





#### Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications

28 October – 8 November 2024 ICTP, Trieste, Italy

#### Lecture 10

#### Phase space files

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Metrology Research Centre National Research Council Canada

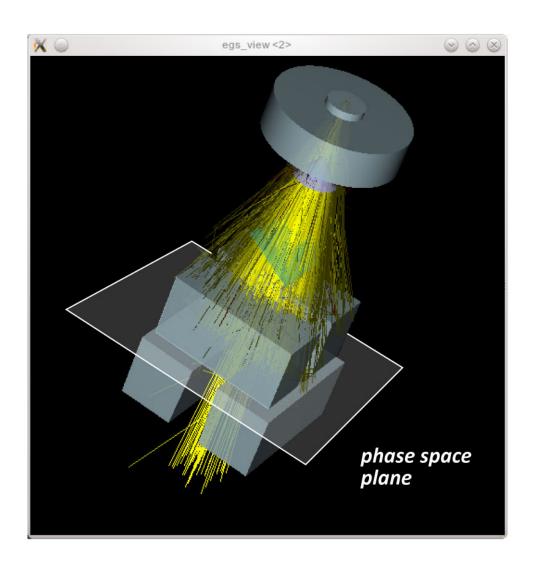




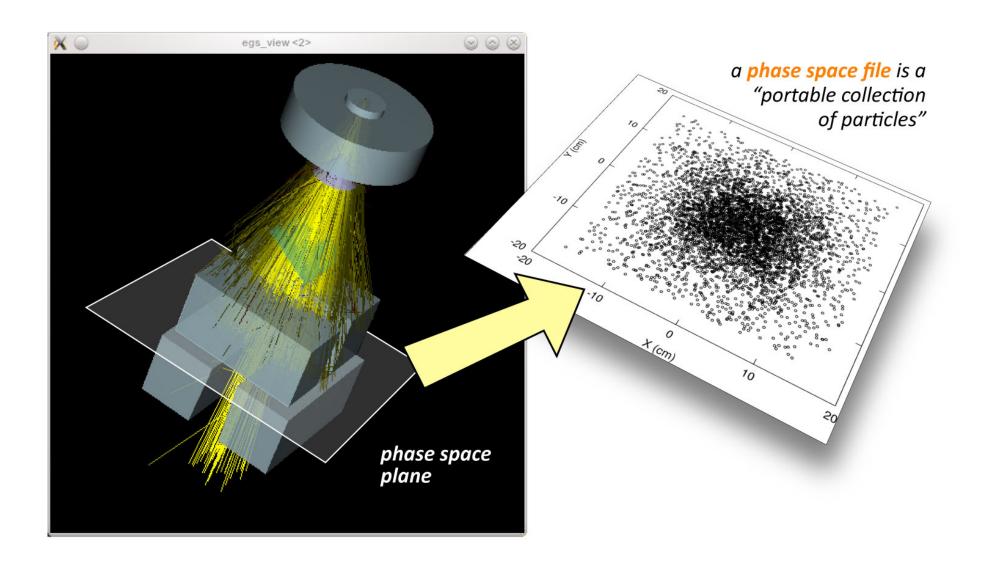




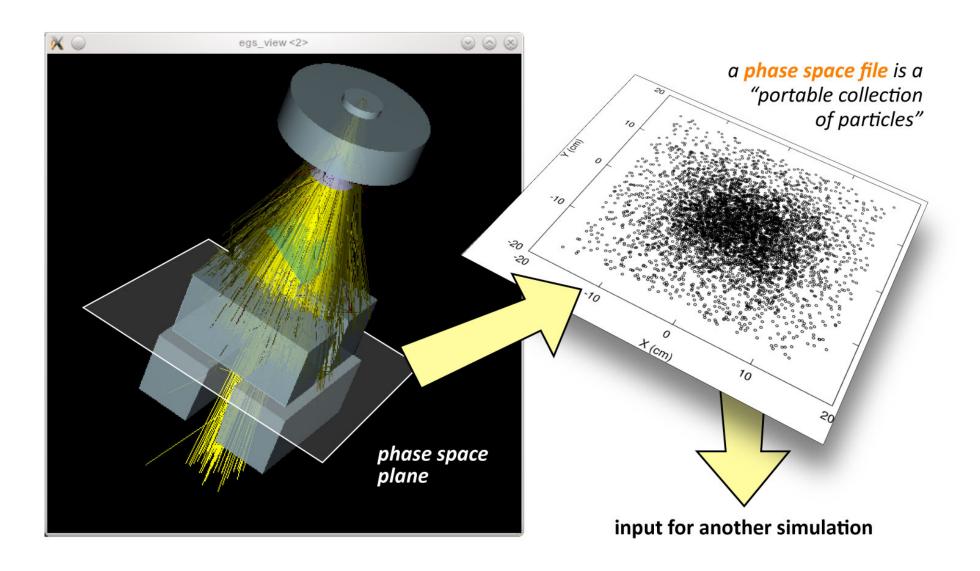
#### The BIG idea



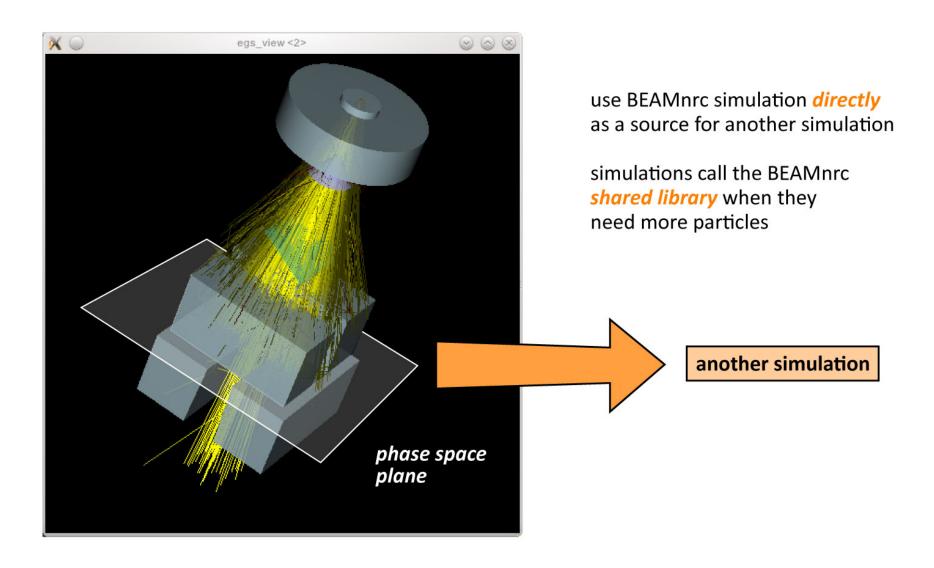
#### The BIG idea



#### The BIG idea

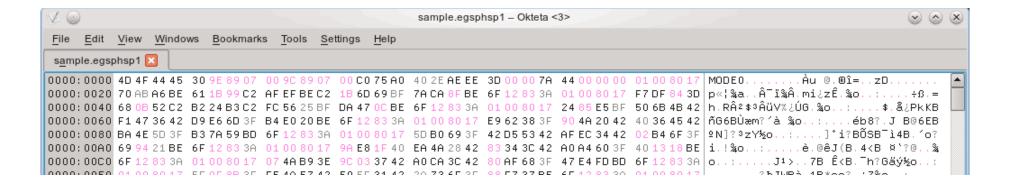


#### The BIGGER idea



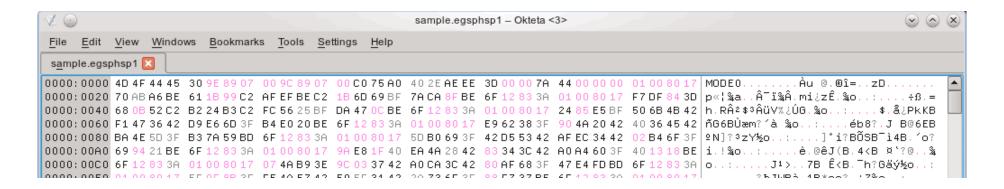
#### Phase space files contain particle data

#### **Binary format :-(**



#### Phase space files contain particle data

#### **Binary format :-(**

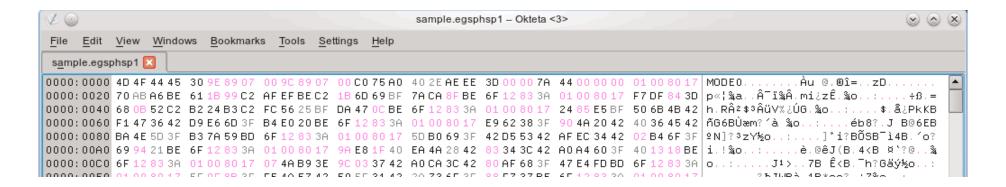


#### There is one phase space file for each scoring plane

```
inputfile.egsphsp#
where #=1,2,3,...
```

#### Phase space files contain particle data

#### **Binary format :-(**



#### There is one phase space file for each scoring plane

```
