Subboxing for independent treatment of asymmetric units

Subboxing and symmetry

Let us first create a tutorial folder:

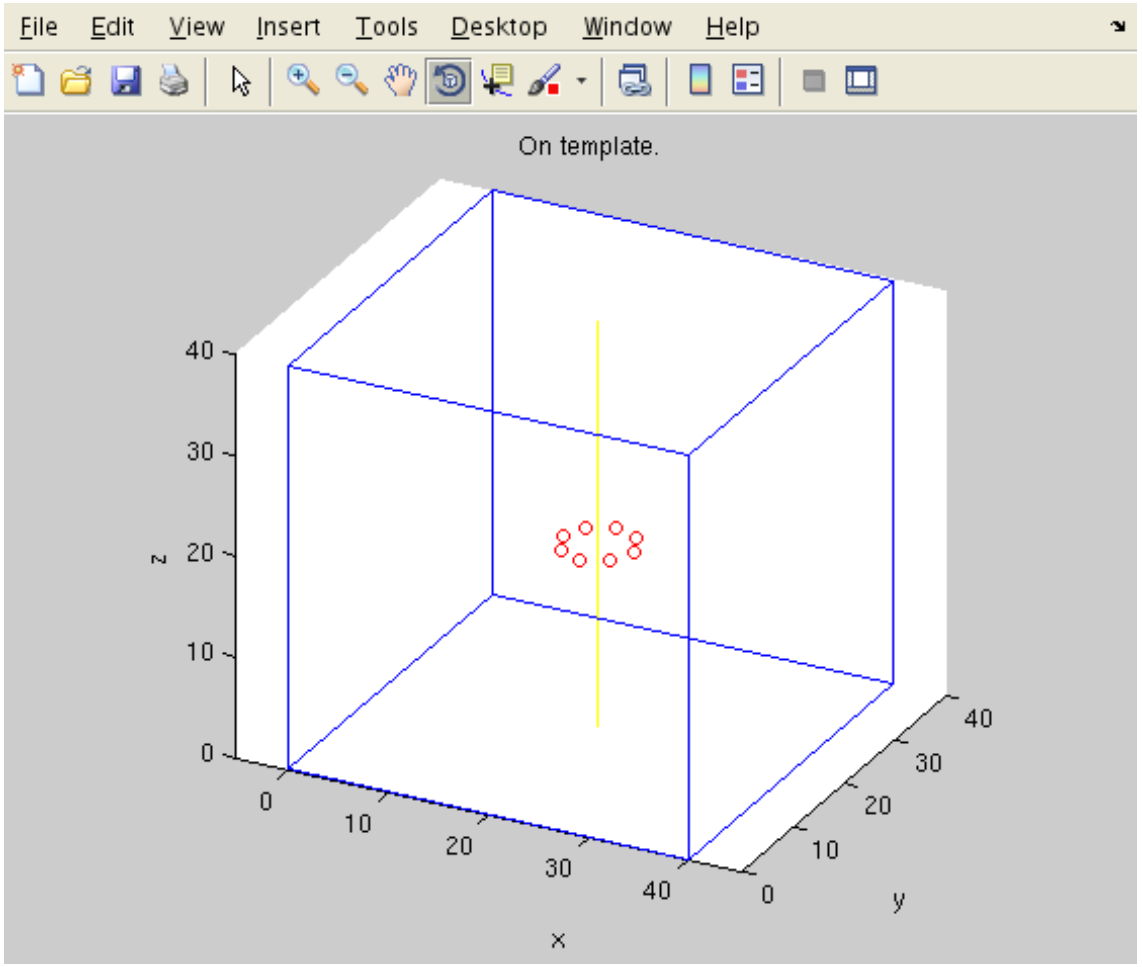
```
dtutorial tsubsym
```

As you know, this tutorial will create inside the folder tsubsym a series of elements (template, data set, real table that aligns the data, an approximative table...)

The template by default reproduces a synthetically generated phantom for a thermosome particle with symmetry C8.

