# Mesh Cells to Augment in Situ Spectroscopy

## MCNP Simulation of Soil Carbon Detection

Jose Andres Cortes, Andrej Korzeniowski, Allen Torbert, Galina Yakubova and Aleksandr Kavetskiy

UT Arlington, USDA-ARS

July 8th, 2025

1. Introduction
2. Soil in MCNP
3. Results
4. Conclusion

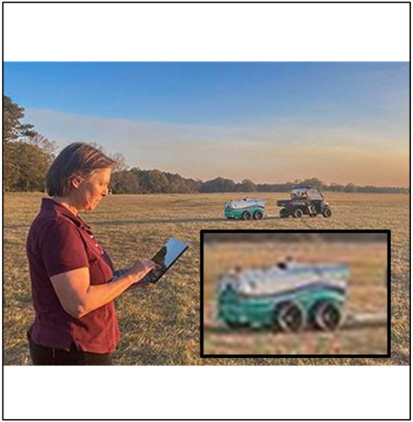
# Background

1. Collaborating with USDA Agriculture Research Service
2. Developing an in situ spectroscopy device for soil analysis

# Core Harvesting

1. Traditional method: “Core Harvesting”
2. Large soil cores extracted and analyzed in lab
3. Time-consuming, labor-intensive

# In Situ Spectroscopy Device



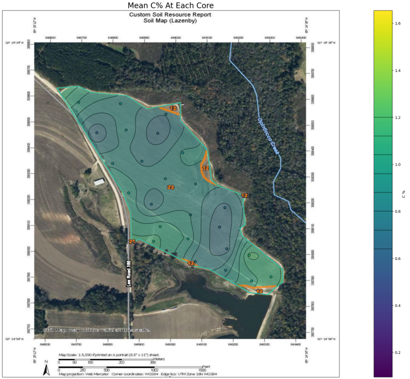
1. Fast, nondestructive, cost-effective alternative
2. “Mobile Inelastic Neutron Scattering System”
3. Uses gamma ray spectroscopy to measure soil composition directly

# Simulation is done in MCNP

1. My role: Mathematical support and simulation
2. Analyze and generate spectroscopy results Simulations performed in MCNP6.2
3. Presenting challenges addressed with MCNP

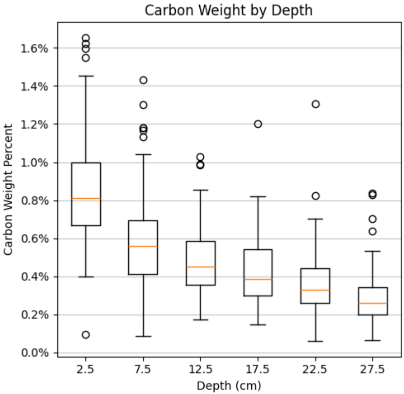
1. Introduction
2. **Soil in MCNP**
3. Results
4. Conclusion

