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Title: Simulating Activation from Underground Nuclear Explosions

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Simulating Activation from Underground Nuclear Explosions

Unstructured Mesh & Space and Earth Science Applications

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ISR-1
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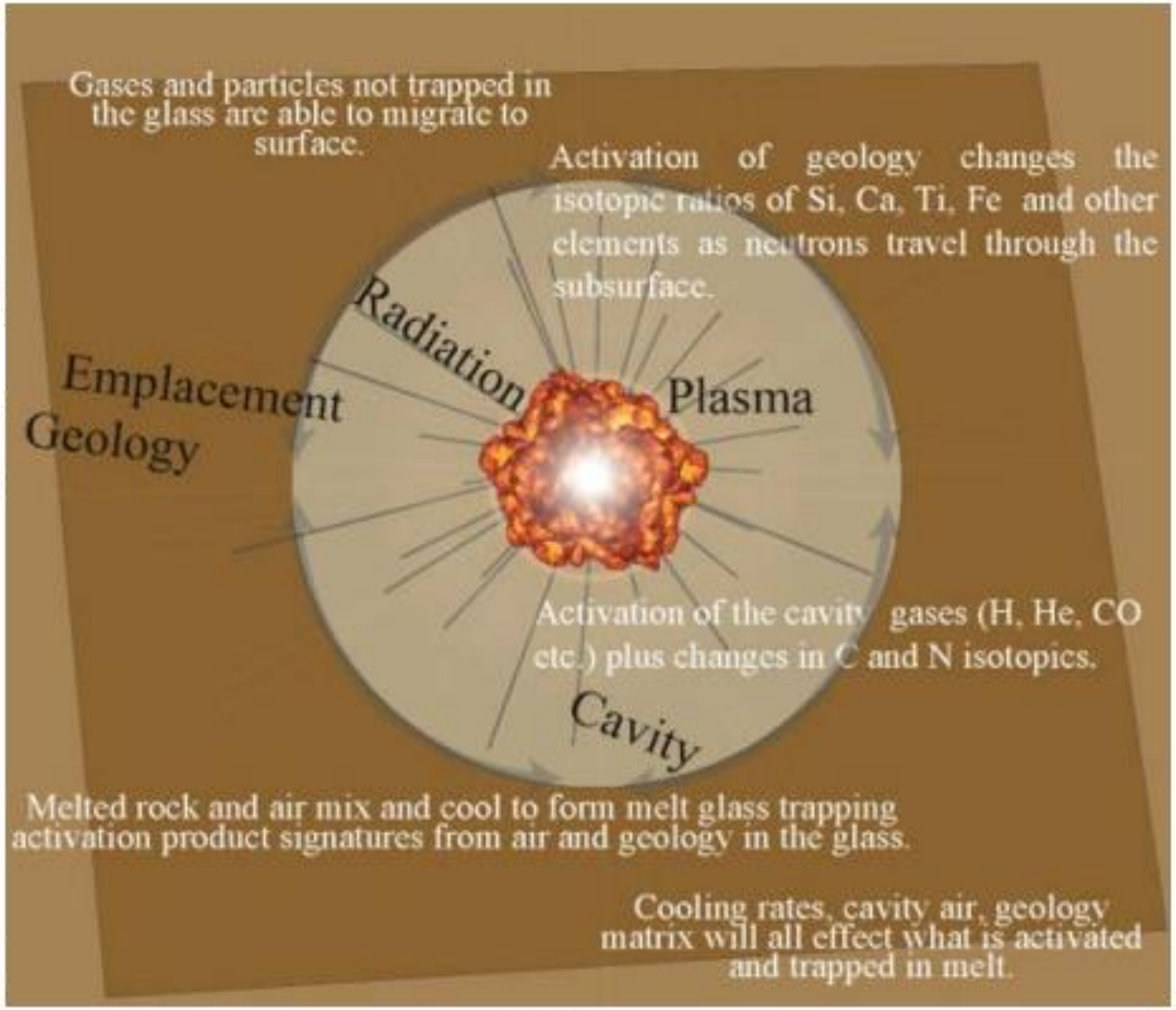
Soil activation from underground testing

- Analyzing Underground Nuclear Explosions (UNE) activation products via MCNP to Study physical and chemical phenomena
- UNE’s create high neutron fluxes in the soil and leaving behind activation products that can be measured
- Couple MCNP with CINDER to obtain atomic densities of nuclides originally present and their activated isotopes.



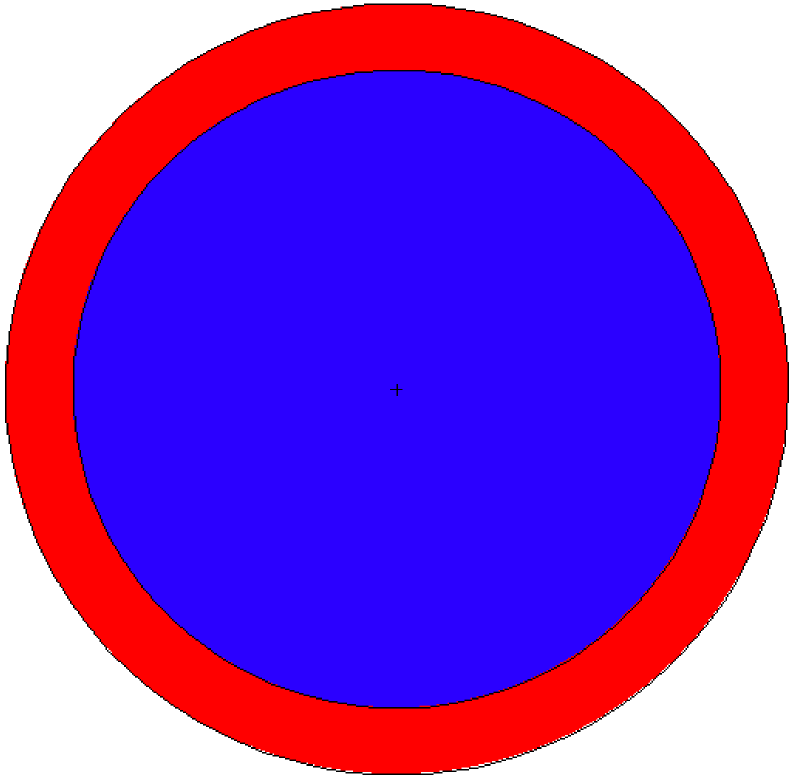
Research approach

Workflow

- In order to model the activated isotopes and resulting dose from a nuclear detonation in an environment, the Activation and Transmutation of Isotopes in an Unstructured Mesh (ACTIUM) Python toolkit has been developed to combine the unstructured mesh based particle transport capability of MCNP6 with the CINDER2008 transmutation code to produce quantities of interest for the post-detonation nuclear forensics and weapons effects communities [1].
- The ACTIUM approach is the first of its kind to couple the latest release of CINDER2008 as a part of the Activation in Accelerator Radiation Environments (AARE) package with MCNP6 and produce transmuted quantities per time step on an unstructured mesh.
  - ACTIUM uses the latest ENDF/B-VIII.0 cross section libraries for the transmutation calculations.
- The legacy eeout file format in ACTIUM has been updated to handle the hdf5 output format now prepared by MCNP.
  - This allows for post processing of the results with ParaView without additional steps.
- Time-steps and neutron energy are selected based off desired UNE interrogation. Soil and air compositions will vary depending on the geological environment where the test is conducted.