inputfile.egsphsp#
where #=1,2,3,...
```

#### Mind the file size!

Phase space files can rapidly grow to fill an entire hard drive. Test for a small number of histories in order to gauge the size of the phase space file for your final simulation.

#### A phase space file starts with a header

MODE\_RW MODE0 (no ZLAST) or MODE2 (with ZLAST)

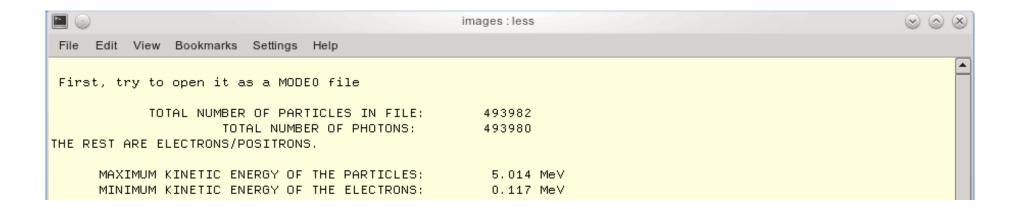
NPPHSP total number of particles in file

NPHOTPHSP total number of photons in file

**EKMAXPHSP** maximum kinetic energy of particles

**EKMINPHSPE** minimum kinetic energy of electrons

NINCPHSP number of particles incident from original source



#### A phase space file is a list of particles

#### For each particle

```
LATCHTMP [-]ESHORT X Y U V W WEIGHTTMP [ZLAST]
```

#### where:

LATCHTMP LATCH value, charge (bits 29-30) and NPASS (bit 31) ESHORT total energy; set negative for new history

X position along X axis (cm)

Y position along Y axis (cm)