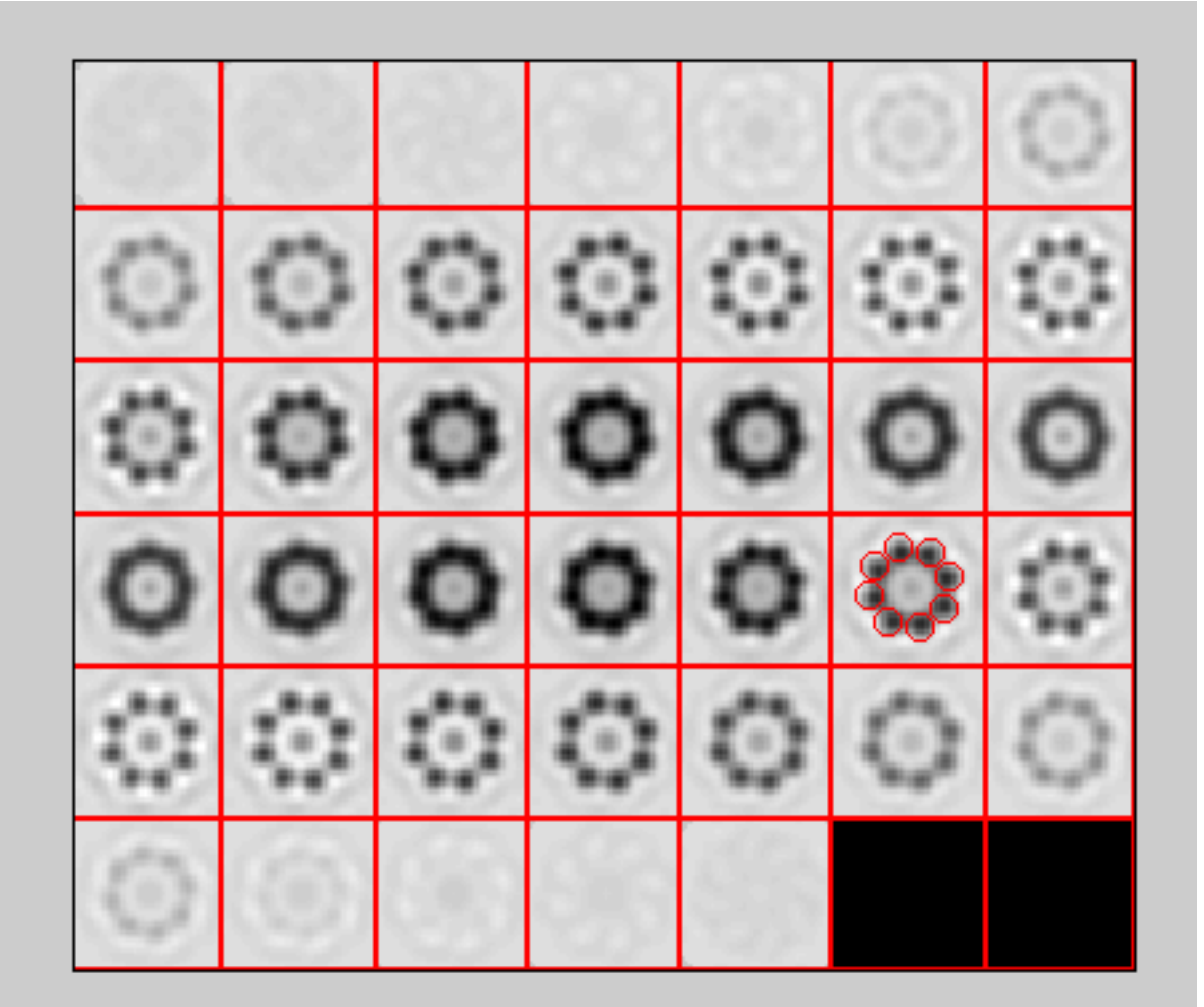
In this case, the “data particles”, which are random orientations of this template will be perfectly symmetric by construction, but in real life the symmetry will not be perfect. Imposition of the symmetry will be a good tool to approach the solution, but finer refinement might benefit from the relaxation of this constraint and the treatment of all subunits stemming from one particle as separated entities.