Setup

MCNP input



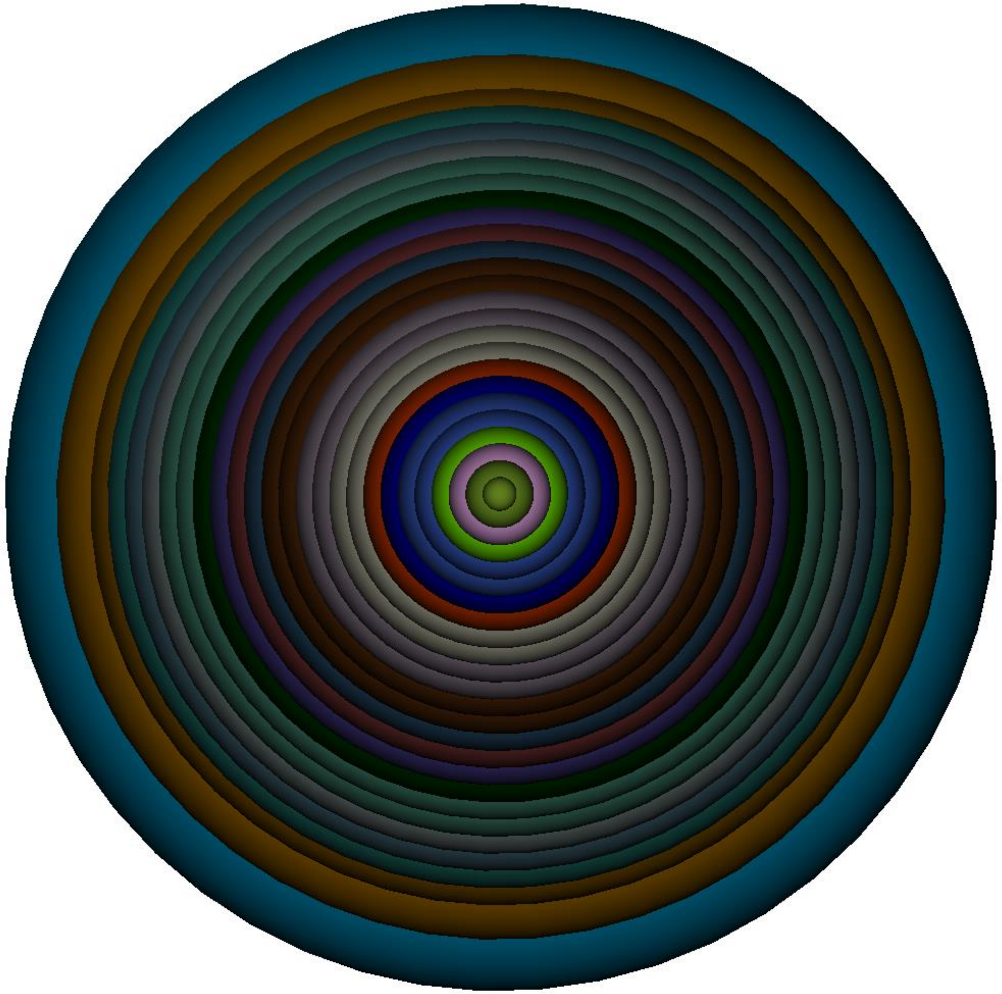
- Sliced view of Air cavity (blue) surrounded by alluvium soil (red)
  - Constructive Solid Geometry (CSG)
  - To be reconstructed using Unstructured Mesh (UM)

- MCNP run with SDEF
  - POS = 0 0 0 WGT=6.022E+23 (Avogadro)
  - At the center of the cavity with a default energy of 14 MeV
  - Characterized to 1 mole
  - NPS 1E8

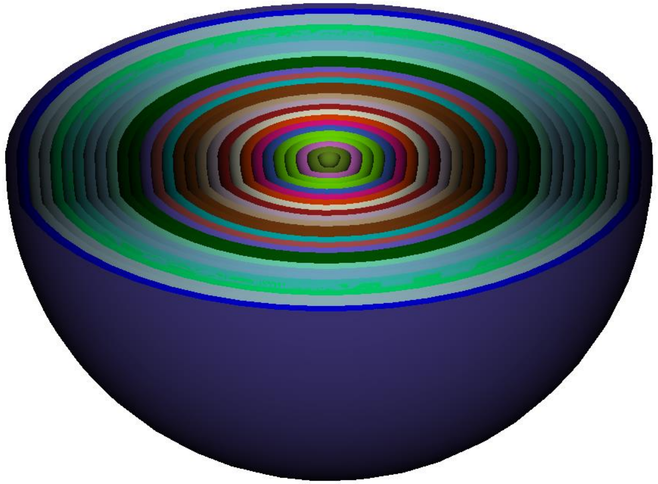
- CINDER activation
  - Time steps of [Instantaneous, 6 min, and 1 yr.]
  - Detonation at initial moment then left to decay up to 1 year

