Comparison of Geant4 Results to EGSnrc and Measured Data in Large Field Electron Dose Distributions

Central axis depth dose curves and dose profiles of 6-21 MeV Primus electron beams were measured for a 40x40 cm field and simulated in EGS4 in work presented at the First McGill International Workshop in 2004. Those Monte Carlo treatment head and water phantom simulations have now been replicated with EGSnrc and the Geant4 Simulation Toolkit (version 8.2.p01). In each case, as with the original EGS4 simulation, source and geometry have been adjusted to best match simulation results to measurement. Geant4 simulations were also shown for case of using the exact same source and geometry parameters used in the EGSnrc simulations.

Work supported in part by the U.S. Department of Energy under contract number DE-AC02-76SF00515 and NIH R01 CA104777-01A2.
The results presented here today are more preliminary than we had hoped, due to an unintended additional experiment that occurred in the middle of our work. So let me briefly describe that experiment first.

A resulting inelastic collision resulted in motion both up and to the right of $bf$.

Moving from left to right in our current frame of reference, we had the combination of two objects: Physicist and Cat.

Moving from the in plane to out of plane axis, we had a smaller object, Cat.

We were unable to precisely measure either the mass energy of Physicist or the kinetic energy of Cat, but the following basic observations were made:

- Cat was able to move away from the Physicist.
- Physicist was carried away.
- Monte Carlo Time of Physicist was substantially reduced.
Previous Related Publication

- Described experiment and simulation using EGS4.
- Showed that source and geometry parameters can be chosen so that EGS4 results match dose distributions nicely, except in bremsstrahlung tail, where dose underestimated.
- Preliminary results demonstrated that the (at that time) recent code, EGSnrc, provided a better match to measurement (electron transport included more accurate multiple scattering).
- We will show final version of those EGSnrc results.
- Helpful to use more than one Monte Carlo code to validate process of using MC simulation along with source and geometry adjustment to determine fluence and to help assess accuracy of calculated fluence.
Objective: Use large-field measurements to validate and compare Monte Carlo codes for treatment head simulation - EGSnrc and Geant4.8

- Source and geometry not known well enough for benchmark
- Accuracy about 2%/2mm

No Applicator!!

40x40 jaws!!

Geometry measurements
Experimental Measurements

• See the paper for full details on the experimental setup.

• Siemens Primus using all energies: 6, 9, 12, 15, 18, 21 MeV
  – Output (dose per monitor unit) measurements done according to AAPM TG-51
  – Diode and Roos for PDD
  – Diode for $d_{\text{max}}$ profiles
  – Thimble ion chamber for $R_{p+}$ profiles
  – Roos vs dose to air for MCRTP, dose to water (TG-21 stopping power ratios) for DOSXYZnrc
  – Roos slow scan, after water waves die down
  – Background defined on CU500E electrometer
  – Foil and chamber position from digital pictures

No Applicator!!
40x40 jaws!!
Measurements and Tweaking

• Starting point of simulation geometry used manufacturer's specs or actual measurements.

• Foil thicknesses come from manufacturer with some tolerance which we don't know.

• Then adjusted various parameters, based on knowledge of what parts can move relative to what.
  – Did not exceed sense of what could reasonably be the actual positions.

• Matching measurement for all beam energies restricted the range of geometry parameters.
  – The beams shared the same exit window, secondary scattering foil, monitor chamber and secondary collimators, so the geometry and position of these components had to be the same in all cases.
  – The thickness of the primary scattering foil had to be the same for the 3 highest energies.

• EGSnrc work involved 30-50 iterations of adjusting geometry and source parameters.
  – Some adjustments could still be done, but remaining mismatches are at extreme edges of field so not of clinical importance.
EGS4 Results - 21 MeV

Dose at depth of maximum dose, dmax

Bremsstrahlung Dose x 10 (13 cm depth)

- Measured In-plane (black line)
- Measured Cross-plane (red line)
- MC In-plane (black histogram)
- MC Cross-plane (red histogram)
EGS4 Results (shown in 2004)
Results: EGSnrc vs Measurement

- EGSnrc gets to 2%/2mm agreement with measurement inside useful field
- 5%/5mm in penumbra and beyond
- bremsstrahlung ($D_e/D_x$) matched to better than 5%
- Better match to diode than parallel plate in build-up region.
- Diode overresponds in the brems region
EGSnrc Results (most recent)

