



Lattice

7th FLUKA Course
NEA Paris, Sept.29-Oct.3, 2008

Lattice

FLUKA geometry has *replication* (lattice) capabilities

Only one level is implemented (No nested lattices are allowed)

In a future release there will be possibility of a second level

- The user defines lattice positions in the geometry and provides transformation rules from the lattice to the prototype region:
 1. in the input with the ROT-DEFI card
 2. in a subroutine (`lattic.f`)

The lattice identification is available for scoring

Transformations should include:

Translation, Rotation and Mirroring.

WARNING:

Do not use scaling or any deformation of the coordinate system

In the geometry

- The regions which constitute the **elementary cell** to be replicated, have to be defined in detail
- The **Lattices** have to be defined as “empty” regions in their correct location.
WARNING: The lattice region should map exactly the outer surface definition of the elementary cell.
- The lattice regions are declared as such with a **LATTICE** card at the end of the geometry input
- In the **LATTICE** card, the user also **assigns lattice names/numbers to the lattices**. These names/numbers will identify the replicas in all FLUKA routines
- Several basic cells and associated lattices can be defined within the same geometry, one **LATTICE** card will be needed for each set
- **Non-replicas carry the lattice number 0**
- Lattices and plain regions can coexist in the same problem

LATTICE card

• After the Regions definition and before the GEOEND card the user can insert the LATTICE cards

- WHAT(1), WHAT(2), WHAT(3)
Container region range (from, to, step)
- WHAT(4), WHAT(5), WHAT(6)
Name/number(s) of the lattice(s)
- SDUM
blank to use the transformation from the lattic routine
ROT#nn to use a ROT-DEFI rotation/translation from input
name use a rotation by names. You can name a rotation using as SDUM in ROT-DEFI any alphanumeric string you like

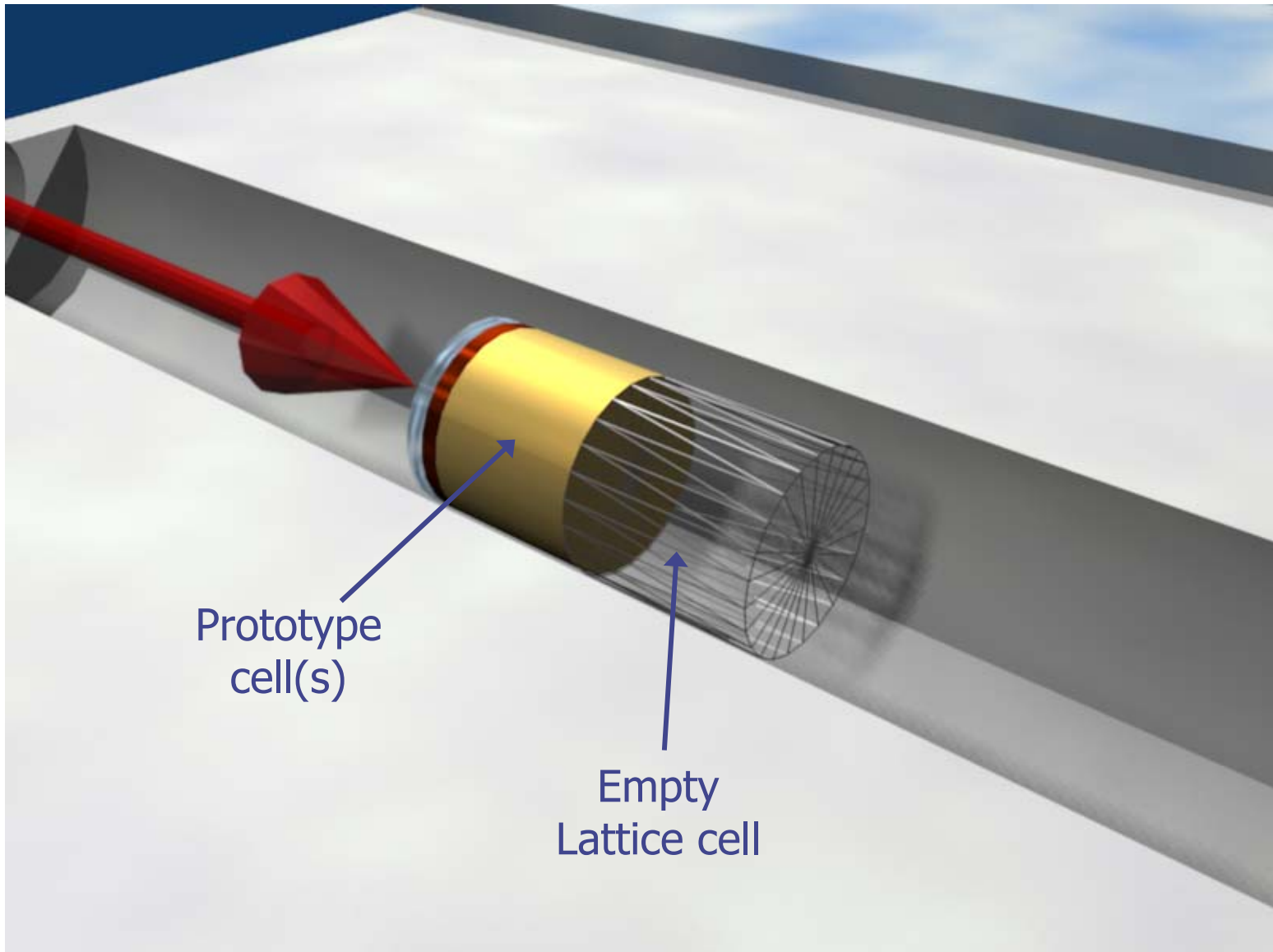
Example

```
*...+...1...+...2...+...3...+...4...+...5...+...6...+...7...+...
LATTICE          6.00000  19.00000          101.0000  114.00
```

