Statistical Errors:

- Can be calculated for single histories, or for batches of several histories
- Distribution of scoring contributions by single histories can be very asymmetric (many histories contribute little or zero)
- Scoring distribution from batches tends to Gaussian for $N \rightarrow \infty$, provided $\sigma^2 \neq \infty$ (thanks to Central Limit Theorem)
- The standard deviation of an estimator calculated from batches or from single histories is an estimate of the standard deviation of the actual distribution ("error of the mean")
- How good is such an estimate depends on the type of estimator and on the particular problem (but it converges to the true value for $N \rightarrow \infty$)

Statistical Errors

- The variance of the mean of an estimated quantity ***x*** (e.g., fluence), calculated in *N* batches, is:

$$\sigma^2_{<x>} = \frac{1}{N-1}\left[\frac{\sum_1^N n_i x_i^2}{n} - \left(\frac{\sum_1^N n_i x_i}{n}\right)^2\right]$$

mean of squares – square of means

N – 1

where:

n_i = number of histories in the i th batch

$n = \Sigma n_i$ = total number of histories in the N batches

x_i = average of x in the i th batch: $x_i = \sum_{j=1}^{n_i} \frac{x_{ij}}{n_i}$

where $\boldsymbol{x_{ij}}$ is the contribution to *x* of the jth history in the ith batch

In the limit N = n, n_i =1, the formula applies to single history statistics

Transport thresholds

In a MC simulation particles are not tracked until they "have lost all their kinetic energy", but until their energy drops to/below a preset transport threshold

When a particle's energy drops below threshold, what happens?

In FLUKA energy is depositedon the spot(for electrons) or ranged out (for heavier projectiles).

General guidelines to set threshold energies?

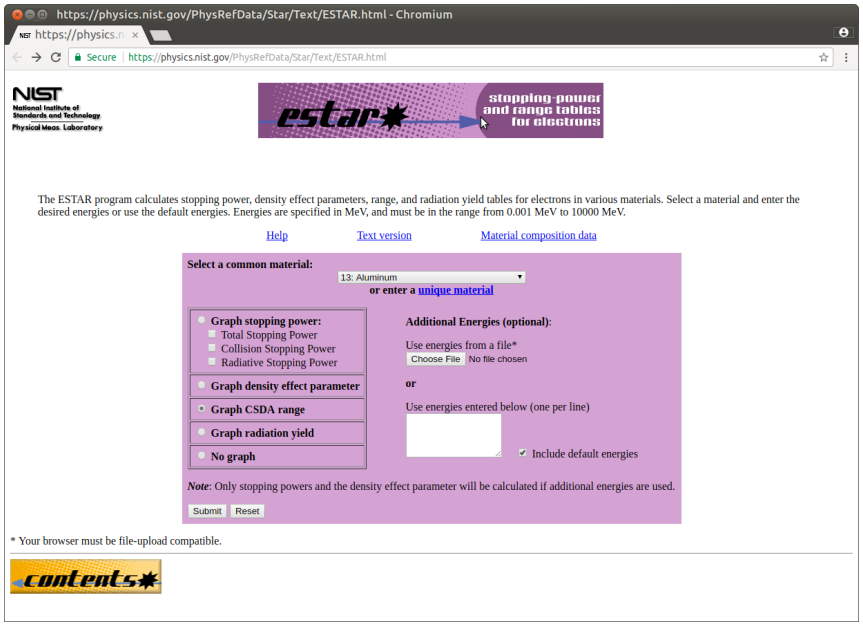
It depends on the "granularity" of the geometry and/or of the scoring mesh. Energy/range tables are very useful.
- Consider the interest in a given region.
- Warning 1: to reproduce correctly electronic equilibrium, neighboring regions should have the same electron energy(NOT range) threshold. To be kept in mind for sampling calorimeters
- Warning 2: Photon thresholds should be lower than electron thresholds (photons travel farther)
- Warning 3: **low thresholds for e-/e+/gammas are CPU eaters**

Transport thresholds - 2

Delta-ray production threshold:
- If production threshold < transport threshold: CPU wasted in producing and dumping particles on the spot
- If production threshold > transport threshold: the latter is increased.

Examine the particle's range

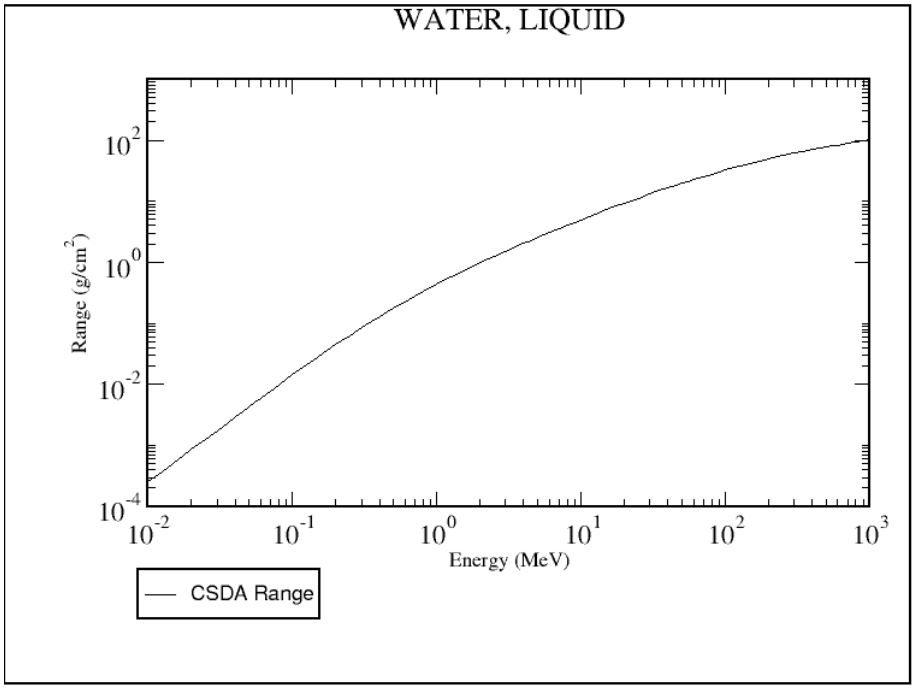
https://physics.nist.gov/PhysRefData/Star/Text/ESTAR.html



Transport thresholds - 3

Range for electrons in water

Water density: 1 g/cm^3 → We may directly read range in cm



Transport threshold at 1 MeV? → 1-MeV e^- range is O(1 mm) = 1000 μm
Depositing/killing them on the spot in a ~50 μm geometry is asking too much...

Transport threshold at 10 keV? →10-keV e^- range is O(10^{-4}) cm = O(1 μm)
Depositing them on the spot in a ~50 μm geometry is fine

Reaction Rate and Cross Section (1/3)

- We call mean free path $\lambda[cm]$ the average distance travelled by a particle in a material before an interaction. Its inverse, $\Sigma\,[cm^{-1}]$ is the probability of interaction per unit distance, and is called macroscopic cross section. Both λ and Σ depend on the material and on the particle type and energy.

- For N identical particles, the number of reactions R occurring in a given time interval will be equal to the total distance travelled l times the probability per unit distance: $\Sigma \quad R = l\Sigma$

- The reaction rate will be $\dot{R} = \mathrm{d}l/\mathrm{d}t\ \Sigma = v\Sigma$, where v is the average particle velocity.

Reaction Rate and Cross Section (2/3)

- Assume now that $n(\boldsymbol{r},v)=dN/dV\ [cm^{-3}]$ be the density of particles with velocity $v=dl/dt\ [cm/s]$, at a spatial position $\boldsymbol{r}$. The reaction rate inside the volume element $\mathrm{d}V$ will be: $\mathrm{d}\dot{R}/\mathrm{d}V = n(\boldsymbol{r},v)v\Sigma$
- The quantity $\dot{\Phi}(\boldsymbol{r},v) = n(\boldsymbol{r},v)v$ is called fluence rate or flux density and has dimensions $[cm^{-3}\ cm\ t^{-1}]=[cm^{-2}\ t^{-1}]$.
- The time integral of the flux density $\Phi(\boldsymbol{r},v) = n(\boldsymbol{r},v)\mathrm{d}l$ is the fluence $[cm^{-2}]$
- Fluence is measured in particles per cm^2 but in reality it describes the density of particle tracks
- The number of reactions inside a volume V is given by the formula:

$$R = \Sigma\Phi V$$

(where both Σ and Φ are integrated over energy or velocity)

Reaction Rate and Cross Section (3/3)

- Dividing the macroscopic cross section by N_0, the number of atoms per unit volume, one obtains the microscopic cross section: $\sigma[barn=10^{-24}cm^2]$

$$\frac{\text{probability/cm}}{\text{atoms/cm}^3} = \frac{\text{probability} \times \text{cm}^2}{\text{atom}} = \text{atom effective area}$$

  i.e., the area of an atom weighted with the probability of interaction (hence the name "cross section");

- But it can also be understood as the probability of interaction per unit length, with the length measured in atoms/cm^2 (the number of atoms contained in a cylinder with a 1 cm^2 base).

- In this way, both microscopic and macroscopic cross section are shown to have a similar physical meaning of "probability of interaction per unit length", with length measured in different units. Thus, the number of interaction can be obtained by both by multiplying by the corresponding particle track-length.

Fluence estimation (1/2)

- Track length estimation:

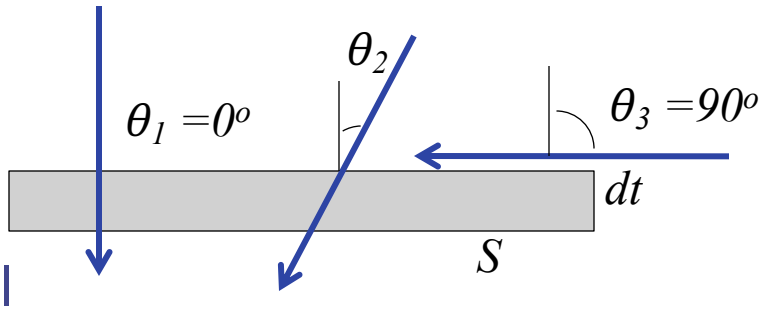
$$\dot{\Phi}(v)\,dt = n(v)\,v\,dt = \frac{dN(v)}{dV}\frac{dl(v)}{dt}\,dt = \lim_{\Delta V \to 0}\frac{\sum_i l_i(v)}{\Delta V}$$

- Collision density estimation:

$$\dot{\Phi}(v) = \frac{\dot{R}(v)}{\sigma(v)\,N_o\Delta V} = \frac{\dot{R}(v)}{\Sigma(v)\Delta V} = \frac{\dot{R}(v)\lambda(v)}{\Delta V}$$

Fluence estimation (2/2)

Surface crossing estimation



- Imagine a surface having an infinitesimal thickness dt A particle incident with an angle θ with respect to the normal of the surface S will travel a segment $dt/cos\theta$.
- Therefore, we can calculate an average surface fluence by adding $dt/cos\ \theta$ for each particle crossing the surface, and dividing by the volume $S\,dt$:

$$\Phi = \lim_{dt \to 0} \frac{\sum_i \frac{dt}{\cos\theta_i}}{S\,dt}$$

- While the current J count the number of particles crossing the surface divided by the surface:

$$J = dN/dS$$

The fluence is independent from the orientation of surface S, while the current is NOT!

In an isotropic field can be easily seen that on a flat surface $J = \Phi/2$

Practical issues for Medical Applications

General problems for MC calculations on CT scans

- How to assign realistic human tissue parameters (= materials) for MC Calculation?
- How to find a good compromise between the number of different HU values (~ 3000-5000) and the materials to be considered in the MC?