A basic tool to visualize the behavior of symmetrical repeats is `dsym_point`




```
dsym_point [18,18,18] c8 -size 40 -show sketch
```

dsym_point [23,10,27] c8 -template tsubsym/original_template.em -show template;



Lets perform a subboxing to extract all the asymmetric subunits separately:

clicked center of an assymetric unit

Symmetry used to compute the positions of the symmetry-related subunits

```
>> ddsubboxing tsubsym/data 32 -r [23,10,27] -t tsubsym/coarse.tbl -st 40  -sym c8 -o symsubs
[data_subboxing] Data contains 8 particles with sidelength 64.
........
------------------------------------------------------------

Subboxing summary:

r                     :  23 10 27
sidelength            :  32
symmetrical repeats   : c8
subbox table          : symsubs/subbox_table.tbl
subbox data folder    : symsubs/data
created subboxes      :  64
skipped subboxes      :  0
original data folder  : tsubsym/data
original table        : tsubsym/coarse.tbl

  [ok]  data_subboxing
```

Resulting subboxing folder containing cropped data (“subparticles”) corresponding to the subunits.

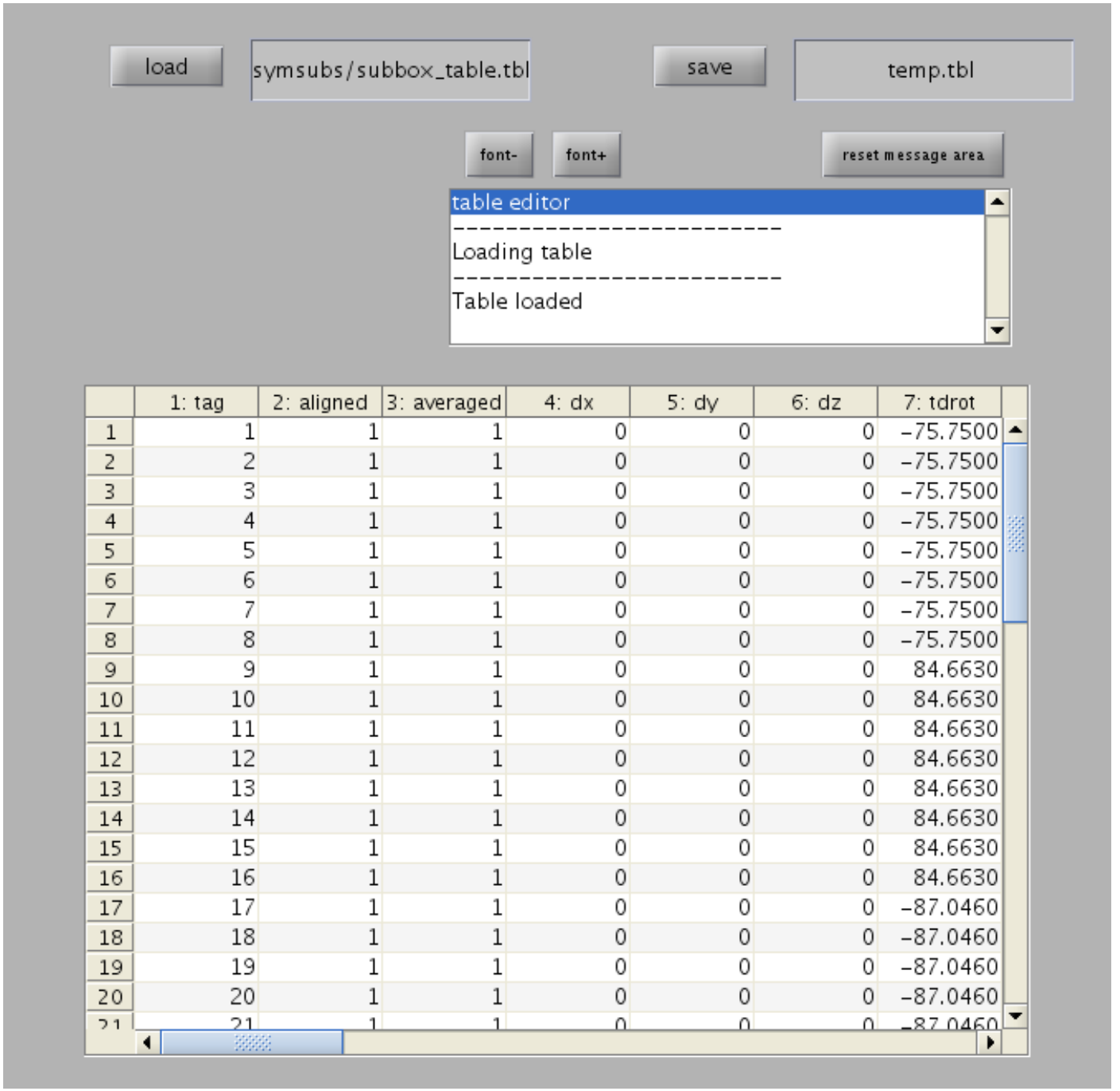
But attention! As we have used a symmetry, the “subboxing data folder” will have more particles than the original data folder (64 = 8 original particles x 8 symmetrical repeats).