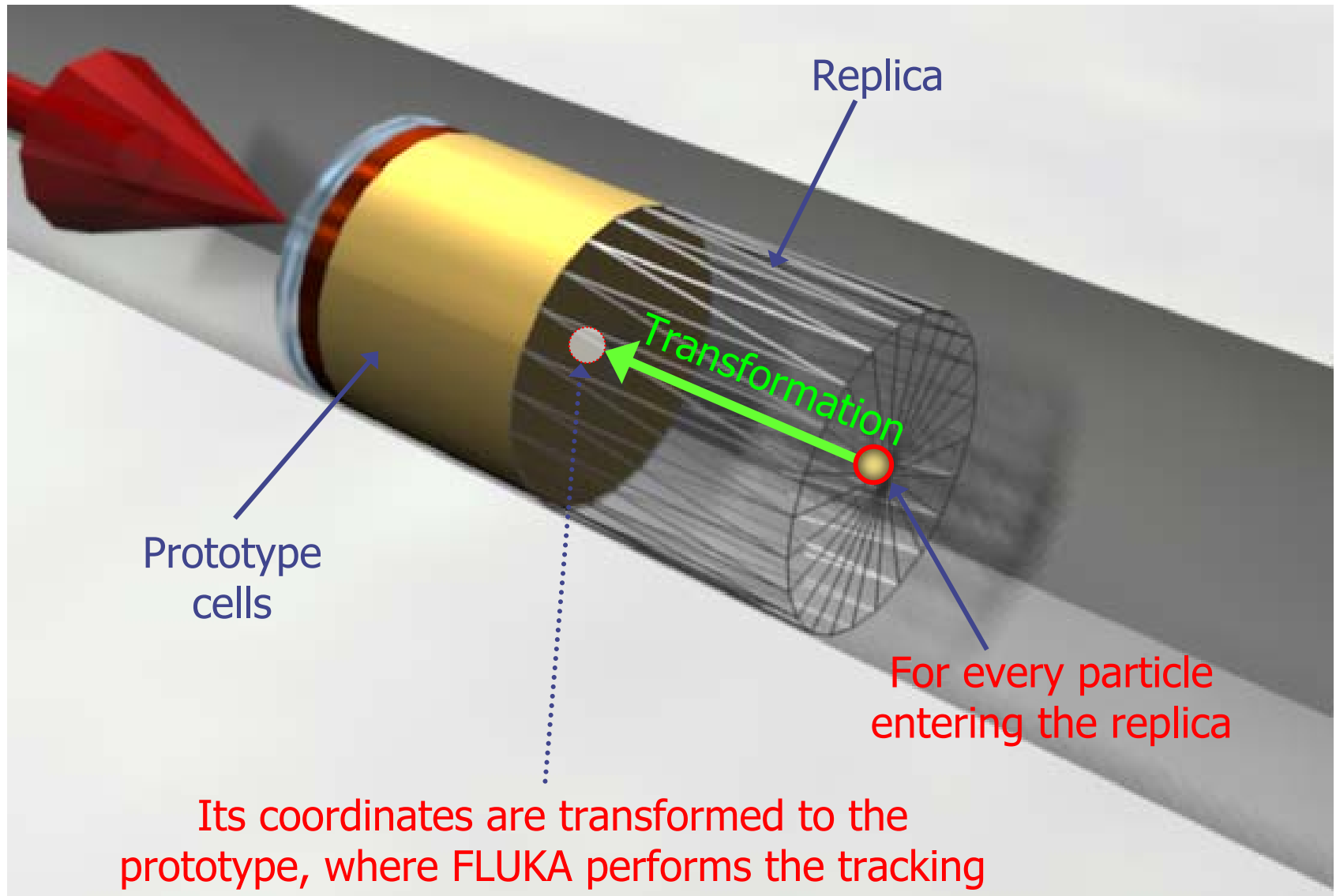
Region # 6 to 19 are the "placeholders" for the first set replicas. We assign to them lattice numbers from 101 to 114

```
LATTICE          TARGRP          TargRep          myRot
TARGRP is the container region using transformation myRot
*          rot. numb.          theta          phi          dx          dy          dz
ROT-DEFI          1.0          0.0          0.0          0.0          0.0          -10.0myRot
```