U direction cosine with respect to X axis

V direction cosine with respect to Y axis

W direction cosine with respect to Z axis

WEIGHTTMP statistical weight of particle, and sign of direction along the Z axis

**ZLAST photons:** Z position of the last interaction;

**electrons:** Z position where electron or its ancestor was

set in motion by a photon

#### A phase space file is a list of particles

|   |             |                  |                  |           |                  |       | images : less          | 3     |   | ⊗ ⊘ ⊗ |
|---|-------------|------------------|------------------|-----------|------------------|-------|------------------------|-------|---|-------|
| File Edit   | t Viev      | w Bookn          | narks Sett       | ings Help | р                |       |                        |       |   |       |
|   |             |                  |                  |           |                  |       |                        |       |   | _     |
| First,  | try t       | o open           | it as a          | MODEO f   | ile              |       |                        |       |   |       |
|   |             |                  |                  |           |                  |       |                        |       |   |       |
|   | Т           | OTAL NU          | IMBER OF         |           |                  |       | 493982                 |       |   |       |
| TOTAL NUMBER OF PHOTONS: 493980   |             |                  |                  |           |                  |       |                        |       |   |       |
| THE REST  | ARE         | ELECTRO          | NS/POSI1         | TRONS.    |                  |       |                        |       |   |       |
| MO.   | V T bal iba |                  | C ENEDGY         | . OF TUE  | DARTIC           | I FO. | E 014                  | Mes / |   |       |
| MAXIMUM KINETIC ENERGY OF THE PARTICLES: 5.014 MeV MINIMUM KINETIC ENERGY OF THE ELECTRONS: 0.117 MeV |             |                  |                  |           |                  |       |                        |       |   |       |
|   |             |                  | CLES FRO         |           |                  |       | 1000.0                 |       |   |       |
|   |             |                  |                  |           |                  |       |                        |       |   |       |
| ENERGY  | IQ          | Х                | Y                | U         | V                | W     | WEIGHT                 | LATO  | CH (set=1, not set=0)                     |       |
|   |             |                  |                  |           |                  |       |                        |       |   |       |
| 0.326   |             |                  | -95.468          |           |                  |       | 1.000E-03              |       | 10000000000000000000001                   |       |
| 0.065   |             |                  | -89.572          |           |                  |       | 1.000E-03              |       | 10000000000000000000001                   |       |
| 1.793   |             | 50.855           | 45.570           |           | -0.157           |       | 1.000E-03              |       | 10000000000000000000001                   |       |
| 0.720   |             | 40.073           | 49.303           |           | -0.053           |       | 1.000E-03              |       | 1000000000000000000001                    |       |
| 0.913<br>2.499  | _           | 52.958<br>42.073 | 45.231<br>47.051 |           | -0.158<br>-0.149 |       | 1.000E-03<br>1.000E-03 |       | 1000000000000000000001<br>100000000000000 |       |
| 0.362   |             | 45.754           | 47.051           |           | -0.149           |       | 1.000E-03              |       | 100000000000000000000000000000000000000   |       |
| 1.086   |             | 53.823           | 44.344           |           | -0.124           |       | 1.000E-03              |       | 100000000000000000000000000000000000000   |       |
| 3.718   | _           | 46.349           | 47.150           |           | -0.123           |       | 1.000E-03              |       | 100000000000000000000000000000000000000   |       |
| 0.176   | 0           | 13.763           | 47.468           | -0.668    | -0.118           | 0.735 | 1.000E-03              | 10111 | 10000000000000000000000000001             |       |
| 1.735   | 0           | 46.113           | 75.410           | 0.660     | 0.695            | 0.285 | 1.000E-03              | 10111 | 1000000000000000000000000001              |       |
| 2.277   | 0           | 57.261           | 32.035           | 0.857     | -0.450           | 0.252 | 1.000E-03              |       | 100000000000000000000000000000000000000   |       |
| 1.012   |             | 41.756           | 46.688           |           | -0.166           |       | 1.000E-03              |       | 1000000000000000000000000001              |       |
| 0.157   |             | 28.377           | 44.695           |           | -0.450           |       | 1.000E-03              |       | 10000000000000000000001                   |       |
| 0.636   |             | 43.376           | 46.380           |           | -0.169           |       | 1.000E-03              |       | 1000000000000000000001                    |       |
| 0.628   |             | 38.449           | 43.908           |           | -0.321           |       | 1.000E-03              |       | 1000000000000000000001                    |       |
| 0.401<br>0.423  |             | 23.484<br>41.789 | 45.936<br>48.657 |           | -0.394<br>-0.079 |       | 1.000E-03<br>1.000E-03 |       | 10000000000000000000001<br>10000000000000 |       |
| 4 254   | 0           | 20 5/4           | 40.007           | 0.002     | 0.079            |       | 4 0005 00              | 10111 | 400000000000000000000000000000000000000   |       |

#### Changing where phase space files are written

**1.** Add the following input to your .egsinp file (either just before or just after the other EGSnrc inputs):

```
:start user inputs:
PHSP OUTPUT DIRECTORY= /full/path/to/new/output/directory
:stop user inputs:
```

2. To change the destination for phase space files globally, edit the file \$OMEGA\_HOME/beamnrc/beamnrc\_user\_macros and change the macro

```
REPLACE {$DIRECTORY-FOR-PHSP} WITH {$cstring(egs_home)//$cstring(user_code)};
```

to read

```
REPLACE {$DIRECTORY-FOR-PHSP} WITH {'/full/path/to/new/output/directory'};
```

Don't forget to recompile your accelerator(s) for this change to take effect!

#### **IAEA** format for phase space files





#### International Advisory Committee (IAC)

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Atomic and nuclear data for medical applications

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Nuclear Data Section

#### > IAEA NAHU/DMRP





#### IAEA NAPC Nuclear Data Section IAEA NAHU Dosimetry and Medical Radiation Physics Section

Project Officer: Roberto Capote

**Objective:** To build a database and disseminate representative <u>phase-space data</u> of accelerators and Co-60 units used in medical radiotherapy by compiling existing data that have been properly validated.

#### **NEWS**

#### **WE ARE WA**



How to produce and submit phase-space data: The IAEA phsp format was designed to cover both phase-space files and event generators (see <a href="https://px.nc.ntents">phsp contents</a>). We have implemented the IAEA phsp format in a set of <a href="read/write routines">read/write routines</a> (Updated: September 2013, see <a href="readme-file">readme-file</a>). Native IAEA phsp format is available in EGSnrc and PENELOPE Monte Carlo codes. Geant4 interface to use the native IAEA phsp format is also <a href="https://available">available</a>. Once the validated phsp data is produced and documentation is published, <a href="https://you.may.submit.your.phsp-for-review">your.phsp-for-review</a> using the <a



**How to download phase-space data:** You have to select a phsp data type among <u>Co-60 source</u>, <u>linac electron</u> or <u>linac photon</u> phsps. For photon and electron PHSPs you may download the header first to decide which data you want to retrieve. Once decided you should download the PHSP data from the corresponding sub-directory. Please note that the first time access to the selected subdirectory could be slow.



#### **IAEA** format for phase space files

- Can make use of the International Atomic Energy Agency (IAEA) online accelerator phase space database: www-nds.iaea.org/phsp/.
- More details on this format are given by Capote et al. in IAEA report INDC (NDS)-0484.
- In order to be able to read and write in IAEA phase space format, EGSnrc and BEAMnrc must be configured on a system with a working C++ compiler.
- If the system is properly configured, then the IAEA phase space handling routines are automatically compiled for you in the shared object

\$HEN\_HOUSE/egs++/dso/iaea\_phsp.so

#### The IAEA format specifies a separate header file

The **text format** . IAEAheader file contains:

```
$CHECKSUM size of phase space file.
```

**\$RECORD\_CONTENTS** description of data stored

**\$RECORD\_CONSTANT** values which are constant, e.g., Z of scoring plane for BEAMnrc

**\$RECORD\_LENGTH** size of each particle data record, in bytes

\$BYTE\_ORDER "1234" for little endian, "4321" for big endian

**\$ORIG\_HISTORIES** number of primary histories

**\$PARTICLES** total number of particles

\$PHOTONS number of photons

\$STATISTICAL\_INFORMATION\_PARTICLES stats for each particle type

\$STATISTICAL\_INFORMATION\_GEOMETRY min/max in X, min/max in Y

#### The IAEA format specifies a separate header file

```
images: less
 File Edit View Bookmarks Settings Help
$IAEA_INDEX:
     // Test header
1000
$TITLE:
PHASESPACE in IAEA format
$FILE_TYPE:
$CHECKSUM:
16296786
$RECORD_CONTENTS:
         // X is stored ?
        // Y is stored ?
       // Z is stored ?
         // U is stored ?
        // V is stored ?
         // W is stored ?
        // Weight is stored ?
       // Extra floats stored ?
        // Extra longs stored ?
        // Incremental history number stored in the extralong array [ 0]
         // LATCH EGS variable stored in the extralong array [ 1]
*RECORD_CONSTANT:
                // Constant Z
    -0.0000
*DECODD LENGTH:
```

