General histogram function:

hist (FileName, InitialTime, FinalTime, SpeciesName)

Description: This function enables users to obtain a histogram during a certain time period of selected species.

Parameters:

* FileName

Acceptable value: String (Must provide)

Description: It is the path to the file (.dat), which is usually named as ‘histogram\_complexes\_time.dat’, representing the histogram data to be analyzed.

Sample: FileName = /Users/UserName/Documents/histogram\_complexes\_time.dat

* InitialTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the initial time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the starting time or exceed the ending time of simulation.

Sample: InitialTime = 0.5

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* FinalTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the final time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the value of InitialTime or exceed the ending time of simulation.

Sample: FinalTime = 1.0

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* SpeciesName

Acceptable value: String (Must provide)

Description: It is the name of species that users want to examine, which should also be identical with the name written in the input (.inp and .mol) files.

Sample: SpeciesName = clat

Function for plotting maximum number of monomers in single complex over time:

max\_complex (FileName, InitialTime, FinalTime, SpeciesName)

Description: This function enables users to obtain a plot indicating maximum number of monomers in single complex molecule during a certain time period.

Parameters:

* FileName

Acceptable value: String (Must provide)

Description: It is the path to the file (.dat), which is usually named as ‘histogram\_complexes\_time.dat’, representing the histogram data to be analyzed.

Sample: FileName = /Users/UserName/Documents/histogram\_complexes\_time.dat

* InitialTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the initial time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the starting time or exceed the ending time of simulation.

Sample: InitialTime = 0.5

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* FinalTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the final time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the value of InitialTime or exceed the ending time of simulation.

Sample: FinalTime = 1.0

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* SpeciesName

Acceptable value: String (Must provide)

Description: It is the name of species that users want to examine, which should also be identical with the name written in the input (.inp and .mol) files.

Sample: SpeciesName = clat

Function for plotting mean number of monomers in single complex over time:

mean\_complex (FileName, InitialTime, FinalTime, SpeciesName, ExcludeNum)

Description: This function enables users to obtain a plot indicating mean number of monomers in single complex molecule during a certain time period.

Parameters:

* FileName

Acceptable value: String (Must provide)

Description: It is the path to the file (.dat), which is usually named as ‘histogram\_complexes\_time.dat’, representing the histogram data to be analyzed.

Sample: FileName = ‘/Users/UserName/Documents/histogram\_complexes\_time.dat’

* InitialTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the initial time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the starting time or exceed the ending time of simulation.

Sample: InitialTime = 0.5

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* FinalTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the final time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the value of InitialTime or exceed the ending time of simulation.

Sample: FinalTime = 1.0

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* SpeciesName

Acceptable value: String (Must provide)

Description: It is the name of species that users want to examine, which should also be identical with the name written in the input (.inp and .mol) files.

Sample: SpeciesName = ‘clat’

* ExcludeNum

Acceptable value: Int (Optional)

Default: 0

Description: In the generated plot, the number of monomers in the complex that are no larger than this number will be excluded and will not be considered into the average calculation.

Sample: ExcludeNum = 1 (which means the monomer will be exclude)

Function for converting histogram\_complexes\_time.dat file to a data frame: hist\_to\_df\_mult(FileName)

Description: This function enables users to convert the raw .dat file to a data frame in python pandas package for multi-species system. Each column in the data frame includes the simulation time and all occurrences of species during the simulation; each row is separated by a different simulation time.

Parameters:

* FileName

Acceptable value: String (Must provide)

Description: It is the path to the file (.dat), which is usually named as ‘histogram\_complexes\_time.dat’, representing the histogram data to be analyzed.

Sample: FileName = /Users/UserName/Documents/histogram\_complexes\_time.dat

Function for creating 3D histogram (histogram with time axis): hist\_3d\_time (FileName, InitialTime, FinalTime, SpeciesName, TimeBins)

Description: This function enables users to generate 3D histogram representing the number of monomers in single complex as simulation time develops. The x-axis is the number of monomers, y-axis is the averaged time and z-axis is the relative occurrence probabilities.

Parameters:

* FileName

Acceptable value: String (Must provide)

Description: It is the path to the file (.dat), which is usually named as ‘histogram\_complexes\_time.dat’, representing the histogram data to be analyzed.

Sample: FileName = ‘/Users/UserName/Documents/histogram\_complexes\_time.dat’

* InitialTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the initial time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the starting time or exceed the ending time of simulation.

Sample: InitialTime = 0.5

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* FinalTime

Acceptable value: Float (Must provide)

Unit: s

Description: It is the final time that users desire to examine and plot on the histogram. The acceptable range should not smaller than the value of InitialTime or exceed the ending time of simulation.

Sample: FinalTime = 1.0

Note: If the InitialTime and FinalTime both input as -1, the entire time range indicated in the reading(.dat) file will be taken as input.

* SpeciesName

Acceptable value: String (Must provide)

Description: It is the name of species that users want to examine, which should also be identical with the name written in the input (.inp and .mol) files.

Sample: SpeciesName = ‘clat’

* TimeBins

Acceptable value: Int (Must provide)

Description: It is the number of bins that users want to divide the selected time period into. The value should be positive integer.