Appendix: Results GPU MC

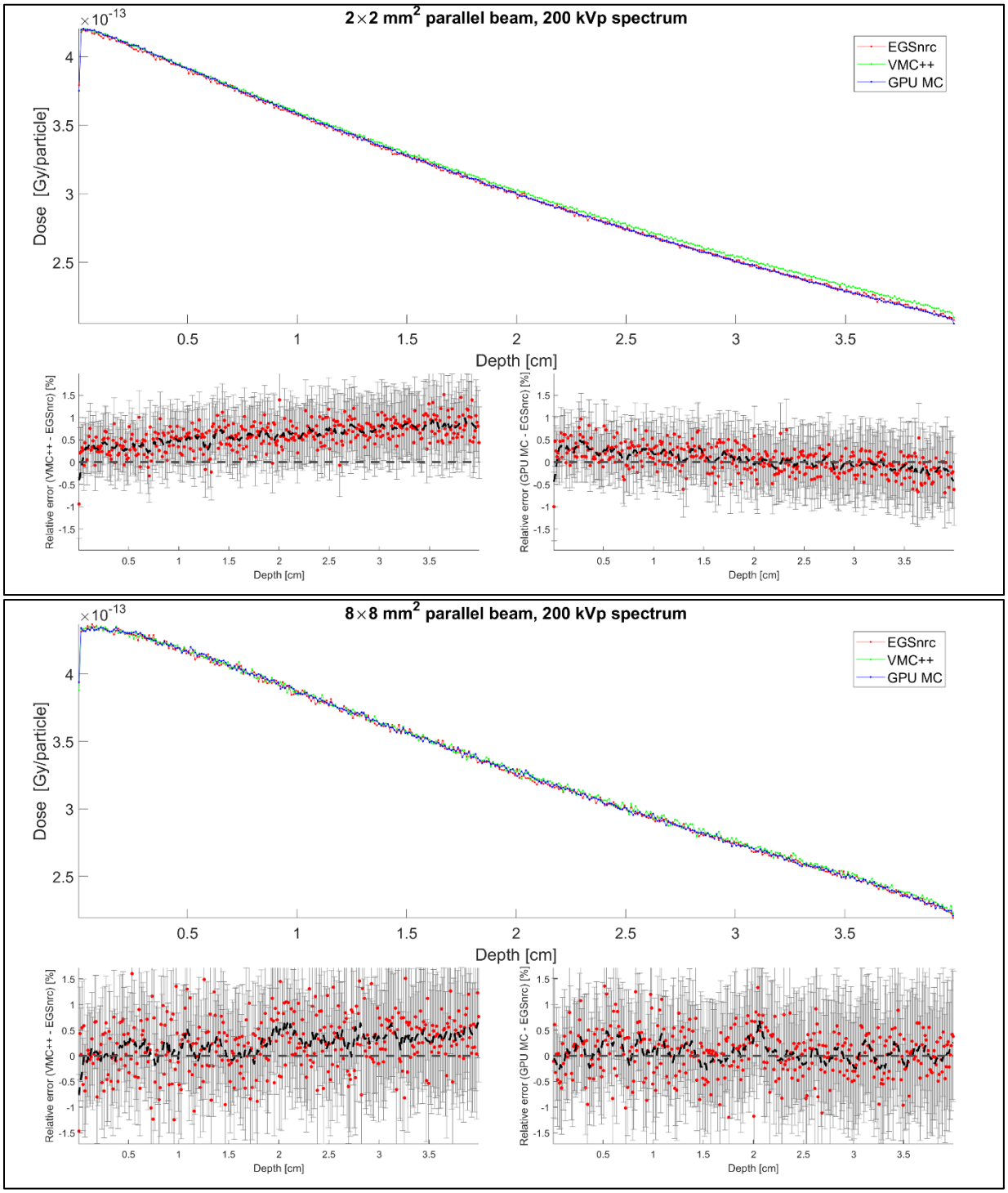
This document contains the corresponding results from *Validation of the analytical irradiator model and Monte Carlo dose engine in the small animal irradiation treatment planning system µ-RayStation 8B* (S. Chiavassa et. al., 2020, Phys. Med. Biol.), but instead of using the VMC++ dose engine, the µ-RayStation in-house GPU MC has been used for all dose calculations.

