Validation of electron, proton and alpha particle ranges

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Aim

- To compare Geant4 and NIST CSDA ranges of electrons (10 keV-1 GeV), protons and alpha particles (1 MeV-1 GeV) in C, Al, Cu, Sn, W, Pb, water, adipose, muscle and bone
- Material definitions from G4NIST database (with I=75 and 78 eV for G4_WATER)
- Three constraints: no secondaries, no msc, no straggling
- 10000 events per energy (no statistical uncertainties)

- Reference physics lists:
  - G4EmStandardPhysics
  - G4EmStandardPhysics_option3
  - G4EmLivermorePhysics (only for electrons)
  - G4EmPenelopePhysics (only for electrons)

Step limitation by ionisation

	electron	proton	alpha
Standard default	0.2, 1 mm	0.2, 1 mm	0.2, 1 mm
Standard option3	0.2, 0.1 mm	0.2, 0.05 mm	0.1, 0.02 mm
Livermore	0.2, 0.1 mm	Standard option3	Standard option3
Penelope	0.2, 0.1 mm	Standard option3	Standard option3

ESTAR uncertainties

From http://physics.nist.gov/PhysRefData/Star/Text/method.html:

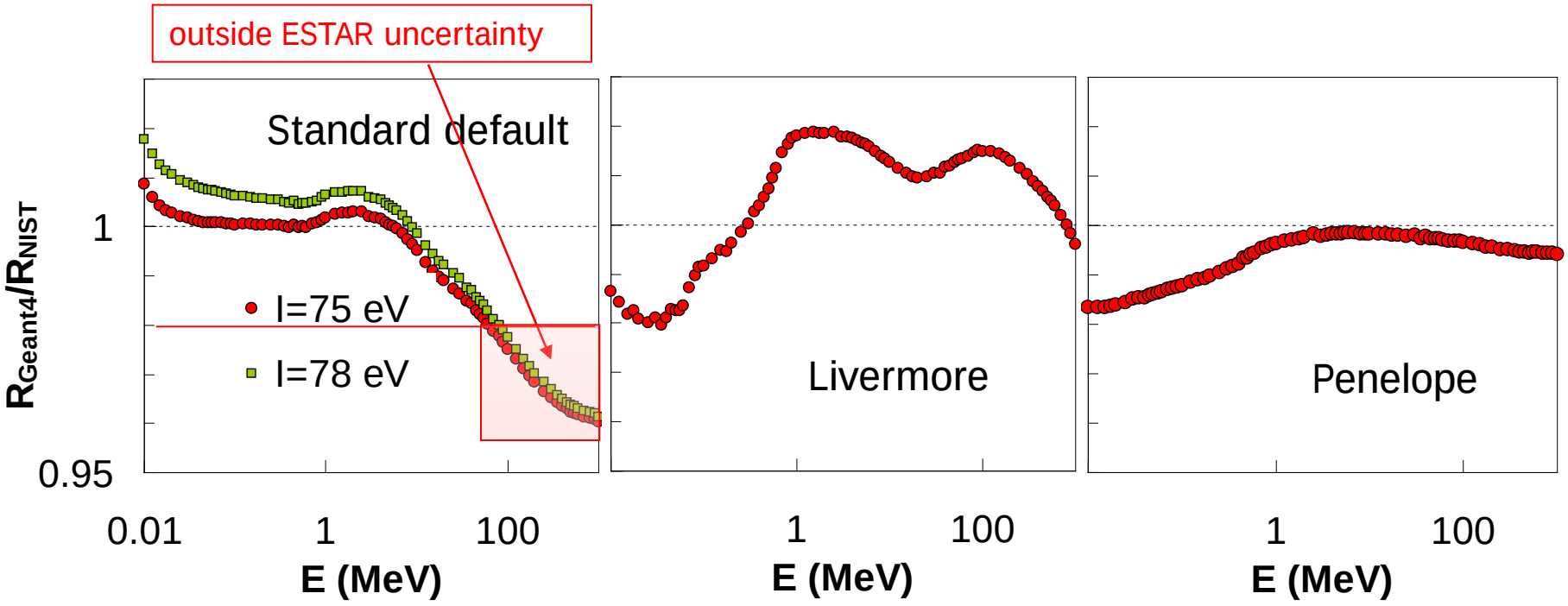
”The uncertainties of the calculated collision stopping powers for electrons are estimated (ICRU, 1984) to be:

- 1 % to 2 % above 100 keV
- 2 % to 3 % (in low-Z materials) between 100 keV and 10 keV
- 5 % to 10 % (in high-Z materials) between 100 keV and 10 keV.

The increasing uncertainties at low energies are due to the lack of shell corrections which are required when the velocity of the incident electron is no longer large compared to the velocities of the atomic electrons, especially those in the inner shells.”

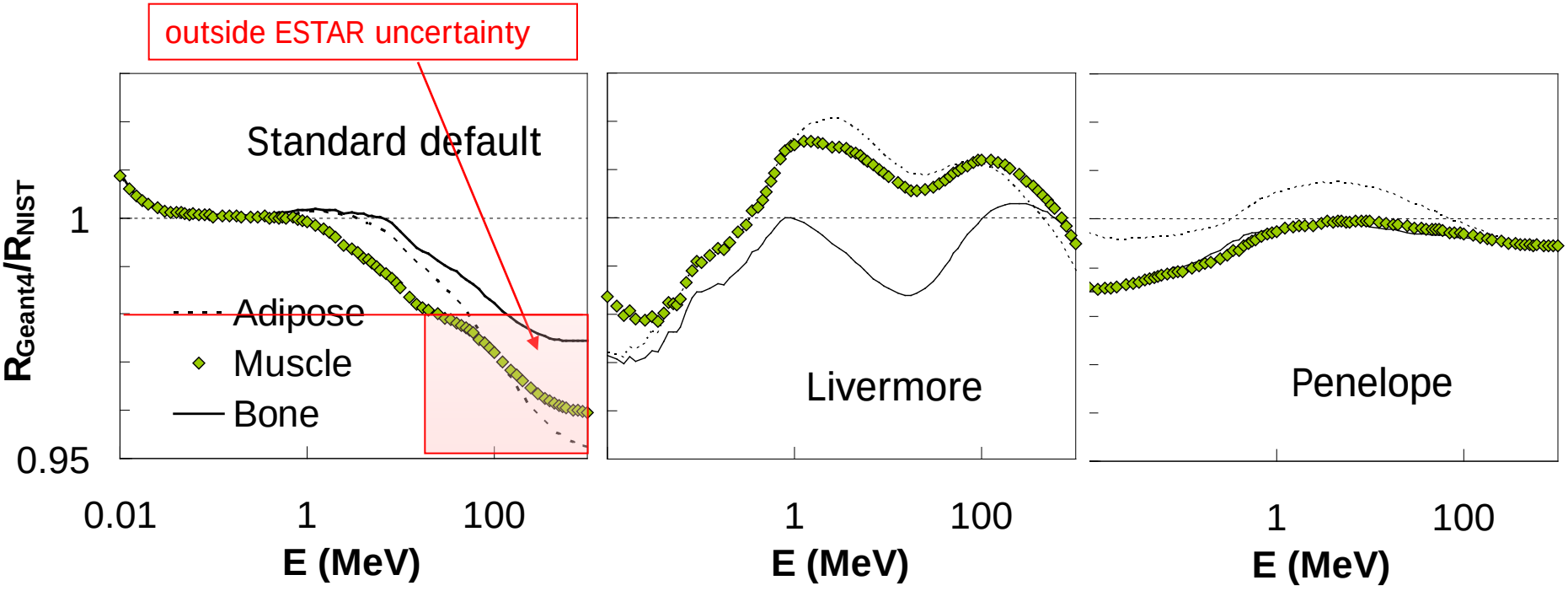
Electrons in water

- All models are within NIST uncertainties, apart from standard for E>60 MeV (I=75 eV), and E>80 MeV (I=78 eV)
- Largest difference G4/NIST = 4%
- Ionisation potential gives a variation of max 1% (at 10 keV)
- Best agreement with NIST: Penelope



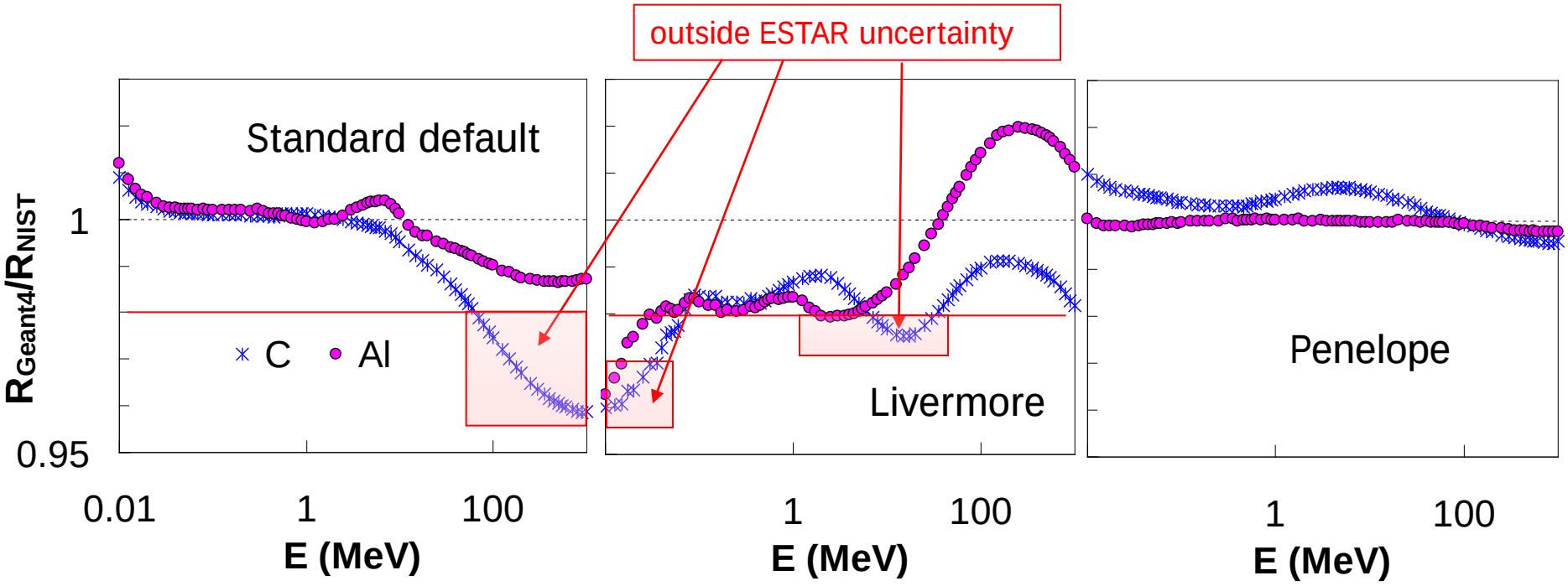
Electrons in adipose, muscle and bone

- All models are within NIST uncertainties, apart from standard for muscle and E>30 MeV, adipose and E>55 MeV, bone and E>150 MeV
- Largest difference G4/NIST = 3% in bone, 4% in muscle, 5% in adipose
- Best agreement with NIST: Penelope