In order to keep a reasonable bookkeeping, the new particles are renumbered

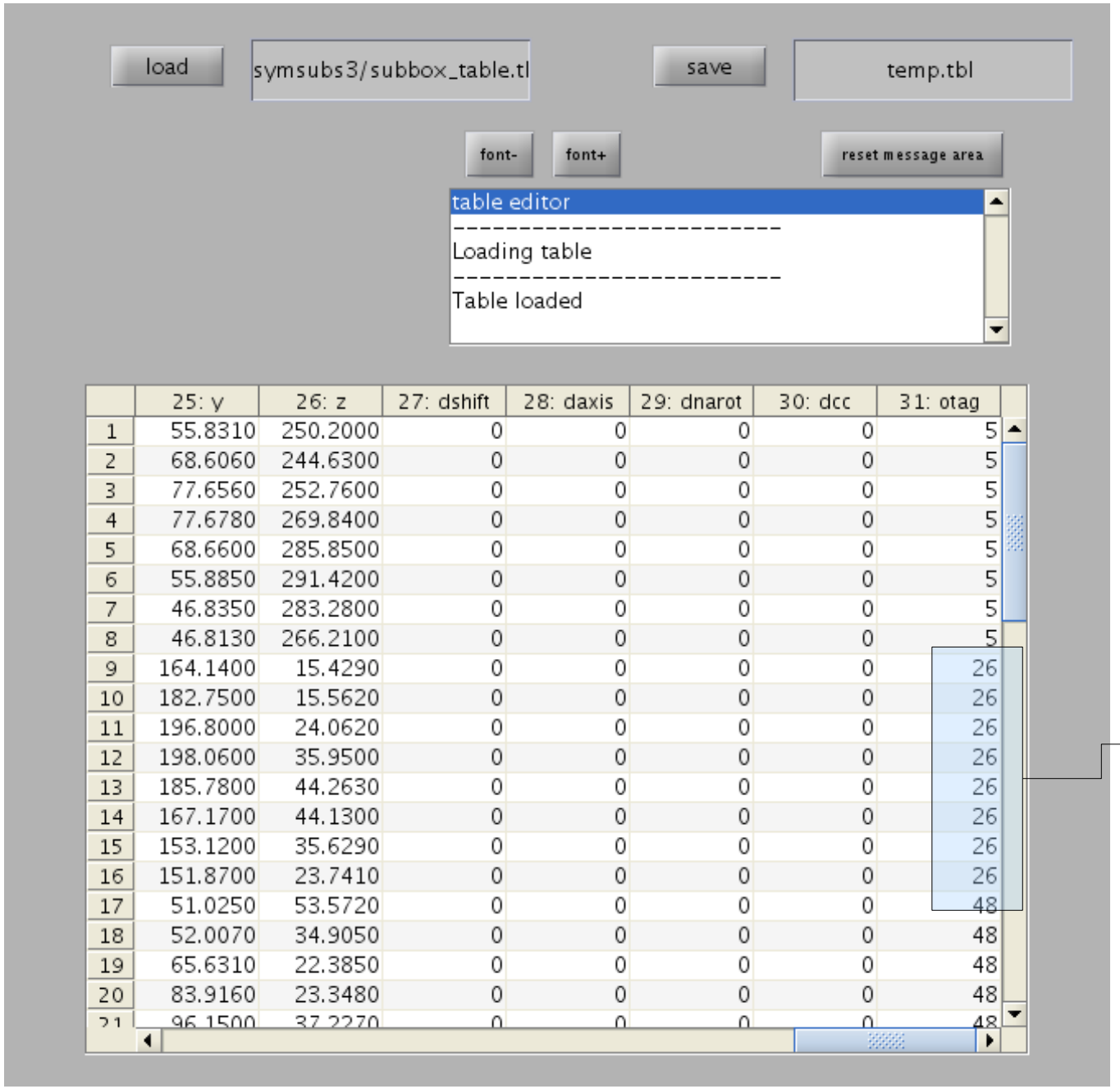
The particles have been renumbered in the new folder.

