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Los Alamos
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MCNP6.3 Electron Energy Deposition Validation with the Lockwood Experiments

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LA-UR-23-32743, Rev. 1

Outline

Introduction & Background

Objective: present the MCNP [1, 2] V&V suite [3] and these extensions to it

- These experiments [4] have been extensively used for validation [5–14]
- Extended-media: sizes beyond CSDA/energy-loss straggling reliability
  - Health physics, space shielding, relativistic electron accelerators
- Motivated by significant experimental/theoretical disagreement
  - Often: normalized, infinite geometries, and/or poor spatial resolution
- Substantial discussion of experimental challenges & configuration
  - Calorimetric measurement methods and theory
  - Data analysis and calibration
  - Apparatus and procedures
- From 40 years ago... time to revisit these?

Numbers given in brackets are hyperlinks to the references at the end of this talk.
CSDA: continuous slowing-down approximation.

Software Testing & the MCNP6.3 V&V Suite: `vnvstats`

- Comprehensive testing for correctness
- Comparison to another code (version)
  - Behavior testing done for every code change during development
  - Full end-to-end testing attempting to isolate behavior(s)/feature(s)
- Comparison to (semi-)analytic results
  - Ensuring the algorithms indeed solve the transport equation
  - Mock problems and data used to isolate code/algorithm implementation
- Comparison to experimental measurements
  - Ensuring the combination of algorithms and data compare well to reality
  - Applies only to application area being tested and compared

More information on the V&V suite is available in [3].

Software Testing & the MCNP6.3 V&V Suite: `vnvstats`

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    - Behavior testing done for every code change during development
    - Full end-to-end testing attempting to isolate behavior(s)/feature(s)
  - Comparison to (semi-)analytic results
    - Ensuring the algorithms indeed solve the transport equation
    - Model problems and data used to validate code/algorithm implementation
  - Comparison to experimental measurements
    - Ensuring the combination of algorithms and data compare well to reality
    - Applies only to applications that can be tested and compared

Regression

Verification

Validation

The MCNP Development Team regularly exercises all of these types of tests.

More information on the V&V suite is available in [3].

Experimental Configuration

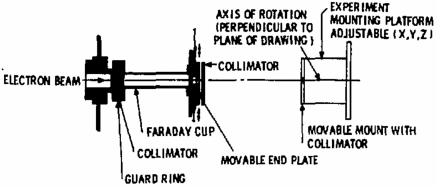


Figure III. 1. Faraday Cup and Experimental Mounting Platform

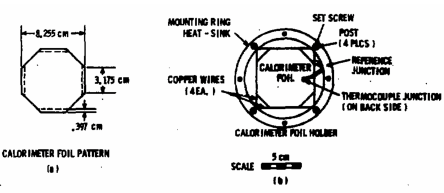


Figure III. 4. Calorimeter Foil

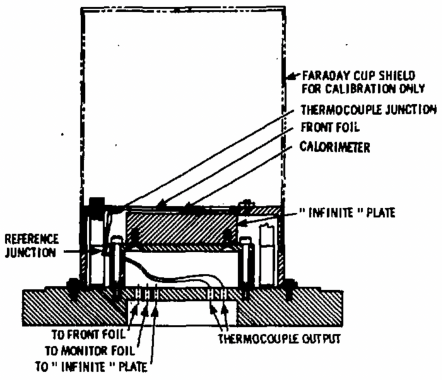
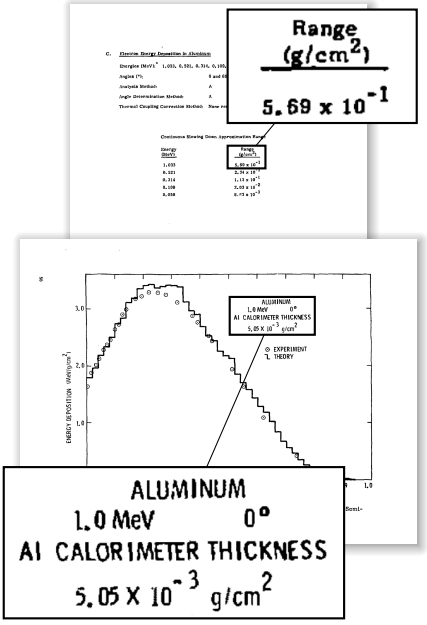


Figure III. 2. Experimental Apparatus

All images from [4].

Fraction of Mean Range (FMR) $\rightarrow$ Foil Thickness



Total thickness of material:

$$\Delta t = \frac{fR}{\rho} = \frac{0.115\left(0.569\ \text{g}\cdot\text{cm}^{-2}\right)}{2.7\ \text{g}\cdot\text{cm}^{-3}} \tag{1}$$

$$\approx 0.0242352\ \text{cm}. \tag{2}$$

Half thickness of the calorimeter foil:

$$\Delta t_{\text{c},\frac{1}{2}} = \frac{\Delta t_{\text{c,a}}}{2\rho} = \frac{5.05\times10^{-3}\ \text{g}\cdot\text{cm}^{-2}}{2(2.7\ \text{g}\cdot\text{cm}^{-3})} \tag{3}$$

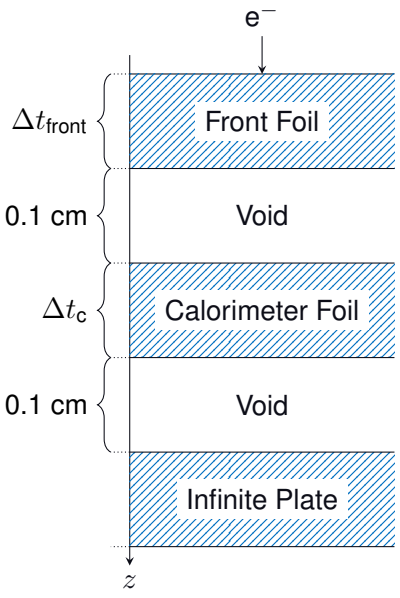
$$\approx 0.000935185\ \text{cm}. \tag{4}$$

Front foil thickness:

$$\Delta t_{\text{front}} = \Delta t - \Delta t_{\text{c},\frac{1}{2}} \approx 0.0233\ \text{cm} \tag{5}$$

Example using FMR index 9, $f = 0.115$, from [4, page 51].
Full calorimeter foil thickness is $\Delta t_{\text{c}} = 2\Delta t_{\text{c},\frac{1}{2}} = 0.00187037$ cm.

