Phenix *Python-based Hierarchical ENvironment for Integrated Xtallography*

Tutorial: Cryo_fit2: Fit Biomolecules into Cryo-EM Maps using dynamics (commandline)

Contents

Overview

This tutorial will show you how to fit biomolecule atomic structures into cryo-EM maps using dynamics simulation with PHENIX commandline

Theory for Cryo_fit2

See the theory notes for cryo_fit2

Install Cryo_fit2

See the installation notes for cryo_fit2

Input

<initial_model>, <target_map> and <map resolution>

The <initial_model> is a guide or template structure (.cif/mmCIF/.pdb) that is close to a <target_map> (.ccp4/.map) structurally.

User can use map_to_model to build the atomic model.

User can use either dock_in_map or UCSF chimera (Tools->Volume Data->Fit in Map) to roughly place the model into a map.

Running the program

At command line:

```
% phenix.cryo_fit2 <initial_model> <target_map> <map resolution in Angstrom>
```

Tutorial command:

```
% Go to <user phenix>/modules/cryo_fit2/tutorial

% source run_me.sh

% (run_me.sh is phenix.cryo_fit2 input/tutorial_cryo_fit2_model.pdb
  input/tutorial_cryo_fit2_map.ccp4 resolution=4)
```

Output

A final cryo_fitted structure: output/cryo_fit2_fitted.pdb

Structures of intermediate steps that can be animated with pymol play button: output/all_states.pdb

In pymol commandline:

```
% load ./user_map.ccp4, map1, 1 , ccp4

% isomesh mesh1, map1, 1.5, (all), 0, 1, 3.0

% cmd.color("blue","mesh1")
```

will show map contour as mesh.

Otherwise, use pymol GUI:

```
% A (action) -> Mesh -> @ Level 3.0
```

will show cryo-EM map contour as mesh.

Options

All options will be used as default if unspecified. e.g. secondary_structure_enabled =True

List of most useful options

Option	Default value	Description of inputs and uses
resolution	none	cryo-EM map resolution (Angstrom) that needs to be specified by a user
start_temperature	300	Start temperature (Kelvin) for molecular dynamics simulation
final_temperature	0	Final temperature (Kelvin) for molecular dynamics simulation
cool_rate	10	Rate of cooling temperature (Kelvin) for MD simulation
number_of_steps	1000	Number of MD simulation steps at each temperature
map_weight	automatically optimized	A weight toward cryo-EM map
secondary_structure.enabled	True	Most MD simulations tend to break secondary structure. Therefore, turning on this option is recommended. If HELIX/SHEET records are present in supplied .pdb file, automatic search of the existing secondary structures in the given input pdb file will not be executed.
secondary_structure.protein.remove_outliers	True	False may be useful for very poor low-resolution structures by ignoring some hydrogen "bond" if it exceed certain distance threshold
output_dir	output	Output folder name prefix
keep_progress_on_screen	True	If True, temp=xx dist_moved=xx angles=xx bonds=xx is shown on screen rather than cryo_fit2.log
keep_origin	True	If True, write out model with origin in original location. If False, shift map origin to (0,0,0)