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Title: Benchmarking Automatic Weight Window Generation in MCATK Against MCNP

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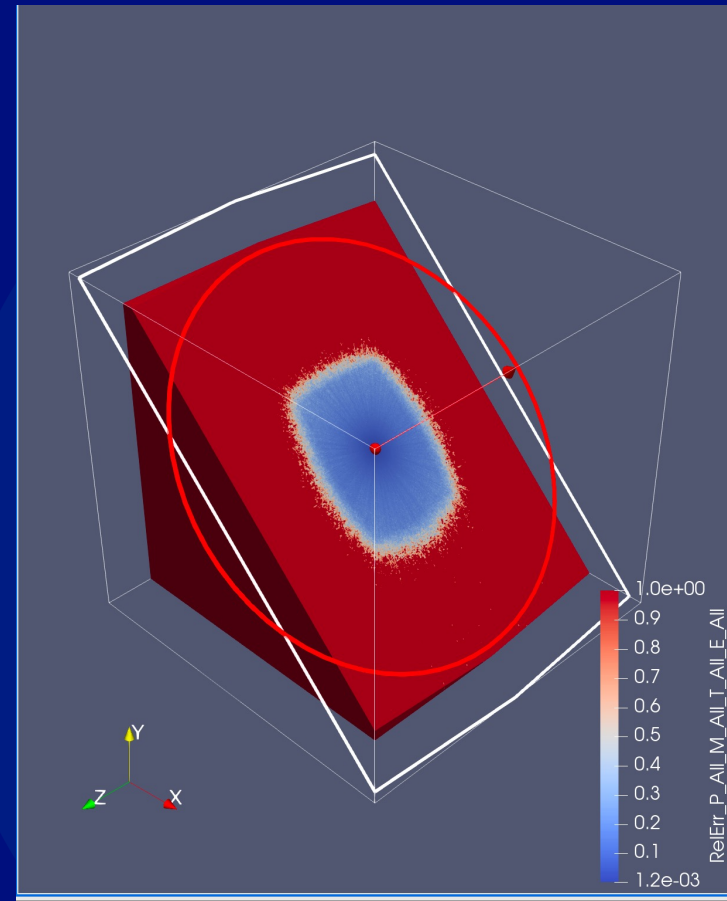
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Benchmarking Automatic Weight Window Generation in MCATK Against MCNP

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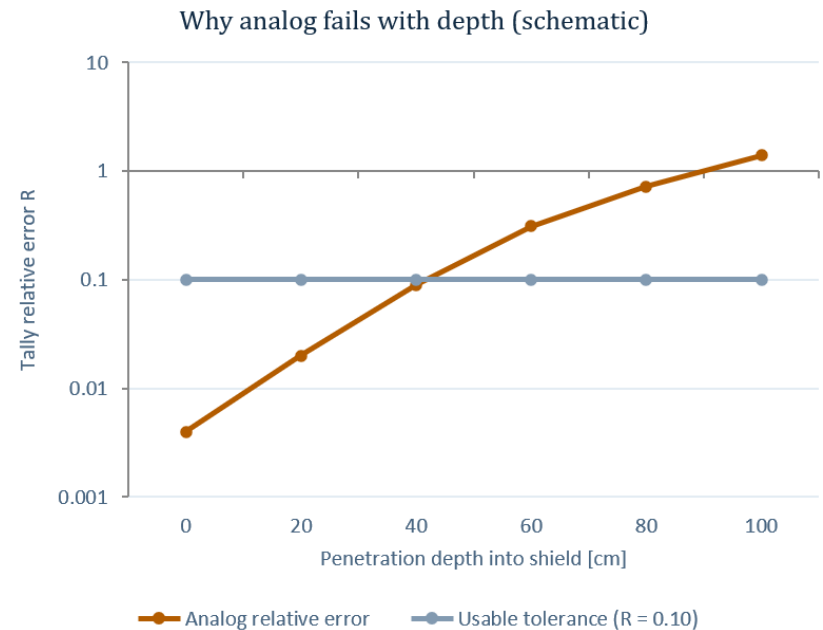
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Monte Carlo and the Need for Variance Reduction

- Monte Carlo (MC) transport is limited by statistical uncertainty from the random walk process
 - Tallies carry inherent noise
 - In deep-penetration problems, almost no histories reach the furthest regions
- Variance reduction (VR) techniques (“games”) modify the random walk to reduce variance while preserving the correct expected value
- **Weight windows (WW):** bias particle sampling toward important regions and away from unimportant ones, reducing the variance on selected tallies
- CADIS/FW-CADIS methods [1] generate importance maps by solving the adjoint transport equation
 - Automates the generation of WW, removing the guesswork of manually defining them



Cartoon schematic depicting the rising relative error of analog MC simulations with penetration depth.

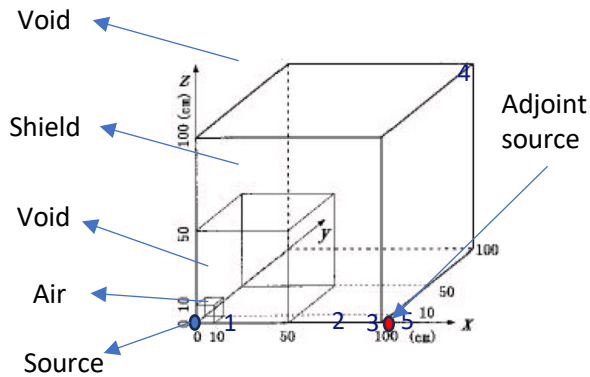
MCATK and PAVR

- The **M**onte **C**arlo **A**pplication **T**ool**K**it (MCATK) [2] is a C++ component-based Monte Carlo particle transport code
- **P**ARTISN-driven **V**ariance **R**eduction (PAVR) code couples the discrete ordinates code PARTISN [3] to MC codes such as MCATK
- Automatic WW generation capabilities using the CADIS formalism have been developed in MCATK within PAVR
 - CADIS optimizes for results at a **specific point in space**, not globally like FW-CADIS
- Testing and benchmarking of this feature is quite limited

Research Objectives

- Demonstrate that MCATK with PAVR enabled runs as intended
- Determine whether PAVR reduces uncertainty and/or the required runtime for estimating tallies for certain benchmark problems
- Compare MCATK results to MCNP [4] results to determine any differences in variance reduction effectiveness between the two codes
 - Demonstrate that Colin Weaver's dawwg-advanced-cadis feature for MCNP works as intended (i.e., it couples PARTISN to MCNP properly)

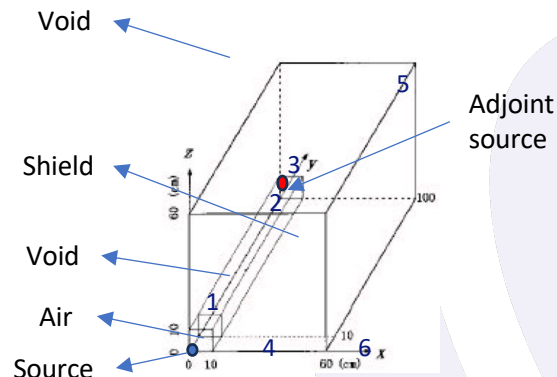
Benchmark Problem Specifications



Problem 1: Shield with Square Void [5]

Pure attenuation. No streaming path; flux falls off smoothly in every direction.

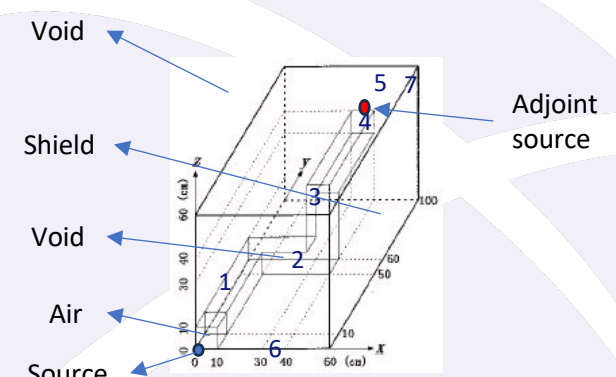
5 detectors



Problem 2: Shield with Void Duct [5]

Streaming through a 10 cm channel. Importance depends on being in the duct, not on radius.

6 detectors



Problem 3: Shield with Dog Leg Void Duct [5]

Three right-angle bends. Angularly peaked flux; CADIS method challenged the most here.