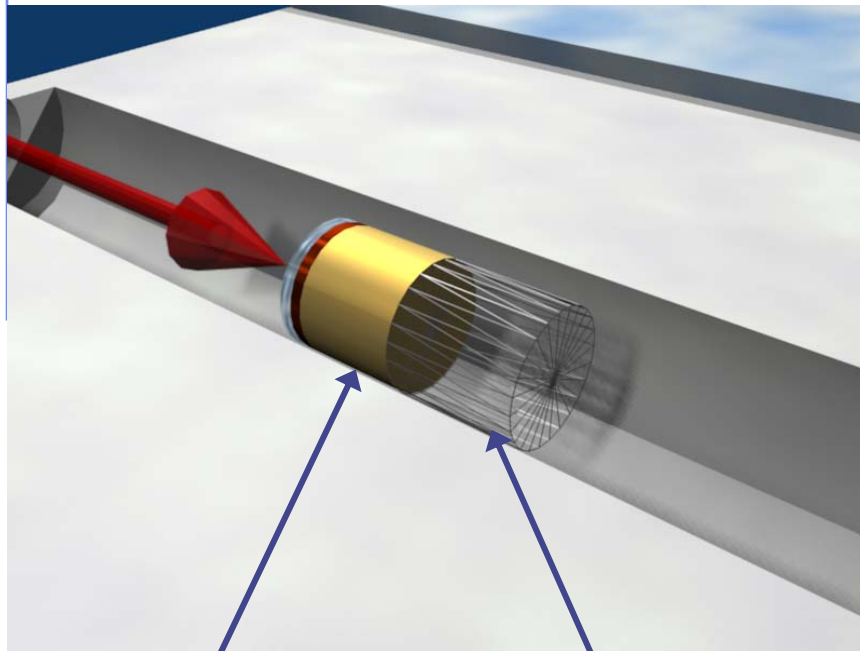
Plot of the Example



Plot of the Example

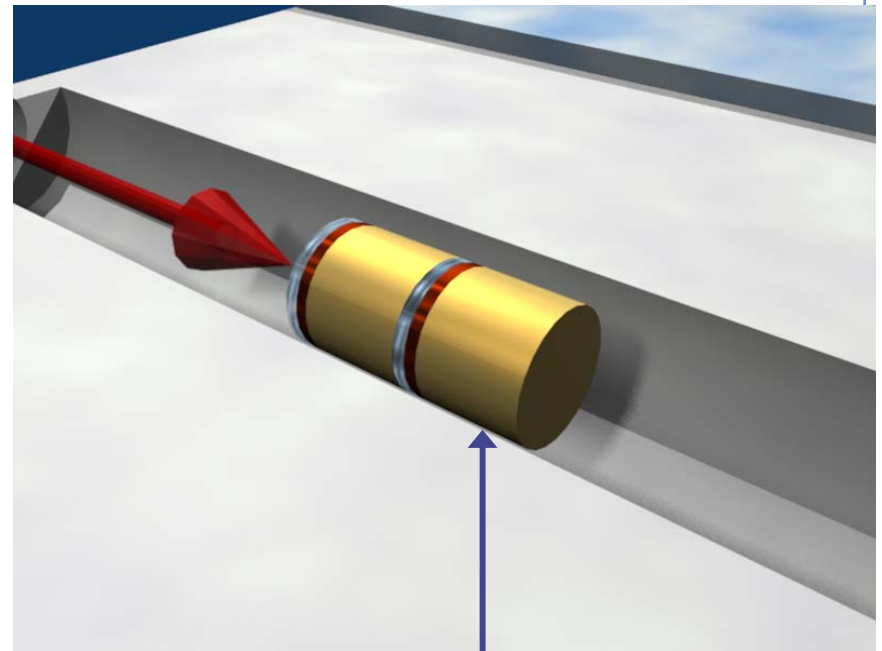


Plot of the Example



Prototype cell

Empty Lattice cell



Final Replica

Transformation by input

- Rotations/Translations can be defined with the **ROT-DEFIni** card
- Can be assigned to a lattice by **name** or with **ROT#nnn** SDUM in the **LATTICE** card
- **ROT-DEFIni** cards can be cascaded (using the same **index** or **name**) to define complex transformations

WARNING:

Since matrix multiplication is not commutative the **order** of the Rotation/Translation operations in 3D is important.

ROT-DEFIni

- The ROT-DEFIni defines roto-translations that can be applied to USRBIN, EVENTBIN and LATTICE. It transforms the position of the tracked particle to place of interest scoring or elementary cell (prototype) with the following order:
 - First applies the translation
 - Followed by the rotation on the azimuthal angle
 - and finally by the rotation on the polar angle.

$$\mathbf{X}_{\text{new}} = \mathbf{M}_{\text{polar}} \times \mathbf{M}_{\text{az}} \times (\mathbf{X} + \mathbf{T})$$

WHAT(1): assigns a transformation index and the corresponding rotation axis
I + J * 100 or I * 1000 + J
I = index of rotation (WARNING: NOTE THE SWAP OF VARIABLES)
J = rotation with respect to axis (1=X, 2=Y, 3=Z)

WHAT(2): Polar angle of the rotation ($0 \leq \vartheta \leq 180^\circ$ degrees)

WHAT(3): Azimuthal angle of the rotation ($-180 \leq \varphi \leq 180^\circ$ degrees)

WHAT(4), WHAT(5), WHAT(6) = X, Y, Z offset for the translation