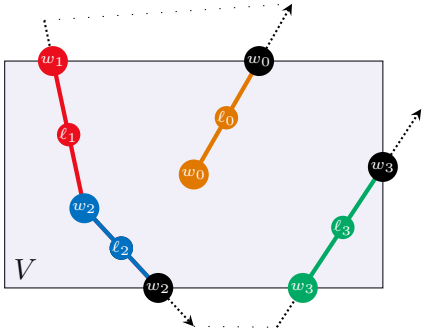
Calculational Configuration



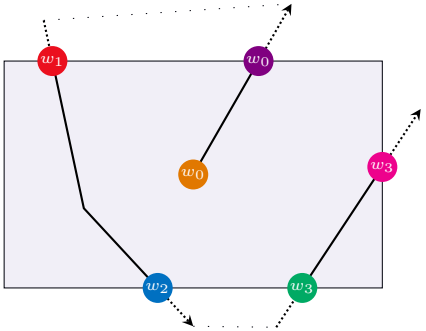

```
Energy deposition for 1.0 MeV electrons in Aluminum at 0deg
1     1  -2.7 100 -101 -200 imp:e=1
2     0            101 -102 -200 imp:e=1
3     1  -2.7 102 -103 -200 imp:e=1
4     0            103 -104 -200 imp:e=1
5     1  -2.7 104 -105 -200 imp:e=1
999   0           -100 :105: 200 imp:e=0

100     pz  0.0
101     pz  0.023300000000000
102     pz  0.123300000000000
103     pz  0.125170370370370
104     pz  0.225170370370370
105     pz  5.0
200     cz  100.0

mode e p
phys:e 1.0 13j 0.001
m1 13000.14p -1
sdef par=3 erg=1.0 x=0. y=0. z=0. vec=0 0 1 dir=1.0
nps 1e6
*f8:e 3
prdmp 2j 1
print
```

Pulse-Height Tally Review

- Different from all other tallies
  - Mimics a pulse-height detector
  - Contribute at surface crossings and source events (cf. track-length tally)



F4 History Score



F8 History Score

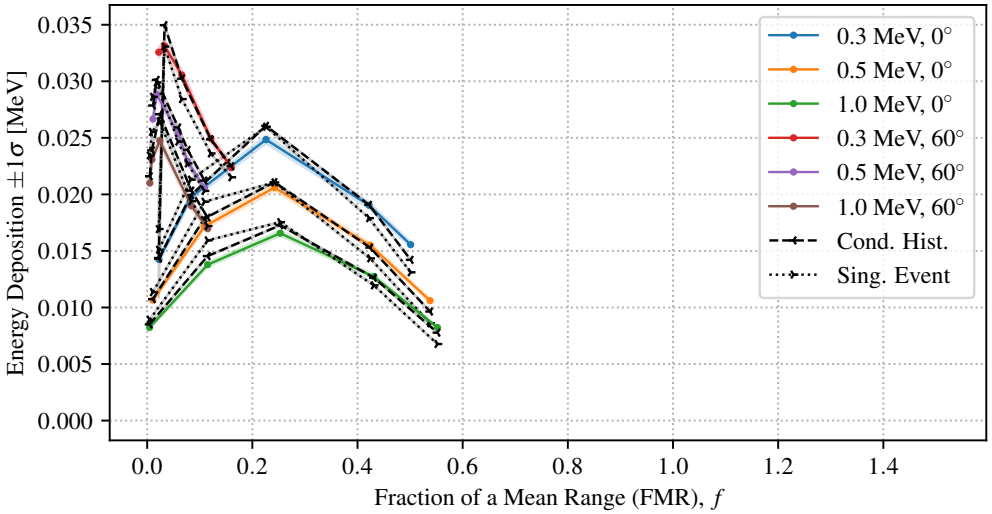
$$x = \frac{w_0\ell_0 + w_1\ell_1 + w_2\ell_2 + w_3\ell_3}{V}$$

$$x = (w_0 + w_1 + w_3) - (w_0 + w_2 + w_3)$$

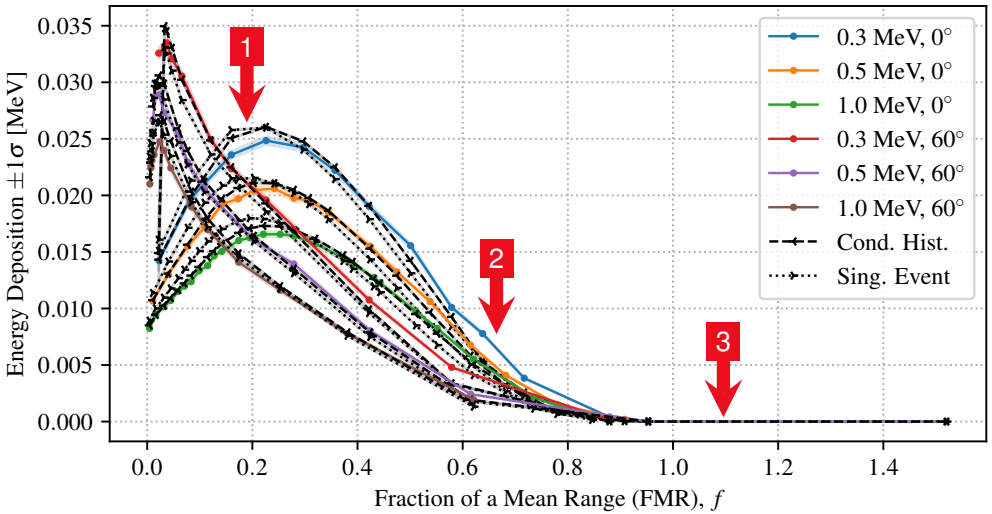
$$x = w_1 - w_2$$

The *F8 tally multiplies energy by weight in the contributions.

