

Mesh Cells to Augment in Situ Spectroscopy

MCNP Simulation of Soil Carbon Detection

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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

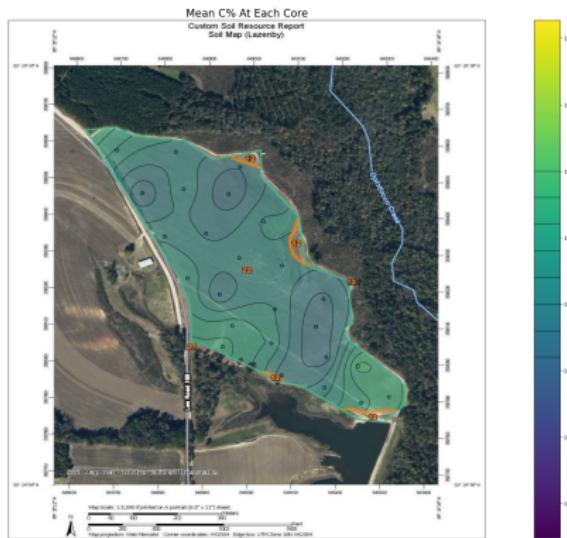
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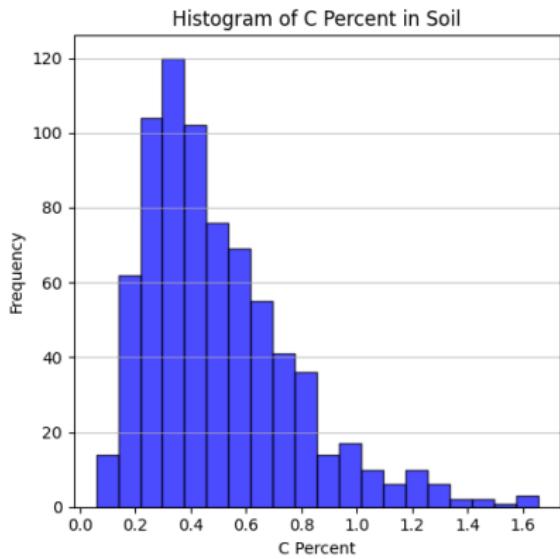
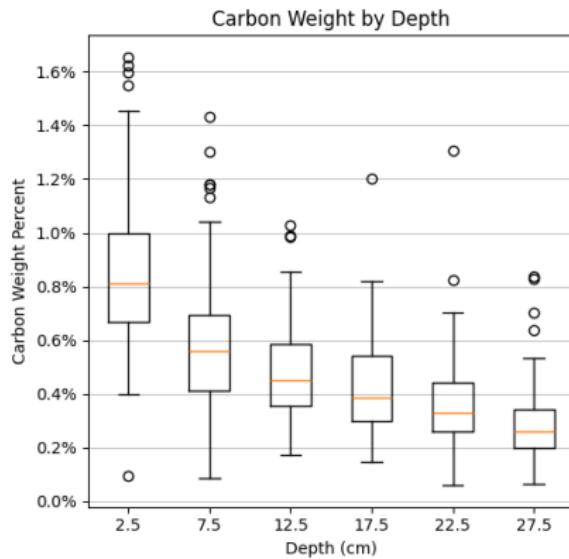
4 Conclusion

Soil is a Nonhomogeneous Material



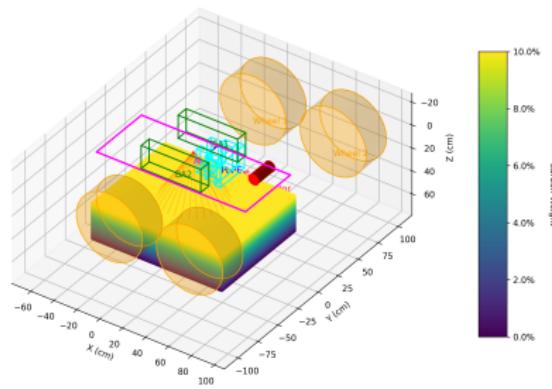
- ① MCNP cells assume homogeneous material
- ② Real soil: heterogeneous