Electrons in C and Al

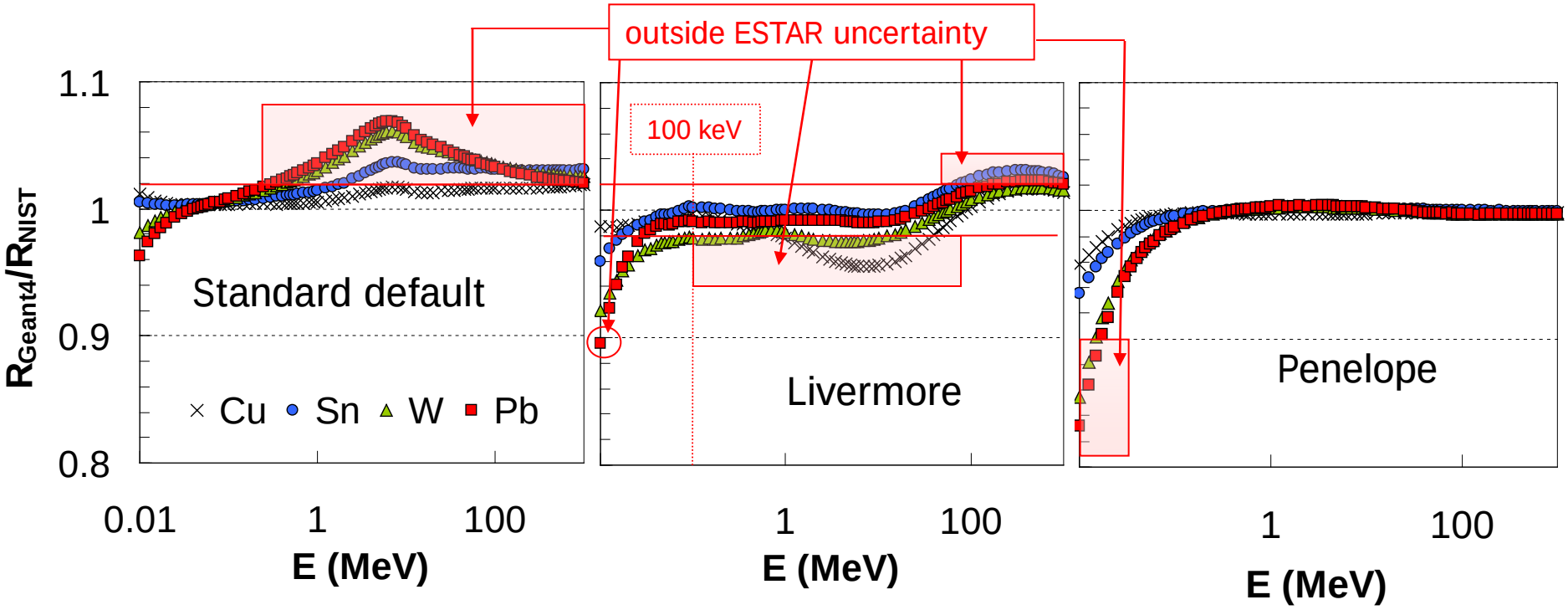
- Penelope is within NIST uncertainties for C, Al
- Standard is within NIST uncertainties for Al, but not for C at E>70 MeV (largest difference from NIST = 4%)
- Livermore deviates from NIST more than 3% for both elements at low energies, and more than 2% at 2-4 MeV for Al and at 7-30 MeV for C
- Best agreement with NIST: Penelope (C, Al) and Standard (Al)



Electrons in Cu, Sn, W and Pb

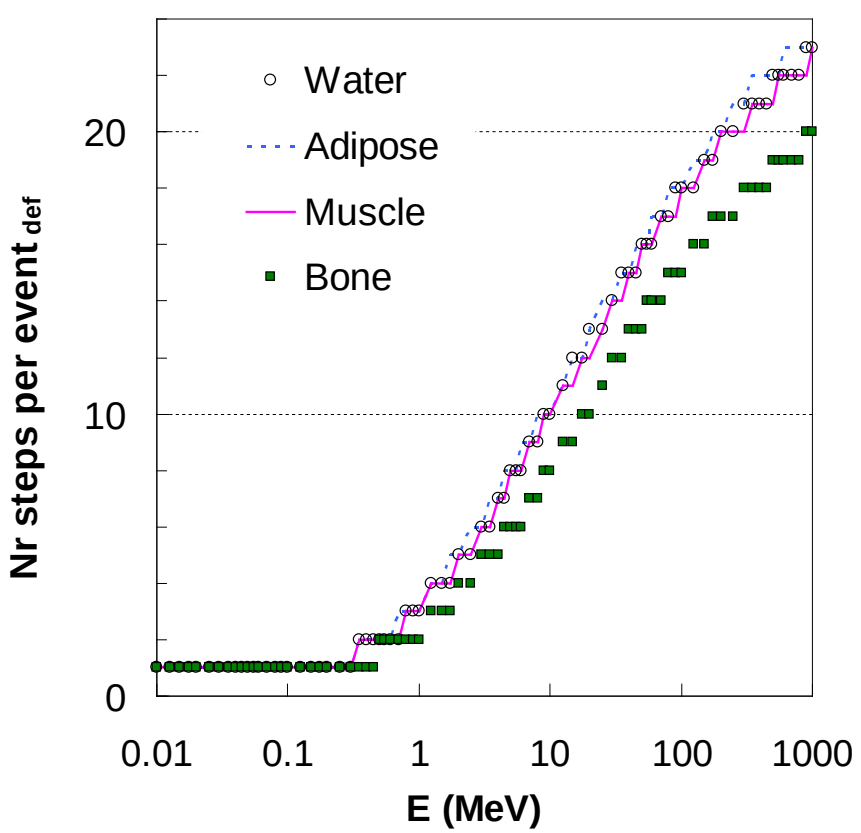
Range of G4/NIST ratio:

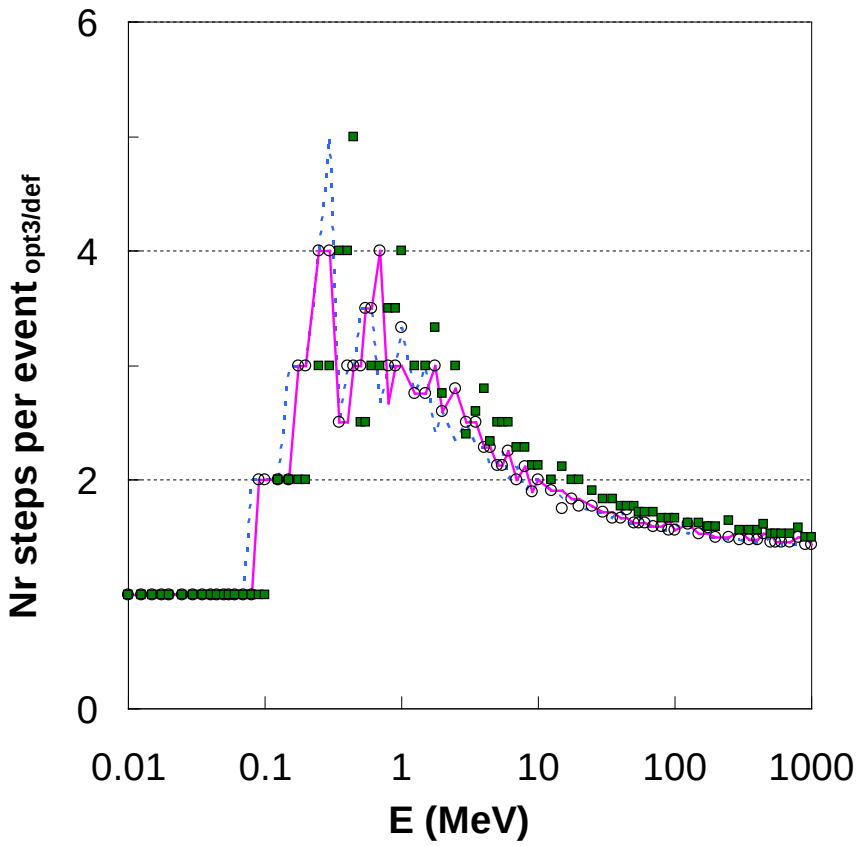
- Cu: 1-1.02 (Standard), 0.96-1.02 (Livermore), 0.95-1 (Penelope)
- Sn: 1-1.04 (Standard), 0.96-1.03 (Livermore), 0.94-1 (Penelope)
- W: 0.98-1.06 (Standard), 0.92-1.02 (Livermore), 0.85-1 (Penelope)
- Pb: 0.96-1.07 (Standard), 0.90-1.02 (Livermore), 0.83-1 (Penelope)
- Best agreement with NIST: Standard



Number of electron steps/event (1)