GPU MC

The new µ-RayStation GPU MC dose algorithm is based on the clinical RayStation in-house GPU MC [RayStation 9B Reference Manual; 2019, which is a Class II algorithm (condensed history) and transports photons, electrons, and positrons. For photons, Compton scattering, photoelectric absorption and pair creation events are simulated. For electrons and positrons, Møller scattering, bremsstrahlung and positron annihilation are simulated as discrete events and multiple scattering using the random hinge condensed history method. It is optimized for 3D dose calculations in voxel-geometries and to avoid traversing each voxel, the fictitious cross section method is used (also known as Woodcock tracking). The idea is that by setting the total cross section to the same in the entire patient, there is no need to step through each voxel. At the site of the interaction it is rejected with a probability that depends on the local cross section.

To make the code suitable for low energies and smaller voxels, lowered transport energy thresholds are used (electron production threshold; 250 → 10 keV, and the multiple scattering to CSDA transport transition threshold; 250 → 35 keV), some technical cross section interpolation issues have been fixed, and Rayleigh scattering has been implemented (missing in VMC++).

The addition of Rayleigh scattering results in slightly more scattering and thus a slightly faster dose fall-off, especially for the lower energies in a typical X-ray beam. Neither the GPU MC, nor VMC++, model the electron binding effect for Compton scattering, which results in slightly too much Compton scattering, and thus a faster dose fall-off. All in all, VMC++ will scatter too little, and the GPU MC a bit too much. To quantify this, the two codes are compared to simulations done in EGSnrc [I. Kawrakow et. al., "*The EGSnrc Code System: Monte Carlo Simulation of Electron and Photon Transport*", NRCC Report PIRS-701 2016]. The results for two parallel square fields, 2×2 mm^2 and 8×8 mm^2 with a 200 kVp energy spectrum, are found in Extra Figure 1. As can be seen, the differences are more pronounced for the smaller field, and larger for VMC++ than for the GPU MC.



Extra Figure 1 [Not from paper]: Central axis depth dose comparison between EGSnrc, VMC++ and the new GPU MC for 2×2 mm^2 and 8×8 mm^2 parallel square fields with a 200 kVp spectrum, top and bottom boxes, respectively. Within each box, the two bottom plots are the relative errors (compared to the maximal EGSnrc dose) for the VMC++ (left) and GPU MC (right) codes, including the statistical uncertainty and a moving average curve (dashed black, width = 9 voxels).

New Results

All the dose distributions from the paper have been recalculated using the same settings and irradiator model as for VMC++. Figures 4-9 and Table 3 from the paper are reproduced with the new doses. In addition to this, result including text sections have been reproduced (in *italic* text) below to the figures they pertain to. The calculation time comparison does not pertain to any figure and is include directly below here.

3.4. Calculation time comparison

For example, a 5 mm anterior beam in water (3×3×4cm³ geometry, calculation grid resolution of 0.2×0.2×0.2mm³ and RSU of 0.3%) requires 302 min with GATE against 5.0 min with μ-RayStation CPU and 1min30sec with μ-RayStation GPU. A typical 3D-conformal treatment (three 5 mm static beams) for the mouse case used in this work (calculation grid resolution of 0.2×0.2×0.2mm³ and RSU of 0.7%) requires 690 min with GATE against 3.7 min with μ-RayStation CPU and 45sec with μ-RayStation GPU. In the same way, a complete arc (5 mm beam) for the mouse (calculation grid resolution of 0.2×0.2×0.2 mm³ and RSU of 1.0%) requires 733 min with GATE against 1.0 min with μ-RayStation CPU and 10 sec with μ-RayStation GPU. The resulting speed-up factors between GATE and μ-RayStation CPU are 60, 180 and 680, respectively. The resulting speed-up factors between GATE and μ-RayStation GPU are 200, 900 and 4400, respectively. Obviously, computing power must be taken into account: GATE calculations were performed on a CPU 8 Core not parallelized (2.3 GHz Intel Core i7), μ-RayStation VMC++ on a CPU 8 Core parallelized (Intel Xeon E5-2667 V3) and the μ-RayStation GPU MC on an M6000 Nvidia GPU.

