Joint ICTP-IAEA Workshop on Monte Carlo Radiation Transport and Associated Data Needs for Medical Applications
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Lecture 5

PEGS4 data sets, *"pegsless"* mode, and examin tool

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Data required by EGSnrc

- Total cross sections
- Differential cross sections
- Stopping powers
- Material information: density, mean ionization energy, atomic mass
- Binding energies
- Atomic relaxation data
- Coherent and incoherent scattering form factors
- Compton profiles
- Particle production thresholds (AE, AP)

Data files are located in folder `$HEN_HOUSE/data/`

PEGS4: Data Preprocessor for EGS4

- Stand-alone MORTRAN code developed to generate simulation data for EGS4 due to efficiency reasons
  (`It was the 70s and 80s!!!`)

- No significant changes for use with EGSnrc:
  - Improved I/O
  - Implicit none
  - Command line options

- Today, EGSnrc requires considerably more data than provided by PEGS4.

- EGSnrc does not rely on PEGS4 to obtain material specific data anymore as these are generated *on-the-fly*. However, the option to use PEGS4 data is still available.

- User can still use PEGS4 data sets.

Photon data

- Three photon cross section compilations are distributed with EGSnrc: Storm&Israel `(si)`, XCOM `(xcom)`, and EPDL `(epdl)`. XCOM is the default. Users can provide arbitrary photon cross section compilations.

- Compton profiles, occupation numbers Z_i and binding energies U_i for all elements (`incoh.data)`.

- Ratio of the bound Compton total cross section to the Klein-Nishina total cross section (`compton_sigma.data)`.

- Radiative Compton corrections (`rad_compton1.data`).

- Coherent scattering molecular form factors (`mff_*.data`) for 15 media.

- Atomic relaxation data (`photo_relax.data)` and elemental photoelectric cross sections (`photo_cs.data)`.

Electron data

- Pre-calculated screened Rutherford multiple elastic scattering data (`msnew.data`)
- Spin rejection data for multiple elastic scattering (`spinms.data`)
- Møller and Bhabha inelastic scattering cross sections for electron and positron
- EII cross sections (`eii_suffix.data` where `suffix` can be casnati, gryzinski, ik, kolbenstvedt, penelope or user-defined)
- Alternative bremsstrahlung cross sections to those by Koch and Motz:
  - NIST (`nist_brems.data`)
  - NRC (`nrc_brems.data`, `nrc_brems_ee.data`, `nrc_brems_en.data`)
- ICRU restricted stopping powers (NIST)

Recent additions:

- Re-normalized DHFS photoelectric cross sections by Sabbatucci and Salvat (`photo_shellwise.data`)
- Full EADL atomic relaxation data (`relax.data`)
- Arbitrary incoherent scattering cross sections (`*_compton.data`)
  - NIST XCOM incoherent cross sections by E. Ali (`xcom_compton.data`) providing a consistent use of the NIST XCOM cross sections in EGSnrc.
- Arbitrary photonuclear cross sections (`*_photonuc.data`)
  - IAEA photonuclear cross sections by E. Ali (`iaea_photonuc.data`) improving accuracy of photon cross sections.

Understanding AE, AP

AE, AP are the secondary particle production thresholds below which energy lost is deposited locally (restricted stopping powers), and this assumption must make sense, i.e.,

$$\text{Range of AE electrons} \ll \text{geometry scale}$$

$$\text{Range of AP photons} \ll \text{geometry scale}$$

The second condition is usually difficult to satisfy. If so, it is also sufficient that

$$\text{Energy lost to sub-AP photons} \ll \text{other energy loss}$$

Note that for the explicit simulation of the photon and electron transport no data is required below AE, AP.