By default the renumbering starts at zero.

(use flag “first_tag” for different settings)



	1: tag	2: aligned	3: averaged	4: dx	5: dy	6: dz	7: tdrot
1	1	1	1	0	0	0	-75.7500
2	2	1	1	0	0	0	-75.7500
3	3	1	1	0	0	0	-75.7500
4	4	1	1	0	0	0	-75.7500
5	5	1	1	0	0	0	-75.7500
6	6	1	1	0	0	0	-75.7500
7	7	1	1	0	0	0	-75.7500
8	8	1	1	0	0	0	-75.7500
9	9	1	1	0	0	0	84.6630
10	10	1	1	0	0	0	84.6630
11	11	1	1	0	0	0	84.6630
12	12	1	1	0	0	0	84.6630
13	13	1	1	0	0	0	84.6630
14	14	1	1	0	0	0	84.6630
15	15	1	1	0	0	0	84.6630
16	16	1	1	0	0	0	84.6630
17	17	1	1	0	0	0	-87.0460
18	18	1	1	0	0	0	-87.0460
19	19	1	1	0	0	0	-87.0460
20	20	1	1	0	0	0	-87.0460
21	21	1	1	0	0	0	-87.0460



	25: y	26: z	27: dshift	28: daxis	29: dnarot	30: dcc	31: otag
1	55.8310	250.2000	0	0	0	0	5
2	68.6060	244.6300	0	0	0	0	5
3	77.6560	252.7600	0	0	0	0	5
4	77.6780	269.8400	0	0	0	0	5
5	68.6600	285.8500	0	0	0	0	5
6	55.8850	291.4200	0	0	0	0	5
7	46.8350	283.2800	0	0	0	0	5
8	46.8130	266.2100	0	0	0	0	5
9	164.1400	15.4290	0	0	0	0	26
10	182.7500	15.5620	0	0	0	0	26
11	196.8000	24.0620	0	0	0	0	26
12	198.0600	35.9500	0	0	0	0	26
13	185.7800	44.2630	0	0	0	0	26
14	167.1700	44.1300	0	0	0	0	26
15	153.1200	35.6290	0	0	0	0	26
16	151.8700	23.7410	0	0	0	0	26
17	51.0250	53.5720	0	0	0	0	48
18	52.0070	34.9050	0	0	0	0	48
19	65.6310	22.3850	0	0	0	0	48
20	83.9160	23.3480	0	0	0	0	48
21	96.1500	37.2270	0	0	0	0	48

But the “subparticles” still remember from which “original particle” they were cropped.

It is recorded in column 31 (“otag” property in a table)

this eight subparticles in the subboxing folder (tags 9 to 16) come from the same particle (with tag “5”) in the original folder

How does the new data of subunits look like?

It is a regular Dynamo data folder, where all the created files obey the naming convention.