#### The IAEA phase space is written in a data file

For each particle, the **binary format** . IAEAphsp data file contains:

```
type
         particle type, and sign of direction cosine with respect to Z
Ε
         KINETIC energy of the particle
X
         position along X axis (cm)
         position along Y axis (cm)
U
         direction cosine with respect to X axis
٧
         direction cosine with respect to Y axis
W
         direction cosine with respect to Z axis
WT
         statistical weight of particle
n_stat number of primary histories since previous particle scored
LATCH
         value of LATCH variable
ZLAST
         photons: Z position of the last interaction;
         electrons: Z position where electron was set in motion;
         This is only output if the input variable IZLAST=1
```

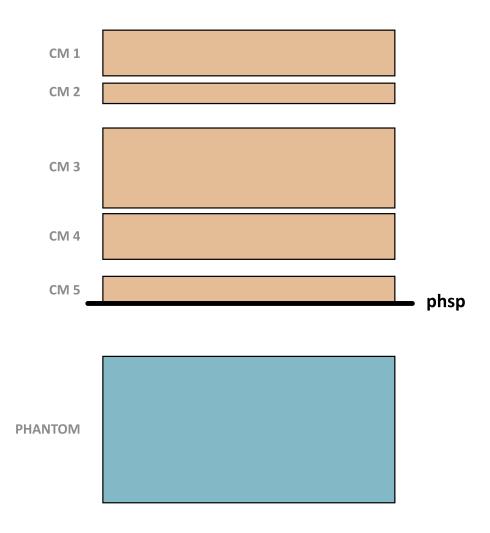
#### Reading and writing IAEA format phase space files

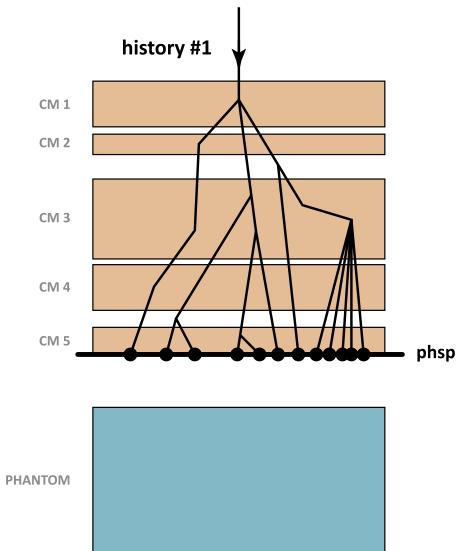
To write IAEA format phase space files from BEAMnrc:

- Set IO\_OPT=4
- Remember that there are **two** files generated for each scoring plane. The naming scheme
  is inputfile.#.IAEAheader and inputfile.#.IAEAphsp, where # is the scoring plane
  number.

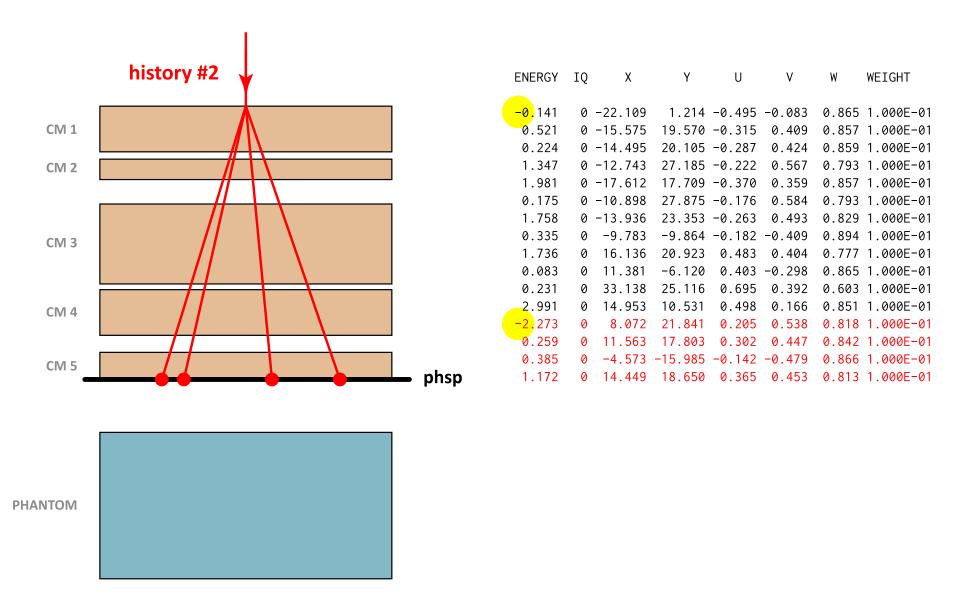
To read IAEA phase space files as sources in BEAMnrc, DOSXYZnrc and other EGSnrc applications:

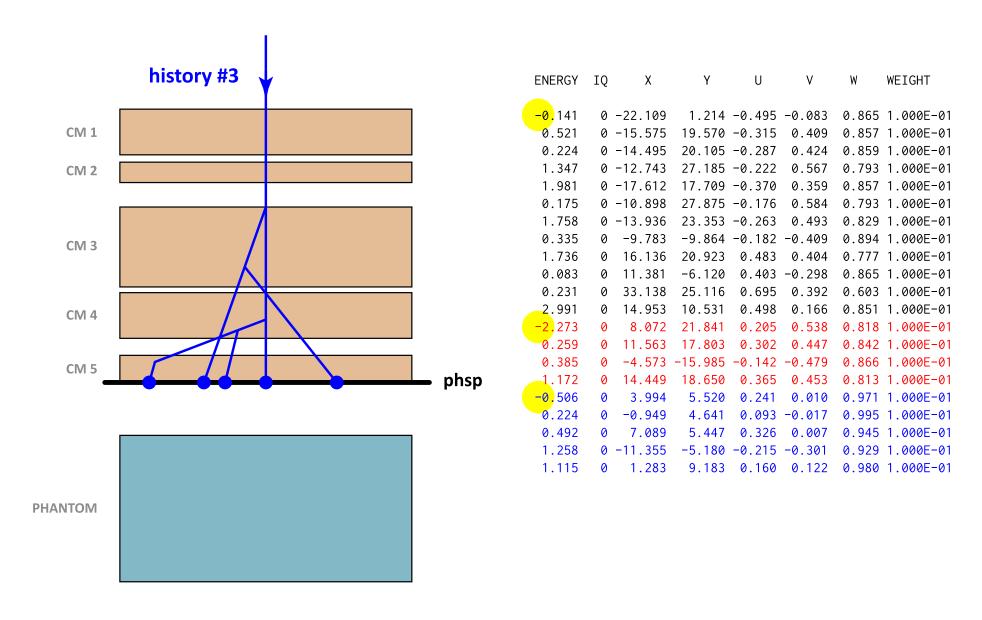
- Input full name of the data file, including the . IAEAphsp extension, and the code takes
  care of the rest.
- Note that the code assumes that the separate . IAEAheader file is in the same directory as the data file.

