Supplemental material to “Intercomparison of Monte Carlo calculated dose enhancement ratios for gold nanoparticles irradiated by X-rays: assessing the uncertainty and correct methodology for extended beams”, Physica Medica, 2021

**Supplementary Table 1**. Monte Carlo simulation programs used in this work and input parameters, number of incident particles, physical models used in programs and computer machines used. (Reproduced from Li et al., Physica Medica 69, 147-169, 2020 with permission of the publisher, license number 5014161479184, license date Feb 22, 2021.)

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Modeler | Code name | Version | Incident photon number | Cut-off energy | | Physics lists and options | | Cross section library | Condensed history or track structure | | Deexcitation | Computer Desktop/super | Computer running system |
|  |  |  |  | photon | electron | Photon | electron |  | Water | Gold |  |  |  |
| PENELOPE#1 | PENELOPE | 2011 | 107 | 50 eV | 50 eV | Coherent and incoherent scattering,  Photoelectric absorption,  Pair production | Inner-shell impact ionization. | Penelope cross section library | Track structure | Track structure | X-ray fluorescence and Auger electrons from K – O1-5 shells and subshells | PC Intel Core i3-2120 CPU @3.30GHz | Windows 7 |
| PENELOPE#2 | PENELOPE | 2014 | 107 | 50 eV | 50 eV | Coherent and incoherent scattering,  Photoelectric absorption,  Pair production | Inner-shell impact ionization | Penelope cross section library | Track structure | Track structure | X-ray fluorescence and Auger electrons from K – O1-5 shells and subshells | PC Intel® Core(TM) i5-6300 U CPU @ 2.40 GHZ | Windows 7 |
| G4/DNA#1 | Geant4/DNA | 10.4.2 | 108 | 50 eV | 10 eV | Coherent and incoherent scattering,  Photoelectric absorption,  Pair production | Inner-shell impact ionization, excitation  Attachment in Geant4-DNA default option for water | EEDL, EPDL and EADL1 | Track structure (Geant4-DNA) Default option and option 7 | Condensed history (Livermore) and multiple scattering | X-ray fluorescence and Auger electrons for KLM shells | PC Intel® Xeon ® CPU E5-2630 U3 @2.40 GHz | Ubuntu 16.04 |
| G4/DNA#2 | Geant4/DNA | 10.0.5 | 107 | 990 eV | 10 eV | Geant4-DNA default physics for Au and H2O | Geant4-DNA default physics for Au and H2O | EEDL, EPDL and EADL | Track structure | Condensed history (Livermore) | Particle induced X-ray emission; complete Auger deexcitation | Virtual machine (VMware Player) ‘G4-10.05-CentOS7\_us’ hosted on an ‘Intel®Core™ i7-3770 CPU@3.40 GHz’ computer containing 32 GB  RAM | CentOS 7, hosted on Windows 7 Enterprise, 64-bit 6.1.7601, Service Pack 1 |
| G4/DNA#3 | Geant4/DNA | 10.4.2 | 109 | 10 eV | 10 eV | Geant4 EM standard physics option 4 for gold and Geant4-DNA default physics for water | Geant4 EM standard physics option 4 for gold and Geant4-DNA default physics for water | EEDL, EPDL and EADL | Track structure | Condensed history (Livermore) | Particle induces x-ray emission, Auger electrons from K-, L- and M-shells and Auger Cascades | PC Intel® Core i5-8500 CPU @4.10GHz  Internal Linux-cluster | Windows 10  Ubuntu 16.04 |
| TOPAS | TOPAS-nBio | 3.1.p3 | 108 | 50 eV | 10 eV | Coherent and incoherent scattering,  Photoelectric absorption,  Pair production | Inner-shell impact ionization, excitation, attachment, Bremsstrahlung | EEDL, EPDL and EADL | Track structure (G4-DNA) | Condensed history (Livermore) | X-ray fluorescence and Auger electrons for KLM shells | ERISOne Linux Cluster | RHEL |
| MCNP6 | MCNP6.1 | 2013 | 108 | 1 keV | 50 eV | coherent and incoherent scattering, photoelectric  absorption, and electron/positron pair production | atomic excitation, electron elastic scattering, subshell  electro-ionization, and bremsstrahlung | ENDF/B VI.8 | single-event method (similar to track structure) | single-event method (similar to track structure) | Relaxation considering as many as 29 subshells and can include almost 3,000 distinct transitions among them. | PC Intel Core i7-7700 CPU@3.60GHz | Windows 10 |
| MDM | MDM | 2006 (water)  2019 (gold) | 1014 | No explicit tracking of photons | Water:  7 eV  Gold:  10 eV | Coherent and incoherent scattering | Water: Elastic scattering BEB Excitations (2 modes) Vibrations (9 modes). Gold: Inelastic: Plasmon excitation BEB  Elastic: ELSEPA  Phonons | Photons: NIST  Auger: EADL | Track structure | Track structure | Full Auger electronic cascade (K to valence band) | Ran at the CCIN2P3 computing center | Linux  CentOS 7.6.1810 |
| PARTRAC | PARTRAC | 2015 | >109 | 100 eV | (H20):10 eV  (Au): 100 eV | Coherent and incoherent scattering,  Photoelectric absorption | Ionization (H2O: 5 shells;  Au: 13 shells and subshells),  Excitation (H2O: 5 levels;  Au: 1 level) | EPDL97,  (photons)  Dingfelder2 (electrons in H2O)  Hantke3 (electrons in Au) | Track structure | Track structure | EADL library | PC Intel-Core i7-3770K CPU @ 3.50 GHz | Linux (openSUSE 12.3) |
| NASIC | NASIC | 2018 | 3×108 | 10 eV | 10 eV | Compton scattering, photoelectric absorption, gamma conversion, Rayleigh scattering. | Water: elastic scattering, ionization, excitation, attachment, vibrational excitation.  Gold: multiple scattering, ionization, bremsstrahlung. | Electron ionization and excitation in liquid water: NASIC cross section library.  Others: Geant4 and Geant4-DNA cross section library. | Track structure | Condensed history | X-ray fluorescence and Auger electrons | PC Intel Core i5-7300HQ CPU @2.50GHz | Windows 10 |

