G4CMP-317 Validation

Michael Kelsey, Wade Lamberson, and Nolan Tenpas

DMC Working Group Meeting

May 12th, 2025

Validation Process

Low Level Validation: Does the algorithm do what we are expecting it to do?

- What is the algorithm doing?
- Where do phonons fail (diffuse fallback)? Why does this happen?

High Level Validation: Does the algorithm give expected macroscopic results?

- Test detector with a 10keV Bulk NR deposit
- Run this detector with 3 orientations: unchanged, rotated, and displaced

Internal Settings: What is the step size and step limit that gives the best results?

Parameter Tuning (not discussed here): Determining the correct probability of diffuse vs specular reflections to better match detector data

Low Level Validation

Sample Information

Sim Information:

Total Events = 1

Energy Deposit = 10keV

Deposit Type = (0,0,0) NR

100% Specular Reflections

QET Abs = 100%

TES Subgap Abs = 100%

Detector Used:

Single Detector = iZIP5

Software Information:

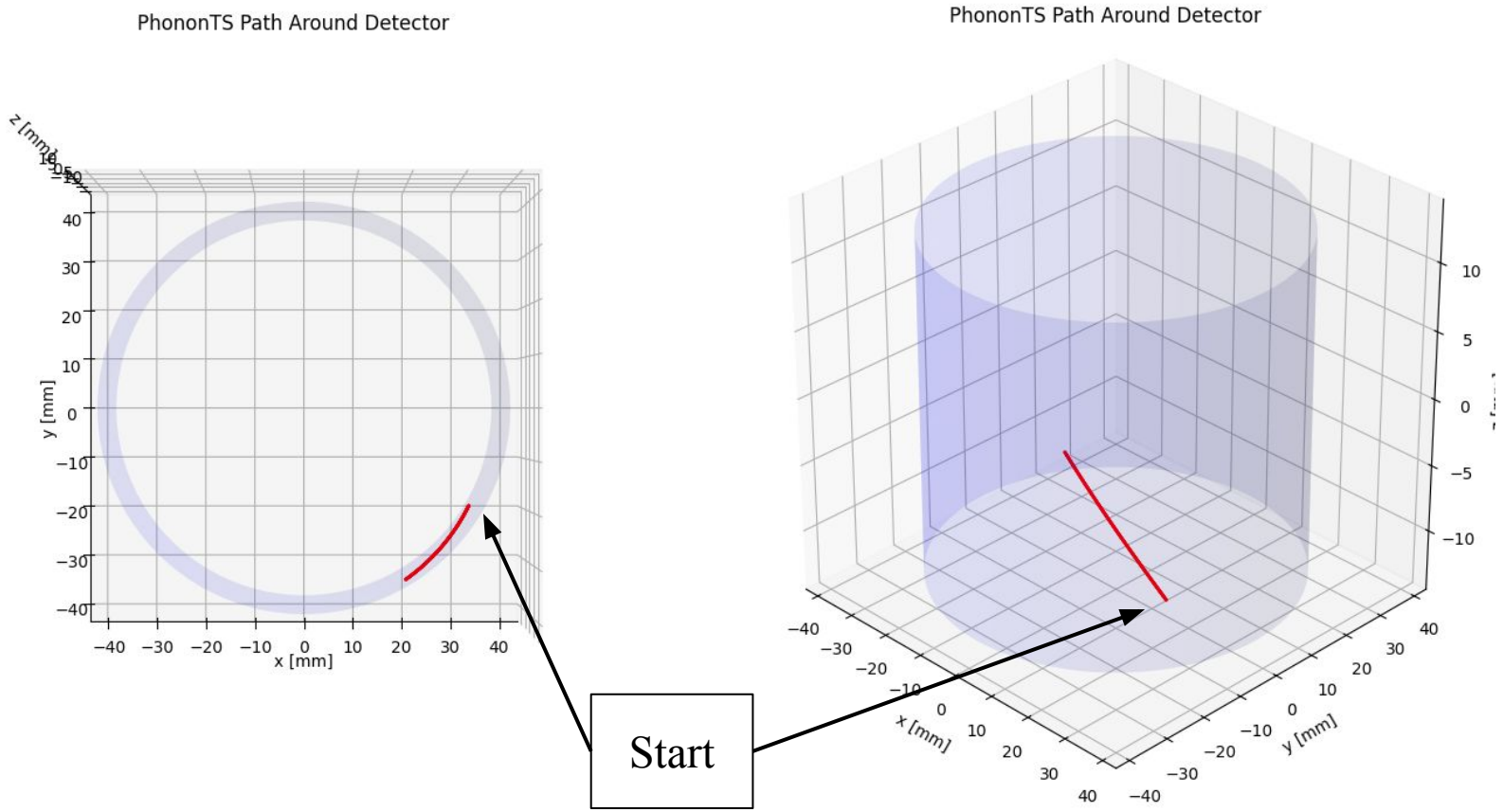
G4CMP : G4CMP-461

Geant4 : geant4-10-07-patch-04 [MT]

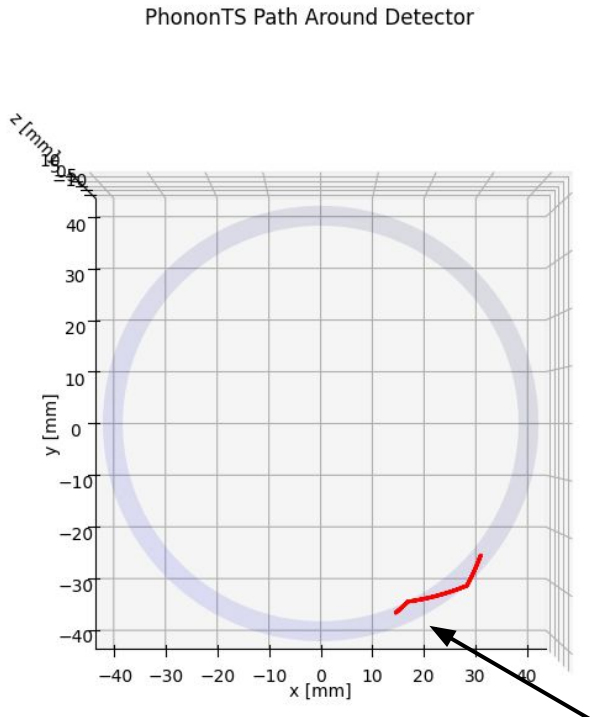
ROOT : 6.28/12

SuperSim : elog/2117-2-g4003271f

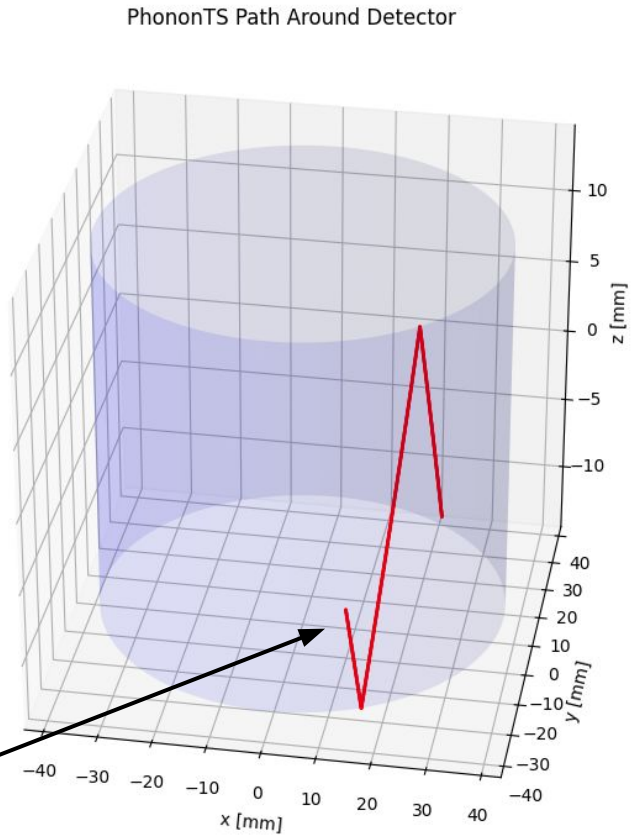
Individual Phonon - Path Around Detector (Simple)