Unstructured Mesh

CUBIT

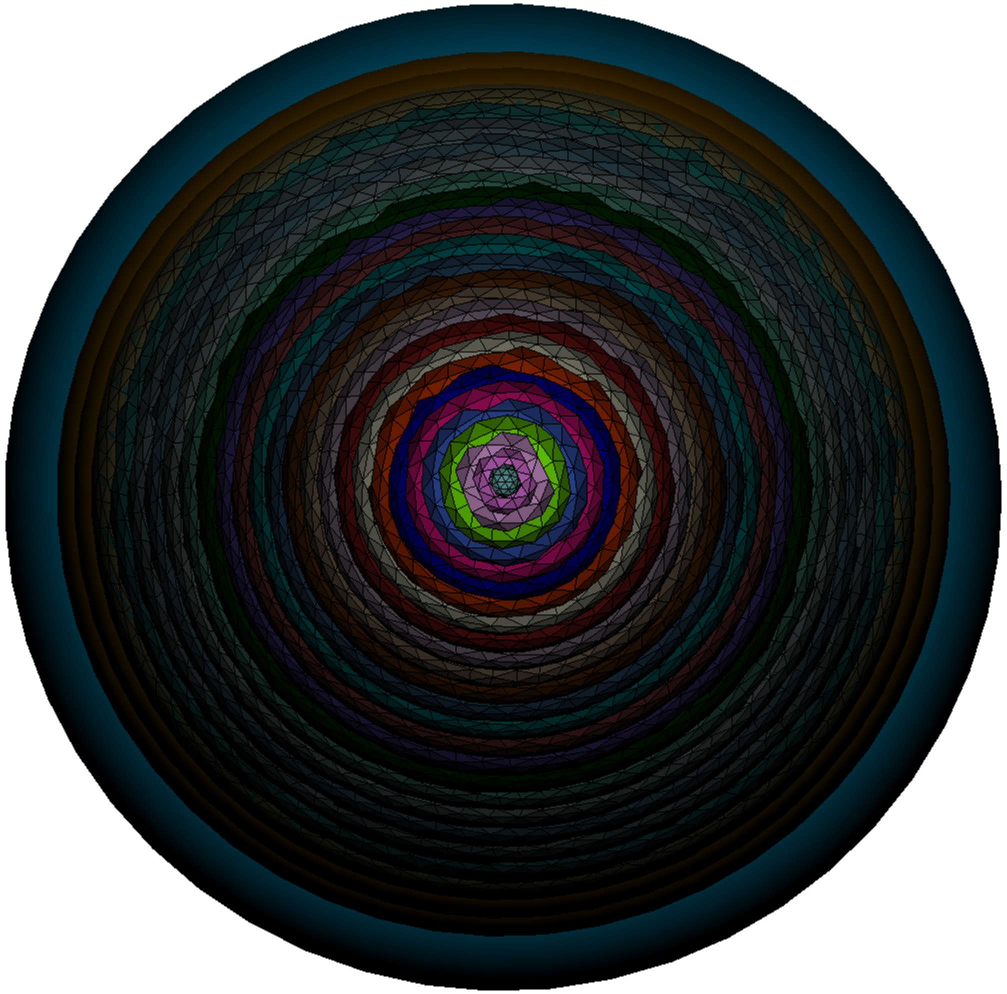


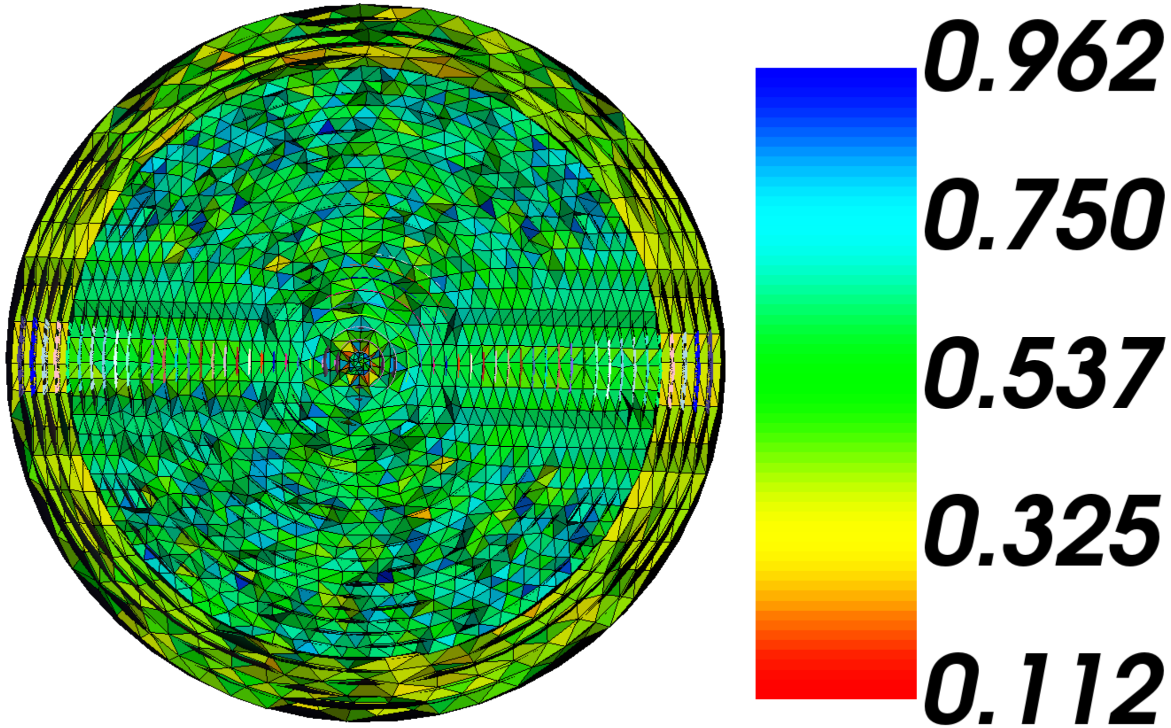
- Air
  - Segmented by 1m radii for a total of 24 layers which are then broken up into individual elements (127,342).
- Soil
  - Segmented by 2 m then 3 m and broken into individual elements (32,305).
- Encompassed (99.799%) of the volume
  - Materials remain unchanged
  - Densities remain unchanged



Mesh Quality

Scaled Jacobian



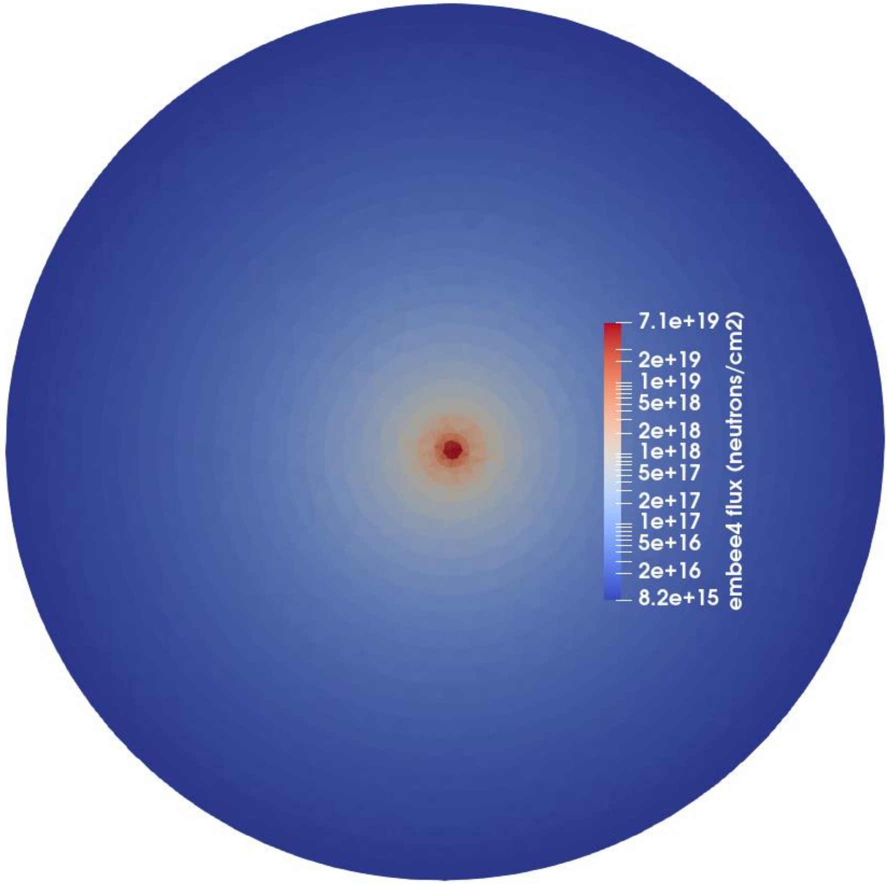


- Air
  - 99.7835% meshed volume
- Soil
  - 99.8204% meshed volume
- Total
  - 159,647 elements

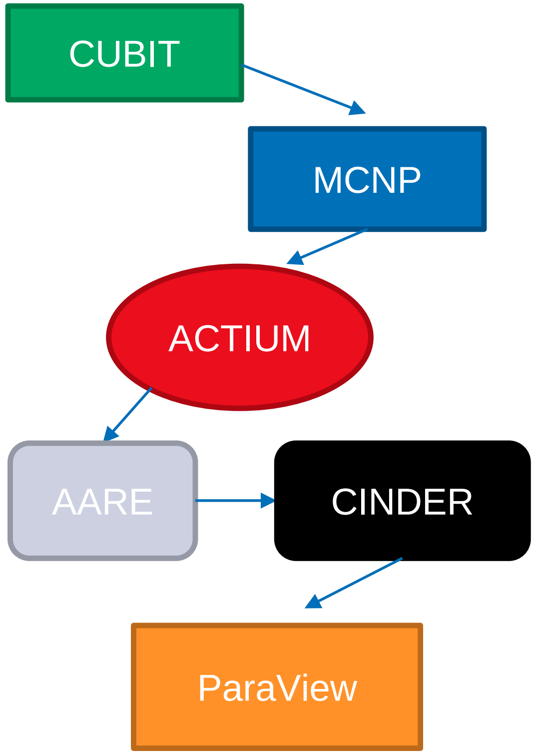
ParaView

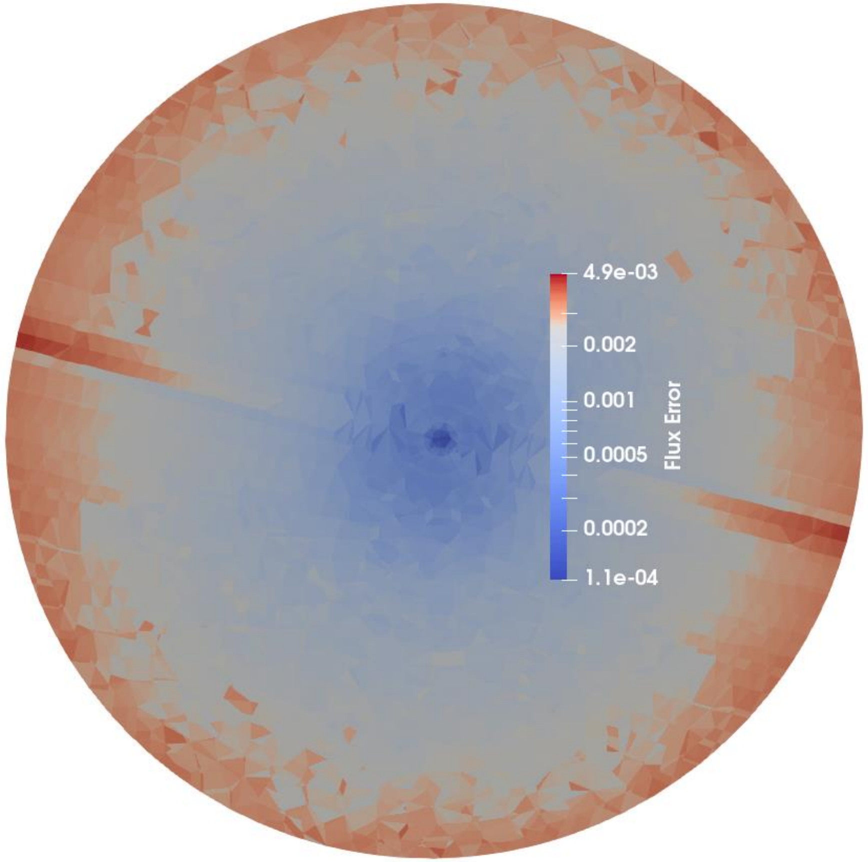
Activation and Transmutation of Isotopes in an Unstructured Mesh (ACTIUM)
Activation in Accelerator Radiation Environments (AARE)

