CTS filament generator tutorial

Extremely basic WIP

To generate filaments, structures need to be supplied as individual subunits. All the normal structure file formats will work. The unit needs to be two things: aligned along the Z axis, and a uniformly repeating monomer or set of monomers.

Starting with a whole filament in a structure editor, align the filament along and centered around the Z axis. This allows the subunits to be rotated if relevant. Then delete all structures except for the repeating subunit (the subunit can be multiple nonuniform structures, and different submodels if desired). Finally, re-center the subunit along the z axis so that its rotational center is 0 along that direction. Make sure not to move the subunit in the X or Y axis – any rotation requires the subunit to maintain its distance and orientation from the Z axis.

Filaments have 4 attributes that determine polymerization behavior in CTS. A GUI will request each value when structure files are loaded.

Helical angle: angle of rotation between consecutive subunits in degrees. Uses a right-hand standard.

Step size: distance between consecutive subunits in angstroms.

Flexibility: maximum angle change in direction between consecutive subunits.

Minimum length: minimum permissible length for the filament. Shorter filaments will not be placed, and longer values also increase the number of placement attempts overall.

Example filaments, with the relevant .fil files in the structures\_filaments folder.

Actin

Angle -166.15 step size 27.3 flexibility 12 min length 20

Cofilactin (cofil\_actin\_split file uses separate classes for actin and cofilin)

Angle -162 step size 24 flexibility 12 min length 20

Microtubules: don’t have a continuous filament structure, so can’t be placed as tubulin dimers. Instead, a full 13-unit loop of dimers was used as the subunit and there is no rotation.

Angle 0 step size 85 flexibility 5 min length 10