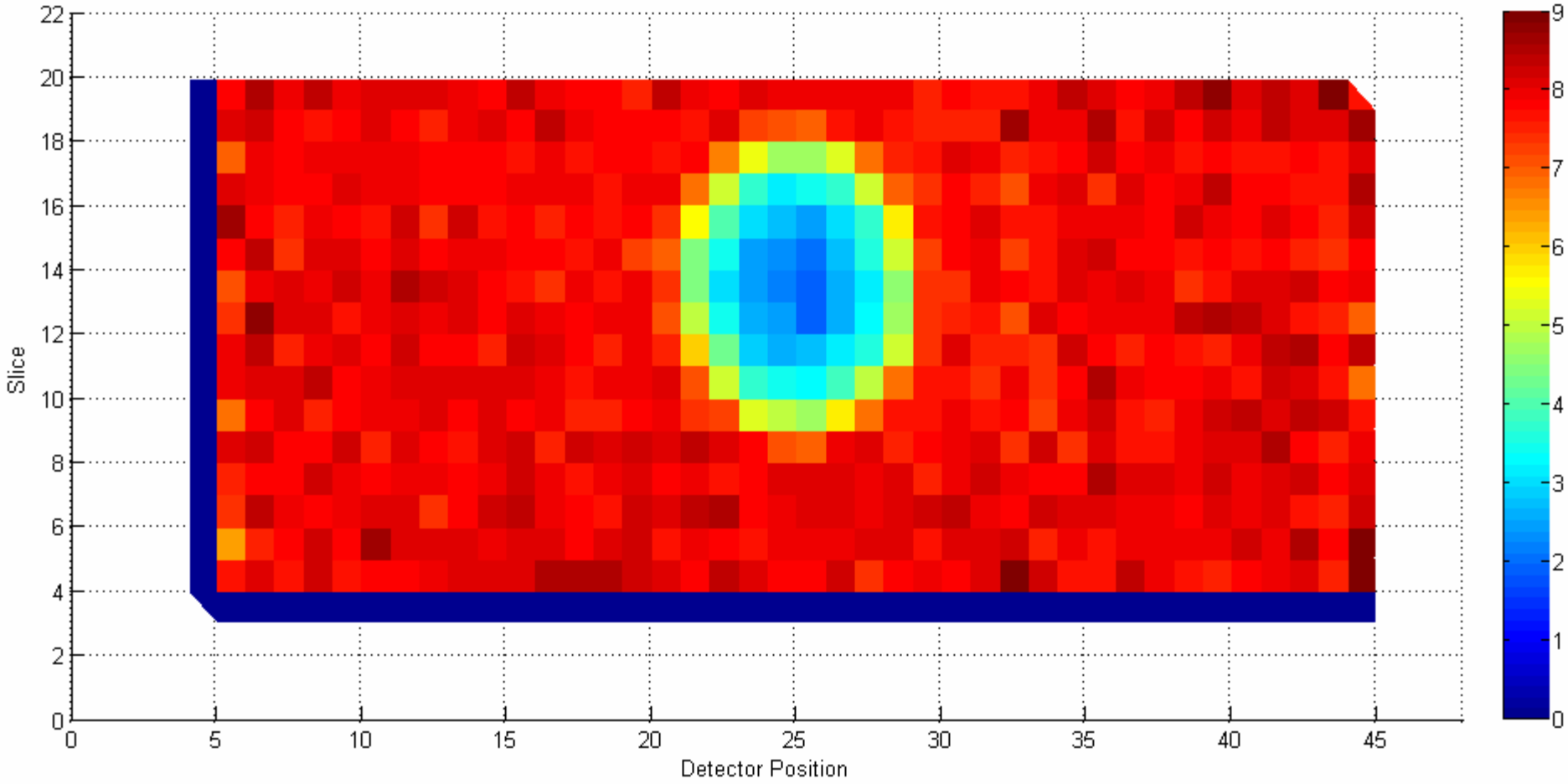
Results – Case 3c Density



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Results

Summary of simulation results

Case number	Measurement time (min)	True mass (kg)	Estimated mass (kg)	Fractional error
1a	3.75	65.812	65.982	+0.0026
1b	15.02	65.812	66.772	+0.0146
1c	37.55	65.812	66.290	+0.0073
2a	3.75	45.339	46.329	+0.0218
2b	15.02	45.339	46.698	+0.0300
2c	37.55	45.339	46.302	+0.0213
3a	3.75	65.502	65.838	+0.0051
3b	15.02	65.502	65.298	–0.0031
3c	37.55	65.502	64.909	–0.0091