  (issues on memory and computation speed when attempting to treat each HU number as a different material !!!)
- How to preserve continuous, HU-dependent information when segmenting the HU numbers into intervals sharing the same “tissue” material ?

  (critical for ion range calculation in hadron therapy !!!)

CT stoichiometric calibration (I)

CT segmentation into 27 materials of defined elemental composition (from analysis of 71 human CT scans)

Air, Lung, Adipose tissue

Soft tissue

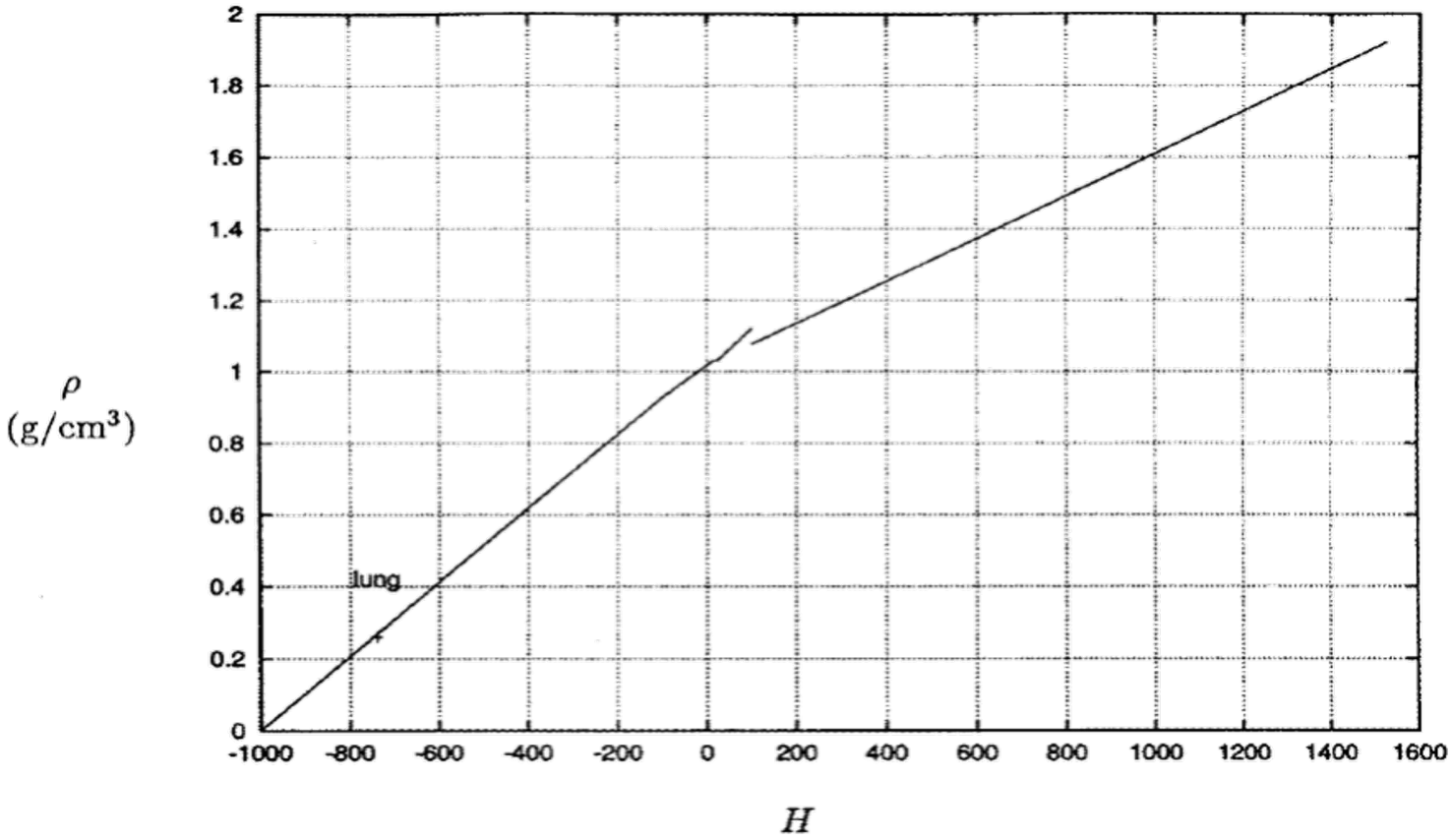
Skeletal tissue

H	w_i (pp)											
	H	C	N	O	Na	Mg	P	S	Cl	Ar	K	Ca
−1000–−950			75.5	23.2						1.3		
−950–−120	10.3	10.5	3.1	74.9	0.2		0.2	0.3	0.3		0.2	
−120–−83	11.6	68.1	0.2	19.8	0.1			0.1	0.1			
−82–−53	11.3	56.7	0.9	30.8	0.1			0.1	0.1			
−52–−23	11.0	45.8	1.5	41.1	0.1		0.1	0.2	0.2			
−22–7	10.8	35.6	2.2	50.9			0.1	0.2	0.2			
8–18	10.6	28.4	2.6	57.8			0.1	0.2	0.2		0.1	
19–80	10.3	13.4	3.0	72.3	0.2		0.2	0.2	0.2		0.2	
80–120	9.4	20.7	6.2	62.2	0.6			0.6	0.3			
120–200	9.5	45.5	2.5	35.5	0.1		2.1	0.1	0.1		0.1	4.5
200–300	8.9	42.3	2.7	36.3	0.1		3.0	0.1	0.1		0.1	6.4
300–400	8.2	39.1	2.9	37.2	0.1		3.9	0.1	0.1		0.1	8.3
400–500	7.6	36.1	3.0	38.0	0.1	0.1	4.7	0.2	0.1			10.1
500–600	7.1	33.5	3.2	38.7	0.1	0.1	5.4	0.2				11.7
600–700	6.6	31.0	3.3	39.4	0.1	0.1	6.1	0.2				13.2
700–800	6.1	28.7	3.5	40.0	0.1	0.1	6.7	0.2				14.6
800–900	5.6	26.5	3.6	40.5	0.1	0.2	7.3	0.3				15.9
900–1000	5.2	24.6	3.7	41.1	0.1	0.2	7.8	0.3				17.0
1000–1100	4.9	22.7	3.8	41.6	0.1	0.2	8.3	0.3				18.1
1100–1200	4.5	21.0	3.9	42.0	0.1	0.2	8.8	0.3				19.2
1200–1300	4.2	19.4	4.0	42.5	0.1	0.2	9.2	0.3				20.1
1300–1400	3.9	17.9	4.1	42.9	0.1	0.2	9.6	0.3				21.0
1400–1500	3.6	16.5	4.2	43.2	0.1	0.2	10.0	0.3				21.9
1500–1600	3.4	15.5	4.2	43.5	0.1	0.2	10.3	0.3				22.5

Schneider et al PMB 45, 2000

CT stoichiometric calibration (II)

Assign to each material a "nominal mean density", e.g. using the density at the center of each HU interval **(Jiang et al, MP 2004)**

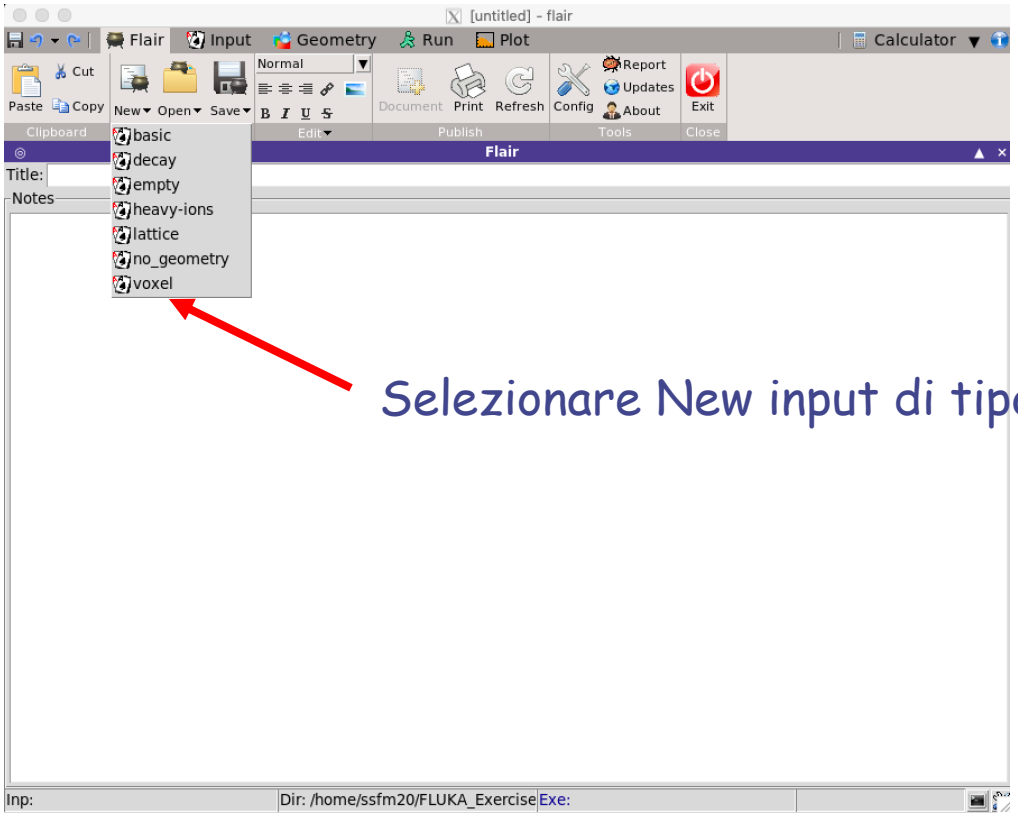


Schneider et al PMB 45, 2000

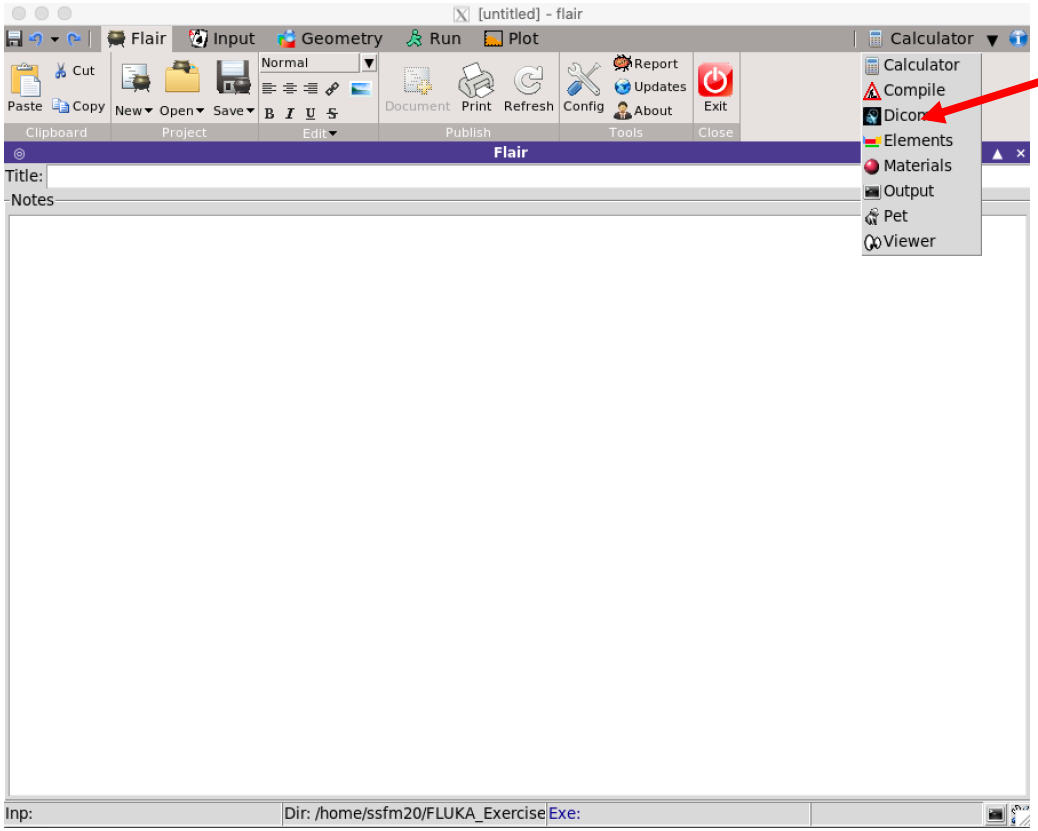
But "real density" (and related physical quantities) varies continuously with HU value !!!

