Scoring physical quantities I

Introduction to built-in estimators

3D distributions (**USRBIN**) & 1D-2D plots

FLUKA scoring

- It is said that Monte Carlo (MC) is a **"mathematical experiment"**; the MC equivalent of the result of a real experiment (*i.e.*, of a **measurement**) is called an **estimator**
- Just as a real measurement, an estimator is obtained by sampling from a statistical distribution and has a **statistical error** (and in general also a **systematic** one)
- There are often several different techniques to measure the same physical quantity: in the same way, **the same quantity can also be calculated using different kinds of estimators**
- FLUKA offers **numerous different estimators**, *i.e.* **scoring** for various quantities of interest can be requested directly from the input file

Definitions

- N : **number of identical particles**

- N_0 : **number of atoms per unit volume**

- λ : **mean free path**, *i.e.* average distance travelled by a particle in a material before an interaction. It depends on the material, particle type and energy

- l : **total distance travelled**

- v : **average particle velocity**

Cross-section

- $\Sigma\,[cm^{-1}] = 1/\lambda\,[cm]$: **macroscopic cross-section**, *i.e.* probability of interaction per unit distance. It depends on the material, particle type and energy.

- $\sigma = \frac{\Sigma}{N_0} = atom\ effective\ area\,, [barn = 10^{-24} cm^2]$: **microscopic cross-section**, *i.e.*
  - the **area of an atom weighted with the probability of interaction** (hence the name “cross-section”)
  - or the **probability of interaction per unit length, with the length measured in atoms/cm^2**

- The microscopic and macroscopic cross-section have a similar physical meaning of “probability of interaction per unit length”, with length measured in different units. Thus, **the number of interactions** can be obtained by multiplying them by the corresponding particle **track-length**

Reaction rate and fluence

- $R = \Sigma\Phi V$: number of reactions in a given time interval inside the volume *V*
(where Φ is the fluence and the product $\Sigma\Phi$ is integrated over energy or velocity)

- $\dot{R} = N\frac{dl}{dt}\Sigma = Nv\Sigma$: **reaction rate**

- $\frac{d\dot{R}}{dV} = \frac{dN}{dV}v\,\Sigma = n(\boldsymbol{r},v)v\Sigma$: reaction rate inside the volume element dV

- $\Phi(\boldsymbol{r},v) = n(\boldsymbol{r},v)dl\,, [cm^{-2}]$: **fluence**, *i.e.* time integral of the flux density
  - Fluence is expressed in **particles per cm^2** but in reality represents the **density of particle tracks [cm / cm^3] !**

- $\dot{\Phi}(\boldsymbol{r},v) = n(\boldsymbol{r},v)v\,, [cm^{-3}cm\,s^{-1}] = [cm^{-2}s^{-1}]$: **fluence rate** or **flux density**

Built-in and user scoring

- Several **pre-defined estimators** can be activated in FLUKA; one usually refers to these estimators as **built-in scoring** capabilities
- Users may build their own custom scoring through **user routines**
- However, **built-in scoring**:
  - covers most **common needs**
  - has been **extensively tested**
  - takes **biasing automatically into account**
  - has **refined algorithms** for track subdivision (apportioning)
  - comes with **utility programs** that allow to evaluate statistical errors
- Therefore users are strongly encouraged to **prefer built-in scorings** wherever possible
- Standard scoring can be adapted by means of simple user routines (**`fluscw.f`**, **`comscw.f`**), activated via **`USERWEIG`** card

FLUKA scoring

What?

Energy deposition and derivatives (dose), fluence or current versus energy, angle or other kinematic variables, time, DPA, residual activity…

Where?

In regions, across boundaries, on region-independent grids

When?

At the end of each cycle or at each event

Output?

Saved in `[inputname]nnn_fort.##` files,
where `nnn` is the cycle number & `##` is the logical unit number chosen by the user

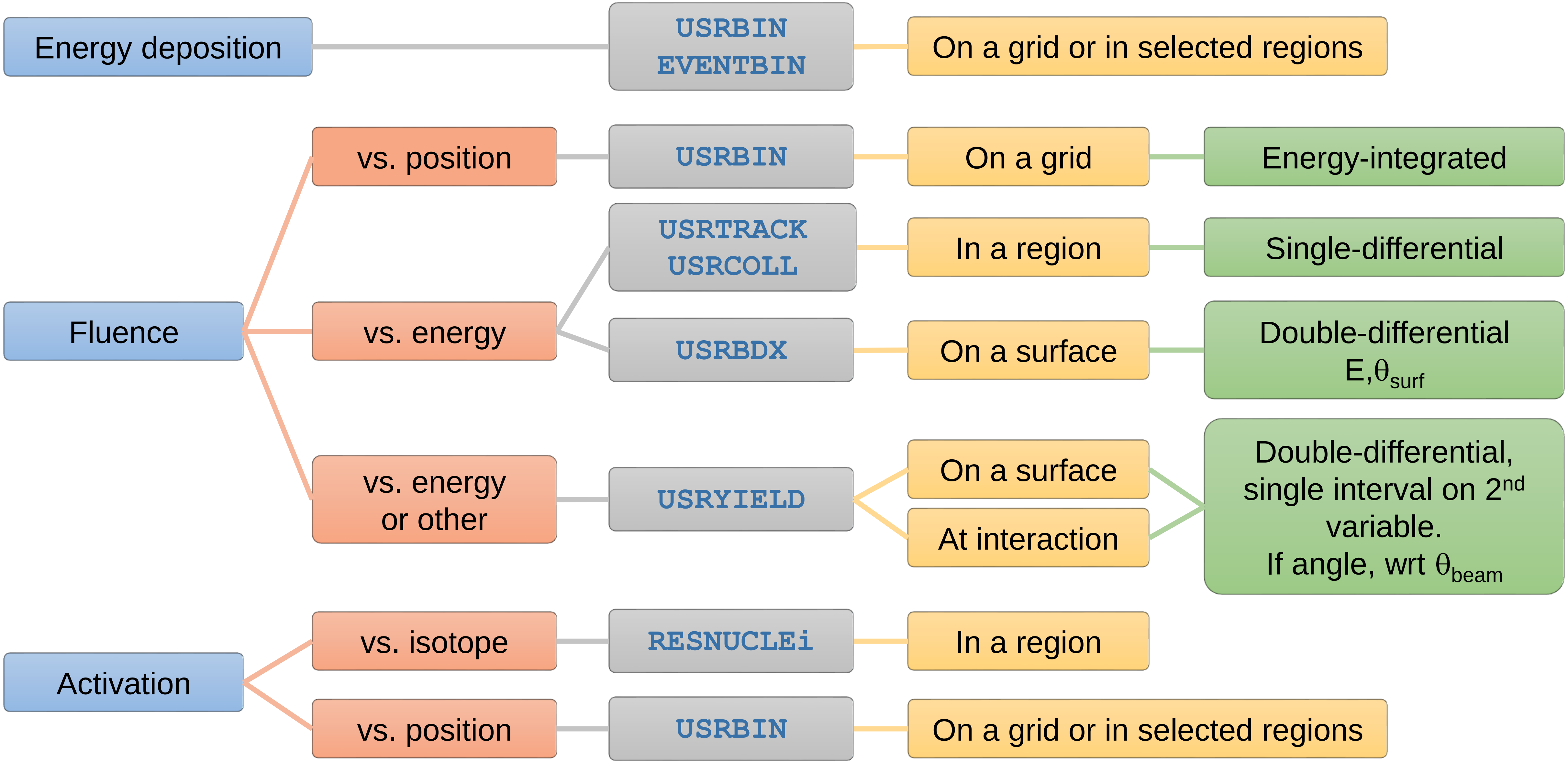
Results?