7 detectors

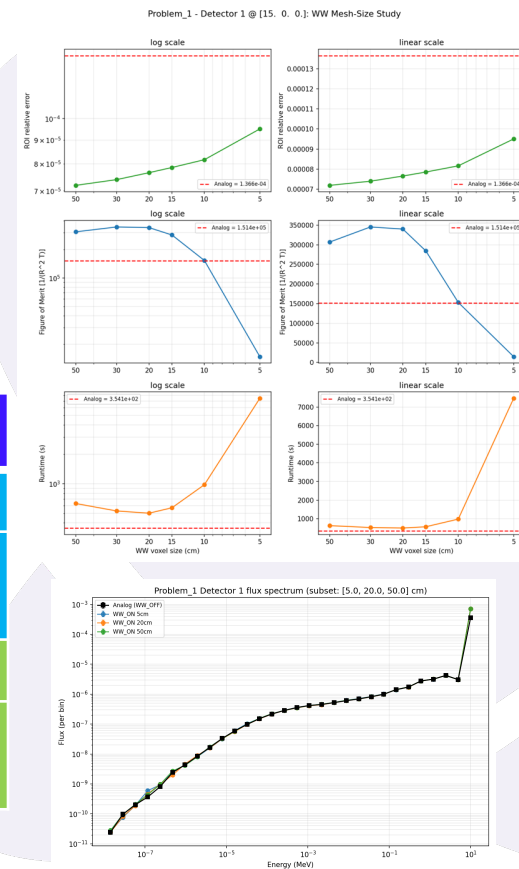
- Geometries reflected across all three coordinate planes (to mimic reflective boundary conditions)
- Void region outside the shield
- Monoenergetic (14.1 MeV), isotropic neutron point source at origin
- Materials: air, void, ordinary concrete

Calculational Setup

- MCATK WW OFF (analog) & WW ON and physics-matched MCNP simulations were performed
- To make fair comparisons of WW effectiveness, Figure of Merit (FOM) is compared:
 - $FOM = 1 / (R^2 * T)$
 - R = relative uncertainty
 - T = total simulation time
- Flux spectra at each detector are calculated for select WW mesh size + analog over 30 logarithmically spaced bins (shown in backup slides)

Code	Configuration	Weight Window Mesh Sizes
MCATK	WW OFF (Analog)	—
MCATK	WW ON	50 cm (only Pr. 1), 30 cm, 20 cm, 15 cm, 10 cm, 5 cm
MCNP	WW OFF (Analog)	—
MCNP	WW ON	50 cm (only Pr. 1), 30 cm, 20 cm, 15 cm, 10 cm, 5 cm

Example MCATK results: Problem 1, detector 1



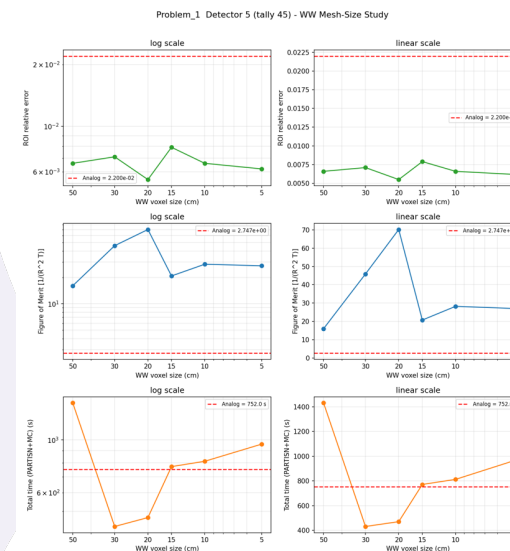
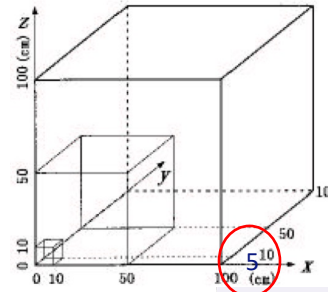
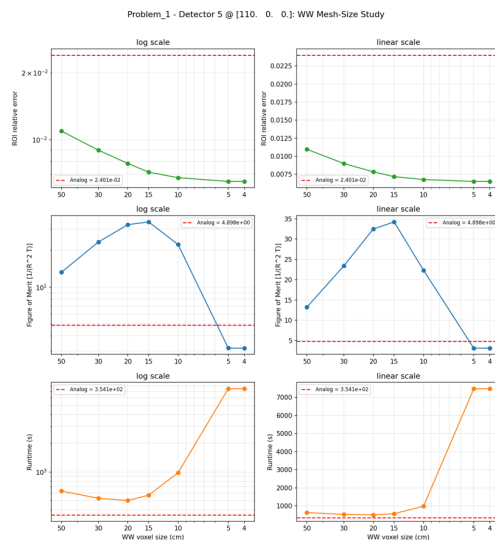
Simulation Specifications

- Deterministic parameters held constant between MCATK and MCNP
 - Caveat: MCNP Problem 1 15 cm, 10 cm, and 5 cm & Problem 2 10 cm simulations use the 21-energy group structure instead of the default 30-group structure (to avoid negative adjoint fluxes)
- 1e6 particles simulated in each MC run
- Every simulation was run in serial (1 core) on Rocinante to keep runtimes consistent
- ENDF/B-VII.1 continuous energy cross section library used for MC transport

Problem 1 Results – Detector 5 (110, 0, 0)

MCATK

MCNP

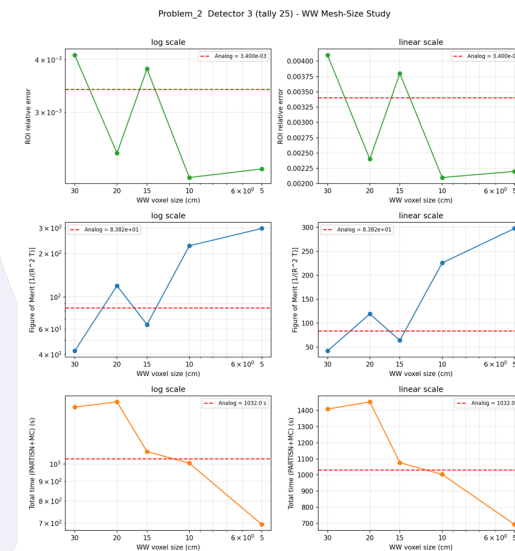
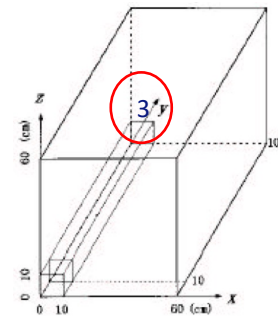
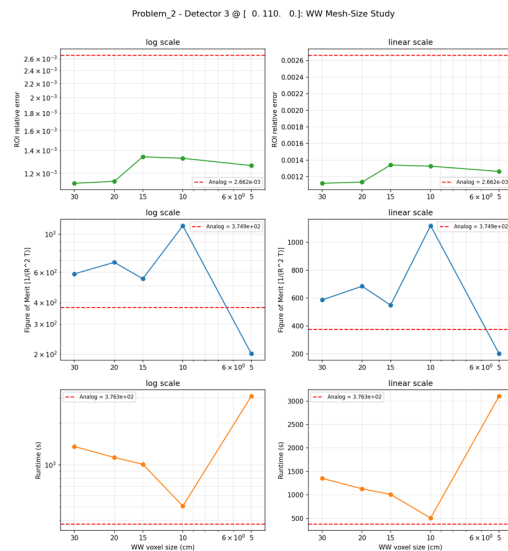


- MCNP wins outright: peak FOM 70.1 at 20 cm vs. MCATK's 34.2 at 15 cm (26x vs. 7x over analog)
- Optimum sits at 15-20 cm for both codes ; MCATK's 15/20 cm points are a flat plateau
- MCATK relative error falls monotonically with mesh refinement ($0.011 \rightarrow 0.0065$); the FOM collapse below 10 cm is entirely a runtime effect, not an accuracy one

Problem 2 Results – Detector 3 (0, 110, 0)

MCATK

MCNP

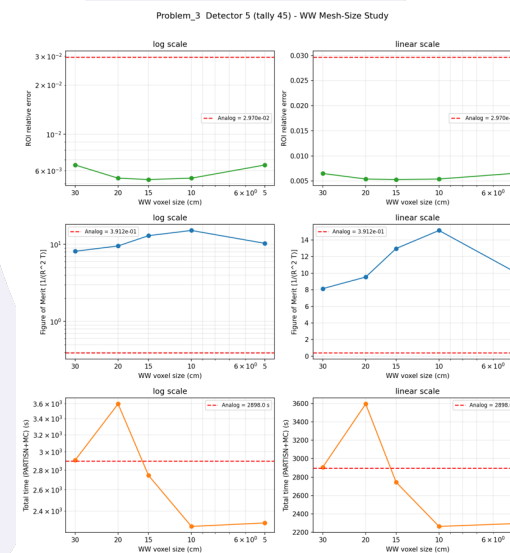
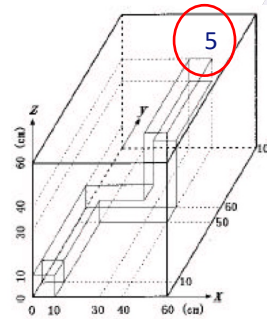
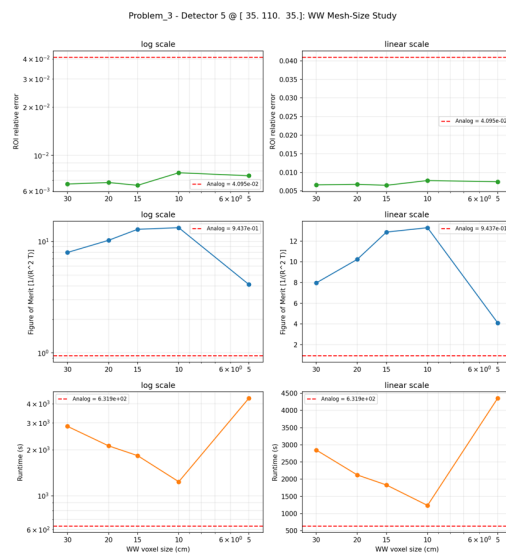


