LA-UR-15-28708
Approved for public release; distribution is unlimited.

Title: Validation of MCNP6 for Electron Energy Deposition in Extended Media

Author(s): Dixon, David A.
Hughes, Henry Grady III

Intended for: 2015 American Nuclear Society Winter Meeting, 2015-11-08/2015-11-12 (Washington D. C., District Of Columbia, United States)

Issued: 2015-11-06

Los Alamos NATIONAL LABORATORY EST.1943

Validation of MCNP6 for Electron Energy Deposition in Extended Media

David A. Dixon and H. Grady Hughes

Los Alamos National Laboratory

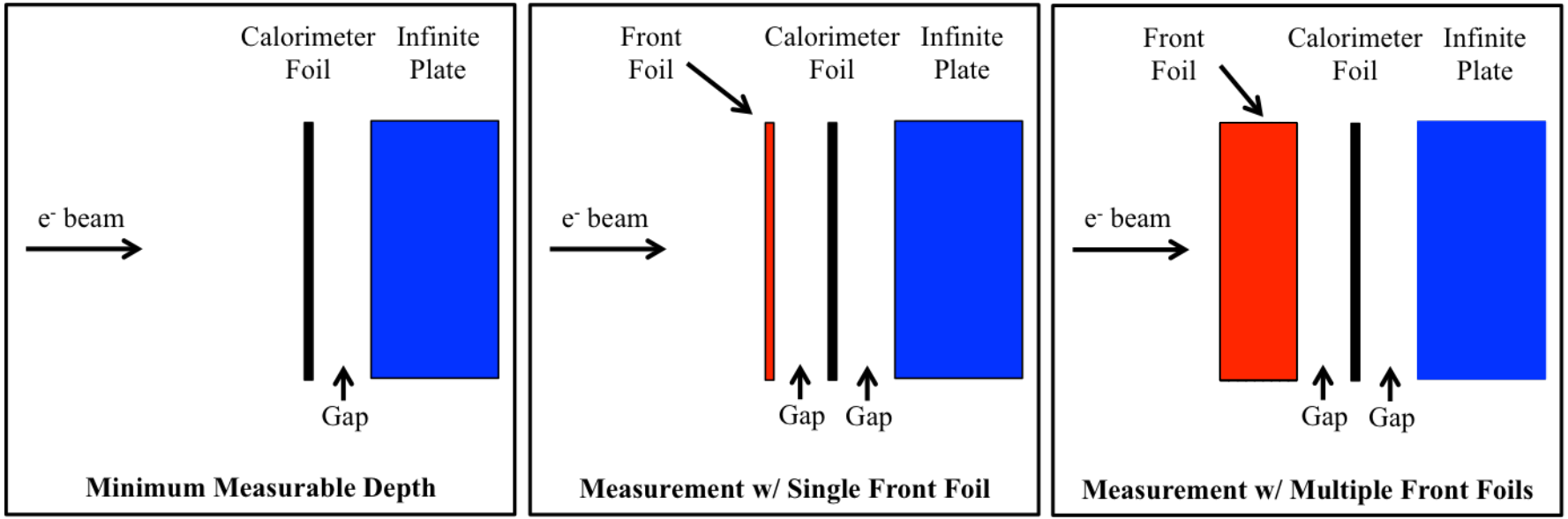
Overview

- Introduction
- Problem setup
- Results
- Conclusions

Introduction

- Gap in MCNP6 electron-photon transport V&V
  - Last edep validation paper written for MCNP4C in 2003
  - No validation since incorporation of new straggling logic
  - First step in a broader V&V effort
- Comparison to Lockwood experiments circa 1987
  - 1-D single- or multi-layer semi-infinite slab
  - Wide range of elemental data (Z=3…79)
  - Source characteristics
    - Monoenergetic pencil beam
    - Energies included: 0.1-, 0.3-, 0.5-, and 1-MeV
    - Angles included: 0°, 30°, and 60°