Post-processing utilities merge cycles, calculate average and rms, provide data files for plotting. Available via **Flair**

Results normalised **per primary**

User code needed for processing of custom scoring!

The FLUKA estimator zoo



Main FLUKA estimators

- **USRBIN** scores the **spatial distribution** of **energy density** or **fluence** (or star* density) in a **selection of regions** or in a **regular mesh** (cylindrical, cartesian) described by the user.
- **USRTRACK** (**USRCOLL**) scores average **$d\Phi/dE$ (differential fluence)** of a given type or family of particles in a **given region**.
- **USRBDX** scores average **$d^2\Phi/dEd\Omega$ (double-differential fluence or current)** of a given type or family of particles on a **given surface**.
- **USRYIELD** scores a **double differential yield** of particles on a **given surface**.
  - The distribution can be with respect to energy and angle, but also other more “exotic” quantities

- All scorings write their results into **logical output units assigned by the user**
  - Unit numbers must be >20.
  - The only exception is SCORE: its output is printed in the **standard output**.

** A star is a hadronic inelastic interaction*

More “special” scoring cards

- `DETECT` scores **energy deposition** for each event (primary history) in coincidence or anti-coincidence with a trigger
- `EVENTBIN` is like `USRBIN`, but prints the binning output **after each event** instead of an average over histories
- `USERDUMP` allows the user to **dump selected information within each primary history**
- `TCQUENCH` sets scoring **time cut-offs** and/or **Birks quenching** parameters for binnings (`USRBIN` or `EVENTBIN`) indicated by the user
- `ROTPRBIN` assigns **rotations/translations** for a given user-defined binning (`USRBIN` or `EVENTBIN`) (and sets the **storage precision**, single or double). Useful with `LATTICEs`
- `AUXSCORE` defines **filters** and **conversion coefficients**
- `RESNUCLEi` scores **stopping nuclei in a given region**
- `DCYSCORE` assigns cooling times

See radiation protection lecture

Standard post-processing programs

- To analyse the results of the different scoring options, several programs are made available
- **Behind the scenes, Flair uses these programs**

- The executables are in `/pathtofluka/bin`, while the sources are available in `/pathtofluka/src/tools` in case modifications are needed
- They assume that the estimator files are **unformatted**, and can calculate standard deviations and average values over many cycles:
  - **`ustsuw.f`** to analyze **`USRTRACK`** and **`USRCOLL`** outputs
  - **`usxsuw.f`** to analyze **`USRBDX`** outputs
  - **`usysuw.f`** to analyze **`USRYIELD`** outputs
  - **`usbsuw.f`** to analyze **`USRBIN`** outputs
  - **`usrsuw.f`** to analyze **`RESNUCLEi`** outputs
  - **`usbrea.f`** to convert **`USRBIN`** outputs to ASCII file

`USRBIN`: Input, visualisation & plotting

USRBIN scoring definition

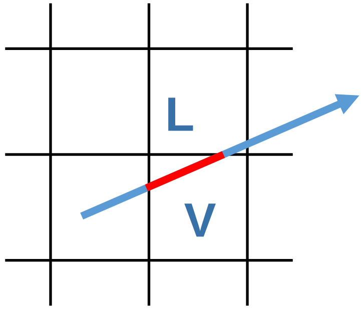
Energy deposition density
(GeV/cm^3 per primary)

Particle fluence
(1/cm^2 per primary)

Energy deposition density in cylindrical mesh
USRBIN Unit: 21 BIN ▾ Name: Edep
Type: R-Φ-Z ▾ Rmin: 0.0 Rmax: 5.0 NR: 50.
Part: ENERGY ▾ X: 0.0 Y: 0.0 NΦ: 1.
Zmin: 0.0 Zmax: 10.0 NZ: 100.

Charged hadron fluence
USRBIN Unit: 31 BIN ▾ Name: ChHad
Type: R-Φ-Z ▾ Rmin: 0.0 Rmax: 5.0 NR: 50.
Part: HAD-CHAR ▾ X: 0.0 Y: 0.0 NΦ: 1.
Zmin: 0.0 Zmax: 10.0 NZ: 100.