This means that you can operate on this folder all the functions foreseen for data viewing or browsing, as:

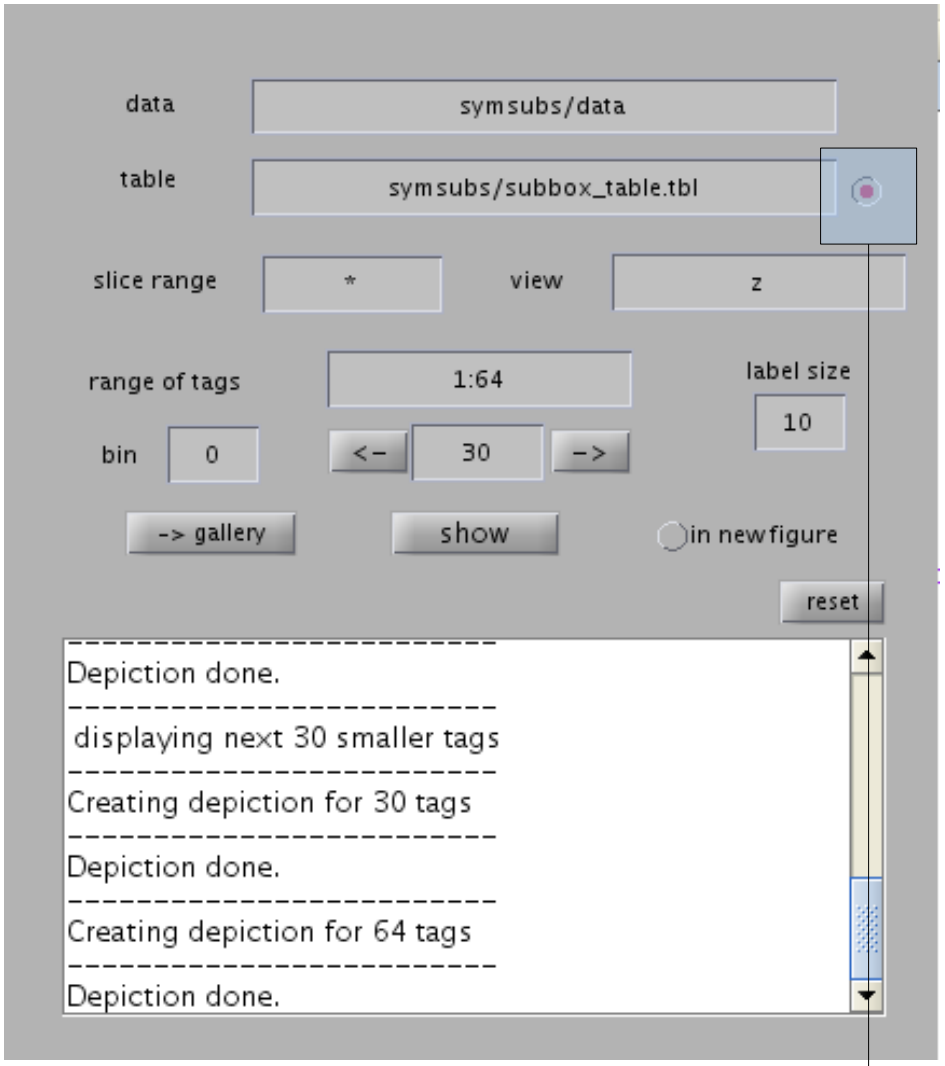
- `dgallery`
- `dslices`
- `ddinfo`
- `ddbrowse`

Let us try this one:

```
ddbrowse -t symsubs/subbox_table.tbl -d  symsubs/data
```

which will open the figure on the right:

After filling the valies as indicated, press [show] to get a snapshot on all the particles (tags 1:64) aligned with the table



Switch this button on to indicate that the particles need to be aligned (according to the table), otherwise unaligned particles will be shown.