Experimental Setup



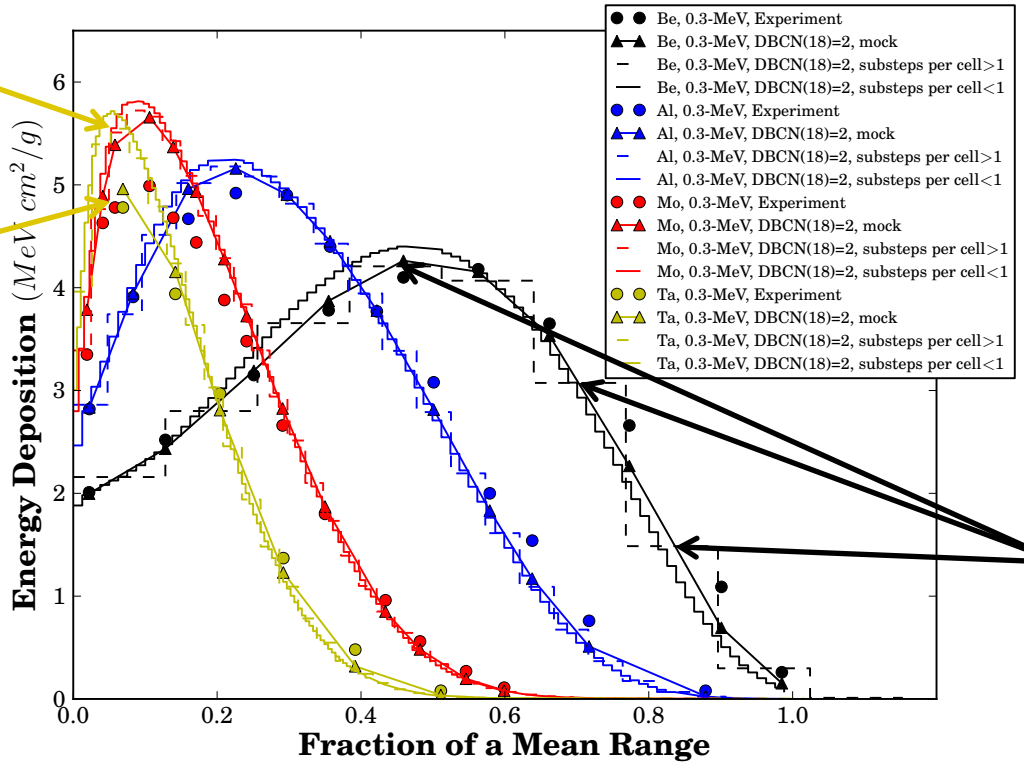
Simulation Characteristics

- Semi-infinite slab simulation
  - Subdivide into cells
  - Histogram results
- “Mock” simulation – closer representation of experiment
  - Reduces boundary crossings
  - Point-wise results (linear or polynomial fits)
- Study impact of
  - Cell size
  - Straggling model
  - ESTEP
  - EFAC

Single-Layer Results (model/cell-size)

Significant overestimation in Ta

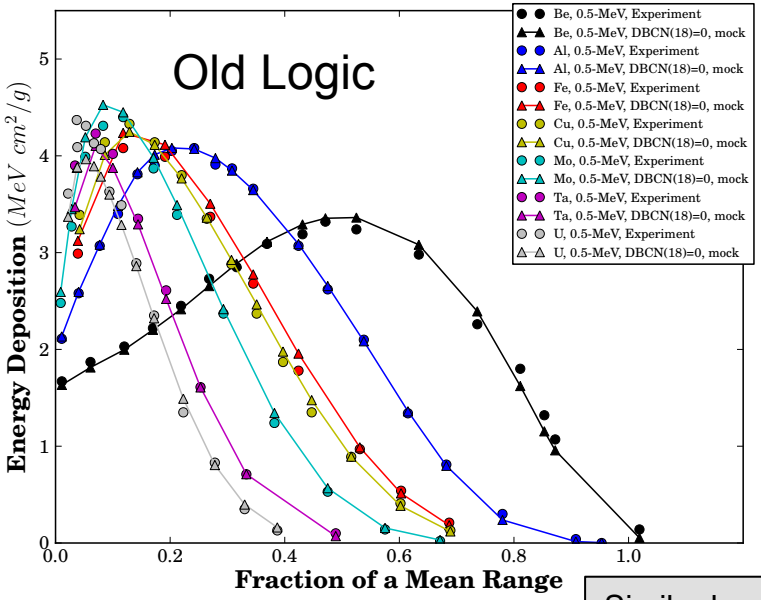
Improved agreement for exp. and "mock" result