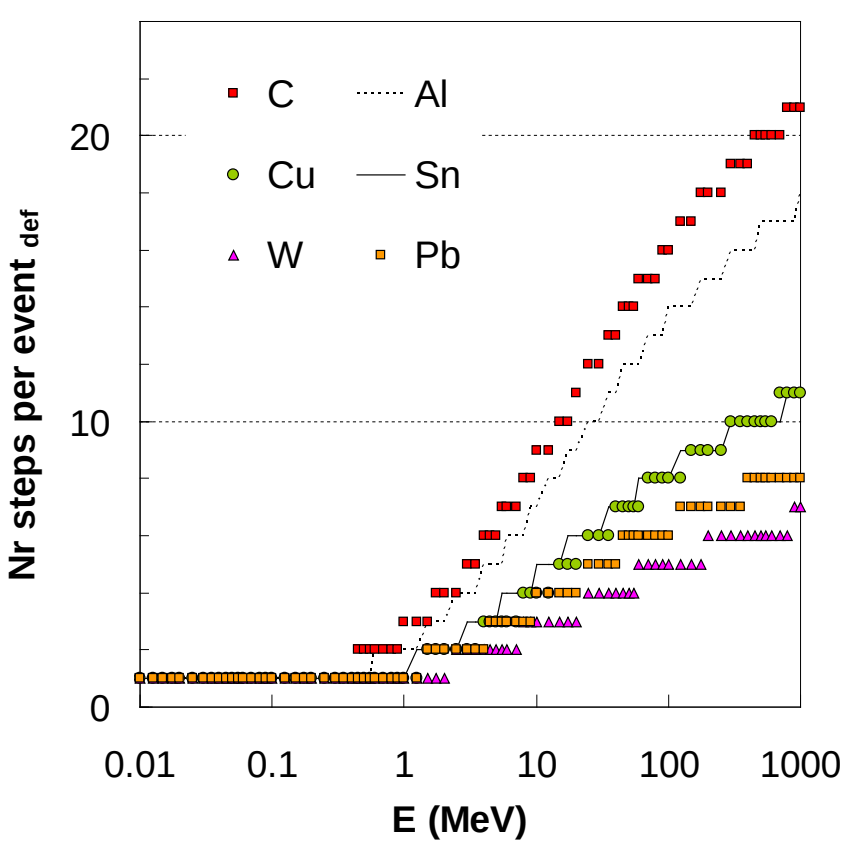
- Standard opt3 and Penelope, Livermore have a similar number of steps/event for all materials
- In water and tissue: only 1 step/event below 0.2 MeV in standard default; step ratio std opt3/def ~ 1.5-2 at E>10 MeV

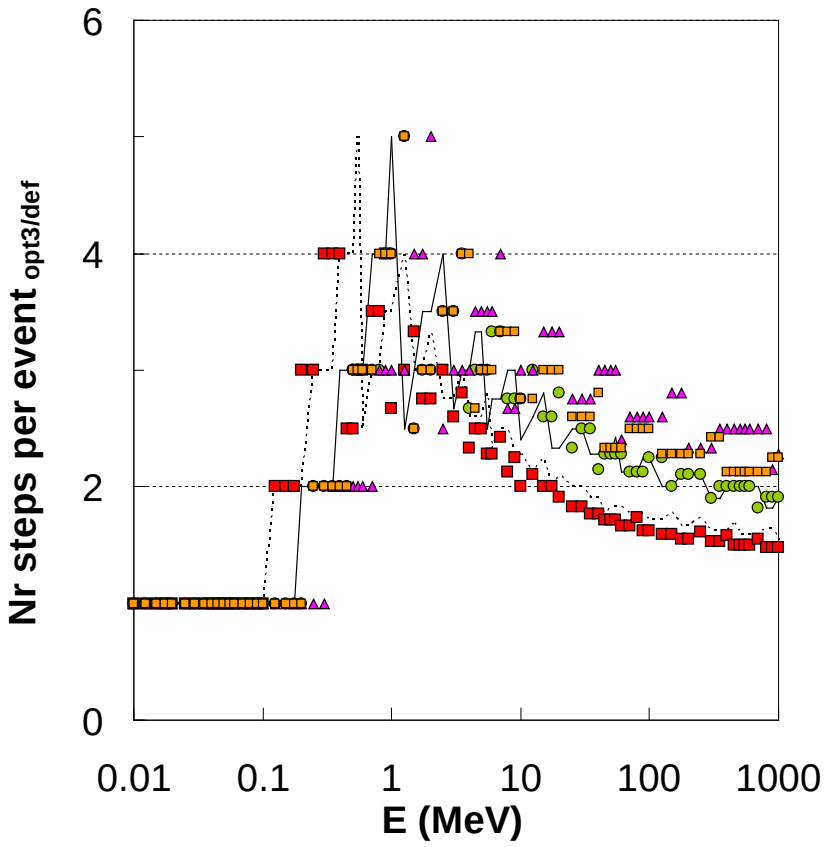




Number of electron steps/event (2)

- In C and Al: 1 step/event below 0.2 MeV in standard default; step ratio std opt3/def ~ 1.5-2 at E>10 MeV
- In Cu, Sn, W and Pb: 1 step/event below ~1 MeV in standard default; step ratio std opt3/def ~ 2-3 at E>10 MeV





PSTAR and ASTAR uncertainties

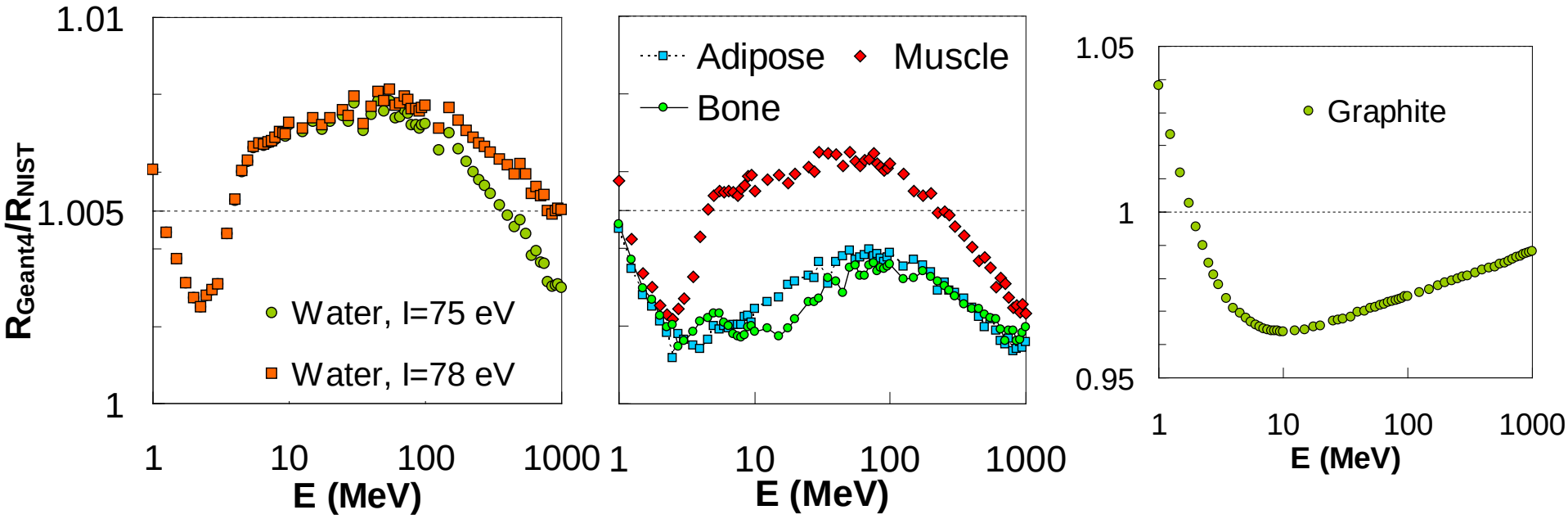
From http://physics.nist.gov/PhysRefData/Star/Text/method.html:

”In ICRU [Report 49] the uncertainties of the collision stopping powers in the high-energy region are stated to be 1 % to 2 % for elements, and 1 % to 4 % for compounds. The uncertainties are more difficult to estimate in the low-energy region. In ICRU (1993) they are estimated to be 2 % to 5 % at 1000 keV, 5 % to 10 % at 100 keV, 10 % to 15 % at 10 keV, and at least 20 % to 30 % at 1 keV. ”

We restricted our simulations to a minimum energy of 1 MeV.
This corresponds roughly to a minimum range of ~10 microns
for protons and of ~1 micron for alphas in the considered absorbers.

