

aiShiftRefine

aiShiftRefine determines an individual shift for each particle and each projection in a tilt series to compensate for alignment inaccuracies.

aiShiftRefine 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 the detected shifts.

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

Type: **string**

Option is mandatory: **true**

ExtraShiftsIn

A shift file with shifts that are to be used as start values.

Type: **string**

Option is mandatory: **true**

LP

Low pass filter value.

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

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

Option is mandatory: **true**

LPS

Low pass filter sigma value.

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

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

Option is mandatory: **true**

HP

High pass filter value.

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

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

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

HPS

High pass filter sigma value.
Argument for command line: **-hps** or **--HPS**
Type: **List<float>**, a list of floating point values
Option is mandatory: **false**
Default value if not set: []

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**

GroupMode

Grouping method for particle projection.

Type: one of [**BY_GROUP**, **MAX_COUNT**, **MAX_DISTANCE**]

Option is mandatory: **true**

Possible notations:

- **BY_GROUP**: ByGroup, BY_GROUP, by_group
- **MAX_COUNT**: MaxCount, MAX_COUNT, max_count
- **MAX_DISTANCE**: MaxDistance, MAX_DISTANCE, max_distance

MaxShift

Maximum shift allowed.

Type: **int**

Option is mandatory: **true**

MaxDist

Maximum distance inbetween particles to form a group.

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

Option is mandatory: **true**

Only applicable if **GroupMode** = **MAX_DISTANCE**.

GroupSize

Number of particles to form a group.

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

Option is mandatory: **true**

Only applicable if **GroupMode** = **MAX_COUNT**.

SpeedupDistance

Assign the same shift to particles in a radius (in unbinned pixels) of this distance instead of computing it individually.

Type: **float**

Option is mandatory: **false**

Default value if not set: **0**

ProjectionMode

Compare the projected reference with the original micrograph or with the particles.

Type: one of [**ORIGINAL**, **PARTICLE**]

Option is mandatory: **true**

Possible notations:

- **ORIGINAL**: Original, ORIGINAL, original
- **PARTICLE**: Particle, PARTICLE, particle

Particles

Filename for the reconstructed particles.

Type: **string**

Option is mandatory: **true**

Only applicable if **ProjectionMode** = **PARTICLE**.

AveragingMode

Defines how to average the group particles: as an entire image or by averaging the CC image.

Type: one of [**CC**, **IMAGE**]

Option is mandatory: **true**

Possible notations:

- **CC**: Cc, CC, cc
- **IMAGE**: Image, IMAGE, image

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**.