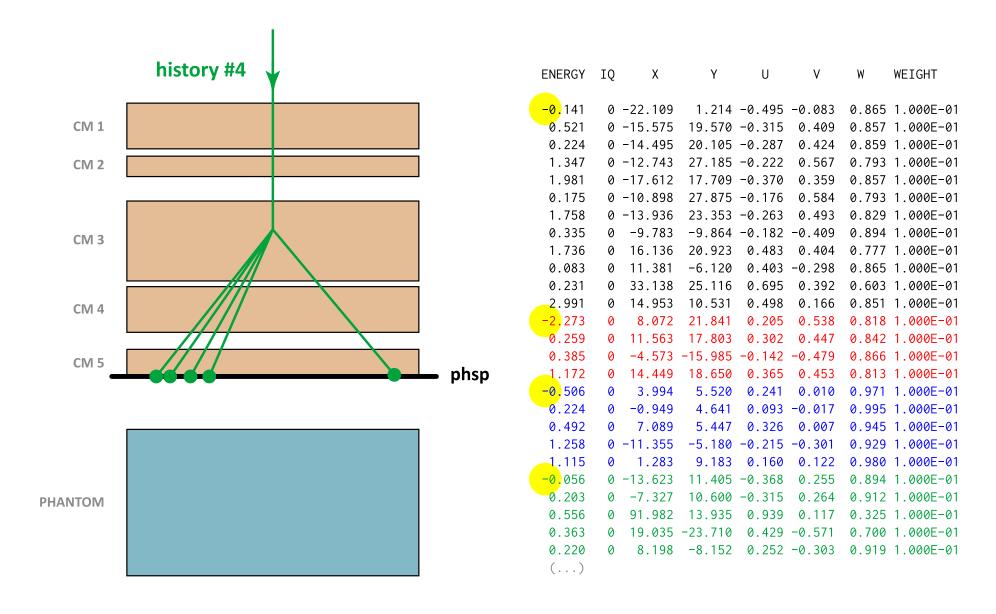


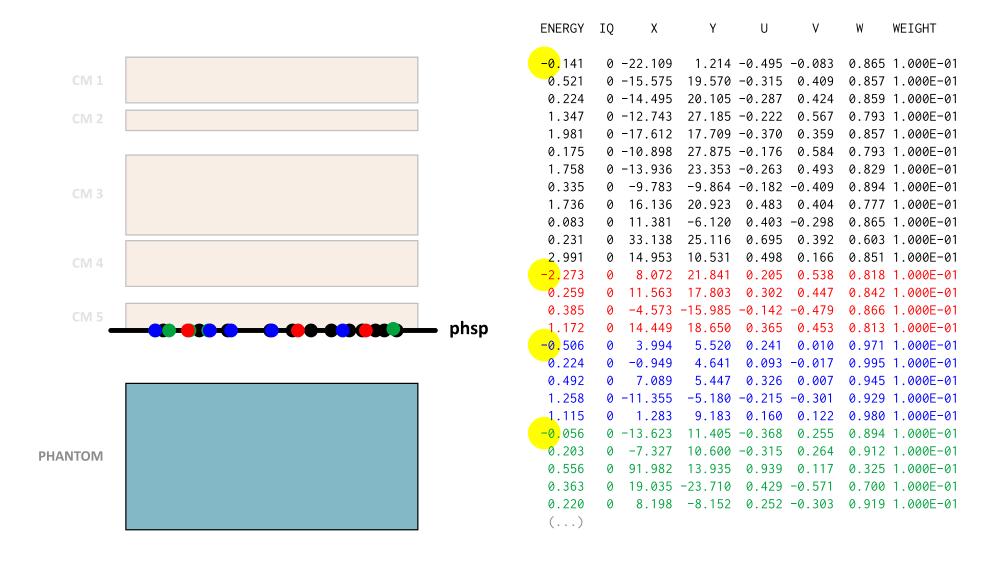


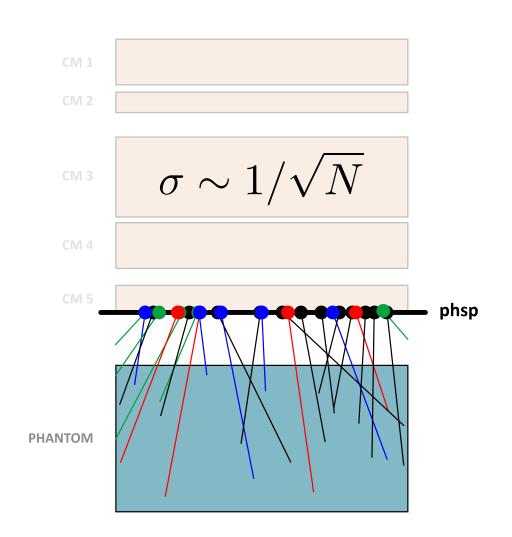
| ENERGY             | IQ | Χ       | Υ      | U      | V      | W     | WEIGHT    |
|--------------------|----|---------|--------|--------|--------|-------|-----------|
|                    |    |         |        |        |        |       |           |
| <del>-0.</del> 141 | 0  | -22.109 | 1.214  | -0.495 | -0.083 | 0.865 | 1.000E-01 |
| 0.521              | 0  | -15.575 | 19.570 | -0.315 | 0.409  | 0.857 | 1.000E-01 |
| 0.224              | 0  | -14.495 | 20.105 | -0.287 | 0.424  | 0.859 | 1.000E-01 |
| 1.347              | 0  | -12.743 | 27.185 | -0.222 | 0.567  | 0.793 | 1.000E-01 |
| 1.981              | 0  | -17.612 | 17.709 | -0.370 | 0.359  | 0.857 | 1.000E-01 |
| 0.175              | 0  | -10.898 | 27.875 | -0.176 | 0.584  | 0.793 | 1.000E-01 |
| 1.758              | 0  | -13.936 | 23.353 | -0.263 | 0.493  | 0.829 | 1.000E-01 |
| 0.335              | 0  | -9.783  | -9.864 | -0.182 | -0.409 | 0.894 | 1.000E-01 |
| 1.736              | 0  | 16.136  | 20.923 | 0.483  | 0.404  | 0.777 | 1.000E-01 |
| 0.083              | 0  | 11.381  | -6.120 | 0.403  | -0.298 | 0.865 | 1.000E-01 |
| 0.231              | 0  | 33.138  | 25.116 | 0.695  | 0.392  | 0.603 | 1.000E-01 |
| 2.991              | 0  | 14.953  | 10.531 | 0.498  | 0.166  | 0.851 | 1.000E-01 |



