Dock3DinDepth

v0.1

biodev.cea.fr/dock3dindepth

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Dock3DinDepth provides the docking of isosurfaces into experimental shape envelopes (AFM, SAXS or cryo-EM).

As envelop input: upload either an atomic force microscopy (AFM) image, a model obtained from SAXS data, or a cryo-EM density map. The AFM image should be saved in ASCII format (.txt) using Gwyddion (including header). For a SAXS envelope a model in PDB format must be provided. And for cryo-EM density maps the formats MAP and MRC are supported.

The object input to be docked can be a structure, providing atomic coordinates in PDB format or an isosurface. The isosurface can be obtained through the tool Adepth also available here: **http://biodev.cea.fr/adepth**. With Adepth, upload the structure in PDB format and generate the isosurface with the desired resolution. The isosurface is determined for all atomic depths, negative (inside structure) or positive (outside), within the boundary indicated. The output from Adepth is a GRID file to be uploaded in Dock3DinDepth.

To dock an isosurface indicate the depth desired, for instance using an AFM envelope its expected to use a positive value which corresponds to a dilation of the structure. Due to computation limitations its also necessary to indicate the density of points in the isosurface to be used, density=1 corresponds to the highest resolution.

Docking the object under an AFM image requires additionally the definition of favorable and forbidden layers: only the atoms inside the favorable region are considered in the scoring. Docking is based on the program DOT 2.0 (SDSC).

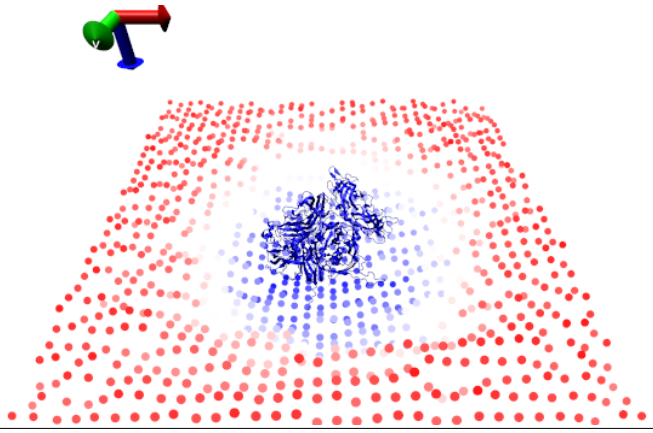
Common to all envelop types, the grid size for docking should embrace the entire envelope for the resolution indicated. And in the case of SAXS and cryo-EM additionally, its required to define the volume of the points in the envelope to fill all the volume for the docking grid selected, using the parameter "node radius".

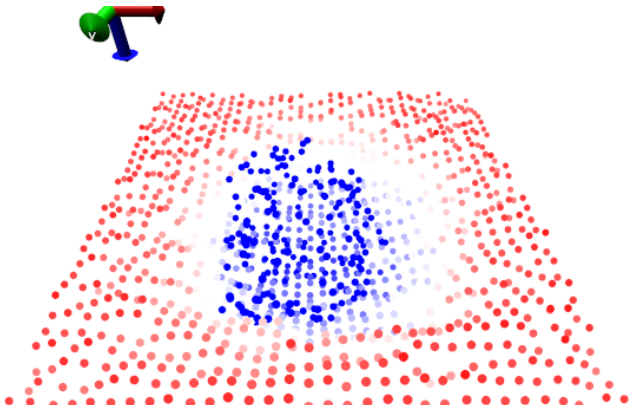
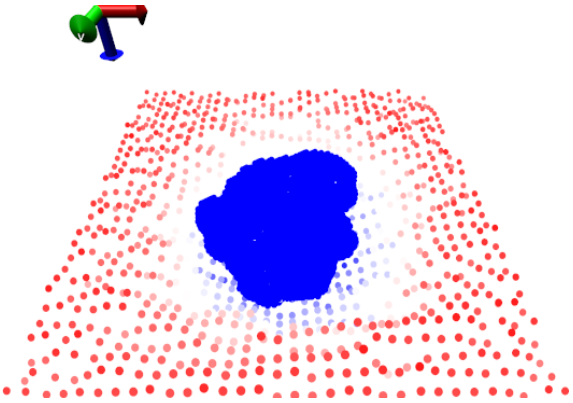
The output will be sent to the email provided.

Any comments, questions, suggestions or corrections please address to us using the link "coordinator".

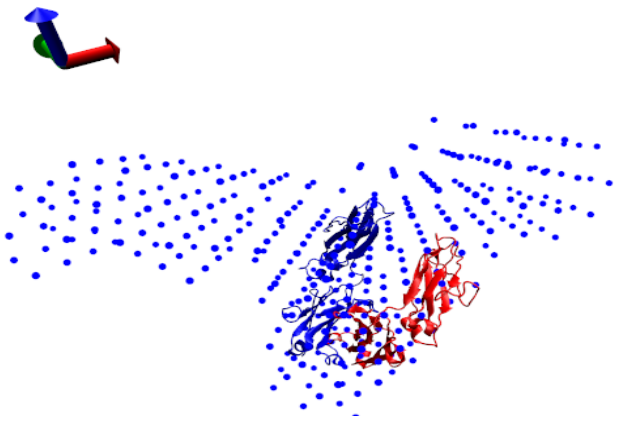
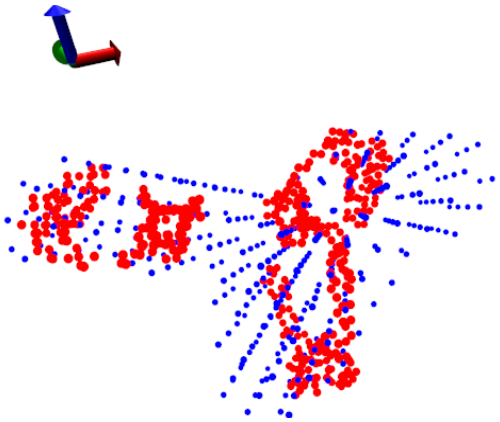
Examples