Results: Aluminum, Before & After

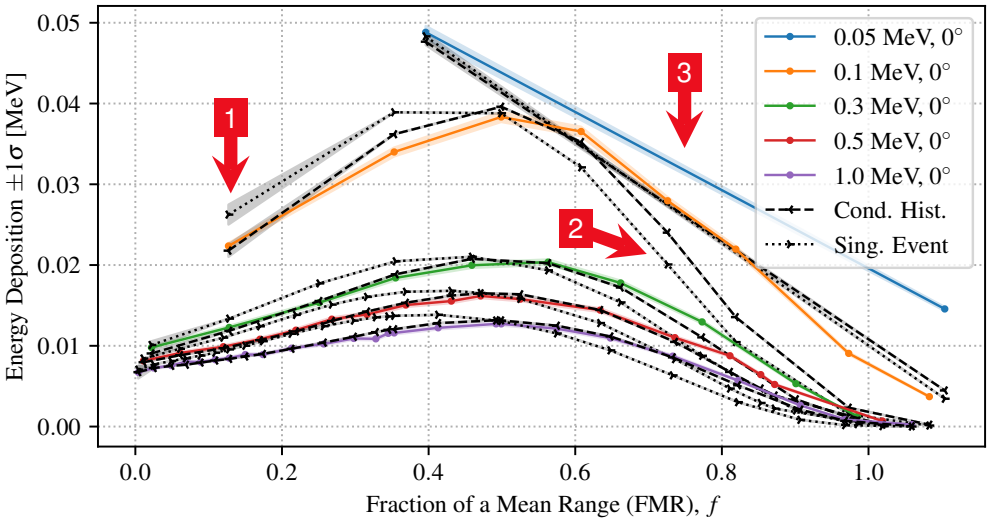


Results: Aluminum, Before & After



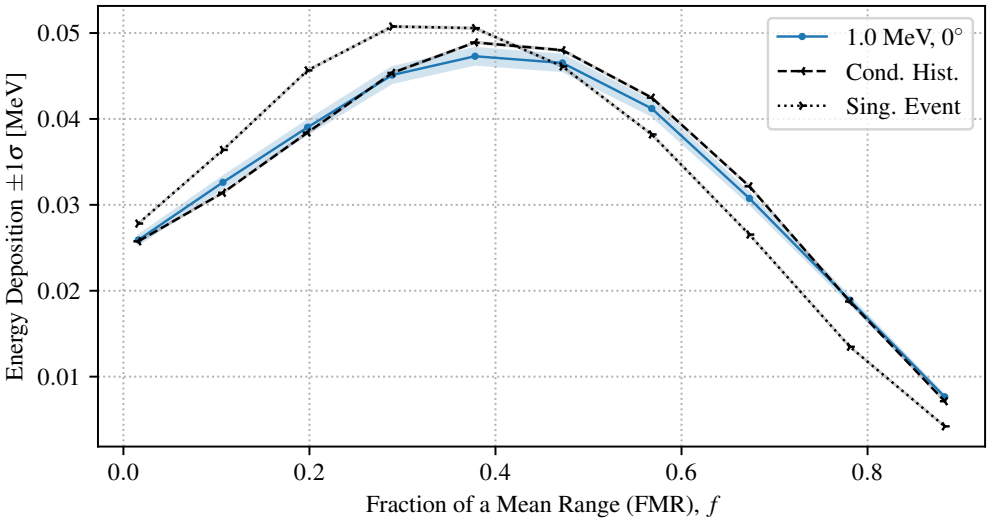
1. Low-energy and low-thickness discrepant region.
2. Low-energy and high-thickness discrepant region.
3. All energy is deposited in the front foil: no temperature rise in calorimeter.

Results: Beryllium

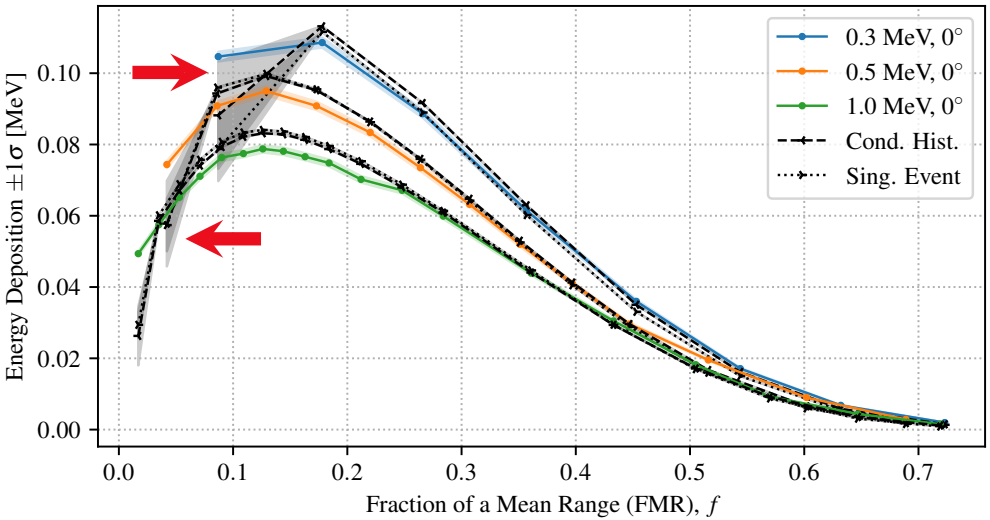


1. Low-energy and low-thickness uncertainty.
2. Low-energy and high-thickness discrepant region.
3. Low-energy discrepancy and coarse FMR points.