Uncertainty Analysis

- **Determine the uncertainty in the results using two methods:**
  - **Propogation of Variance**
  - **Monte Carlo**
- **Compare the fractional uncertainty to the fractional error (previous slide) in order to check for systematic error.**

Uncertainty Analysis

- **Estimate the range of the ‘true’ (population) mean mass, μ, using the measured mass.**
- **In this case, the sample size is 1, and the mean is the estimated mass from the simulation.**
- **The uncertainty in the mass estimate depends on the uncertainty in each of the 3,168 correlation measurements.**
- **The uncertainty in the number of correlations can be modeled using a Normal distribution with mean and variance equal to the measured number of correlations (counting statistics).**

Propagation of Variance

- **Gaussian error approximation:**

$$\sigma_u^2 = \left(\frac{\partial u}{\partial x}\right)^2 \sigma_x^2 + \left(\frac{\partial u}{\partial y}\right)^2 \sigma_y^2 + \left(\frac{\partial u}{\partial z}\right)^2 \sigma_z^2 + \ldots$$

- **Rewriting the equation for density in terms of correlations:**

$$\rho_{i,j} = \frac{\ln\left(\frac{C_U^{i,j}}{N_U^{i,j}}\right) - \ln\left(\frac{C_0^{i,j}}{N_0^{i,j}}\right)}{\ln\left(\frac{C_8^{i,j}}{N_8^{i,j}}\right) - \ln\left(\frac{C_0^{i,j}}{N_0^{i,j}}\right)} \rho_8 = \frac{\ln\left(C_U^{i,j}\right) - \ln\left(C_0^{i,j}\right) - \ln\left(N_U^{i,j}\right) + \ln\left(N_0^{i,j}\right)}{\ln\left(C_8^{i,j}\right) - \ln\left(C_0^{i,j}\right) - \ln\left(N_8^{i,j}\right) + \ln\left(N_0^{i,j}\right)} \rho_8$$

Propagation of Variance

- **Applying the Gaussian Error Approximation to the density formula yields:**

$$s_\rho^2 = \left(\frac{\partial \rho}{\partial C_U}\right)^2 s_{C_U}^2 + \left(\frac{\partial \rho}{\partial C_0}\right)^2 s_{C_0}^2 + \left(\frac{\partial \rho}{\partial C_8}\right)^2 s_{C_8}^2$$

- **Solving for the variance in density:**

$$s_\rho^2 = \frac{C_0 \cdot C_8 \cdot \ln^2\left(\frac{C_8 \cdot N_0}{C_0 \cdot N_8}\right) + C_U \cdot C_8 \cdot \ln^2\left(\frac{C_U \cdot N_8}{C_8 \cdot N_U}\right) + C_U \cdot C_0 \cdot \ln^2\left(\frac{C_U \cdot N_0}{C_0 \cdot N_U}\right)}{C_U \cdot C_0 \cdot C_8 \cdot \ln^4\left(\frac{C_8 \cdot N_0}{C_0 \cdot N_8}\right)} \rho_8^2$$

Propagation of Variance

- **Remember that the mass was:**

$$M = V \sum_{i=1}^{22} \sum_{j=1}^{48} f_{i,j} \cdot \rho_{i,j}$$

- **Applying the Gaussian Error Approximation to this equation yields:**

$$s_M^2 = V^2 \sum_{i=1}^{22} \sum_{j=1}^{48} f_{i,j}^2 \cdot s_{\rho_{i,j}}^2$$

Propagation of Variance

- **The standard deviation (uncertainty) in the mass estimate is the square root of the variance:**

$$s_M = V\sqrt{\sum_{i=1}^{22}\sum_{j=1}^{48} f_{i,j}^2 \cdot s_{\rho_{i,j}}^2}$$