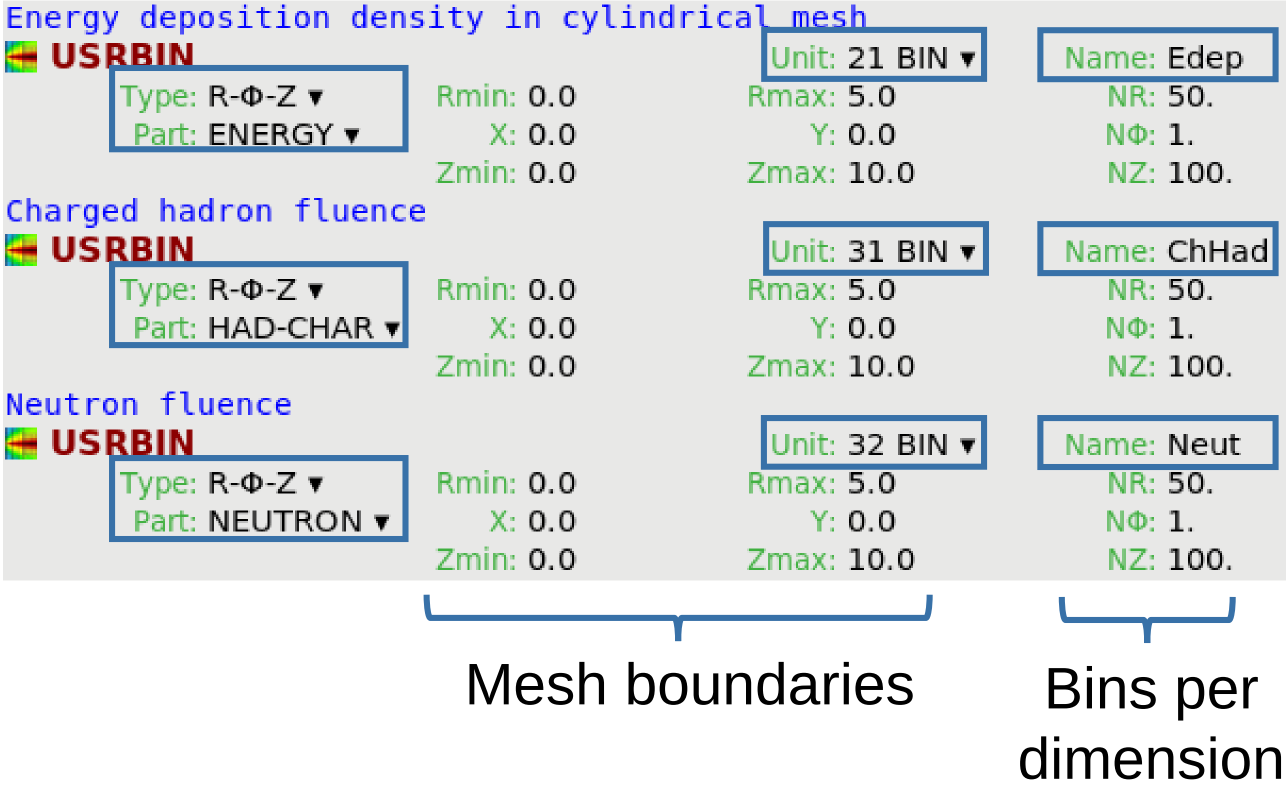
Neutron fluence
USRBIN Unit: 32 BIN ▾ Name: Neut
Type: R-Φ-Z ▾ Rmin: 0.0 Rmax: 5.0 NR: 50.
Part: NEUTRON ▾ X: 0.0 Y: 0.0 NΦ: 1.
Zmin: 0.0 Zmax: 10.0 NZ: 100.



Path length **L** [cm] inside the bin divided by the bin volume **V** [cm^3] → cm / cm^3 = 1/cm^2

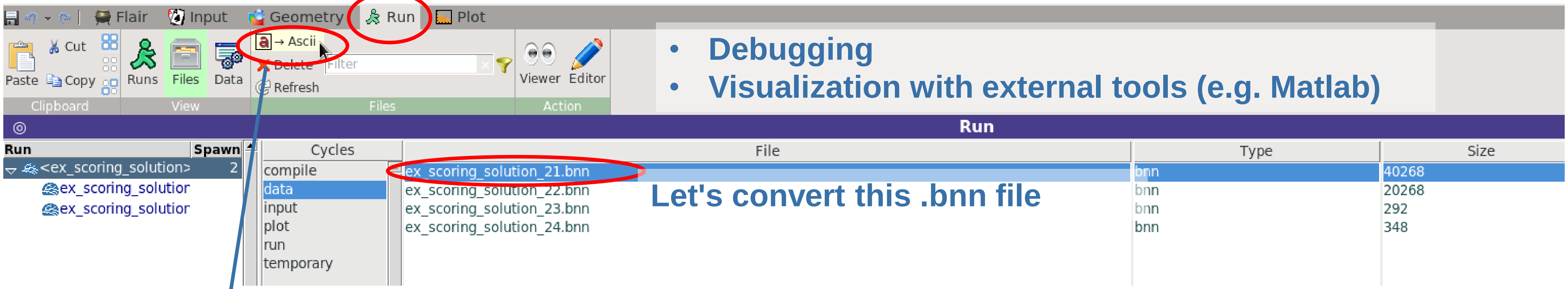
`USRBIN` input card

- **Type**:
  - * X-Y-Z: cartesian mesh
  - * R-Φ-Z: cylindrical mesh
  - * per region
  - * …
- **Part**: generalised particle
- **Unit**: logical output unit
  - **BIN** (binary): unformatted output
    Can be converted to ASCII
    or directly post-processed via Flair.
  - **ASC** (ASCII): formatted output
    Cannot be post-processed via Flair.
- **Name**: 8-character limit



Note on "Type":
Do not choose the **"point"** versions,
which do not return e.g. fluence when a particle is selected,
but density of stars produced by the particles.

Convert `USRBIN` bnn file to ASCII (3D mesh data)



- **Debugging**
- **Visualization with external tools (e.g. Matlab)**

Result: bnn.lis file
Always 10 columns per line

```
1
  R - Z     binning n.   1  "EneSmall  " , generalized particle n.  208
      R coordinate: from  0.0000E+00 to  5.0000E+00 cm,    50 bins ( 1.0000E-01 cm wide)
      Z coordinate: from  0.0000E+00 to  1.0000E+01 cm,   100 bins ( 1.0000E-01 cm wide)
      axis coordinates: X = 0.0000E+00, Y =  0.0000E+00 cm
      Data follow in a matrix A(ir,iz), format (1(5x,1p,10(1x,e11.4)))

      accurate deposition along the tracks requested
        2.3867E-01  1.8430E-04  1.6286E-05  9.9585E-06  3.3918E-07  2.1157E-06  7.4462E-06  6.5266E-06  6.3637E-06  4.9691E-06
        0.0000E+00  0.0000E+00  1.6428E-06  3.8209E-06  4.4210E-06  3.7473E-06  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
        0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.1102E-06
        1.8253E-08  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
        0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
        2.3794E-01  3.4083E-04  5.7607E-05  2.7670E-05  2.7495E-05  2.0694E-05  0.0000E+00  0.0000E+00  0.0000E+00  2.5324E-06
        3.5606E-06  3.5531E-06  1.8965E-06  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
        0.0000E+00  0.0000E+00  2.7077E-09  0.0000E+00  0.0000E+00  0.0000E+00  6.8063E-08  0.0000E+00  0.0000E+00  0.0000E+00
        0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  6.1228E-08  0.0000E+00  0.0000E+00  0.0000E+00  2.7059E-07  0.0000E+00
        0.0000E+00  0.0000E+00  4.4389E-11  0.0000E+00  1.6188E-10  2.2633E-14  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
```