Generally, when AE, AP $\downarrow$, accuracy $\uparrow$ and CPU time $\uparrow$

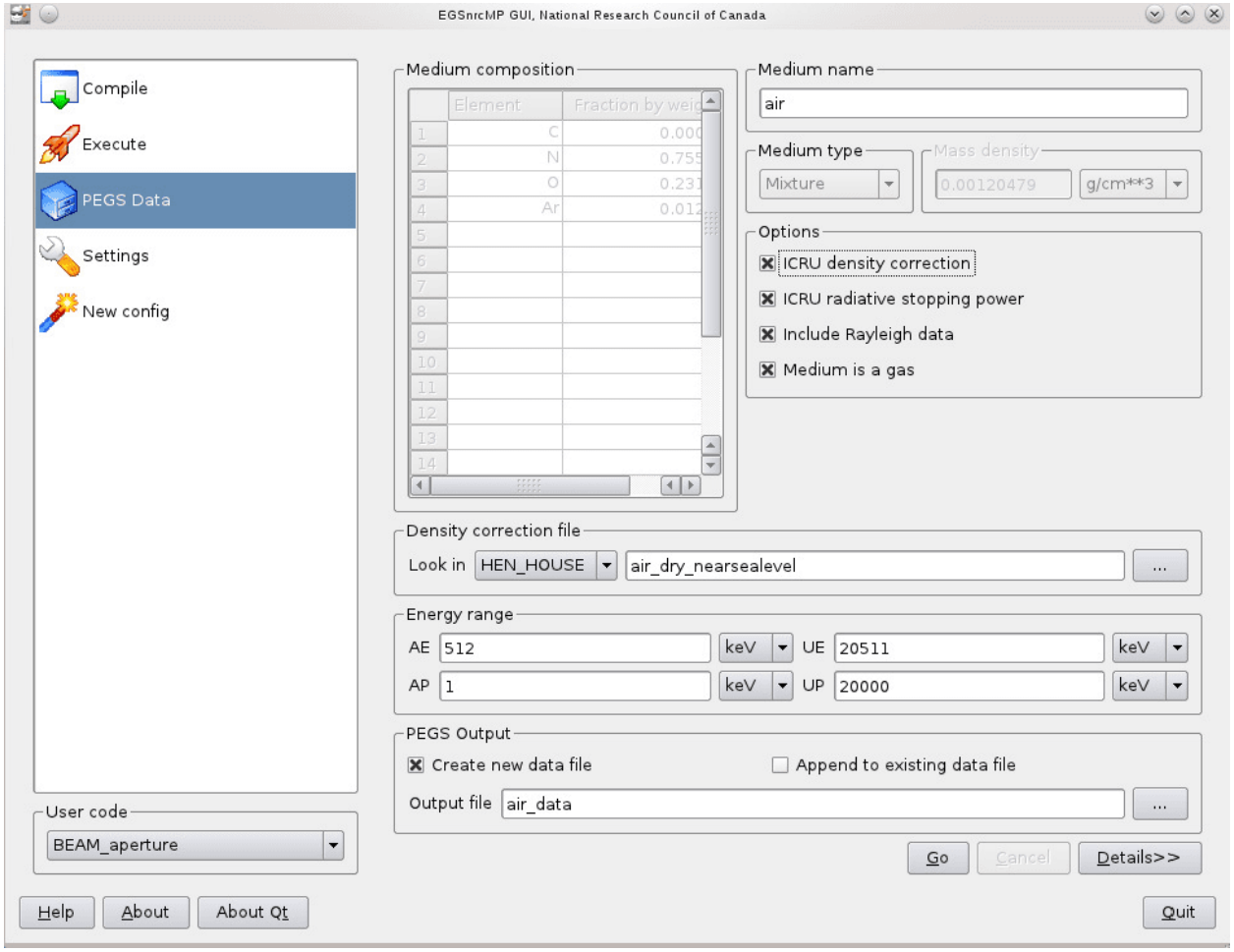
Running PEGS4 on the command line

Typing pegs4.exe -h or –help describes the different command line options:

```
pegs4.exe -i ifile [-o ofile] [-a] [-d density] [-x CrossSectData] [-e HEN_HOUSE]

 -i ifile         => ifile.pegs4inp is the input file
 -o ofile         => if present output file is
                     $EGS_HOME/pegs4/data/ofile.pegs4dat
                     & if not present output  is
                     $EGS_HOME/pegs4/data/ifile.pegs4dat
 -a               => if present that output is appended to
                     [i|o]file.pegs4dat
 -d density       => if present density effect is in
                     density.density
 -x CrossSectData => if present use
                     $HEN_HOUSE/pegs4/CrossSectData as
                     cross section file instead of
                     $HEN_HOUSE/pegs4/pgs4pepr.dat
 -e HEN_HOUSE     => if present store data on
                     $HEN_HOUSE/pegs4/data
                     rather than $EGS_HOME/pegs4/data
 -h or --help     => print this help screen
```

See PEGS4 manual in chapter 6 of PIRS-701 for more details.

Creating PEGS4 data sets using `egs_gui`



Use egs_gui: It is much simpler, and handles almost everything!!! (except IUNRST not equal zero)

The IUNRST options (in ENER namelist)

- `IUNRST = 0` default restricted radiative and collisional stropping powers and ‘normal’ mfp to electron interactions
- `IUNRST = 1` unrestricted collision stopping power.
- `IUNRST = 2` CSDA data set for CSDA calculation with all of the brem energy deposited locally. Stopping power is unrestricted total (collision + radiative) and distances to discrete electron interactions are infinite.
- `IUNRST = 3` CSDA calculation with brem interactions. Stopping powers are unrestricted collision plus restricted radiative stopping power. Distance to discrete interactions takes into account only brem events.
- `IUNRST = 4` CSDA calculation with delta-ray interactions. Stopping powers are restricted collision plus unrestricted radiative stopping powers. Distance to discrete interactions takes into account only creation of knock-on electrons.
- `IUNRST = 5` unrestricted radiative stopping power for comparison to published radiative stopping powers.
- `IUNRST = 6` restricted radiative stopping power.
- `IUNRST = 7` restricted collision stopping powers.

PEGS4less mode

- Since the 2013 release, EGSnrc can be used in “pegsless” mode thanks to Blake Walters.
- No PEGS4 file needed to obtain material specific data. These are generated *on-the-fly*.
- Materials can be defined in the input file or in a general material file. In the latter case the name of the material definition file must be provided in the input file.
- The information required is similar to the one provided to PEGS4 such as particle production thresholds, material composition, density, *etc*.
- Described in chapter 7 of PIRS-701

Media definition via a general material file

```
:start media definition:

    AE=0.521
    UE=50.511
    AP=0.01
    UP=50.

    # If all required media in the file below, nothing else needed

    material data file=/home/username/HEN_HOUSE/pegs4/data/material.dat

:stop media definition:
```