- **And the fractional uncertainty is calculated by dividing the standard deviation by the mass:**

$$\tilde{s}_M = \frac{s_M}{M}$$

Propagation of Variance - Results

Summary of propagation of variance uncertainties

Case number	True mass (kg)	Estimated mass (kg)	Uncertainty (kg)	Fractional uncertainty	Fractional error
1a	65.812	65.982	0.259	0.0039	+0.0026
1b	65.812	66.772	0.132	0.0020	+0.0146
1c	65.812	66.290	0.085	0.0013	+0.0073
2a	45.339	46.329	0.220	0.0047	+0.0218
2b	45.339	46.698	0.112	0.0024	+0.0300
2c	45.339	46.302	0.072	0.0016	+0.0213
3a	65.502	65.838	0.262	0.0040	+0.0051
3b	65.502	65.298	0.131	0.0020	–0.0031
3c	65.502	64.909	0.085	0.0013	–0.0091

Monte Carlo Uncertainty Analysis

- **As with PoV, the Monte Carlo method assumes that each input variable (correlation) is normally distributed with a variance equal to its mean.**
- **Randomly select a value of each input variable from this normal distribution.**
- **Compute a mass estimate using these values.**
- **Repeat many times (10^6 in this case)**
- **Calculate the variance of the result using these 10^6 estimates.**

Monte Carlo Uncertainty Analysis

- **Random normals were selected using the formula:**

$$\left[\sum_{k=1}^{12} j_k - 6\right] \sim Norm(0,1)$$

- **Thus each correlation input was selected using:**

$$\hat{C}_m = C + \sqrt{C}\left[\sum_{k=1}^{12} j_k - 6\right]$$

- **The standard deviation of 'q' estimates was then:**

$$s_M = \sqrt{\frac{q}{q-1}\left[\sum_{m=1}^{q} \hat{M}_m^2 - \left(\sum_{m=1}^{n} \hat{M}_m\right)^2\right]}$$

Monte Carlo Uncertainty Analysis - Results

Summary of Monte Carlo uncertainties

Case number	True mass (kg)	Estimated mass (kg)	Mean mass (kg)	MC uncertainty (kg)	MC fractional uncertainty	PoV fractional uncertainty	Fractional error
1a	65.812	65.982	66.493	0.268	0.0040	0.0039	+0.0026
1b	65.812	66.772	66.898	0.133	0.0020	0.0020	+0.0146
1c	65.812	66.290	66.340	0.086	0.0013	0.0013	+0.0073
2a	45.339	46.329	46.922	0.224	0.0048	0.0047	+0.0218
2b	45.339	46.698	46.907	0.112	0.0024	0.0024	+0.0300
2c	45.339	46.302	46.418	0.072	0.0015	0.0016	+0.0213
3a	65.502	65.838	66.369	0.272	0.0041	0.0040	+0.0051
3b	65.502	65.298	65.425	0.133	0.0020	0.0020	–0.0031
3c	65.502	64.909	64.960	0.086	0.0013	0.0013	–0.0091

Testing for systematic error

- **Calculate the z-score for each mass estimate using the formula:**

$$z = \frac{\varepsilon_M}{\tilde{s}_M}$$

- **where**

$$\varepsilon_M = \frac{M_{measured} - M_{true}}{M_{true}}$$

- **This value represents the number of standard deviations the estimated mass is from the true mass.**
- **Using the cdf of the standard normal distribution, determine the probability the mass estimate would be randomly selected from an unbiased distribution.**
- **Null Hypothesis:** $H_0 : \hat{M} \in Normal(\mu, s_M^2)$

