RADDOSE-3D GUI

TRY our new GUI written by Josh Dickerson (jdickerson@mrc-lmb.cam.ac.uk)!!

To run RADDOSE-3D for MX, SMX, SAXS (whichever you like!), RADDOSE-XFEL (+ Monte-Carlo simulations) or RADDOSE-ED

Step 1: Download and unzip the RADDOSE-3D GUI from:

GitHub - GarmanGroup/RADDOSE-3D

There are versions for a PC (Windows_release.zip) and for Linux (Linux_release.zip).

If you have a MAC, there is no new GUI yet, but you can run a limited capability RADDOSE-3D from the WWW sit*:

raddo.se (click on 'manual interface' and run the test example first. Then edit the input for a case you would like to try)

To run the GUI you need to have Java installed which you can get free at

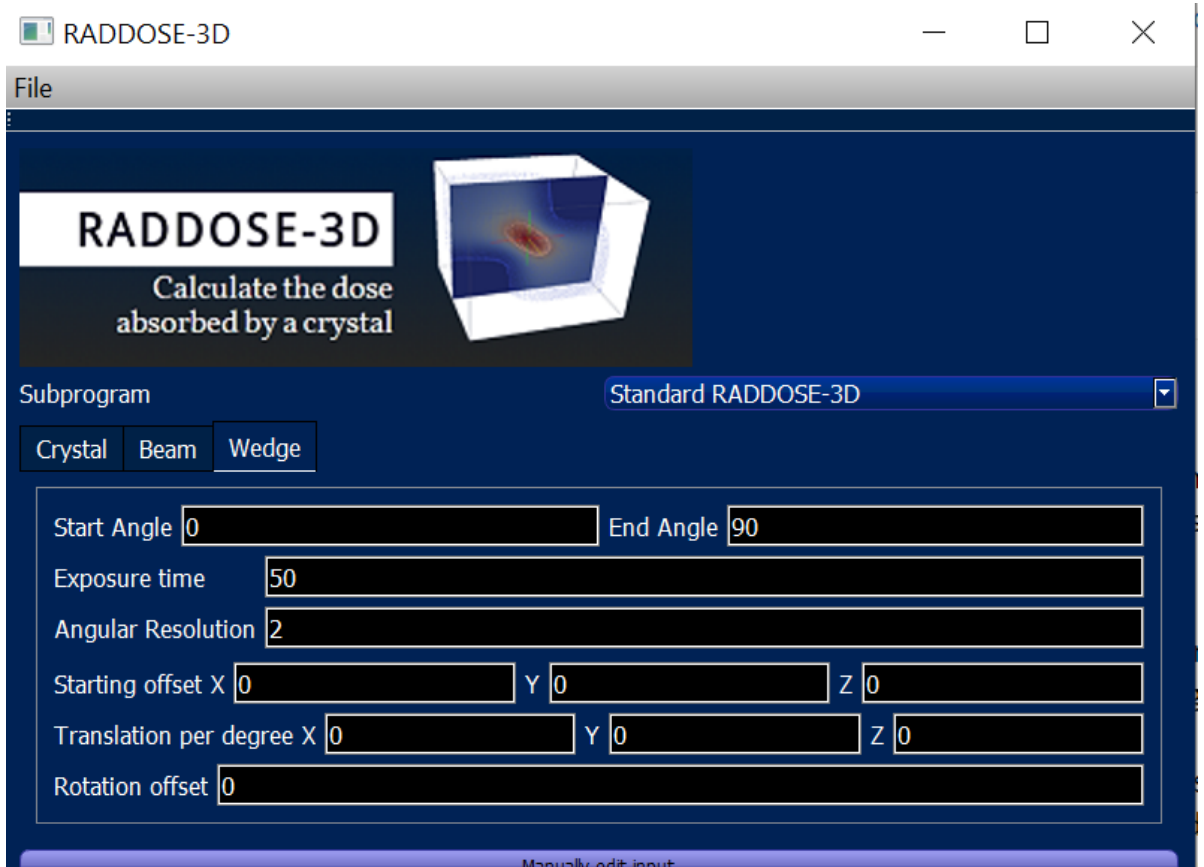
https://www.java.com/download/ie_manual.jsp

Also, if you have R (https://www.r-project.org/) installed, from the RADDOSE-3D output you will be able to produce 3D representations of the dose distribution in your sample.

- **Step 2:** Unzip the file you have downloaded. On Windows machines Josh recommends the best place to install the executable (e.g. Documents versus Program Files) is in Documents as he tends to avoid putting programs in Program Files unless he is using an installer, to avoid the need for admin privileges and to keep things self-contained.

