

# Workflow session Summary

February 14, 2012

## **Aim**

Standards for data Interchange in single particles.

## **Summary**

In this session we agreed on:

1. Which data should be interchange
2. How to “represent” this data
3. Data format to be used in the data interchange
4. Create a web site with:
  - (a) description of the interchange format including conventions
  - (b) tests to check conversion utilities

## **Which data should be interchange**

1. Information related with “particle picking”: list of coordinates
2. “Simplified” CTF description: defocus, astigmatism, etc
3. Information related with Alignment in 2D and 3D
4. information related with:
  - (a) classes
  - (b) figures of merit
  - (c) comments
  - (d) disable/enable flags

## **How to “represent” this data**

The data would be represented through a collection of pairs label/value. Of course these labels may be used to interchange information different from the one described in the section “Which data should be interchange”

### **List of label, units, definitions:**

Label names has been selected so they adjust to the “star format philosophy” and existing EM dictionary.

### **class emx\_micrograph**

Data items in the emx\_micrograph category describe all parameters associated with an electron micrograph.

label name	data type/units	definition
emx_micrograph.url	string	pointer to image containing the micrograph
emx_micrograph.magnification	float	Describes the microscope magnification at which the micrograph was taken. Together with the detector or scanner pixel size the nominal pixel size can be calculated.
emx_micrograph.scanner_pixel_size	float/micron per pixel	describes the detector or scanner pixel size in microns. Together with the magnification the nominal pixel size can be calculated.
emx_micrograph.defocusU	float/Å	Underfocus positive. For underfocus micrographs this must be the major axis
emx_micrograph.defocusV	float/Å	Underfocus positive. For underfocus micrographs this must be the minor axis
emx_micrograph.astigmatism_angle	float/degrees	describes the astigmatism angle for the micrograph as measured from the x axis to the defocusU, counter-clockwise, in degrees
emx_micrograph.voltage	float/kVolt	describes the acceleration voltage used to take the electron micrograph in kilovolts
_emx_micrograph.Cs	float/mm.	describes the spherical aberration coefficient
emx_micrograph.amplitude_contrast	float	describes the amplitude contrast contribution for the micrograph as a fraction
emx_micrograph.FOM	float	quality index. 0 worst case, 1 best case

### CTF equation

$$CTF = -w \cos(\chi) - \sqrt{1 - w^2} \sin(\chi)$$

$$\chi = \frac{2\pi}{\lambda} \left( \frac{\Delta f \Theta^2}{2} - \frac{C_s \Theta}{4} \right)$$

$$\Theta = \frac{\lambda}{d}$$

Note: In order to apply the above eq.  $d$ ,  $\Delta f$ ,  $C_s$  and  $\lambda$  should be in the same units.

**Example: set of two ctfs**

```
# This file contains two ctfs
data_
loop_
_emx_micrograph.url
_emx_micrograph.magnification
_emx_micrograph.scanner_pixel_size
_emx_micrograph.defocusU
_emx_micrograph.defocusV
_emx_micrograph.astigmatism_angle
_emx_micrograph.voltage
_emx_micrograph.Cs
_emx_micrograph.amplitude_contrast
mg_1.mrc 45000 6.5 1.523 1.423 23.8 300 2.2 0.07
mg_2.mrc 39000 7.0 0.543 0.444 56.2 200 2 0.10
```

**class emx\_particle**

contains image pointer, alignment information and selection information

label name	data type/units	definition
emx_particle.url	string	pointer to file containing particle. Either file name or index@filename for stacks. index starts at 1
_emx_particle.coordinate_x	float	describes the x-coordinate of the center of a particle in a micrograph. Starts in 0
_emx_particle.coordinate_y	float	describes the y-coordinate of the center of a particle in a micrograph. Starts in 0
emx_particle.transformation_matrix_1_1	float	describes the first element of the transformation matrix.
emx_particle.transformation_matrix_1_2	float	describes the second element of the transformation matrix.
emx_particle.transformation_matrix_1_3	float	describes the third element of the transformation matrix.
emx_particle.transformation_matrix_offset_x	float	describes the 4th element of the transformation matrix.
emx_particle.transformation_matrix_2_1	float	describes the 5th element of the transformation matrix.
emx_particle.transformation_matrix_2_2	float	describes the 6th element of the transformation matrix.
emx_particle.transformation_matrix_2_3	float	describes the 7th element of the transformation matrix.
emx_particle.transformation_matrix_offset_y	float	describes the 8th element of the transformation matrix.
emx_particle.transformation_matrix_3_1	float	describes the 9th element of the transformation matrix.
emx_particle.transformation_matrix_3_2	float	describes the 10th element of the transformation matrix.
emx_particle.transformation_matrix_3_3	float	describes the 11st element of the transformation matrix.
emx_particle.transformation_matrix_offset_z	float	describes the 12sd element of the transformation matrix.
emx_particle.active_flag	binary	if =0 ignore this particle, any other value particle is active
emx_particle.FOM	float	quality index. 0 worst case, 1 best case

**Transformation Matrix:**

A11 A12 A13 Xoff

A21 A22 A23 Yoff

A31 A32 A33 Zoff

A full description of the transformation matrix will be include in the Electron Microscopy exchange web site (under construction).

**Example: set coordinates**

```
# Particle picking for micrograph mg_1.mrc and mg_2.mrc
data_1
  _emx_micrograph.url mg_1.mrc
loop_
  _emx_particle.coordinate_x
  _emx_particle.coordinate_y
49.000 49.000
49.000 49.000
data_2
  _emx_micrograph.url mg_2.mrc
loop_
  _emx_particle.coordinate_x
  _emx_particle.coordinate_y
42.000 49.000
43.000 49.000
```

**Example: projection matching output**

```
# Particle alignment
data_
loop_
  _emx_particle.url                               _emx_particle.transformation_matrix_1_1 _emx_part
1@part.mrc  1 0 0 0 1 0 0 0 1 0.54 1.22 -0.54
2@part.mrc  0 0.5 0.5 0 1 0.2 0.6 0 1 -1.54 1.22 -0.54
```

**class emx\_class**

groups images.

label name	data type/units	definition
emx_class.id	string	class identifier

**Example: classification**

```
# particle classification
data_1
  _emx_class.id 1
loop_
  _emx_particle.url
1@filename.mrc
2@filename.mrc
data_2
  _emx_class.id 2
```

loop\_  
\_emx\_particle.url  
11@filename.mrc  
22@filename.mrc