Carbon by Depth



- ① Carbon often decreases exponentially with depth

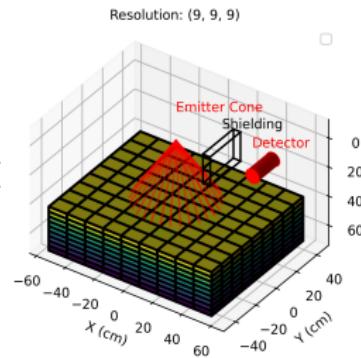
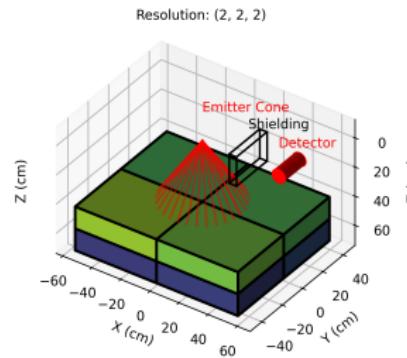
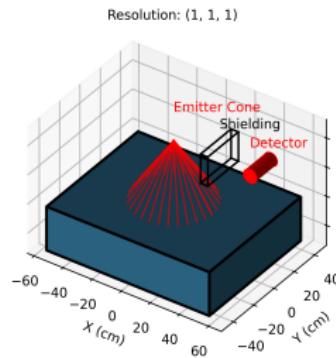
Functionally Defined Soil



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

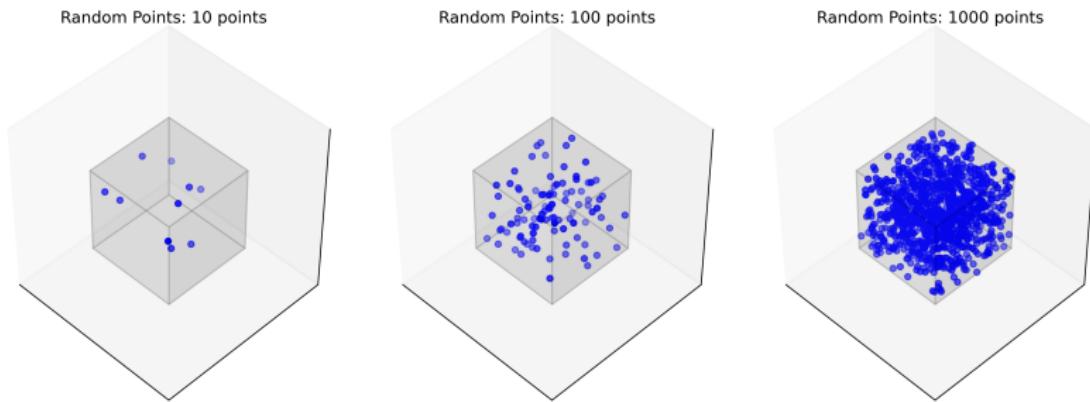
Mesh Cells

Carbon Levels as Cells increased



- ➊ Divide soil into a mesh of smaller cells Approximate functional characteristics in discrete space
- ➋ 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

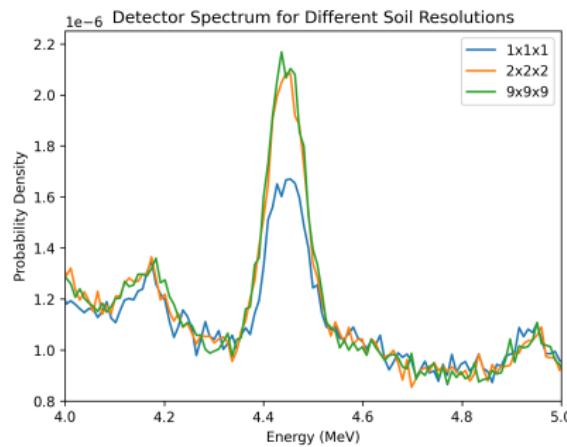
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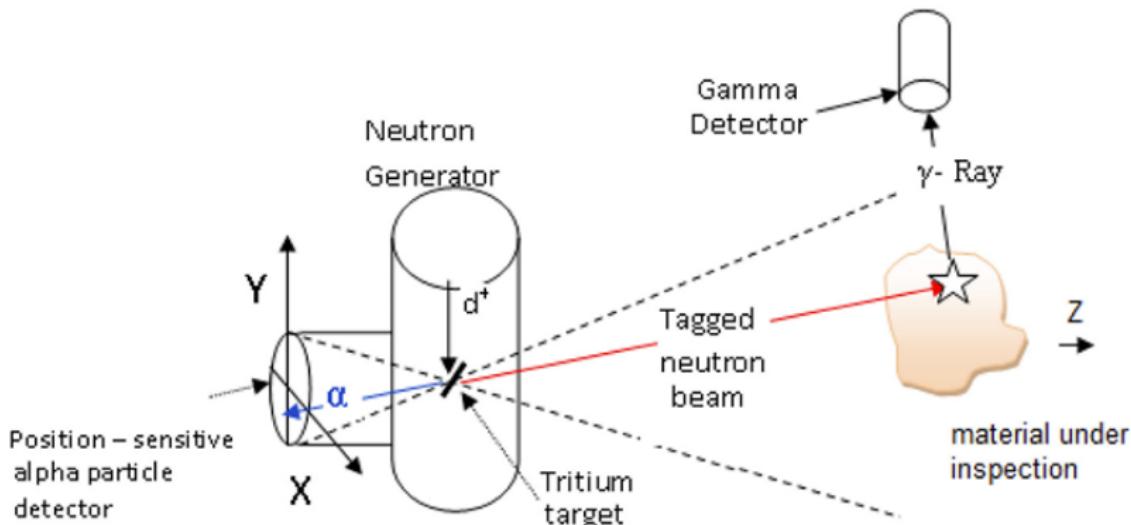
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effects on detection