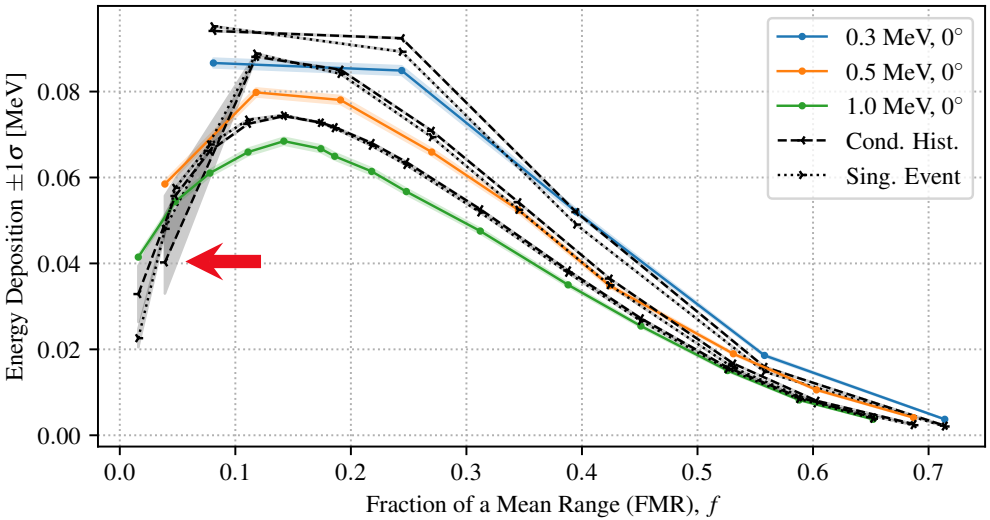
Results: Carbon



Results: Copper

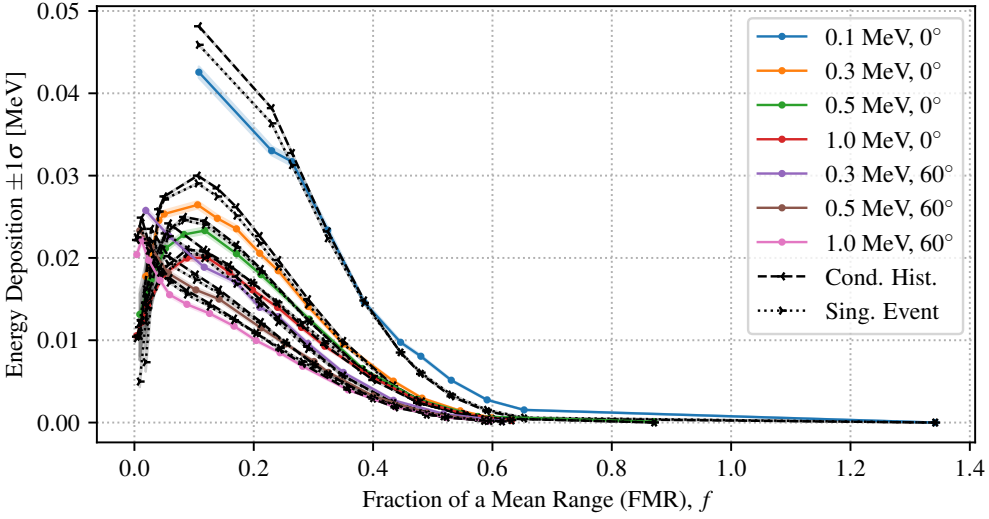


Results: Iron

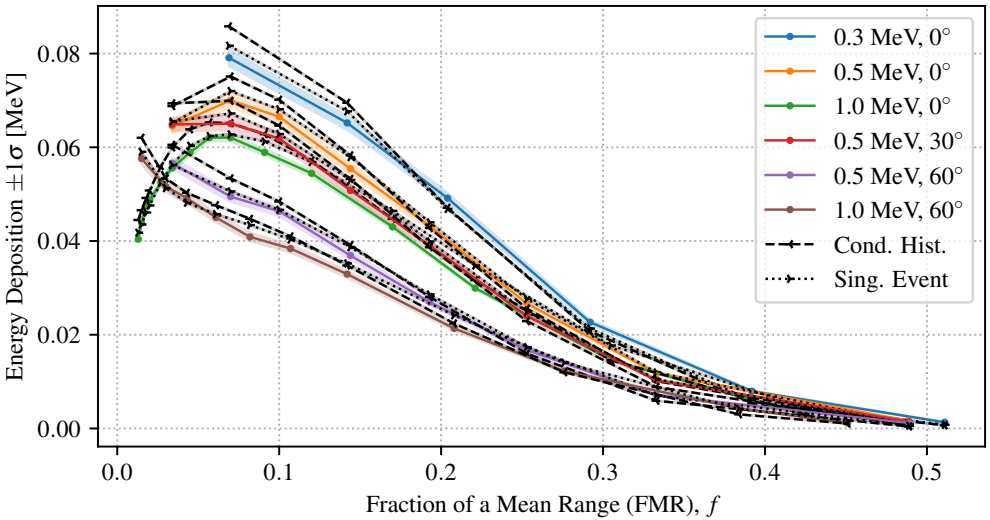


Why such uncertainty for these cases in particular?

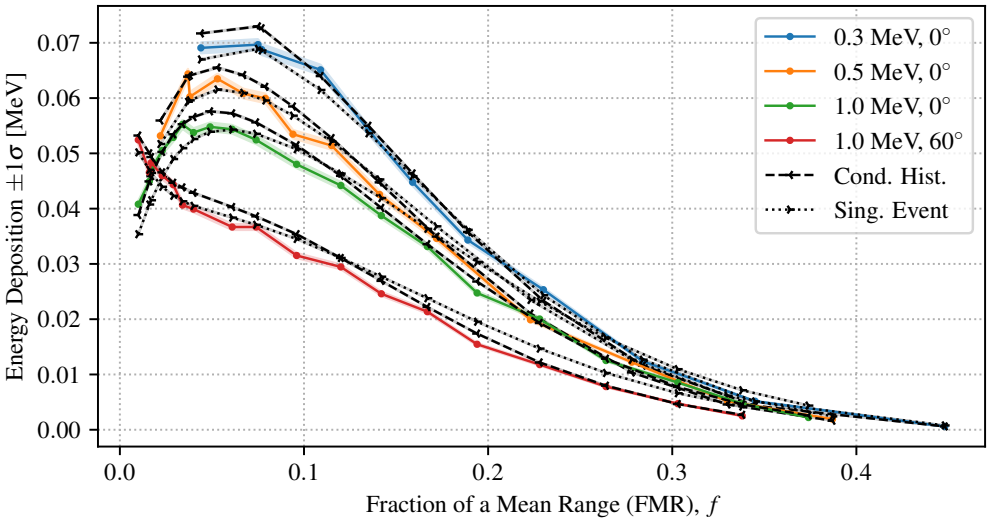
Results: Molybdenum



Results: Tantalum



Results: Uranium



Summary & Future Work

Summary

- Discussed MCNP6.3 V&V suite status and direction
- Demonstrated foil thickness calculating from FMR
- Showed extended set of homogenous-foil results

Open Questions

- Low-energy discrepancies?
- Why such coarse FMR points and disagreement?

Future Work

- Extend V&V suite to include “sandwich” configurations
  - Be/Au/Be, C/Cu/C, C/Ta/C, C/Au/C, C/U/C, Al/Au/Al, Ta/Al
- Extend V&V suite to include unstructured mesh representations
- Should “we” pursue this experiment again for other materials, FMRs, etc.?

Questions?