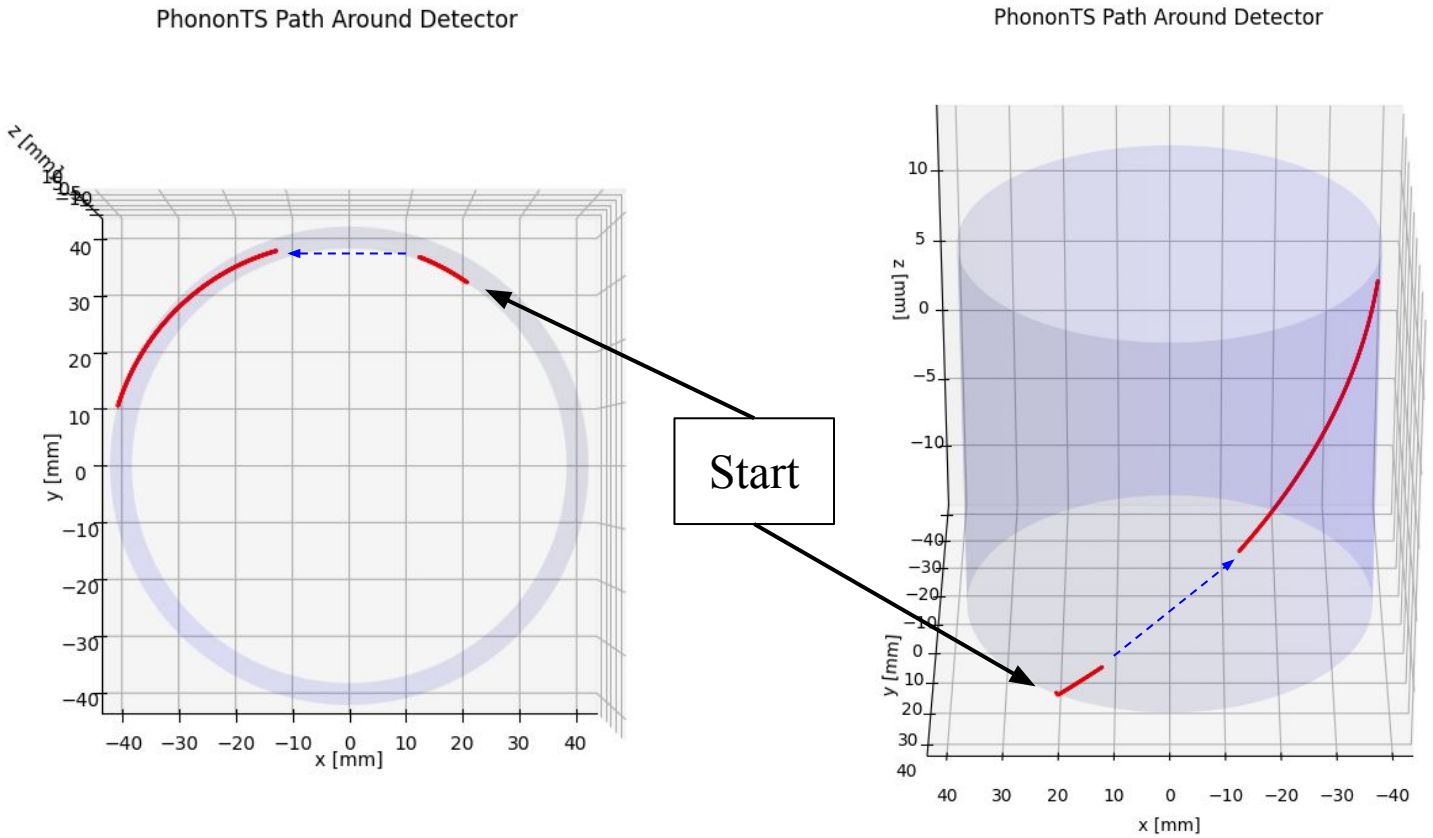
Individual Phonon - Path Around Detector (Edge Reflection)



Start

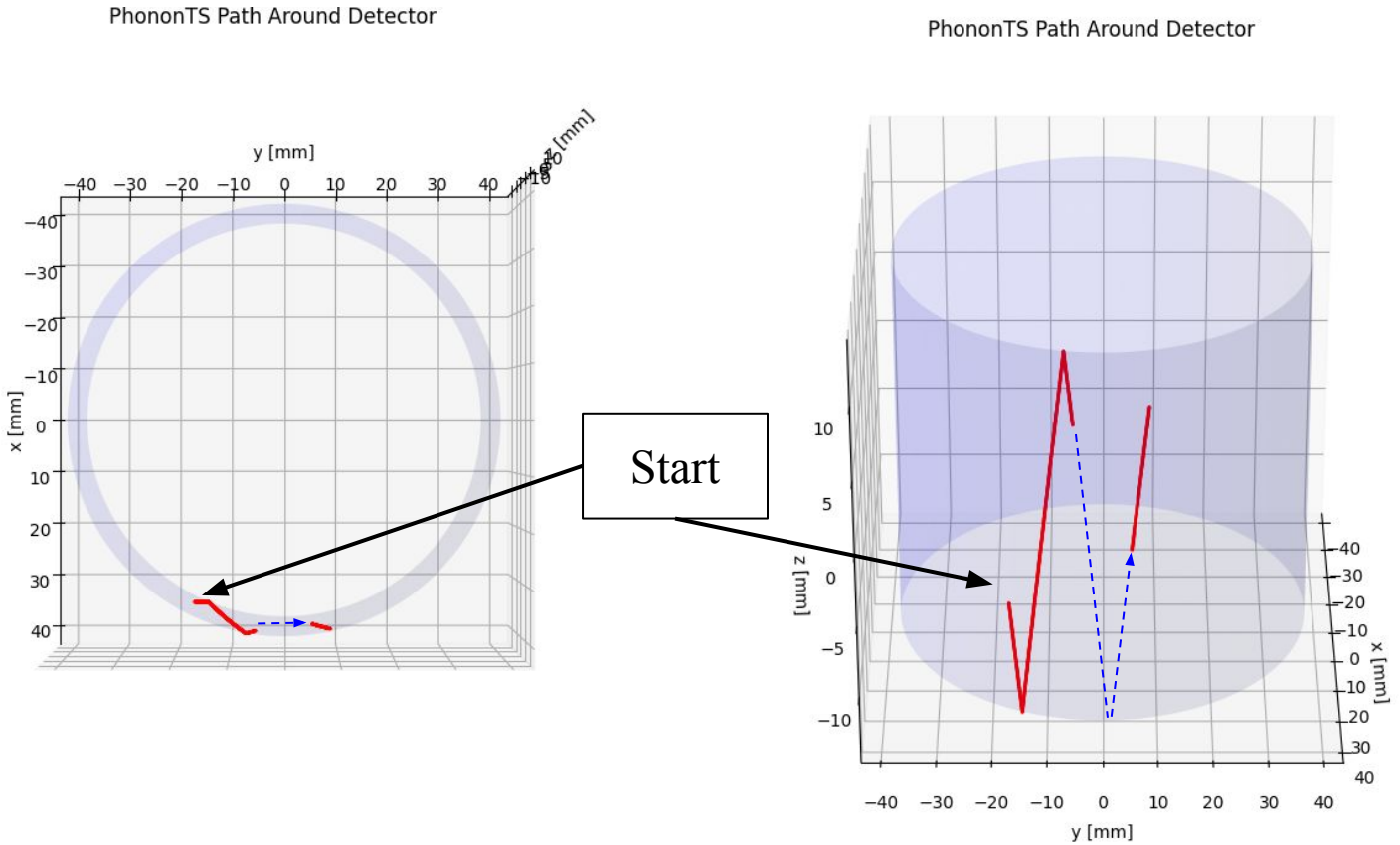


Individual Phonon - Path Around Detector (Skip Flats)



These are scatter plots - The gap is due to the displacement across the flat taking 0 steps

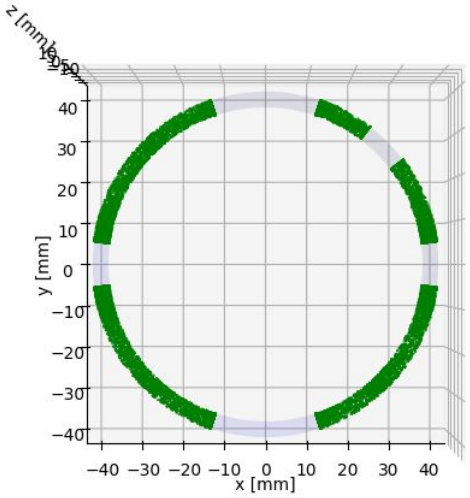
Individual Phonon - Path Around Detector (Skip Flats + Edge Reflection)



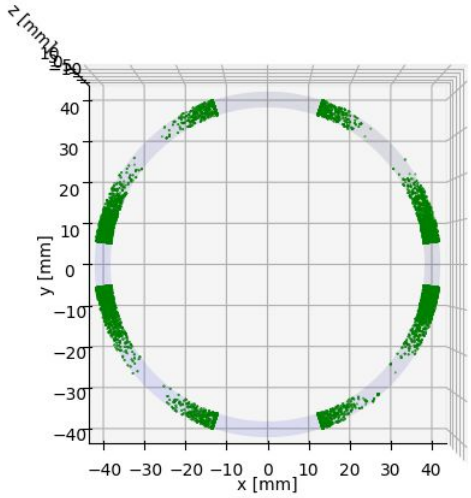
These are scatter plots - The gap is due to the displacement across the flat taking 0 steps

Plotting Successful Reflection Locations

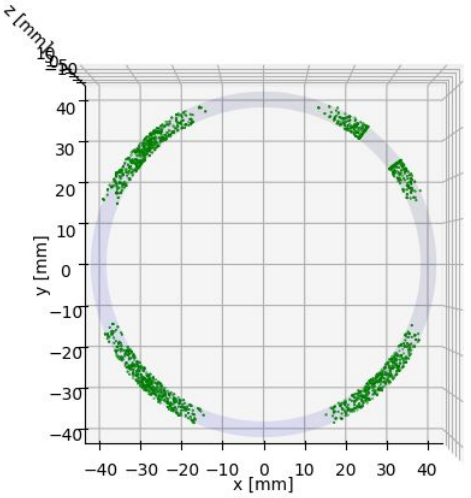
PhononTS Successful Reflections Position Distribution
G4CMP-317