Air Flux embee4



- Flux average in individual elements and along with their respective errors

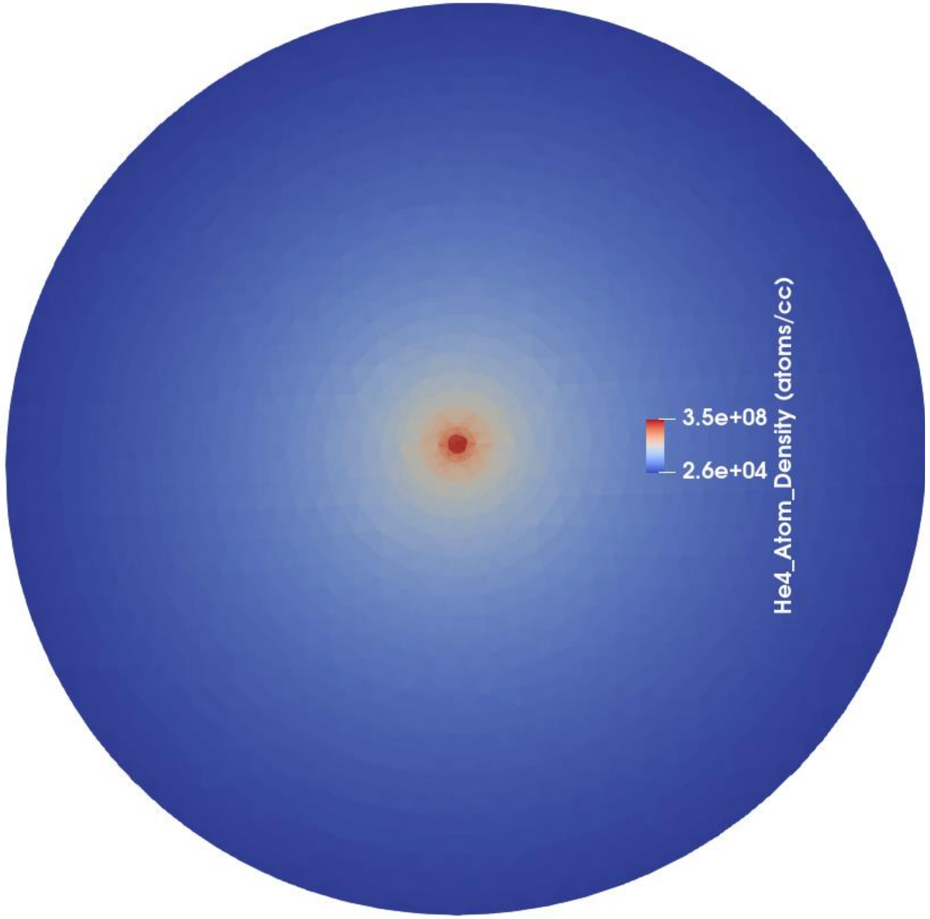




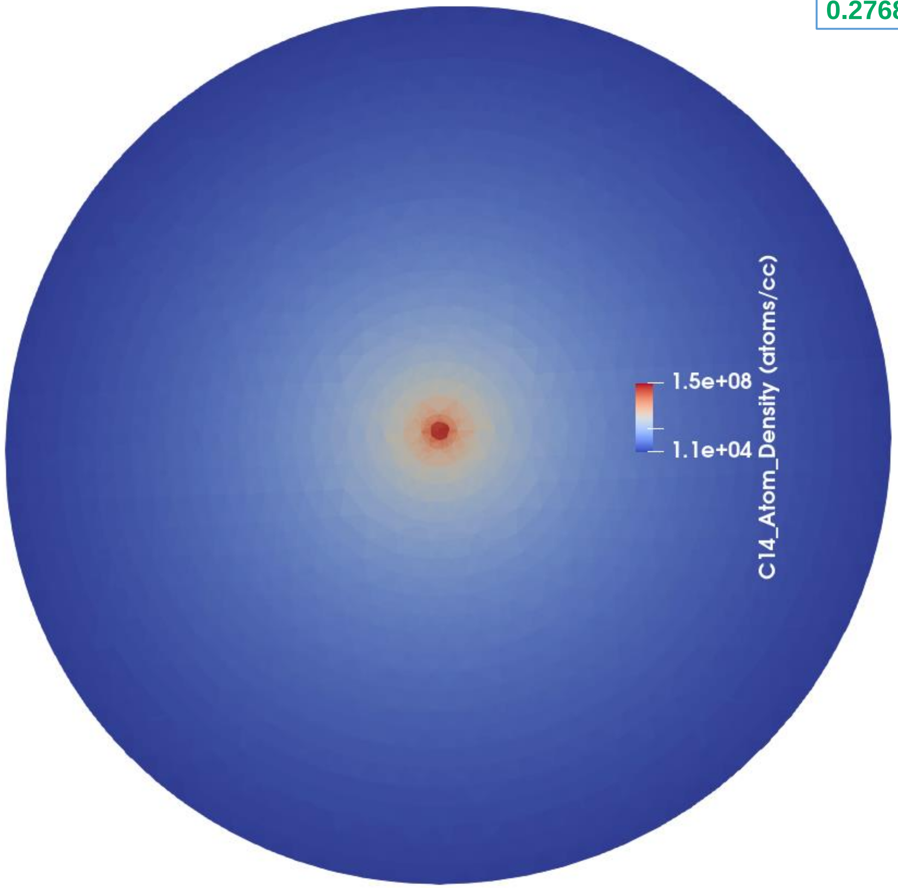
Activation Analysis

Air Atom Density per Mole immediately post event

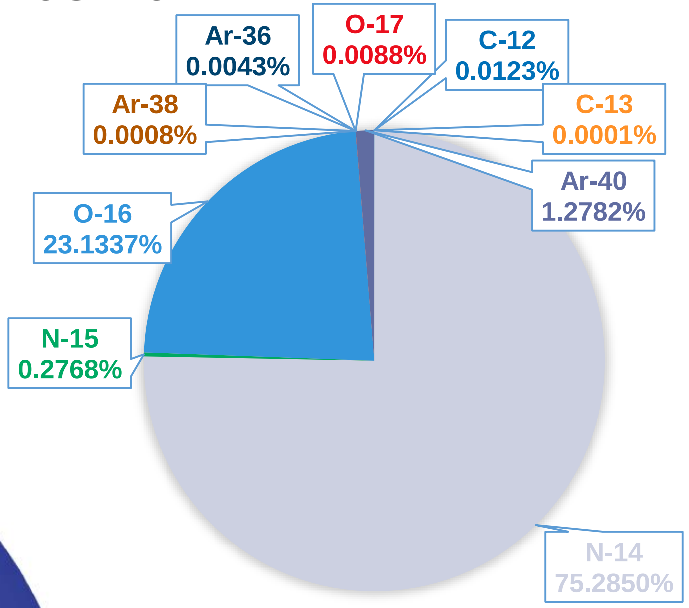
- ${}^{4}_{2}He$ seen in air



- ${}^{14}_{6}C$ from activation in air



AIR COMPOSITION



${}^{4}_{2}He$ alpha from decay and activation resulting from neutron capture

${}^{14}_{6}C$ results from:

$${}^{13}_{6}C(n,\gamma){}^{14}_{6}C$$

$${}^{14}_{7}N(n,p){}^{14}_{6}C$$

$${}^{15}_{7}N(n,d){}^{14}_{6}C$$

$${}^{16}_{8}O(n,\,{}^{3}_{2}He){}^{14}_{6}C$$

$${}^{17}_{8}O(n,a){}^{14}_{6}C$$

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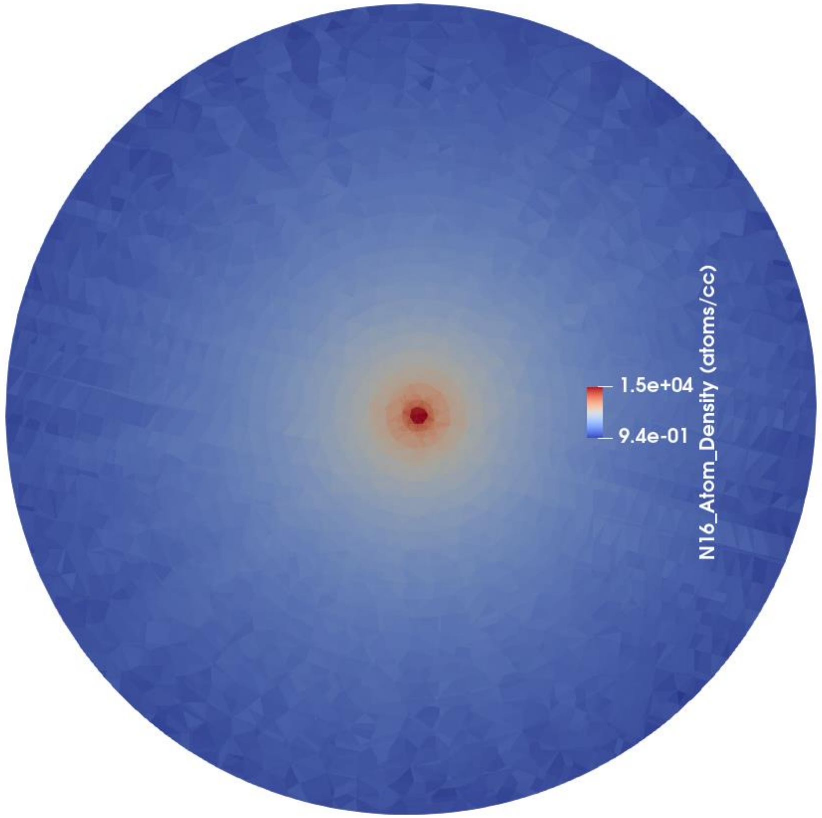
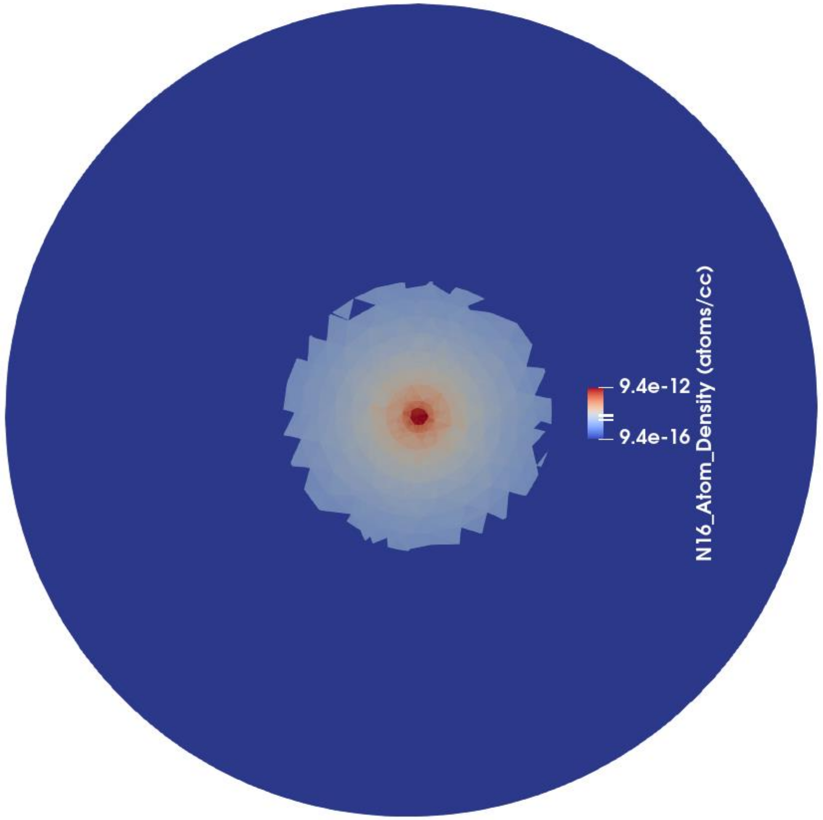
Activation Analysis

Air Atom Density per Mole post event

- $^{16}_{7}N$ from activation in air (instantaneously)



- $^{16}_{7}N$ from activation in air (6 min after)



Most of the air (>75%)

Is made up of Nitrogen

N-16 has a half-life of 7.13 seconds

After a year there is no trace of N-16

Dispersion of activated isotope and respective decay can be tracked throughout the air over their life time.

Activation Analysis

Air Atom Density per Mole post event (1 yr)

- After a year post detonation, approximately half of all the elements in the air have activated and decayed.
- The remaining isotopes remain as a trace corresponding to the 14 MeV neutron flux seen within the cavity.
- This air cavity is assumed to remain contained within the soil throughout the simulation.

Material	Atomic Fraction
C-12	1.488E-04
C-13	1.485E-06
N-14	7.819E-01
N-15	2.685E-03
O-16	2.105E-01
O-17	7.523E-05
Ar-36	1.733E-05
Ar-38	3.096E-06
Ar-40	4.657E-03

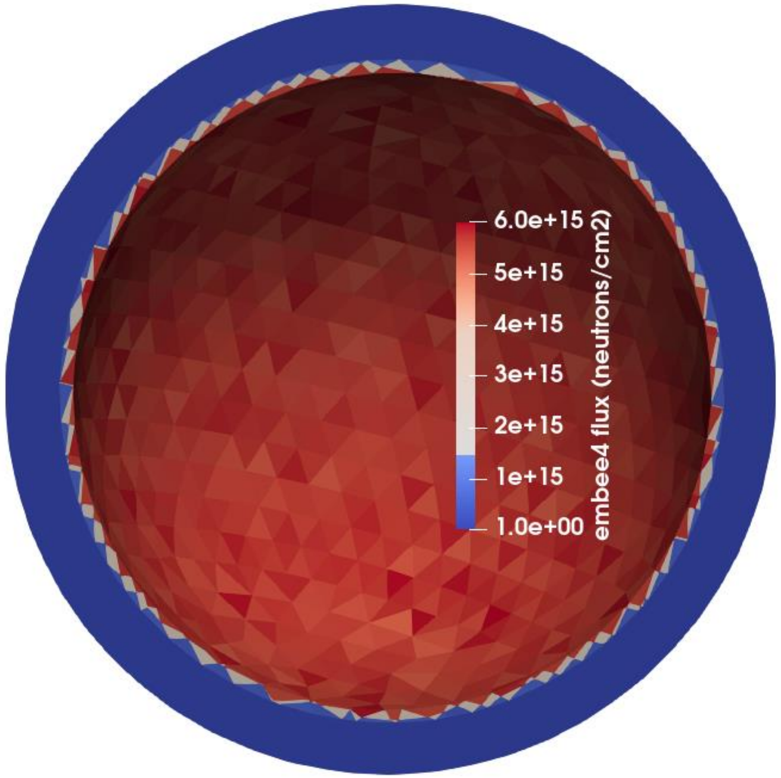
Isotopes present in the Air after a year

Ar	36	37	38	39	40
B	10	11			
Be	9	10			
C	12	13	14		
Cl	35	36	37		
H	1	2			
He	3	4			
K	39	41			
Li	6	7			
N	14	15			
O	16	17	18		
P	31	33			
S	32	33	34	35	36
Si	29	30			