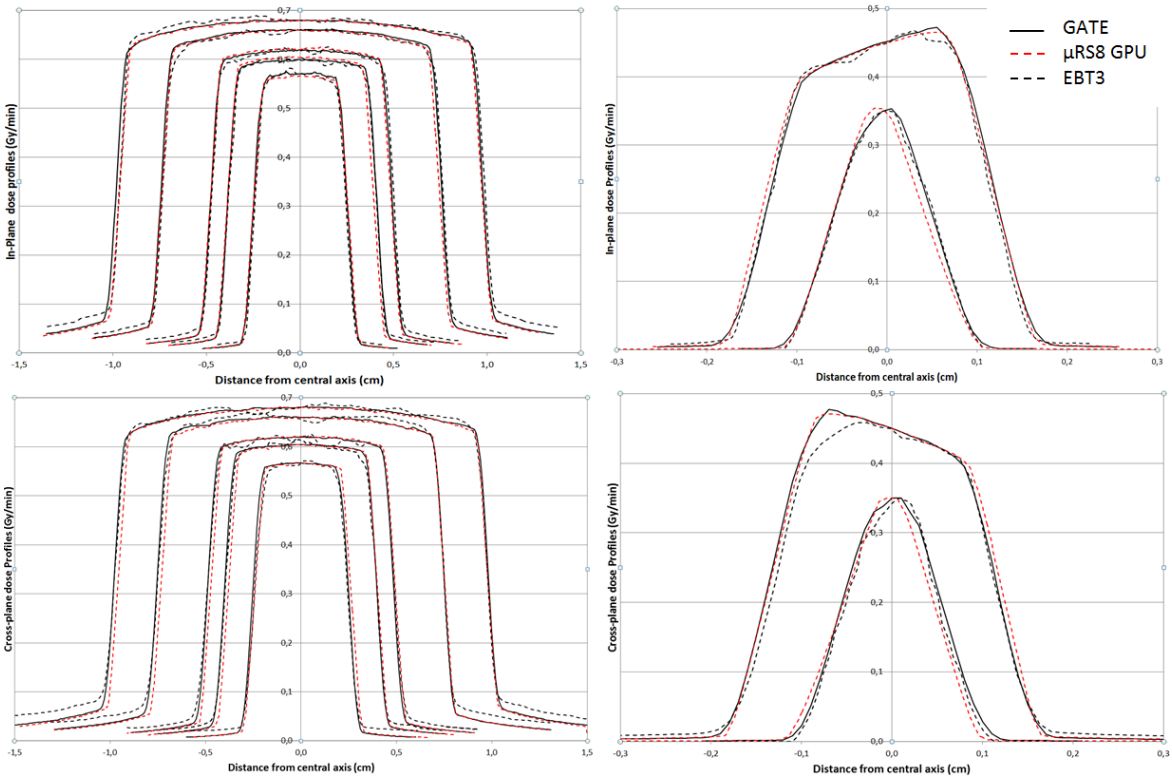


Figure 4: Measured (EBT3) and calculated (μ-RayStation 8B GPU and GATE) In-plane (top) and Cross-plane (bottom) off-axis profiles for (left) the five collimators with a diameter greater than the focal spot size (5, 8, 10, 15 and 20 mm in diameters) and (right) the two collimators with a diameter smaller than the focal spot (2.5 and 1 mm in diameters). EBT3 uncertainty was 3.2%. RSU was below 0.5% for GATE and below 0.2% for μ-RayStation 8B GPU. Data were normalized at the central axis.

The maximal distance-to agreement (DTA) at 50% of the central dose between μ-RayStation 8B GPU and both EBT3 measurements and GATE was 0.19 mm for all beams.