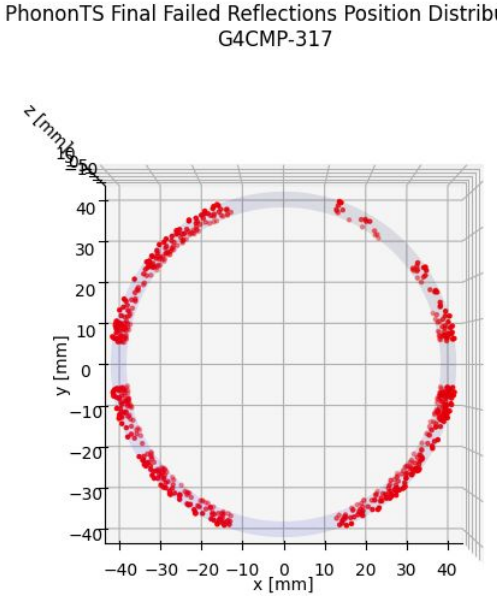
PhononTF Successful Reflections Position Distribution
G4CMP-317



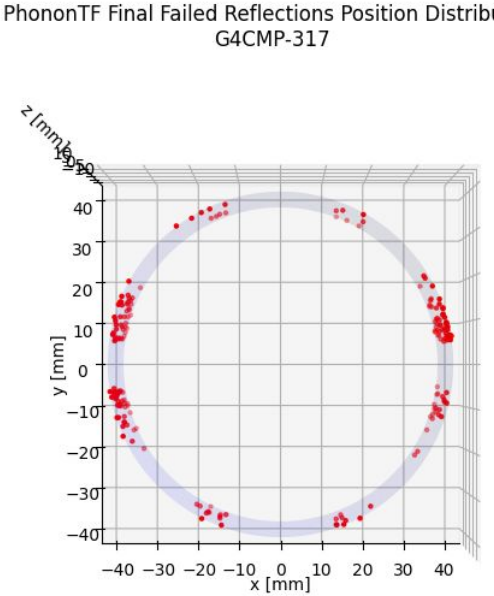
PhononL Successful Reflections Position Distribution
G4CMP-317



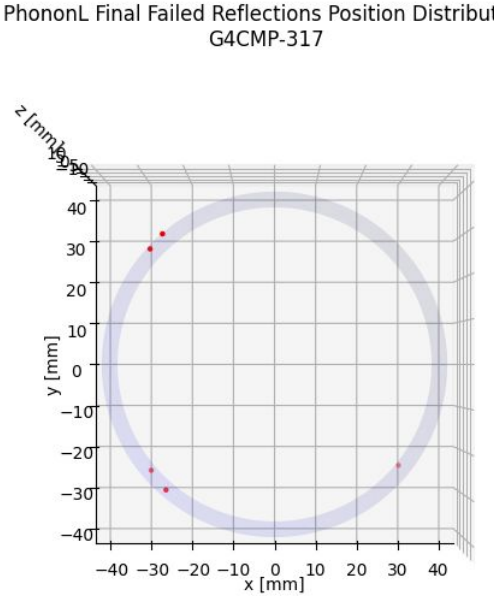
Plotting Diffuse Reflection Locations



Total phonons displaced: 19290
Failed reflections on walls: 633



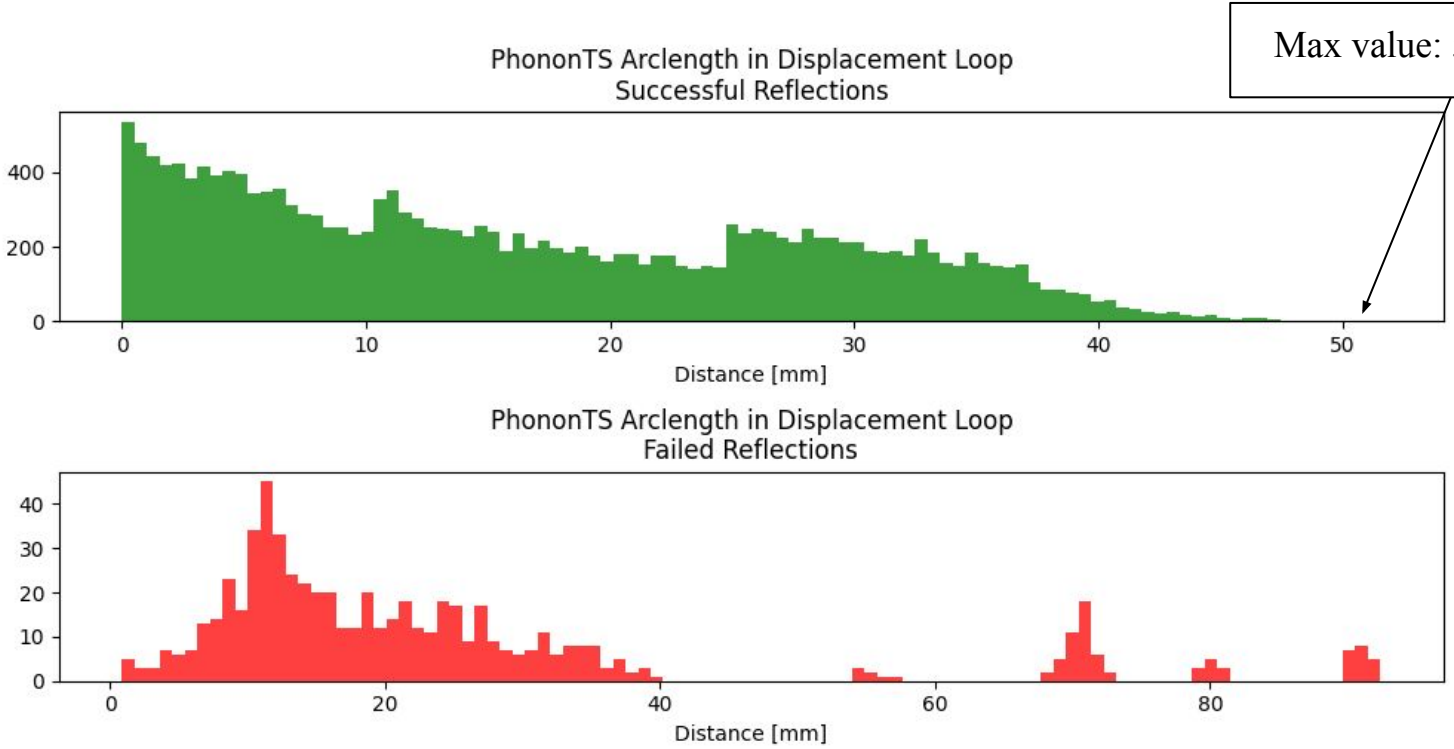
Total phonons displaced: 9950
Failed reflections on walls: 193



Total phonons displaced: 1691
Failed reflections on walls: 5

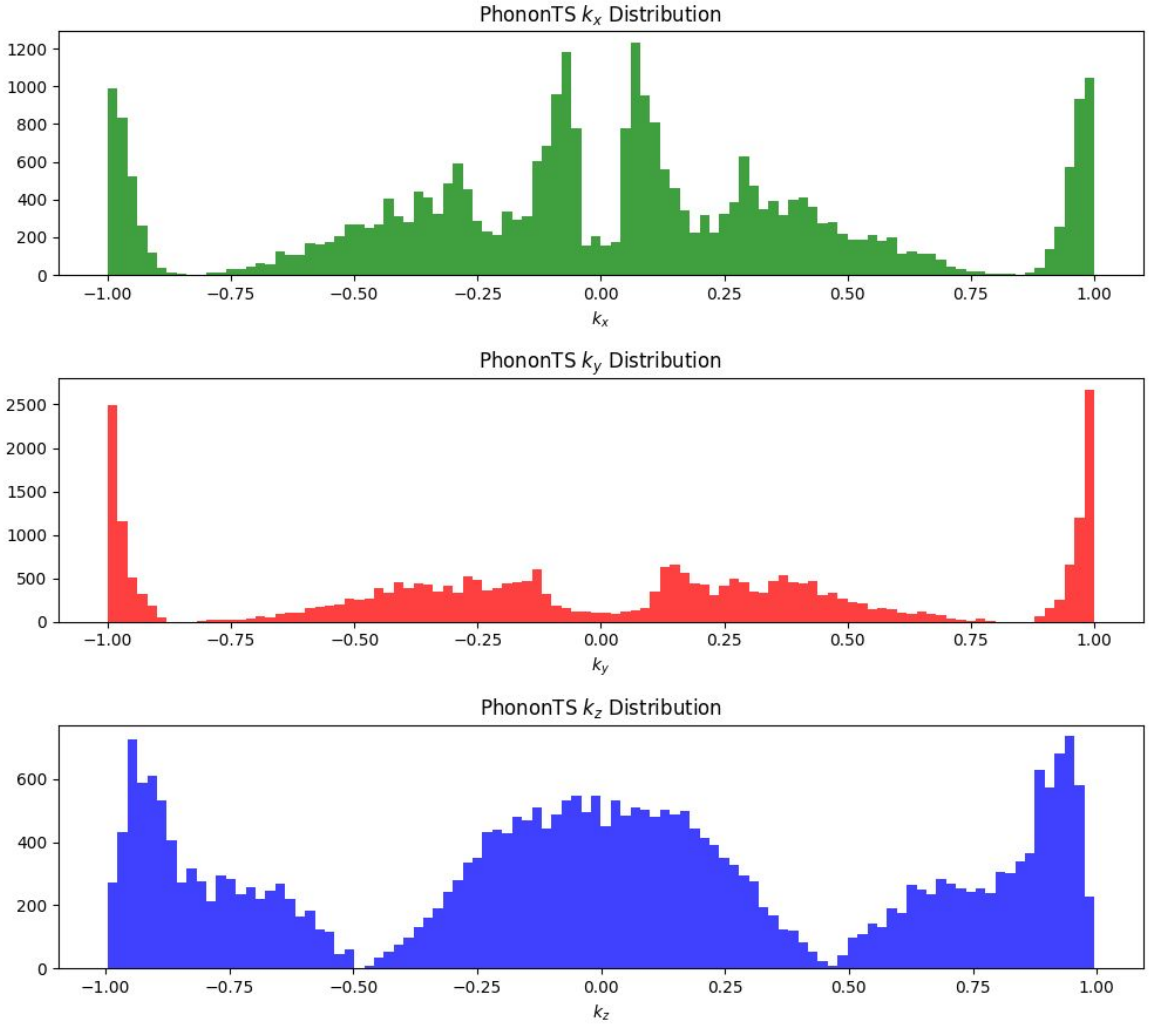
Total Displaced Reflections: 30931; Total Diffuse Reflections: 838
→ 2.7% Displaced phonons ended up diffuse
→ 7 phonons didn't reach 1000 steps