Caricamento di una immagine Dicom e produzione di una geometria a voxel

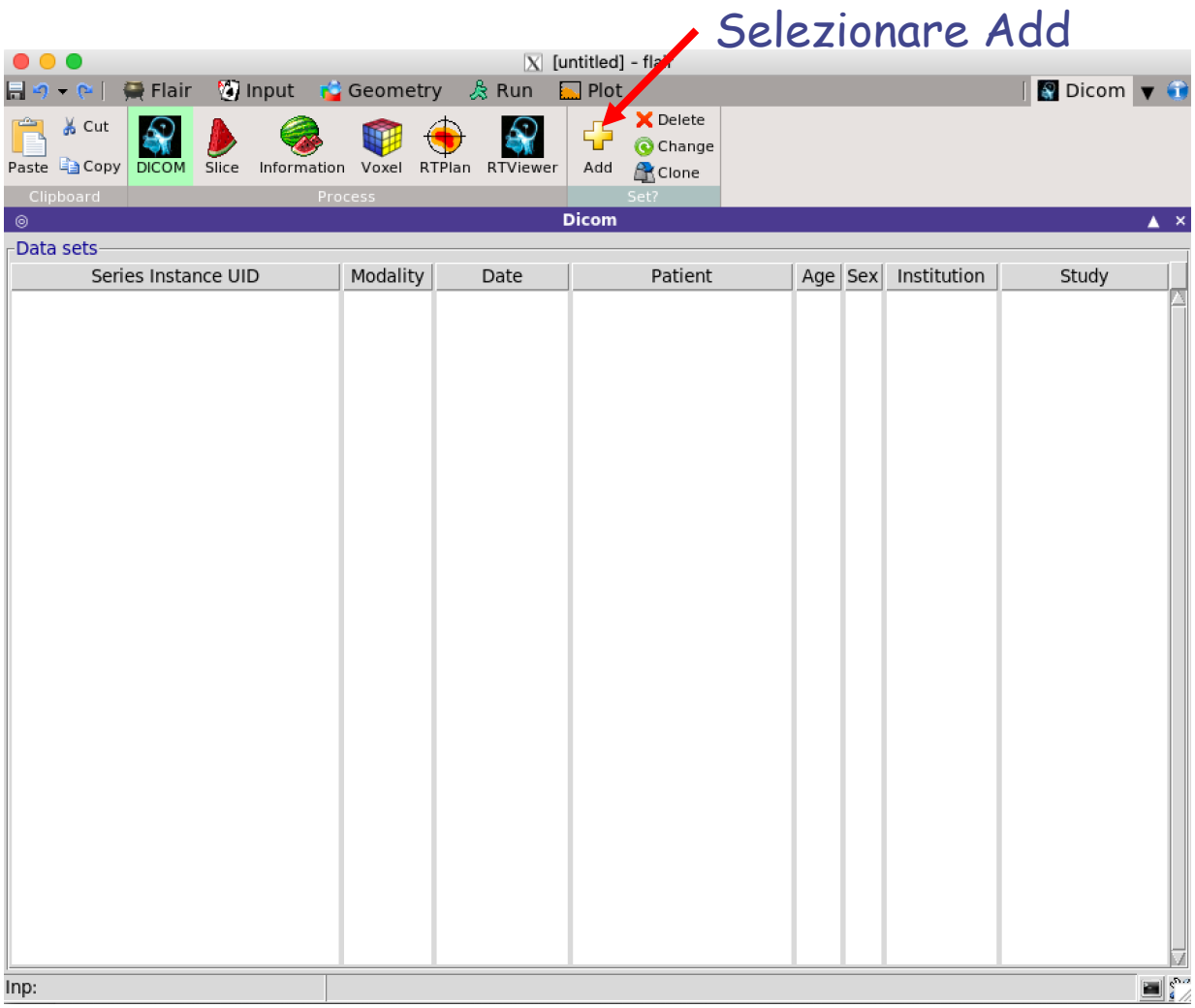
cd FLUKA_Exercises
cd Dicom
flair

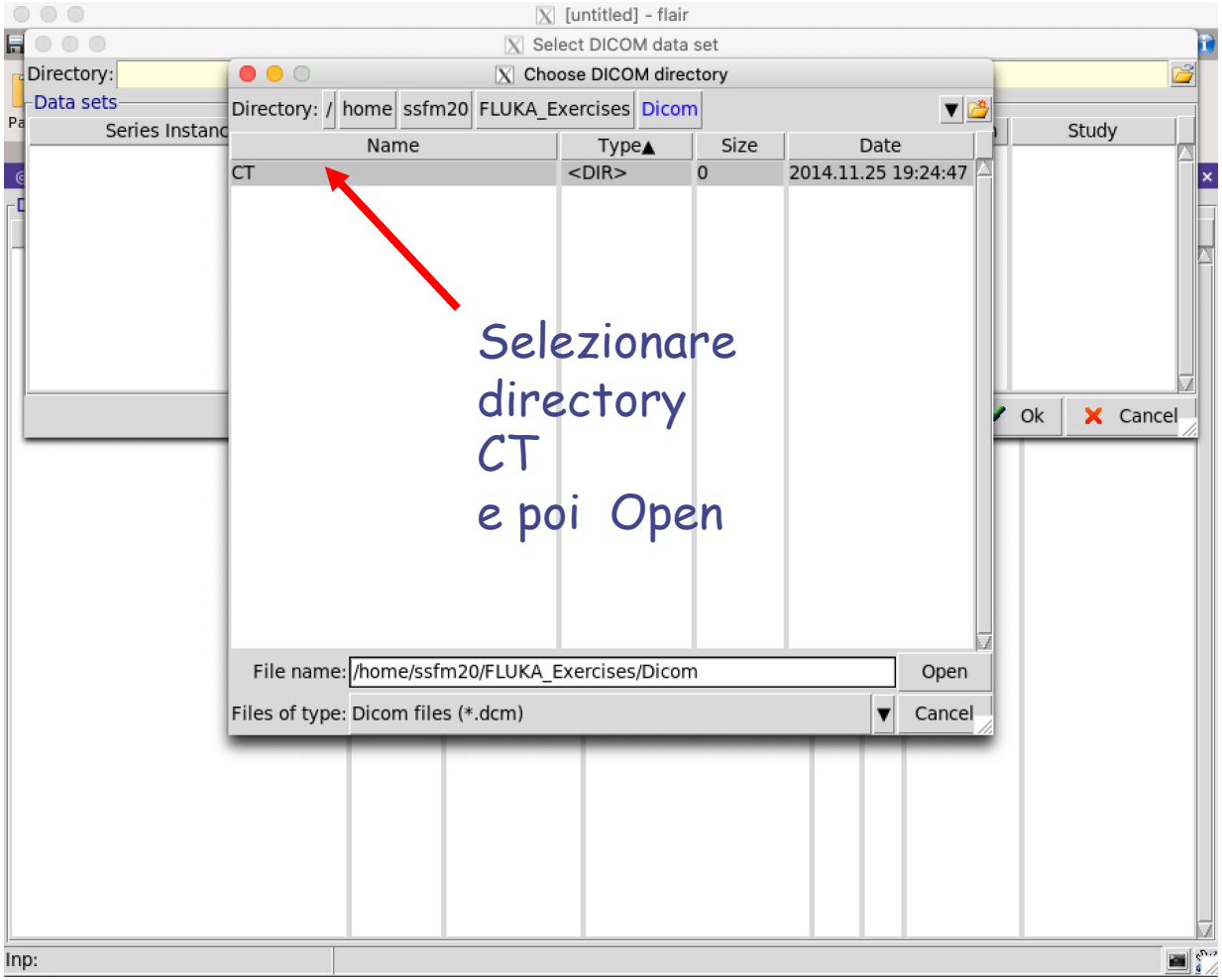


Selezionare New input di tipo voxel

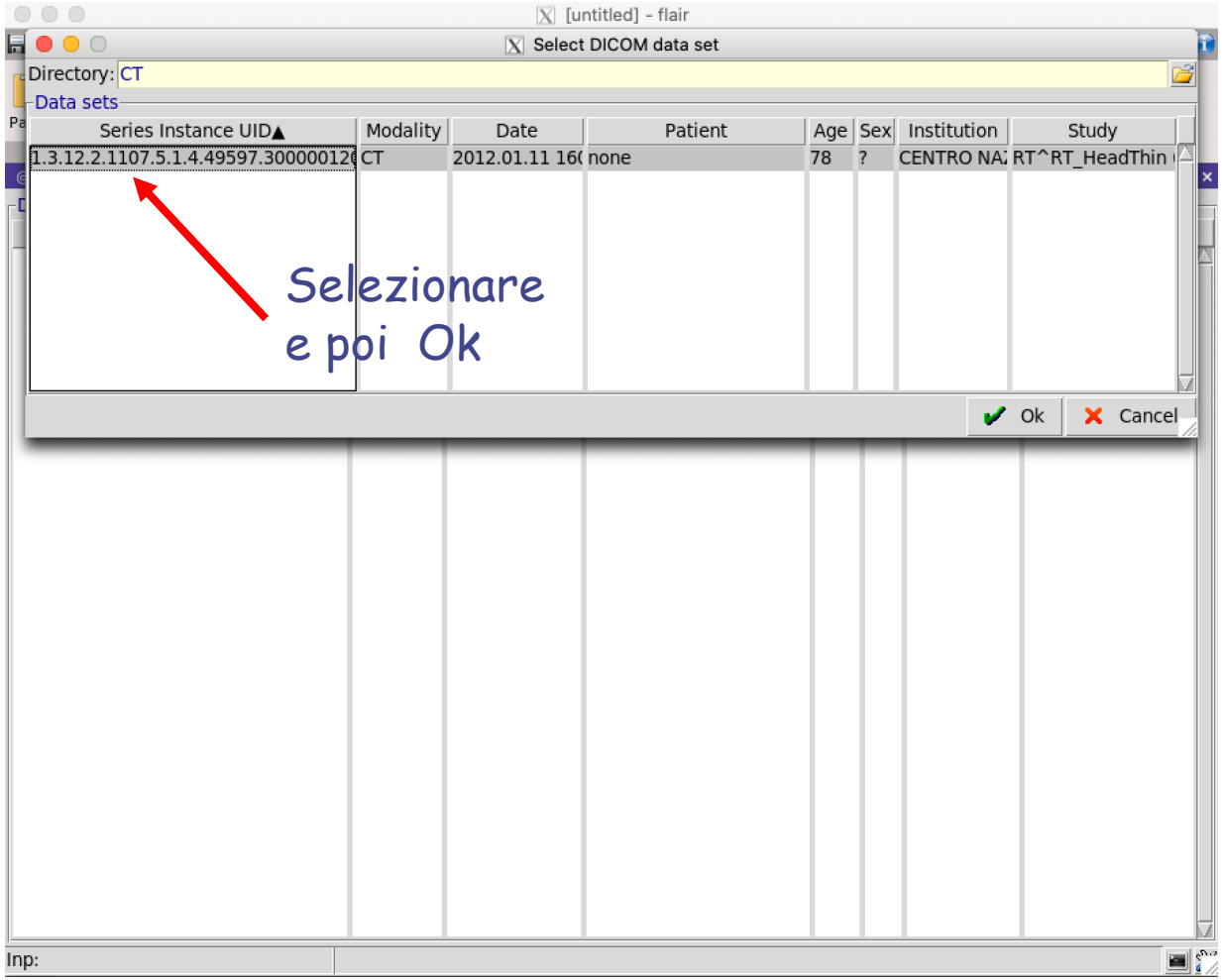


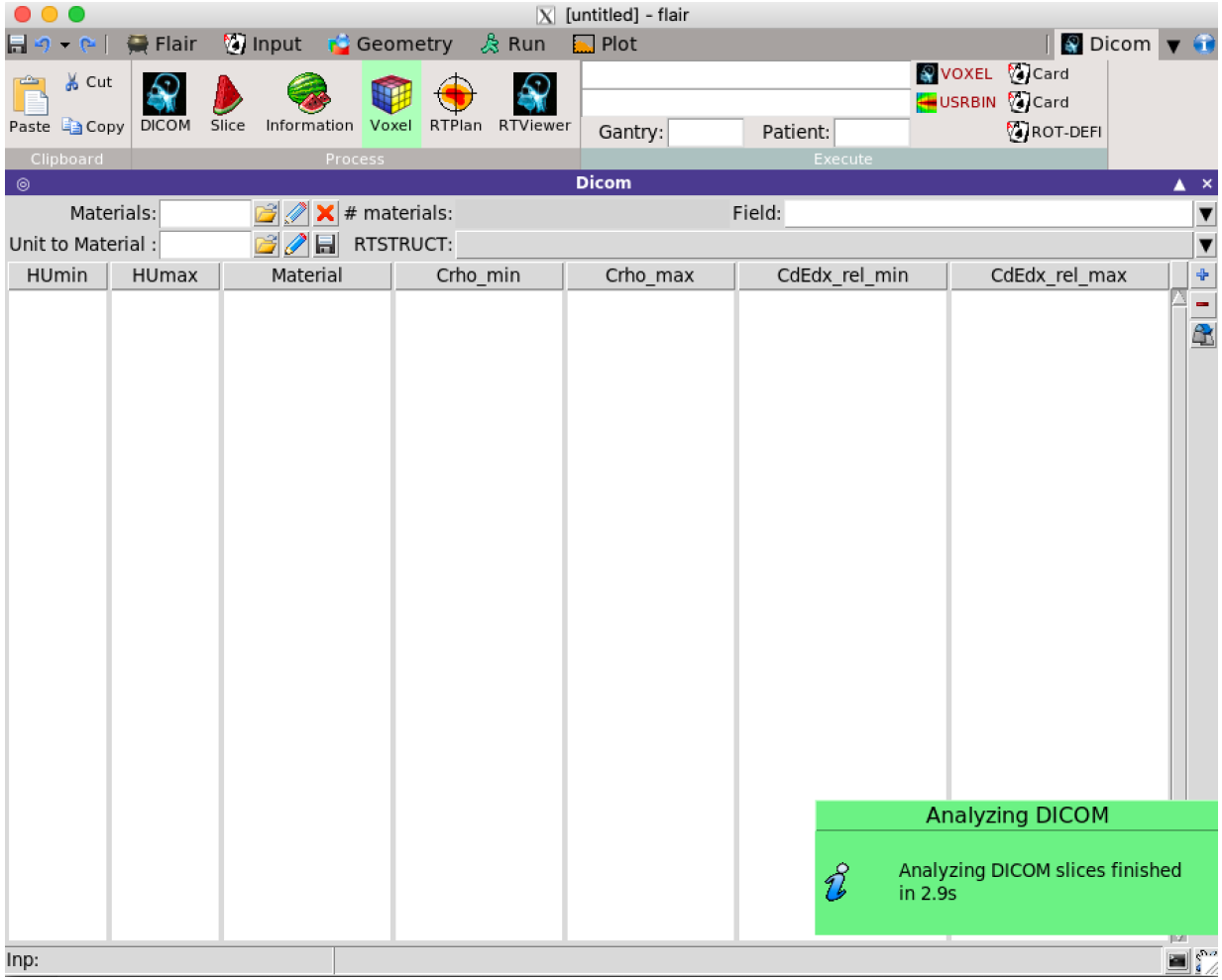
Selezionare Dicom


Selezionare Add
[untitled] - flair
Flair
Input
Geometry
Run
Plot
Dicom
Cut
Copy
Paste
DICOM
Slice
Information
Voxel
RTPlan
RTViewer
Add
Delete
Change
Clone
Clipboard
Process
Set?
Dicom