- 6 MeV
  - 1.3 cm depth, dose@5 cm x 100
  - 2.7 cm depth, dose@8 cm x 25

- 9 MeV
  - 2 cm depth, dose@7 cm x 50
  - 3 cm depth, dose@10 cm x 10

- 12 MeV
  - 2.1 cm depth, dose@12 cm x 10

- 15 MeV
  - 1.9 cm depth, dose@13 cm x 10

- 18 MeV

Distance off axis (cm)
Results: Geant4 vs Measurement

- Geant4 gets to 3%/2mm agreement with measurement inside useful field
- 6%/6mm in penumbra and beyond
- bremsstrahlung ($D_e/D_x$) high by about 6%, but we are not finished tweaking
- Better match to parallel plate than diode in build-up region.
Results: Geant4 vs Measurement

[Graph showing dose distributions for different depths and energies, with annotations for dose values and energy levels.]
Geant4 Version: 8.2.p01

- No modifications were made to the Geant4 source.
- Materials were taken from NIST definitions built into Geant4.
  - This feature added in Geant4.7.1 helps assure that accepted standard NIST definitions are used for materials.
  - The only non-NIST materials were the Stainless Steel and the beam vacuum.
- Scored on a 60cm x 60cm x 15cm water target treated as 200 x 200 x 75 voxels each of size 3x3x2 mm.
  - Made use of the new nested parameterization feature added in Geant4.8.0 and discussed in Makoto Asai’s talk yesterday.
  - The earlier, 3D parameterization technique in Geant4 causes this example to require over 1GB of memory due to the large number of voxels in the target (3 million).
  - The new Nested Parameterization gets this down to about a 25M executable.
  - Geant4 Scoring was simplified by using the new Geant4 MultiFunctionalDetector and PrimitiveScorers.
  - This new feature added in Geant4.8.0 eliminates the need for the user to define their own detector sensitivity classes for standard scoring application such as are most common in medical physics.
  - See Geant4 example RE02.
Geant4 Geometry

- Initially set up according to same schematic as EGSnrc.

<table>
<thead>
<tr>
<th>Energy</th>
<th>6</th>
<th>9</th>
<th>12</th>
<th>15</th>
<th>18</th>
<th>21</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean energy</td>
<td>6.77</td>
<td>9.86</td>
<td>12.52</td>
<td>16.11</td>
<td>18.83</td>
<td>21.79</td>
</tr>
<tr>
<td>IP direction cosine</td>
<td>0.003</td>
<td>0.002</td>
<td>0.000</td>
<td>0.007</td>
<td>0.002</td>
<td>-0.001</td>
</tr>
<tr>
<td>CP direction cosine</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>Foil thickness change</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
<td>0%</td>
<td>5%</td>
<td>5%</td>
</tr>
</tbody>
</table>

- Energy spectra from Parmella, shifted to mean energy
- Spot shape Gaussian: FWHM of 0.2 cm, or sigma of 0.085 cm.
- Foil shift (IP,CP): (0.02 cm, -0.006 cm)
- Monitor chamber shift (IP,CP): (0.22 cm, -0.016 cm)
- Patient coordinates (PC) and beam coordinates (BC)...
- BEAM (BC), and MCRTP (PC) coordinates: (IP,CP)=(xBC,yBC)=(xPC,yPC)
- Geant4 coordinates: (IP,CP)=(xBC,yBC)=(xPC,yPC)

Secondary collimators (Y-Jaw and X-MLC) are composed of tungsten. Lateral transport limited to 16 cm width square from downstream surface of ion chamber to downstream surface of X-MLC (35.36 cm). Lateral transport limited to 20 cm width square from downstream of X-MLC (35.36 cm) to 40 cm, 30 cm width square to isocenter at 99.54 cm from source, i.e, at water surface.

<table>
<thead>
<tr>
<th>Collimator</th>
<th>Coordinate in direction of motion</th>
<th>Z of upstream surface</th>
<th>Range of open region</th>
<th>Z of downstream surface</th>
<th>Range of open region</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jaw</td>
<td>IP</td>
<td>19.27</td>
<td>-3.996</td>
<td>3.846</td>
<td>27.07</td>
</tr>
<tr>
<td>MLC</td>
<td>CP</td>
<td>27.80</td>
<td>-5.652</td>
<td>5.652</td>
<td>35.36</td>
</tr>
</tbody>
</table>