Slow-Transverse Arc Length Traveled



→ 551 failed reflections have arc length < 40mm

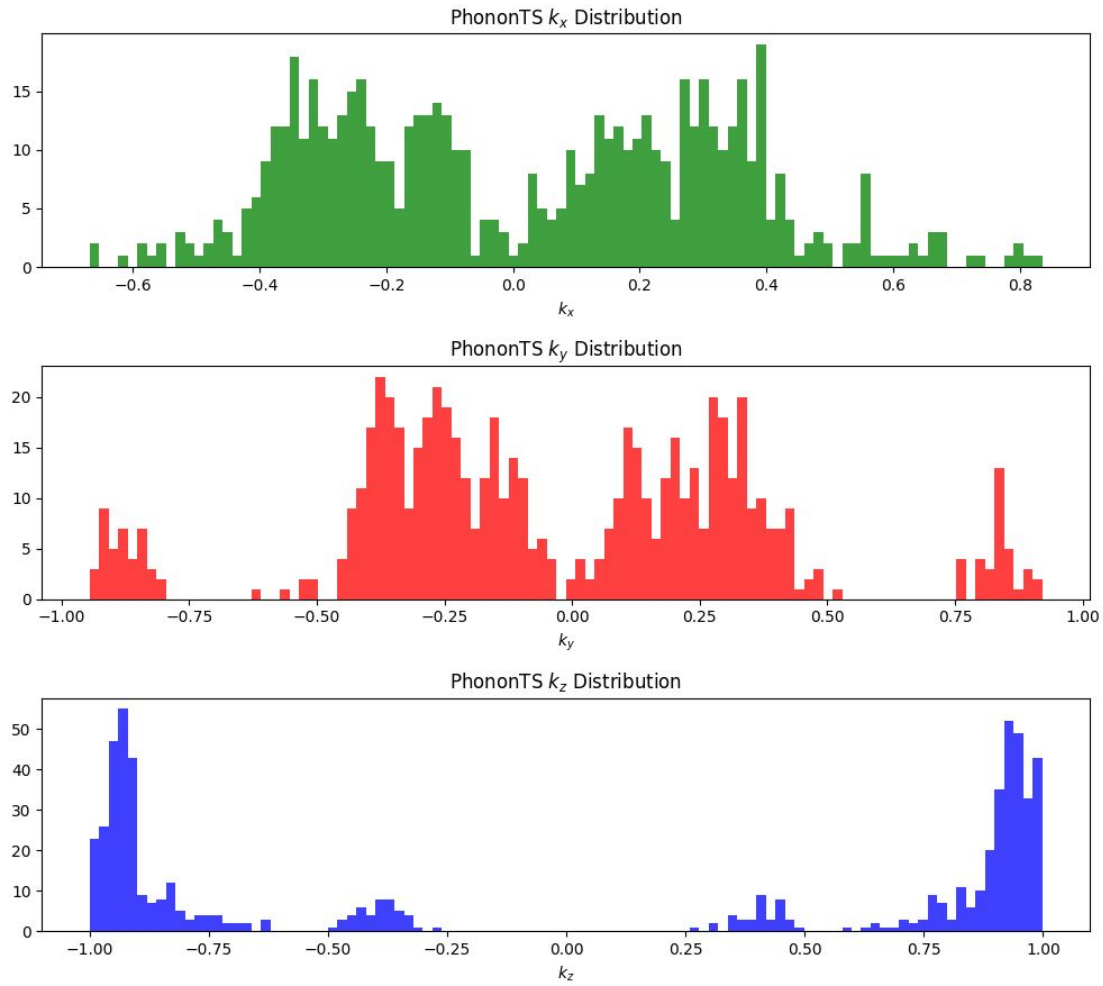
Slow-Transverse Wave Vector Distribution - Successful Reflections



Slow-Transverse Wave Vector Distribution - Failed Reflections

This means a majority of failures are bouncing back and forth between the top and bottom Z faces, and not moving far enough azimuthally to get an inward group velocity

This can be handled by increasing the number of steps taken (see Internal Settings)



Low Level Validation: Notes and Observations

The code is doing what we expect it to do!

As shown in the previous slides, we see that the phonons are successfully stepping along the curved sidewall, reflecting as needed against the Z surfaces

We have seen phonons enter onto the detector flat and “skip” across it; maintaining the expected k-tangent trajectory, handling the reflections against the Z surfaces as needed

The remaining diffuse reflections are due to phonons with a large k_Z component, which cause the phonons to bounce between the Z surfaces instead of moving a sufficient angular distance to find an inward group velocity

- This can be further reduced by adjusting the internal displacement loop settings (shown in the Internal Settings section)

High Level Validation

Sample Information

Sim Information:

Total Events = 1

Energy Deposit = 10keV

Deposit Type = Bulk NR

100% Specular Reflections

QET Abs = 100%

TES Subgap Abs = 100%

Autoseed off

Detectors Used:

Single Detector = HV100mm

Software Information:

G4CMP : G4CMP-480

Geant4 : geant4-10-07-patch-04 [MT]

ROOT : 6.28/12

SuperSim : elog/2117-2-g4003271f

Results

Detector Orientation	Number of Diffuse Reflections
Normal	1033
Rotated (120 degree)	991
Displaced (.5 .5 .5 m)	1023
Rotated (120 degree) & Displaced (.5 .5 .5 m)	974

All events had 100% collection efficiency

Differences between the rotated and unrotated simulations are likely due to numerical errors by applying repetitive transforms

High Level Validation: Notes and Observations

Overall, things look very good. We have thoroughly tested this branch with several phonon burst jobs, each with 100% collection efficiency

- We no longer have the killed phonon messages from before this work (G4CMP-310)
- The displaced phonons have the correct volume assignment and don't escape to the world

We believe that the differences between the normal and rotated detector jobs are due to numerical inaccuracies. If the same phonon enters the displacement loop with a slightly different position or wavevector, this difference will compound on itself as the phonon bounces around

When running single phonon jobs, we saw very little differences for ~30 steps between the normal and rotated detector. At 30 steps, the X position was different by a little more than 1pm. This difference gradually grew as the phonon bounced around. Details have been described in G4CMP-480

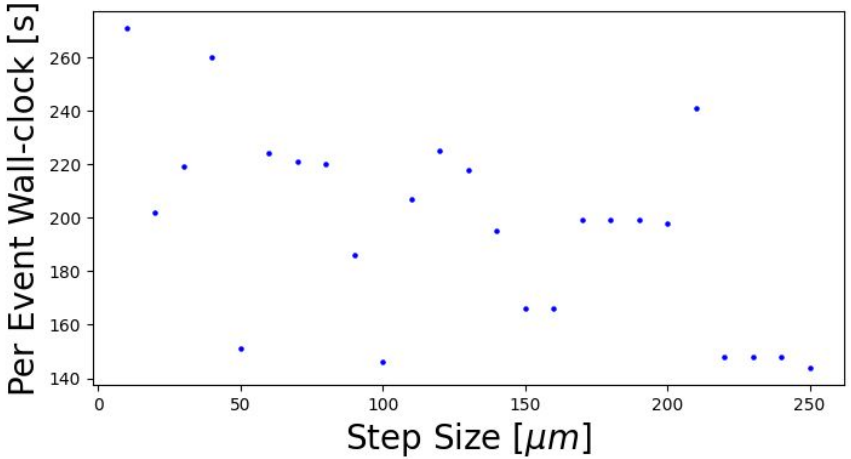
Internal Settings

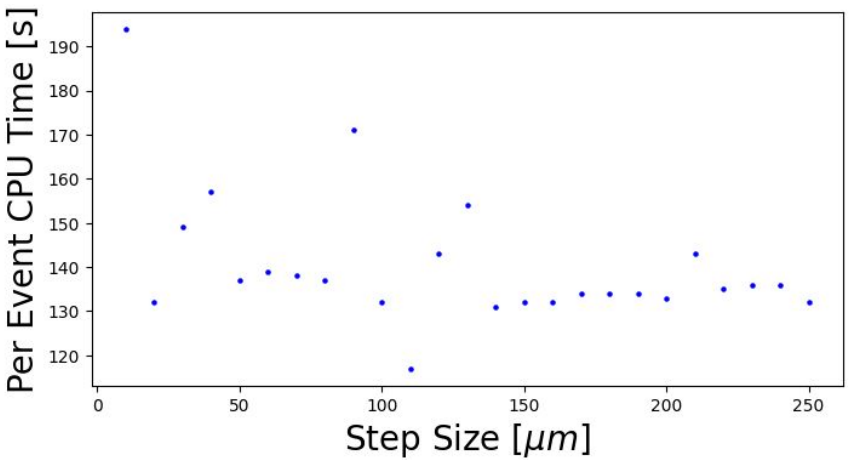
What are the Internal Settings?

