Phenix *Python-based Hierarchical ENvironment for Integrated Xtallography*

Cryo_fit1 FAQ

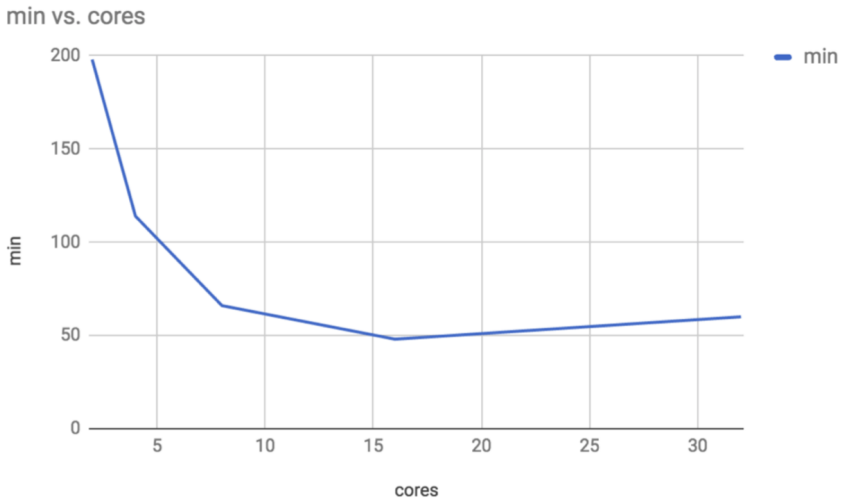
Contents

How long does it take to run cryo_fit?

How long does it take to run cryo_fit?

- CentOS with 2 cores (2.7 Ghz)
  - tRNA (6,000 atoms) : 2.5 minutes
  - Nucleosome (26,000 atoms): 1 hr
  - Beta-galactosidase (64,000 atoms): 2.5 hrs
  - ribosome (386,000 atoms): 3~7 hrs
- macOS
  - 24 cores (2.7 Ghz)
    - (4~16 cores would give similar/better performance)
    - Beta-galactosidase (64,000 atoms): 3.9 hrs
  - 4 cores (3.1 Ghz)
    - Beta-galactosidase (64,000 atoms, 50,000 cryo_fit steps): 5.8 hrs

Benchmark with ribosome (same linux machine, 10k emsteps, 50k number_of_steps, 3x emweight)



- Based on this result, number of cores is recommended up to 16

How to generate and record movie?

Generate_record_movie_by_cryo_fit1

I see an error message at my 1_make_gro step.

- If a user sees "Fatal error: Atom xx in residue xx xxx was not found in rtp entry xx with xx atoms while sorting atoms." on his/her screen,
  - please remove/fix wrong atoms. Running real_spaace_refine via phenix GUI will show which atoms need to be removed/fixed.

I see "Fatal error: A charge group moved too far between two domain decomposition steps. This usually means that your system is not well equilibrated" at my 8_cryo_fit step.

- Using macOS 10.13.6 helped rather than using Ubuntu 16.04. Maybe macOS has better numerical stability.

- One gromacs expert suggested to try smaller time_step_for_cryo_fit.
- However but for Doonam, simply using macOS solved the problem.

I see "Fatal error: Number of grid cells is zero. Probably the system and box collapsed." at my 8_cryo_fit step.