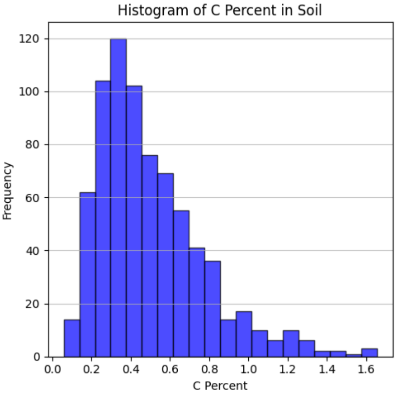
# Soil is a Nonhomogeneous Material




1. MCNP cells assume homogeneous material
2. Real soil: heterogeneous

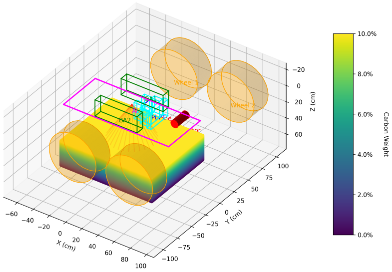
# Carbon by Depth



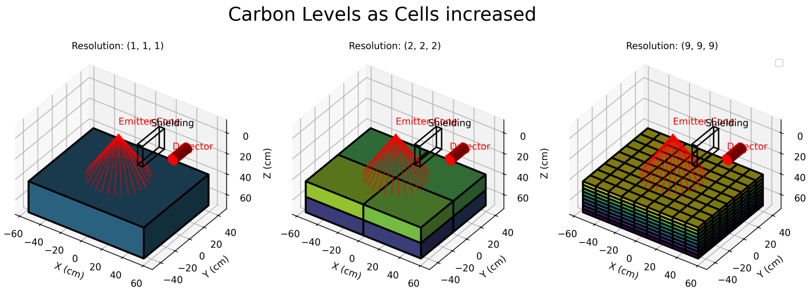

1. Carbon often decreases exponentially with depth

# Functionally Defined Soil



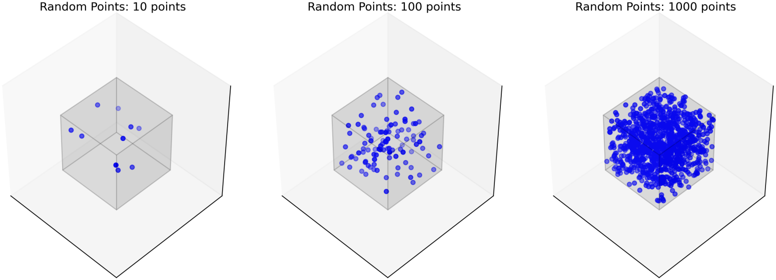

1. Soil characteristics can be described as functions of 3D space
2. Needed a way to translate this into MCNP input

# Mesh Cells




1. Divide soil into a mesh of smaller cells Approximate functional characteristics in discrete space
2. Higher mesh resolution = more accurate representation

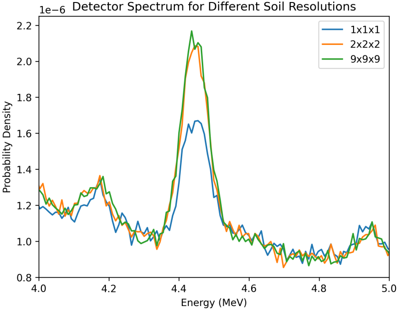
# Defining cell characteristics




1. Use Monte Carlo sampling to average properties in each mesh cell
2. Assign average values to each cell

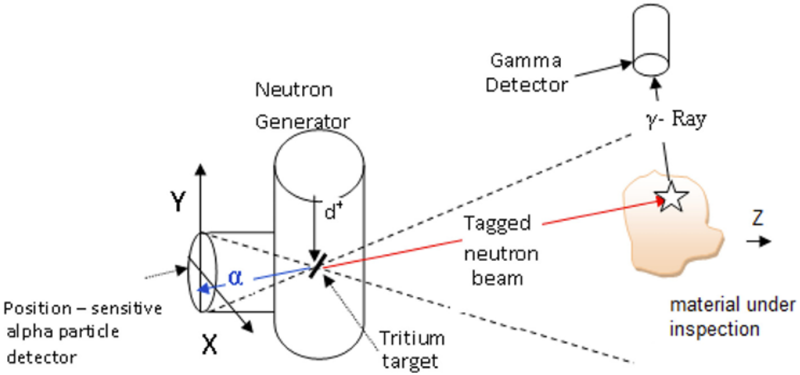
1. Introduction
2. Soil in MCNP
3. Results
4. Conclusion

# effects on detection



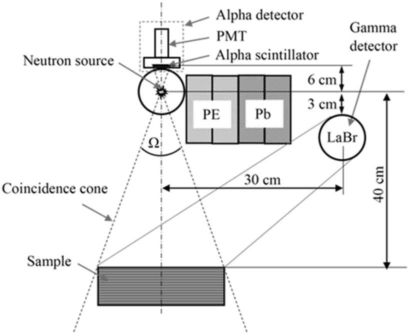

1. As mesh resolution increases, carbon density approaches true function
2. Effects on spectral readings around key energy ranges (e.g., 4.4 MeV)