Background

Software Testing & the MCNP6.3 V&V Suite

Experimental & Calculational Configuration

Results

Summary & Future Work

Backup Slides

Outline

References

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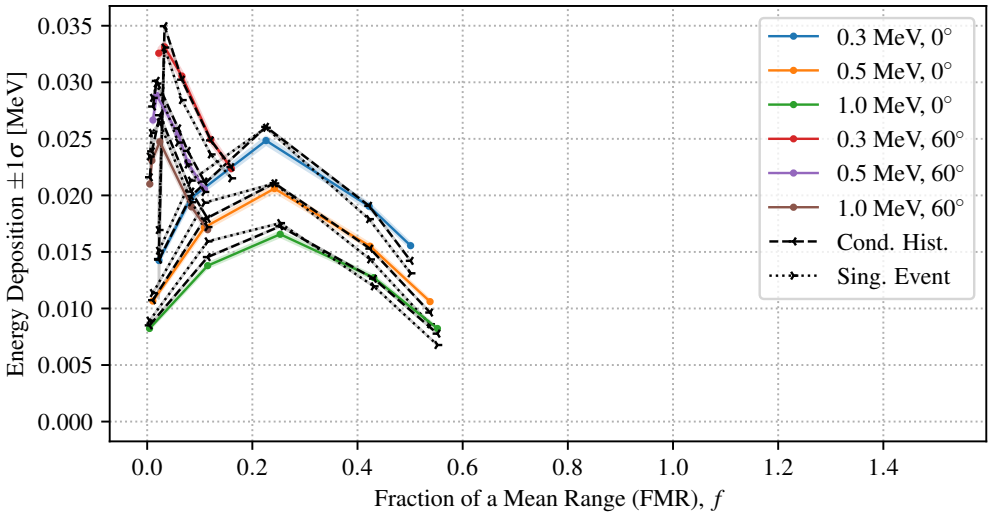
Results: Aluminum, Before & After



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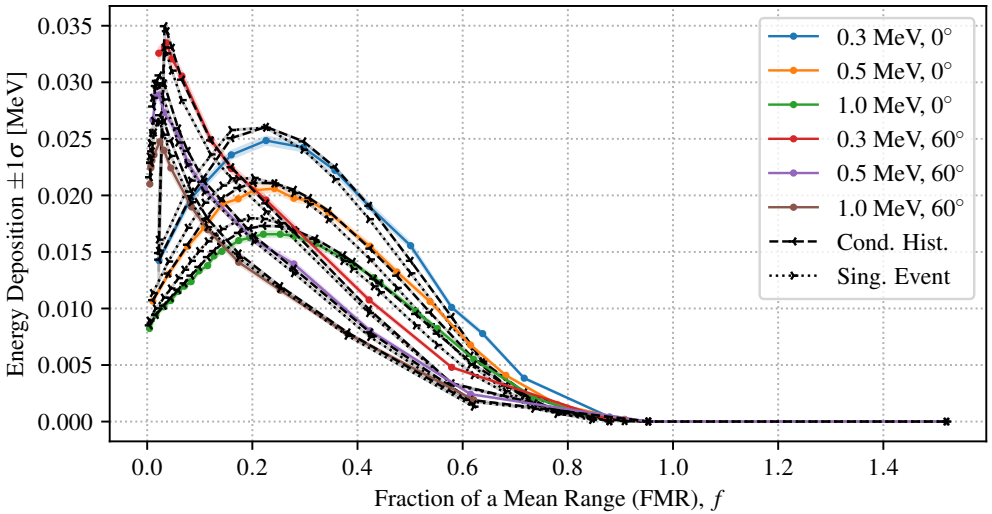
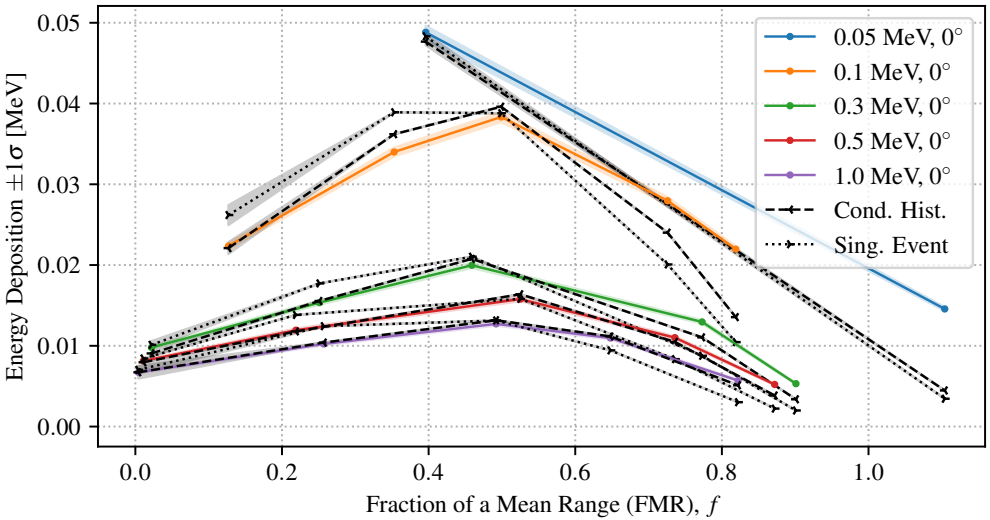
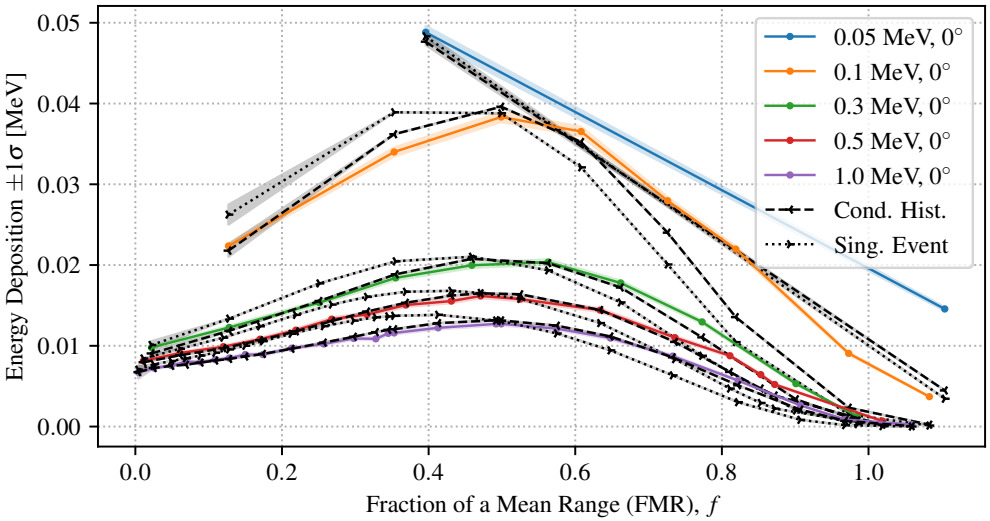


