# Anacor.preprocess\_lite

parser.add\_argument(

"--dataset" ,

type = str ,

help = "dataset number " ,

)

parser.add\_argument(

"--store-dir" ,

type = str ,

default = "./" ,

help = "the store directory " ,

)

parser.add\_argument(

"--segimg-path" ,

type = str ,

required = True ,

help = "the path of segmentation images" ,

)

parser.add\_argument(

"--rawimg-path" ,

type = str ,

default = None ,

help = "the path of raw flat-field images" ,

)

parser.add\_argument(

"--store-calculation" ,

type = str2bool ,

default = False ,

help = "whether store the path lengths to calculate with different absorption coefficients" ,

)

parser.add\_argument(

"--refl-filename" ,

type = str ,

required = True ,

help = "the path of the reflection table" ,

)

parser.add\_argument(

"--expt-filename" ,

type = str ,

required = True ,

help = "the path of the experimental file" ,

)

parser.add\_argument(

"--model-storepath" ,

type = str ,

default = None ,

help = "the storepath of the 3D model built by other sources in .npy" ,

)

parser.add\_argument(

"--create3D" ,

type = str2bool ,

default = True ,

help = "whether the reconstruction slices need to be vertically filpped to match that in the real experiment" ,

)

parser.add\_argument(

"--coefficient" ,

type = str2bool ,

default = False ,

help = "whether the reconstruction slices need to be vertically filpped to match that in the real experiment" ,

)

parser.add\_argument(

"--coefficient-auto" ,

type = str2bool ,

default = True ,

help = "whether calculating the best estimate of the flat-field image to calculate absorption coefficient "

"automatically" ,

)

parser.add\_argument(

"--coefficient-orientation" ,

type = int ,

default = 0 ,

help = "the orientation of the flat-field image to match the 3D model in degree"

"normally this is 0 degree" ,

)

parser.add\_argument(

"--coefficient-viewing" ,

type = int ,

default = 0 ,

help = "the viewing angle of the 3D model to have the best region to determine absorption coefficient"

"in degree" ,

)

parser.add\_argument(

"--model-name" ,

type = str ,

default = None ,

help = "the optional 3D model name, otherwise it would be {dataset}\_.npy" ,

)

parser.add\_argument(

"--full-reflection" ,

type = str2bool ,

default = False ,

help = "whether cutting some unwanted data of the reflection table"

"before calculating" ,

)

parser.add\_argument(

"--dials-dependancy" ,

type = str ,

required = True ,

help = "the path to execute dials package"

"e.g. module load dials" "e.g. source /home/yishun/dials\_develop\_version/dials" ,

)

# Anacor.mp\_lite

parser.add\_argument(

"--num-cores" ,

type = int ,

default = 20 ,

help = "the number of cores to be distributed" ,

)

parser.add\_argument(

"--store-dir" ,

type = str ,

default = "./" ,

help = "the store directory " ,

)

parser.add\_argument(

"--dataset" ,

type = str , required = True ,

help = "dataset number default is 13304" ,

)

parser.add\_argument(

"--offset" ,

type = float ,

default = 0 ,

help = "the orientation offset" ,

)

parser.add\_argument(

"--sampling" ,

type = int ,

default = 5000 ,

help = "sampling for picking crystal point to calculate" ,

)

parser.add\_argument(

"--store-lengths" ,

type = str2bool ,

default = False ,

help = "whether store the path lengths to calculate with different absorption coefficients" ,

)

parser.add\_argument(

"--crac" ,

type = float , required = True ,

help = "the absorption coefficient of the crystal and it is needed" ,

)

parser.add\_argument(

"--loac" ,

type = float , required = True ,

help = "the absorption coefficient of the loop and it is needed" ,

)

parser.add\_argument(

"--liac" ,

type = float , required = True ,

help = "the absorption coefficient of the liquor and it is needed" ,

)

parser.add\_argument(

"--buac" ,

type = float , default = 0 ,

help = "the absorption coefficient of the bubble and it is not necessarily needed" ,

)

parser.add\_argument(

"--refl-filename" ,

type = str ,

default = '' ,

help = "the filenames of the reflection table" ,

)

parser.add\_argument(

"--expt-filename" ,

type = str ,

default = '' ,

help = "the filenames of the experimental table" ,

)

parser.add\_argument(

"--python-dependancy" ,

type = str ,

default = '' ,

help = "the python version that is to be executed" ,

)

parser.add\_argument( "--time" , nargs = '\*' , type = int ,

help = "List of time for the cluster job"

"e.g. 01 10 10 is 1hour 10minute 10seconds" )

# Anacor.postprocess\_lite

parser.add\_argument(

"--store-dir" ,

type = str ,

default = "./" ,

help = "the store directory " ,

)

parser.add\_argument(

"--dataset" ,

type = str , required = True ,

help = "dataset number " ,

)

parser.add\_argument(

"--save-note" ,

type = str , default = 'anacor',

help = "note of the saving" ,

)

parser.add\_argument(

"--refl-filename" ,

type = str ,

default = '' ,

help = "the filenames of the reflection table" ,

)

parser.add\_argument(

"--expt-filename" ,

type = str ,

default = '' ,

help = "the filenames of the experimental table" ,

)

parser.add\_argument(

"--dials-dependancy" ,

type = str ,

default = '' ,

help = "the dials version that is to be executed" ,

)

parser.add\_argument(

"--mtz2sca-dependancy" ,

type = str ,

default = '' ,

help = "the dependancy to convert mtz into sca files" ,

)

parser.add\_argument(

"--full" ,

type = str2bool ,

default = False ,

help = "prerejection for better computational efficiency no: 1, yes: 1" ,

)

parser.add\_argument(

"--with-scaling" ,

type = str2bool ,

default = True ,

help = "absorption correcction within the scaling process true: 1 , false: 0" ,

)