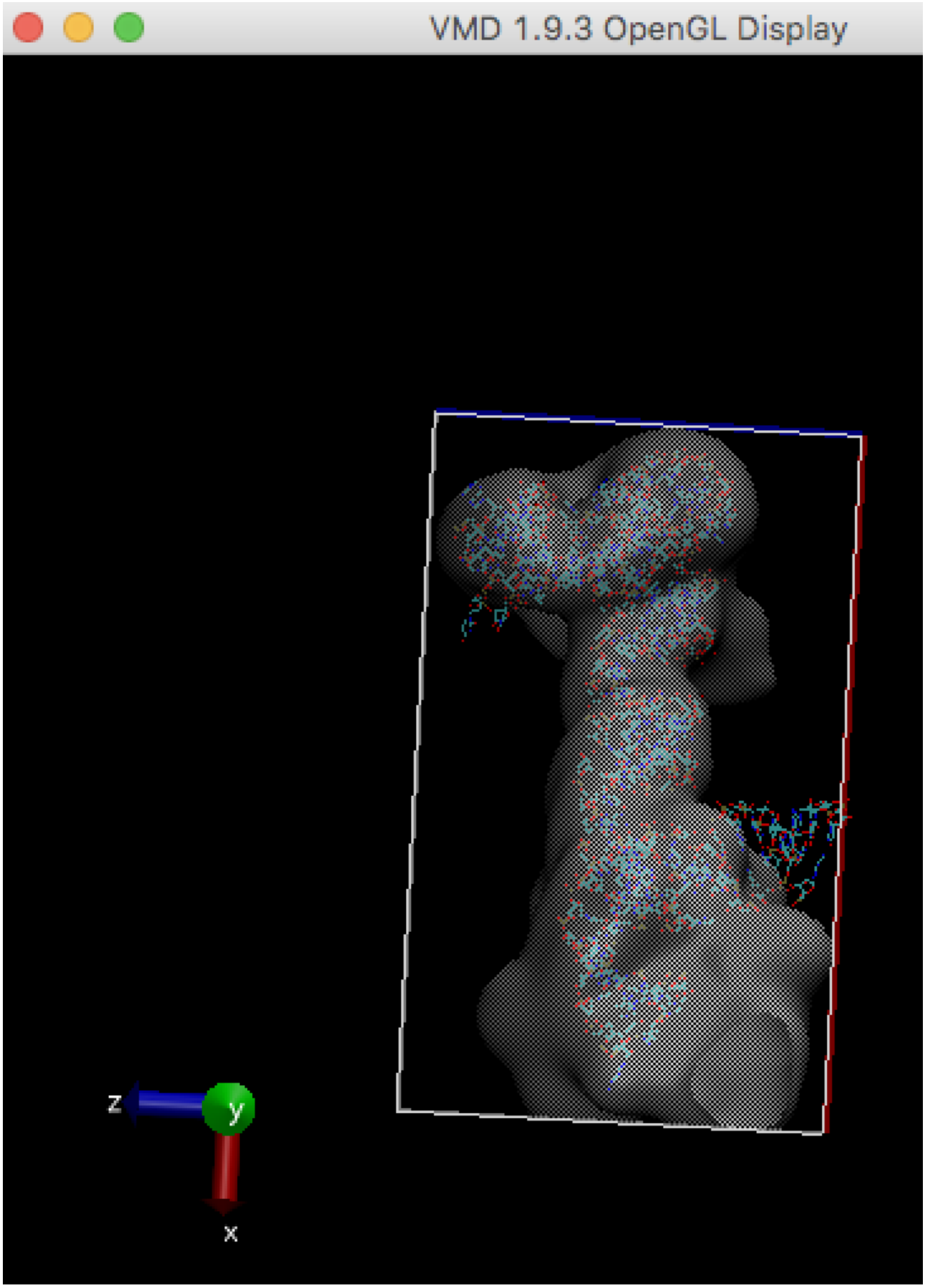
- step_8 may be full of stepxb_nx.pdb.
- Most likely, this means that initial cc is too low for MD simulation.
- When Doonam ran real_space_refine first, then run real_space_refined atomic model in cryo_fit, it was solved.
- Alternatively, UCSF Chimera's 'fit in map' or UCSF ChimeraX's isolde may improve initial cc.
- Less likely, but still a possible case is when the map weight is too high, lowering emweight_multiply_by may help.

I see "step 0 correlation coefficient: nan" at my 8_cryo_fit step.