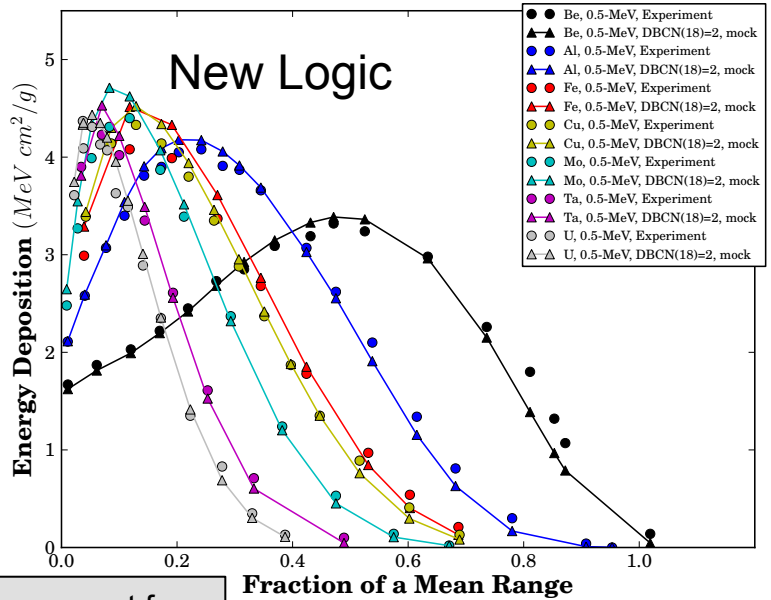


Profile is slightly sensitive to substeps per cell <1

Agreement between "mock" and histogram results where substeps per cell > 1

Single-Layer Results (Straggling)





Similar levels of agreement for different straggling models with exception of Fe, Mo, and U

Single-Layer Results (ESTEP)

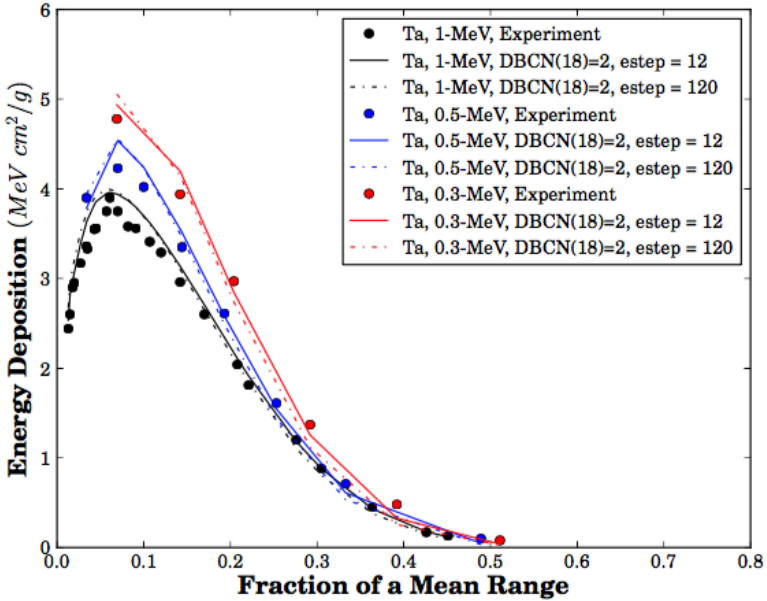
M(Z) by element: Z is an average the of atomic number in a mixture:

M(Z=1…5) = 2	M(Z=6…9) = 3	M(Z=10…12) = 4
M(Z=13…21) = 5	M(Z=22…28) = 6	M(Z=29…39) = 7
M(Z=40…49) = 8	M(Z=50…54) = 9	M(Z=55…64) = 10
M(Z=65…69) = 11	M(Z=70…78) = 12	M(Z=79…84) = 13
M(Z=85…91) = 14	M(Z=92…100) = 15	

M(Z) can be increased, if desired:

m13 1000. 2. 8000. 1. estep = 5

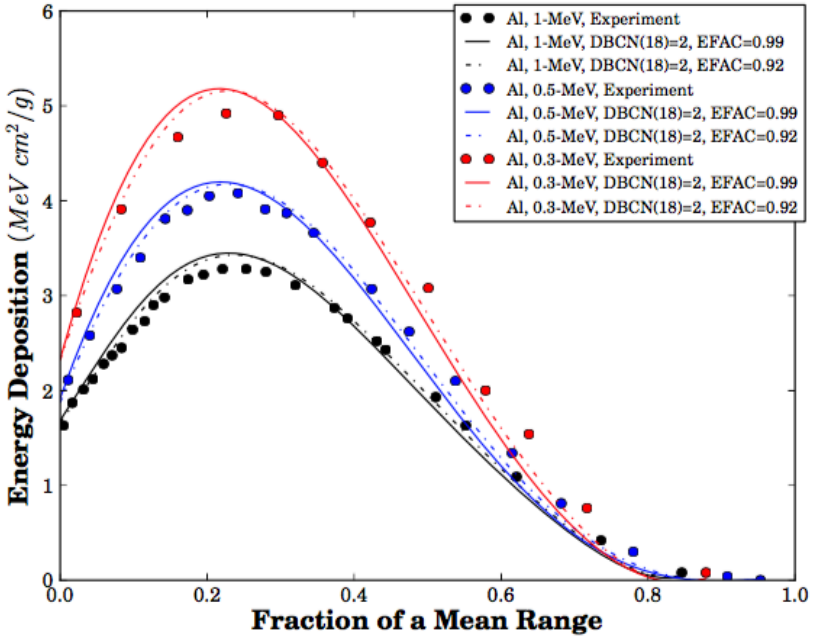
Results relatively insensitive to ESTEP – USE THE DEFAULTS



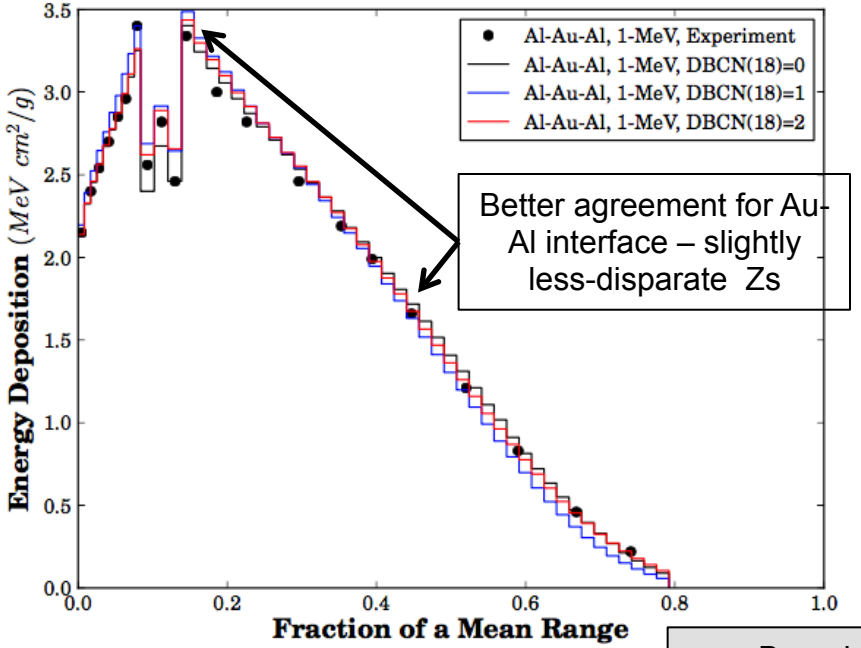
Single-Layer Results (EFAC)