Data sets
Series Instance UID
Modality
Date
Patient
Age
Sex
Institution
Study
Inp:

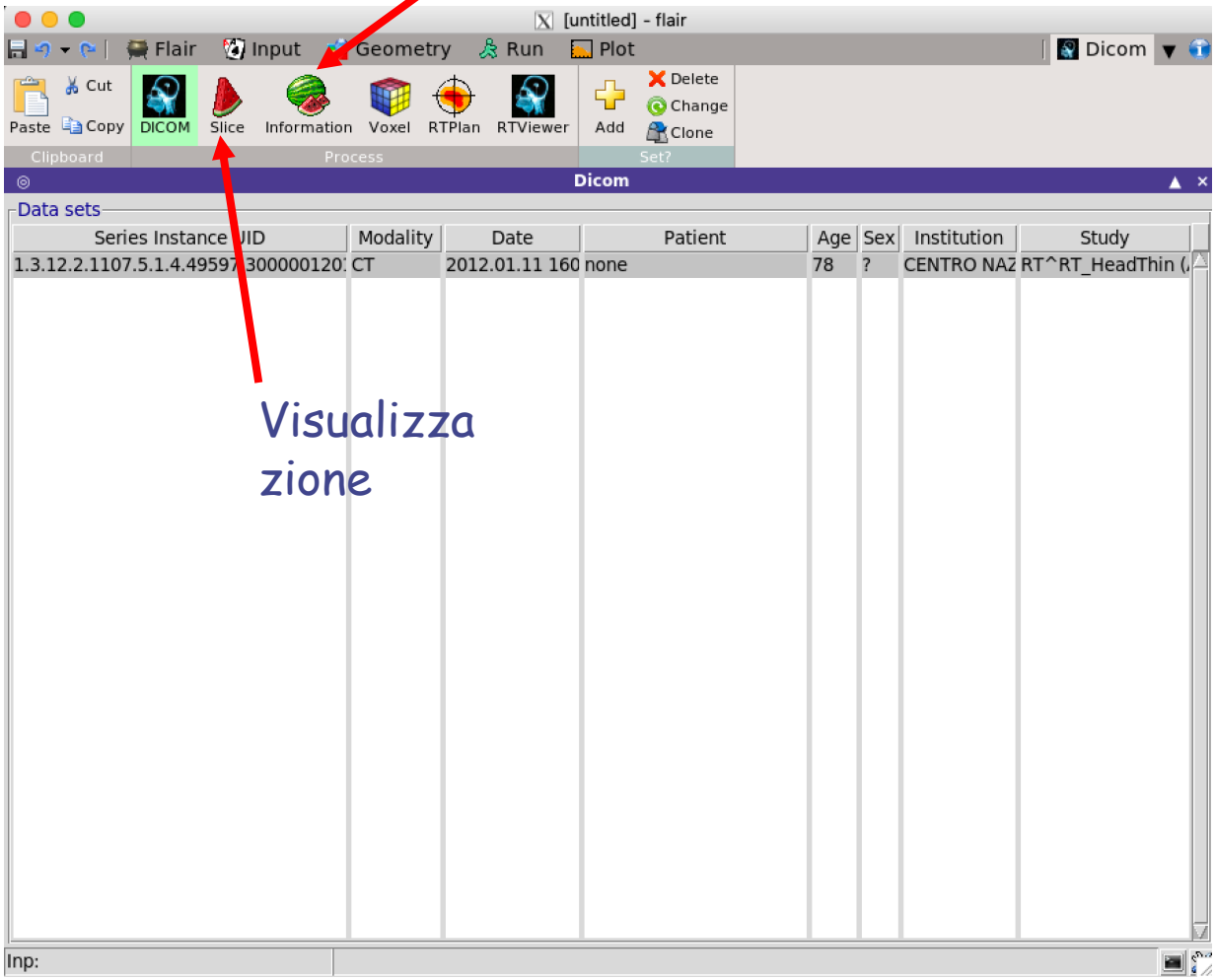


La directory CT contiene tutti i files di una dicom (anonimizzata) di un paziente

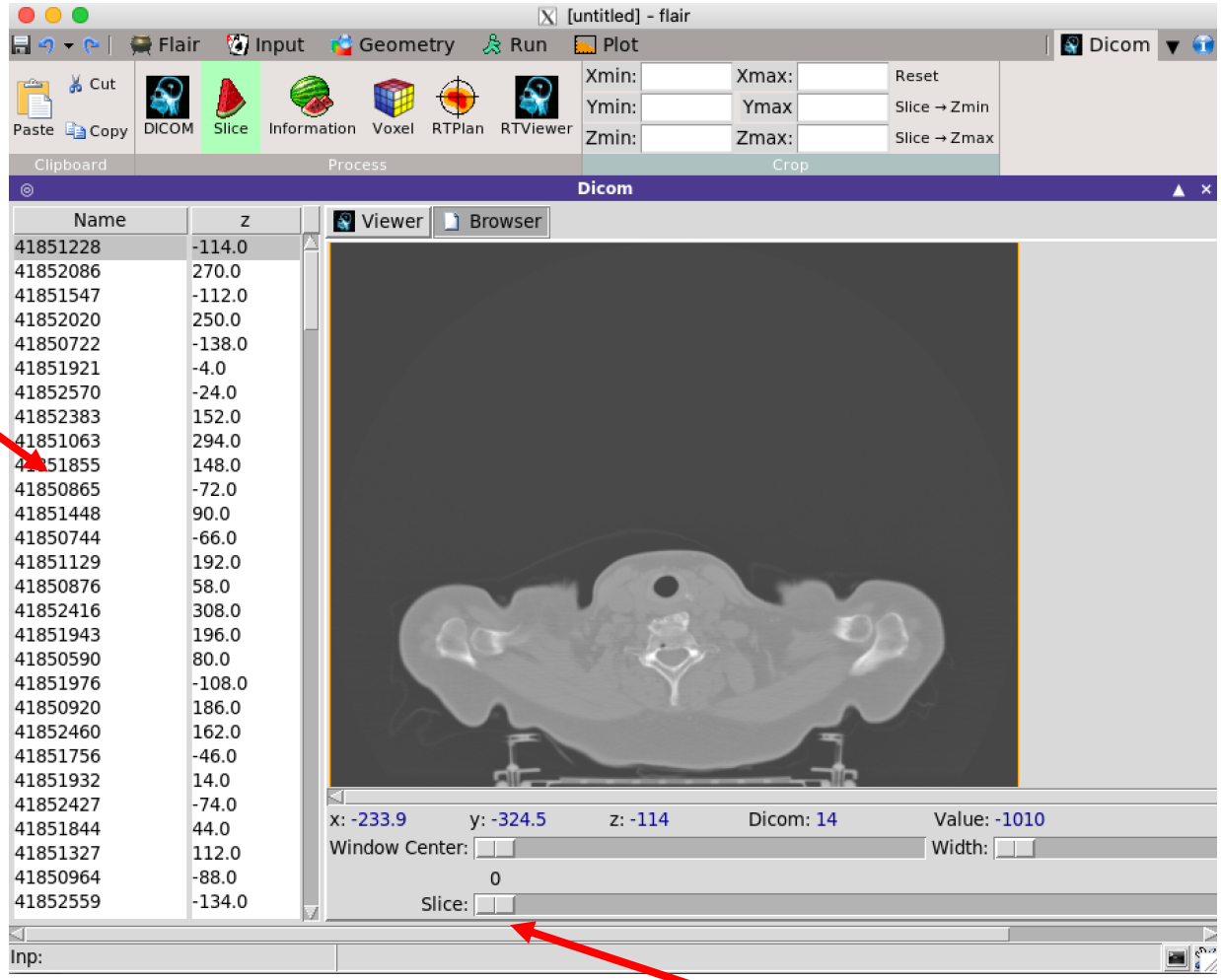

[untitled] - flair
Select DICOM data set
Directory: CT
Data sets
Series Instance UID▲
Modality
Date
Patient
Age
Sex
Institution
Study
1.3.12.2.1107.5.1.4.49597.300000126
CT
2012.01.11 16(
none
78
?
CENTRO NA
RT^RT_HeadThin
Selezionare
e poi Ok
Ok
Cancel
Inp:


[untitled] - flair
Flair
Input
Geometry
Run
Plot
Dicom
Paste
Cut
Copy
DICOM
Slice
Information
Voxel
RTPlan
RTViewer
VOXEL
Card
USRBIN
Card
ROT-DEFI
Gantry:
Patient:
Clipboard
Process
Execute
Dicom
Materials:
materials:
Field:
Unit to Material :
RTSTRUCT:
HUmin
HUmax
Material
Crho_min
Crho_max
CdEdx_rel_min
CdEdx_rel_max
Analyzing DICOM
Analyzing DICOM slices finished in 2.9s
Inp:

Accesso alle informazioni



Visualizza zione



Lista delle slices

Cursore per scorrimento slices

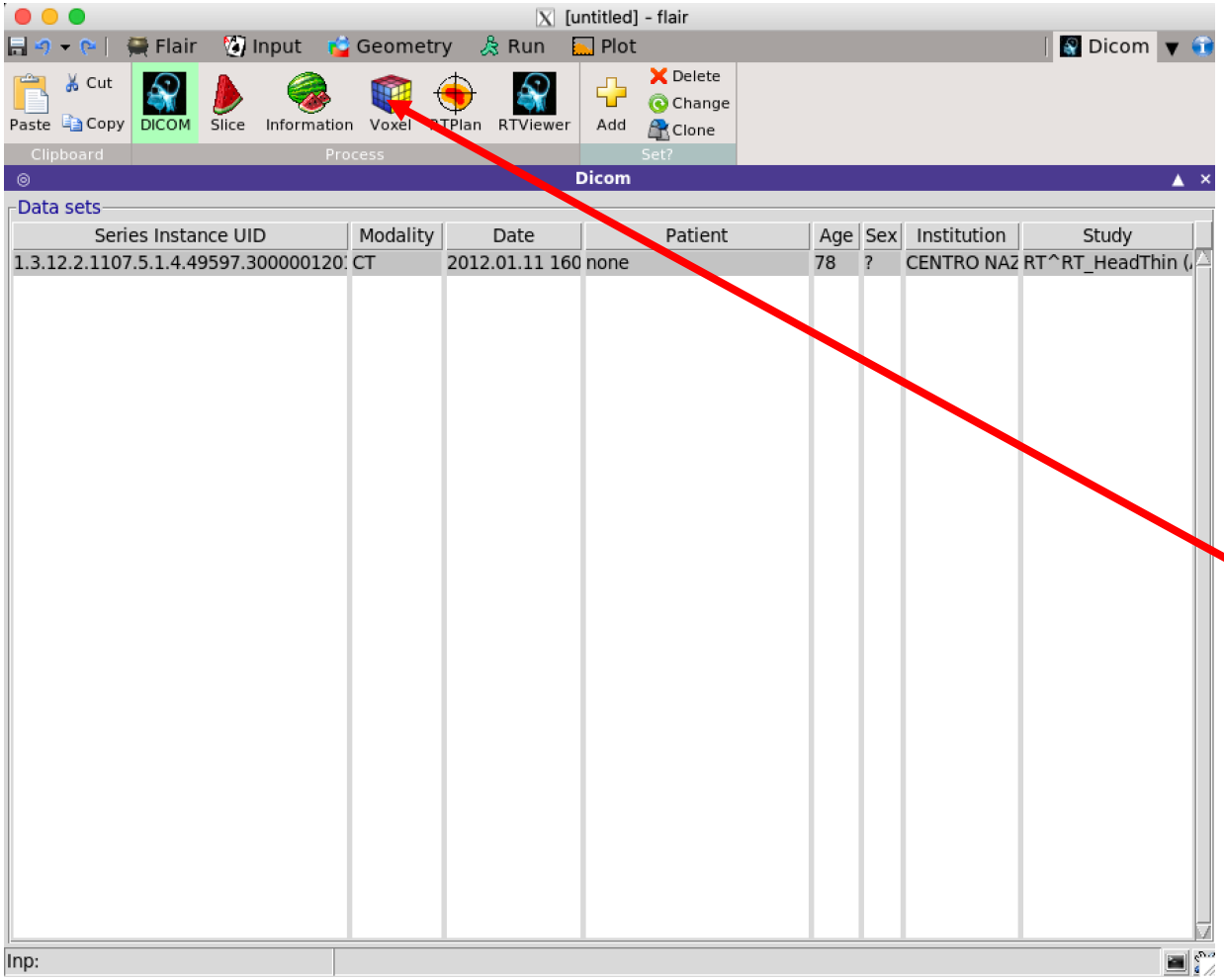
From CT to FLUKA Voxel Geometry

We will use loosely the word "organ" to indicate a group o fvoxels (or even more than one group) made of the same "tissue" material (same HU value or in a given HU interval)

1. Assign an organ index to each voxel. In many practical cases, the user will have a continuum of CT values (HU), and may have to group these values in intervals
2. Each organ is identified by a unique integer≤32767. The organ numbering does not need to be contiguous i.e. "holes" in the numbering sequence a are allowed.
3. One of the organs must have number **0** and plays the role of the medium surrounding the voxels (usually vacuum or air).
4. Assign to each NON ZERO organ a voxel-region number. The voxel-region numbering has to be contiguous and starts from1 .