Material file format

```
...
medium=170C521ICRU
rho=1.7
elements=C
number of atoms=1
bremsstrahlung correction=NRC
density correction file= carbon_graphite_1.700g_cm3

medium=H2O521ICRU
rho=1.0
elements=H,O
number of atoms=2,1
bremsstrahlung correction=NRC
density correction file= water_liquid
...
medium=ICRPBONE521ICRU
rho=1.85
elements=H,C,N,O,MG,P,S,CA,ZN
mass fractions=4.72340E-02,1.44330E-01,4.19900E-02,4.46096E-01,2.20000E-03,
               1.04970E-01,3.15000E-03,2.09930E-01,1.00000E-04
bremsstrahlung correction=NRC
density correction file= bone_cortical_icrp
...
```

Input file syntax for elements and compounds

```
:start media definition:
    AE=0.521
    UE=50.511
    AP=0.01
    UP=50.

    # Medium name is case sensitive:
    # H2O521ICRU is different than h2o521ICRU
    :start H2O521ICRU:
        elements=H,O
        number of atoms=2,1
        rho=1.0
    :stop H2O521ICRU:
    ...
    :start another:
      ...
    :stop another:
:stop media definition:
```

Input file syntax for mixtures

```
:start media definition:
    AE=0.521
    UE=50.511
    AP=0.01
    UP=50.

    :start AIR521ICRU:
        elements=C,N,O,AR
        mass fractions=1.24000E-04,7.55200E-01,2.31800E-01,1.28300E-02
        rho=1.2048E-03
        gas pressure = 1.0
    :stop AIR521ICRU:
    ...
    :start another:
      ...
    :stop another:
:stop media definition:
```

Input file syntax: further options

```
:start media definition:
    AE=0.521
    UE=50.511
    AP=0.01
    UP=50.
    :start H2O521ICRU:
        elements=H,O
        number of atoms=2,1
        rho=1.0
        stopping powers=restricted total # IUNRST
        bremsstrahlung correction=NRC    # IAPRIM
        density correction file=water_liquid
    :stop H2O521ICRU:
    ...
    :start another:
      ...
    :stop another:
:stop media definition:
```

Medium definition via density correction file

```
:start media definition:
    AE=0.521
    UE=50.511
    AP=0.01
    UP=50.

    :start H2O521ICRU:
        density correction file=water_liquid
    :stop H2O521ICRU:

    :start AIR521ICRU:
        density correction file= air_dry_nearsealevel
    :stop AIR521ICRU:
    ...
    :start another:
      ...
    :stop another:
:stop media definition:
```

Combining media from material and input file

```
:start media definition:
    AE=0.521
    UE=50.511
    AP=0.01
    UP=50.

    # If all required media in the file below, nothing else needed
    material data file=/home/username/HEN_HOUSE/pegs4/data/material.dat

    # Define new media below or modify media in material.dat
    # Medium name is case sensitive:
    # H2O521ICRU is different than h2o521ICRU
    :start H2O521ICRU:
        elements=H,O
        number of atoms=2,1
        rho=1.0
    :stop H2O521ICRU:
    ...
    :start another:
      ...
    :stop another:
:stop media definition:
```