- Both codes either peak or show a strong local peak at 10 cm, exactly the duct width
- MCATK holds a 5x absolute FOM advantage at that optimum (1120 vs. 228)
- Normalized gains are the smallest in this case (3x and 2.7x); this detector has by far the highest analog FOM (375 and 84), so there is less room for improvement
- MCNP falls below analog at 30 cm and 15 cm; MCATK falls below analog at 5 cm

Problem 3 Results – Detector 5 (35, 110, 35)

MCATK

MCNP



- Cleanest cross-code agreement in the study: both peak at 10 cm, absolute FOM 13.3 vs. 15.0 (within 13%), relative error curves nearly coincident at 0.005-0.008
- MCNP's much larger normalized gain (39x vs. 14x) comes entirely from a worse analog FOM baseline (0.391 vs. 0.944), not better weight windows
- Both codes suppress relative error $\sim 6\times$ below analog across every mesh size

Overall Takeaways

- **Weight windows cut relative error several-fold versus analog at each code's optimal mesh, enough to reach the same precision with far fewer histories**
- Optimal WW voxel size is **10-20 cm** across all three problems and both codes (i.e., 1-2 shield mean free paths). The finest mesh is never optimal for PAVR
- PAVR wins on absolute FOM in Problem 2 (5x) and ties in Problem 3 (13%); MCNP wins in Problem 1 (2x). No code dominates
- **PAVR degrades sharply at 5 cm in all three problems** (FOM drops to 0.5-4x), while MCNP holds 3.6-26x at 5 cm. The single most consistent difference between the codes

The Fine-Mesh Runtime Penalty

- MCATK runtime at 5 cm exceeds its own optimum-mesh runtime by 15x (P1), 6x (P2), and 3.5x (P3)
- MCNP runtime at 5 cm is at or near its minimum in all three problems (827 s, 575 s, 2160 s)
- Relative error keeps improving or stays flat for MCATK at 5 cm. The FOM collapse is purely cost, not degraded windows
- Good optimization target: PAVR's per-voxel overhead (during MC transport, window lookup, split/roulette bookkeeping, etc.) rather than the underlying importance map

Conclusions & Future Work

Conclusions

- 3 benchmark problems constructed in MCATK and MCNP
- Simulations were run without WW and with WW of varying mesh sizes
- It was determined that PAVR does indeed reduce the uncertainty of specified tallies compared to analog MC and performs comparably to MCNP's automatic weight window generation
- Verified that Colin Weaver's dawwg-advanced-cadis feature works as intended

Future Work

- Run simulations with multiple cores and determine impact on FOM
- Figure out why PARTISN in MCNP was generating negative adjoint fluxes in some instances
- Further explore the memory limitations of fine meshes (< 5 cm)
- Implement FW-CADIS in MCATK

References

- [1] Haghghat, A., & Wagner, J. C. (2003). Monte Carlo variance reduction with deterministic importance functions. *Progress in Nuclear Energy*, 42(1), 25-53. [https://doi.org/10.1016/S0149-1970\(02\)00002-1](https://doi.org/10.1016/S0149-1970(02)00002-1)
- [2] Jeremy Sweezy, Tim Burke, Terry Adams, Simon Bolding, Jesse Giron, Alex Long, Steven Nolen, Corey Skinner, Aaron Tumalak, Tony Zukaitis, Austin McCartney, Travis Trahan, 2024 MCATK Status, EPJ Nuclear Sci. Technol. **11**, 49 (2025). <https://doi.org/10.1051/epjn/2025035>.
- [3] R. E. Alcouffe and R. S. Baker. "PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System", LA-UR-08-07258 (March 2009).
- [4] Kulesza, J. A. (Ed.). (2024). *MCNP® code version 6.3.1 theory & user manual* (Tech. Rep. No. LA-UR-24-24602, Rev. 1). Los Alamos National Laboratory. <https://mcnp.lanl.gov/manual.html> [1, 2, 3, 4]
- [5] Toth, B., & Brown, F. B. (2003). *MCNP5 benchmark calculations for 3-D radiation transport in simple geometries with void regions* (Report No. LA-UR-03-5974). Los Alamos National Laboratory. https://mcnp.lanl.gov/pdf_files/TechReport_2003_LANL_LA-UR-03-5974_TohtBrown.pdf

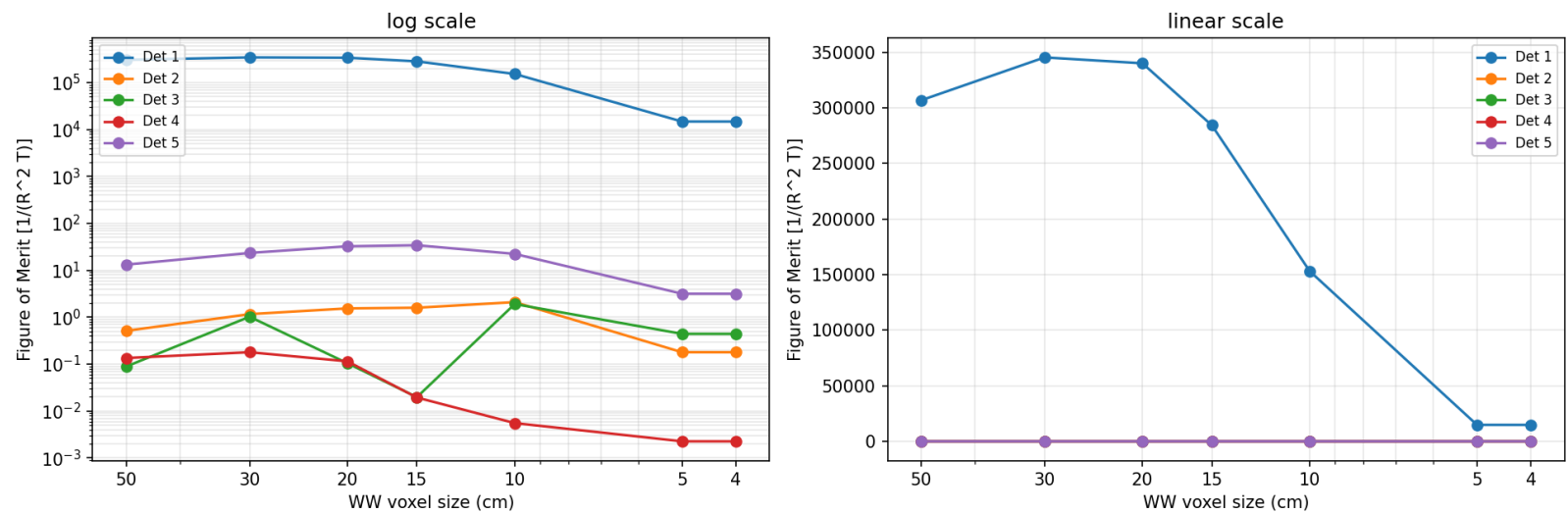
Acknowledgements

- Aaron Tumulak
- Simon Bolding
- Colin Weaver
- ASC Transport Project for providing the funding for my work this summer.

Backup Slides

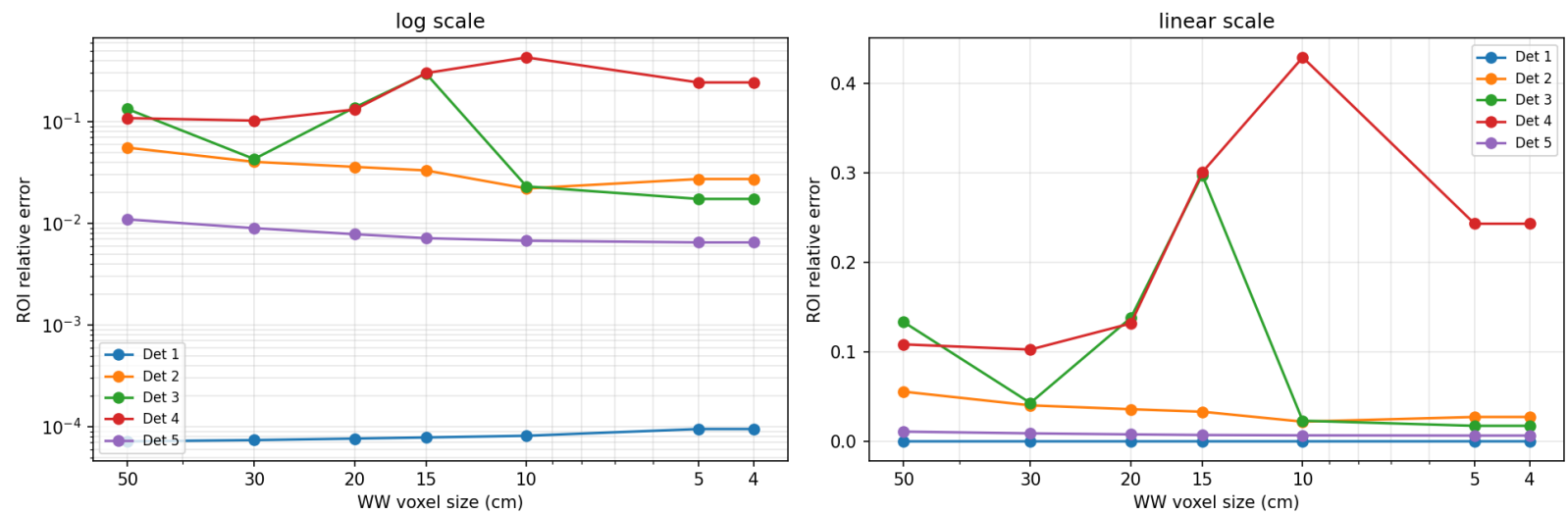
MCATK Problem 1 FOM All Detectors Overlay