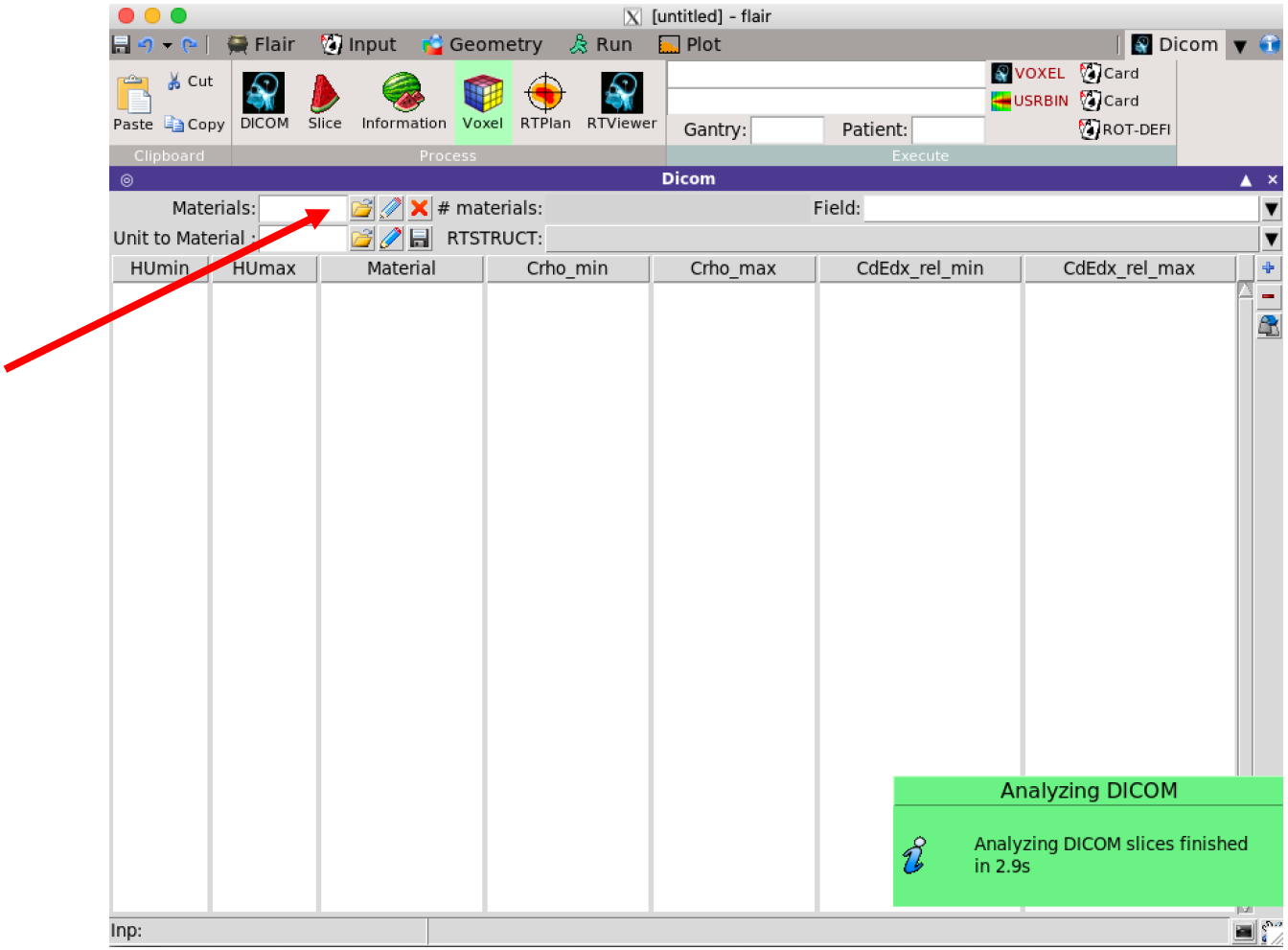
The FLUKA voxel geometry

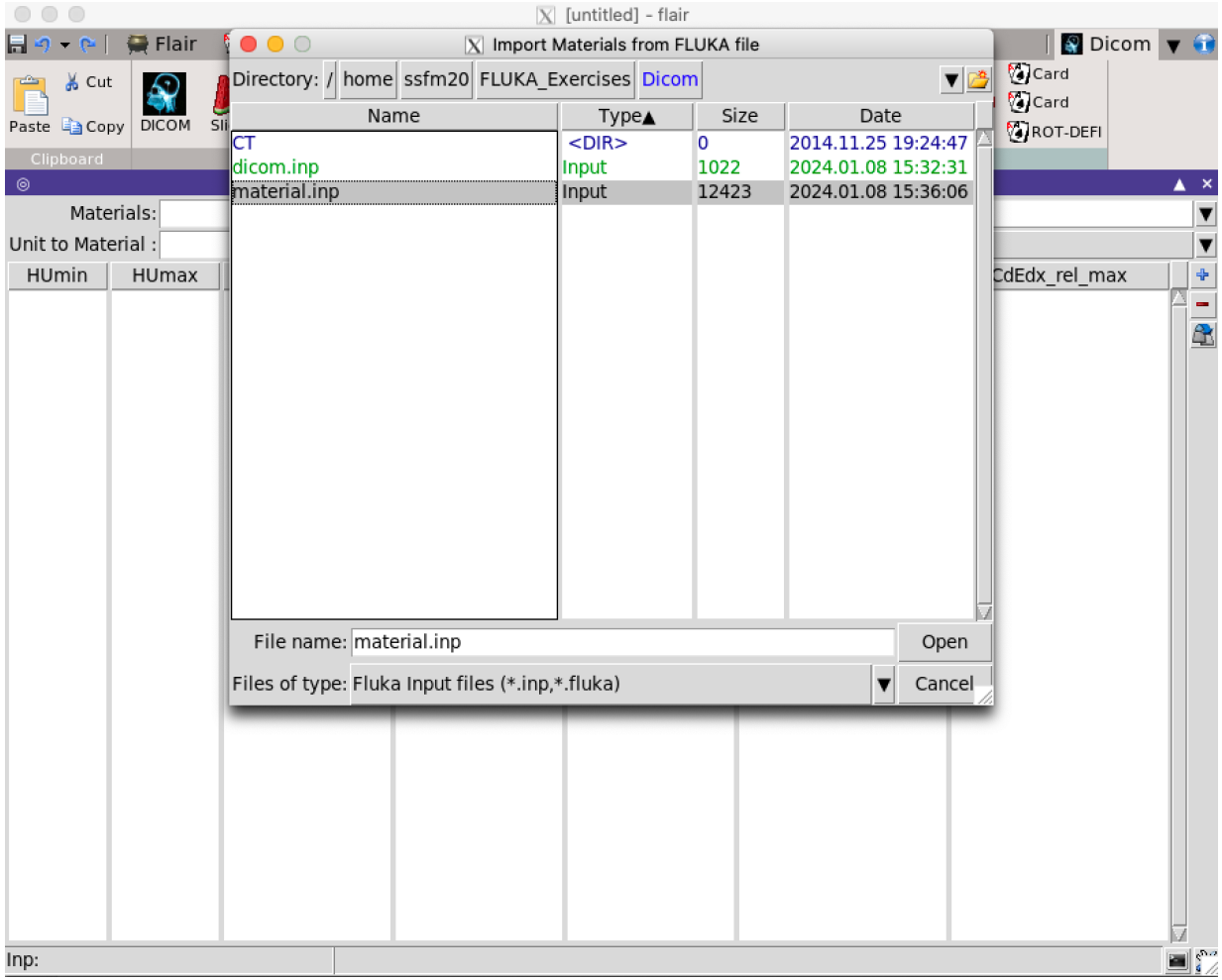
- All CT information can be given as input to FLUKA through a special file *vxl containing:
  - The number of voxels in each coordinate
  - The number of voxel-regions, and the maximum organ number
  - The voxel dimension in each coordinate
  - A list of the organ corresponding to each voxel
  - A list of the voxel-region number corresponding to each organ
  - Definition of Regions of Interests (ROI) A list of the ROIs for each voxel
- The code handles each organ as a Comb Geo region, possibly in addition to other conventional "non-voxel"r egions defined by the user
- The voxel structure can be complemented by parts written in the standard Combinatorial geometry
- The code assumes that the voxel structure is contained in a parallelepiped. This RPP is automatically generated from the voxel information.

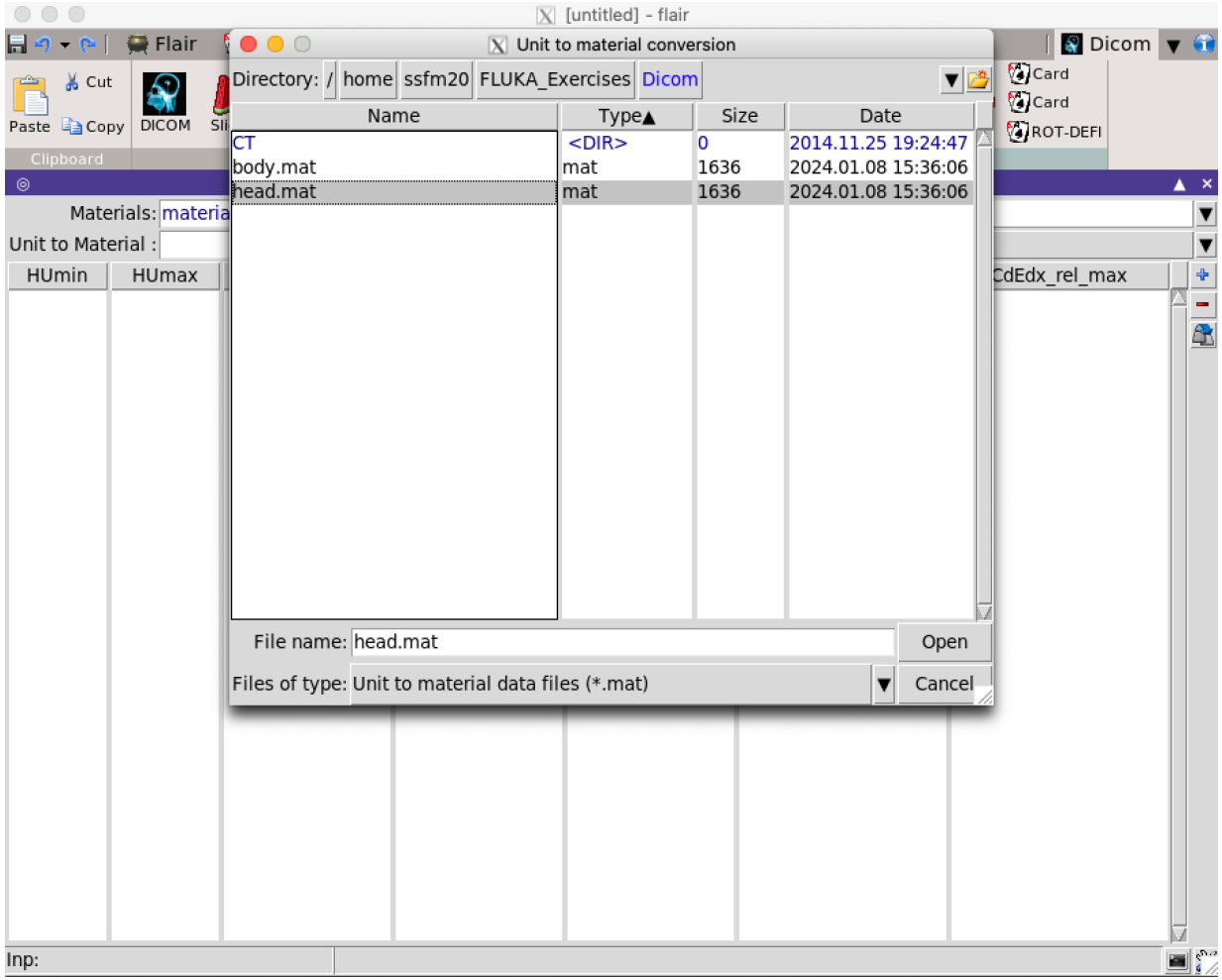


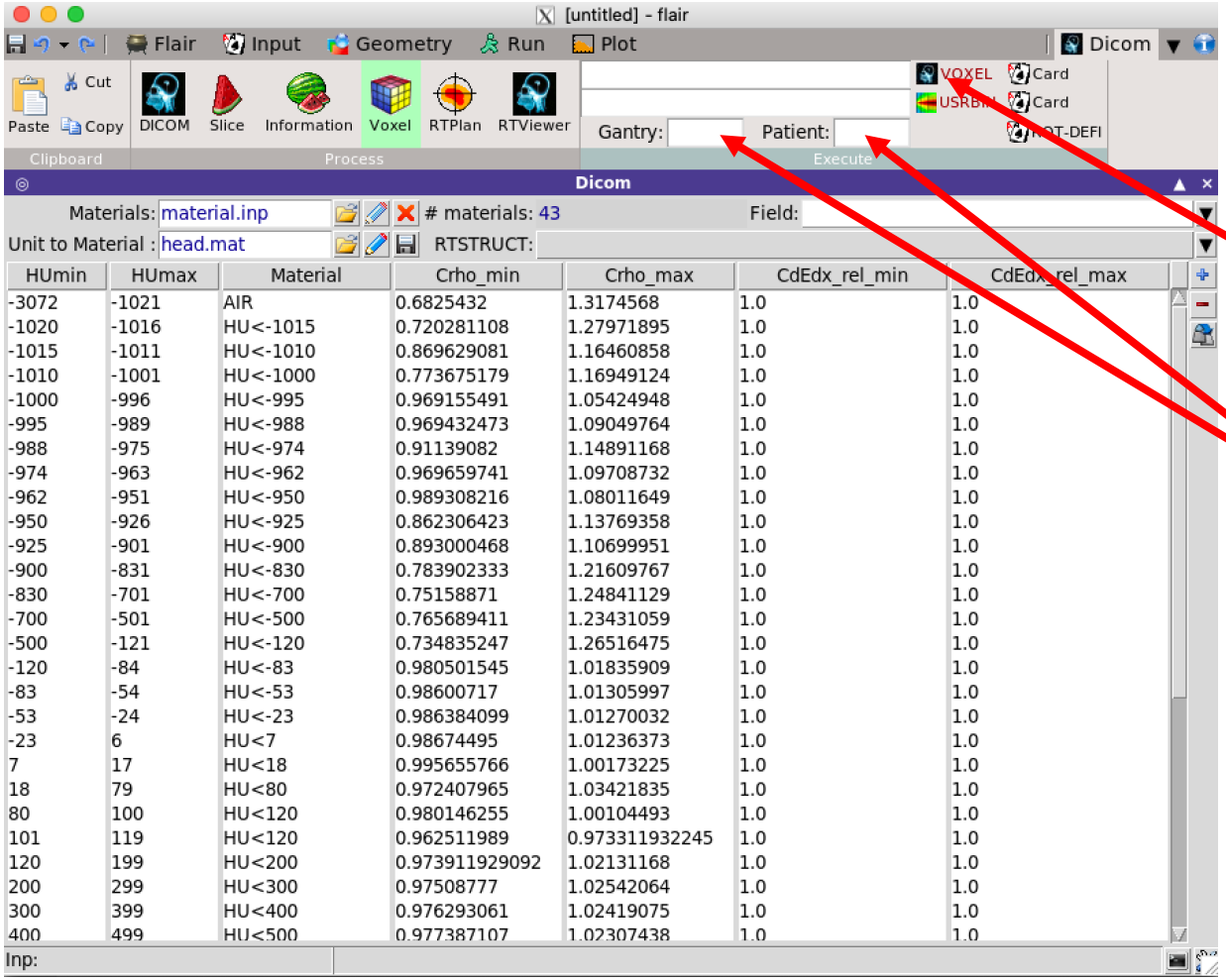
Seleziona re Voxel

Occorre caricare la conversione da numeri HU a materiali (2 files)




[untitled] - flair
Flair
Dicom
Cut
Copy
Paste
DICOM
Clipboard
Card
Card
ROT-DEFI
Import Materials from FLUKA file
Directory: / home ssfm20 FLUKA_Exercises Dicom
Name
Type▲
Size
Date
CT
<DIR>
0
2014.11.25 19:24:47
dicom.inp
Input
1022
2024.01.08 15:32:31
material.inp
Input
12423
2024.01.08 15:36:06
File name: material.inp
Open
Files of type: Fluka Input files (*.inp,*.fluka)
Cancel
Materials:
Unit to Material :
HUmin
HUmax
CdEdx_rel_max
Inp:


[untitled] - flair
Flair
Dicom
Cut
Copy
Paste
DICOM
Clipboard
Card
Card
ROT-DEFI
Unit to material conversion
Directory: / home ssfm20 FLUKA_Exercises Dicom
Name
Type▲
Size
Date
CT
<DIR>
0
2014.11.25 19:24:47
body.mat
mat
1636
2024.01.08 15:36:06
head.mat
mat
1636
2024.01.08 15:36:06
File name: head.mat
Open
Files of type: Unit to material data files (*.mat)
Cancel
Materials:
Unit to Material :
HUmin
HUmax
CdEdx_rel_max
Inp:



HUmin	HUmax	Material	Crho_min	Crho_max	CdEdx_rel_min	CdEdx_rel_max
-3072	-1021	AIR	0.6825432	1.3174568	1.0	1.0
-1020	-1016	HU<-1015	0.720281108	1.27971895	1.0	1.0
-1015	-1011	HU<-1010	0.869629081	1.16460858	1.0	1.0
-1010	-1001	HU<-1000	0.773675179	1.16949124	1.0	1.0
-1000	-996	HU<-995	0.969155491	1.05424948	1.0	1.0
-995	-989	HU<-988	0.969432473	1.09049764	1.0	1.0
-988	-975	HU<-974	0.91139082	1.14891168	1.0	1.0
-974	-963	HU<-962	0.969659741	1.09708732	1.0	1.0
-962	-951	HU<-950	0.989308216	1.08011649	1.0	1.0
-950	-926	HU<-925	0.862306423	1.13769358	1.0	1.0
-925	-901	HU<-900	0.893000468	1.10699951	1.0	1.0
-900	-831	HU<-830	0.783902333	1.21609767	1.0	1.0
-830	-701	HU<-700	0.75158871	1.24841129	1.0	1.0
-700	-501	HU<-500	0.765689411	1.23431059	1.0	1.0
-500	-121	HU<-120	0.734835247	1.26516475	1.0	1.0
-120	-84	HU<-83	0.980501545	1.01835909	1.0	1.0
-83	-54	HU<-53	0.98600717	1.01305997	1.0	1.0
-53	-24	HU<-23	0.986384099	1.01270032	1.0	1.0
-23	6	HU<7	0.98674495	1.01236373	1.0	1.0
7	17	HU<18	0.995655766	1.00173225	1.0	1.0
18	79	HU<80	0.972407965	1.03421835	1.0	1.0
80	100	HU<120	0.980146255	1.00104493	1.0	1.0
101	119	HU<120	0.962511989	0.973311932245	1.0	1.0
120	199	HU<200	0.973911929092	1.02131168	1.0	1.0
200	299	HU<300	0.97508777	1.02542064	1.0	1.0
300	399	HU<400	0.976293061	1.02419075	1.0	1.0
400	499	HU<500	0.977387107	1.02307438	1.0	1.0

Selezionare Voxel per generare il file di geometria e caricarlo nell'input

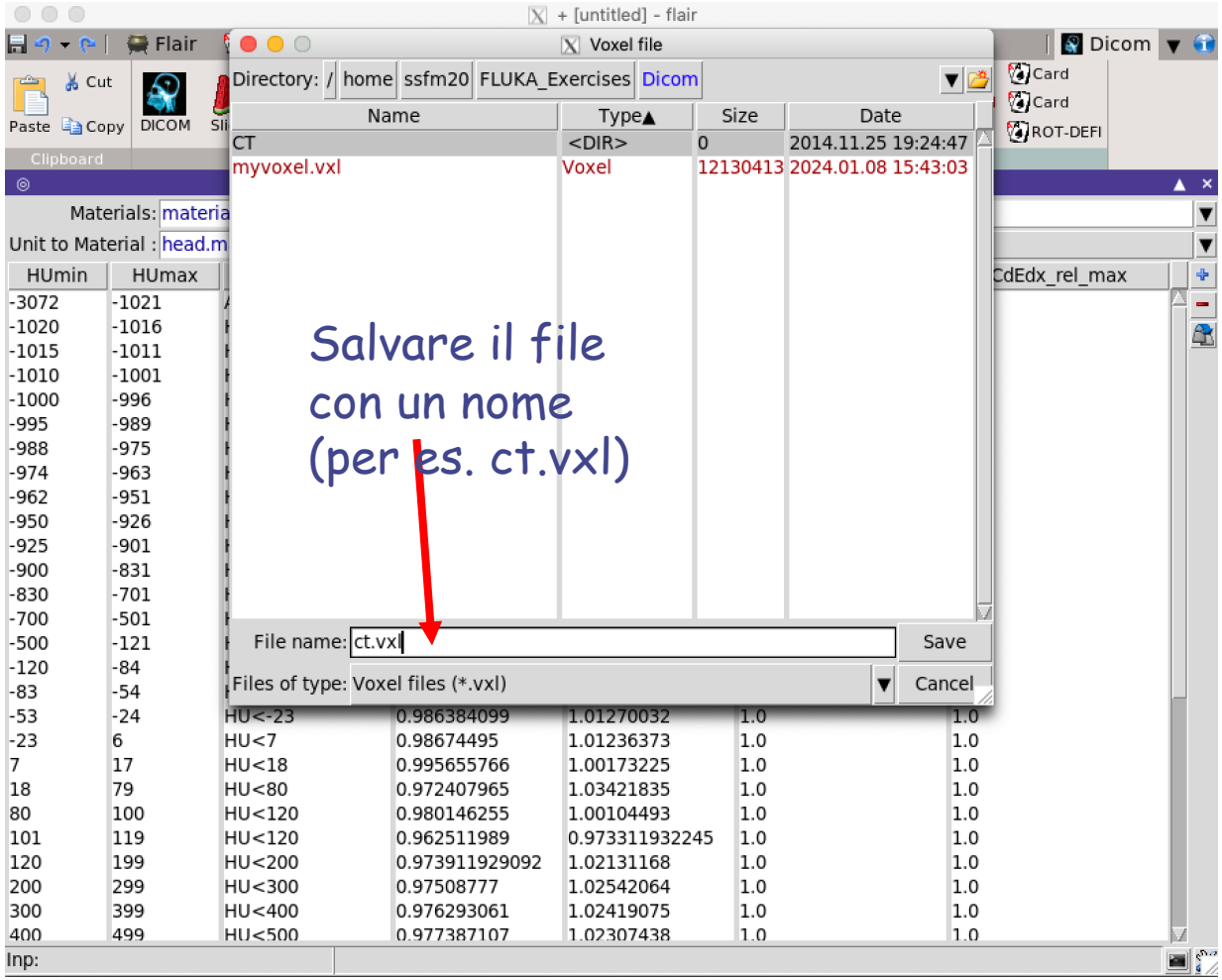
E' possibile introdurre angoli di rotazione e coordinate di traslazione

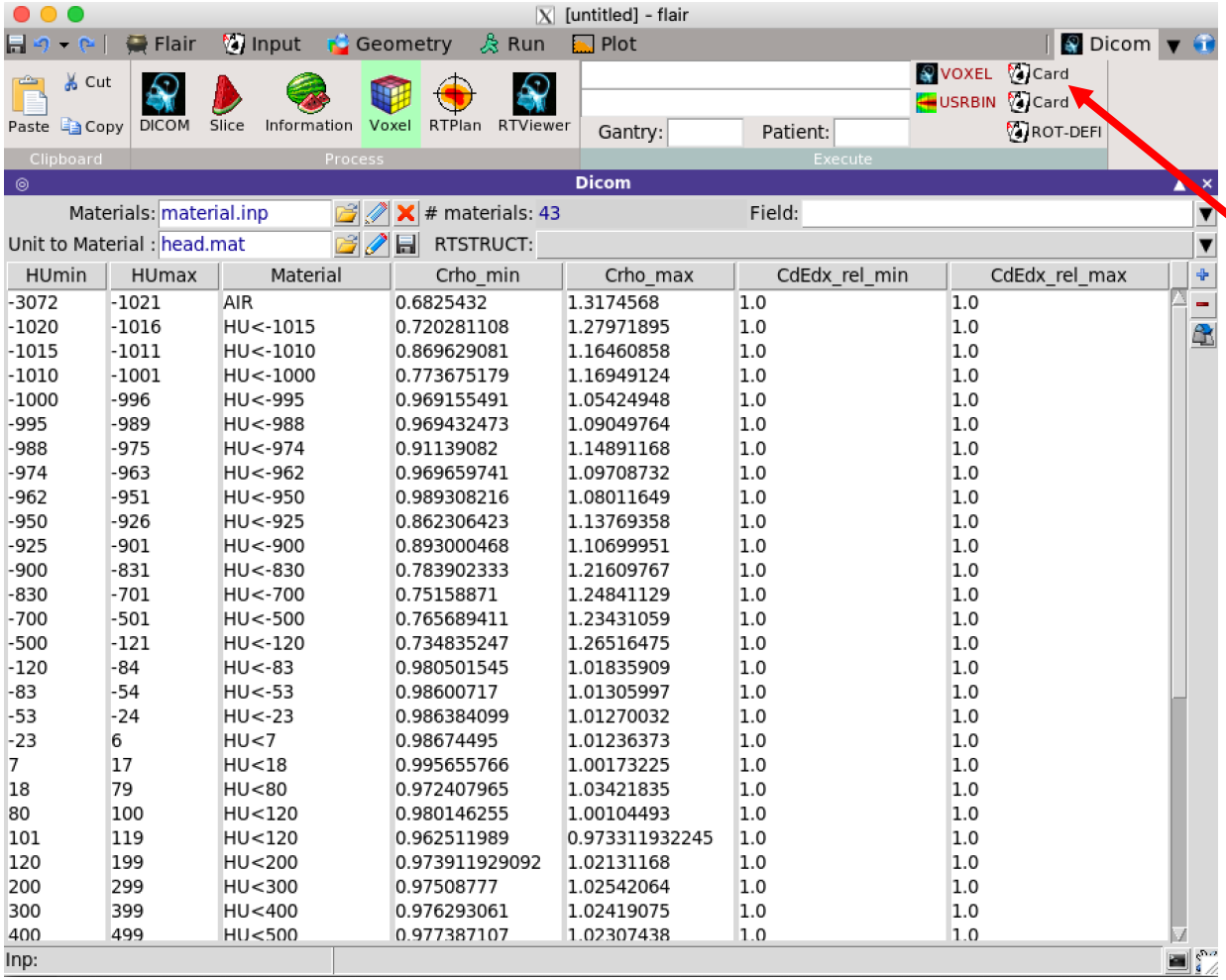
- <= Unit: specify the upper limit of the range. Every entry will correspond to a range from the previous upper limit+1 until the current upper limit.
- Material: select any of the predefined FLUKA materials defined previously.