Pegsless execution from the command line

- Running application app interactively

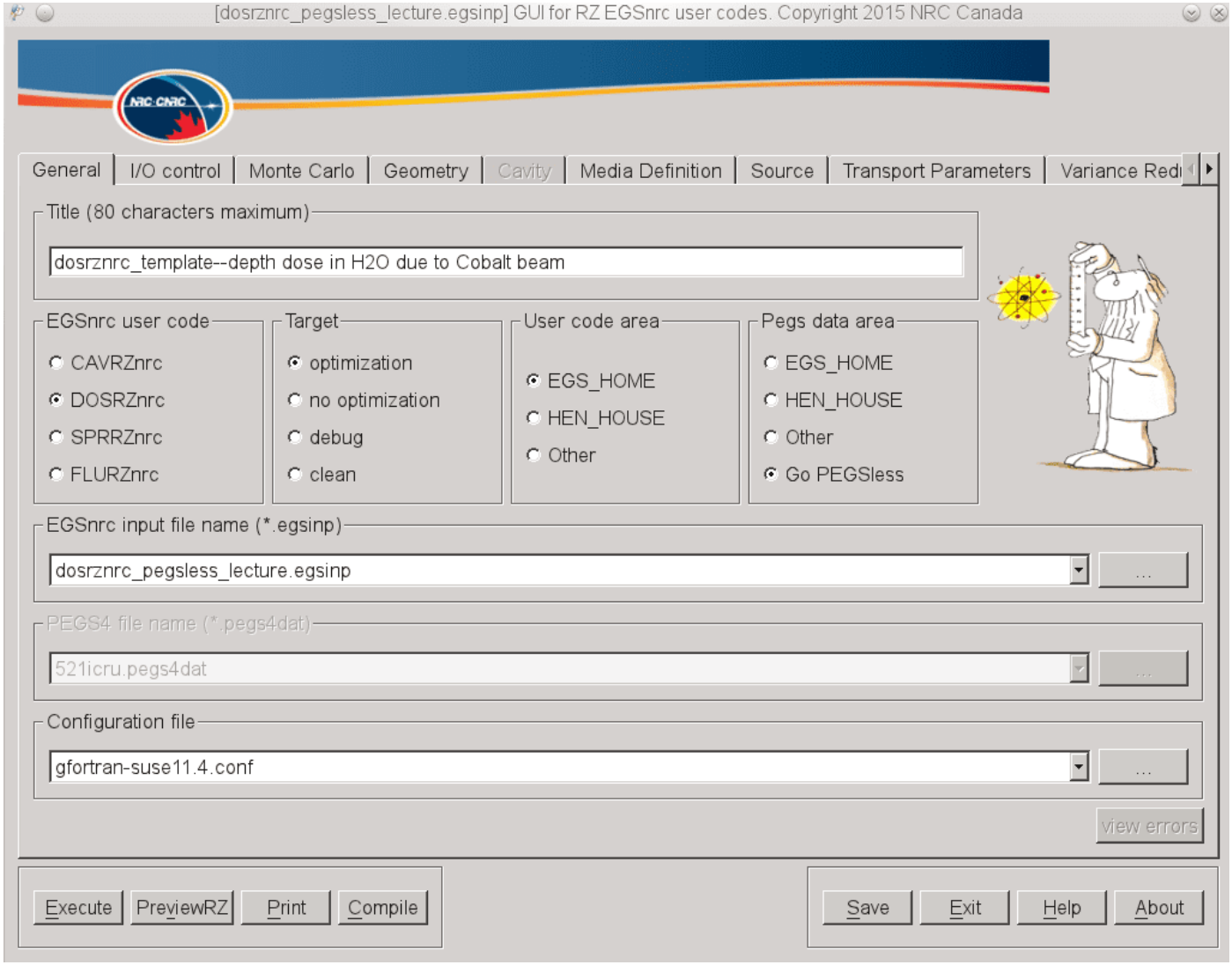
  ```
  $ app -i input_file
  ```

- Script for parallel execution requires `pegsless` keyword instead of a pegs4 file name:

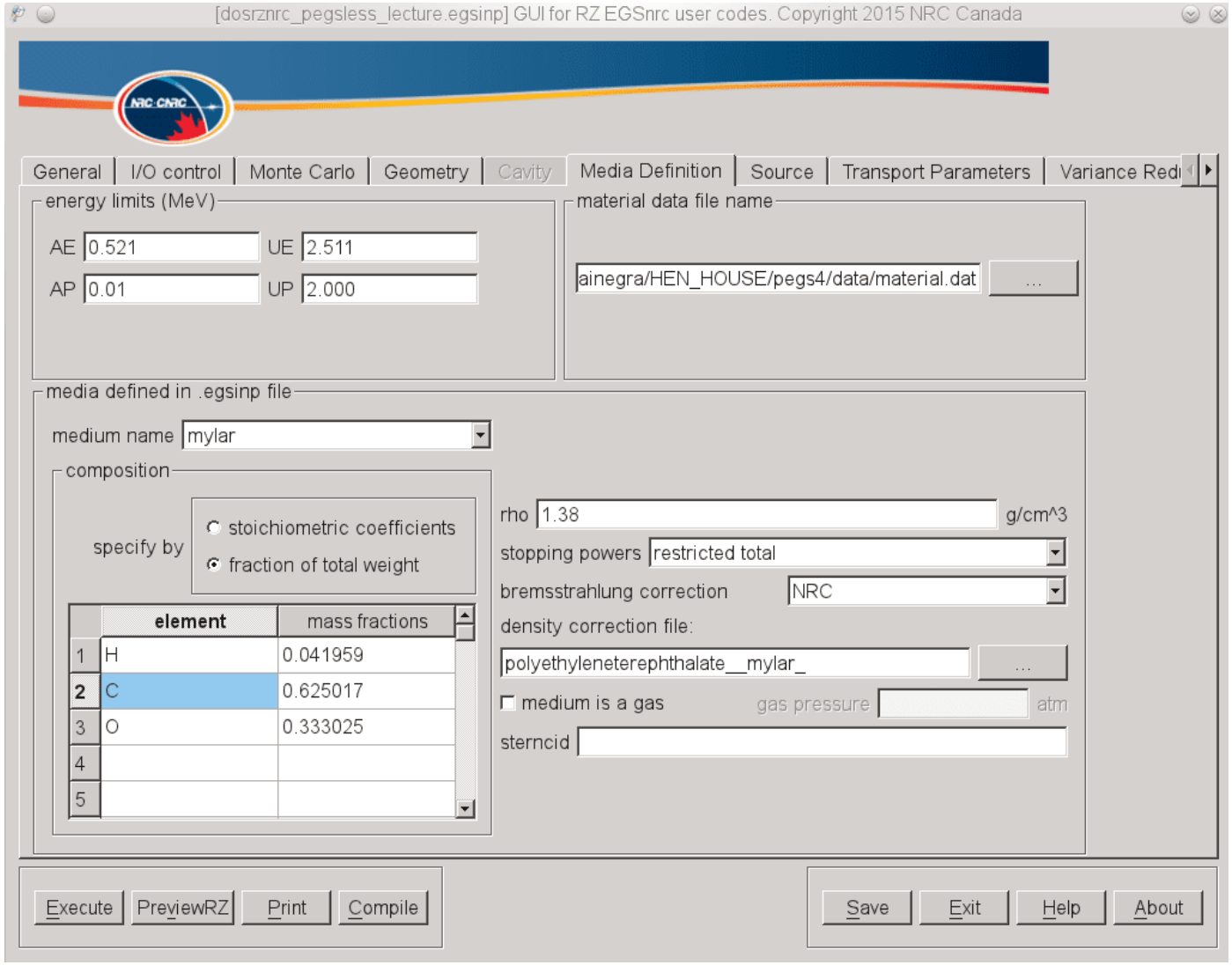
  ```
  $ exb app input_file pegsless [queue] ...
  ```