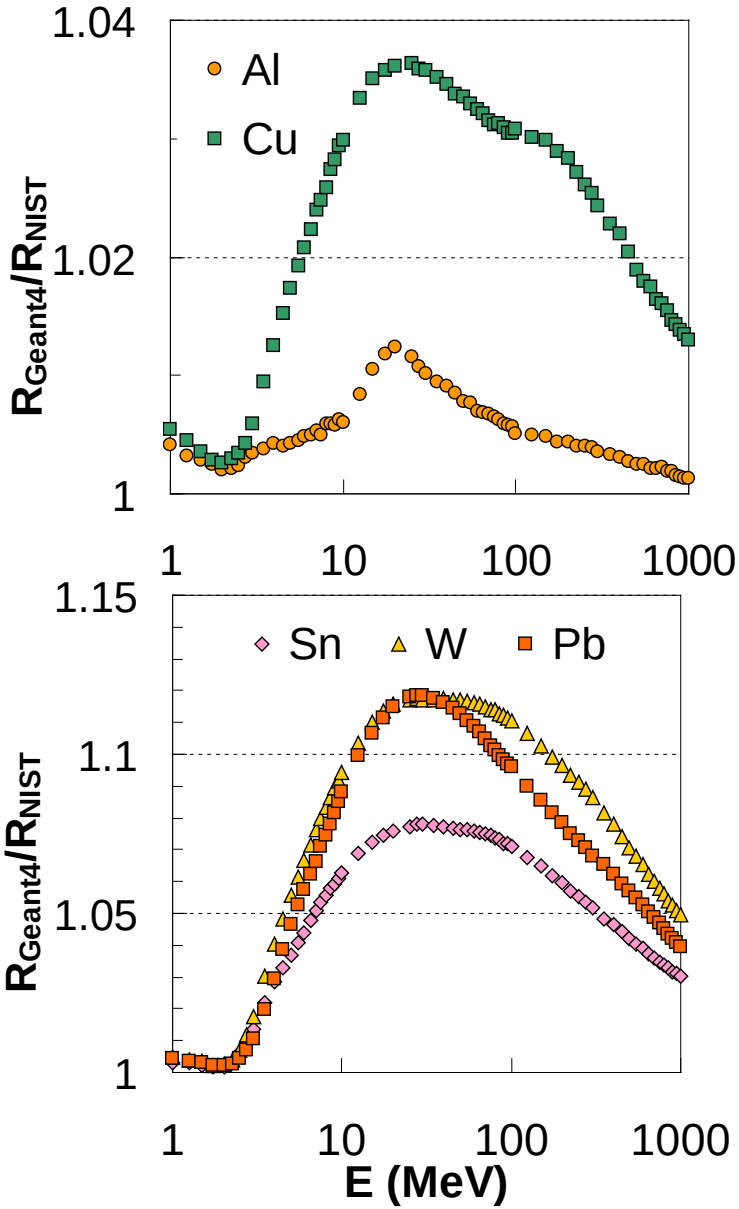
Protons in light absorbers

- Excellent agreement between Standard default and NIST for water, adipose, muscle and bone (1%)
- G4 deviates ±5% from NIST for graphite (NIST uncertainty ~2%)
- The effect of the ionisation potential in water is very small (~0.2%)



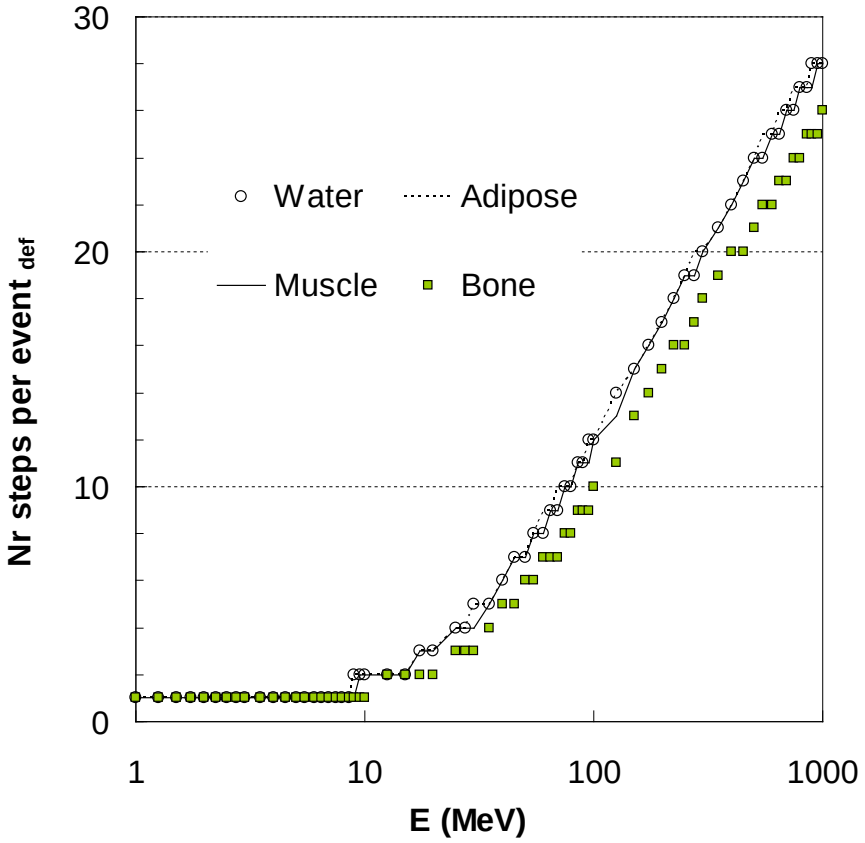
Protons in Cu, Al, Sn, W, Pb (std def)

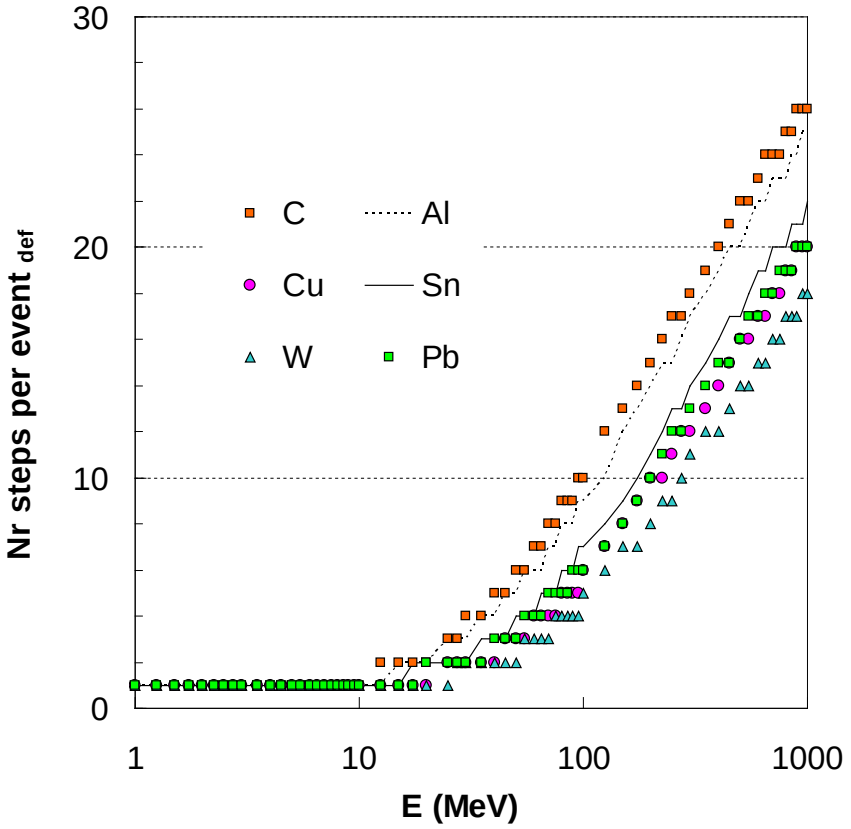
- G4/NIST is within NIST uncertainties (2%) only for Al
- Discrepancies between G4 and NIST are seen mainly in the energy interval 10-100 MeV
- Maximal deviations from NIST:
  - Al: 1.2%
  - Cu: 3.5%
  - Sn: 8%
  - W, Pb: 12%



Number of proton steps/event

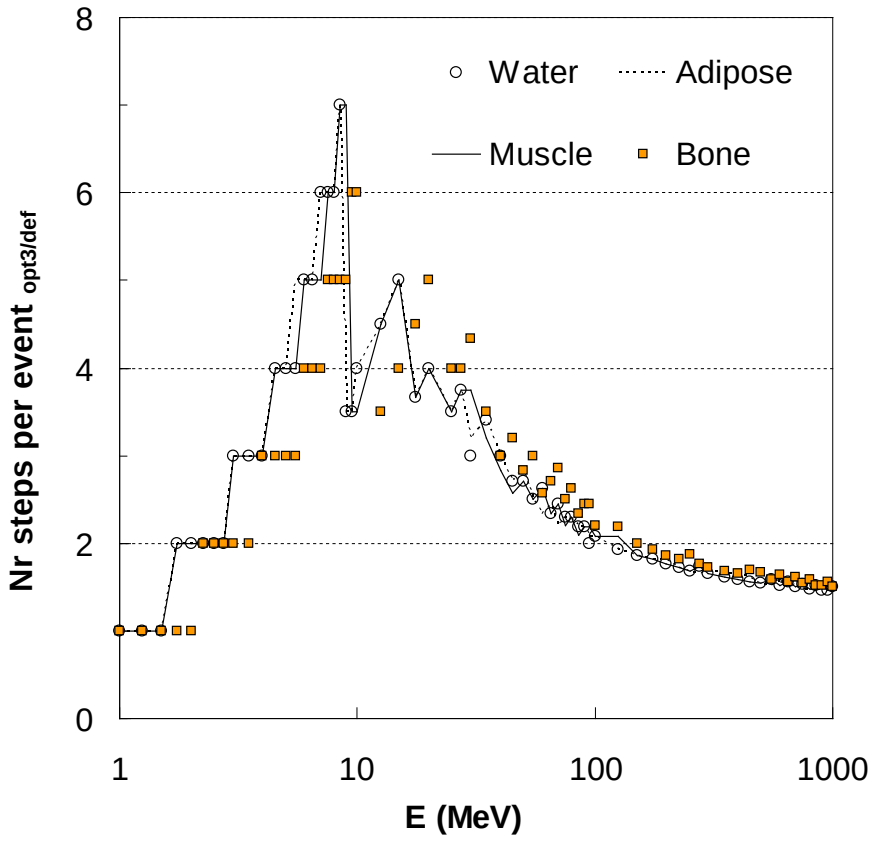
- only 1 step/event below ~10 MeV for all absorbers
- The number of steps/event in the region 10-100 MeV is less than 10