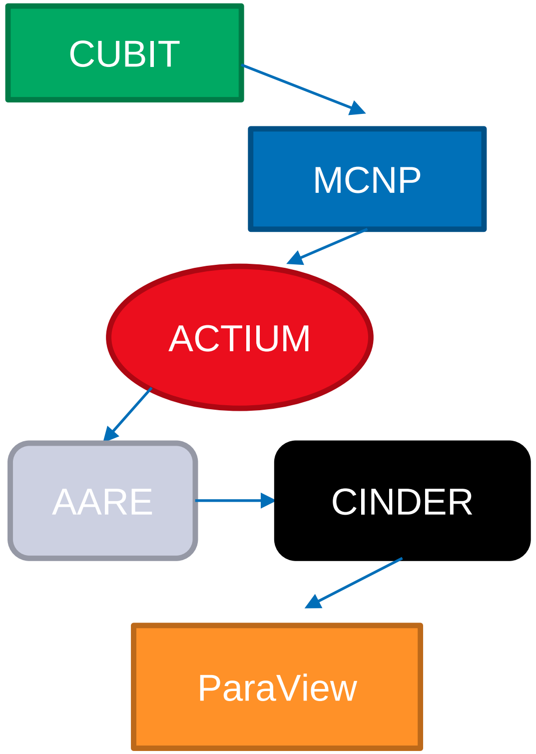
ParaView

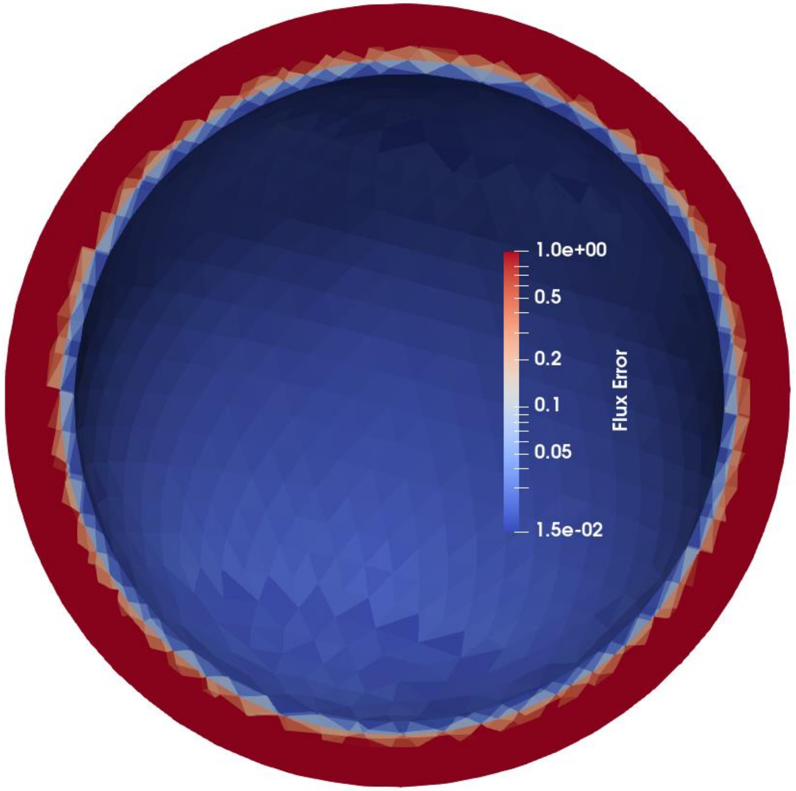
Activation and Transmutation of Isotopes in an Unstructured Mesh (ACTIUM)
Activation in Accelerator Radiation Environments (AARE)

Soil Flux embee4



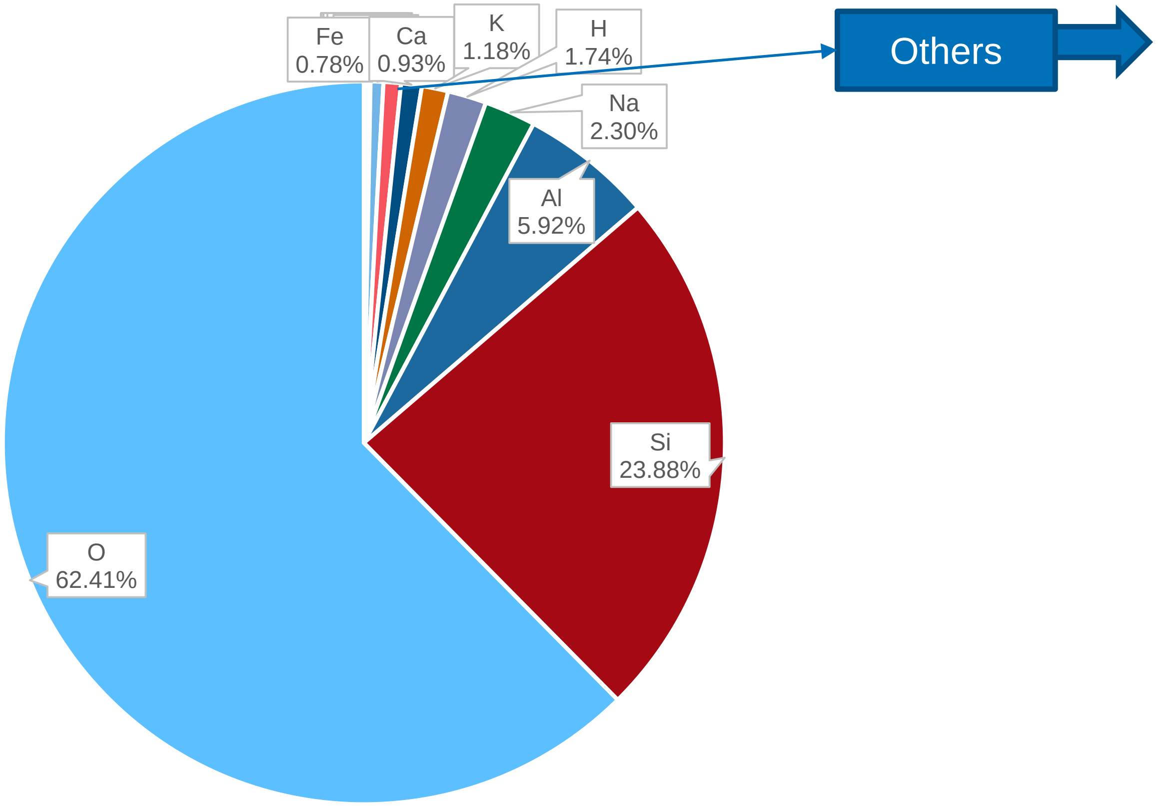
The flux is not penetrating past 2m of soil. Showing that it is a good representation of a cavity.





Activation Analysis

Soil Composition and Mass Fraction

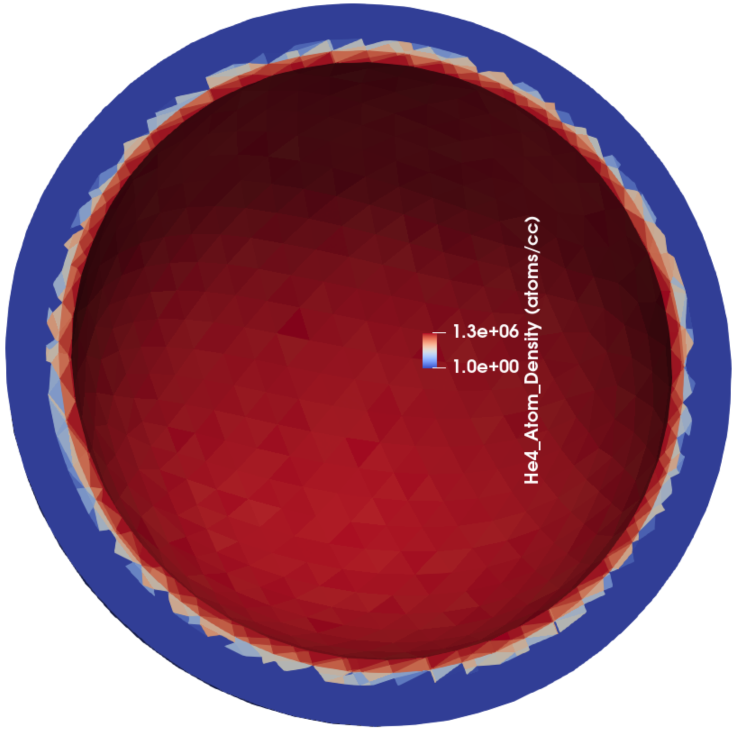


Element	Percent
Lu	0.000002%
Tm	0.000002%
Ta	0.000003%
Tb	0.000004%
Ho	0.000004%
U	0.000009%
Yb	0.000011%
Eu	0.000012%
Er	0.000012%
Mo	0.000017%
W	0.000018%
Dy	0.000022%
Gd	0.000034%
Th	0.000035%
Cs	0.000042%
Sm	0.000042%
Pr	0.000065%
Nb	0.000085%
Ar	0.000140%
Pb	0.000166%
Y	0.000208%
La	0.000265%
Co	0.000274%
Sc	0.000288%
Cu	0.000289%
Zr	0.000420%
Ce	0.000576%
Ni	0.001272%
Zn	0.001302%
Rb	0.001316%
V	0.001920%
V	0.001920%
Cr	0.002121%
N	0.010907%
Sr	0.012195%
Ba	0.014337%
Mn	0.020090%
P	0.037800%
C	0.084997%
Ti	0.100734%
Mg	0.574120%