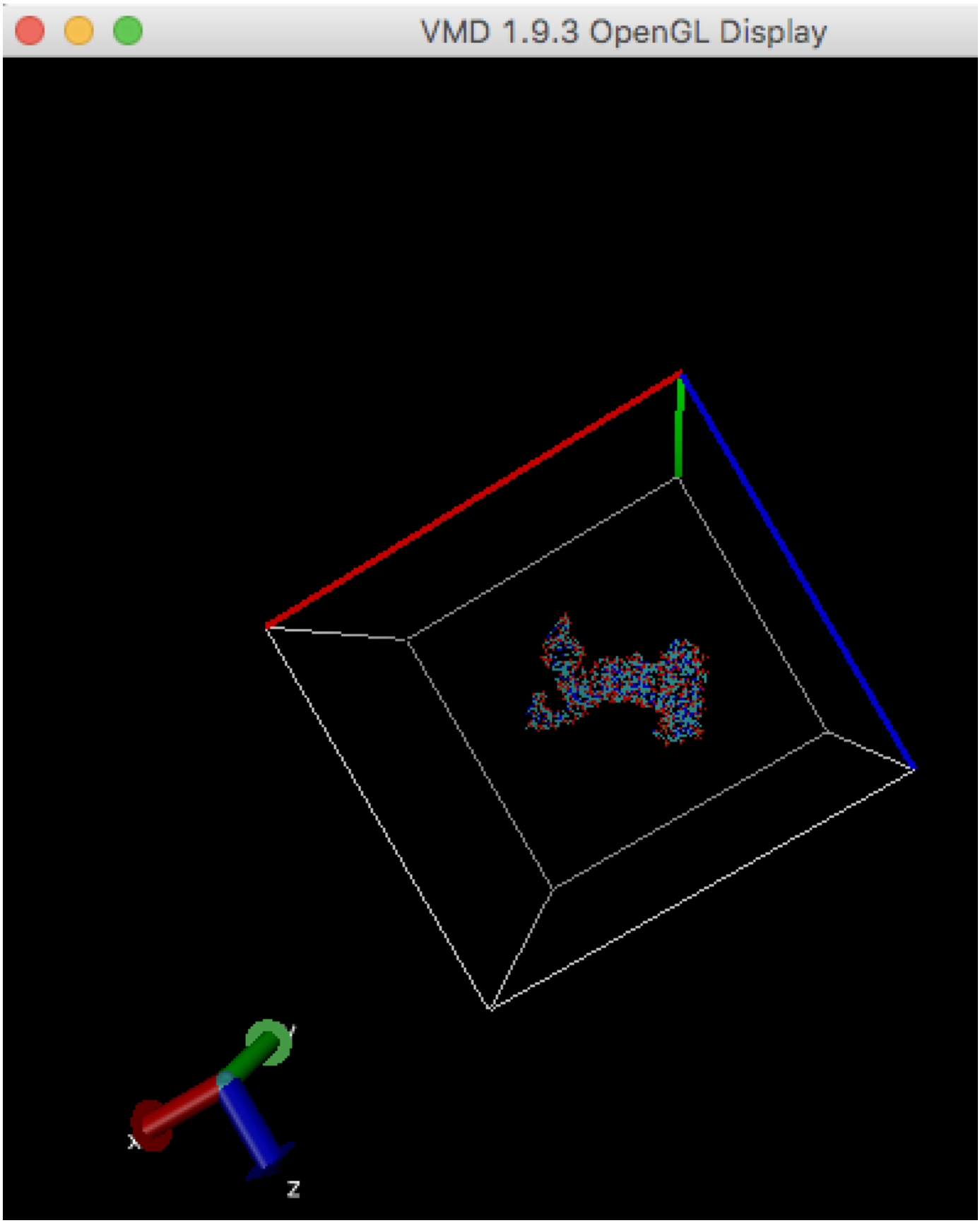
- This often indicates that the initial atomic model is not placed into a cryo-EM map.
- Try dock_in_map or UCSF Chimera's fit in map, and provide refitted atomic model to cryo_fit

I see "step 0 correlation coefficient: nan" and "Range checking error: Explanation: During neighbor searching, we assign each particle to a grid based on its coordinates. If your system contains collisions or parameter errors that give particles very high velocities you might end up with some coordinates being +- Infinity or NaN (not-a-number). Obviously, we cannot put these on a grid, so this is usually where we detect those errors. Make sure your system is properly energy-minimized and that the potential energy seems reasonable before trying again." at my 8_cryo_fit step.

- When a user used a partical map region ("boxed map") by phenix.map_box , cryo_fit's automatic mrc to sit map format conversion may not work properly.
- Therefore, please use situs map2map to convert your mrc format map to situs format map. You can convert by "map2map user.mrc user.sit" then enter 1 for "Convert to classic Situs (auto)*". Then, provide this user.sit file to your cryo_fit. For example, phenix.cryo_fit user.pdb user.sit
- When Doonam provided situs made sit map file, the cryo_fit ran smoothly again.
- When a user didn't use phenix.map_box, it means that the map dimensions need to be larger.
- Like other MD simulations, gromacs need enough map box size to cover the atomic model to run (ziggle and wiggle). Refer Waters seems to be out of the box
- For example, stuck-out red oxygen atoms outside the right edge of the box are the problem.



- In order to run any MD simulation (including cryo_fit), a box should be large enough like

- 

- Make map box dimensions larger, and run cryo_fit again. You can check map box size by VMD.