  where exb is an alias to `$HEN_HOUSE/scripts/run_user_code_batch`

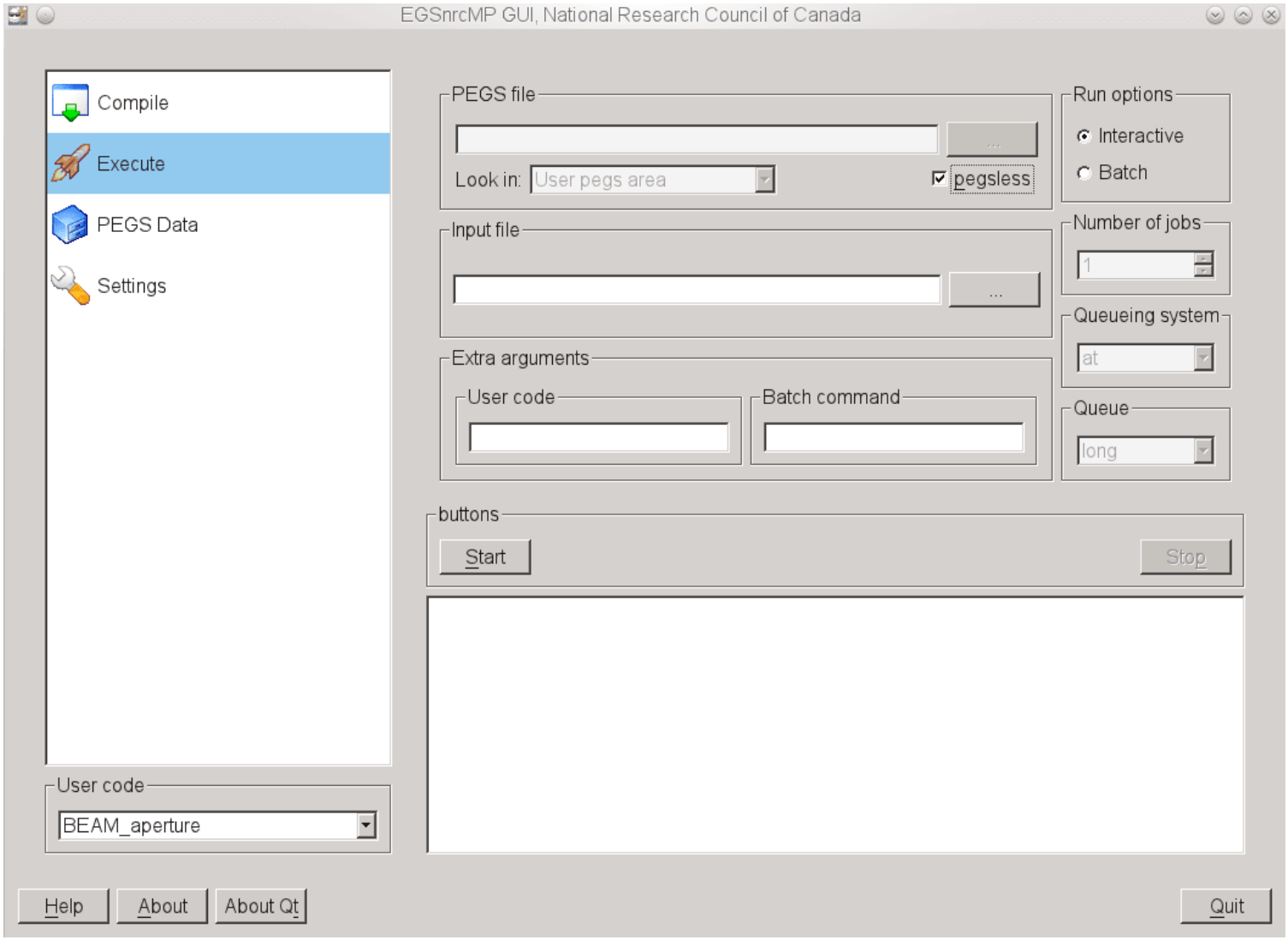
Pegsless mode from the `egs_inprz` GUI



Defining media from the `egs_inprz` GUI



PEGS4less mode from the `egs_gui` GUI



EXAMIN

- `examin` is an EGSnrc application which allows the user to examine the main cross sections used by EGSnrc. It allows various options regarding output, including a graphical output.

- Using `examin` requires a PEGS4 data file.

- Provides a working example of how to extract the cross sections from EGSnrc if you need them for your own purposes.

- Can be used on Windows if the macros `$Call_xvgr` and `$list_pegs4_media` are reset to their null versions. In this case graphical output is disabled and no listing of PEGS4 media will be available during execution.