AFM

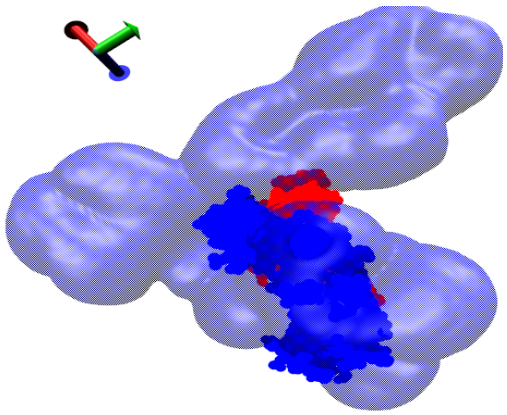
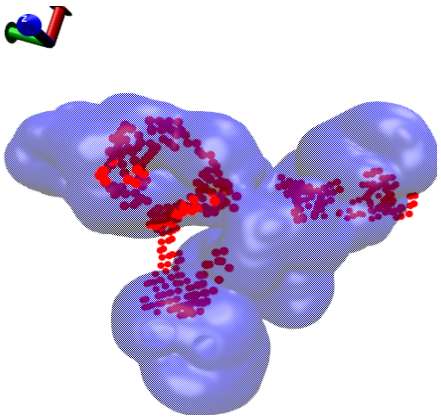
AFM+PDB
envelope = image.txt (not eroded, z = 0 Å) object = structure.pdb   favorable = 20 (Å) forbidden = 20 (Å) grid size = 32 resolution XY Z = 10 10 (Å) rotation = 12 (deg)
expected output:

offset_XYZ_A.txt = 1.375 -15.457 46.364 Energy_kcal.mol-1.txt = -12.1000

AFM+ISO (a)	AFM+ISO (b)
envelope = image.txt (not eroded, z = 0 Å) object = fva.pdb__adepth_probe.1.5A_grid.3.3.3A_boundary20A.grid input/object.grid atomic depth = **10** (Å) surface density = **20** favorable = 20 (Å) forbidden = 20 (Å) grid size = 32 resolution XY Z = 10 10 (Å) rotation = 12 (deg)	envelope = image.txt (not eroded, z = 0 Å) object = fva.pdb__adepth_probe.1.5A_grid.3.3.3A_boundary20A.grid input/object.grid atomic depth = **10** (Å) surface density = **1** favorable = 20 (Å) forbidden = 20 (Å) grid size = 32 resolution XY Z = 10 10 (Å) rotation = 12 (deg)
expected output:	
	
offset_XYZ_A.txt = -5.569 18.190 27.012 Energy_kcal.mol-1.txt = -5.9000	offset_XYZ_A.txt = -5.511 8.853 23.412 Energy_kcal.mol-1.txt = -15.7000

SAXS

SAXS+PDB	SAXS+ISO
envelope = MCA_011_1.pdb object = SBTN_Fc.pdb grid size = 32 resolution XY Z = 6.5 (Å) rotation = 12 (deg) 3D node radius = 6.5 (Å)	envelope = MCA_011_1.pdb object = 1HZH_SBTN.cen.noh.pdb__adepth_probe.2A_grid.4.4.4A_boundary5A.grid atomic depth = **-8** (Å) surface density = **1** grid size = 32 resolution XY Z = 6.5 (Å) rotation = 12 (deg) 3D node radius = 6.5 (Å)
expected output:	
	
offset_XYZ_A.txt = 5.033 -18.650 -12.325 Energy_kcal.mol-1.txt = -40.0000	offset_XYZ_A.txt = -8.448 -1.683 -1.671 Energy_kcal.mol-1.txt = -25.7000

cryo-EM

cryo-EM+PDB	cryo-EM+ISO
envelope = emd_2285.map object = SBTN_Fc.pdb grid size = 32 resolution XY Z = 6.5 (Å) rotation = 12 (deg) 3D node radius = 6.5 (Å)	envelope = emd_2285.map object = 1HZH_SBTN.cen.noh.pdb__adepth_probe.2A_grid.4.4.4A_boundary5A.grid atomic depth = **-8** (Å) surface density = **1** grid size = 32 resolution XY Z = 6.5 (Å) rotation = 12 (deg) 3D node radius = 6.5 (Å)
expected output:	
	
offset_XYZ_A.txt = -19.596 -20.613 -7.778 Energy_kcal.mol-1.txt = -40.5000	offset_XYZ_A.txt = -0.301 -24.049 -4.504 Energy_kcal.mol-1.txt = -27.7000