SDUM: Optional (but recommended) name for the transformation

The lattic routine

- The actual transformation from the lattice cell (container) to the elementary cell (prototype) can also be provided through the **LATTIC** routine (if the **SDUM** is left blank)

SUBROUTINE LATTIC (XB, WB, DIST, SB, UB, IR, IRLTGG, IRLT, IFLAG)

- IRLTGG is the current **lattice number** (.. from the **LATTICE** card..)
- XB, WB are vectors with the **current particle position and direction**
- the routine must give back SB, UB, i.e. **position and direction transported to the elementary cell**

- The

ENTRY LATNOR (UN, IRLTNO, IRLT)

must provide the transformation for **normal vectors** to boundaries (UN is both the in and out vectors)

- To convert into the index number the lattice/region name to be accessed, use the following routines:

GEOL2N(LATTICE, NAME, ERR)

Lattice # to Lattice Name

GEON2L(LATTICE, NAME, ERR)

Lattice Name to Lattice #

GEOR2N(NREGION, NAME, ERR)

Region # to Region Name

GEON2R(NREGION, NAME, ERR)

Region Name to Region #

- It is always a good practice to call these functions only the first time the routine is accessed and save the index for later use

The lattic routine-example

In our example:

```
LOGICAL LFIRST
DATA LFIRST / .TRUE. /
SAVE LFIRST, IREP
IF (LFIRST) THEN ! Find replica's lattice number
    CALL GEON2L("TargRep", IREP, IERR)
    LFIRST = .FALSE.
END IF
IF ( IRLTGG .EQ. IREP ) THEN
    SB (1) = XB (1)
    SB (2) = XB (2)
    SB (3) = XB (3) - 10.0
    UB (1) = WB (1)
    UB (2) = WB (2)
    UB (3) = WB (3)
END IF
```