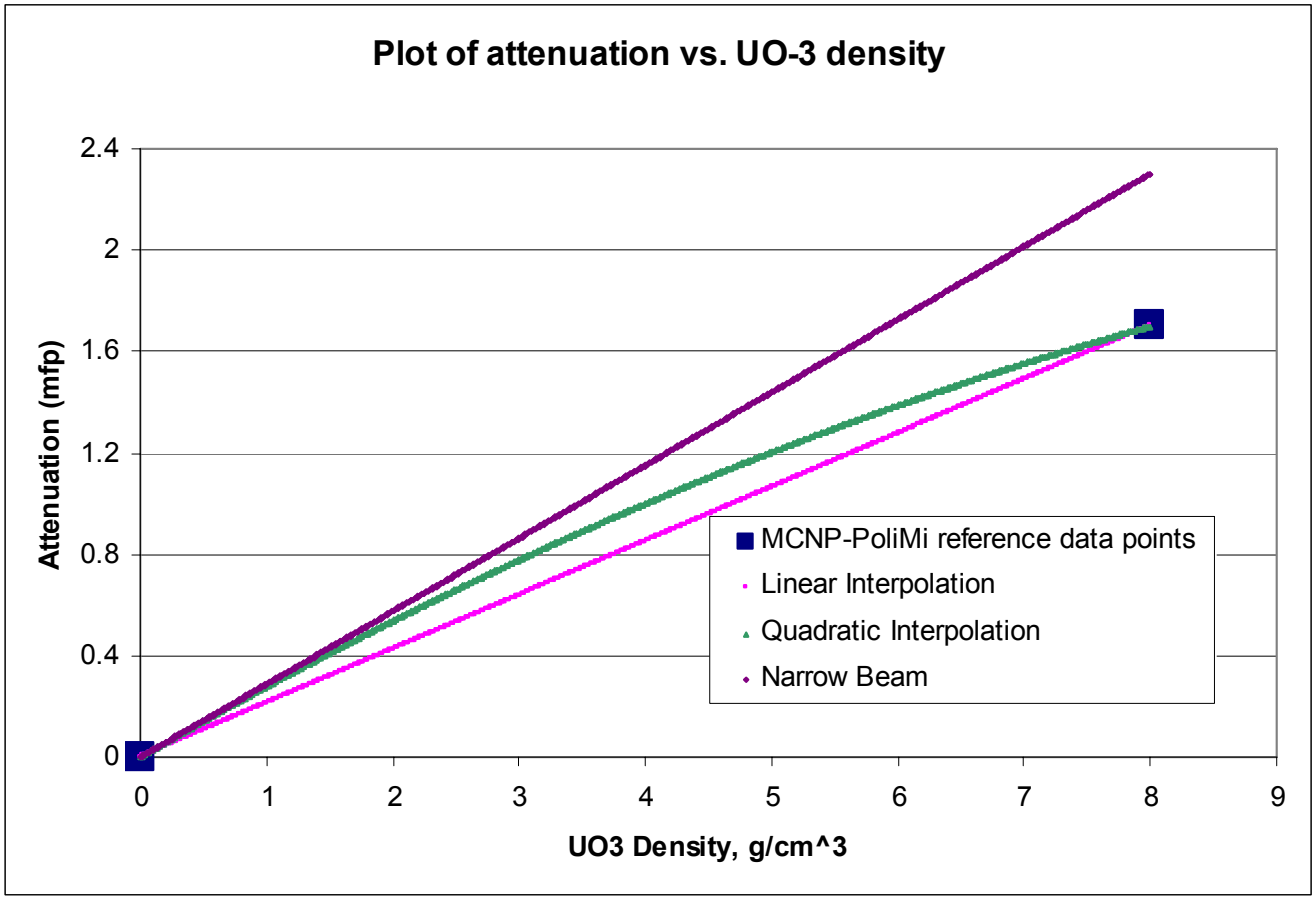
Summary of Uncertainty Analysis

Summary of simulation results and uncertainty analysis

Case number	True mass (kg)	Estimated mass (kg)	Fractional uncertainty	Fractional error	z-score	Probability of random
1a	65.812	65.982 ± 0.268	0.0040	+0.0026	+0.60	0.5485
1b	65.812	66.772 ± 0.133	0.0020	+0.0146	+7.30	<0.0001
1c	65.812	66.290 ± 0.086	0.0013	+0.0073	+5.62	<0.0001
2a	45.339	46.329 ± 0.224	0.0048	+0.0218	+4.54	<0.0001
2b	45.339	46.698 ± 0.112	0.0024	+0.0300	+12.50	<0.0001
2c	45.339	46.302 ± 0.072	0.0015	+0.0213	+14.20	<0.0001
3a	65.502	65.838 ± 0.272	0.0041	+0.0051	+1.24	0.2150
3b	65.502	65.298 ± 0.133	0.0020	–0.0031	–1.55	0.1211
3c	65.502	64.909 ± 0.086	0.0013	–0.0091	–7.00	< 0.0001

- **The measurements in red are highly significant, indicating the presence of systematic error → Reject H_0.**

Possible Sources of Systematic Error



- **The effective attenuation was assumed to fall off linearly with density.**

Possible Sources of Systematic Error

- **The effective attenuation was assumed to be the same for any two pixels with the same average density.**

Conclusions

- **In each case, the simulated mass estimates were within 3% of the true mass.**
- **Because of the presence of systematic errors, longer measurement times did not produce more accurate results.**
- **It is hoped that these results can be validated with experimental measurements.**