

## aiCTFRefine

After a first round of sub-tomogram averaging, aiCTFRefine refines the CTF parameters for every tilt in a tilt series by projecting each particle on each micrograph. Searching for the CTF parameters only based on the real particle position allows for precise defocus and astigmatism determination.

aiCTFRefine needs a configuration file provided by the **-u** argument. Some options can be overwritten using command line arguments.

Options are:

### CudaDeviceIDs

The deviceIDs of the GPUs to use.

Argument for command line: **-d** or **--CudaDeviceIDs**

Type: **List<int>**, a list of integer values

Option is mandatory: **true**

### Input

The file to process.

Argument for command line: **-i** or **--Input**

Type: **string**

Option is mandatory: **true**

### ExtraShifts

The file name for additional particle shifts.

Argument for command line: **-o** or **--ExtraShifts**

Type: **string**

Option is mandatory: **true**

### LP

Low pass filter value.

Argument for command line: **-lp** or **--LP**

Type: **float**

Option is mandatory: **true**

### LPS

Low pass filter sigma value.

Argument for command line: **-lps** or **--LPS**

Type: **float**

Option is mandatory: **true**

### HP

High pass filter value.

Argument for command line: **-hp** or **--HP**

Type: **float**

Option is mandatory: **false**

Default value if not set: **0**

## HPS

High pass filter sigma value.

Argument for command line: **-hps** or **--HPS**

Type: **float**

Option is mandatory: **false**

Default value if not set: **0**

## DeadPixelRemoval

Enables removal of dead pixels based on thresholding. If set to 'relative', the threshold is X times the STD + MEAN of the image.

Argument for command line: **-deadPixel** or **--DeadPixelRemoval**

Type: one of [**ABSOLUTE**, **NONE**, **RELATIVE**]

Option is mandatory: **false**

Default value if not set: **NONE**

Possible notations:

- **ABSOLUTE**: ABSOLUTE, Absolute, absolute
- **NONE**: NONE, None, none
- **RELATIVE**: RELATIVE, Relative, relative

## DeadPixelThreshold

Threshold above which a pixel is considered invalid.

Argument for command line: **-threshold** or **--DeadPixelThreshold**

Type: **float**

Option is mandatory: **true**

Only applicable if

- **DeadPixelRemoval** = ABSOLUTE or
- **DeadPixelRemoval** = RELATIVE

## ReconstructionSettings

The file name for the file with reconstruction settings.

Argument for command line: **-rec** or **--ReconstructionSettings**

Type: **string**

Option is mandatory: **true**

## CtfCorrectionType

The type of CTF correction to perform.

Type: one of [**NONE**, **PHASE\_FLIP**, **WIENER\_FILTER**]

Option is mandatory: **true**

Possible notations:

- **NONE**: NONE, None, none, FALSE, false, False, NO, No, no
- **PHASE\_FLIP**: PHASEFLIP, PhaseFlip, phaseflip, PHASE\_FLIP, Phase\_Flip, phase\_flip
- **WIENER\_FILTER**: WIENERFILTER, WienerFilter, wienerfilter, WIENER\_FILTER, Wiener\_Filter, wiener\_filter

## CTFSliceThickness

The thickness of a CTF slice for 3D-CTF-Correction in nanometer.

Type: **float**

Option is mandatory: **true**

Only applicable if

- **CtfCorrectionType** = PHASE\_FLIP or
- **CtfCorrectionType** = WIENER\_FILTER

## SwitchCTFDirection

Inverses the defocus offset value (experimental, do not use).

Type: **bool**

Option is mandatory: **false**

Default value if not set: **false**

Only applicable if

- **CtfCorrectionType** = PHASE\_FLIP or
- **CtfCorrectionType** = WIENER\_FILTER

## IgnoreZShiftForCTF

Ignore possible Z-Shift of the reconstruction volume for defocus offset.

Type: **bool**

Option is mandatory: **false**

Default value if not set: **true**

Only applicable if

- **CtfCorrectionType** = PHASE\_FLIP or
- **CtfCorrectionType** = WIENER\_FILTER

## ProjectionNormalization

Projection normalization method to use before reconstruction.

Type: one of [MEAN, NONE, STANDARD\_DEV]

Option is mandatory: **true**

Possible notations:

- **MEAN**: MEAN, Mean, mean
- **NONE**: NONE, none, None
- **STANDARD\_DEV**: STD, std, StandardDeviation, STANDARD\_DEV

## DebugImages

Save temporary images to disk for debugging.

Type: **bool**

Option is mandatory: **false**

Default value if not set: **false**

## Binning

Bin the tilt series images prior to reconstruction.