R-Z binning: (ir, iz)
First loop on ir,
[then on iphi (if exists),]
then on iz

Cartesian binning: (ix, iy, iz)
First loop on ix,
then on iy,
then on iz

First 50 values (first 5 lines) are $\{val_{(ir,\ iz=1)}\}$, with **ir ∈ ⟦1, 50⟧**. **Next 50 values** are $\{val_{(ir,\ iz=2)}\}$, with **ir ∈ ⟦1, 50⟧**. And so on, **for each iz** ∈ ⟦**1, 100**⟧.

USRBIN mesh geometry check

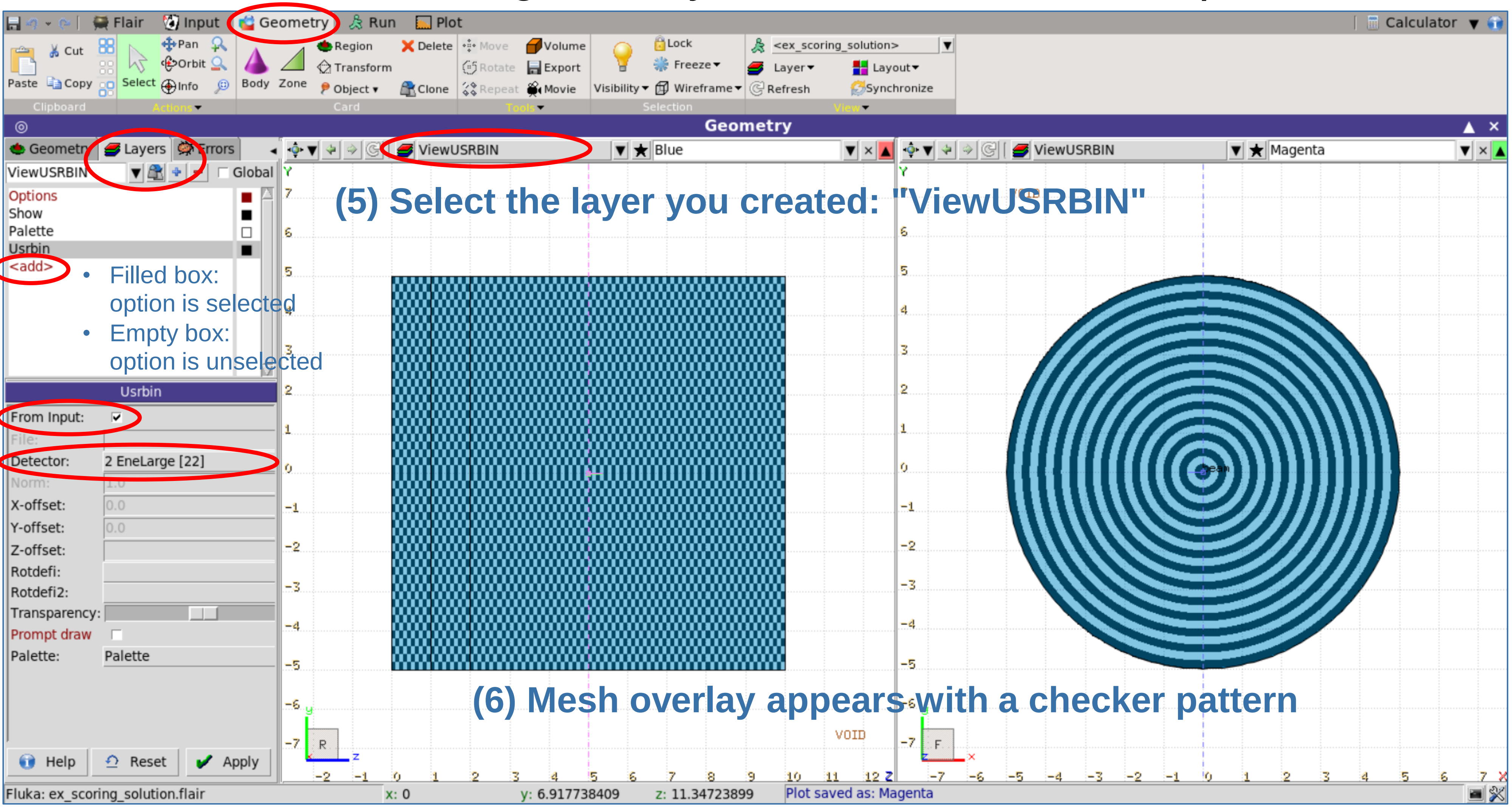
- A defined mesh can be overlaid on the geometry to check that it is well-positioned

(1) Click "+"
to create a new layer.
Here for example,
we name it "ViewUSRBIN".