Example use of EXAMIN

```
~/production/egs_home/examin @develop]$ examin -p tutor_data -o water_xcom_p_e
================================================================================
EGSnrc version 4 for linux64                          Wed May 18 19:28:40 2016
================================================================================
configuration.....................................linux64
user code.........................................examin
pegs file.........................................tutor_data on HEN_HOUSE
using host........................................irs15
output file(s)....................................water_xcom_p_e
================================================================================
 Media available in this data file are:
 MEDIUM=TA                      ,STERNCID=TA
 MEDIUM=NAI                     ,STERNCID=NAI
 MEDIUM=SI                      ,STERNCID=SI
 MEDIUM=H2O                     ,STERNCID=H2O
 MEDIUM=GE                      ,STERNCID=GE
 MEDIUM=PB                      ,STERNCID=PB
 Material identifier: H2O
 Title after  H2O                Example for EGSnrc course at Health Canada

 Electrons and photons(0), only electrons(1) or photons(2): 0
 Select photon cross section data base!
 ENTER defaults to: xcom
 Photon xsections [si, xcom, epdl, pegs4, user-defined]:
 Include Rayleigh(coherent)scattering(1) or not(0): 1
 Compton xsections (default, xcom, user-defined) [default]:xcom
 Include bound Compton(1) or not(0): 1
 Include radiative Compton corrections(1) or not(0): 1
```

Example use of EXAMIN (cont'd)

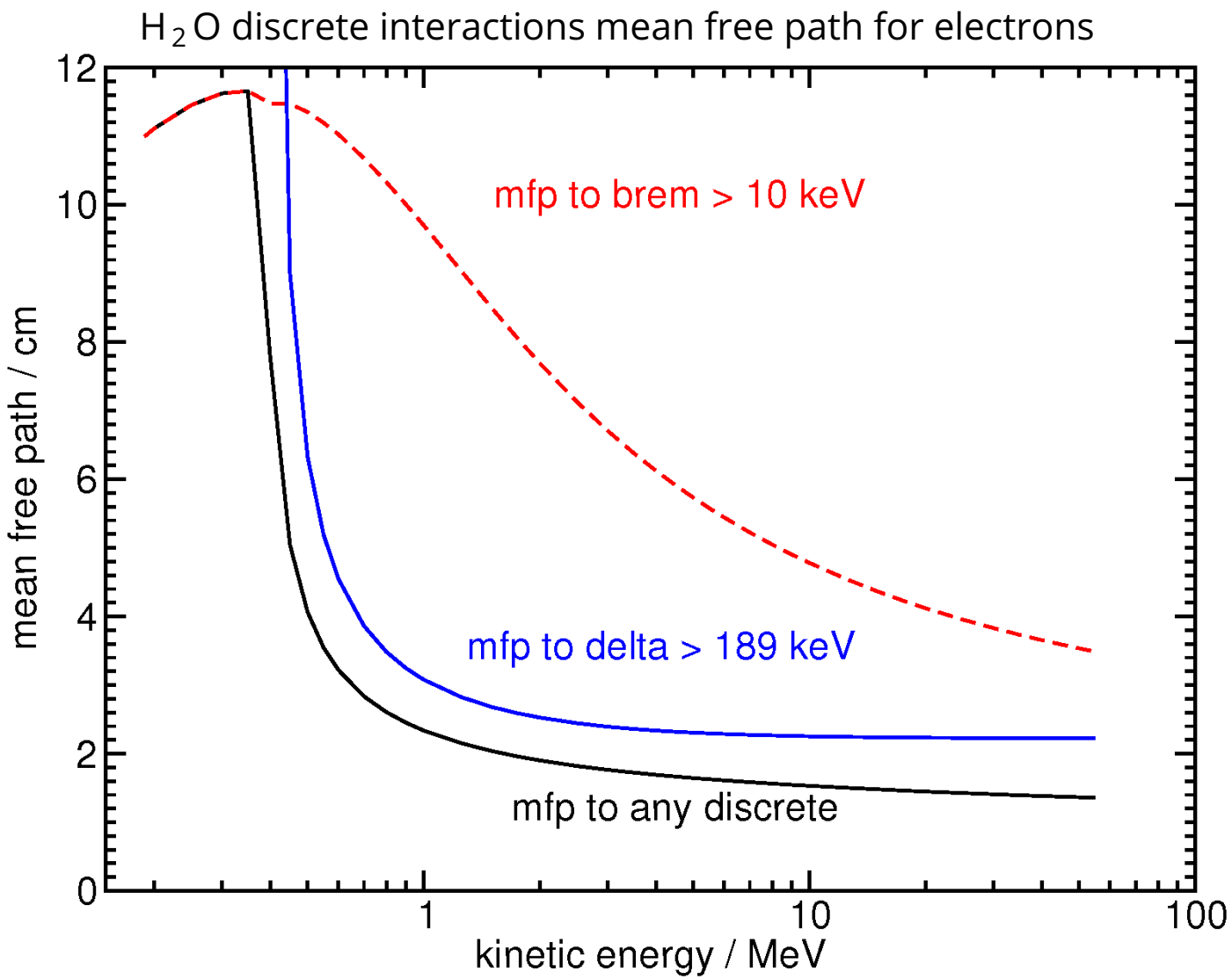
```
 Call HATCH
 RAYLEIGH OPTION REQUESTED FOR MEDIUM NUMBER  1

 Rayleigh data available for medium  1 in PEGS4 data set.

(Re)-initializing photon cross section data
Using data files from the series xcom

Photon cross sections: xcom Compton cross sections: xcom
Using Compton cross sections from /home/mainegra/production/HEN_HOUSE/data/xcom_compton.data

Working on medium   1 ...  \n  ->          100  atomic ff values computed!
      preparing data for Rayleigh sampling ... done
OK
Reading screened Rutherford MS data ..............  done
Bound Compton scattering requested, reading data ......  Done
Reading photo-absorption data ..... Done
Reading relaxation data ..... Done
Reading photo cross section data ..... Done

Reading EADL relaxation data ......
-> Element Z =   1 has  1 shells
-> Element Z =   8 has  4 shells
...... Done.

EGSnrc SUCCESSFULLY 'HATCHED' FOR ONE MEDIUM.
Call to HATCH completed
```