Problem_1: Figure of Merit [$1/(R^2 T)$] vs WW mesh (all detectors)



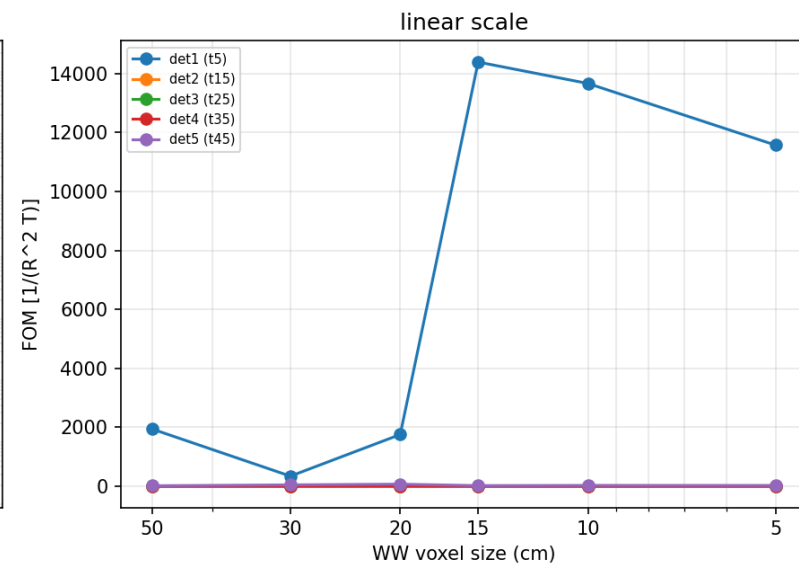
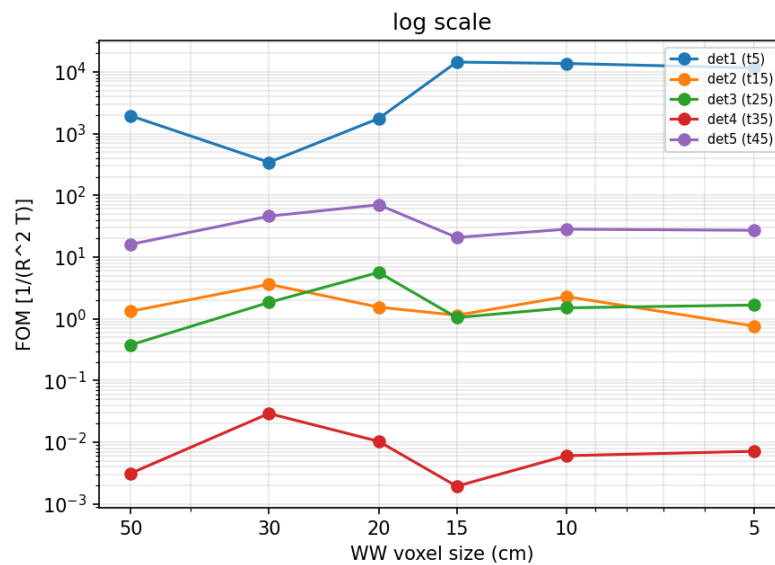
MCATK Problem 1 Relative Error All Detectors Overlay

Problem_1: ROI relative error vs WW mesh (all detectors)



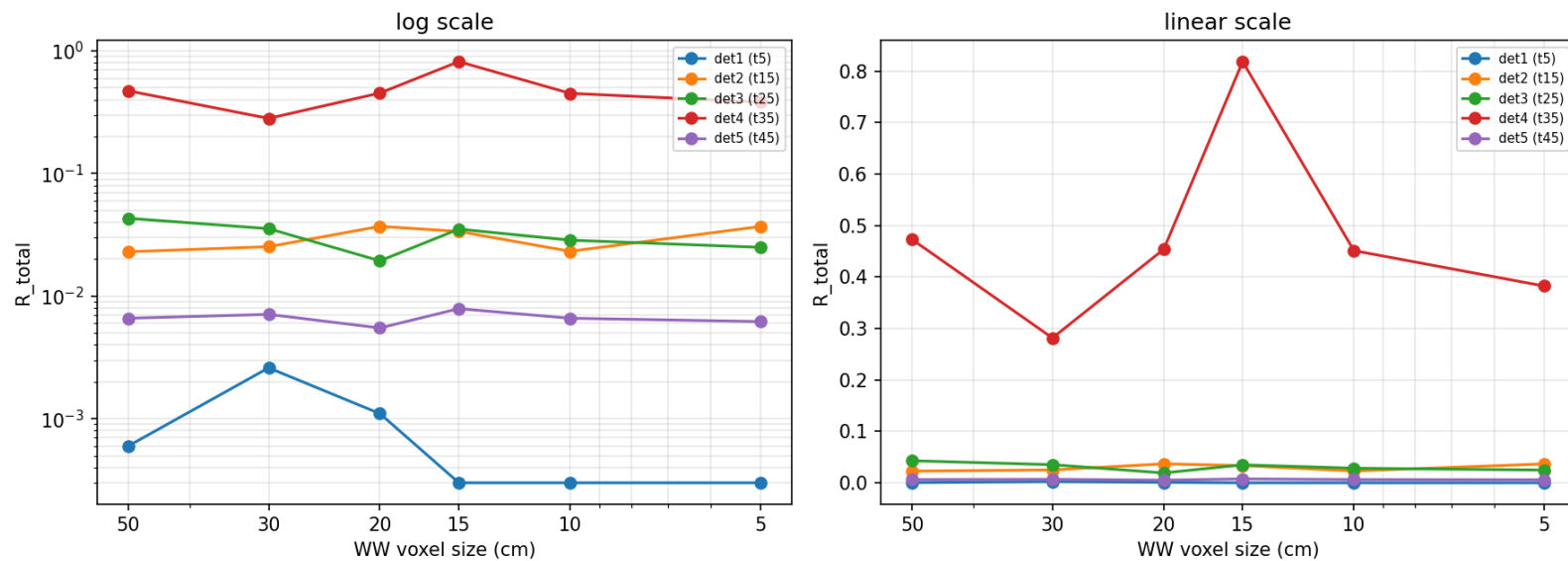
MCNP Problem 1 FOM All Detectors Overlay

Problem_1 FOM vs WW mesh - all detectors



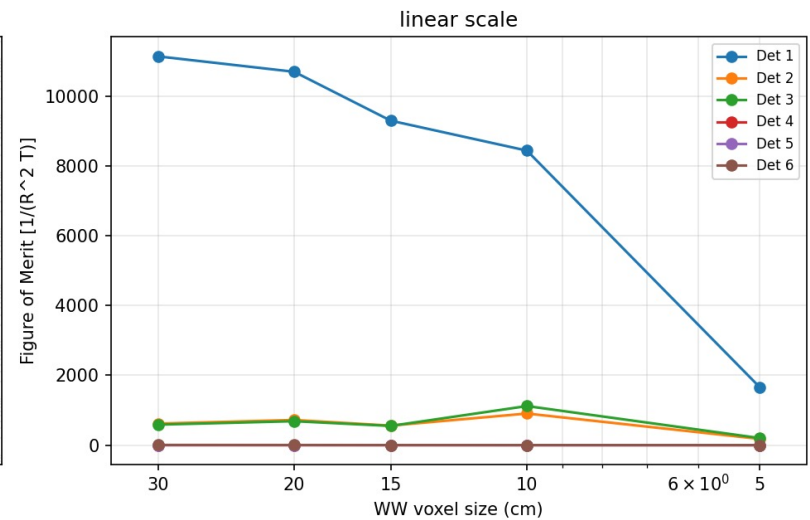
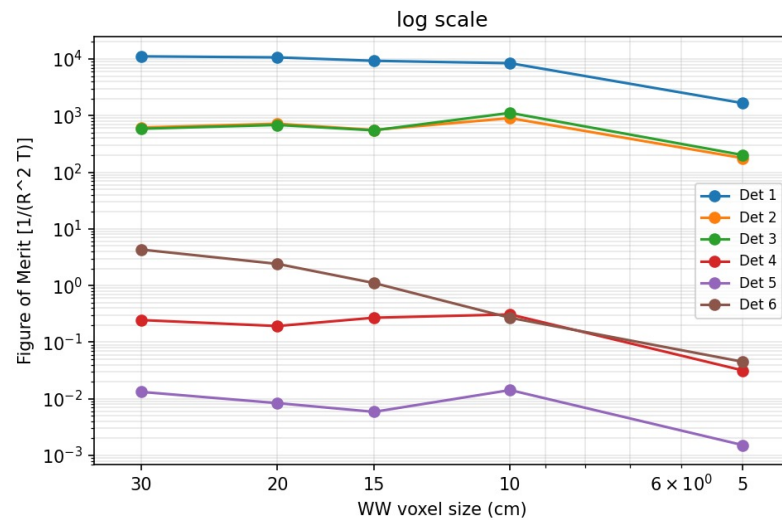
MCNP Problem 1 Relative Error All Detectors Overlay