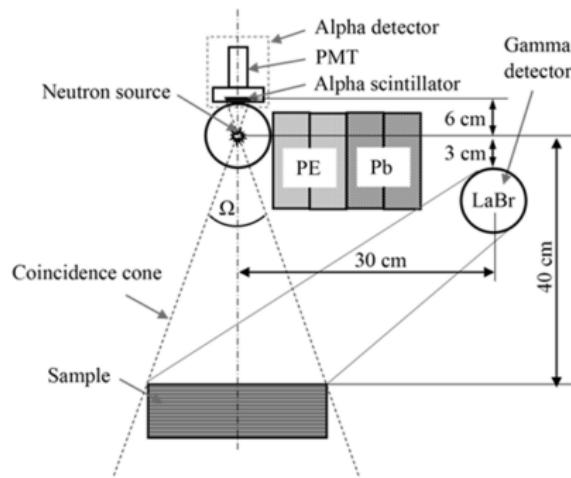
- ① As mesh resolution increases, carbon density approaches true function
- ② Effects on spectral readings around key energy ranges (e.g., 4.4 MeV)

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 91 56 JMESH= -45 91 45 KMESH= 0 91 20
(ix1x1)
F836:p,n 101
E836 0 1e-5 932i 8.4295
FU836 9000000 10000000000
FT836 TAG 3

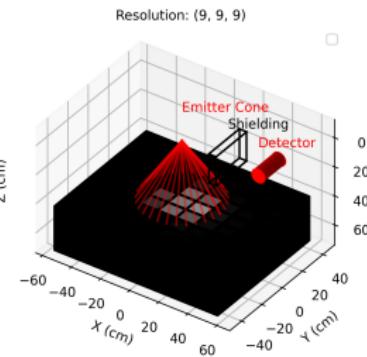
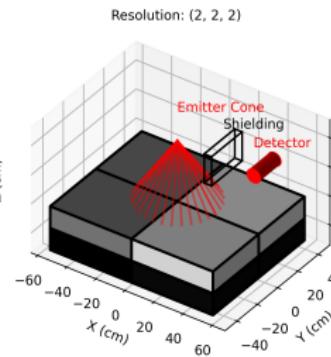
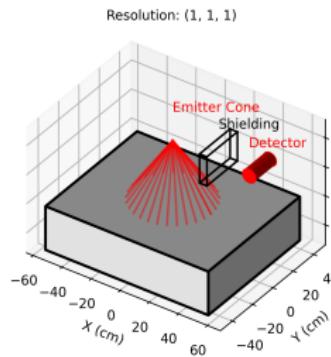
(2x2x2)
F836:p,n 101
E836 0 1e-5 932i 8.4295
FU836 900000 9100000 9200000 9300000 9400000 9500000 9600000 9700000 10000000000
FT836 TAG 3

(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

Detection Influence as Cells increased

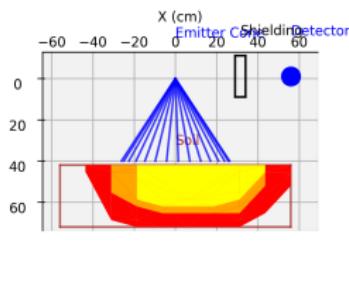


- ① Treat mesh cells as independent
- ② U card: bins tally by cell of interaction
- ③ Allows investigation of where detections originate