1 EEDL – Evaluated Electrons Data Library; EPDL – Evaluated Photon Data Library; EADL – Evaluated Atomic Data Library.

2 Data from Dingfelder et al. [53]

3 Data not published

**Supplementary Table 2**. Comparison of the codes for the modelers used in this work and in Li et al., Physica Medica 69, 147-169, 2020.

|  |  |
| --- | --- |
| This work | Li et al., Physica Medica 69, 147-169, 2020 |
| G1 | G4/DNA#1 |
| G2 | G4/DNA#2 |
| G3 | G4/DNA#3 |
| M1 | MCNP6 |
| M2 | MDM |
| N | NASIC |
| P1 | PARTRAC |
| P2 | PENELOPE#1 |
| P3 | PENELOPE#2 |
| T | TOPAS |

**Supplementary Table 3**. Photon energy spectra used in the simulations. (The given photon energies are the lower bin boundaries.)

| **50 kVp** | | **100 kVp** | |
| --- | --- | --- | --- |
| photon energy / keV | spectral density / keV-1 | photon energy / keV | spectral density / keV-1 |
| 5 | 1.59912E-90 | 10 | 1.154E-13 |
| 5.5 | 2.34087E-72 | 10.5 | 2.468E-12 |
| 6 | 3.43669E-54 | 11 | 5.578E-11 |
| 6.5 | 1.12659E-44 | 11.5 | 5.551E-10 |
| 7 | 3.70716E-35 | 12 | 5.546E-09 |
| 7.5 | 1.24503E-29 | 12.5 | 2.963E-08 |
| 8 | 4.19206E-24 | 13 | 1.586E-07 |
| 8.5 | 1.00901E-20 | 13.5 | 5.714E-07 |
| 9 | 2.43388E-17 | 14 | 2.072E-06 |
| 9.5 | 3.77834E-15 | 14.5 | 5.444E-06 |
| 10 | 5.88942E-13 | 15 | 1.436E-05 |
| 10.5 | 1.44822E-11 | 15.5 | 3.042E-05 |
| 11 | 3.62077E-10 | 16 | 6.472E-05 |
| 11.5 | 3.66218E-09 | 16.5 | 1.155E-04 |
| 12 | 3.7102E-08 | 17 | 2.065E-04 |
| 12.5 | 1.95927E-07 | 17.5 | 3.242E-04 |
| 13 | 1.03574E-06 | 18 | 5.101E-04 |
| 13.5 | 3.60639E-06 | 18.5 | 7.329E-04 |
| 14 | 1.25991E-05 | 19 | 1.055E-03 |
| 14.5 | 3.19856E-05 | 19.5 | 1.409E-03 |
| 15 | 8.136E-05 | 20 | 1.885E-03 |
| 15.5 | 0.00016654 | 20.5 | 2.382E-03 |
| 16 | 0.00034126 | 21 | 3.012E-03 |
| 16.5 | 0.000589575 | 21.5 | 3.637E-03 |
| 17 | 0.001019336 | 22 | 4.398E-03 |
| 17.5 | 0.001553442 | 22.5 | 5.133E-03 |
| 18 | 0.002368697 | 23 | 5.993E-03 |
| 18.5 | 0.0033084 | 23.5 | 6.798E-03 |
| 19 | 0.004622752 | 24 | 7.717E-03 |
| 19.5 | 0.006015967 | 24.5 | 8.513E-03 |
| 20 | 0.007831297 | 25 | 9.393E-03 |
| 20.5 | 0.009652096 | 25.5 | 1.024E-02 |
| 21 | 0.01189854 | 26 | 1.117E-02 |
| 21.5 | 0.014042297 | 26.5 | 1.197E-02 |
| 22 | 0.016574235 | 27 | 1.283E-02 |
| 22.5 | 0.018929227 | 27.5 | 1.360E-02 |