Materials:
- Al, pure aluminum, density 2.699 g/cm³
- H₂O, density 1.000 g/cm³, H and O in 2:1 ratio by number
- Air, density 1.205e-03 g/cm³, C, N, O, O₂ in proportion of 0.000124, 0.756, 0.232, 0.0128 by weight
- W, pure tungsten, density 19.3 g/cm³
- Au, pure gold, density 19.32 g/cm³
- Ti, pure titanium, density 4.54 g/cm³
- Kapton, density 1.42 g/cm³, H, C, N, O in 10:22:2:5 ratio by number
- Stainless steel, density 8.06 g/cm³, C, Si, Cr, Mn, Fe, Ni, in proportion of 0.001, 0.007, 0.18, 0.01, 0.712, 0.09 by weight
Geant4 Geometry

- Checked using Geant4 visualization output through HepRAp graphical browser.
Geant4 Geometry - Close Up

- HepRApp's measuring tool is helpful for checking that placements are as
Geant4 Geometry

- 100 Histories - Red e+, Blue e-, Green Gamma
Geant4 Geometry

- 100 Histories - Red e+, Blue e-, Green Gamma
Geant4 Physics Lists

• Because Geant4 is a general purpose tool designed to simulate almost any physics, the user must specify a specific list of what physics processes are to be simulated for what particle types for their specific application. This is done by constructing a Geant4 class called a physics list.

• For our application, we took the lists from one of the standard Geant4 electromagnetic examples, TestEM7.

• For most of our work, we used the list that TestEM7 calls PhysListEmStandard. It included the following physics:

  • Gamma:
    – PhotoElectricEffect
    – ComptonScattering
    – GammaConversion

  • Electron
    – MultipleScattering
    – eIonisation
    – eBremsstrahlung

  • Positron
    – MultipleScattering
    – eIonisation
    – eBremsstrahlung
    – eplusAnnihilation

  • Muon
    – hMultipleScattering
    – MuIonisation
    – MuBremsstrahlung
    – MuPairProduction

  • Alpha or Ion
    – hMultipleScattering
    – ionIonisation

  • All others charged particles except geantino
    – hMultipleScattering
    – hIonisation
Geant4 Range Cuts

• Geant4 has the user specify a "range cut" rather than a production threshold.
  – Threshold for secondary production.

• This is a balancing act:
  – need to go low enough to get the physics you're interested in
  – can't go too low because some processes have infrared divergence causing CPU time to skyrocket

• The traditional Monte Carlo solution is to impose an absolute cutoff in energy
  – particles are stopped when this energy is reached
  – remaining energy is dumped at that point

• In Geant4, this threshold is a distance, not an energy
  – the primary particle loses energy by producing secondary electrons or gammas
  – if primary no longer has enough energy to produce secondaries which travel at least the specified (range cut) distance, two things happen:
    • discrete energy loss ceases (no more secondaries produced)
    • the primary is tracked down to zero energy using continuous energy loss

• Applies only to particles that have infrared divergence.
Effect of Range Cuts

- We used both "default" range cut, 1mm, and some tighter range cuts.
- We set same range cut for e+, e- and gamma, though Geant4 allows one to set different cuts for different particles.

Effect of Physics List choice and Range Cut choice on processing time:
- Normalizing to speed for EM Standard with 1.0 mm range cut (at 12 MeV),
  - EM Standard Range Cut 1.0 mm: 1.0
  - EM Standard Range Cut 0.1 mm: 1.05 x
  - EM Standard Range Cut 0.01 mm: 1.4 x
  - EM Standard Range Cut 1 micron: 3.6 x
  - EM Low Energy Range Cut 1.0 mm: 1.7 x
  - EM Low Energy Range Cut 1 micron: 19. x

Effect of physics list choice and range cut choice on match to experiment:
- Bruce - may have better comparison data by Tuesday
  - Standard physics with range cut 1mm:
    - electron scatter is fine
    - but minor problem in Brems.
  - Can fix this by going to either:
    - standard physics list with 1micron range cut (maybe just need in primary foil)
    - or low energy physics and keep 1mm range cut
Geant4 Processing

• Processing was done on a cluster of 64-bit AMD Opteron processors running Linux Redhat 4.

• We ran 50M histories for each of six energies for a total of 300M histories.
  – Same number of histories that was used for the comparable EGS4 and EGSnrc studies.

• For each energy, the work was split into 10, 20 or 30 separate jobs so that each job would run in about one day.

