Visualizing the surface routine in MPMC

Specifying the keyword “surf_output” in the input file will turn on the printing of geometries at certain stages of the surface generation routine. As there are a huge number of geometries constructed, this output can fill an entire disk rather quickly :) To suppress the output, a cryptic file is written. This output file must be decoded, and inflated, *via* the “surface_traj_decode.py” python script, which resides in the /tools/ directory. A new file, “surface_trajectory.pqr” will be created, which is readable by VMD. It is recommended to feed this file into VMD using the -pdb flag, as *vmd -pdb surface_trajectory.pqr*.

Within the MPMC input file:

surf_output	[FILE]
surf_print_level	[integer, 1-6] (default = 3)

In /mc/surface.c, there is 6 nested loops. This is where the isotropic averaging occurs. The amount of output requested will depend on the value of surf_print_level set (default = 3). A value of 1 will result in minimal input, while a value of 6 will result in an obnoxiously large output file (setting a value of 6 should only be used for visual debugging purposes).