Phenix *Python-based Hierarchical ENvironment for Integrated Xtallography*

CryoFit2: Fitting to a Cryo-EM Map using Phenix Dynamics

Contents

Overview

Still developing for automatic parameter optimization!

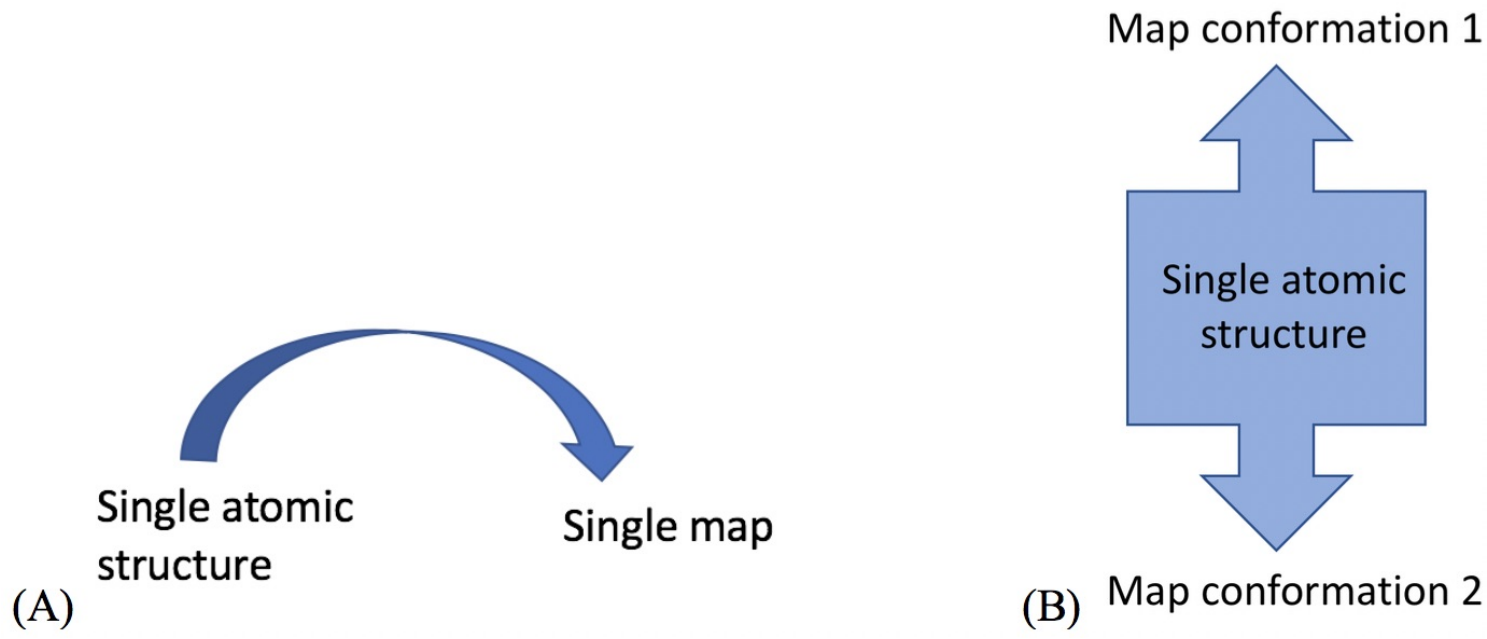
Unlike Cryo_fit1 that uses gromacs, CryoFit2 runs within phenix suite. Therefore, it doesn't require gromacs installation and is faster to execute. It suits the need not only traditional "static" fitting but also "dynamic" fitting.

Theory

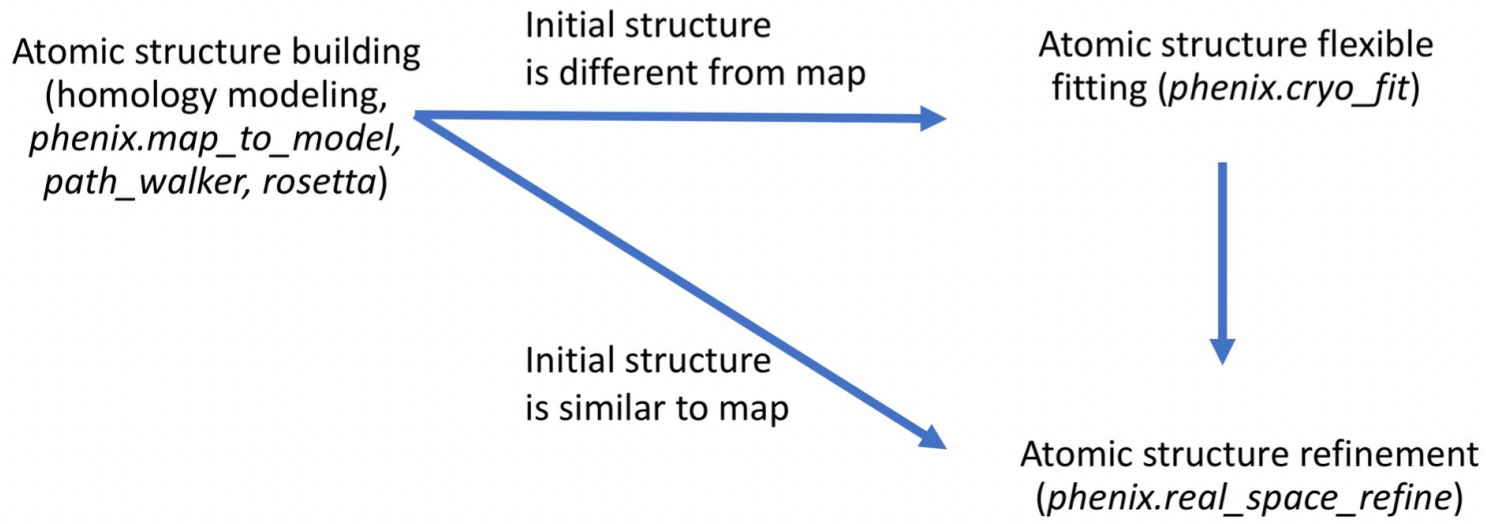
This program uses phenix dynamics written by Pavel.

Temperature gradient descent rather than simulated annealing is carried out by default to minimize the objection function T (=T_target_map * wx + T_geom * wc). wx is cryo-EM map weight and wc is geometry keeping weight.

Traditional "static" fitting (A) versus "dynamic" fitting (B)



Cryo_fit 1 & 2 are recommended when the initial structure is different from map



How to Run Cryo_fit2

See the tutorial notes for cryo_fit2

Limitation

If wx is too small like 5, it may break starting secondary structure. When wx is 100, it kept starting helix structure. If wx is too big, angle change for each step maybe too big (~30 degree), so pdb validation later (like molprobity) may raise a red flag. We will add real_space_refine style wx, wc auto-optimization module soon.

As described in phenix dynamics, cryo_fit2 doesn't use electrostatic interaction. Therefore, it does not fully capture all physical forces. Cryo_fit1 also omitted electrostatic interaction so that md simulation runs faster.

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