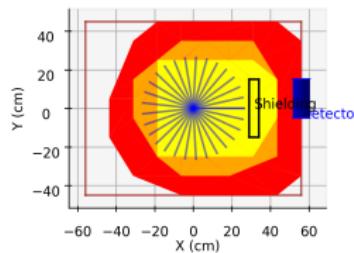
Cell influence clouds

Tracking Tally Signal

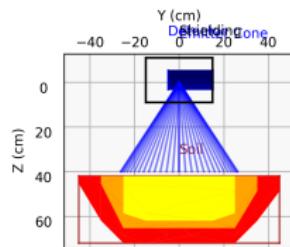
Side View



Top View



Front View

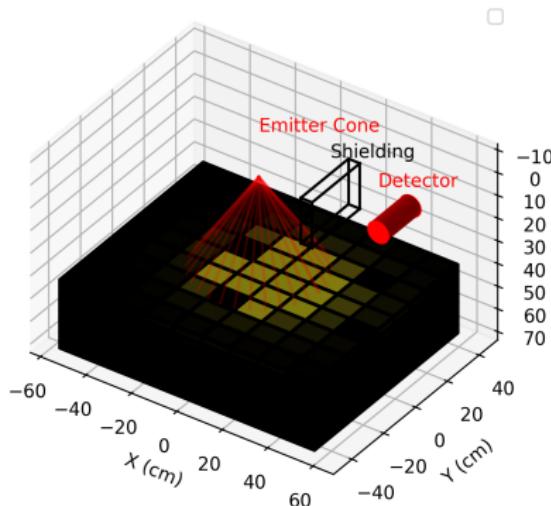


- ① Cells can be grouped into "clouds" by influence
- ② 90, 95, 99 percent detection influence

Measured Characteristic

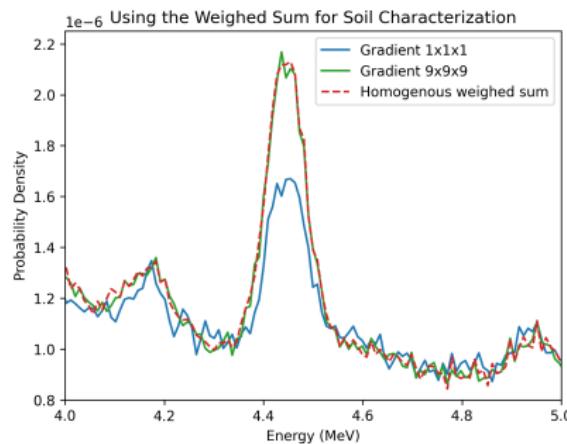
Influence * Carbon Level

Resolution: (9, 9, 9)



- ① $\text{Sum}(\text{Cell detector influence} * \text{Cell Carbon weight}) = \text{Measured Carbon}$

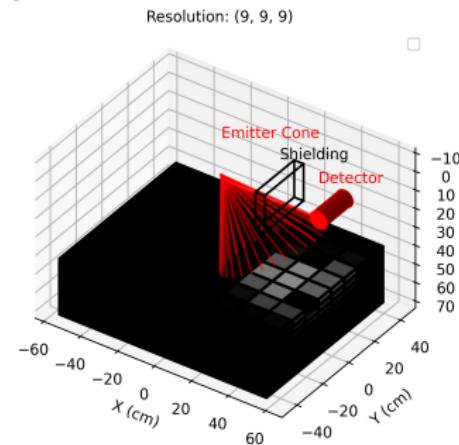
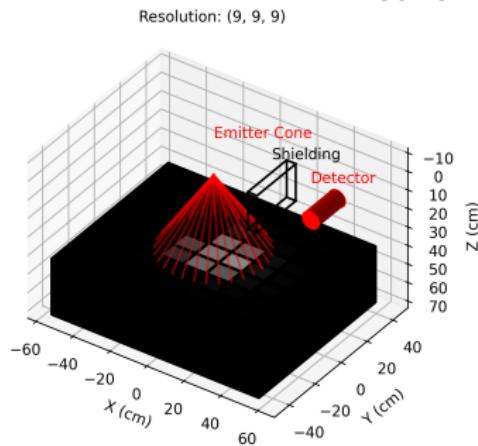
Gradient vs Homogeneous Characteristic from Gradient Weighed Avg



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

Usage Example

Reorienting The Emitter



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

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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

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- 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/summer-schools/2013/introduction-to-neutron-scattering/>

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