

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

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Overview

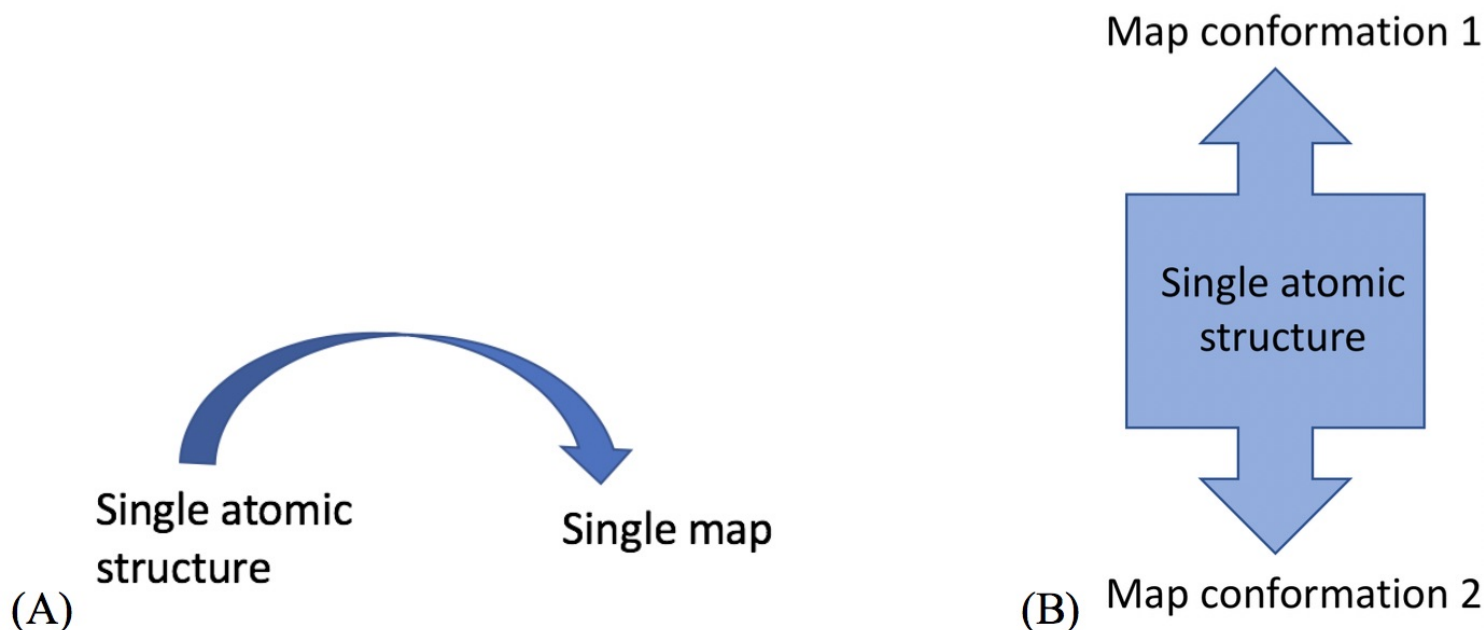
Unlike [Cryo_fit1](#) that uses gromacs, CryoFit2 runs within phenix suite. Therefore, it doesn't require gromacs installation and is faster to execute. It suits the need not only traditional "static" fitting but also "dynamic" fitting.

Theory

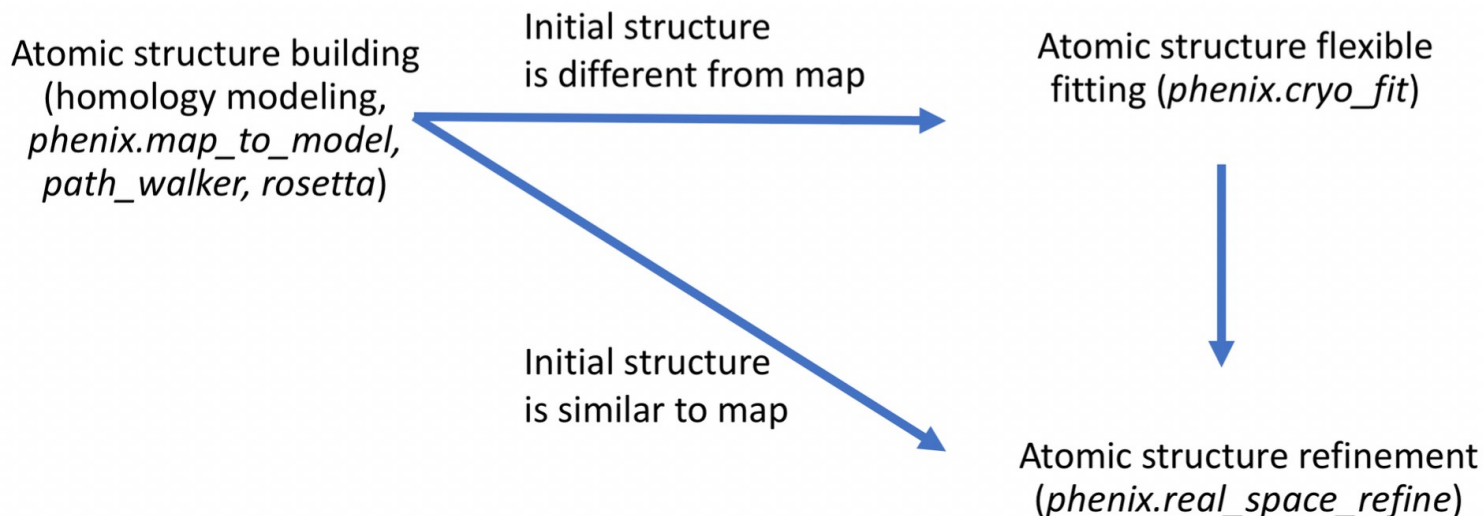
This program uses [phenix dynamics](#) written by Pavel.

Temperature gradient descent rather than simulated annealing is carried out by default to minimize the objection function $T (=T_{\text{target_map}} * wx + T_{\text{geom}} * wc)$. 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 molprobtity) may raise a red flag.

We will add *real_space_refine* style *wx*, *wc* auto-optimization module soon.

Author

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