- EFAC
  - Controls energy grid density
  - E_i-1 = EFAC*(E_i)
  - Valid EFAC's: 0.1-0.99
  - Default is 0.92
  - Increasing EFAC increases run time

Changing EFAC does not improve agreement and increases run time – USE THE DEFAULT

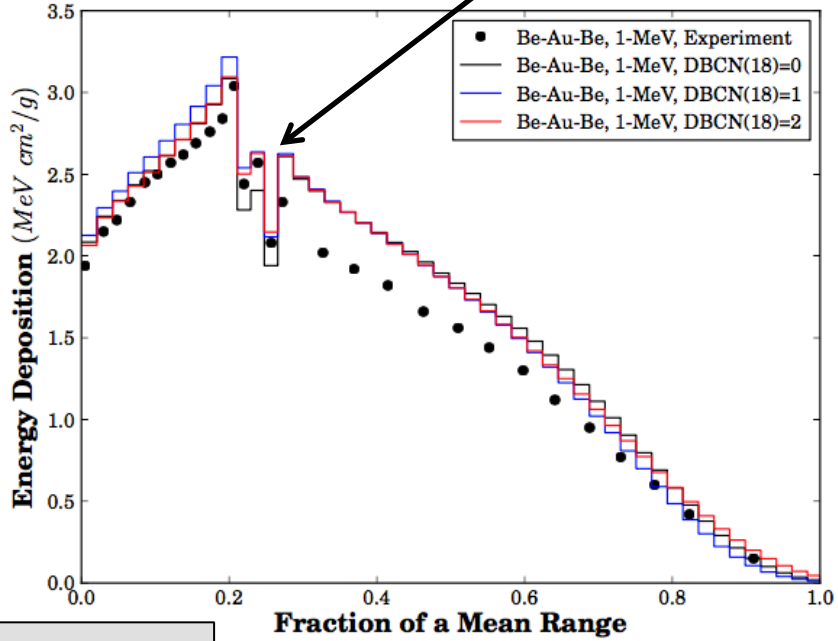


Multi-Layer Results



Better agreement for Au-Al interface – slightly less-disparate Zs

Significant overestimation of EDEP after high-z-low-z interface



Boundary crossing approximations remain an issue, but severity is problem dependent

Suggestions for users

- Pay attention to smallest dimensions
  - Check print table 85 for estep range (need ***print*** option in input)
  - Divide estep range by number of substeps and compare
- Use the default
  - Straggling model
  - ESTEP
  - EFAC
- Bottom line – allow for margin of error
  - Be conservative in problems with small cells (< 1 substep)
  - Or for source energies below 0.3-MeV

Conclusions

- Confidence in integrated dose
- No significant improvements in local agreement
- Boundary crossings remain an issue
- Similar validations indicate MCNP6 is competitive with:
  - ITS (CLASS I)
  - PENELOPE (hybrid)
  - EGSnrc (hybrid)
  - Geant4 (hybrid)