(2) Click "add"
and select "Usrbin"

(3) Select "From input"

(4) Select the
USRBIN card name
from your input file

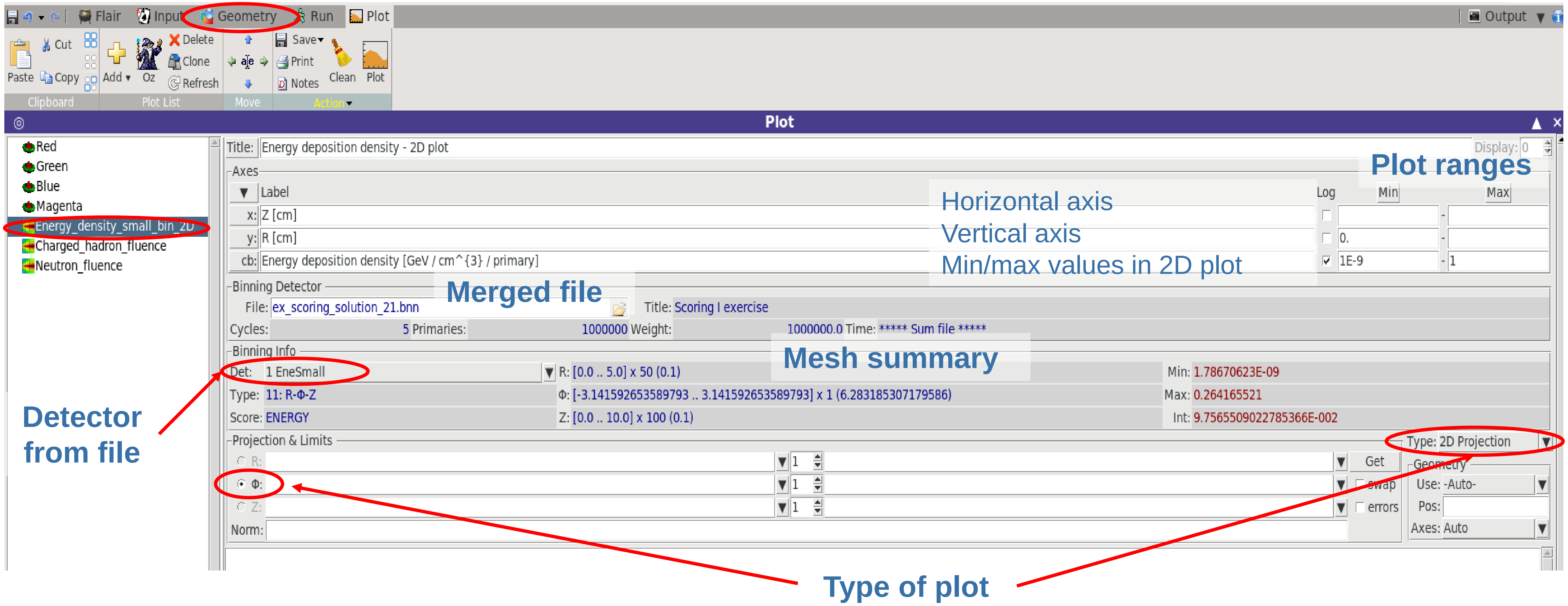


Volume normalisation

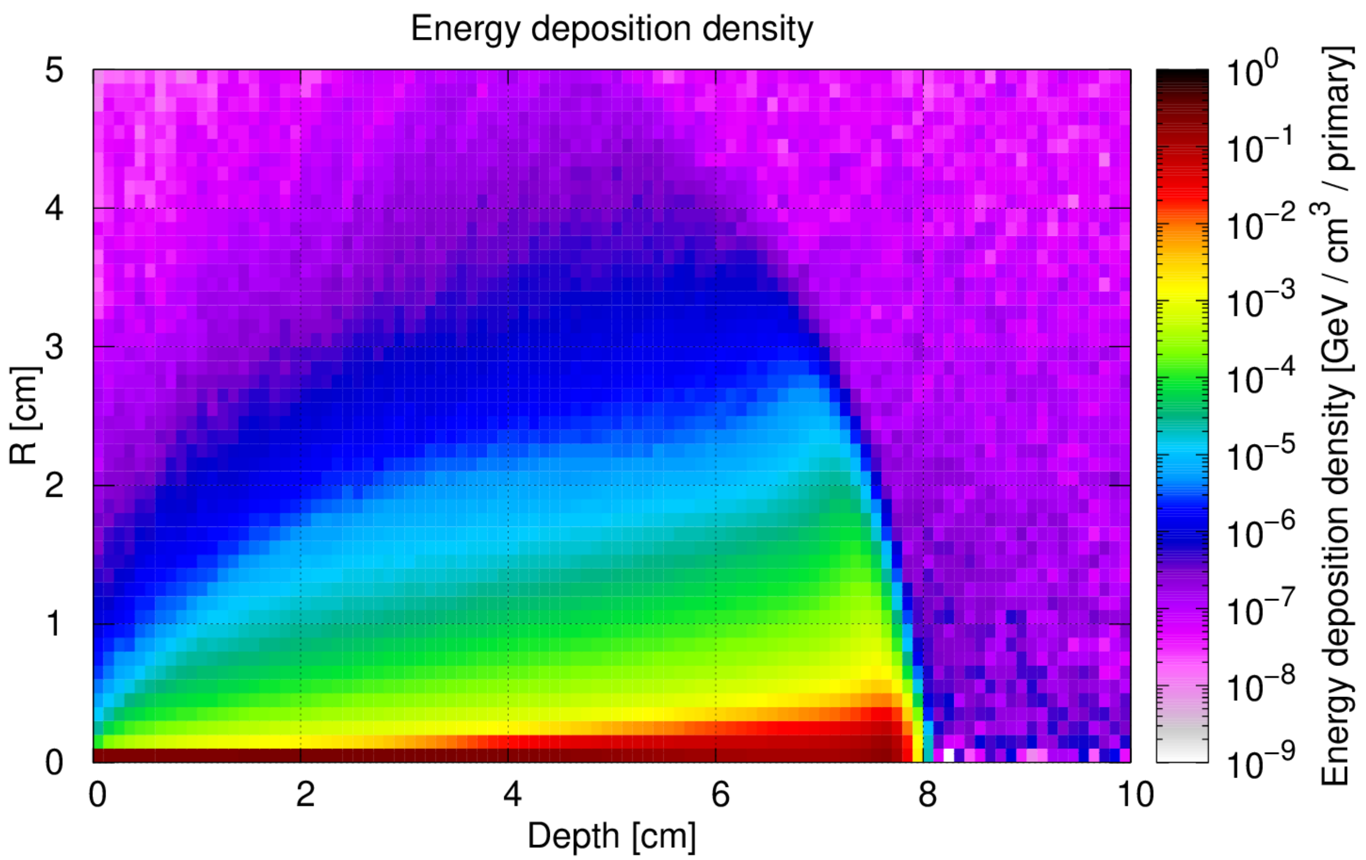
- **USRBIN region: FLUKA results are NOT normalized by volume.**
  When scoring particle *fluence* (e.g. NEUTRON) *or energy density* (ENERGY) with USRBIN
  by region, FLUKA results are *total track-length and energy deposition*, respectively.
  - Indeed, FLUKA does not calculate regions volumes (which can be arbitrarily complex!).
  - Results are provided assuming the region has a volume equal to 1 cm^3 .
  - The user needs to divide by the region volume to get the intended quantities.