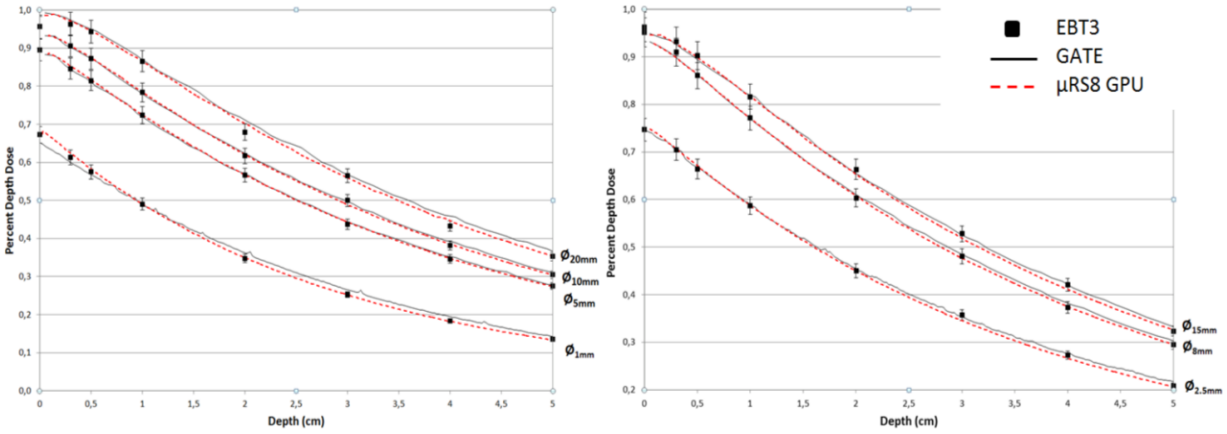


Figure 5: Measured (EBT3) and calculated (µ-RayStation 8B GPU and GATE) PDD for collimators of diameters 1, 5, 10 and 20 mm (left), and 2.5, 8 and 15 mm (right). PDD are weighted by OF. EBT3 uncertainty was 3.2%. µ-RayStation RSU was below 0.4%. GATE mean statistical uncertainties were below 1%.

Relative comparison between µ-RayStation 8B GPU and measurement on the one hand, and µ-RayStation 8B GPU and GATE on the other hand, was made considering respectively measurement and GATE calculation at 1 cm depth as reference. Between µ-RayStation 8B GPU and measurement, mean absolute error were 1.2%, 0.9%, 0.8%, 0.8%, 0.5%, 0.6% and 0.9% for collimators with a field diameter of 20, 15, 10, 8, 5, 2.5 and 1 mm respectively (global mean error 0.8%). Corresponding comparison between µ-RayStation 8B GPU and GATE were 0.5%, 0.6%, 0.6%, 0.8%, 0.5%, 0.6% and 0.9% (global mean error 0.7%). In all cases, the maximal absolute error was 3.3%. Measured reference dose in water and relative OF were used to determine collimator specific dose scaling adjustments for the model.