# Lab spectroscopy can cover entire sample




1. Investigate detection range of the device
2. Lab: detector covers entire sample

# Soil is a Semi-Infinite Sample



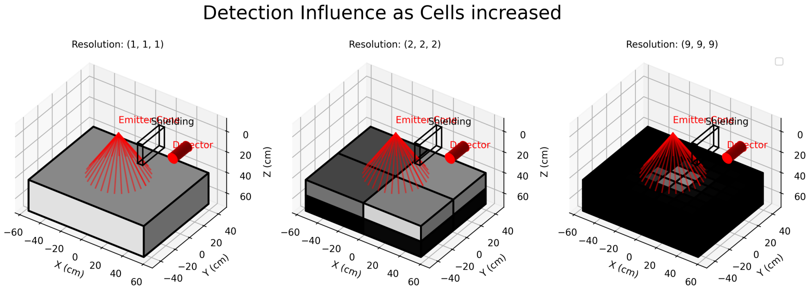

1. Investigate detection range of the device
2. Field: soil is semi-infinite, detection range is finite

# Cell Mesh vs FMESH

```
(FMESH
FMESH836:p,n ORIGIN= 0 0 42 IMESH= -56 9i 56  JMESH= -45 9i 45 KMESH= 0 9i 20

(1x1x1)
F836:p,n 101
E836 0 1e-5 932i 8.4295
FU836 9000000 10000000000
FT836 TAG 3


(2x2x2)
F836:p,n 101
E836 0 1e-5 932i 8.4295
FU836 9000000 9100000 9200000 9300000 9400000 9500000 9600000 9700000 10000000000
FT836 TAG 3

(9x9x9)
F836:p,n 101
E836 0 1e-5 932i 8.4295
FU836 900000000 900100000 900200000 900300000 900400000
        900500000 900600000 900700000 900800000 900900000 901000000
        901200000 901300000 901400000 901500000 901600000 901700000
        901800000 901900000 902000000 902100000 902200000 902300000
        902500000 902600000 902700000 902800000 902900000 903000000
        903100000 903200000 903300000 903400000 903500000 903600000...
```

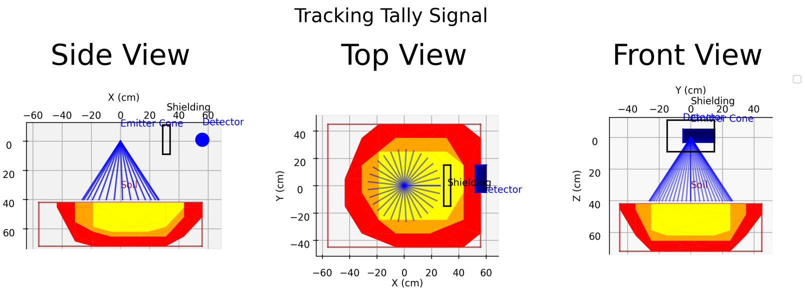
1. MCNP FMESH: tally results in mesh bins (for imaging, range studies)
2. Cell meshes: can also tally per cell
3. Both methods help analyze detection range

# Independent Cell Functionality



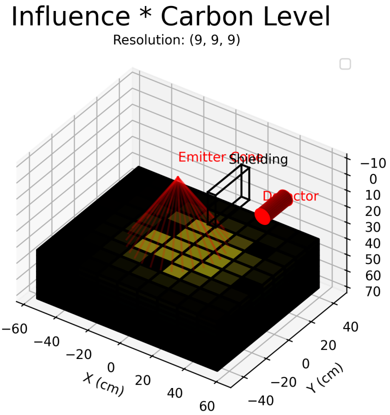

1. Treat mesh cells as independent
2. U card: bins tally by cell of interaction
3. Allows investigation of where detections originate