• The same binary was used for all jobs. Difference was only that each job ran with a different Geant4 macro specifying:
  – beam spectrum (different for each of six Primus setups of MeV 6, 9, 12, 15, 18 and 21)
  – beam direction (different for each of six Primus setups)
  – primary foil material
  – primary foil thickness
  – starting random number seed (MTwist engine)
  – range cut (either 1 mm or 1 micron)
  – number of histories
Parallelization

- We were fortunate to have access to a 120 processor cluster such that we could run all of the jobs in parallel, enabling one day turnaround for the entire set of jobs (for a given choice of physics list and range cut except for the most time-consuming combination of Low Energy physics list with 1 micron range cut).
- Given the availability of this resource, we ran with no variance reduction techniques.
  - (This will be a useful baseline for future validations of such techniques).
- Geant4.8.2.p01 was run exactly as it comes from Geant4 - no modifications.
- Parallelization was straightforward.
- Only caveat is to make sure not to enable Geant4's feature that writes the current random number out at each event. Doing so with 120 processors causes a bottleneck as each processor tries to write to the same disk at a rate of 100 events per second for a total of 12K writes per second.
- If you need to save the ending random number seed, do so only at end of run (do the main run, then issue commands to turn on random seed saving, then run a single additional history).
CPU Time

- Jobs were compiled in 32 bit mode.
  - Later tests showed a 13 % speedup if jobs were compiled in 64 bit mode, but as some jobs had already been begun it was decided to continue all work in 32 bit to avoid an extra variable in this study.
  - Additional speedups may also have been possible had we used special compiler flags for the AMD Opteron, but none of these were used for the present study.

- CPU time to produce 50M history data sets were as follows
  - AMD Opteron, 1.8MHz, Redhat 4, compiled in 32-bit mode, no special compiler flag:

<table>
<thead>
<tr>
<th>Standard EM, range cut 1.0 mm:</th>
<th>Standard EM, range cut 0.01 mm:</th>
<th>LowEnergy EM, range cut 1.0 mm:</th>
</tr>
</thead>
<tbody>
<tr>
<td>MeV06</td>
<td>150 Ksec</td>
<td>MeV06</td>
</tr>
<tr>
<td>MeV09</td>
<td>180 Ksec</td>
<td>MeV09</td>
</tr>
<tr>
<td>MeV12,</td>
<td>210 Ksec</td>
<td>MeV12,</td>
</tr>
<tr>
<td>MeV15</td>
<td>180 Ksec</td>
<td>MeV15</td>
</tr>
<tr>
<td>MeV18</td>
<td>230 Ksec</td>
<td>MeV18</td>
</tr>
<tr>
<td>MeV21</td>
<td>290 Ksec</td>
<td>MeV21</td>
</tr>
</tbody>
</table>

- Standard EM, range cut 0.1 mm:

<table>
<thead>
<tr>
<th>Standard EM, range cut 1 micron:</th>
<th>LowEnergy EM, range cut 1 micron:</th>
</tr>
</thead>
<tbody>
<tr>
<td>MeV06</td>
<td>160 Ksec</td>
</tr>
<tr>
<td>MeV09</td>
<td>190 Ksec</td>
</tr>
<tr>
<td>MeV12</td>
<td>220 Ksec</td>
</tr>
<tr>
<td>MeV15</td>
<td>190 Ksec</td>
</tr>
<tr>
<td>MeV18</td>
<td>250 Ksec</td>
</tr>
<tr>
<td>MeV21</td>
<td>310 Ksec</td>
</tr>
</tbody>
</table>

- Comparable EGSnrc jobs, ~12 hrs = 43 Ksec
  - So Geant4 here slower by factor of 4 for Standard 1.0mm, more for other physics lists or range cuts
  - Comparison very rough (not same machine, includes DOSExyz?), Geant4 tuning still very preliminary

- Not clear yet which range cut value really needed. Study still in progress.
  - Probably only need fine range cut in region of primary scattering foil.
Source and Geometry Tuning

- Geant4 jobs were initially run with exactly the same geometry as was used for the EGSnrc study.
- It should be noted the source and geometry had been specifically tuned to give best results in the EGSnrc study.
- Subsequent rounds of Geant4 jobs were done with source and geometry adjusted to give better results.
- Number of iterations for this tuning was somewhat limited due to constraints on physicist time (see slide 1 on bf-cat inelastic collision).
- Thus far, we have had considerably fewer iterations than had been done for the EGSnrc result shown here (but Geant4 tuning had benefit of being able to start from the EGSnrc values).
Tweaking Non-Energy-Dependent Params

**Used for EGSnrc Simulation**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian focal spot FWHM</td>
<td>0.2 cm</td>
</tr>
<tr>
<td>Primary foil and foil ring inplane lateral shift</td>
<td>0.02 cm</td>
</tr>
<tr>
<td>Primary foil and foil ring crossplane lateral shift</td>
<td>-0.006 cm</td>
</tr>
<tr>
<td>Monitor chamber inplane lateral shift</td>
<td>0.22 cm</td>
</tr>
<tr>
<td>Monitor chamber crossplane lateral shift</td>
<td>-0.016 cm</td>
</tr>
</tbody>
</table>