- **USRBIN meshes: FLUKA results are normalized by volume.**
  Conversely, as USRBIN scoring on regular (Cartesian, cylindrical) meshes
  is requested, *particle fluence and energy density* will be automatically provided.
  - Results are already normalized by the bins volume(s).
  - Indeed, FLUKA can easily compute the mesh bins volume(s). In addition, it would not make sense for the user to calculate each cylindrical mesh bin volume (varying radially)!

Plotting – Energy deposition density (USRBIN mesh)

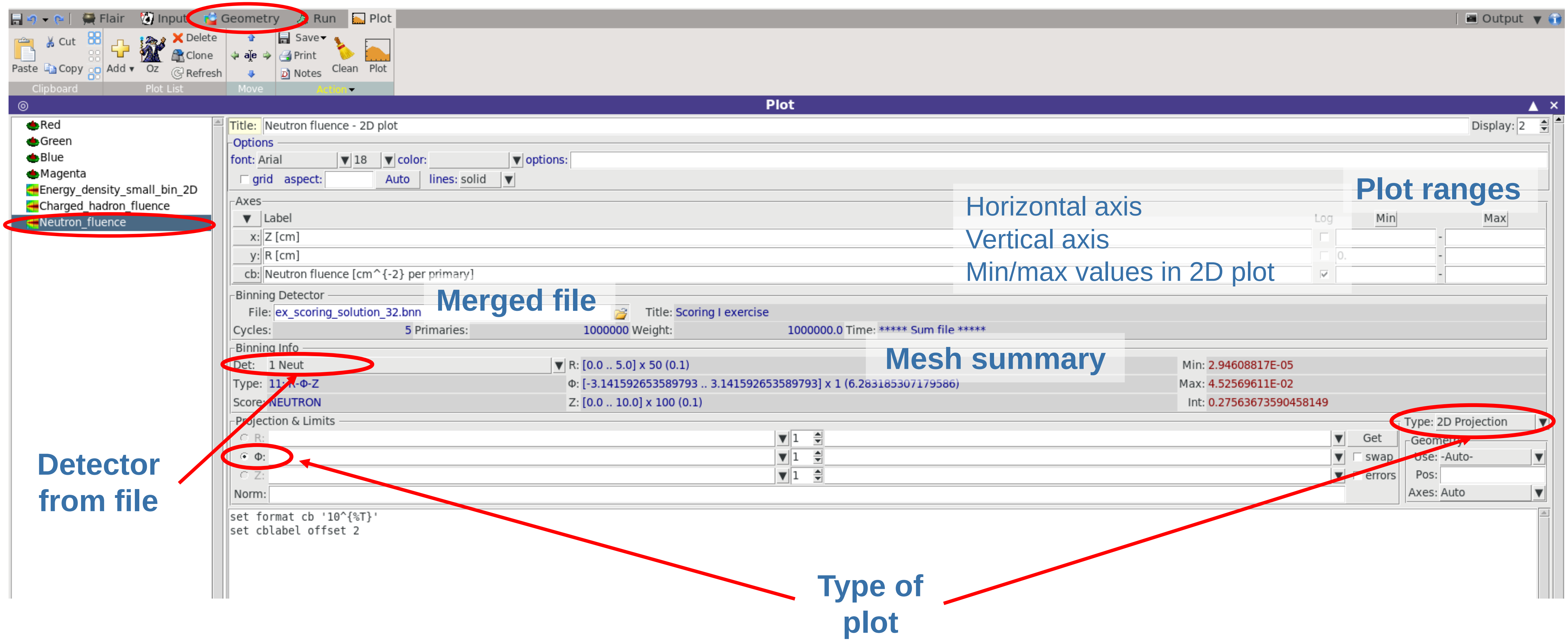


Plot result – Energy deposition density (USRBIN mesh)