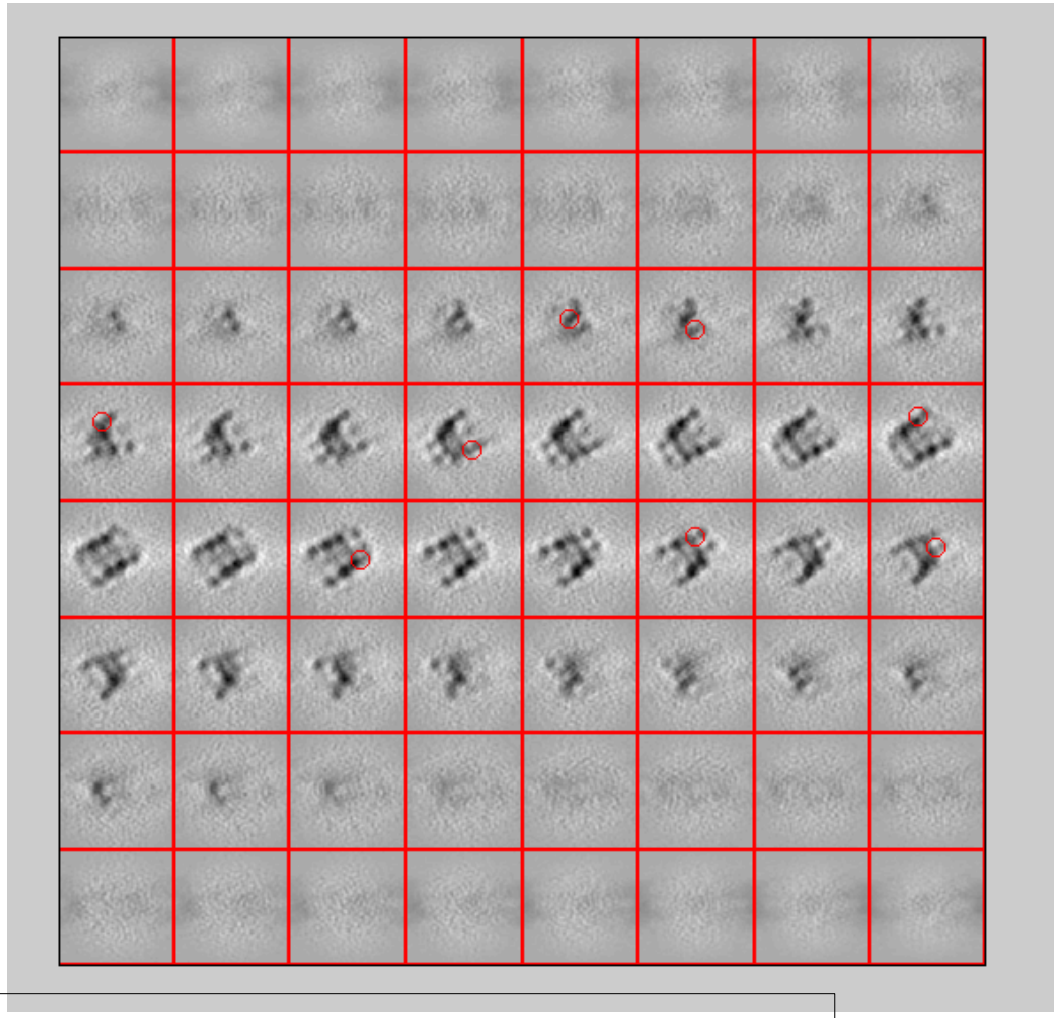
In the new data set, the “particles” are centered on each subunit

Now that you have data and table, you can create an appropriate project.

* The subcropping sidelength here is probably too big:
  in a real experiment you would probably repeat the subboxing command with
  a smaller sidelength

* Remember that you can use the tool dynamo_vpr_subboxing to ease the creation
  projects in subboxing folders.
  This is however not strictly necessary.

Note that you can check where the subboxing centes of the subunits are on each of the data particles:



original tutorial folder

produces a density map visualization for a particle (instead of a template)

```
dsym_point [23,10,27] c8 -size 40 -t tsubsym/coarse.tbl -d tsubsym/data -tag 5 -show particle;
```