- Note that installing a third party executable by direct download rather than through an installer might lead to your antivirus software to complain.

Step 3: Find the file RD3D_GUI.EXE and if on a PC click on it. For Linux run it however you usually run executable files. The GUI should open, and you can enter input on 3 tabs: crystal, beam and wedge. See the RADDOSE-3D Manual (link on raddo.se) if yu are not familiar with the required input.



RADDOSE-3D run

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Wedge 1:

Collecting data for a total of 50.0s from phi = 0.0 to 90.0 deg.

Crystal coefficients calculated with RADDOSE-3D.
Photelectric Coefficient: 3.21e-04 /um.
Inelastic Coefficient: 1.86e-05 /um.
Elastic Coefficient: 2.10e-05 /um.
Attenuation Coefficient: 3.61e-04 /um.
Density: 1.14 g/ml.

Average Diffraction Weighted Dose        : 6.238509 MGy
Last Diffraction Weighted Dose           : 10.508146 MGy
Elastic Yield                            : 2.27e+11 photons
Diffraction Efficiency (Elastic Yield/DWD): 3.64e+10 photons/MGy
Average Dose (Whole Crystal)             : 5.921152 MGy

Average Dose (Exposed Region)            : 5.921152 MGy
Max Dose                                 : 37.291488 MGy
Average Dose (95.0 % of total absorbed energy threshold (2.85 MGy)): 9.501849 MGy
Dose Contrast (Max/Threshold Av.)        : 3.92
Used Volume                              : 100.0%
Absorbed Energy (this Wedge)             : 6.88e-03 J.
Dose Inefficiency (Max Dose/mJ Absorbed)  : 5.4 1/g
Dose Inefficiency PE (Max Dose/mJ Deposited): 5.5 1/g

Final Dose Histogram:
Bin  1,  0.0 to  0.1 MGy: 16.6 %
Bin  2,  0.1 to  3.4 MGy: 26.1 %
Bin  3,  3.4 to  6.7 MGy: 21.0 %
Bin  4,  6.7 to 10.1 MGy: 16.0 %
Bin  5, 10.1 to 13.4 MGy:  9.4 %
Bin  6, 13.4 to 16.7 MGy:  5.0 %
Bin  7, 16.7 to 20.0 MGy:  1.8 %
Bin  8, 20.0 to 23.4 MGy:  1.6 %
Bin  9, 23.4 to 26.7 MGy:  1.0 %
Bin 10, 26.7 to 30.0 MGy:  1.2 %
Bin 11, 30.0 MGy upwards:  0.3 %

RADDOSE-3D terminated after 0.9 seconds
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Plot dose histogram

Back

Step 4: Understanding the output! DOSE = ENERGY ABSORBED/MASS

Photoelectric Coefficient: 6.35e-04 /um.
Inelastic Coefficient: 1.87e-05 /um.
Elastic Coefficient: 2.36e-05 /um.
Attenuation Coefficient: 6.77e-04 /um.
Density: 1.16 g/ml.

Average Diffraction Weighted Dose : 11.887135 MGy
Last Diffraction Weighted Dose : 20.040846 MGy
Elastic Yield : 2.51e+11 photons
Diffraction Efficiency (Elastic Yield/DWD): 2.11e+10 photons/MGy
Average Dose (Whole Crystal) : 11.271797 MGy
Average Dose (Exposed Region) : 11.271797 MGy
Max Dose : 71.040785 MGy

Step 4: Understanding the output! DOSE = ENERGY ABSORBED/MASS

Average Dose (95.0 % of total absorbed energy threshold (5.36 MGy)): 18.088188 MGy
Dose Contrast (Max/Threshold Av.) : 3.93
Used Volume : 100.0%
Absorbed Energy (this Wedge) : 1.33e-02 J.
Dose Inefficiency (Max Dose/mJ Absorbed) : 5.3 1/g
Dose Inefficiency PE (Max Dose/mJ Deposited): 5.5 1/g

NB: some dose is escaping with photoelectrons emerging from crystal so Max dose/energy absorbed is less than Max dose/energy deposited)

RADDOSE-3D References

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6) Doses for experiments with microbeams and microcrystals :Monte Carlo simulations in RADDOSE-3D. Joshua L. Dickerson and Elspeth F. Garman. *Protein Science* (2021) 30, 8–19.

7) RADDOSE-XFEL: Femtosecond time-resolved dose estimates for macromolecular XFEL experiments. Joshua L. Dickerson, Patrick T.N. McCubbin and Elspeth F. Garman.

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