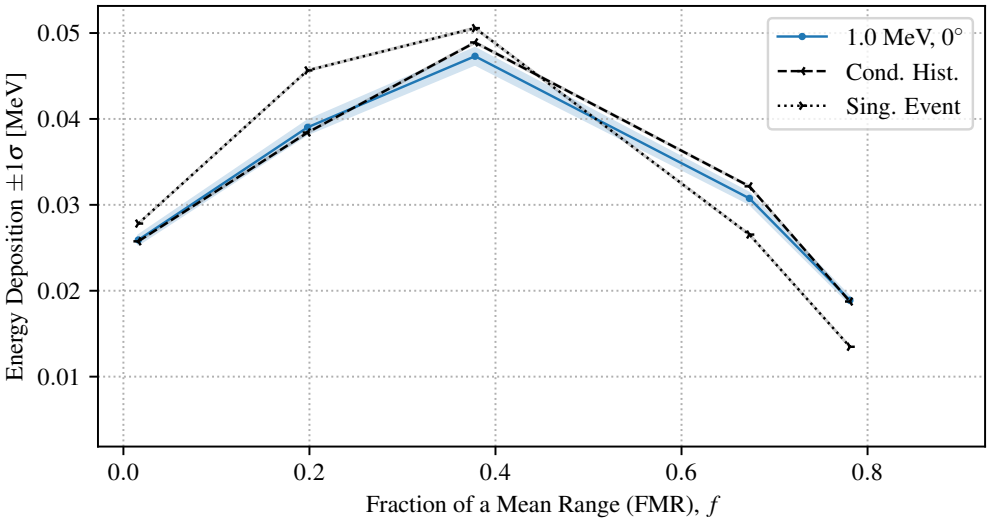
Results: Beryllium, Before & After



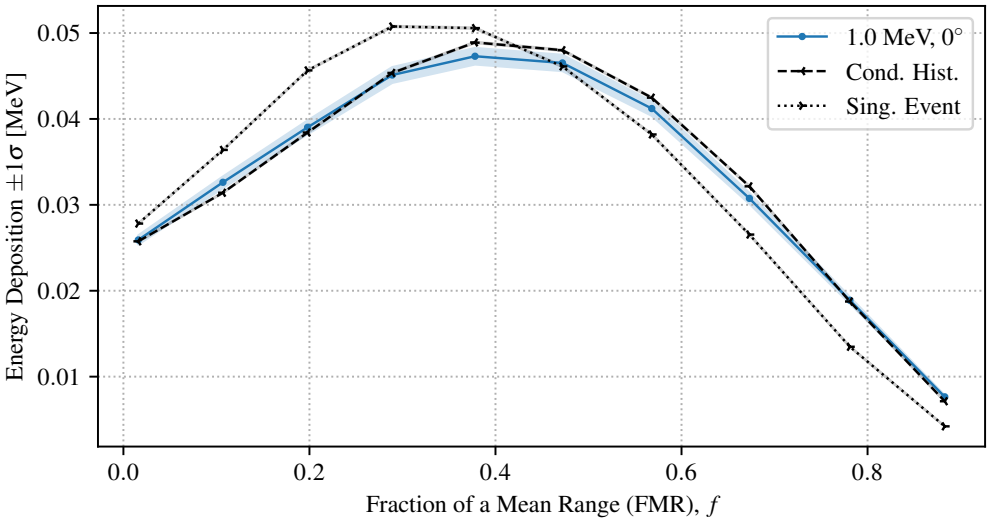
Results: Beryllium, Before & After



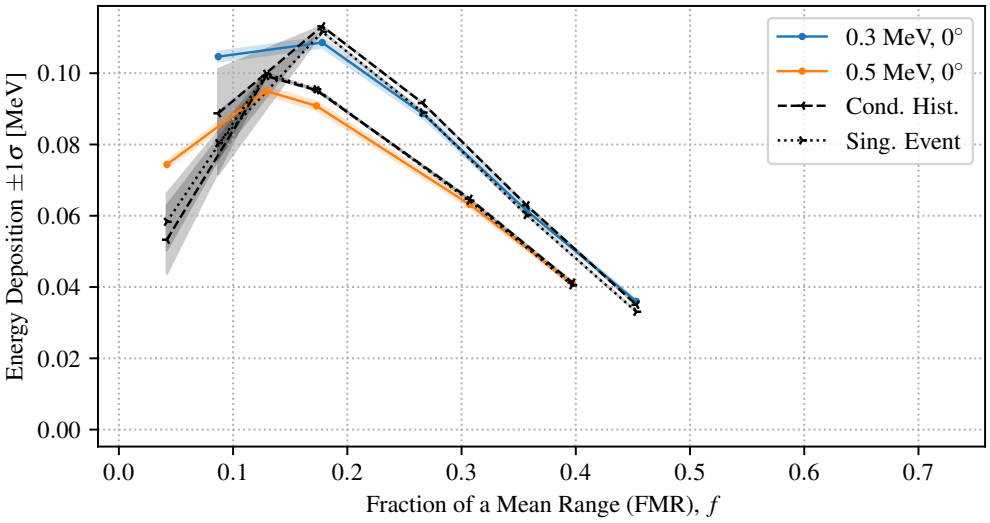
Results: Carbon, Before & After



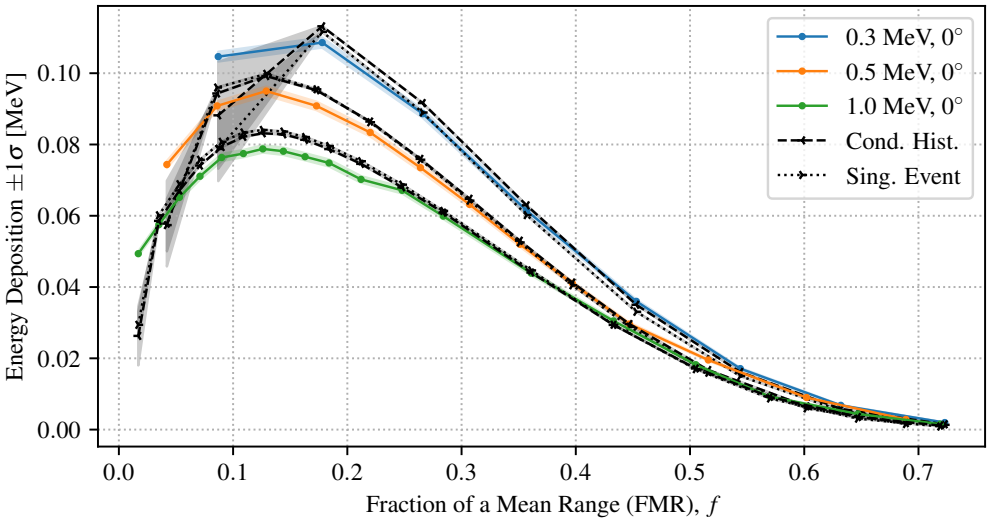
Results: Carbon, Before & After