Outputs from EXAMIN

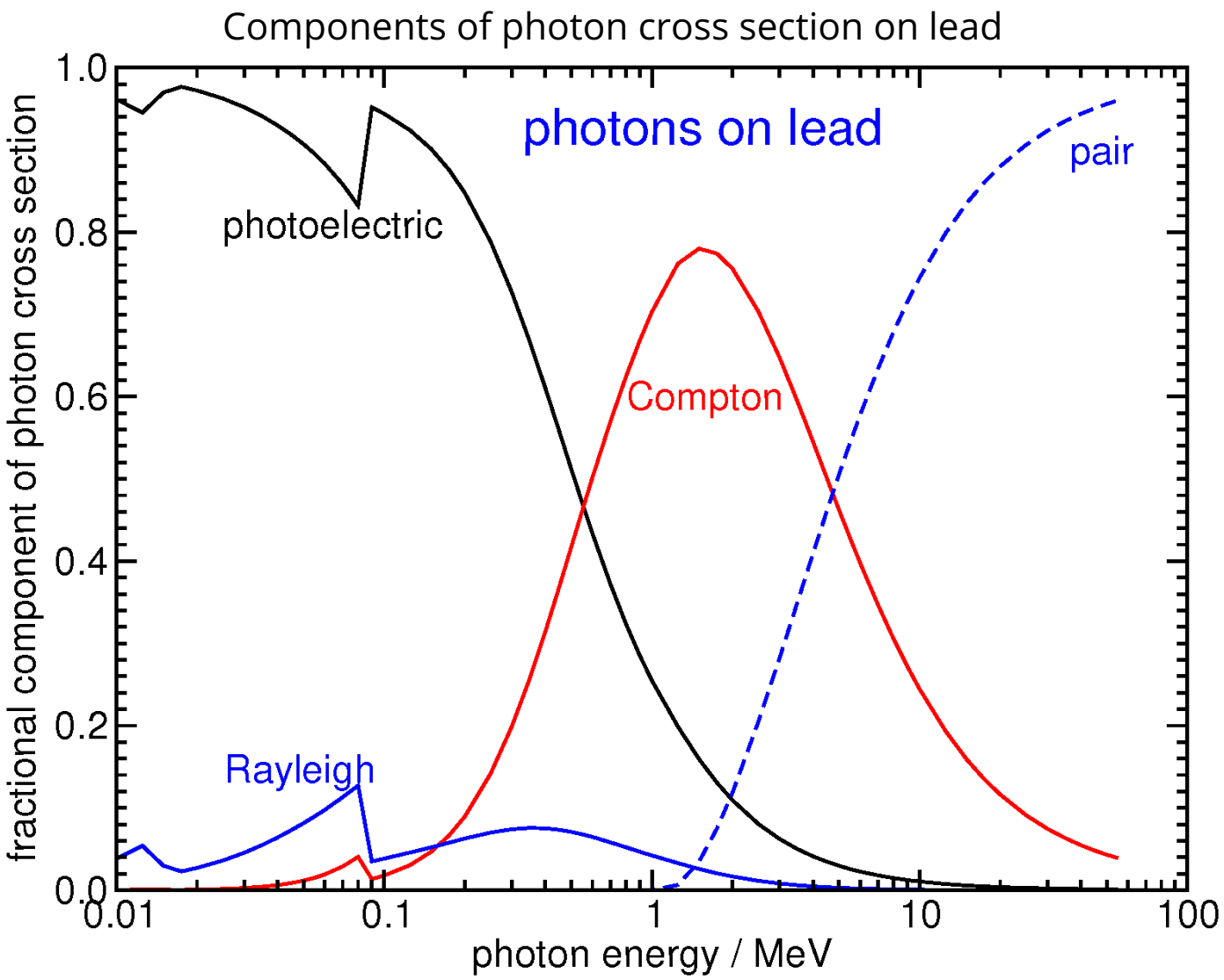
The run on the previous page produces two types of output on area `$EGS_HOME/examin` :

- During the run it interactively creates `xmgrace` graphs if the plot option is selected.
- The second output is a file called `output_file.examin`
  (In this case `water_xcom_p_e.examin` since we used the output option
  `-o water_xcom_p_e`) which tabulates electron and photon cross sections.

EXAMIN graphical output for xmgrace



EXAMIN graphical output for xmgrace



EXAMIN output: Photon data

```
Summary of photon data: MEDIUM = H2O        Title= Example for EGSnrc course at Health Canada
Wed May 18 19:34:34 2016
 ============================================================================

 Electron kinetic energy range:          0.189      50.000 MeV
 Photon energy range:                    0.010      50.000 MeV

 Radiation length =                   36.086300 cm
 Density =                             1.000000 g/cm**3
 Photon data set: xcom (absolute components)
 Incoherent scatter data: xcom
 Will print .xsections file
```