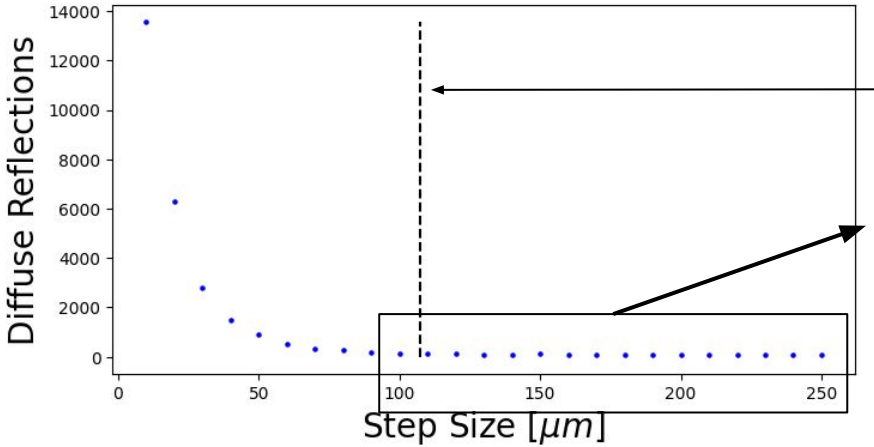
In this model, we use two settings to “tune” the algorithm to reduce the number of diffuse reflection fallbacks:

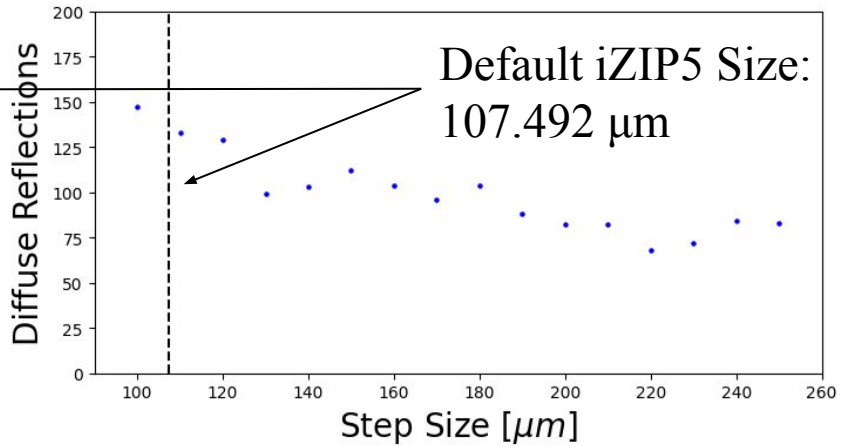
1) **Step Size** - The linear distance displaced (prior to surface adjustment) while stepping around the detector
    a) Set with the macro command: /g4cmp/phononSurfStepSize N <unit>
    b) Default value: (Diagonal distance of the solid bounding box) / 1000
2) **Step Limit** - The number of steps taken around the detector until we use the diffuse fallback
    a) Set with the macro command: /g4cmp/phononSurfStepLimit N
    b) Default value: 5000

Results - Changing Step Size (1000 Step Limit)

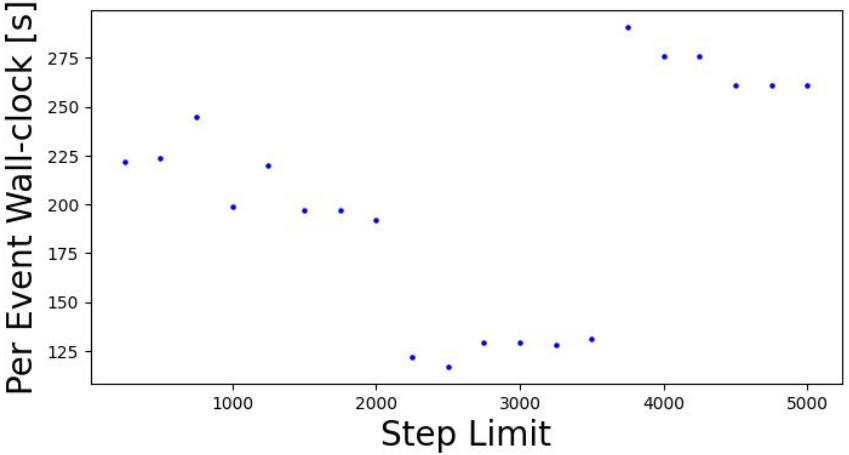


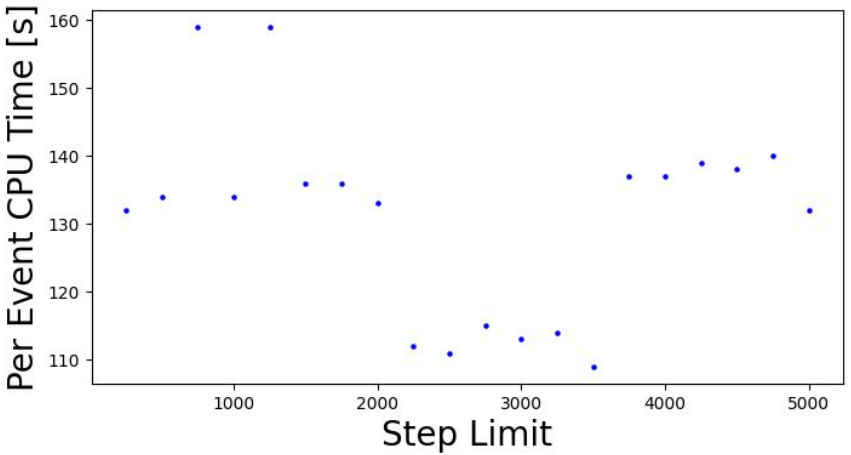


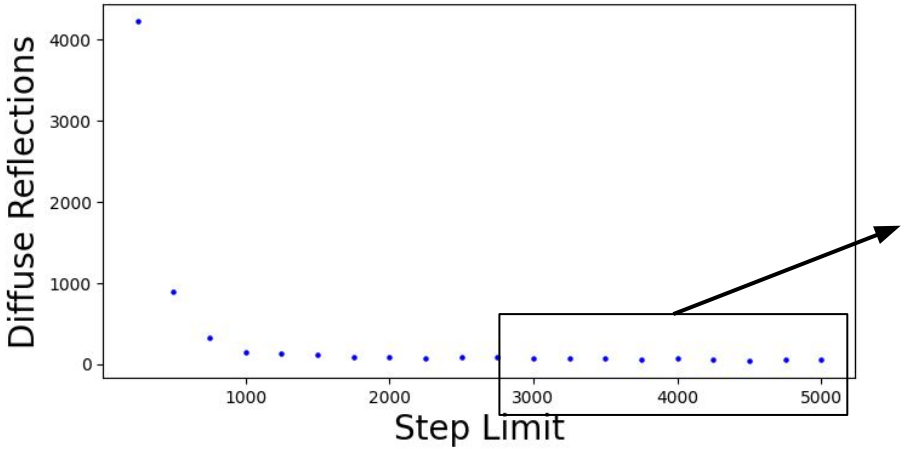


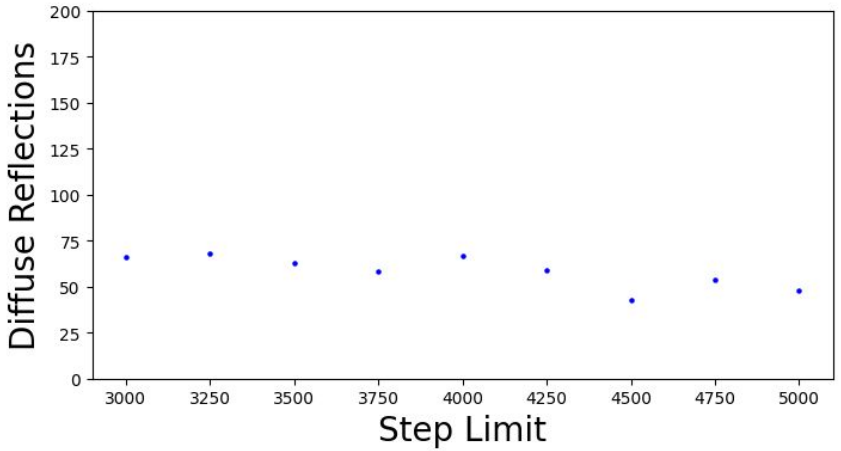


Results - Changing Step Limit (100µm Step Size)









Internal Settings: Notes and Observations

We can see that increasing the step size and number of steps in the displacement algorithm decreases the number of diffuse reflection fallbacks without a noticeable impact on the per-event runtime (the variations shown are due to cluster file system issues)