| 23 | 0.021619908 | 28 | 1.442E-02 |
| 23.5 | 0.024029276 | 28.5 | 1.510E-02 |
| 24 | 0.026706846 | 29 | 1.582E-02 |
| 24.5 | 0.02889123 | 29.5 | 1.639E-02 |
| 25 | 0.031252149 | 30 | 1.699E-02 |
| 25.5 | 0.033434127 | 30.5 | 1.751E-02 |
| 26 | 0.035764131 | 31 | 1.804E-02 |
| 26.5 | 0.037643778 | 31.5 | 1.849E-02 |
| 27 | 0.03961538 | 32 | 1.897E-02 |
| 27.5 | 0.041219448 | 32.5 | 1.933E-02 |
| 28 | 0.042934617 | 33 | 1.971E-02 |
| 28.5 | 0.044179307 | 33.5 | 2.000E-02 |
| 29 | 0.045470705 | 34 | 2.029E-02 |
| 29.5 | 0.046299676 | 34.5 | 2.050E-02 |
| 30 | 0.047128273 | 35 | 2.072E-02 |
| 30.5 | 0.047711906 | 35.5 | 2.086E-02 |
| 31 | 0.048284088 | 36 | 2.101E-02 |
| 31.5 | 0.048636121 | 36.5 | 2.111E-02 |
| 32 | 0.048968747 | 37 | 2.120E-02 |
| 32.5 | 0.049013005 | 37.5 | 2.125E-02 |
| 33 | 0.049031997 | 38 | 2.130E-02 |
| 33.5 | 0.048805248 | 38.5 | 2.128E-02 |
| 34 | 0.048550655 | 39 | 2.127E-02 |
| 34.5 | 0.048102127 | 39.5 | 2.123E-02 |
| 35 | 0.047625483 | 40 | 2.120E-02 |
| 35.5 | 0.046997966 | 40.5 | 2.112E-02 |
| 36 | 0.046342731 | 41 | 2.104E-02 |
| 36.5 | 0.045537942 | 41.5 | 2.093E-02 |
| 37 | 0.044706961 | 42 | 2.082E-02 |
| 37.5 | 0.043762419 | 42.5 | 2.069E-02 |
| 38 | 0.042793292 | 43 | 2.056E-02 |
| 38.5 | 0.041699036 | 43.5 | 2.041E-02 |
| 39 | 0.040583516 | 44 | 2.026E-02 |
| 39.5 | 0.039412726 | 44.5 | 2.009E-02 |
| 40 | 0.03822114 | 45 | 1.992E-02 |
| 40.5 | 0.036936009 | 45.5 | 1.974E-02 |
| 41 | 0.035633122 | 46 | 1.957E-02 |
| 41.5 | 0.034252674 | 46.5 | 1.938E-02 |
| 42 | 0.032856857 | 47 | 1.918E-02 |
| 42.5 | 0.031404683 | 47.5 | 1.897E-02 |
| 43 | 0.02993824 | 48 | 1.877E-02 |
| 43.5 | 0.028409098 | 48.5 | 1.857E-02 |
| 44 | 0.026866845 | 49 | 1.836E-02 |
| 44.5 | 0.025254876 | 49.5 | 1.814E-02 |
| 45 | 0.023631253 | 50 | 1.793E-02 |
| 45.5 | 0.02194061 | 50.5 | 1.771E-02 |
| 46 | 0.020238105 | 51 | 1.749E-02 |
| 46.5 | 0.018444242 | 51.5 | 1.726E-02 |
| 47 | 0.01663912 | 52 | 1.704E-02 |
| 47.5 | 0.014599238 | 52.5 | 1.682E-02 |
| 48 | 0.012551527 | 53 | 1.660E-02 |
| 48.5 | 0.010525564 | 53.5 | 1.638E-02 |
| 49 | 0.008470459 | 54 | 1.616E-02 |
| 49.5 | 0.004222889 | 54.5 | 1.593E-02 |
| 50 | 0 | 55 | 1.571E-02 |
|  |  | 55.5 | 1.548E-02 |
|  |  | 56 | 1.526E-02 |
|  |  | 56.5 | 1.504E-02 |