Optionally you can specify correction factors for the density and dE/dx

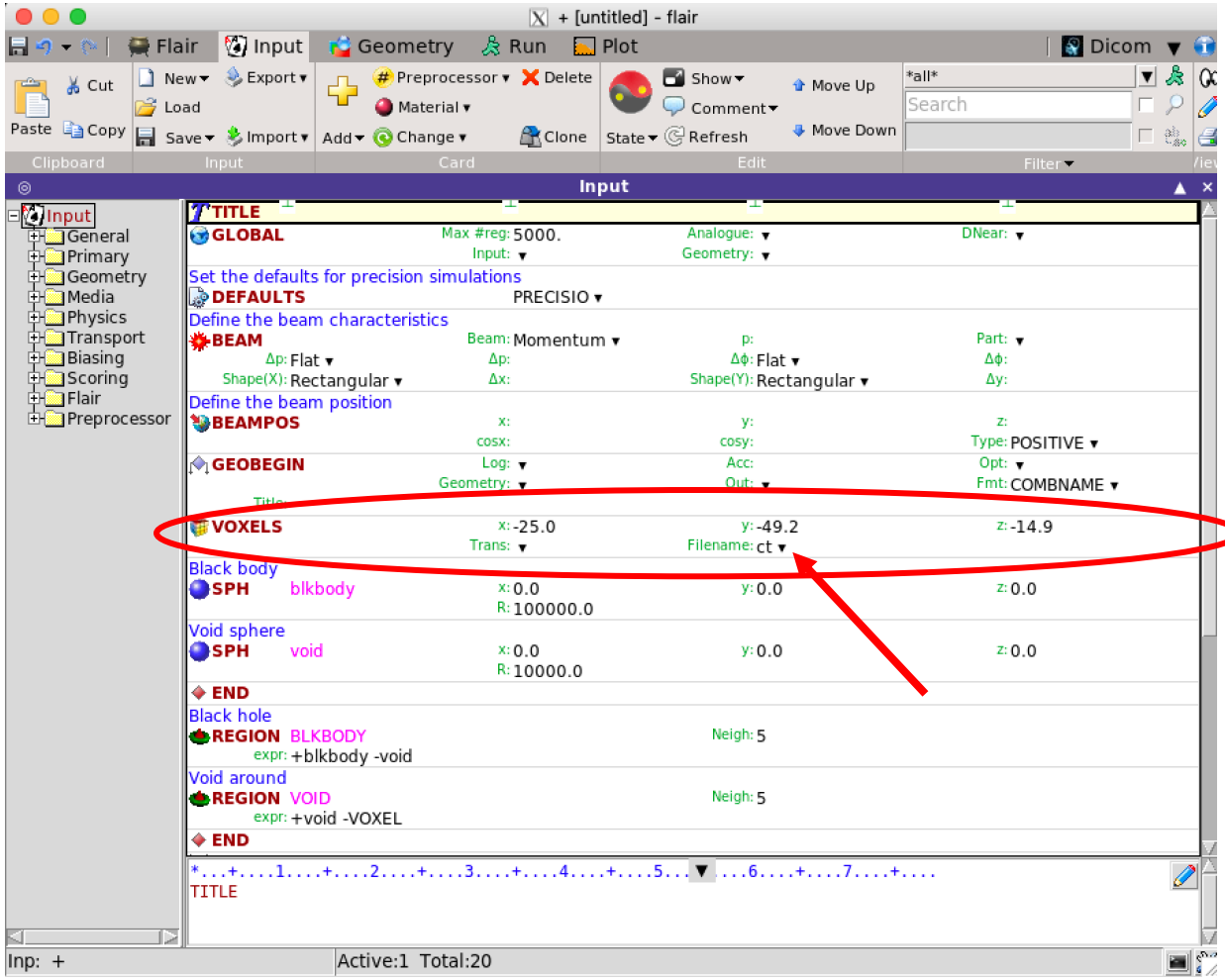
- Crho_min/Chro_max: density correction factors to be applied on the lower/upper limit of the unit range (see next slides).
- CdEdx_rel_min/CdEdx_rel_max: relative correction factors on dE/dx for minimum/maximum unit in the range (see next slides)

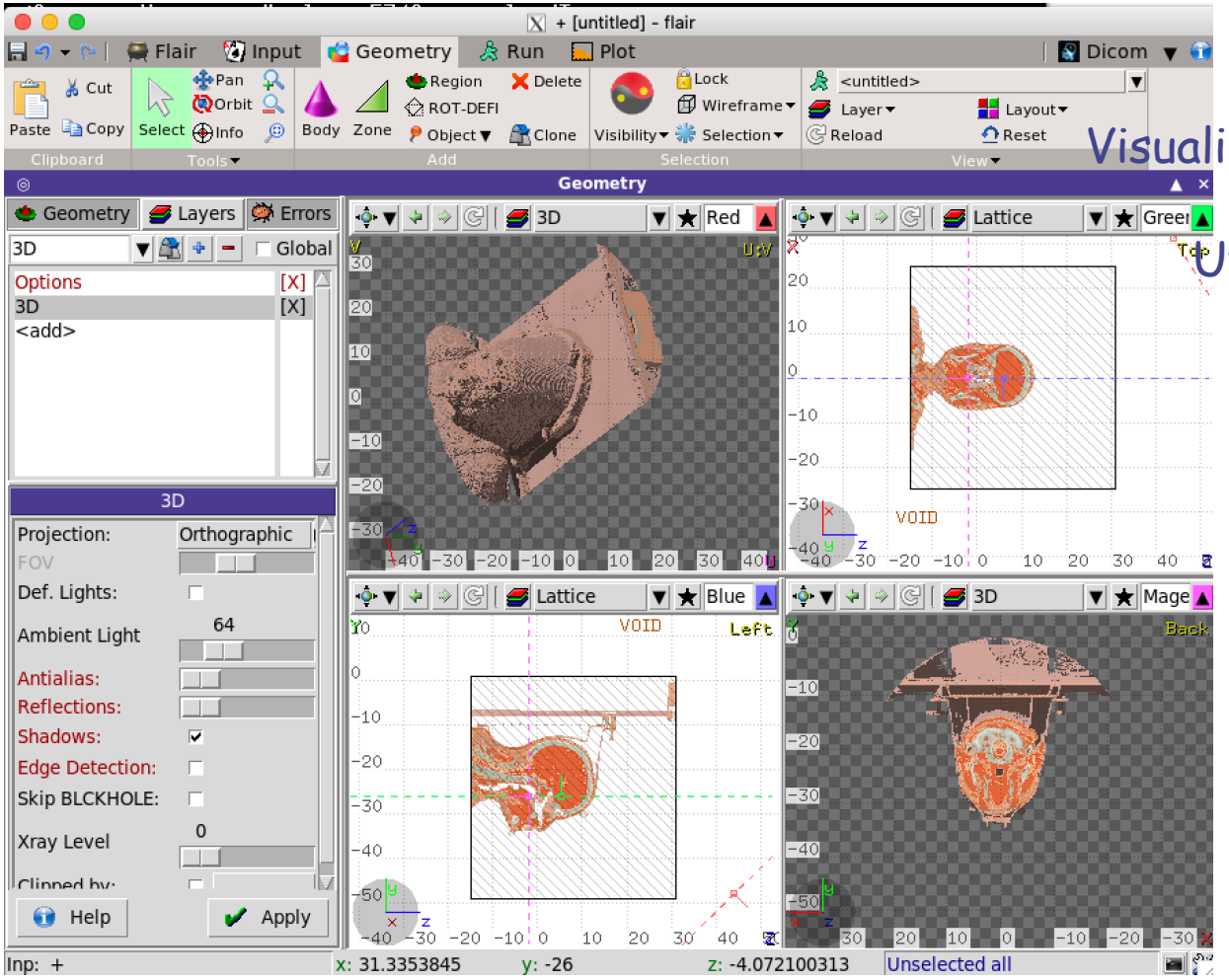
≤ Unit	Material	Crho_min	Crho_max	CdEdx_rel_min	CdEdx_rel_max
-1020	AIR	0.6825432	1.3174568	1.0	1.0
-1015	HU<-1015	0.720281108	1.27971895	1.0	1.0
-1010	HU<-1010	0.869629081	1.16460858	1.0	1.0
-1000	HU<-1000	0.773675179	1.16949124	1.0	1.0
-995	HU<-995	0.969155491	1.05424948	1.0	1.0
-988	HU<-988	0.969432473	1.09049764	1.0	1.0
-974	HU<-974	0.91139082	1.14891168	1.0	1.0
-962	HU<-962	0.969659741	1.09708732	1.0	1.0
-950	HU<-950	0.989308216	1.08011649	1.0	1.0
-925	HU<-925	0.862306423	1.13769358	1.0	1.0
-900	HU<-900	0.893000468	1.10699951	1.0	1.0
-830	HU<-830	0.783902333	1.21609767	1.0	1.0
-700	HU<-700	0.75158871	1.24841129	1.0	1.0
-500	HU<-500	0.765689411	1.23431059	1.0	1.0
-120	HU<-120	0.734835247	1.26516475	1.0	1.0
-83	HU<-83	0.980501545	1.01835909	1.0	1.0
-53	HU<-53	0.98600717	1.01305997	1.0	1.0


+ [untitled] - flair
Flair
Dicom
Cut
Copy
Paste
DICOM
Clipboard
Card
Card
ROT-DEFI
Voxel file
Directory: / home ssfm20 FLUKA_Exercises Dicom
Name
Type
Size
Date
CT
<DIR>
0
2014.11.25 19:24:47
myvoxel.vxl
Voxel
12130413
2024.01.08 15:43:03
Salvare il file
con un nome
(per es. ct.vxl)
File name: ct.vxl
Save
Files of type: Voxel files (*.vxl)
Cancel
Materials:
Unit to Material :
HUmin
HUmax
CdEdx_rel_max
-3072 -1021
-1020 -1016
-1015 -1011
-1010 -1001
-1000 -996
-995 -989
-988 -975
-974 -963
-962 -951
-950 -926
-925 -901
-900 -831
-830 -701
-700 -501
-500 -121
-120 -84
-83 -54
-53 -24 HU<-23 0.986384099 1.01270032 1.0 1.0
-23 6 HU<7 0.98674495 1.01236373 1.0 1.0
7 17 HU<18 0.995655766 1.00173225 1.0 1.0
18 79 HU<80 0.972407965 1.03421835 1.0 1.0
80 100 HU<120 0.980146255 1.00104493 1.0 1.0
101 119 HU<120 0.962511989 0.973311932245 1.0 1.0
120 199 HU<200 0.973911929092 1.02131168 1.0 1.0
200 299 HU<300 0.97508777 1.02542064 1.0 1.0
300 399 HU<400 0.976293061 1.02419075 1.0 1.0
400 499 HU<500 0.977387107 1.02307438 1.0
Inp:



Selezionare Card per aggiungere in input l'istruzione di carcicare il file voxel appena generato


+ [untitled] - flair
Flair
Input
Geometry
Run
Plot
Dicom
Paste
Cut
Copy
New
Load
Save
Export
Import
Preprocessor
Material
Add
Change
Delete
Clone
Show
Comment
State
Refresh
Move Up
Move Down
all
Search
Clipboard
Input
Card
Edit
Filter
Input
Input
General
Primary
Geometry
Media
Physics
Transport
Biasing
Scoring
Flair
Preprocessor
TITLE
GLOBAL
Max #reg: 5000.
Input:
Analogue:
Geometry:
DNear:
Set the defaults for precision simulations
DEFAULTS
PRECISIO
Define the beam characteristics
BEAM
Beam: Momentum
p:
Part:
Δp: Flat
Δp:
Δϕ: Flat
Δϕ:
Shape(X): Rectangular
Δx:
Shape(Y): Rectangular
Δy:
Define the beam position
BEAMPOS
x:
y:
z:
cosx:
cosy:
Type: POSITIVE
GEOBEGIN
Log:
Acc:
Opt:
Geometry:
Out:
Fmt: COMBNAME
VOXELS
x: -25.0
y: -49.2
z: -14.9
Trans:
Filename: ct
Black body
SPH blkbody
x: 0.0
y: 0.0
z: 0.0
R: 100000.0
Void sphere
SPH void
x: 0.0
y: 0.0
z: 0.0
R: 10000.0
END
Black hole
REGION BLKBODY
Neigh: 5
expr: +blkbody -void
Void around
REGION VOID
Neigh: 5
expr: +void -VOXEL
END
*...+....1....+....2....+....3....+....4....+....5....+....6....+....7....+....
TITLE
Inp: +
Active:1 Total:20



Visualizzazione nel tab Geometry di

Utilizzare i layers Lattice o 3D

A questo punto si potrà def

- Fascio e sua direzione/pos
- Energia
- Scoring
- ecc. ecc.