Problem_1 Relative error vs WW mesh - all detectors



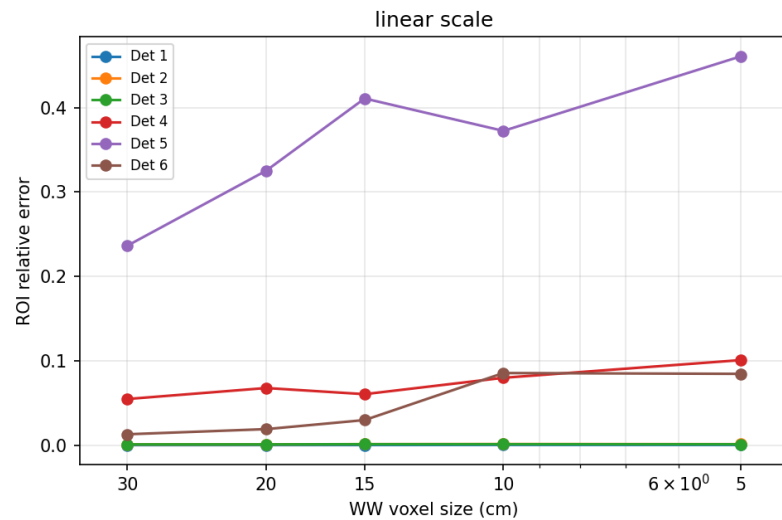
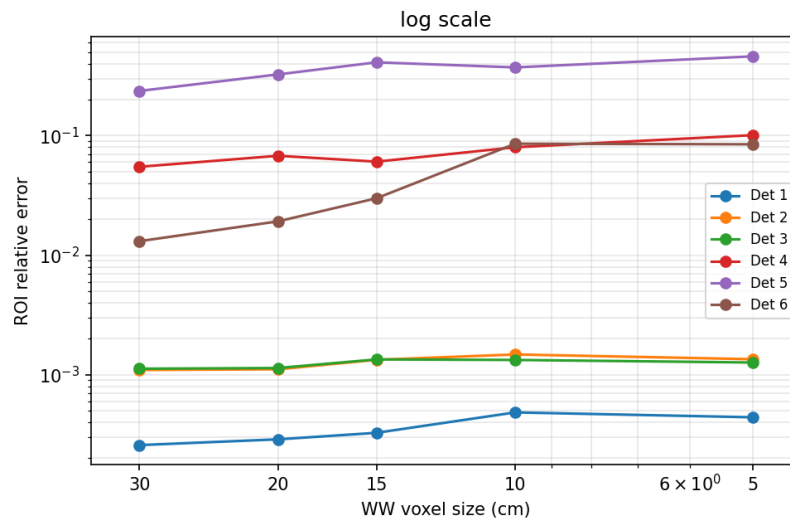
MCATK Problem 2 FOM All Detectors Overlay

Problem_2: Figure of Merit [$1/(R^2 T)$] vs WW mesh (all detectors)



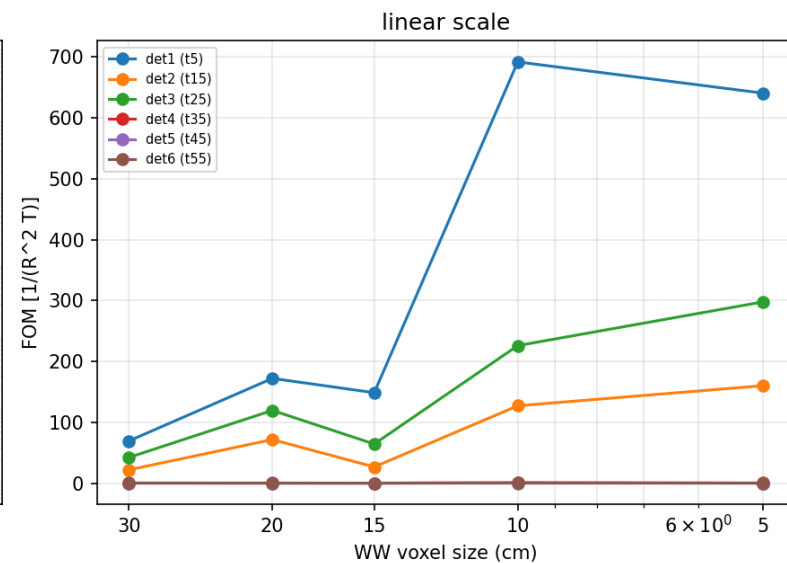
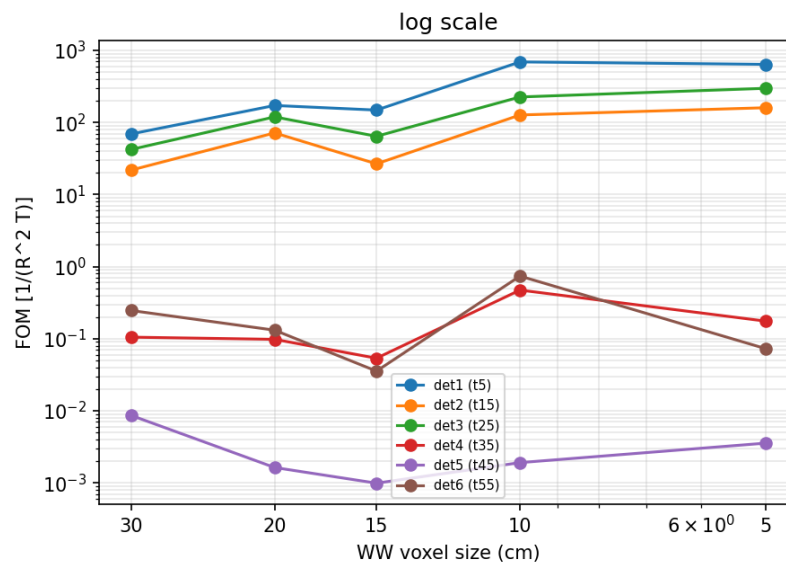
MCATK Problem 2 Relative Error All Detectors Overlay

Problem_2: ROI relative error vs WW mesh (all detectors)



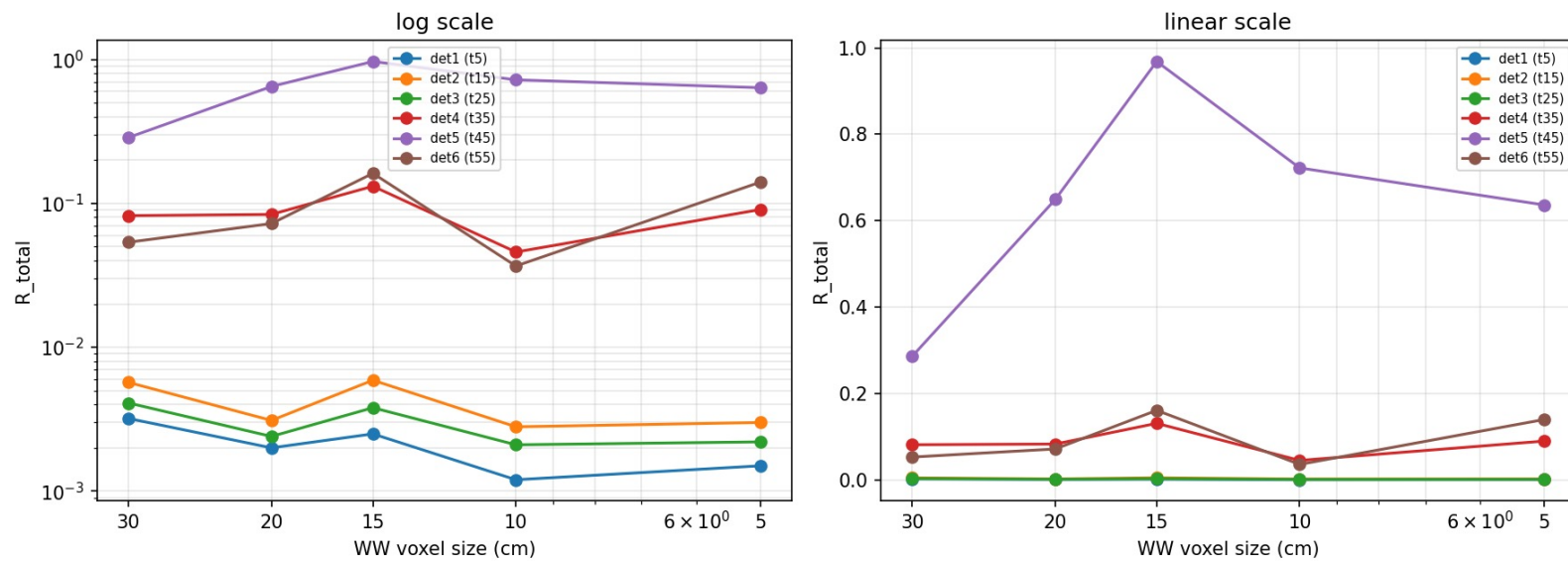
MCNP Problem 2 FOM All Detectors Overlay