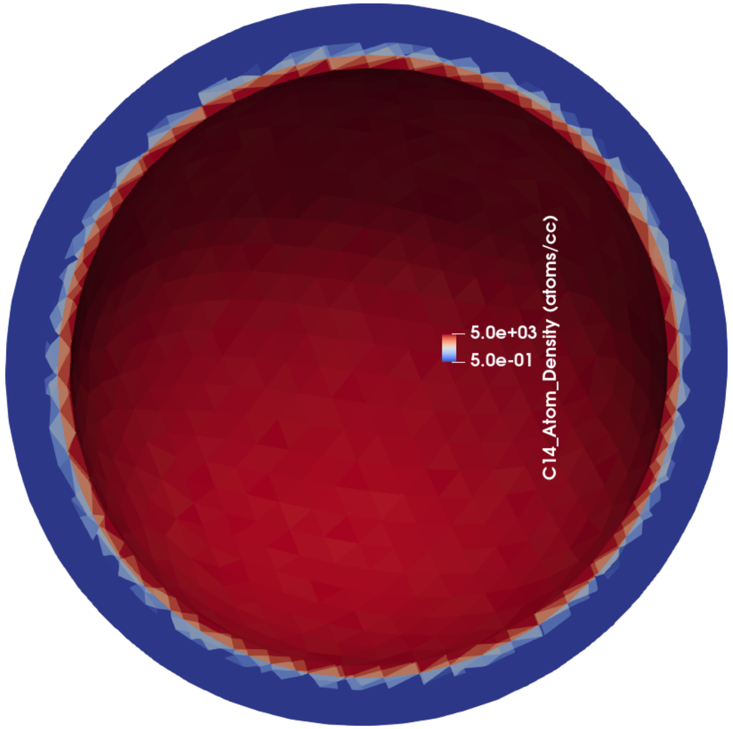
Activation Analysis

Soil Atom Density per Mole immediately post event

- ${}^{4}_{2}He$ seen in the soil



- ${}^{14}_{6}C$ from activation in the soil



- C14 does not change in concentration within this decay time.
- While there are a few more **α** particles formed (2.48E+07) atoms per cm^3 on average by the end of 1 year.
- At the initial detonation there is no formation of a few isotopes that are eventually produced:
  - ${}^{180}_{72}Hf$
  - ${}^{228}_{88}Ra$

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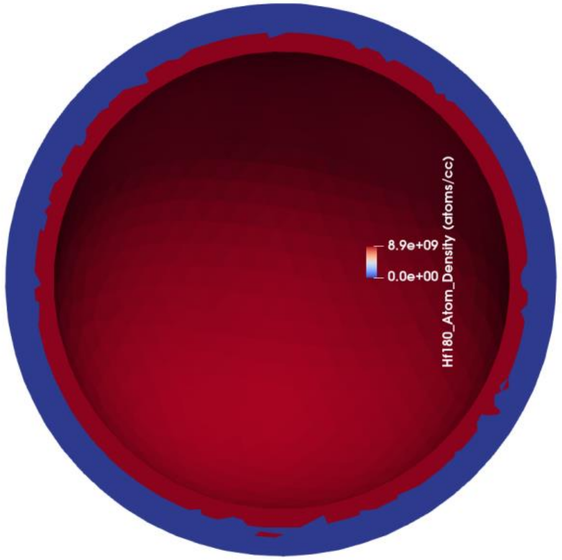
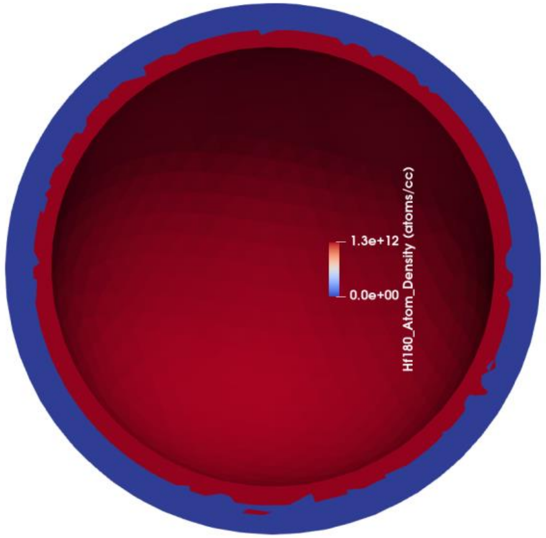
Decay Products

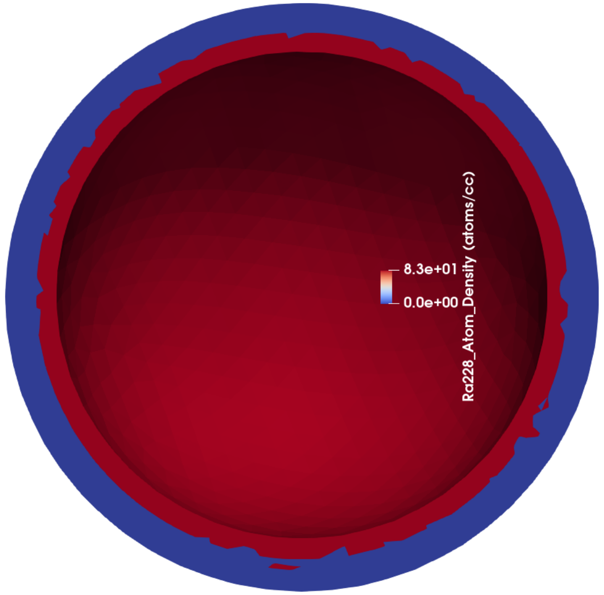
- $^{180}_{72}Hf$ (6 min)



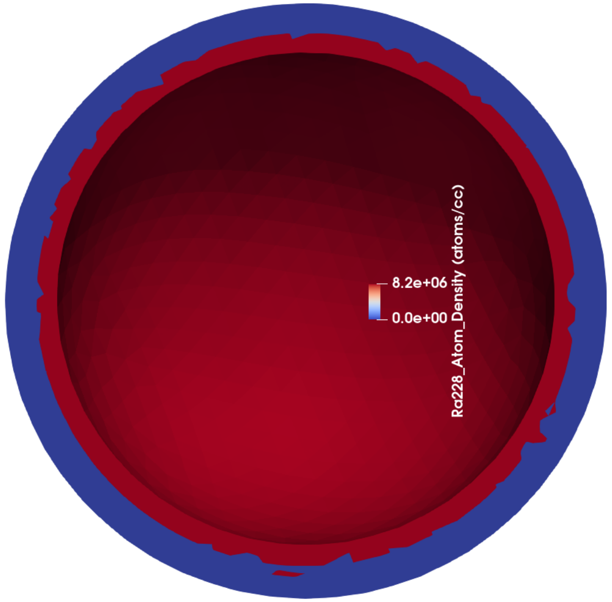
- $^{180}_{72}Hf$ (1 year)

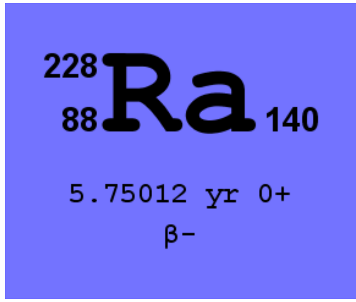


- $^{228}_{88}Ra$ (6 min)