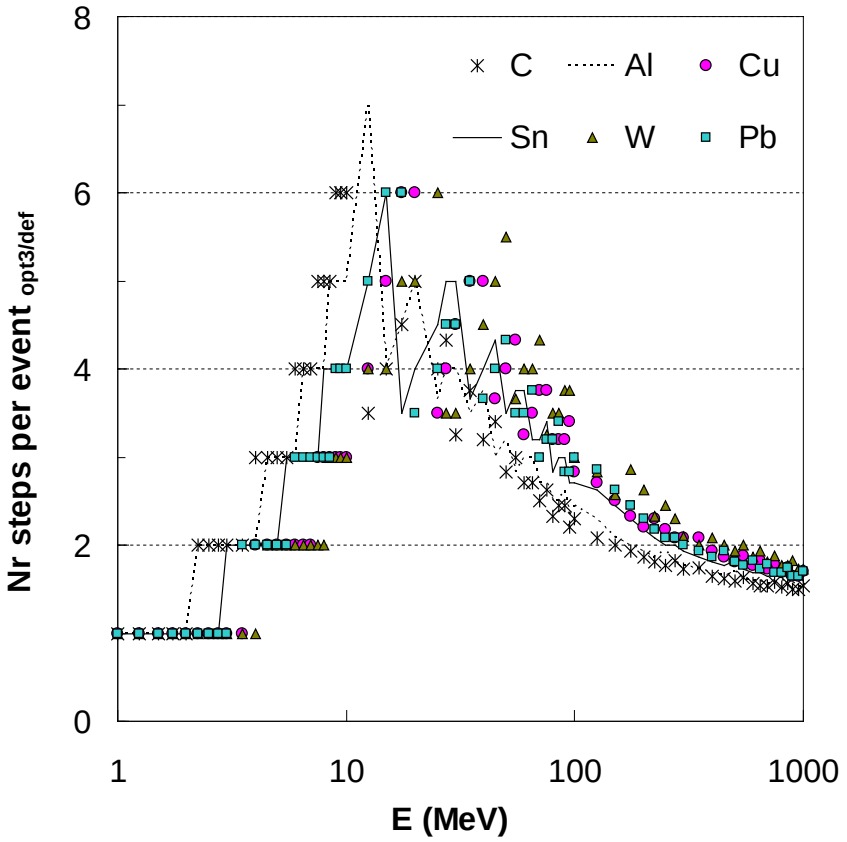




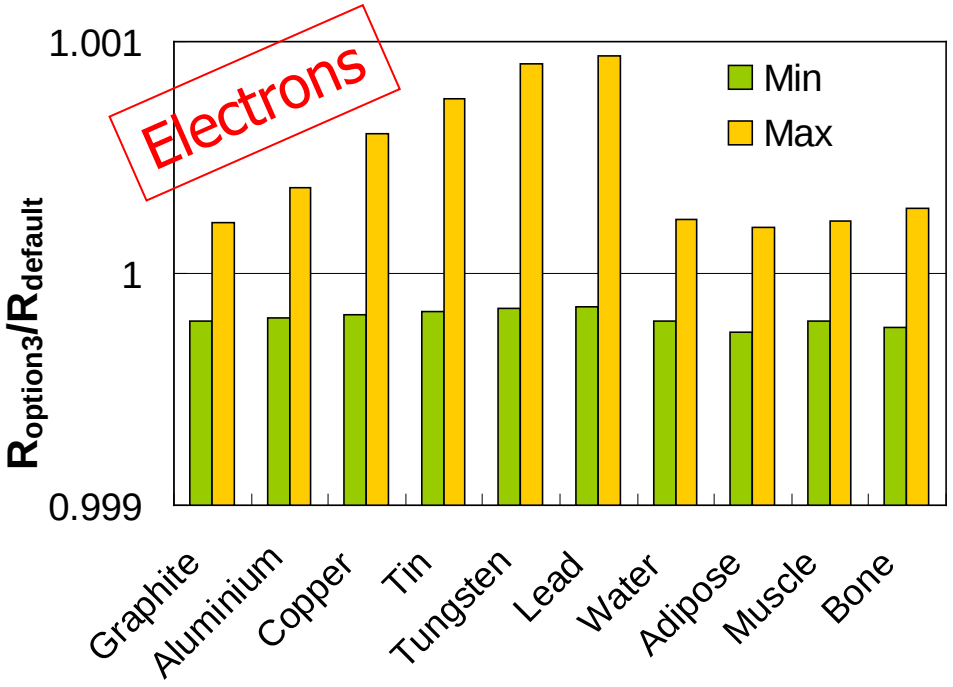
Number of proton steps/event: opt3/def

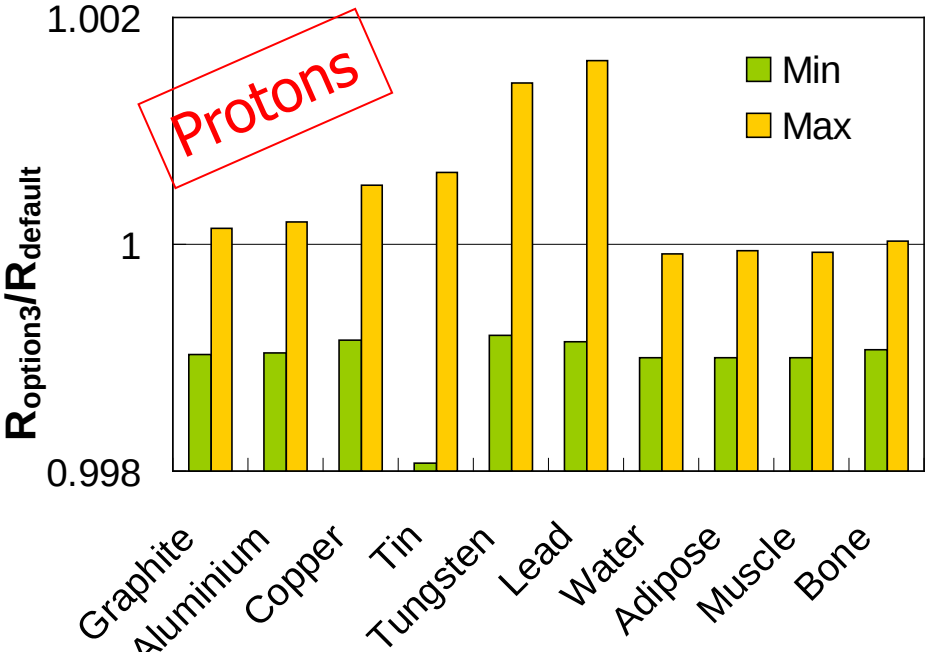
- In the region 10-100 MeV, the number of steps/event increases by a factor 2-7 between default and opt3
- At energies above 100 MeV, opt3 has about 1.5x (light absorbers) and 2x (heavier absorbers) more steps than default





Electron and proton range: Standard default vs Standard option3



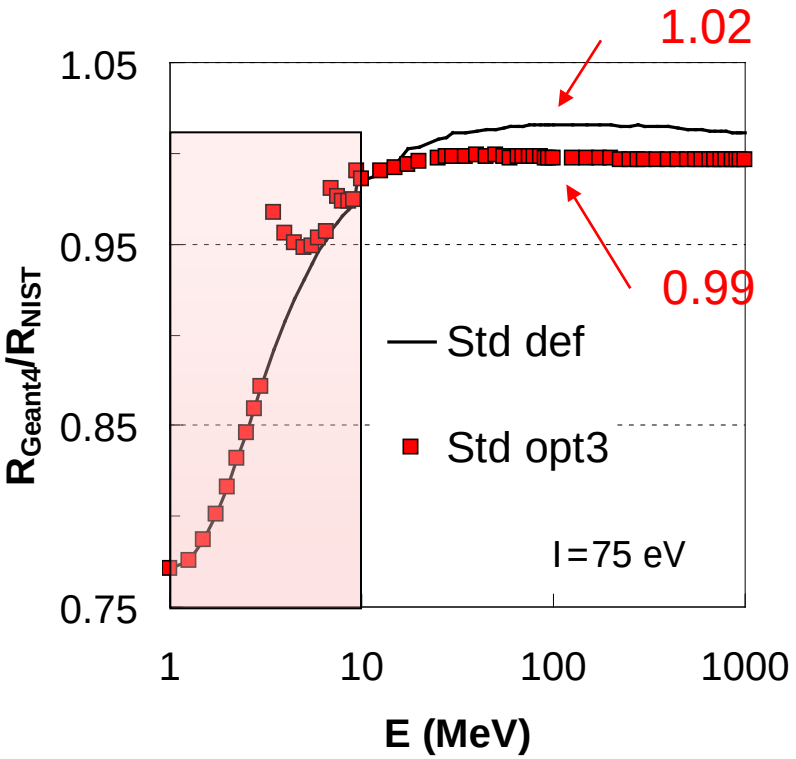


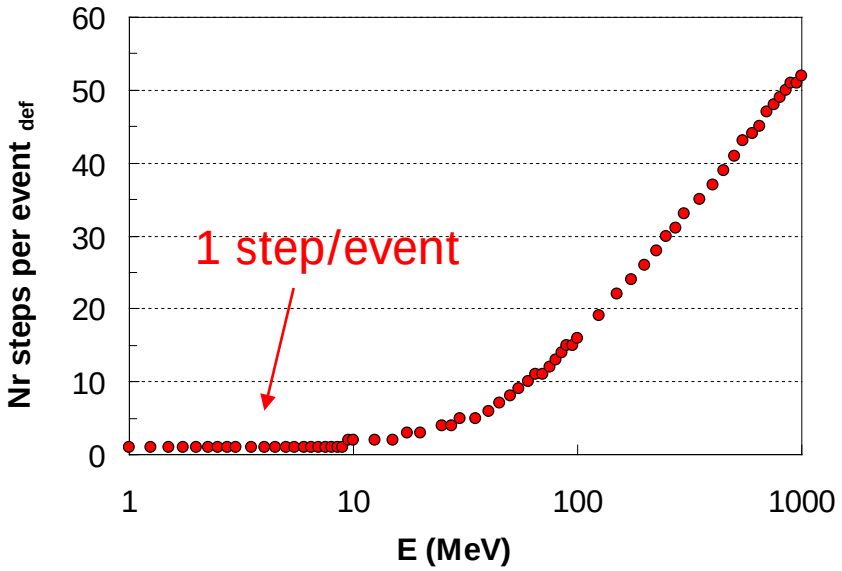
The two options of the Standard physics list calculate the same CSDA ranges within 0.1% for electrons and 0.2% for protons in spite of the differences in number of steps/event

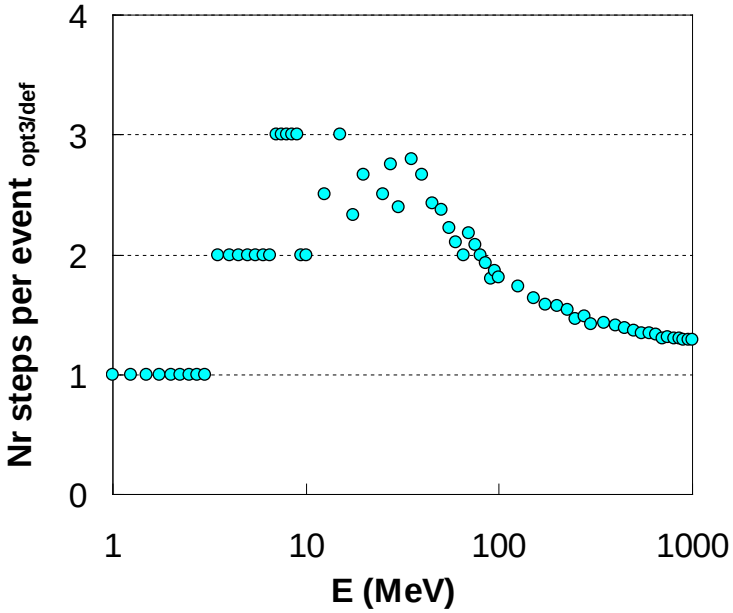
Alphas in water

The number of steps/event matters for alphas!