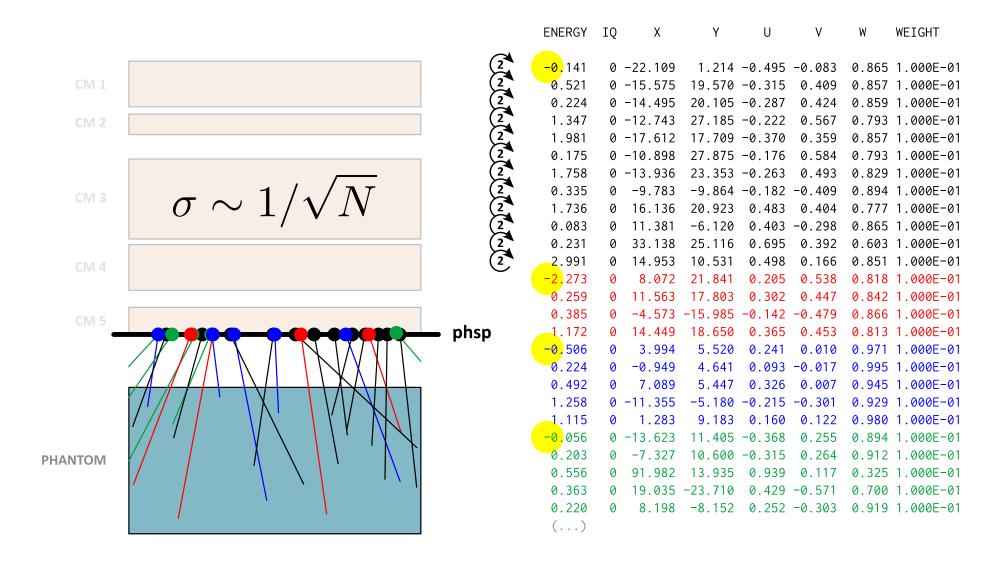


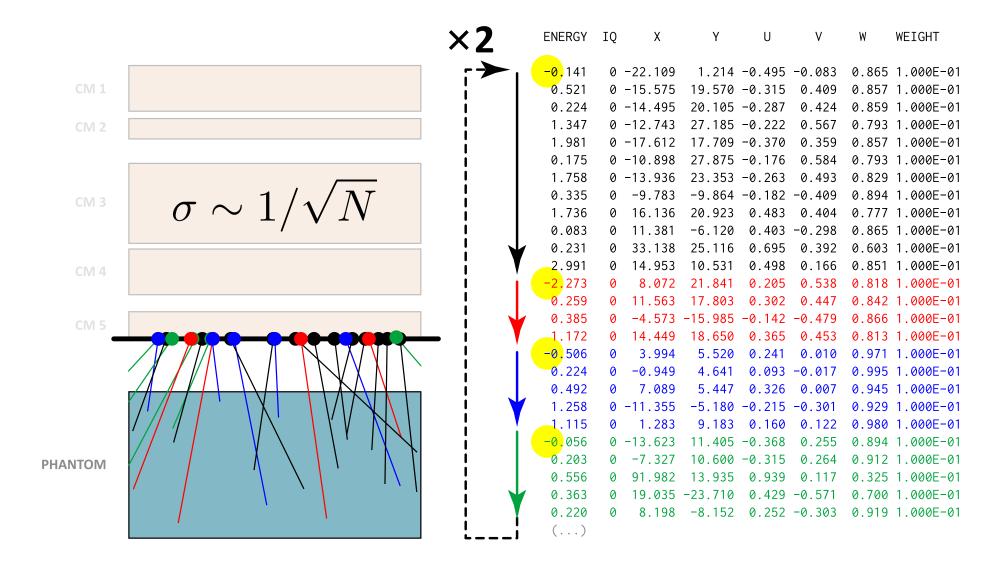






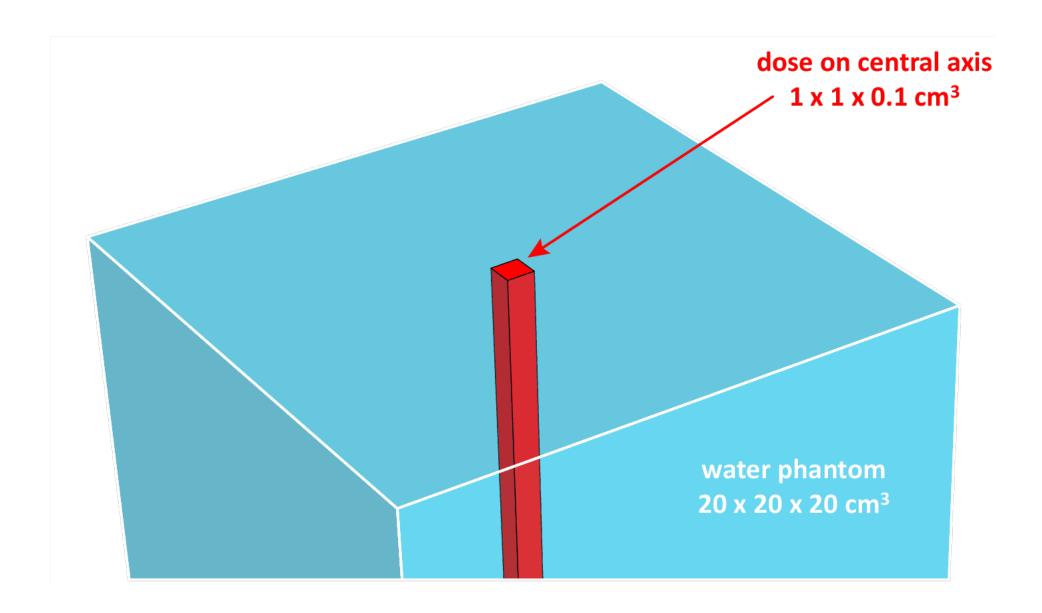
```
ENERGY IQ
                Χ
                        Υ
                               U
                                       ٧
                                                  WEIGHT
<del>-0</del>.141
          0 -22.109
                      1.214 -0.495 -0.083
                                            0.865 1.000E-01
 0.521
          0 -15.575
                     19.570 -0.315
                                     0.409
                                            0.857 1.000E-01
 0.224
          0 - 14.495
                     20.105 -0.287
                                     0.424
                                            0.859 1.000E-01
 1.347
          0 - 12.743
                     27.185 -0.222
                                     0.567
                                            0.793 1.000E-01
 1.981
          0 -17.612 17.709 -0.370
                                     0.359
                                            0.857 1.000E-01
 0.175
          0 - 10.898
                     27.875 -0.176
                                     0.584
                                            0.793 1.000E-01
 1.758
          0 -13.936
                     23.353 -0.263
                                     0.493
                                            0.829 1.000E-01
 0.335
            -9.783
                     -9.864 -0.182 -0.409
                                            0.894 1.000E-01
 1.736
          0 16.136
                     20.923
                            0.483
                                    0.404
                                            0.777 1.000E-01
 0.083
            11.381
                     -6.120
                             0.403 -0.298
                                            0.865 1.000E-01
 0.231
            33.138
                     25.116
                             0.695
                                     0.392
                                            0.603 1.000E-01
 2.991
            14.953
                     10.531
                             0.498
                                     0.166
                                            0.851 1.000E-01
-2.273
             8.072
                     21.841
                             0.205
                                     0.538
                                            0.818 1.000E-01
 0.259
            11.563
                    17.803
                            0.302
                                    0.447
                                            0.842 1.000E-01
 0.385
            -4.573 -15.985 -0.142 -0.479
                                            0.866 1.000E-01
 1.172
            14.449
                     18.650
                             0.365
                                     0.453
                                            0.813 1.000E-01
<del>-0.</del>506
             3.994
                      5.520
                             0.241
                                     0.010
                                            0.971 1.000E-01
 0.224
            -0.949
                      4.641
                             0.093
                                   -0.017
                                            0.995 1.000E-01
 0.492
             7.089
                             0.326
                                     0.007
                                            0.945 1.000E-01
                      5.447
 1.258
          0 -11.355
                     -5.180 -0.215 -0.301
                                            0.929 1.000E-01
 1.115
             1.283
                      9.183
                             0.160
                                     0.122
                                            0.980 1.000E-01
-0.056
                     11.405 -0.368
          0 - 13.623
                                    0.255
                                            0.894 1.000E-01
 0.203
            -7.327
                     10.600 -0.315
                                     0.264
                                            0.912 1.000E-01
                     13.935
 0.556
            91.982
                             0.939
                                     0.117
                                            0.325 1.000E-01
 0.363
            19.035 -23.710
                             0.429 - 0.571
                                            0.700 1.000E-01
 0.220
             8.198
                     -8.152 0.252 -0.303
                                            0.919 1.000E-01
 (...)
```