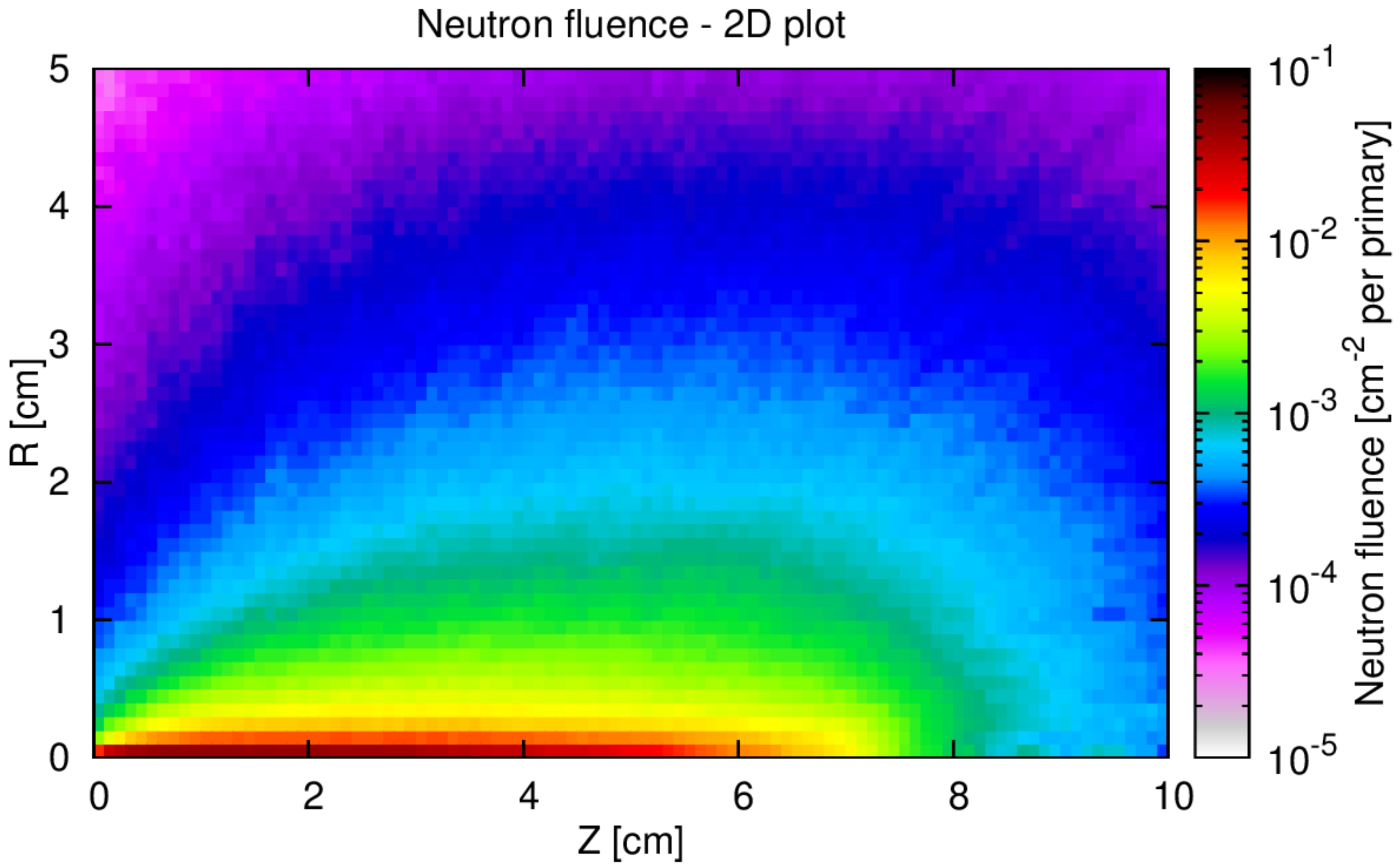


- This plot is a **2D projection** of a 3D structure
  → **the result is the volume-weighted** average **over the 3rd coordinate** (Φ in this case)
- The 2D limits, and the range on which to perform the average, can be set in Flair

Plot result – Neutron fluence (USRBIN mesh)



Plotting – Neutron fluence (`USRBIN` mesh)



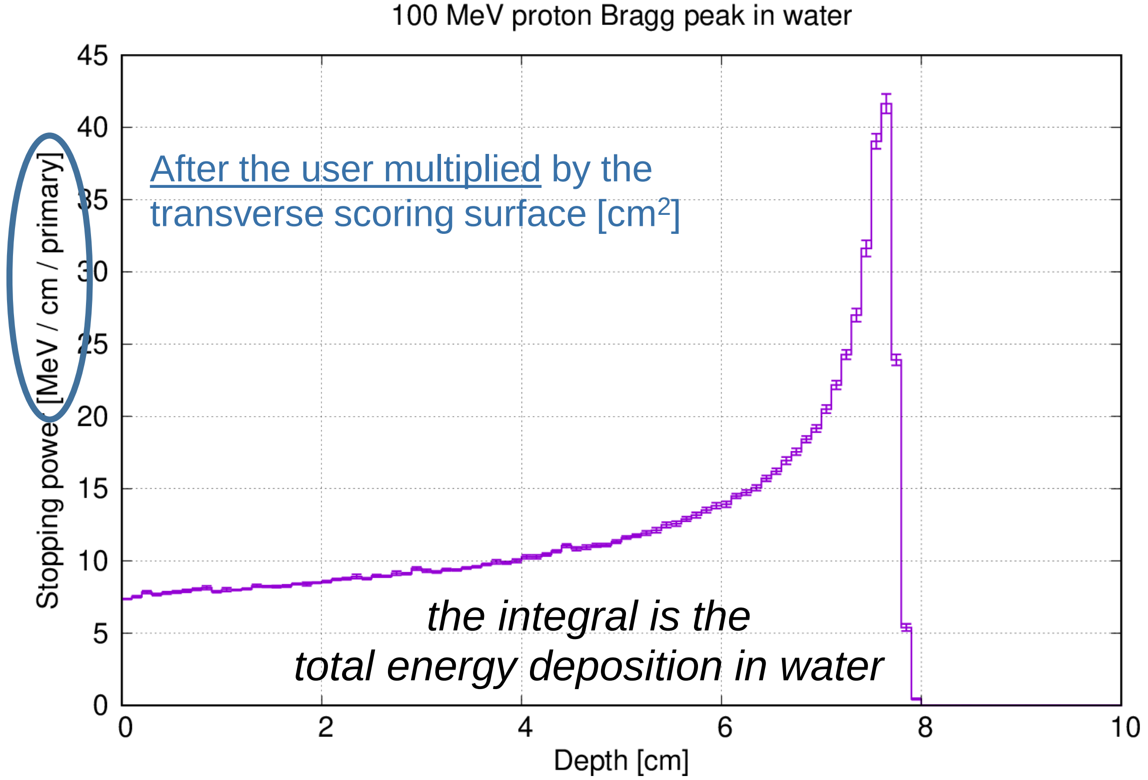
- This plot is a **2D projection** of a 3D structure
  → **the result is the volume-weighted** average **over the 3rd coordinate** (Φ in this case)
- The 2D limits, and the range on which to perform the average, can be set in Flair

One dimensional plots

- 1D plots can be obtained from 3D **USRBIN** meshes, e.g. (for an R-Φ-Z mesh):