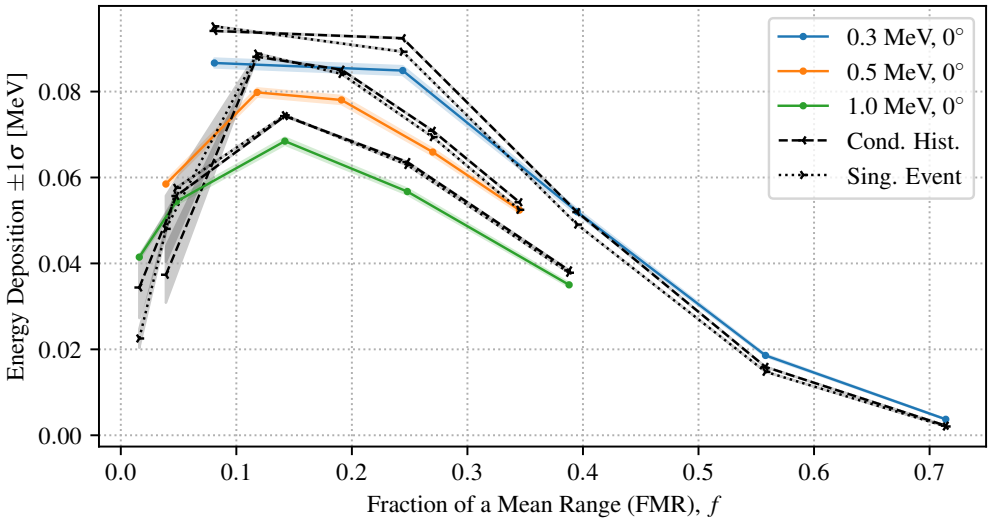
Results: Copper, Before & After



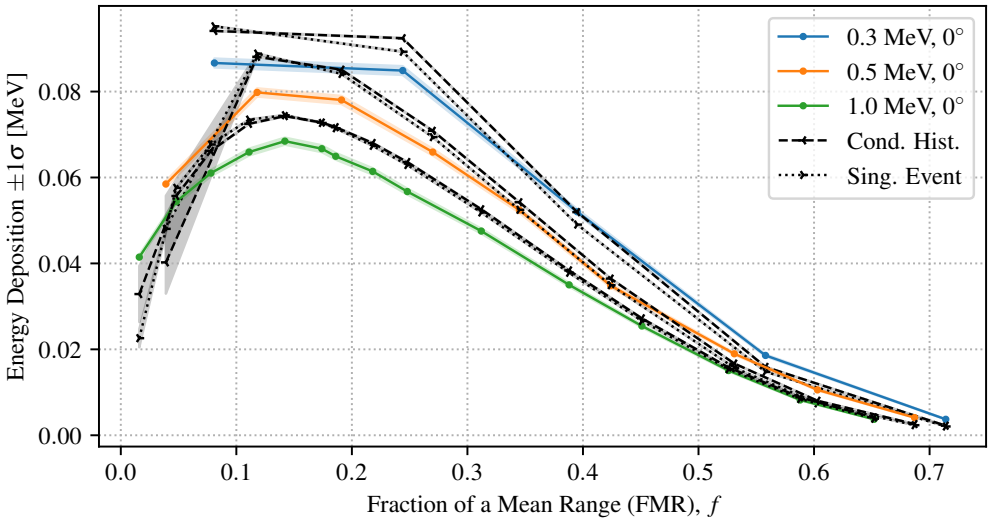
Results: Copper, Before & After



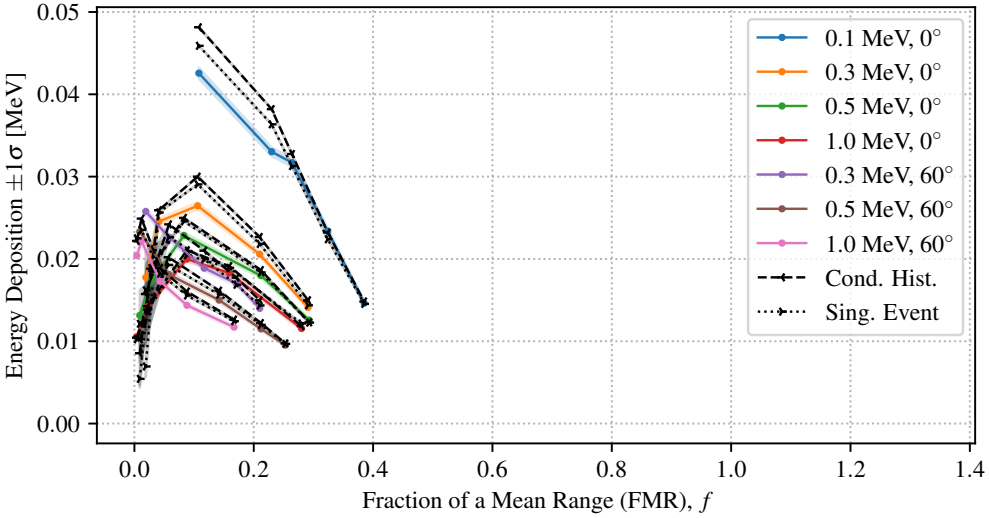
Results: Iron, Before & After



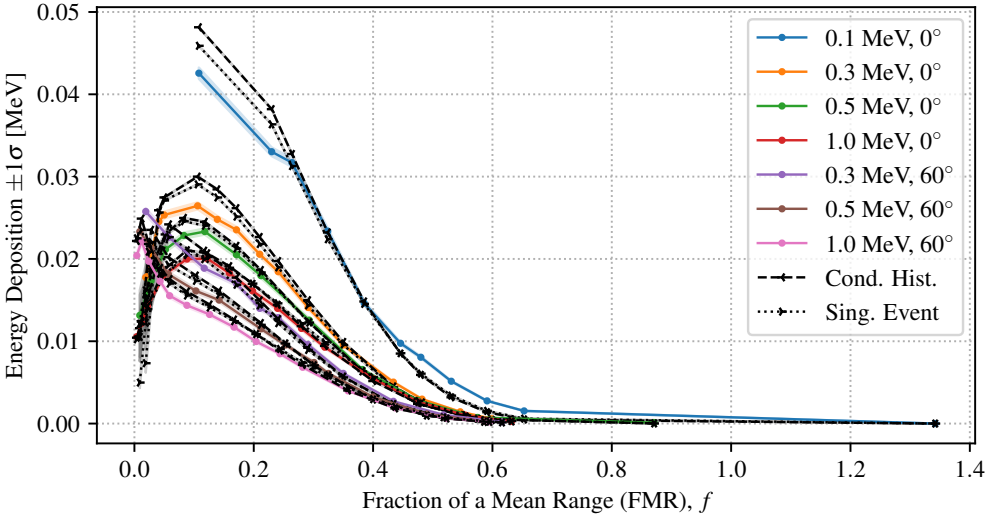
Results: Iron, Before & After



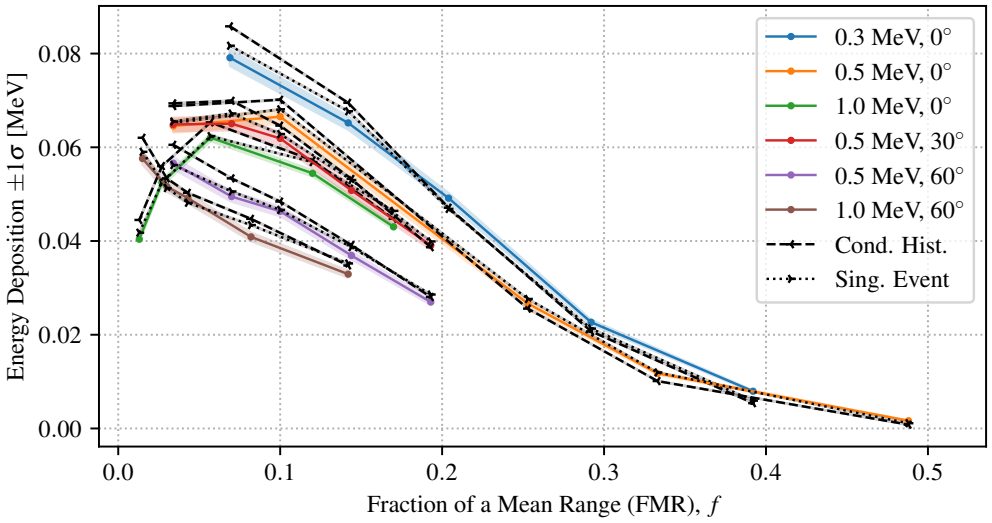
