## SIMPLE 2.0 command line dictionary

acf autocorrelation function

amsklp automask low-pass limit (in Å)

bin binarize (yes|no)

box image size in pixels (image assumed to be box\*box array)

boxpd padded box size (default is 2\*box)

center center(yes|no)

clsdoc Spider format clustering document

cure cure or not (yes|no), for curing NaN:s and normalize

cwd current working directorydebug debug mode (yes|no)

deterministicdeterministic search (yes|no)discretediscrete option (yes|no)doaligndo alignment (yes|no)

dopcado PCA (yes|no)doprintdo print (yes|no)e1first Euler anglee2second Euler anglee3third Euler angle

edge edge size for softening molecular envelope (in pixels)

eo even-odd test (yes|no)

even (yes|no)

fbody file body (<body>.ext)

filterfilter (yes|no)fracfraction [0,1]frompfrom particle indexfromsfrom state index

gw Gaussian half width (in pixels)

hphigh-pass limit (in Å)kmeansdo kmeans (yes|no)locallocal refinement (yes|no)lplow-pass limit (in Å)

matched use matched Wiener filter (yes|no)
maxits maximum number of iterations

*minp* minimum number of particle images (in a cluster)

moldiam molecular diameter (in Å)

msk circular or spherical mask radius (in pixels)

mskfile external mask file (\*.spi)

mul multiplication (scaling) factor (for shifts)

mwmolecular weight (in kD)navgsnumber of averagesnclsnumber of clusters

ndiscrete number of discrete (orientations)

*ndocs* number of documents

newbox new box size

noise noise (yes|no)

norisnumber of orientationsnormnormalize (yes|no)npartnumber of partitions

npeaks number of peaks (=number of nonzero orientation weights)

nptcls number of particle images

*nran* number of images in random sample

*nspace* number of projection directions in search space

*nstates* number of discrete state groups *nthr* number of openMP threads

*nvars* number of eigenvectors or hidden variables

*nvox* number of voxels

oritab SIMPLE orientations file (\*.txt)
outfile SIMPLE output file (\*.txt)

outstkoutput Spider image stack (\*.spi suffix required)outvoloutput Spider volume (\*.spi suffix required)

part partition number

pgrp point-group symmetry (c1, c2, c3, ..., or d1, d2, d3, ...)

phrand phase randomize (yes|no)

phranlp phase randomization low-pass limit (in Å)

ppca probabilistic pca (yes|no)

ring1 inner ring in polar image representation outer ring in polar image representation

rnd random (yes|no)

roalgn rotational alignment (yes|no)
shalgn shift alignment (yes|no)
smpd sampling distance (in Å)
snr signal-to-noise ratio
space space (real|fourier)

startit starting iteration (if different than 1)

state discrete state group

stk spider image stack name (\*.spi suffix required)

stk2second spider image stack name (\*.spi suffix required)stk3third spider image stack name (\*.spi suffix required)

tau temperature parameter time\_per\_image per particle time indicator

topto particle indextosto state indextresthreshold

trs origin shift search range parameter [-trs,trs]

*trsstep* translation step size *utst* unit test number

*var* variance

vol1spider volume 1 name (\*.spi suffix required)wfunweighting function or interpolation kernel

winsz window size for interpolation