Problem_2 FOM vs WW mesh - all detectors



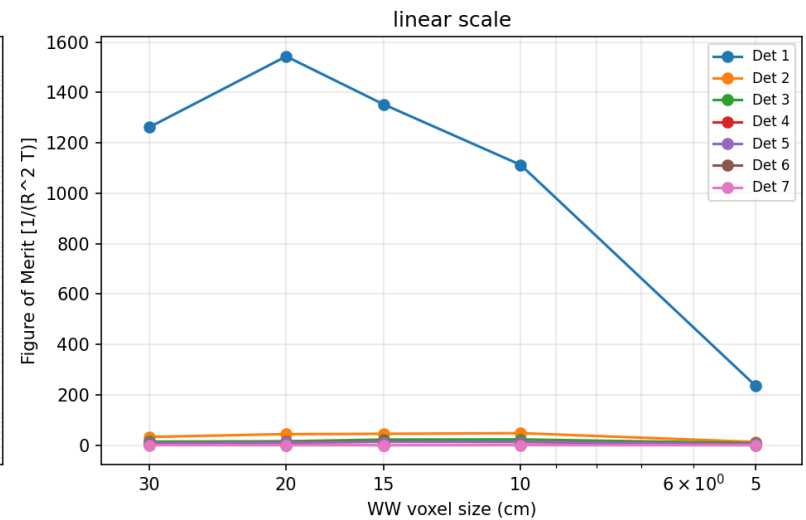
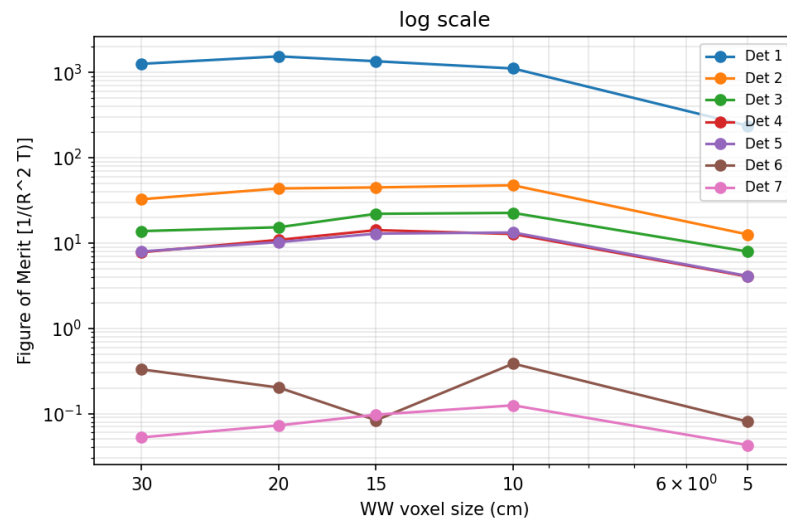
MCNP Problem 2 Relative Error All Detectors Overlay

Problem_2 Relative error vs WW mesh - all detectors



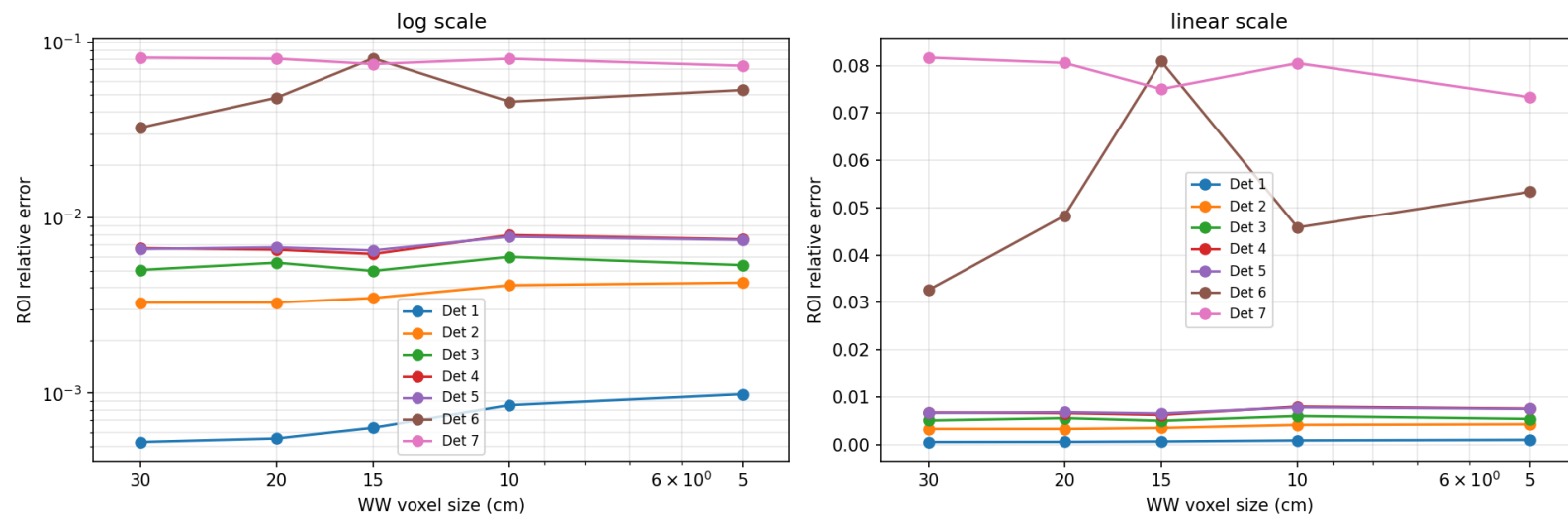
MCATK Problem 3 FOM All Detectors Overlay

Problem_3: Figure of Merit [$1/(R^2 T)$] vs WW mesh (all detectors)



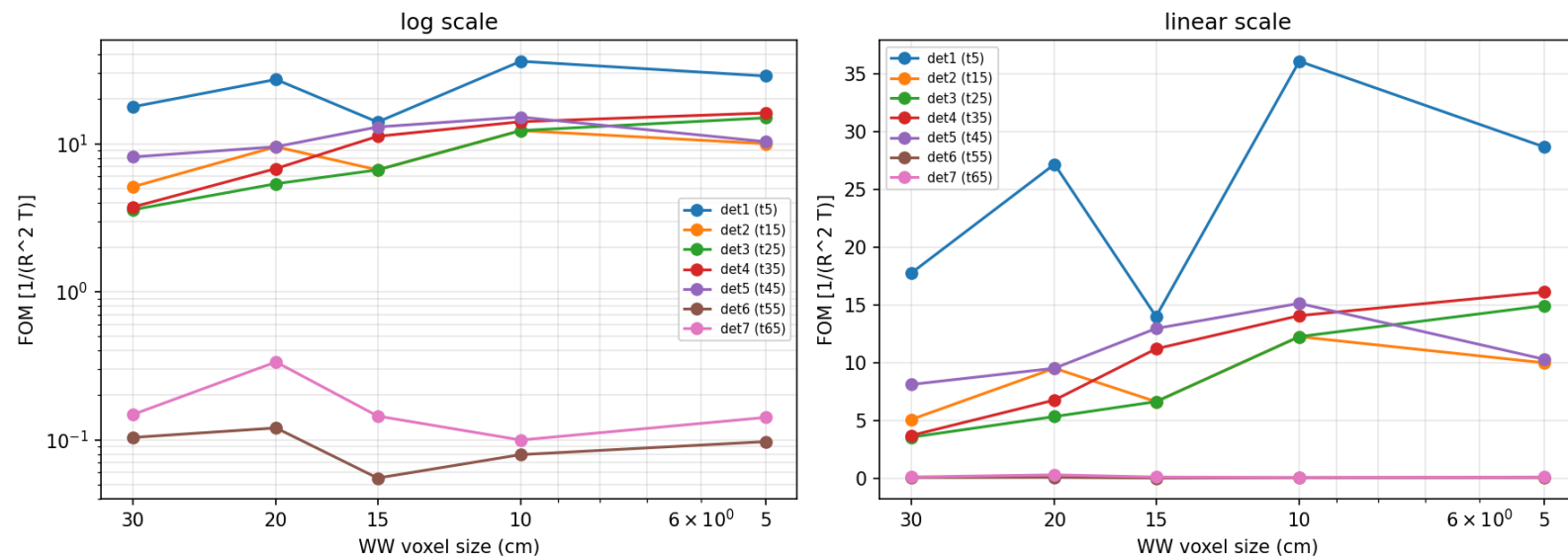
MCATK Problem 3 Relative Error All Detectors Overlay