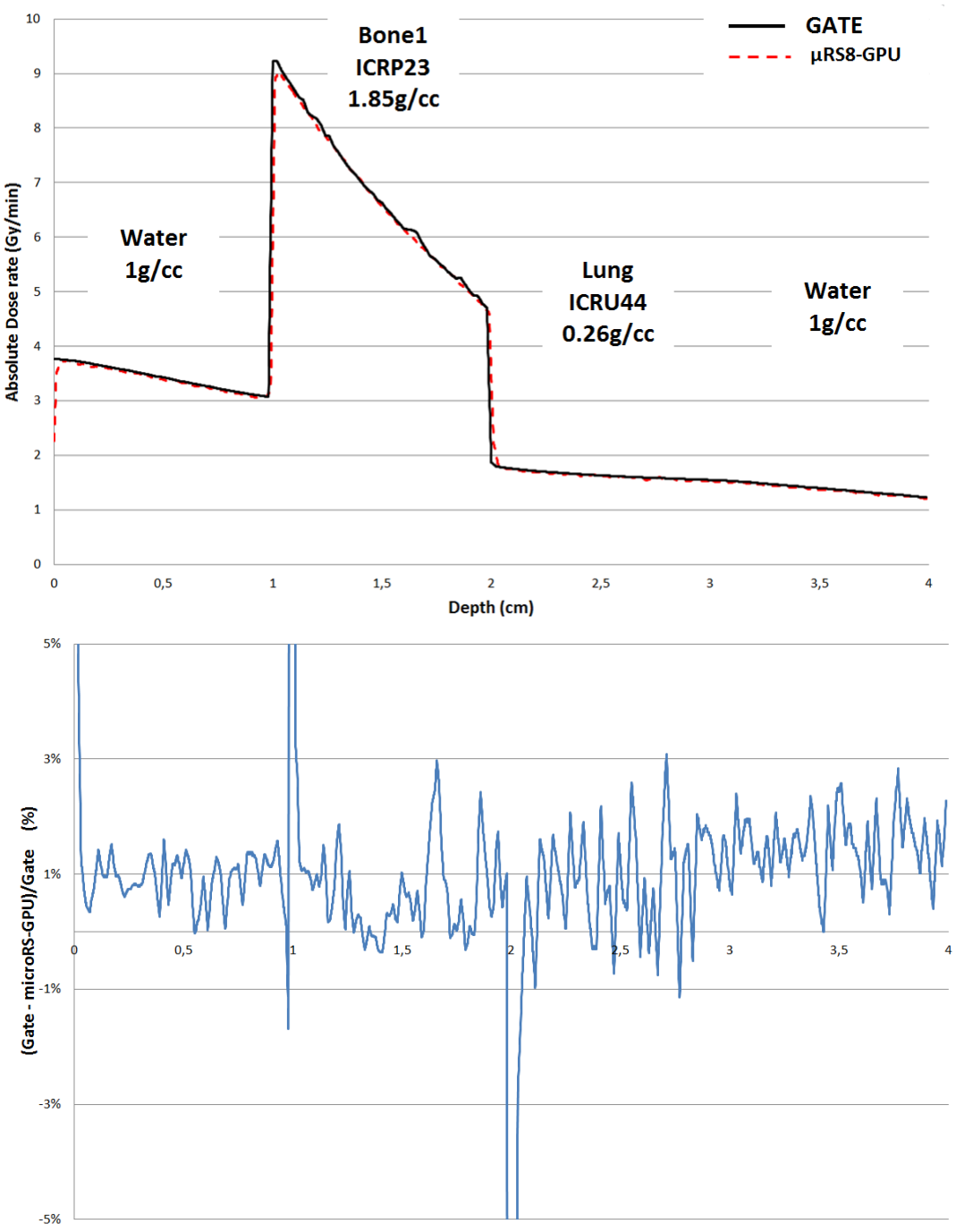


Figure 6: Absolute Dose rate (Gy/min) in depth in calculated heterogeneous slabs with GATE and µ-RayStation 8B GPU (top). Relative error (%) between GATE and µ-RayStation GPU in depth (bottom). Relative statistical uncertainty was 0.87% in GATE and 0.20% in µ-RayStation GPU.

GATE and µ-RayStation GPU provide closely matching dose distributions, with a mean absolute error of 1.0%, 0.7%, 1.0% and 1.5% for slabs of water, bone, lung, and water, respectively. Interfaces present slight deviations with a DTA of 0.1 mm, corresponding to one voxel.