Results: Molybdenum, Before & After



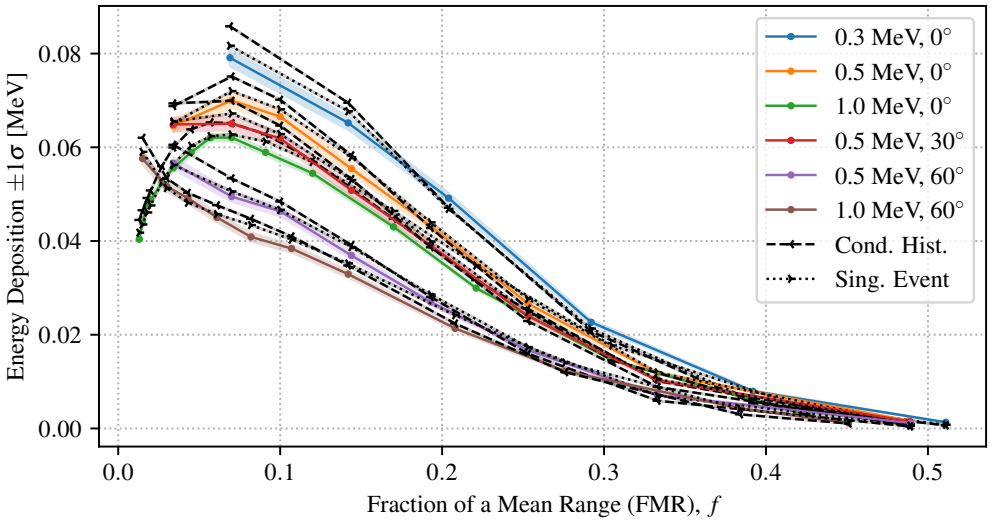
Results: Molybdenum, Before & After



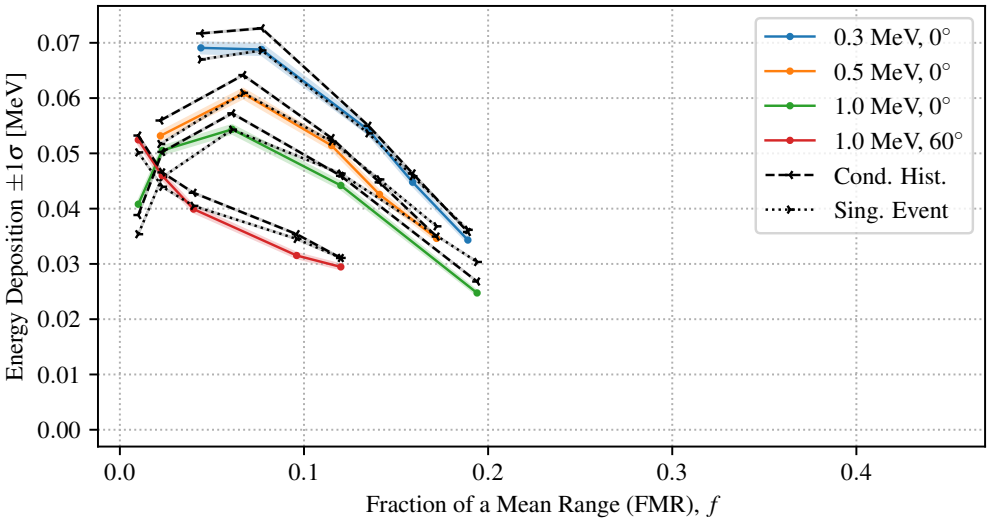
Results: Tantalum, Before & After



Results: Tantalum, Before & After



Results: Uranium, Before & After



Results: Uranium, Before & After