Problem_3: ROI relative error vs WW mesh (all detectors)



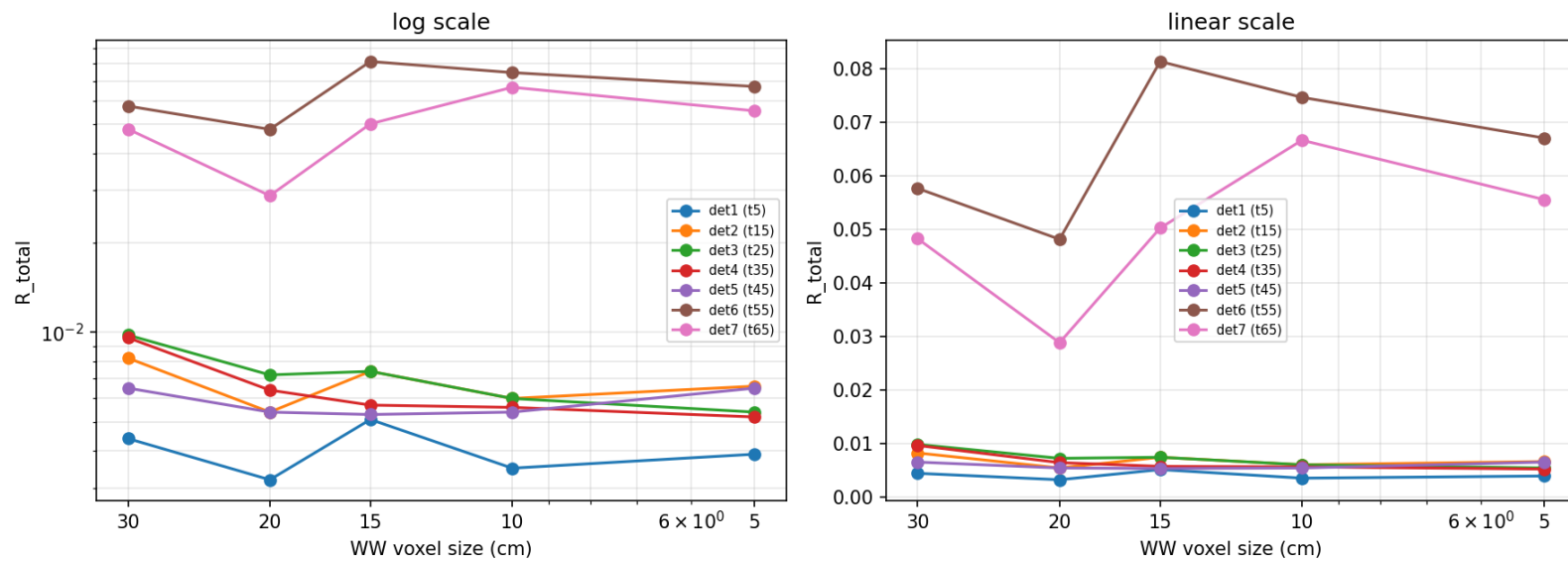
MCNP Problem 3 FOM All Detectors Overlay

Problem_3 FOM vs WW mesh - all detectors

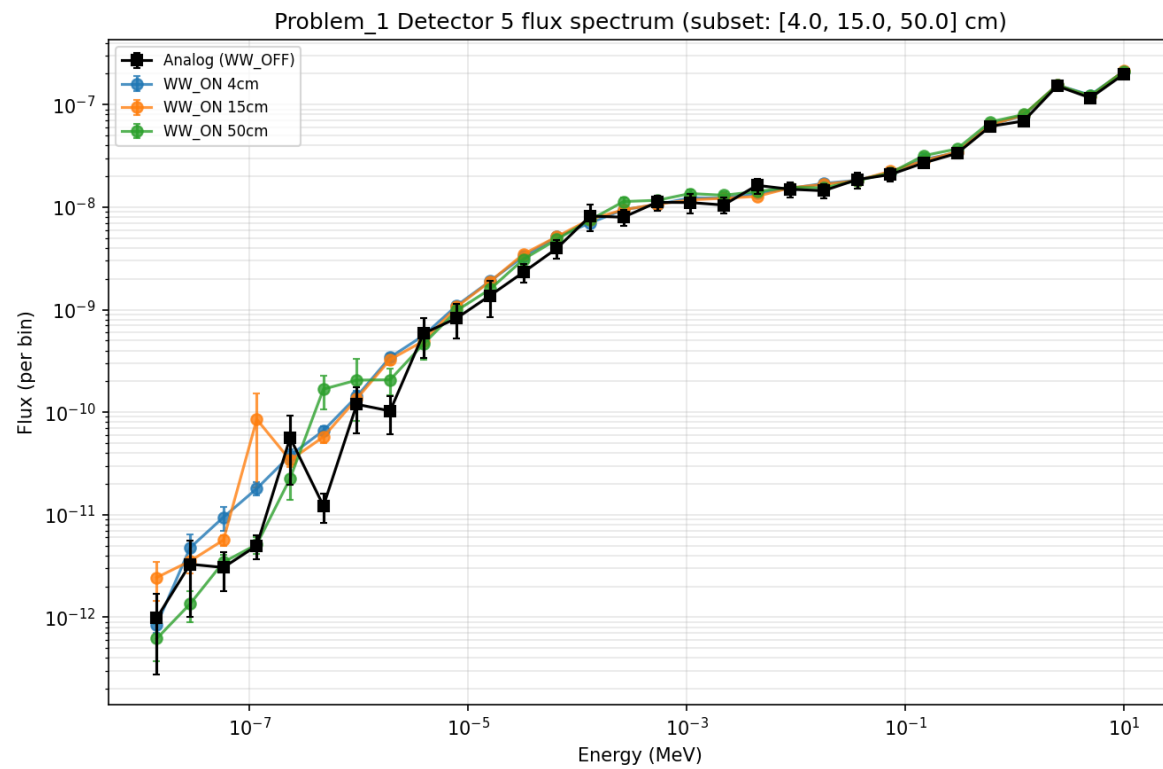


MCNP Problem 3 Relative Error All Detectors Overlay

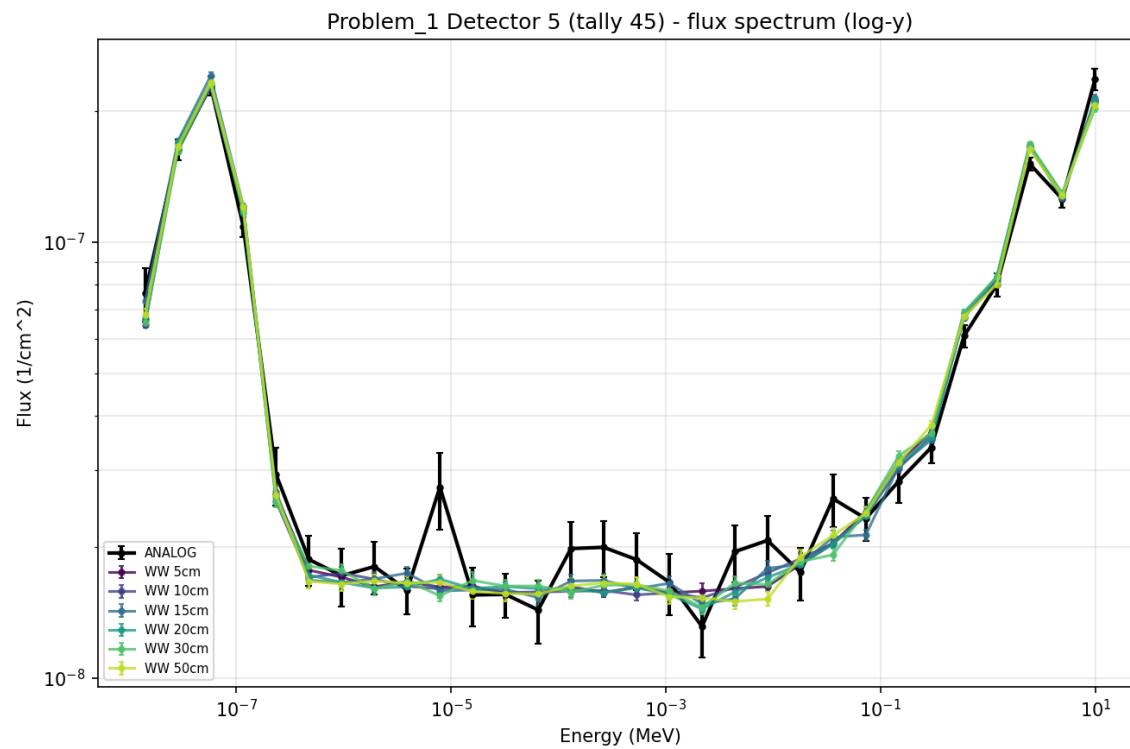
Problem_3 Relative error vs WW mesh - all detectors