# Cell influence clouds



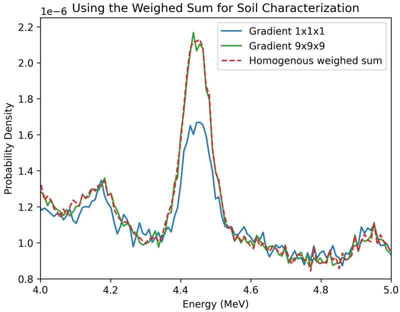

1. Cells can be grouped into ”clouds” by influence
2. 90, 95, 99 percent detection influence

# Measured Characteristic



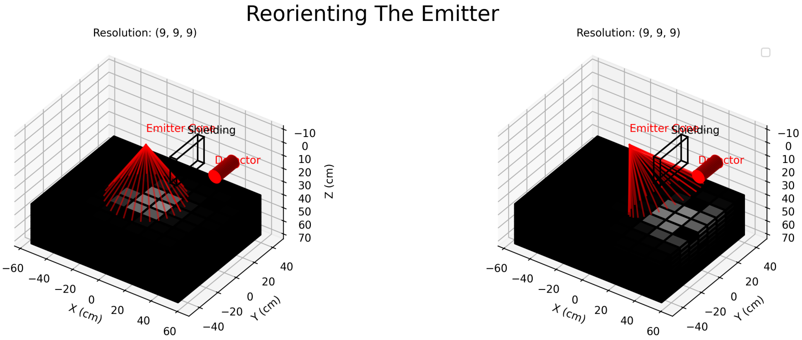

1. Sum(Cell detector influence * Cell Carbon weight) = Measured Carbon

# Gradient vs Homogeneous Characteristic from Gradient Weighed Avg




1. Weighted sum of homogeneous cell returns similar results to heterogeneous mesh

# Usage Example




1. When machine design changes, simulate new detection results
2. Range can be re-evaluated
3. Example: pointing emitter under detector changes detection range

# Summary

1. Mesh cells allow for detailed soil modeling in MCNP
2. Enables accurate simulation of in situ spectroscopy
3. Helps understand detection range and sensitivity

# Future Work

1. Further refine mesh resolution for improved accuracy (theoretical limit of 10,000 cells)
2. Explore additional soil characteristics (hydration)
3. Accurate comparison with core harvesting results

# Contact

1. Jose Andres Cortes
2. Email: jose.cortes@uta.edu
3. linkedin.com/in/cortesjoseandres

# Acknowledgements

1. Thanks to my advisors for guiding me through this process.
2. Thank you to UTA and USDA-ARS for funding my research

# References 1


1. Yakubova et al. - 2014 - Field Testing a Mobile Inelastic Neutron Scattering System to Measure Soil Carbon.
2. d2399-1 by USDAgov is licensed under CC BY 2.0.
3. J. Copley, Introduction to Neutron Scattering, presented at the Summer School on the Fundamentals of Neutron Scattering, NIST Center for Neutron Research, Jul. 17, 2013. Available: https://www.ncnr.nist.gov/summ

# References 2


1. C. J. Werner et al., MCNP User's Manual Code Version 6.2. Los Alamos National Laboratory Tech. Rep. LA-UR-17-29981, Los Alamos, NM, USA, Oct. 2017.
2. C. R. Bates, S. R. Bolding, C. J. Josey, J. A. Kulesza, C. J. Solomon Jr., and A. J. Zukaitis, "The MCNPTools Package: Installation and Use," Los Alamos National Laboratory Tech. Rep. LA-UR-22-28935, Los Alamos, NM, USA, Aug. 2022, doi: https://doi.org/10.2172/1884737.
3. A. G. Kavetskiy, G. N. Yakubova, S. A. Prior, and H. A. Torbert III, "Monte-Carlo simulations for soil content determinations on Atlas," SCINet Newsletter, 2024. Available: https://scinet.usda.gov/news/newsletter

# References 3


1. R. J. Gehl and C. W. Rice, "Emerging technologies for in situ measurement of soil carbon," Climatic Change, vol. 80, pp. 43–54, 2007, doi: https://doi.org/10.1007/s10584-006-9150-2.
2. L. Wielopolski, A. Chatterjee, S. Mitra, and R. Lal, "In situ determination of Soil carbon pool by inelastic neutron scattering: Comparison with dry combustion," Geoderma, vol. 160, no. 3, pp. 394–399, 2011, doi: https://doi.org/10.1016/j.geoderma.2010.10.009.

# References 4


1. I. Matejovic, “Determination of carbon and nitrogen in samples of various soils by the dry combustion,” Communications in Soil Science and Plant Analysis, vol. 28, no. 17–18, pp. 1499–1511, 1997.
2. A. Kavetskiy, G. Yakubova, S. A. Prior, and H. A. Torbert, ‘Neutron gamma analysis of soil carbon: Post-irradiation physicochemical effects’, Environmental Technology  Innovation, vol. 31, p. 103219, Aug. 2023, doi: 10.1016/j.eti.2023.103219.