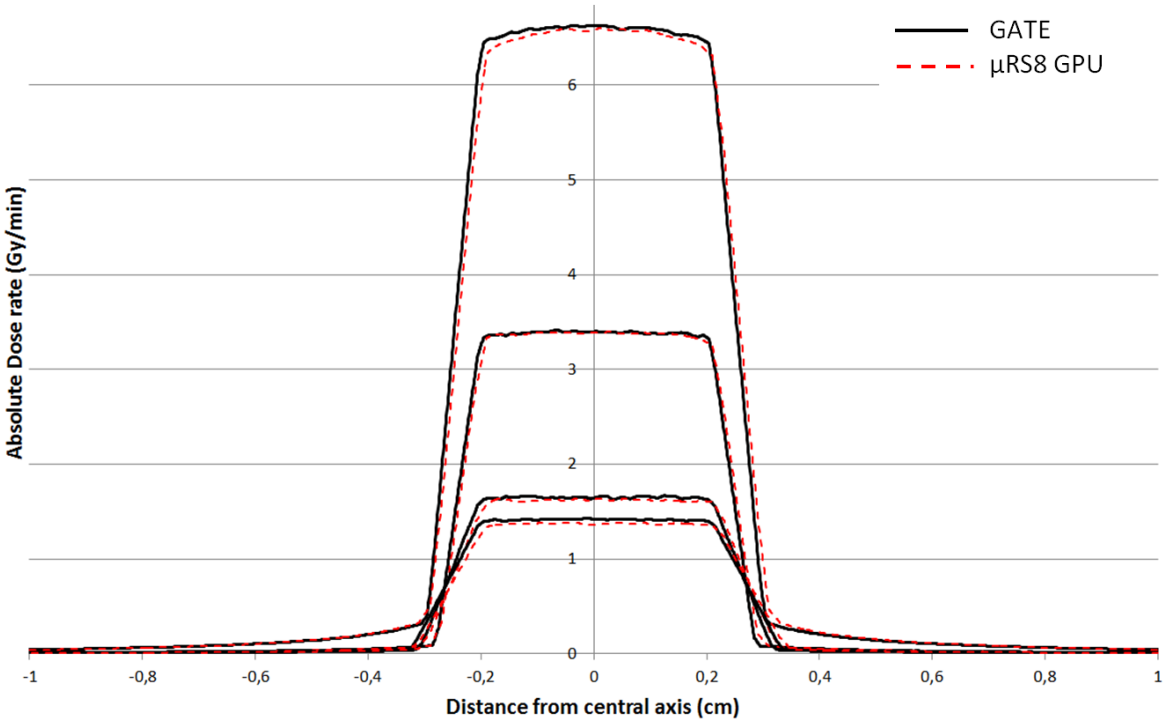


Figure 7: Dose rate profiles in anode/cathode direction calculated with GATE and µ-RayStation 8B GPU in the heterogeneous phantom. Profiles are extracted at depth 0.5cm (water), 1.5cm (bone), 2.5cm (lung) and 3.5cm (water).

DTA between GATE and µ-RayStation GPU at 50% of the central dose are 0.05mm, 0.07mm, 0.06mm and 0.09mm on the anode side and 0.04mm, 0.06mm, 0.08mm and 0.06mm on the cathode side for depths 0.5cm, 1.5cm, 2.5cm and 3.5cm respectively. DTA obtained for the same collimator in water at 2 cm depth were 0.07 mm and 0.1 mm.

Table 3: 2D Gamma-local analysis between µ-RayStation GPU and GATE calculation in mouse. The axial, coronal and sagittal planes intersect the beam isocenter.

% pixels local-γ passed criteria	3 static beams - spine 5mm collimator			Arc plan - spine 5mm collimator			6 static beams - lung 1mm collimator		
	axial	coronal	sagittal	axial	Coronal	sagittal	axial	coronal	sagittal
1%/0.3mm	99.7	99.4	99.5	99.3	99.7	100	99.3	99.5	99.4
1%/0.2mm	94.8	94.6	97.6	96.6	97.8	98.7	98.5	99.5	97.6