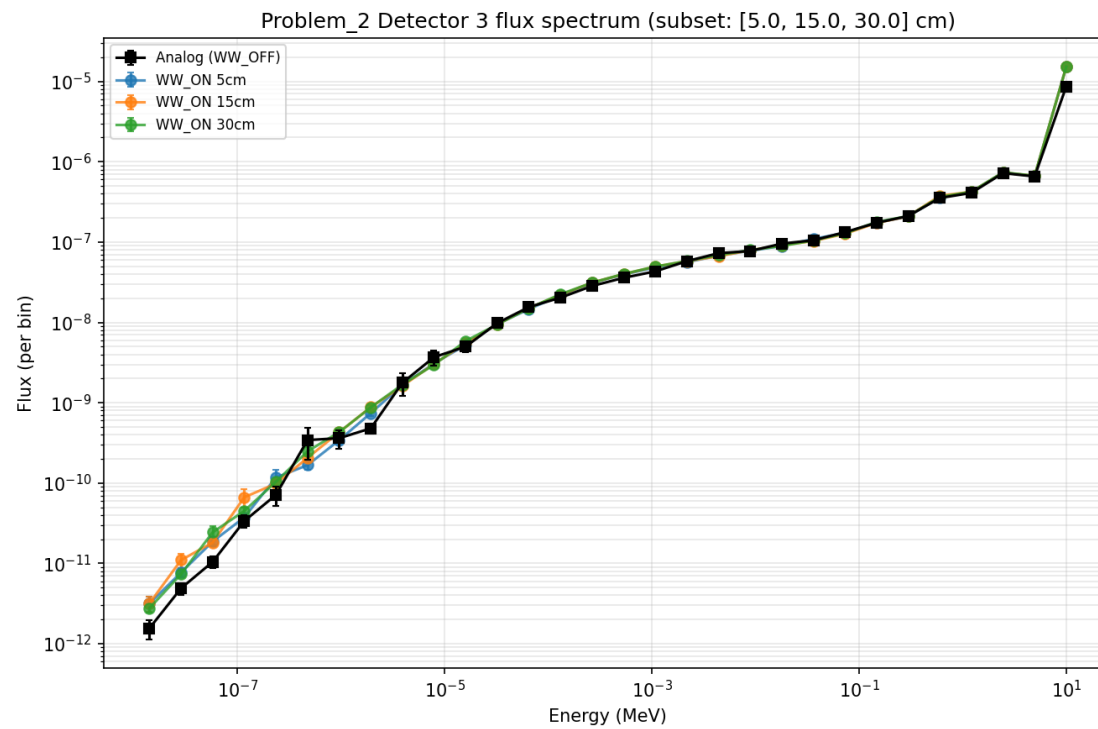
MCATK Problem 1 Detector 5 Flux Spectra



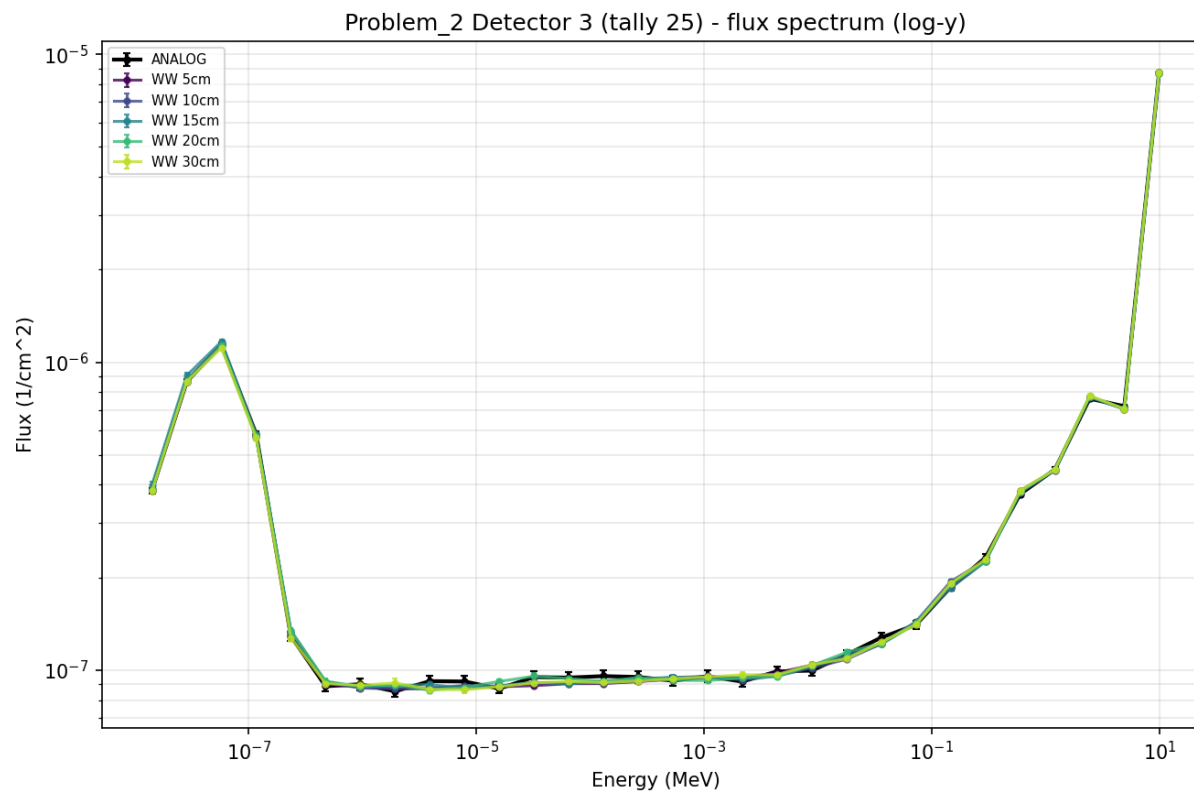
MCNP Problem 1 Detector 5 Flux Spectra



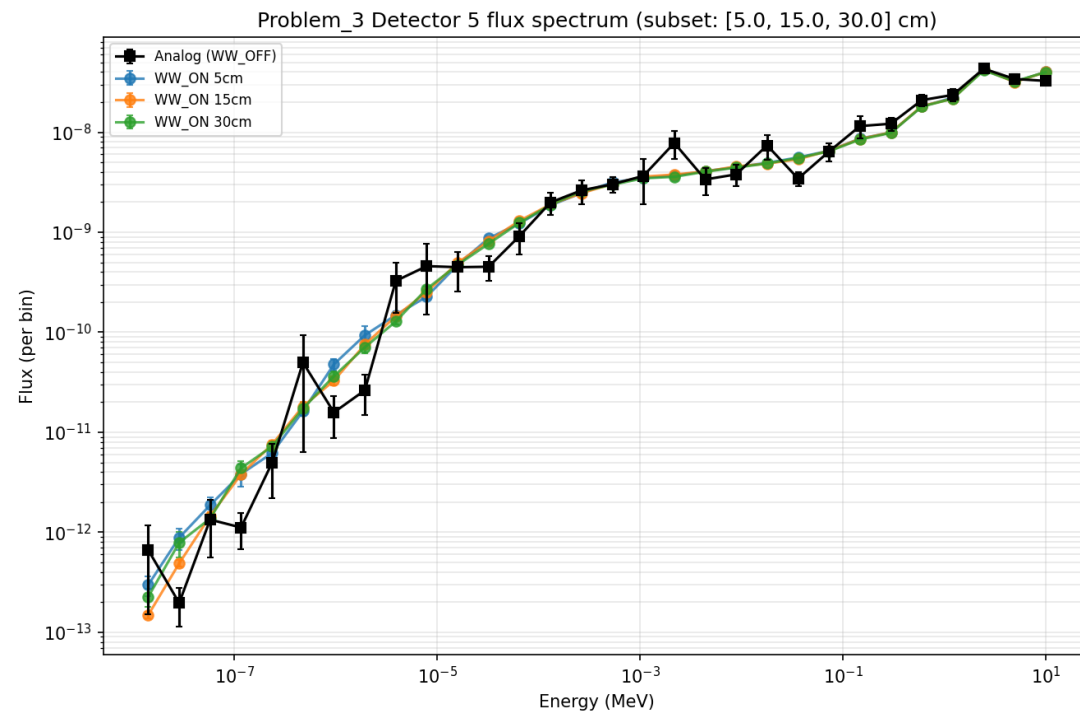
MCATK Problem 2 Detector 3 Flux Spectra



MCNP Problem 2 Detector 3 Flux Spectra



MCATK Problem 3 Detector 5 Flux Spectra



MCNP Problem 3 Detector 5 Flux Spectra