|  |  | 57 | 1.482E-02 |
|  |  | 57.5 | 1.460E-02 |
|  |  | 58 | 5.251E-02 |
|  |  | 58.5 | 1.417E-02 |
|  |  | 59 | 1.395E-02 |
|  |  | 59.5 | 8.038E-02 |
|  |  | 60 | 1.352E-02 |
|  |  | 60.5 | 1.331E-02 |
|  |  | 61 | 1.310E-02 |
|  |  | 61.5 | 1.289E-02 |
|  |  | 62 | 1.269E-02 |
|  |  | 62.5 | 1.248E-02 |
|  |  | 63 | 1.227E-02 |
|  |  | 63.5 | 1.207E-02 |
|  |  | 64 | 1.188E-02 |
|  |  | 64.5 | 1.167E-02 |
|  |  | 65 | 1.147E-02 |
|  |  | 65.5 | 1.128E-02 |
|  |  | 66 | 1.109E-02 |
|  |  | 66.5 | 1.089E-02 |
|  |  | 67 | 3.307E-02 |
|  |  | 67.5 | 1.051E-02 |
|  |  | 68 | 1.032E-02 |
|  |  | 68.5 | 1.014E-02 |
|  |  | 69 | 1.581E-02 |
|  |  | 69.5 | 9.774E-03 |
|  |  | 70 | 9.007E-03 |
|  |  | 70.5 | 8.850E-03 |
|  |  | 71 | 8.694E-03 |
|  |  | 71.5 | 8.542E-03 |
|  |  | 72 | 8.393E-03 |
|  |  | 72.5 | 8.242E-03 |
|  |  | 73 | 8.092E-03 |
|  |  | 73.5 | 7.942E-03 |
|  |  | 74 | 7.795E-03 |
|  |  | 74.5 | 7.647E-03 |
|  |  | 75 | 7.500E-03 |
|  |  | 75.5 | 7.351E-03 |
|  |  | 76 | 7.204E-03 |
|  |  | 76.5 | 7.061E-03 |
|  |  | 77 | 6.917E-03 |
|  |  | 77.5 | 6.776E-03 |
|  |  | 78 | 6.637E-03 |
|  |  | 78.5 | 6.494E-03 |
|  |  | 79 | 6.351E-03 |
|  |  | 79.5 | 6.210E-03 |
|  |  | 80 | 6.071E-03 |
|  |  | 80.5 | 5.931E-03 |
|  |  | 81 | 5.791E-03 |
|  |  | 81.5 | 5.657E-03 |
|  |  | 82 | 5.525E-03 |
|  |  | 82.5 | 5.388E-03 |
|  |  | 83 | 5.250E-03 |
|  |  | 83.5 | 5.113E-03 |
|  |  | 84 | 4.979E-03 |
|  |  | 84.5 | 5.173E-02 |
|  |  | 85 | 4.708E-03 |
|  |  | 85.5 | 4.576E-03 |
|  |  | 86 | 4.445E-03 |
|  |  | 86.5 | 4.312E-03 |
|  |  | 87 | 4.178E-03 |
|  |  | 87.5 | 4.047E-03 |
|  |  | 88 | 3.918E-03 |
|  |  | 88.5 | 3.782E-03 |
|  |  | 89 | 3.647E-03 |
|  |  | 89.5 | 3.517E-03 |
|  |  | 90 | 3.388E-03 |
|  |  | 90.5 | 3.252E-03 |
|  |  | 91 | 3.117E-03 |
|  |  | 91.5 | 2.985E-03 |
|  |  | 92 | 2.856E-03 |
|  |  | 92.5 | 2.719E-03 |
|  |  | 93 | 2.581E-03 |
|  |  | 93.5 | 2.447E-03 |
|  |  | 94 | 2.314E-03 |
|  |  | 94.5 | 2.166E-03 |
|  |  | 95 | 2.018E-03 |
|  |  | 95.5 | 1.871E-03 |
|  |  | 96 | 1.726E-03 |
|  |  | 96.5 | 1.581E-03 |
|  |  | 97 | 1.436E-03 |
|  |  | 97.5 | 1.294E-03 |
|  |  | 98 | 1.154E-03 |
|  |  | 98.5 | 8.611E-04 |
|  |  | 99 | 5.687E-04 |
|  |  | 99.5 | 2.819E-04 |
|  |  | 100 | 0.000E+00 |