At E<10 MeV, both default and opt3 have a small number of steps/event → large differences between G4 and NIST

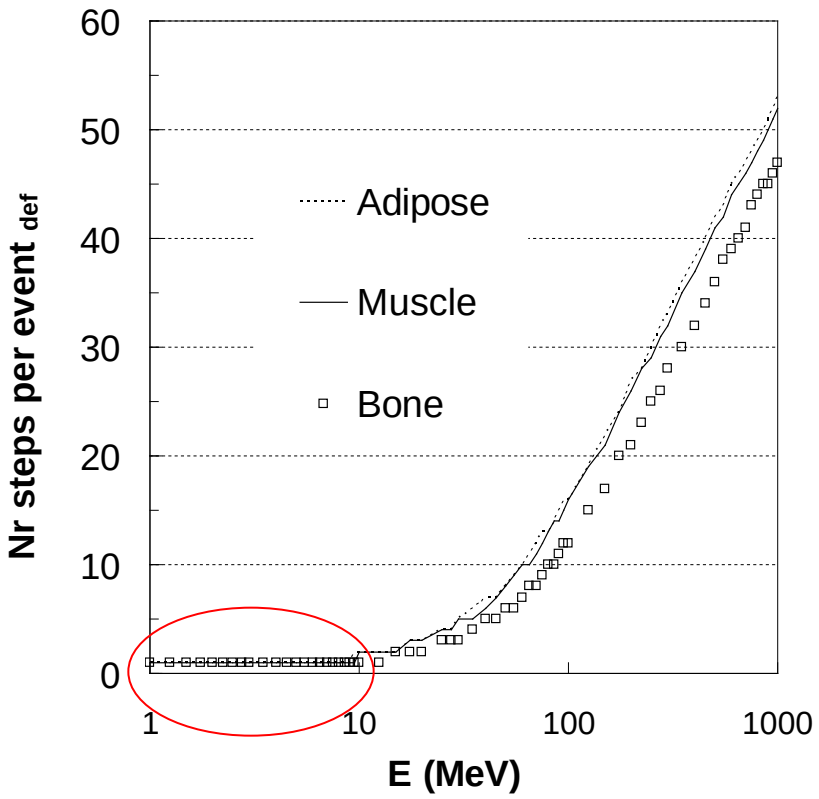


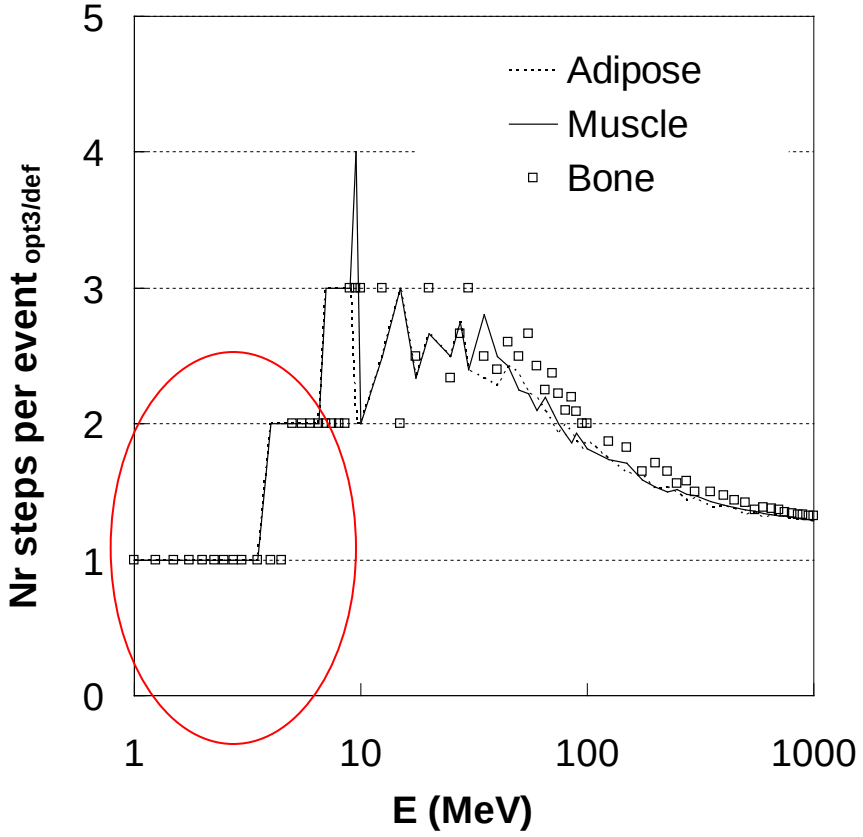




Number of alpha steps/event (1)

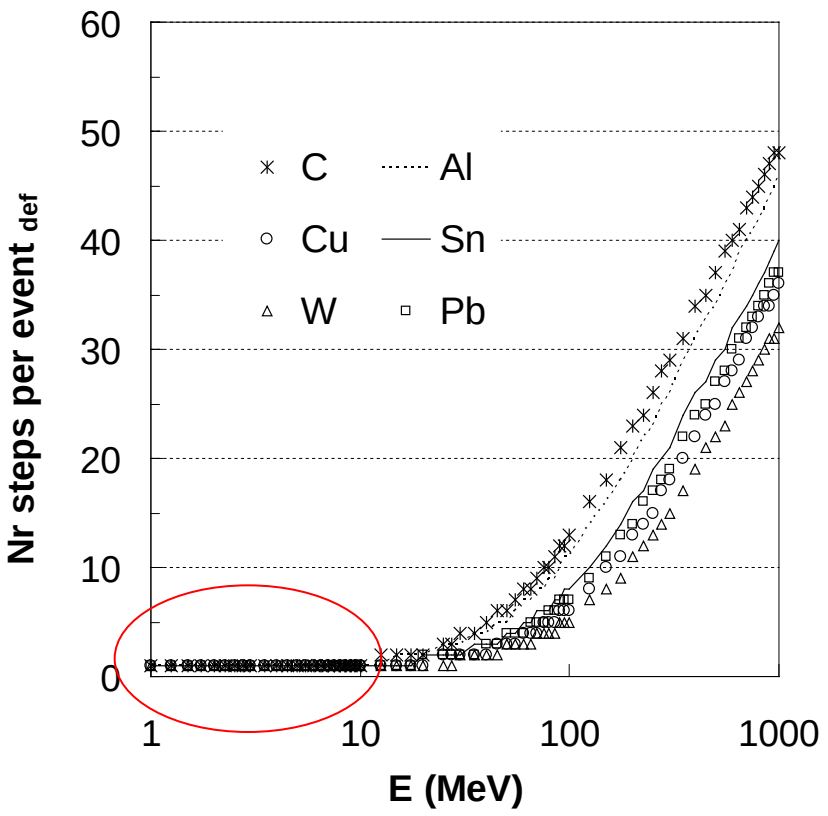
Adipose, muscle and bone have about the same #steps/event as water...