Questions?

```
 warning.  material      100 has been set to a conductor.
1range table for material      100 (condensed)                                                    print table 85

 electron substeps per energy step =   3,  default =   3.  mean ionization energy = 7.80000E+01 ev.

 density effect data
 conductor
   z =   6
    occ no, be(ev) pairs
       2.    288.000       2.     16.590      -2.     11.260
       plas(ev)       wt       tmin(mev)
       21.68718     2.78282     0.00000

         energy           stopping power           range    radiation   beta**2   density   rad/col   e-step    dyield
   n                collision radiation   total                yield              corr                range
          mev      mev cm2/g mev cm2/g mev cm2/g   g/cm2                        mev cm2/g             g/cm2

  107  1.0265E-03  1.045E+02 2.522E-03 1.045E+02 5.059E-06 1.931E-06  4.005E-03 1.858E-03 2.413E-05 7.937E-07 1.983E-09
  106  1.1194E-03  9.890E+01 2.569E-03 9.890E+01 5.974E-06 3.850E-06  4.367E-03 1.863E-03 2.598E-05 9.142E-07 2.328E-09
  105  1.2207E-03  9.351E+01 2.614E-03 9.351E+01 7.028E-06 5.769E-06  4.761E-03 1.869E-03 2.796E-05 1.054E-06 2.732E-09
  104  1.3312E-03  8.833E+01 2.658E-03 8.833E+01 8.244E-06 7.699E-06  5.190E-03 1.875E-03 3.009E-05 1.216E-06 3.207E-09
  103  1.4517E-03  8.337E+01 2.699E-03 8.337E+01 9.649E-06 9.653E-06  5.657E-03 1.882E-03 3.238E-05 1.405E-06 3.763E-09
  102  1.5831E-03  7.863E+01 2.739E-03 7.863E+01 1.127E-05 1.164E-05  6.167E-03 1.890E-03 3.483E-05 1.623E-06 4.415E-09
  101  1.7263E-03  7.411E+01 2.776E-03 7.411E+01 1.315E-05 1.367E-05  6.723E-03 1.898E-03 3.746E-05 1.878E-06 5.180E-09
  100  1.8826E-03  6.980E+01 2.812E-03 6.980E+01 1.532E-05 1.577E-05  7.328E-03 1.907E-03 4.029E-05 2.174E-06 6.075E-09
```

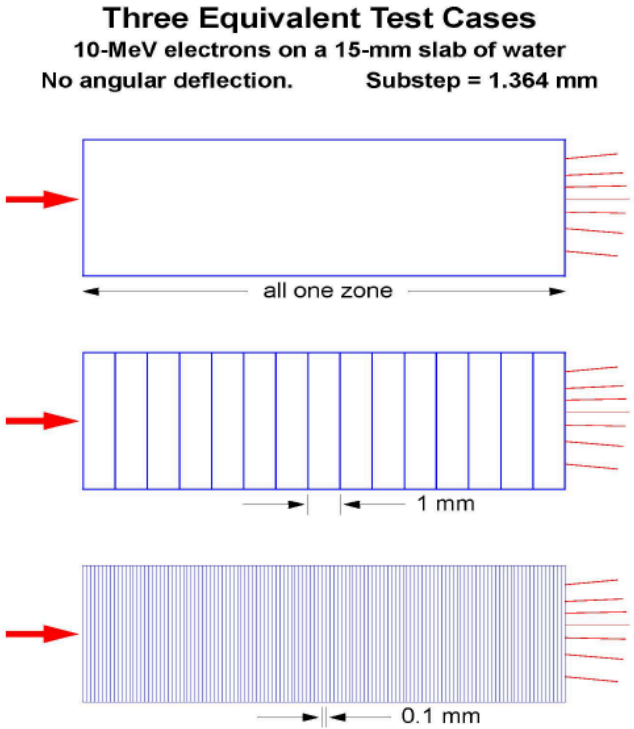
Summary of Results

- Energy deposition profiles
  - Relatively insensitive to straggling logic
  - Nevertheless, there are clear benefits to new logic
  - Boundary crossing artifacts remain
- Total energy deposition
  - Generally, good agreement
  - 70% of results within 5% of experiment
- Overall performance satisfactory

Future work

- Algorithmic
  - Max number of terms in multiple-scattering distributions
  - Boundary crossing approximation – new interpolation
- Verification and validation
  - Fano cavity test (in process)
  - Faddegon scattering experiment (in process)
  - Reproduce Gierga & Adams work from MCNP4
  - Tabata charge deposition experiments

MCNP6 Straggling Logic



MCNP6 Straggling Logic