Type: **float**

Option is mandatory: **false**

Default value if not set: **1**

## CompensateImageRotation

Rotate the image before applying the WBP filter so that the WBP is not interpolated.

Type: **bool**

Option is mandatory: **false**  
Default value if not set: **false**

## MotiveList

The motive list with alignment information for each particle.

Type: **string**

Option is mandatory: **true**

## References

Reference filename. Naming convention: filename\_RefNr\_IterationNr.em/mrc.

Type: **string**

Option is mandatory: **true**

## Masks

Mask filename. Naming convention: filename\_MaskNr.em/mrc.

Type: **string**

Option is mandatory: **true**

## DefocusMin

Begin of search range in [nm] for each iteration. The value is added to the initial defocus value.

Argument for command line: **-defMin** or **--DefocusMin**

Type: **List<float>**, a list of floating point values

Option is mandatory: **true**

## DefocusMax

End of search range in [nm] for each iteration. The value is added to the initial defocus value.

Argument for command line: **-defMax** or **--DefocusMax**

Type: **List<float>**, a list of floating point values

Option is mandatory: **true**

## DefocusStep

Search step in [nm] for defocus in each iteration.

Argument for command line: **-defStep** or **--DefocusStep**

Type: **List<float>**, a list of floating point values

Option is mandatory: **true**

## Astigmatism

If true, the astigmatism parameters are included in the search.

Argument for command line: **-astig** or **--Astigmatism**

Type: **bool**

Option is mandatory: **false**

Default value if not set: **false**

## AstigmatismMin

Begin of search range for astigmatism in [nm] for each iteration. The value is added to the initial value.

Argument for command line: **-astigMin** or **--AstigmatismMin**

Type: **List<float>**, a list of floating point values

Option is mandatory: **true**  
Only applicable if **Astigmatism** = true.

### **AstigmatismMax**

End of search range for astigmatism in [nm] for each iteration. The value is added to the initial value.  
Argument for command line: **-astigMax** or **--AstigmatismMax**  
Type: **List<float>**, a list of floating point values  
Option is mandatory: **true**  
Only applicable if **Astigmatism** = true.

### **AstigmatismStep**

Search step for astigmatism in each iteration.  
Argument for command line: **-astigStep** or **--AstigmatismStep**  
Type: **List<float>**, a list of floating point values  
Option is mandatory: **true**  
Only applicable if **Astigmatism** = true.

### **AstigmatismAngleMin**

Begin of search range for astigmatism angle in [degree] for each iteration. The value is added to the initial value.  
Argument for command line: **-astigAngMin** or **--AstigmatismAngleMin**  
Type: **List<float>**, a list of floating point values  
Option is mandatory: **true**  
Only applicable if **Astigmatism** = true.

### **AstigmatismAngleMax**

End of search range for astigmatism in [degree] for each iteration. The value is added to the initial value.  
Argument for command line: **-astigAngMax** or **--AstigmatismAngleMax**  
Type: **List<float>**, a list of floating point values  
Option is mandatory: **true**  
Only applicable if **Astigmatism** = true.

### **AstigmatismAngleStep**

Search step for astigmatism angle in each iteration.  
Argument for command line: **-astigAngStep** or **--AstigmatismAngleStep**  
Type: **List<float>**, a list of floating point values  
Option is mandatory: **true**  
Only applicable if **Astigmatism** = true.

### **FrameMetadata**

Frame metadata for a tilt series can be stored inside the tilt series metadata file or in an additional file.  
Argument for command line: **-meta** or **--FrameMetadata**  
Type: **string**  
Option is mandatory: **false**  
Default value if not set: ""

## ReduceGoldBeadArtifacts

Reduces artifacts due to the high contrast of gold beads in the tomogram.

Type: **bool**

Option is mandatory: **false**

Default value if not set: **false**

## ReduceGoldBeadArtifactStrength

The strength factor for gold bead artifact reduction. The value has to be in range [0..1] and is usually  $> 0.5$ .

Type: **float**

Option is mandatory: **true**

Only applicable if **ReduceGoldBeadArtifacts** = true.

## GoldBeadSize

The size of the goldbeads used in the tilt series in nm. (With a small additional margin of 1 to 2 nm and if multiple sizes are used, the larger one.)

Type: **float**

Option is mandatory: **true**

Only applicable if **ReduceGoldBeadArtifacts** = true.

## DoseLimit

Only tilt with a total dose lower than this limit are refined.

Type: **float**

Option is mandatory: **false**

Default value if not set: **0**