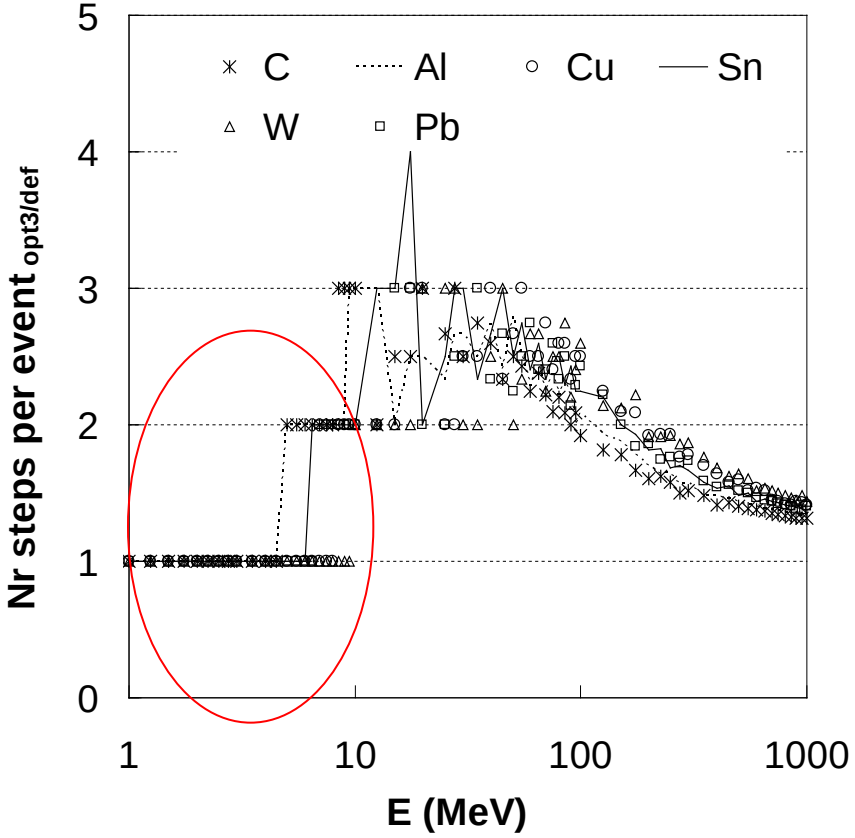


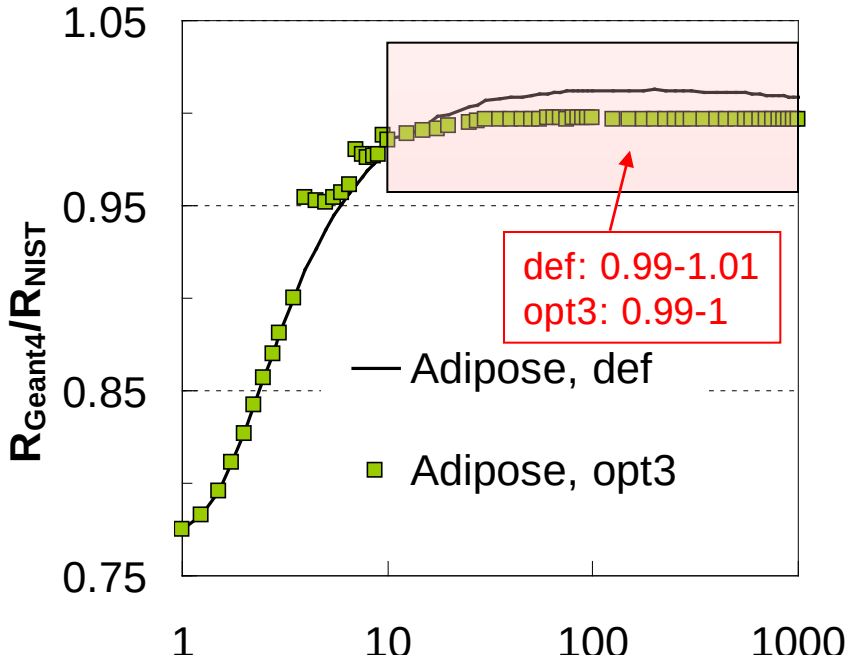


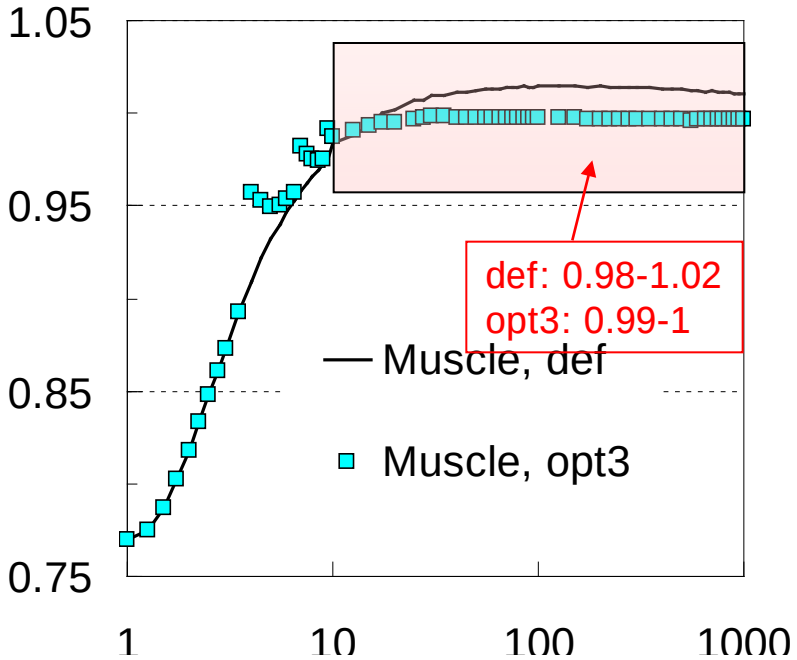
Number of alpha steps/event (2)

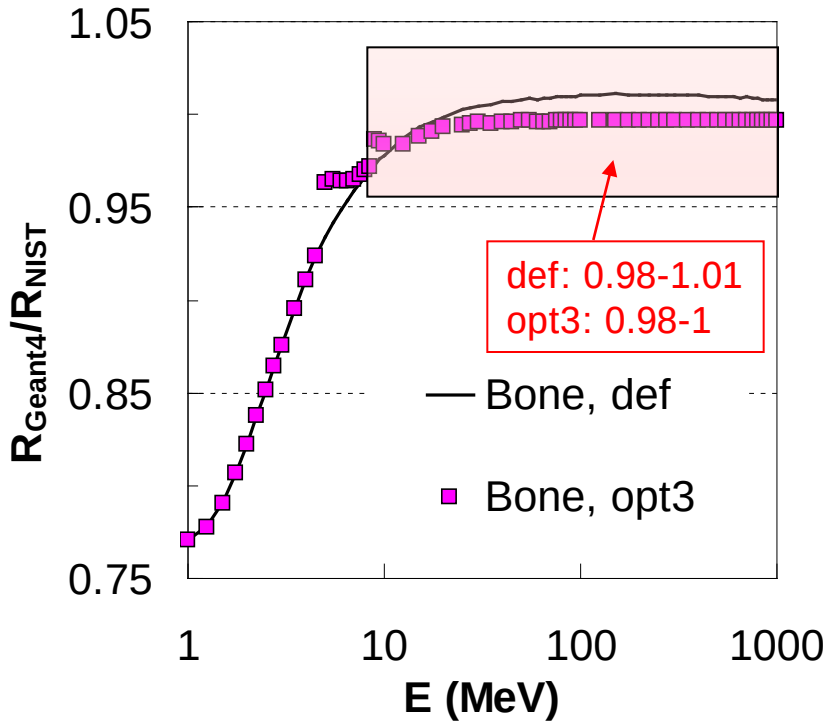
...and so do the heavier absorbers for energies below 10 MeV...