And the **UN** transformation is the identity

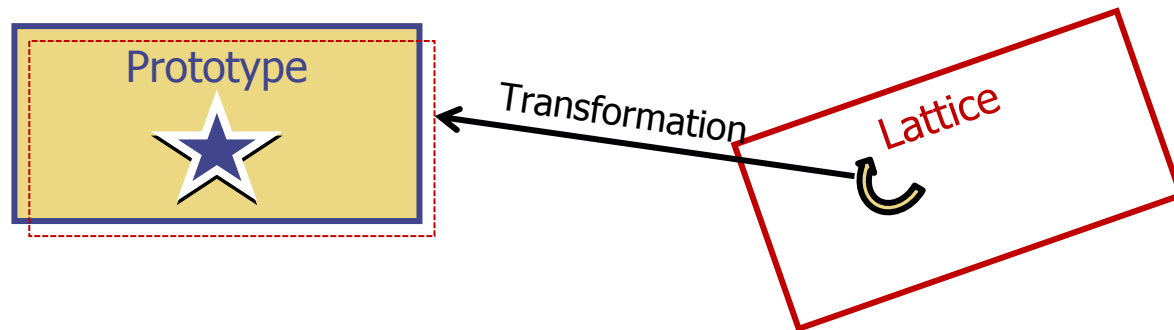
More complex cases can involve reflections and rotations.

For instance, for a reflection around the z axis :

```
UN (1) = UN (1)
UN (2) = UN (2)
UN (3) = -UN (3)
```

Numerical Precision

- Due to the nature of the floating point operations in CPU even if the transformation is correct the end result could be problematic



This small misalignment between lattice/transformation/prototype could lead to geometry errors

- Use as many digits as possible to describe correctly the prototype and lattice cells as well as the transformation.
Is important that the lattice with the transformation corresponds EXACTLY to the prototype
- In case of need use a **FREE** and **FIXED** card before and after the **ROT-DEFI** to use more than 10 digits
- **GEOBEGIN WHAT(2)** will relax the geometry errors (**USE WITH CAUTION**)

Input file, and output quantities

- Materials and other properties have to be assigned only to the regions constituting the basic cell(s).
- In all (user) routines the region number refers to the corresponding one in the elementary cell.
- This applies also to the summary output in the .out file, and in the scoring by regions (i.e. the results for a prototype region include also the contribution from its replicas).
- The lattice identity can be recovered by the *lattice number*, as set in the LATTICE card, or by GEON2L subroutine if is defined by name
- In particular, the LUSRBL routine allows to manage the scoring on lattices in the special USRBIN/EVENTBIN structure.

The USRBIN/EVENTBIN special binning

EVENTBIN or **USRBIN** with **WHAT(1)=8** :

Special user-defined 3D binning. Two variables are discontinuous (e.g. region number), the third one is continuous, but not necessarily a space coordinate.

Variable	Type	Default	Override Routine
1 st	integer	region number	MUSRBR
2 nd	integer	lattice cell number	LUSRBL
3 rd	float	pseudorapidity	FUSRBV

Tips & Tricks [1/2]

- Always remember that the **transformation** refers to the **particles** and not to the geometry!
- You can always divide a transformation into many **ROT-DEFI** cards for easier manipulation.
- Rotations are always around the center of the **geometry**, **and not the center of the object**.
 - To rotate an object, first translate the object to the origin of the axes
 - Perform the rotation
 - Final translation to the requested position.
Of course with the inverse order since everything should apply to the particle

Tips & Tricks [2/2]

- The **Geometry transformation editor in flair** can read and write **ROT-DEFI** cards with the transformation requested
- An easy way of creating a replica and the associated transformation is the following:
 1. Select the body defining the outer cell of the prototype
 2. Clone it with (**Ctrl-D**) and change the name of the clones. Click on "**No**" when you are prompted to change all references to the original name.
 3. Open the Geometry transformation dialog (**Ctrl-T**)
 4. Enter the transformation of the object in the listbox
 5. Click on "**Transform**" to perform the transformation on the clone bodies
 6. Click on "**Invert**" button to invert the order of the transformation
 7. Enter a name on the "**ROT-DEFIni**" field and click "**Add to Input**" to create the **ROT-DEFIni** cards
 8. Now you have to create manually the correct **regions** and the **LATTICE** cards