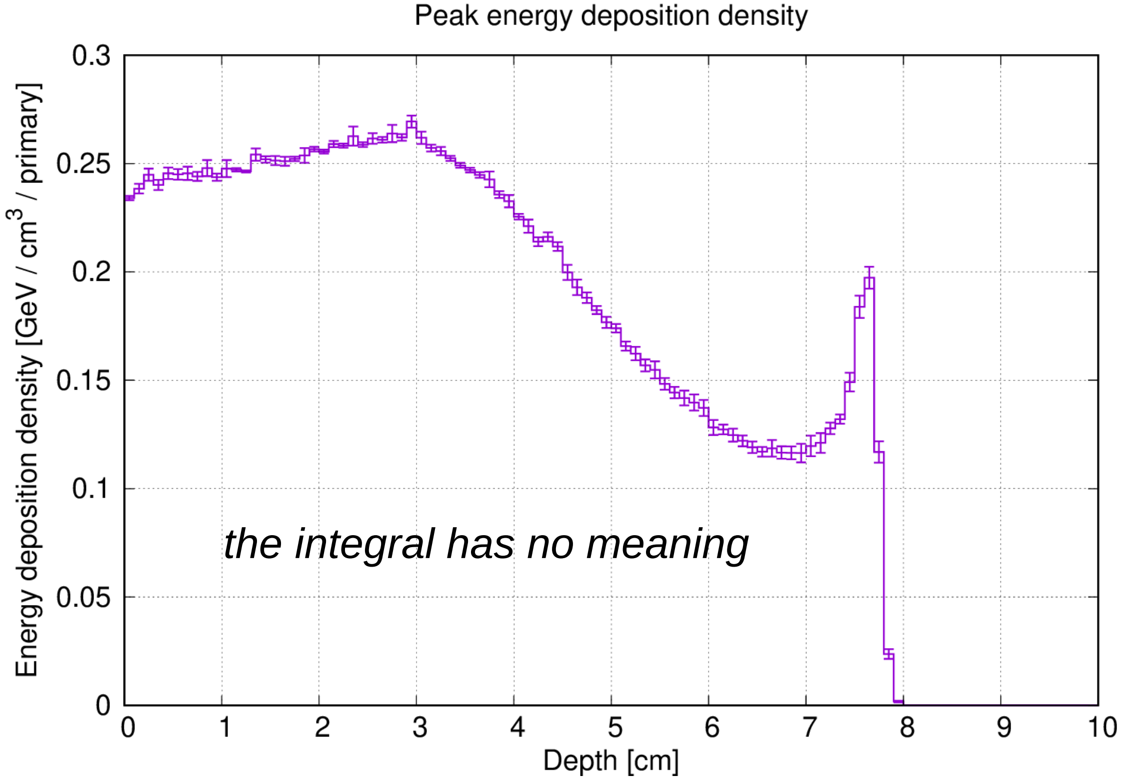
1D Projection

- For each z bin:
  average over all {R, Φ} bins



1D Max

- For each z bin:
  highest over all {R, Φ} bins



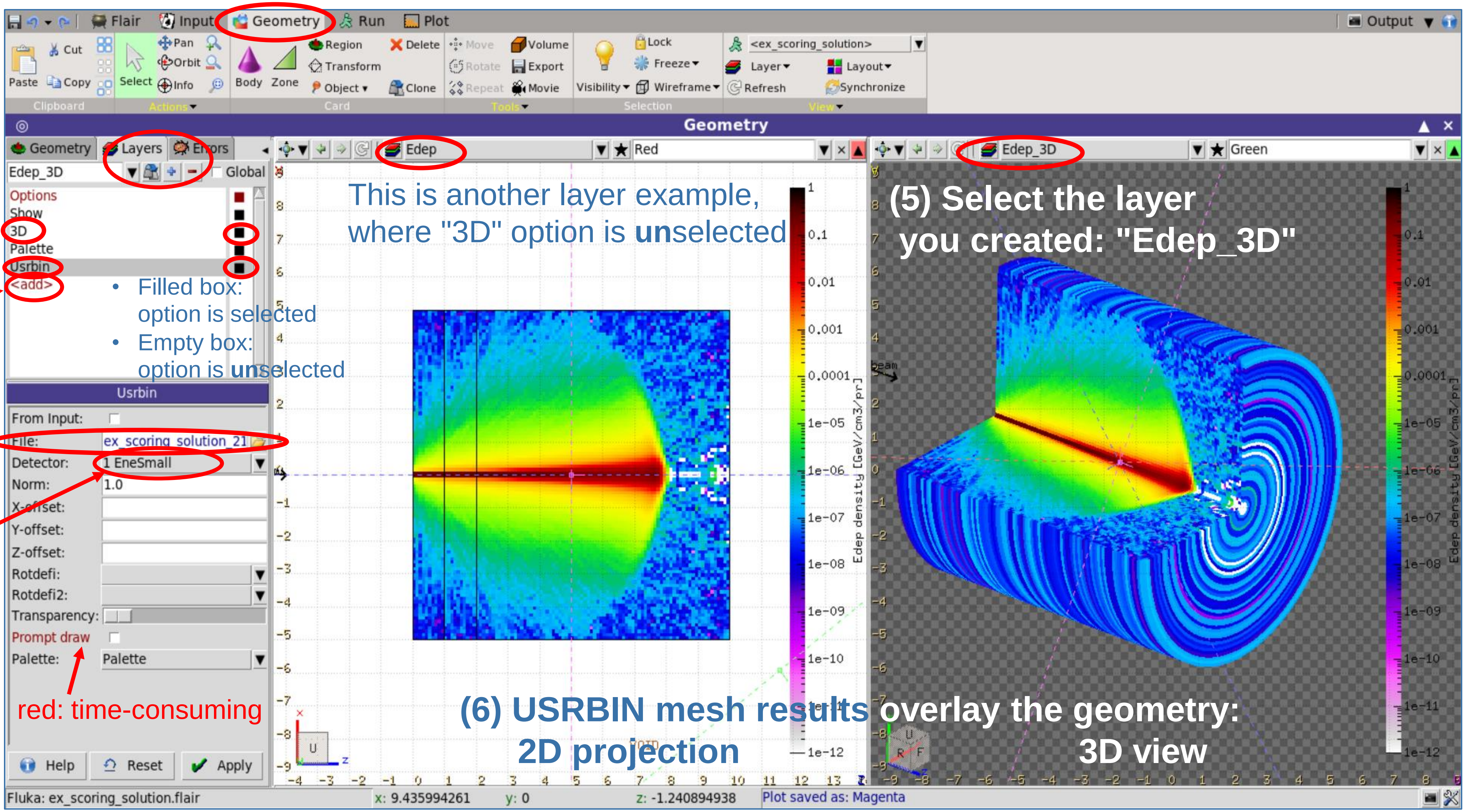
Overlaying USRBIN mesh results on 2D/3D geometry

(1) Click "+" to create a new layer.
Here for example, we name it "Edep_3D".

(2) Click "add" and select "Usrbin". Also add "3D".

(3) Select merged file from run results

(4) Select the USRBIN card name from your input file



FLUKA