**Used for Geant4 Simulation**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gaussian focal spot FWHM</td>
<td>no change</td>
</tr>
<tr>
<td>Beam window thickness</td>
<td>3 % thicker</td>
</tr>
<tr>
<td>Foil and foil ring inplane lateral shift</td>
<td>no change</td>
</tr>
<tr>
<td>Foil and foil ring crossplane lateral shift</td>
<td>no change</td>
</tr>
<tr>
<td>Distance from primary foil to secondary foil</td>
<td>-0.1 cm</td>
</tr>
<tr>
<td>Monitor chamber inplane lateral shift</td>
<td>no change</td>
</tr>
<tr>
<td>Monitor chamber crossplane lateral shift</td>
<td>no change</td>
</tr>
</tbody>
</table>
Tweaking Energy-Dependent Params

- Used for EGSnrc Simulation
  - Energy spectra from Parmella, shifted to mean energy
  - 15 MeV, 18 Mev and 21 MeV used the same foil

<table>
<thead>
<tr>
<th>Nominal energy</th>
<th>6 MeV</th>
<th>9 MeV</th>
<th>12 MeV</th>
<th>15 MeV</th>
<th>18 MeV</th>
<th>21 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean energy (MeV)</td>
<td>6.77</td>
<td>9.86</td>
<td>12.52</td>
<td>16.11</td>
<td>18.83</td>
<td>21.79</td>
</tr>
<tr>
<td>Inplane direction cosine</td>
<td>0.005</td>
<td>0.003</td>
<td>0.001</td>
<td>0.008</td>
<td>0.003</td>
<td>0.000</td>
</tr>
<tr>
<td>Crossplane direction cosine</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
<td>0.003</td>
</tr>
<tr>
<td>Primary foil thickness change</td>
<td>0%</td>
<td>0%</td>
<td>-8%</td>
<td>-7%</td>
<td>-7%</td>
<td>-7%</td>
</tr>
</tbody>
</table>

- Used for Geant4 Simulation
  - blank means no change from above

<table>
<thead>
<tr>
<th>Nominal energy</th>
<th>6 MeV</th>
<th>9 MeV</th>
<th>12 MeV</th>
<th>15 MeV</th>
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<th>21 MeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean energy (MeV)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Inplane direction cosine</td>
<td>0.003</td>
<td>0.002</td>
<td>0.000</td>
<td>0.007</td>
<td>0.002</td>
<td>-0.001</td>
</tr>
<tr>
<td>Crossplane direction cosine</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Primary foil thickness change</td>
<td>0%</td>
<td>13%</td>
<td>2%</td>
<td>-1%</td>
<td>3%</td>
<td>3%</td>
</tr>
</tbody>
</table>
Results: Geant4 vs EGSnrc

- Monte Carlo simulation and measurement match to 2%/2mm
- Mismatch between parallel-plate and diode under investigation
- EGSnrc agrees best with diode
- Geant4 agrees best with parallel-plate
Comparison of $d_{\text{max}}$ Profiles

- Measurement: black lines
- EGSnrc matches measurement
- Geant4 differs from EGSnrc with same parameters by 4%/4mm
- Geant4 matches measurement after tweak
Comparison of $R_{p^+}$ Profiles

- Measurement: black lines
- EGSnrc matches bremsstrahlung dose
- Geant4 differs from EGSnrc with same parameters by 4%
- Geant4 with parameters adjusted overestimates x-ray dose by 5%
- Further adjustment may improve Geant4 result
Conclusions

- Established match to large-field measurements for 6-21 MeV electron beams with 2 Monte Carlo codes.
- EGSnrc matched to 2%/2mm in treatment part of beam, 5%/5mm outside, x-ray dose relative electron dose to better than 5%.
- Geant4 matched to 3%/2mm in treatment part of beam, 6%/6mm outside, x-ray dose relative to electron dose overestimated by 6%.
- Required modest differences in source and geometry parameters. Difference in calculated dose distributions is of modest clinical significance (4%/4mm).

- Geant4 Results are Preliminary
  - Input of source and geometry details is not trivial in any code.
  - We need to make sure we did all of this correctly one more time!
  - That is, the results are subject to change after further intense scrutiny.
  - Look for publications!