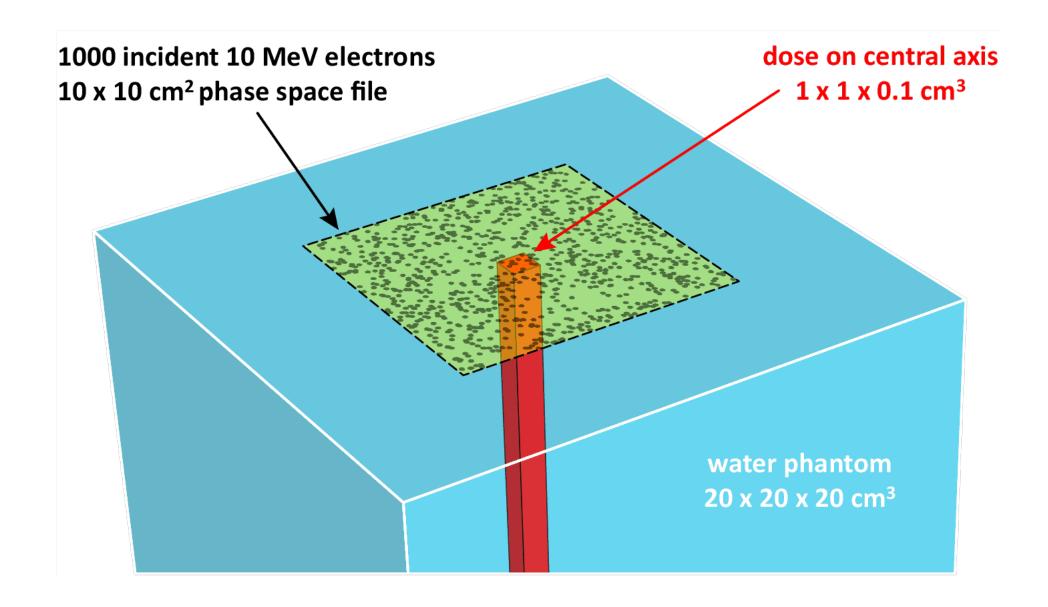


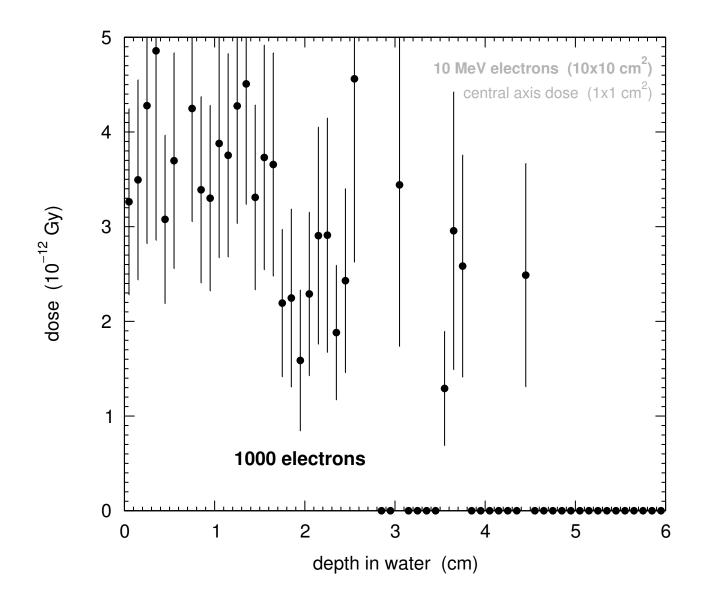


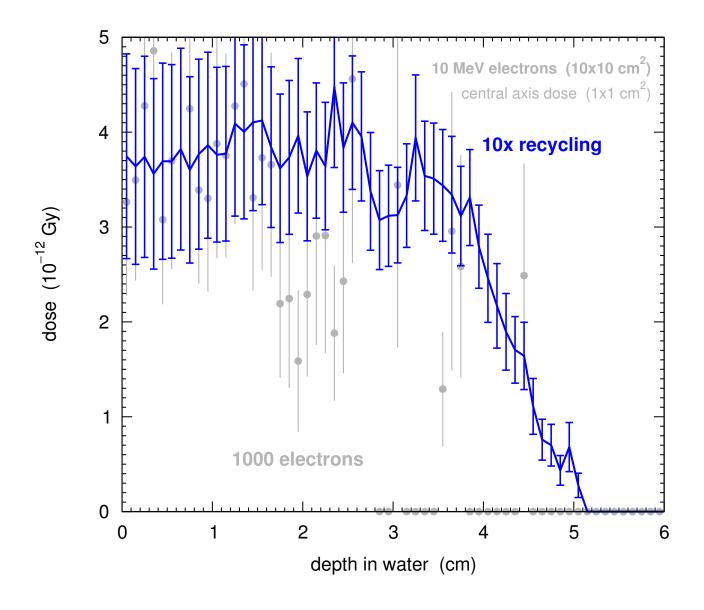
#### Executive summary (if you *must* reuse particles)