We can attribute a majority of the computation time to the different custom functions used in the edge finding algorithm (used for reflections against the Z-surfaces on the curved sidewalls)

The number of diffuse reflections continues to decrease as the step limit is increased, but remains relatively constant after 3000 steps:

- Ranges from 68-43 diffuse reflections for 3000 - 5000 steps
- Average: 58.44 +/- 8.23

Summary and Conclusions

The simplified surface mode model is working as expected! We have shown a variety of edge cases, such as reflecting against the Z-surfaces and skipping across the detector flats

The number of diffuse reflections can be further reduced by increasing the number of steps that we take around the detector in the displacement algorithm

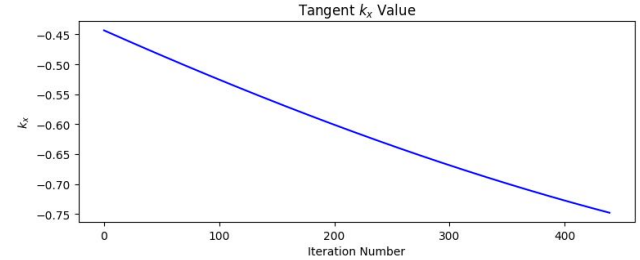
Two custom classes were created as part of this work that could be useful for future G4CMP development: **G4CMPSolidUtils** and **ParticleChangeForPhonon**

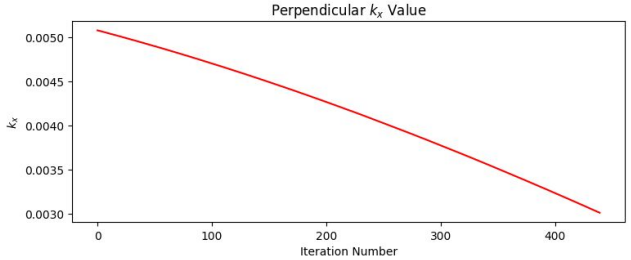
The remaining tasks are underway:

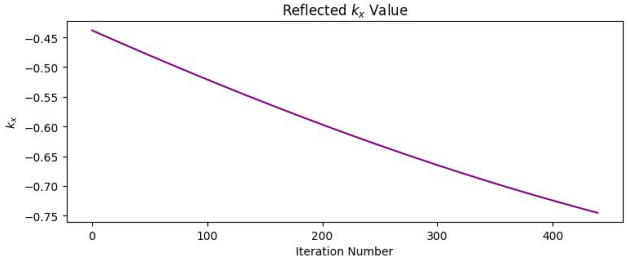
- Probability of Specular vs Diffuse reflections (Rik B. @ A&M for CDMSlite)
- Final code review for merging 317 onto develop

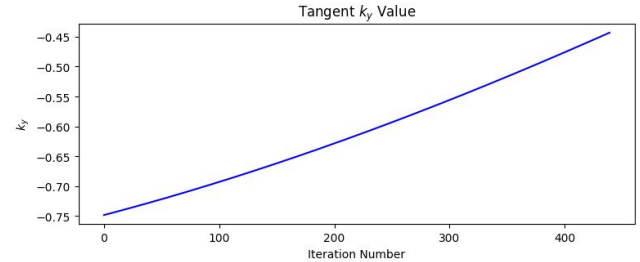
Backup Slides

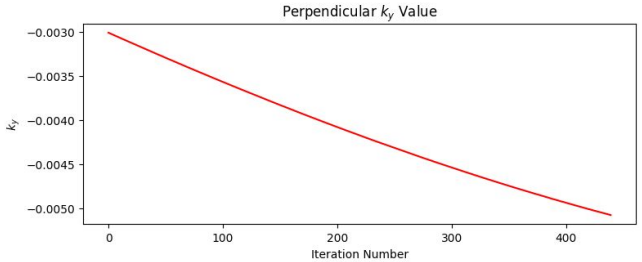
Individual Phonon - Wave vector (Simple)

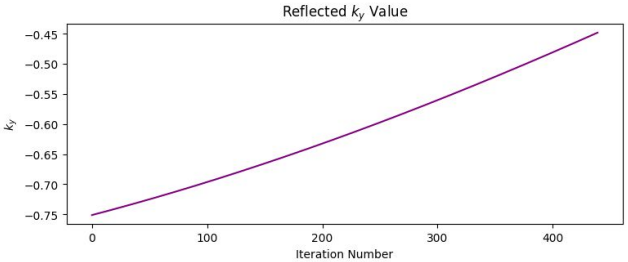


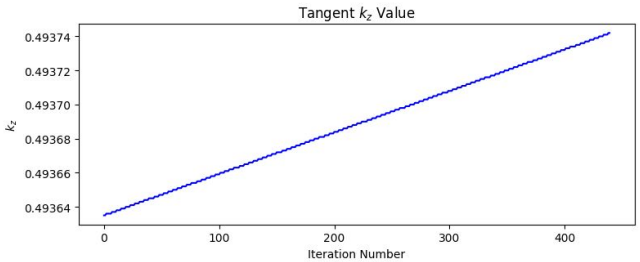


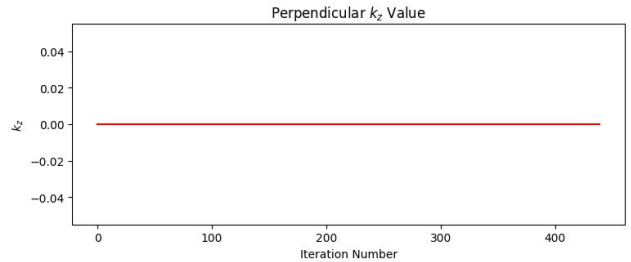


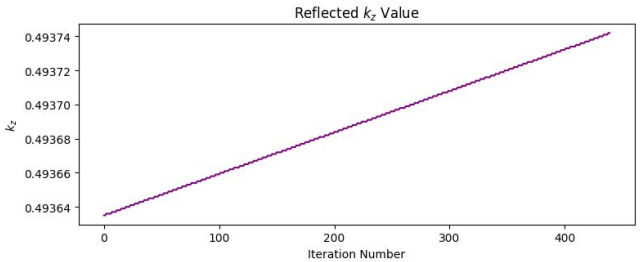




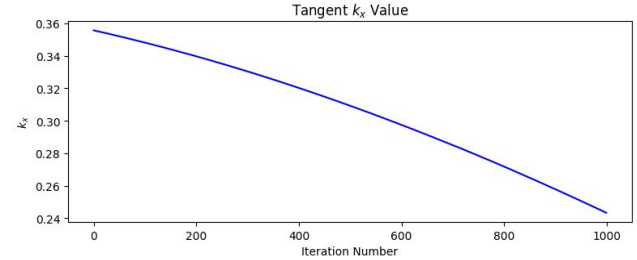


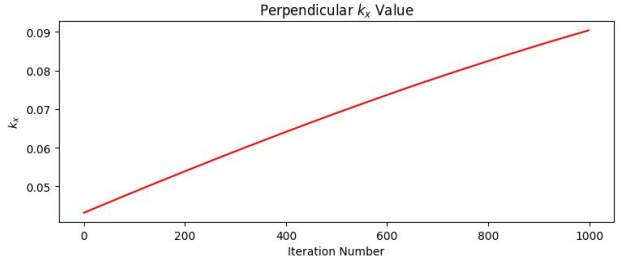


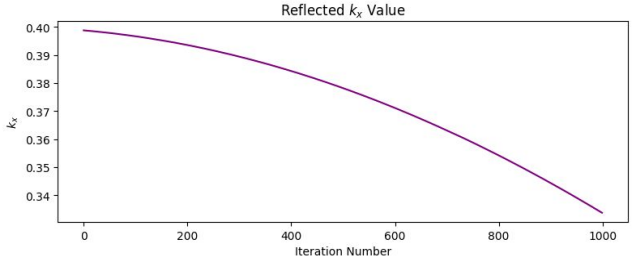


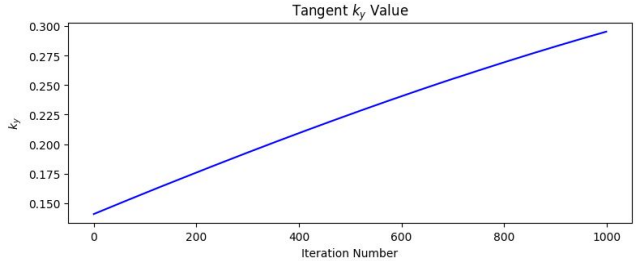


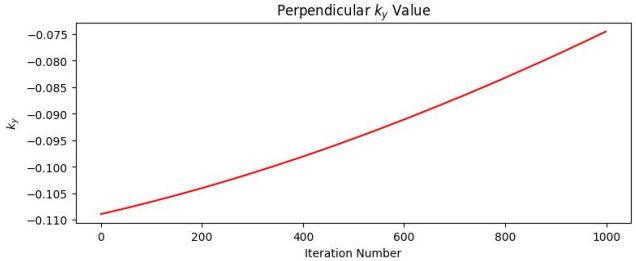
Individual Phonon - Wave vector (Edge Reflection)