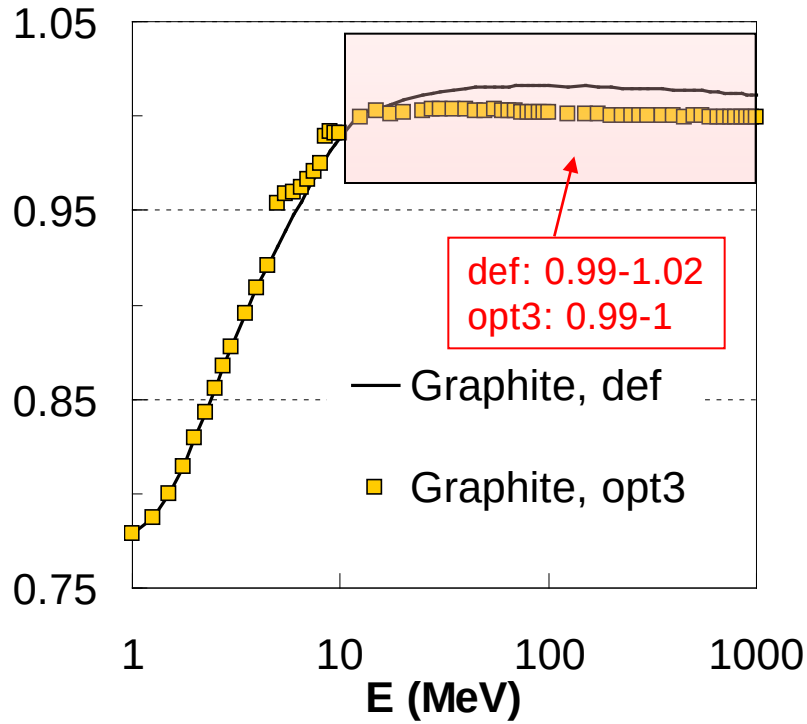


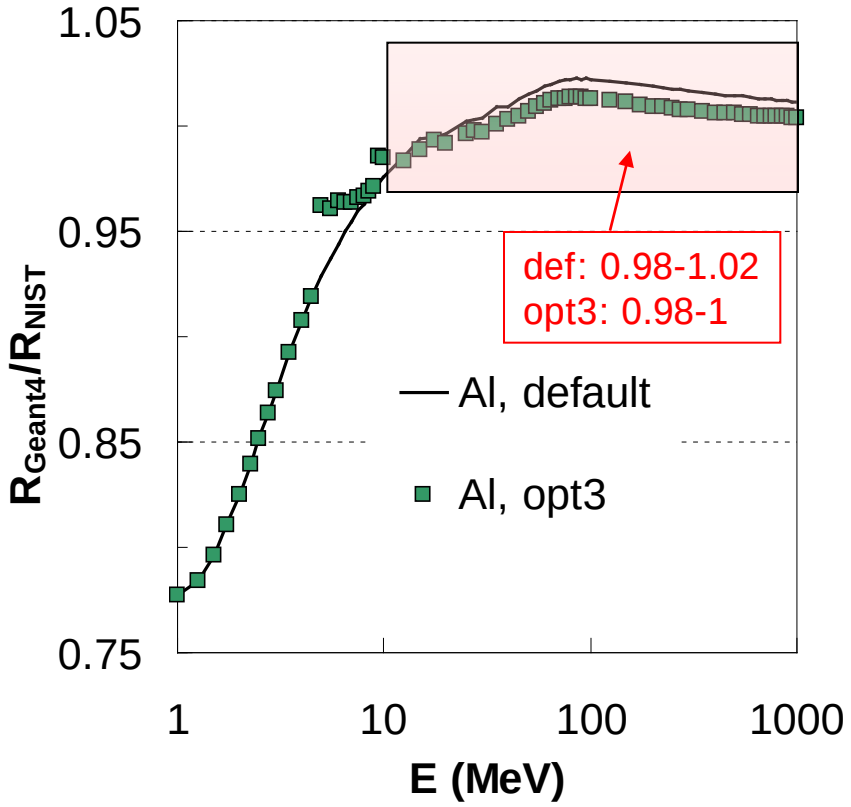


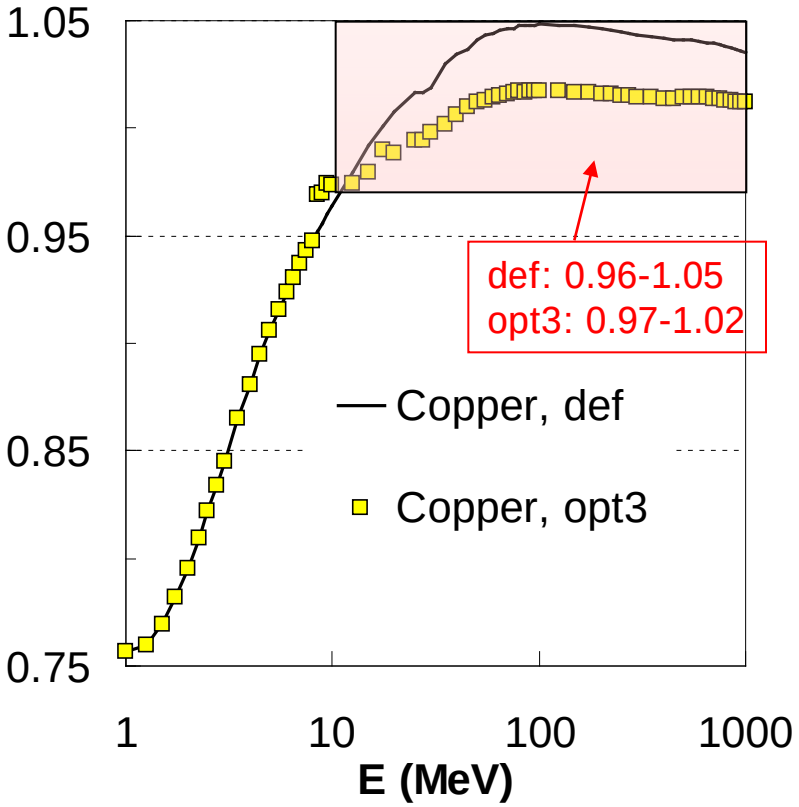

1.05
0.95
0.85
0.75
R_{Geant4}/R_{NIST}
def: 0.99-1.01
opt3: 0.99-1
Adipose, def
Adipose, opt3
1
10
100
1000


1.05
0.95
0.85
0.75
def: 0.98-1.02
opt3: 0.99-1
Muscle, def
Muscle, opt3
1
10
100
1000


1.05
0.95
0.85
0.75
R_{Geant4}/R_{NIST}
def: 0.98-1.01
opt3: 0.98-1
Bone, def
Bone, opt3
1
10
100
1000
E (MeV)

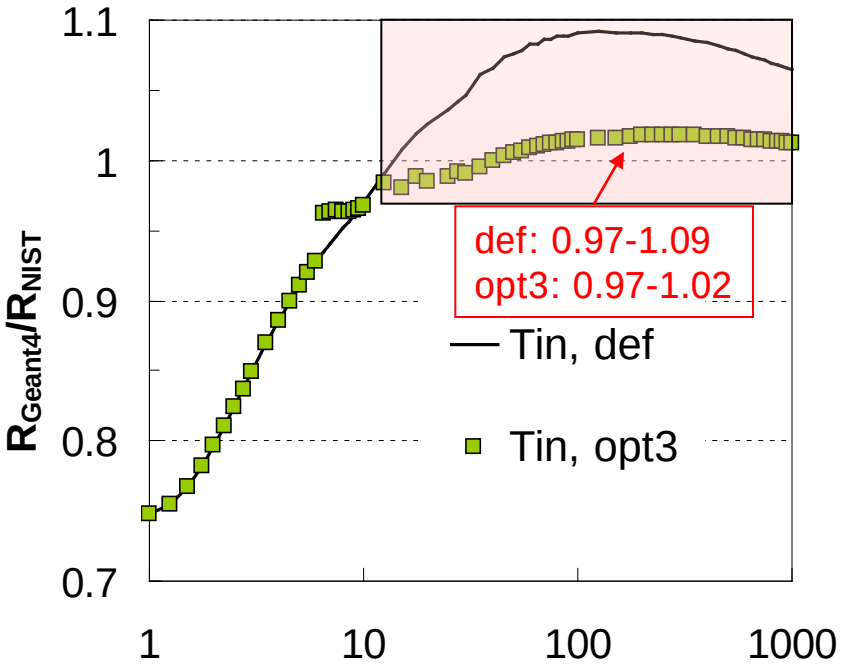

1.05
0.95
0.85
0.75
def: 0.99-1.02
opt3: 0.99-1
Graphite, def
Graphite, opt3
1
10
100
1000
E (MeV)

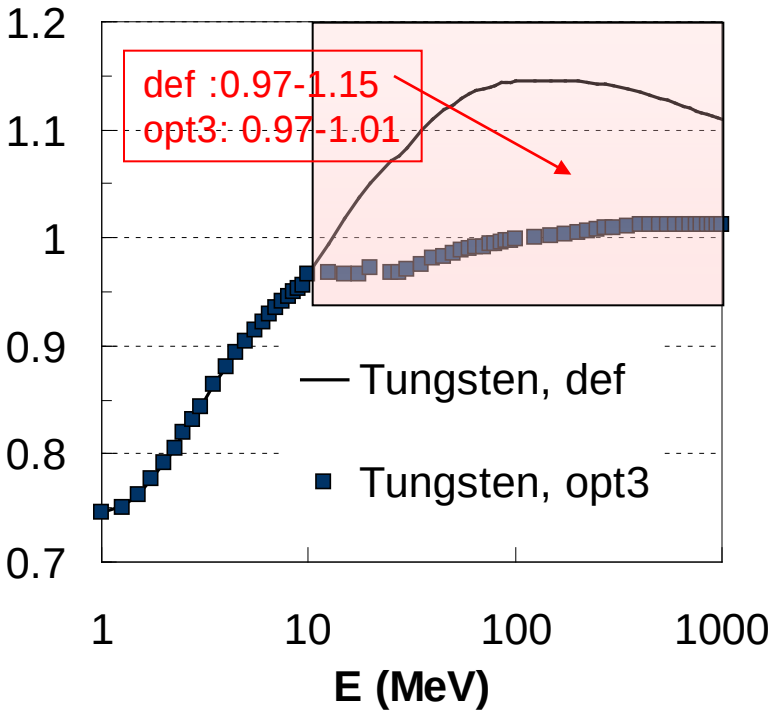


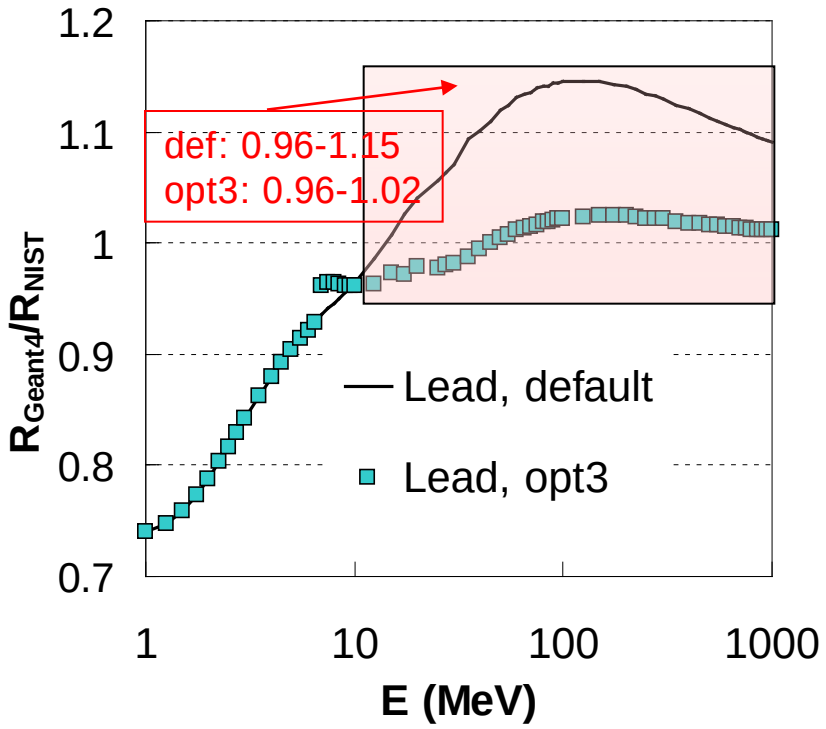


Above 10 MeV:

- water, adipose, muscle, bone, graphite and aluminium are within NIST uncertainties (2%) for def and opt3
- copper G4/NIST ranges are between -4% and +5% for def and between -3% and 2% for opt3







Above 10 MeV and for opt3:

- Sn and W are within 3% from NIST
- Pb is within 4% from NIST

Max deviations for default:
9% for Sn, 15% for W and Pb

Summary (1)

Electrons:

- Penelope gives the best agreement with NIST for light absorbers (water, adipose, muscle, bone, graphite, aluminium), with G4 ranges varying by 0.98-1.01 from NIST
- Standard gives the best agreement with NIST for heavier absorbers (copper, tin, tungsten, lead), with G4 ranges varying by 0.96-1.07 from NIST

Protons:

- Excellent agreement G4/NIST (1%) for water, adipose, bone, muscle
- Larger deviations for graphite (5%) and heavier elements (max deviation for W and Pb: 12%)

Summary (2)

Alphas:

- The number of steps/event has a significant effect on range calculation
- Below 10 MeV, the simulation makes 1 step (def) or 2-3 steps (opt3) – this results in large deviations from NIST (25%)
- Above 10 MeV, def and opt3 ranges are in good agreement with NIST for light absorbers (within 5%)
- Above 10 MeV, tin, tungsten and lead differ by 10-15% from NIST for default, but the differences are smaller for opt3 (3-4%)
- Fine-tuning of alpha ranges for low energy application require using additional step limitation