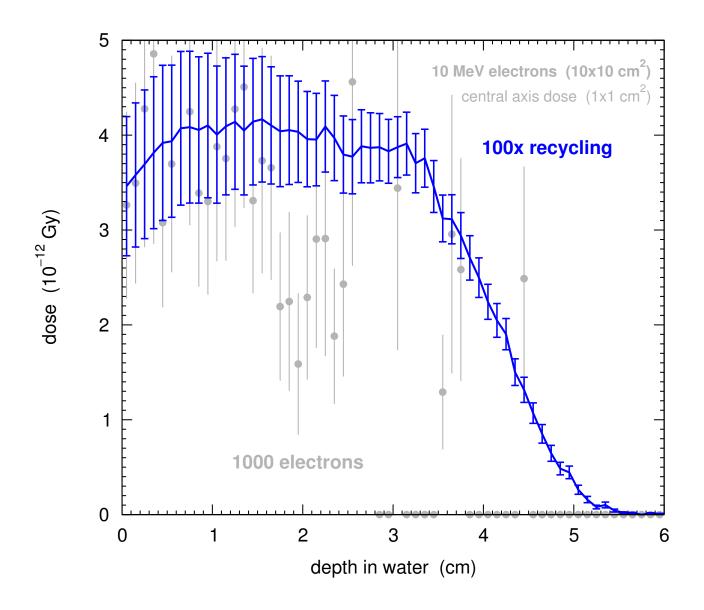
## Recycling is good Restarting is bad

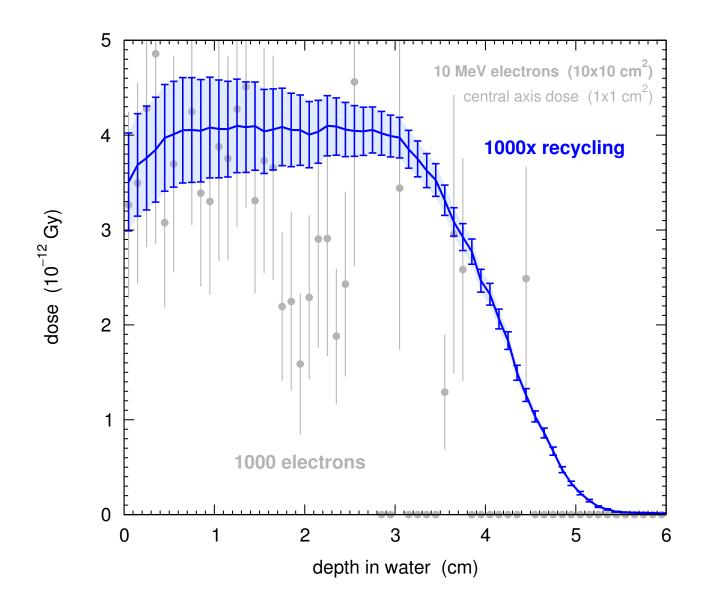


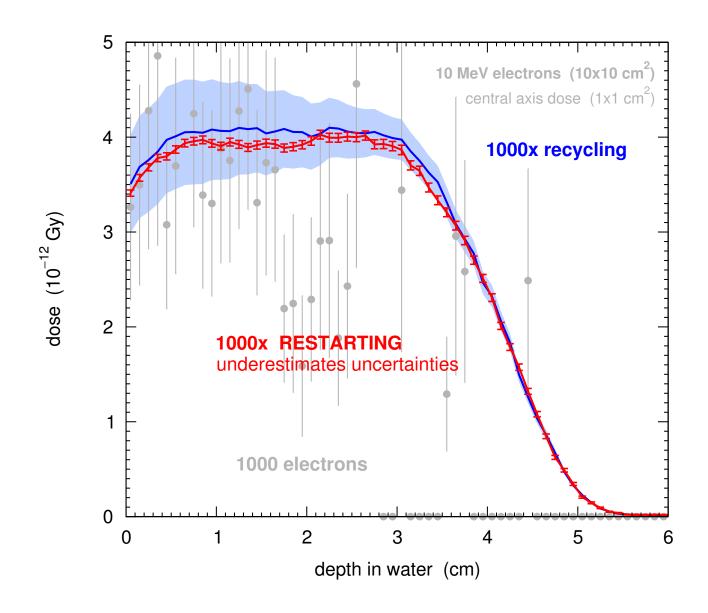


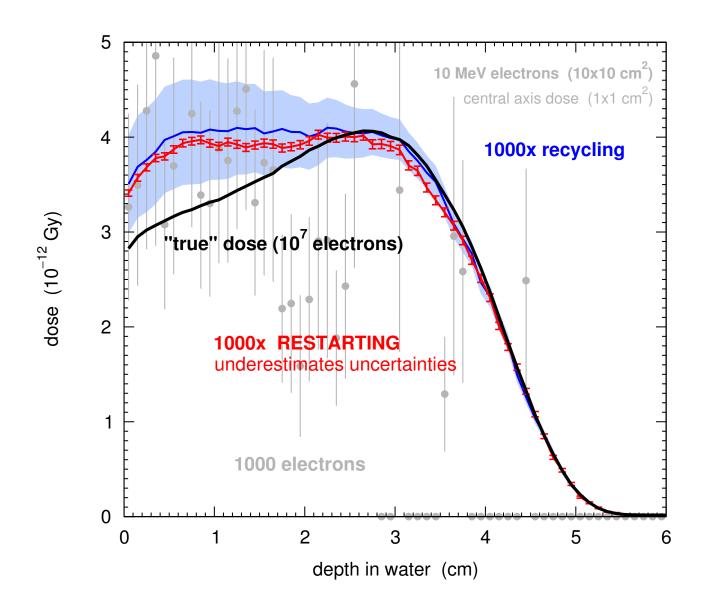












#### **Conclusion**

### Restarting: stop.

#### Conclusion

# Restarting: stop. Recycling: slow down...

#### Conclusion

# Restarting: stop. Recycling: slow down... More particles: go!