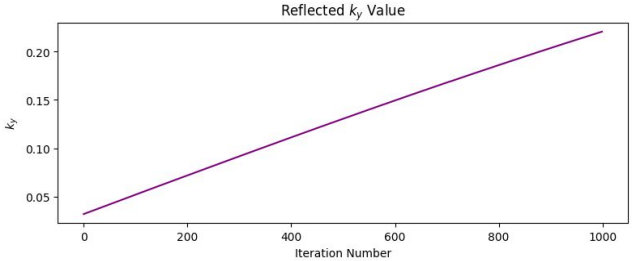


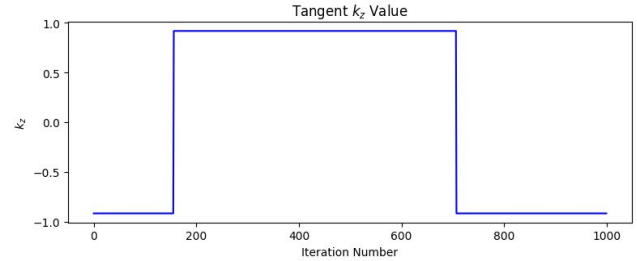


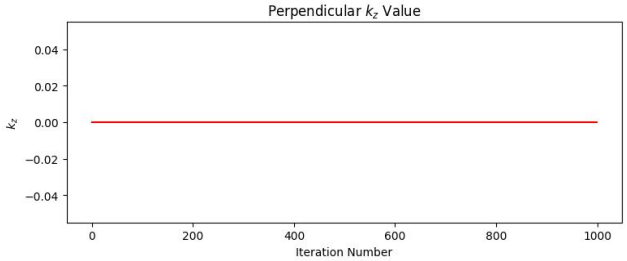


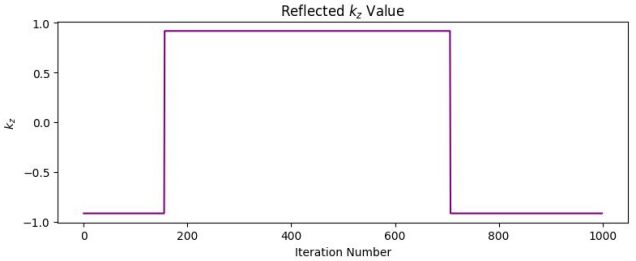




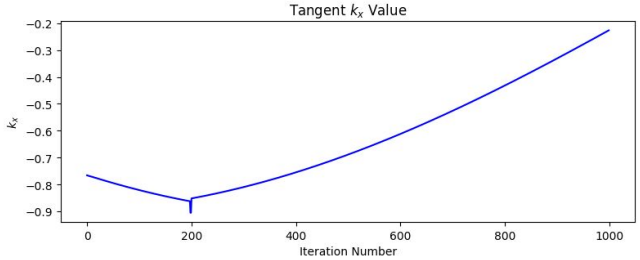


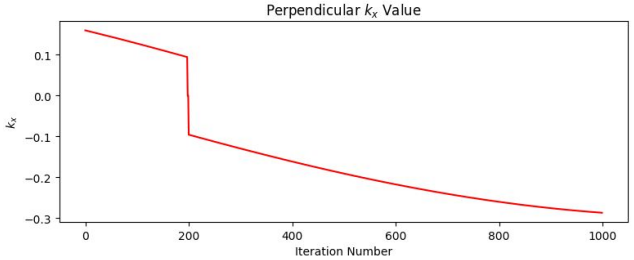


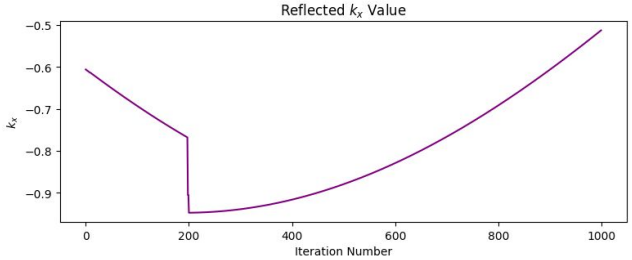


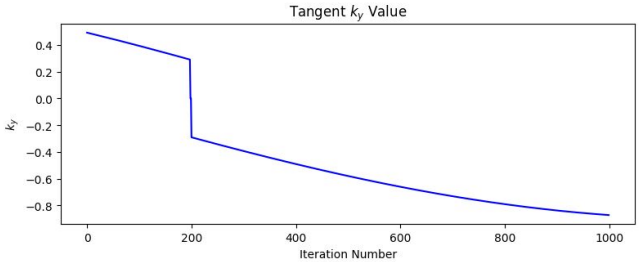


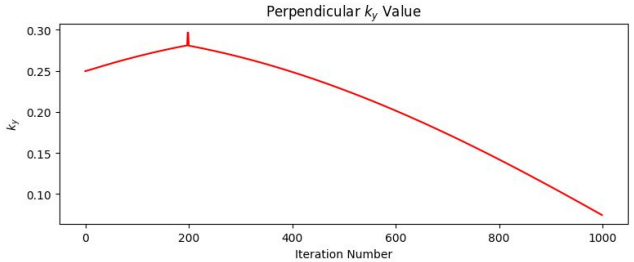
Individual Phonon - Wave vector (Skip Flats)

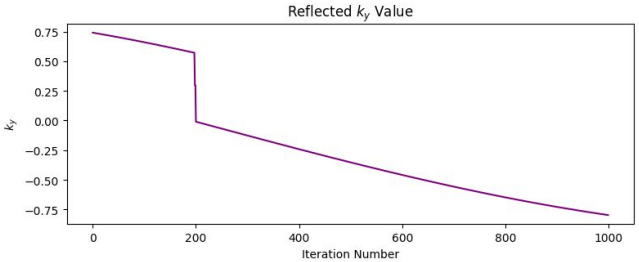


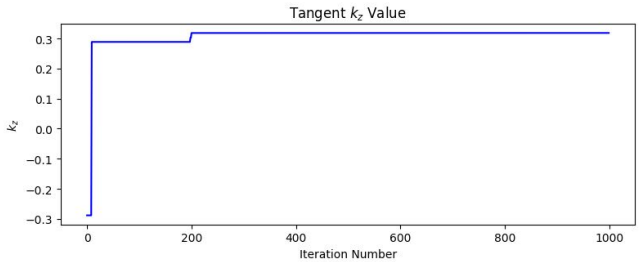


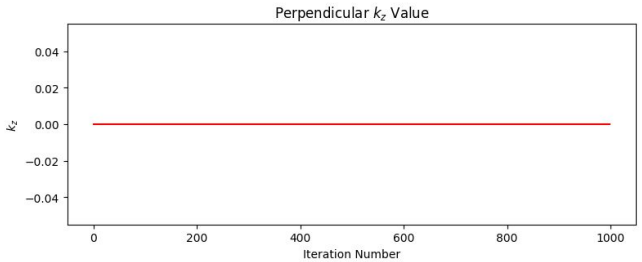


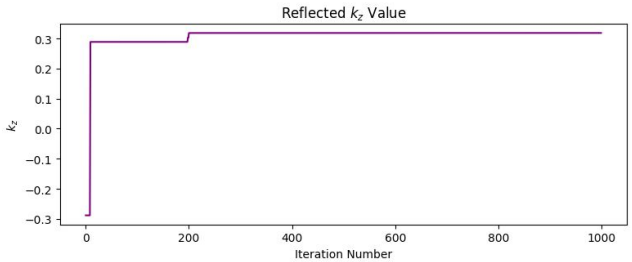




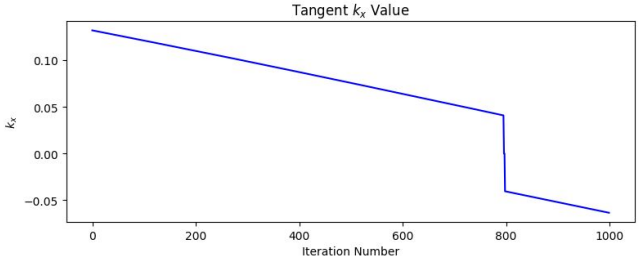


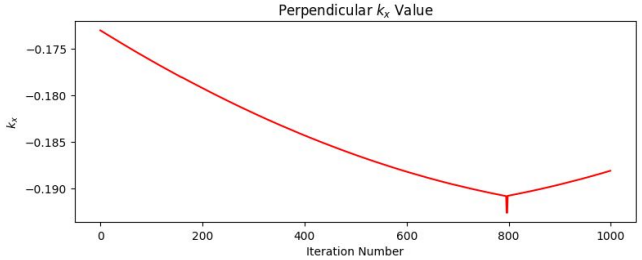


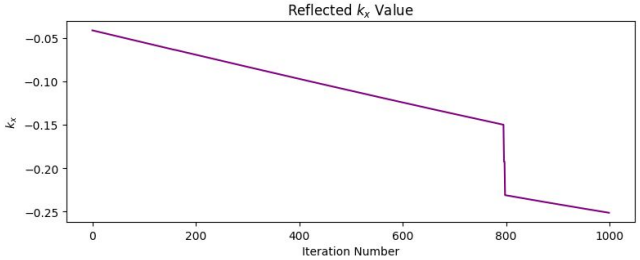


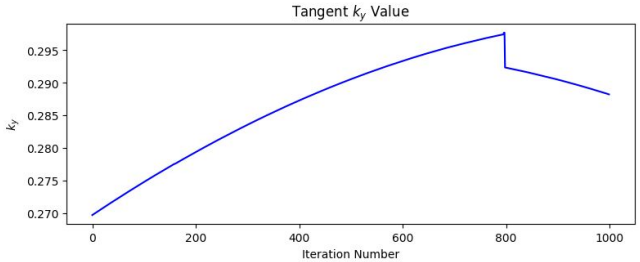


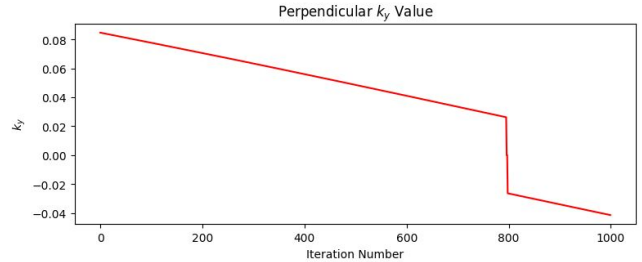
Individual Phonon - Path Around Detector (Skip Flats + Edge Reflection)