Photon En	GMFP (cm)	Rayleigh cm**2/g	Photoelec cm**2/g	Compton cm**2/g	Pair cm**2/g	Total cm**2/g	cm**-1
1.000E-02	1.876E-01	2.305E-01	4.944E+00	1.549E-01	0.000E+00	5.329E+00	5.3297E+00
1.250E-02	3.597E-01	1.708E-01	2.445E+00	1.638E-01	0.000E+00	2.779E+00	2.7799E+00
1.500E-02	5.979E-01	1.332E-01	1.369E+00	1.699E-01	0.000E+00	1.672E+00	1.6724E+00
1.750E-02	8.949E-01	1.074E-01	8.358E-01	1.741E-01	0.000E+00	1.117E+00	1.1174E+00
2.000E-02	1.234E+00	8.855E-02	5.438E-01	1.772E-01	0.000E+00	8.097E-01	8.0974E-01
2.500E-02	1.967E+00	6.298E-02	2.639E-01	1.811E-01	0.000E+00	5.081E-01	5.0813E-01
3.000E-02	2.662E+00	4.698E-02	1.457E-01	1.827E-01	0.000E+00	3.755E-01	3.7552E-01
3.500E-02	3.253E+00	3.624E-02	8.796E-02	1.831E-01	0.000E+00	3.073E-01	3.0737E-01
4.000E-02	3.727E+00	2.877E-02	5.679E-02	1.827E-01	0.000E+00	2.682E-01	2.6828E-01

EXAMIN output: Electron data

```
Summary electron data: MEDIUM=H2O        Title:Example for EGSnrc course at H
Wed May 18 19:34:34 2016
 ================================================================================
 Electron kinetic energy range:          0.189      50.000 MeV
 Photon energy range:                    0.010      50.000 MeV

 Radiation length =                   36.086300 cm
 DENSITY =                             1.000000 g/cm**3
 200.*TEFFO =                          0.531838 cm

 Koch and Motz radiative stopping
 Standard PEGS4 density effect for collision stopping
 Standard PEGS4 data set (restricted collision + radiative (IUNRST=0))

 FIXTMX HAS ALTERED THE STEP SIZES USING ESTEPE=   0.250

 Kin En     e(-),     e(+) dE/drhoX  e(-),e(+) Mean free path (brem fraction)
    MeV         MeV/(g/cm**2)                          cm
    0.189    2.8710       2.9222    1.103E+01 (1.00000)   4.838E+00 (0.43849)
    0.200    2.7936       2.8346    1.086E+01 (1.00000)   4.456E+00 (0.41050)
    0.250    2.5285       2.5351    1.019E+01 (1.00000)   3.621E+00 (0.35536)
    0.300    2.3553       2.3391    9.680E+00 (1.00000)   3.282E+00 (0.33903)
    0.350    2.2351       2.2023    9.267E+00 (1.00000)   3.086E+00 (0.33301)
    0.400    2.1402       2.1026    6.479E+00 (0.73147)   2.951E+00 (0.33067)
    0.450    2.0608       2.0273    4.401E+00 (0.51086)   2.847E+00 (0.32983)
    0.500    2.0001       1.9692    3.603E+00 (0.43038)   2.762E+00 (0.32967)
    0.550    1.9492       1.9201    3.171E+00 (0.38889)   2.690E+00 (0.32981)
```

Some notes on EXAMIN output

- The electron cross-sections vary with AE and AP but the photon cross sections are independent of these values.
- One could get PEGS4 to generate the unrestricted stopping powers and list or plot them.
- The electron and positron mean free paths are the mfps in cm to the next discrete interaction above the thresholds specified. Note that the range may be much less than the mfp, which only means that there are going to be very few such interactions.
- The number in brackets specifies the fraction of the discrete events which are from bremsstrahlung events as opposed to the creation of a secondary electron.

Data sets on distribution ($HEN_HOUSE/pegs4/data)

```
2074683 Nov  6  2015 521icru.pegs4dat     for ion chamber calns

1764782 Nov  6  2015 700icru.pegs4dat     for phantom calns

  61576 Nov  6  2015 ge.pegs4dat          element data example

  12832 Nov  6  2015 material.dat         pegsless material information

  61576 Nov  6  2015 pb.pegs4dat          element data example

 300462 Nov  6  2015 tutor_data.pegs4dat  for tutorial codes
```

show_data script

```
irs15> show_data tutor_data
show_data will list materials in tutor_data.pegs4dat
 MEDIUM=TA                          ,STERNCID=TA
 MEDIUM=NAI                         ,STERNCID=NAI
 MEDIUM=SI                          ,STERNCID=SI
 MEDIUM=H2O                         ,STERNCID=H2O
 MEDIUM=GE                          ,STERNCID=GE
 MEDIUM=PB                          ,STERNCID=PB

 MEDIUM=TA                          ,STERNCID=TA
 ELEM,RHO= 1.6600E+01,NE= 1
 ASYM=TA,Z=73.,A=  180.948,PZ= 1.00000E+00,RHOZ= 1.80948E+02
    4.10759E-01   7.0000E-01   1.0000E-02   5.0511E+01   5.0000E+01
--
 MEDIUM=NAI                         ,STERNCID=NAI
 COMP,RHO= 3.6700E+00,NE= 2
 ASYM=NA,Z=11.,A=   22.990,PZ= 1.00000E+00,RHOZ= 2.29898E+01
 ASYM=I ,Z=53.,A=  126.904,PZ= 1.00000E+00,RHOZ= 1.26904E+02
    2.58633E+00   7.0000E-01   1.0000E-02   5.0511E+01   5.0000E+01
```

Take-away message

- Users are not limited to the materials provided on the distribution
- Users have complete freedom to create simulation data for their own materials as long as the composition is known!

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