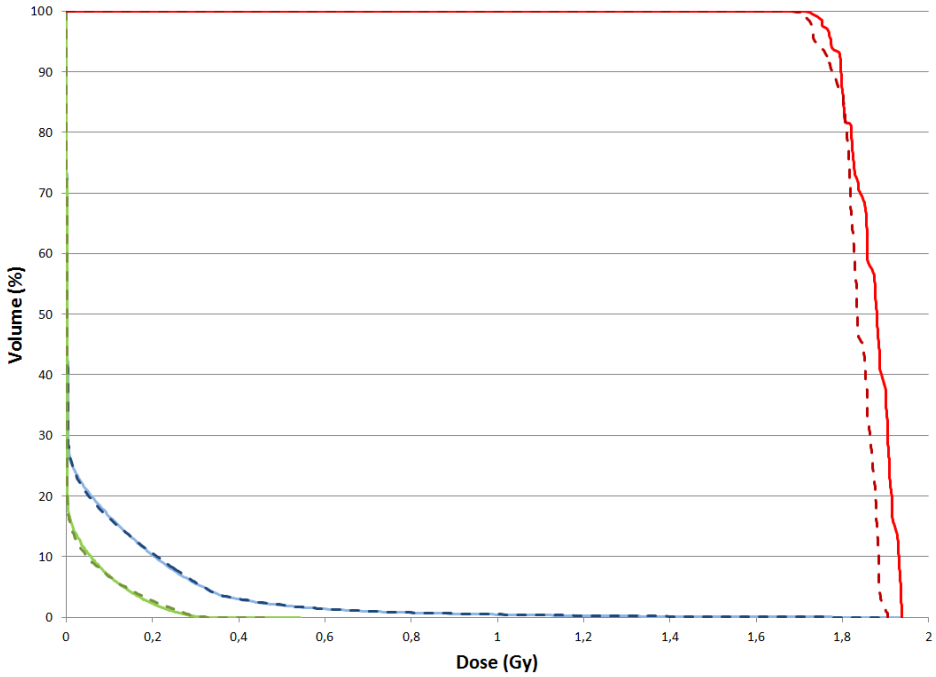


Figure 8: Dose-volume histogram of left lung (green), right lung (blue) and tumor (red) calculated in µ-RayStation from µ-RayStation V8 GPU calculation (solid lines) and GATE (dotted lines).

Figure 8 shows dose-volume histogram comparison for the lung target. Relative difference for average and maximal doses in tumor calculated by µ-RayStation GPU and GATE were 1.6% and 2% respectively. No significant dose difference was found in right and left lungs.

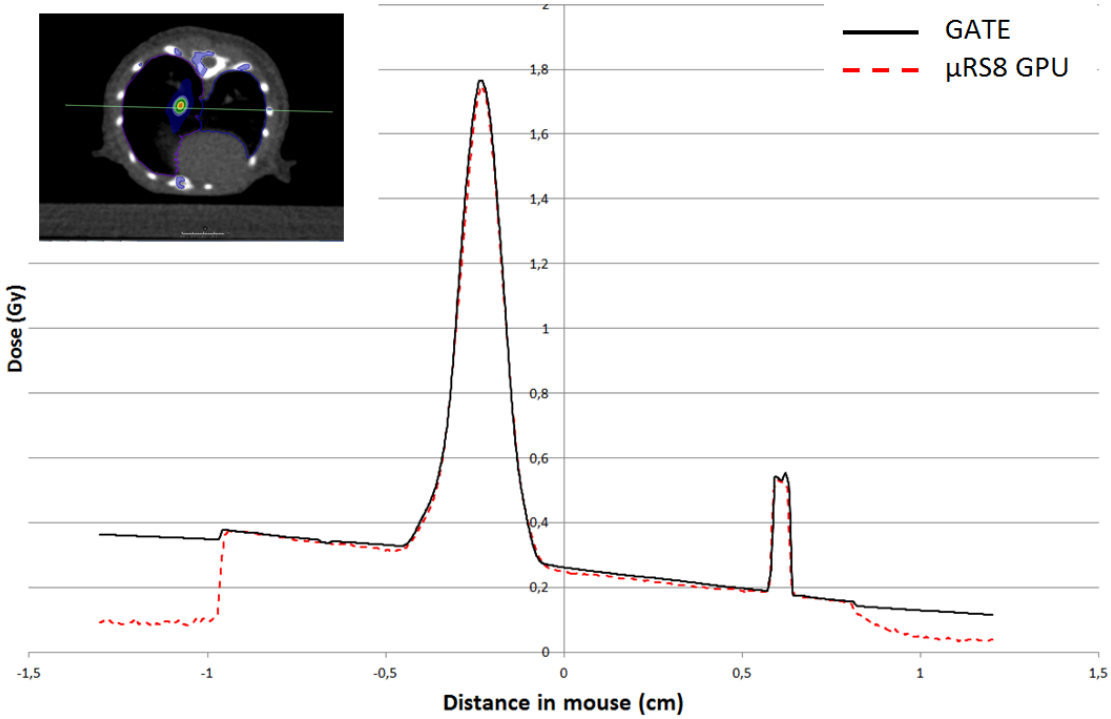


Figure 9: profiles extracted from µ-RayStation V8 GPU and GATE calculation in mouse lung. Profile position is represented on the mouse in the top left figure.