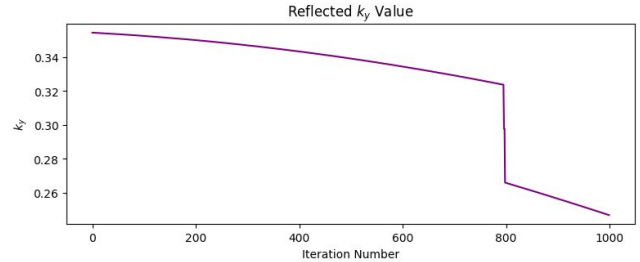


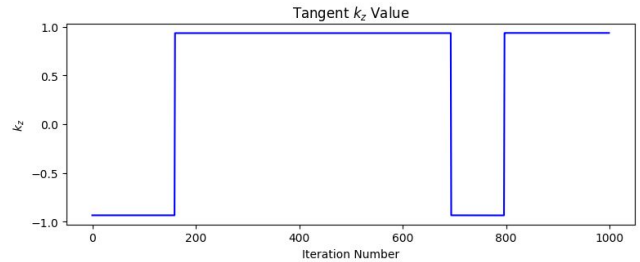


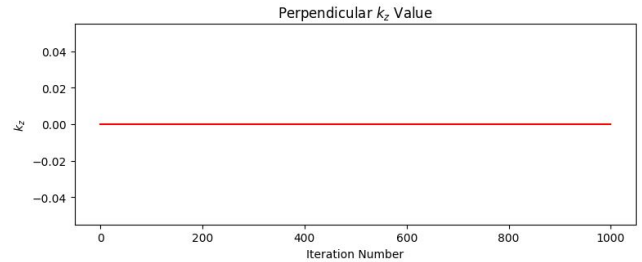


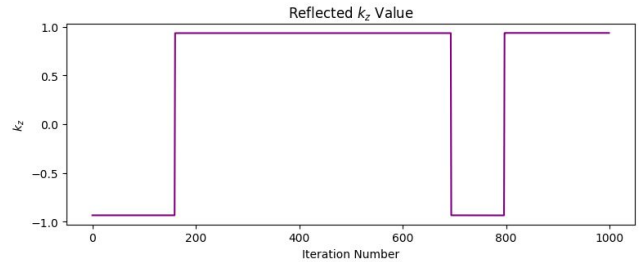




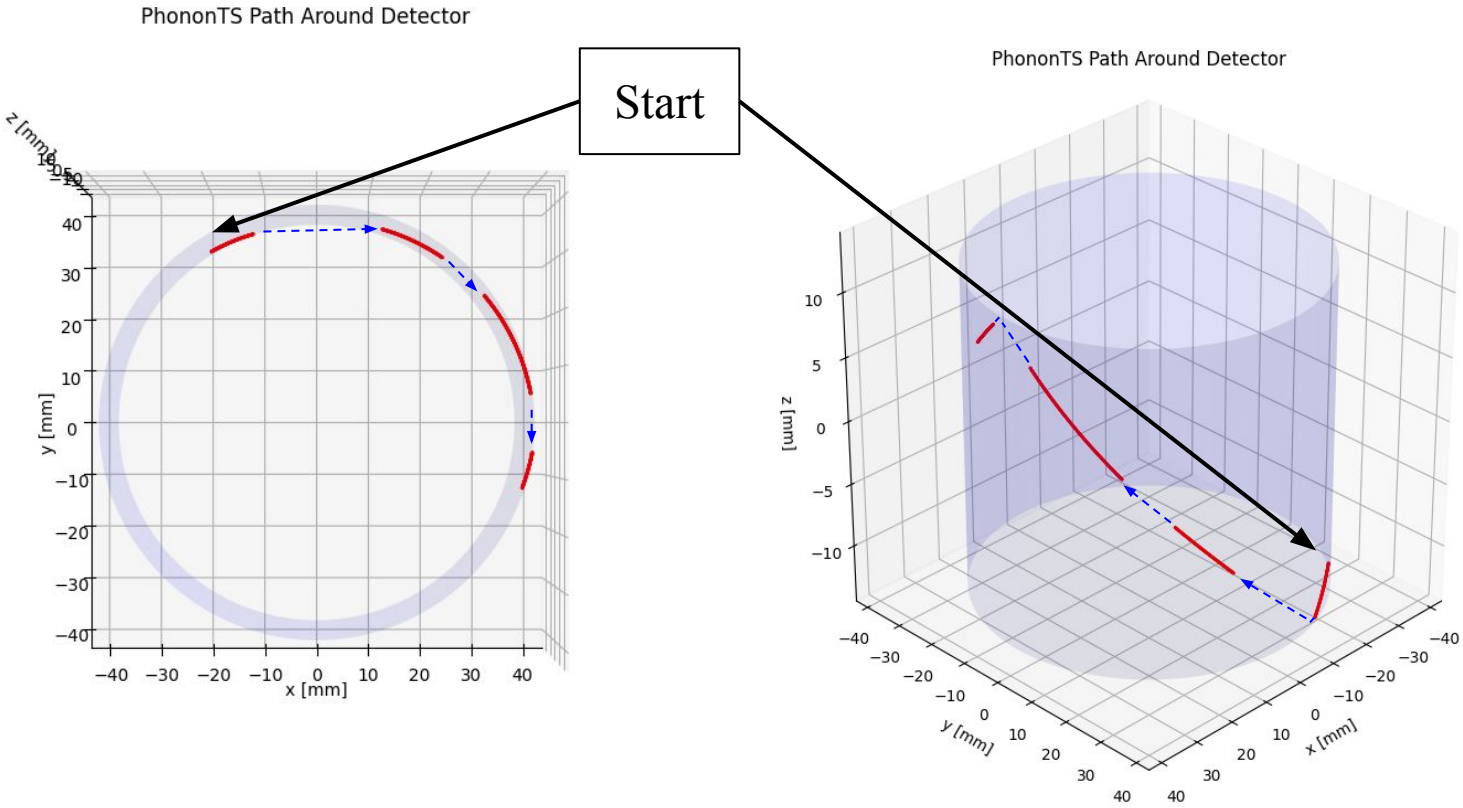








Failed Reflection - Long Arclength



These are scatter plots - The gap is due to the displacement across the flat taking 0 steps

Initial High Level Results → G4CMP-480

Single Detector:	**Rotated Detector (120 deg):**	**Displaced Detector:**
Collection Efficiency: 100%	Collection Efficiency: 100%	Collection Efficiency: 100%
Number of diffuse reflections:	Number of diffuse reflections:	Number of diffuse reflections:
Job 0: 15779	Job 0: 25217	Job 0: 13400
Job 1: 13659	Job 1: 23570	Job 1: 13311
Job 2: 15498	Job 2: 28885	Job 2: 17989
Job 3: 18651	Job 3: 26587	Job 3: 16416
Job 4: 17802	Job 4: 28836	Job 4: 18897
Total: 81,389	Total: 133,095	Total: 80,013
Diffuse reflections per event: 814	Diffuse reflections per event: 1331	Diffuse reflections per event: 800

The rotated detector indicates a problem with the transforms → G4CMP-480

High Level Results (After G4CMP-480)

Single Detector:	**Rotated Detector (120 deg):**	**Displaced Detector:**
Collection Efficiency: 100%	Collection Efficiency: 100%	Collection Efficiency: 100%
Number of diffuse reflections:	Number of diffuse reflections:	Number of diffuse reflections:
Job 0: 14798	Job 0: 14582	Job 0: 14137
Job 1: 14835	Job 1: 16932	Job 1: 19684
Job 2: 20441	Job 2: 14554	Job 2: 18008
Job 3: 17423	Job 3: 12468	Job 3: 18391
Job 4: 17226	Job 4: 15812	Job 4: 18897
Total: 84723	Total: 74348	Total: 89117
Diffuse reflections per event: 848	Diffuse reflections per event: 744	Diffuse reflections per event: 892

All events had 100% collection efficiency

High Level Results (After G4CMP-480)

Single Detector:	**Rotated & Displaced Detector:**
Collection Efficiency: 100%	Collection Efficiency: 100%
Number of diffuse reflections:	Number of diffuse reflections:
Job 0: 14798	Job 0: 20253
Job 1: 14835	Job 1: 14898
Job 2: 20441	Job 2: 21722
Job 3: 17423	Job 3: 13573
Job 4: 17226	Job 4: 16061
Total: 84723	Total: 86507
Diffuse reflections per event: 848	Diffuse reflections per event: 866

All events had 100% collection efficiency