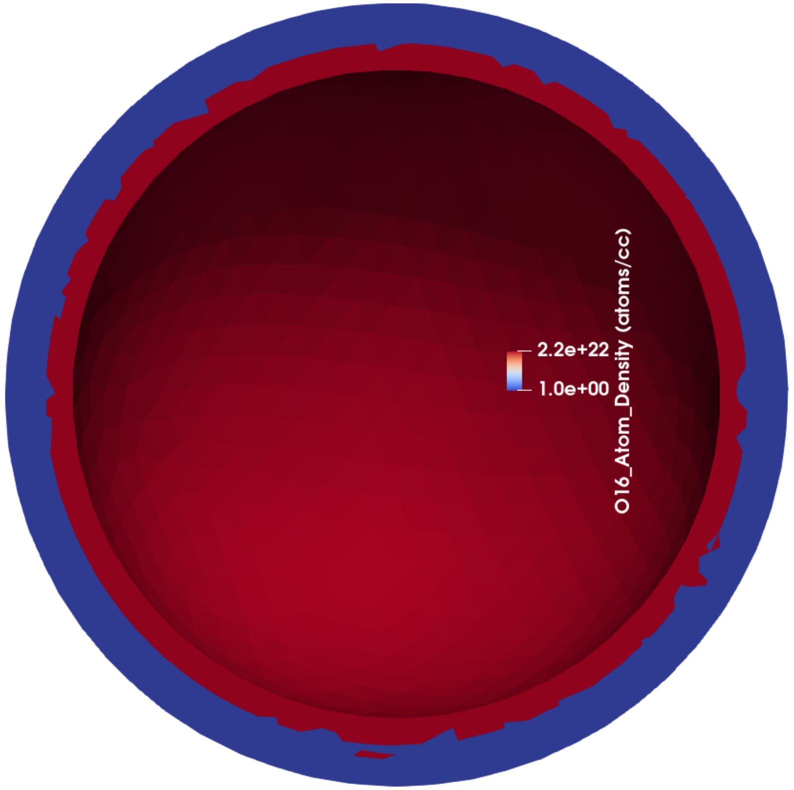
- $^{228}_{88}Ra$ (1 year)

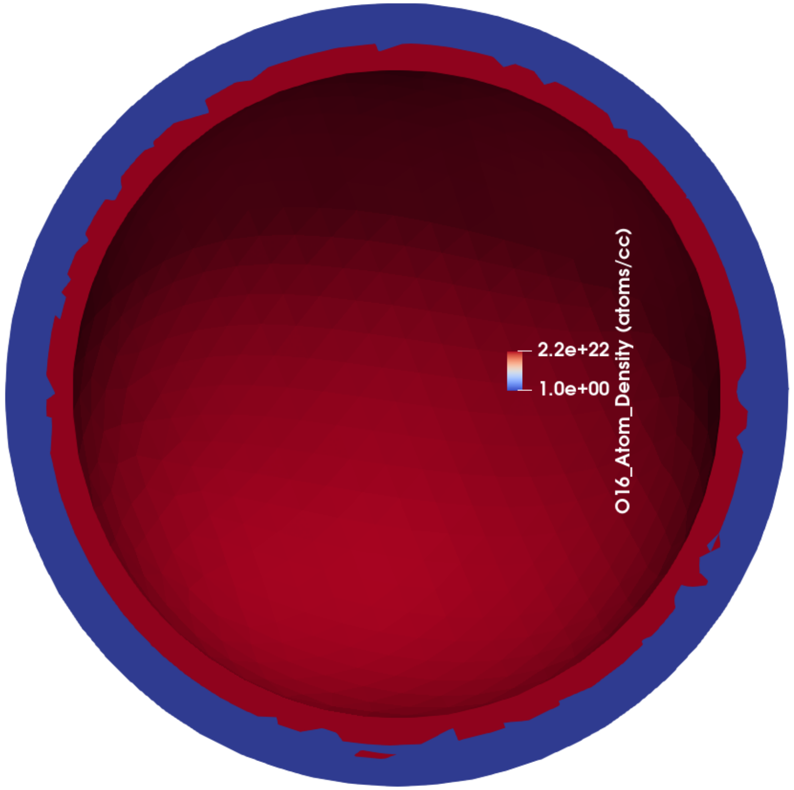


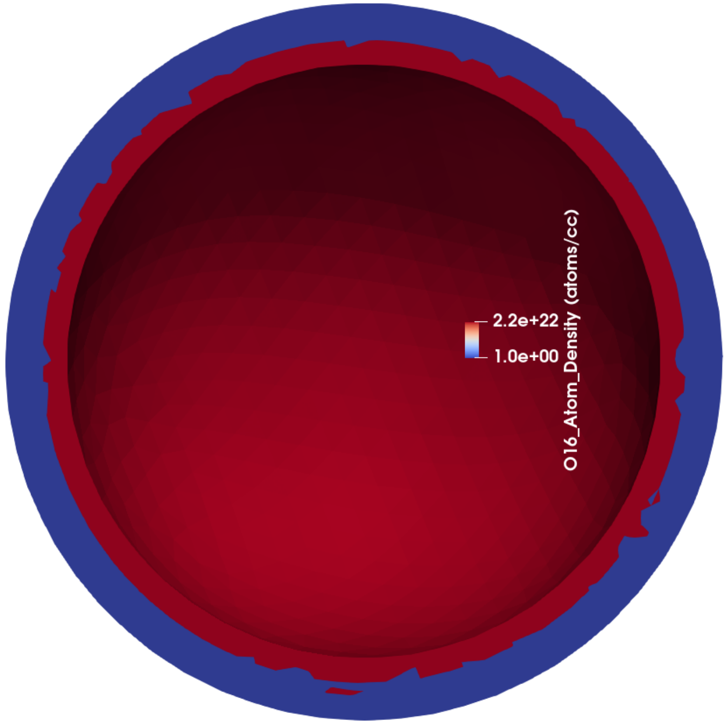


Activation Analysis Continued.

- (immediately)
- (6 min)
- (1 year)







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Summary

Underground Nuclear Explosions and Activation Analysis

- Developing a process for activation calculation and analysis on unstructured mesh geometry.

- Having a subdivided geometry allows for higher fidelity flux calculations in comparison with CSG models.

- This process enables more intricate cavity setups to be modeled, with either varying material/air compositions and specifically subdivided geometry to focus the analysis on an individual area of interest.

[1] *McClanahan, Tucker Caden, "Study of the Production of Isotopes in an Urban Nuclear Post-Detonation Environment." PhD diss., University of Tennessee, 2020.*

Project supported by 20210215DR

Average prompt energy release per fission is 200 MeV

Fission

Released for 1 kt of TNT

- 4.184×10^{12} J [joules]
  - A kiloton of TNT can be visualized as a cube of TNT 8.46 meters on a side.

- 200 MeV released per fission resulting from U^{235}
  - 200 MeV *1.60218E-13 (MeV to J)
    - = 3.20436E-11 J
  - $\frac{4.184E12\ J}{3.20436E\text{-}11\ J} = 1.30572\text{E}23$
  - the average number of neutrons produced per fission = 2.455
    - 1.30572E23 * 2.455 = 3.9079E23 neutrons per fission in 1 kt of TNT

Comparison: 1kt of Trinitrotoluene (TNT) is equivalent to 3.9079E23 neutrons per fission

On the order of Avogadro's number (6.02204E23) particles per mole

Energy

Released per 1 mole

Molecular Weight of U^{235}: 235.044 g/mol

$$\frac{235.044\ g/mol}{6.02204E23\ mol^{-1}} = 3.88*10^{-22}\ \mathrm{gram/nucleus}$$

- 6.02204E23 Avogadro's number
  - The number of particles in 1 mole

- Weight of 1 nucleus of Uranium-235 is $3.88*10^{-22}$ gram/nucleus
  - 200 MeV released per atom of U^{235}
  - 200E6 eV *4.8E-10 (electron charge) / 300
    - = 3.2E-4 erg/nucleus
  - $\frac{2.7E-4\ erg/nucleus}{3.88E-22\ gram/nucleus} = 8.24742\mathrm{E17\ erg/gram}$

A volt is $\frac{1}{300th}$ of the electrostatic unit of voltage

Comparison: 1g of Trinitrotoluene (TNT) is equivalent to 4.184E10 erg/gram

Uranium-235 Energy Release is a factor of 1.97E07 greater than TNT