



*Python-based **H**ierarchical **E**Nvironment for **I**ntegrated **X**tallography*

Cryo_fit1 FAQ

Contents

- [How long does it take to run cryo_fit?](#)
- [How to generate and record movie?](#)
- [I see an error message at my 1 make_gro step.](#)
- [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.](#)
- [I see "Fatal error: Number of grid cells is zero. Probably the system and box collapsed." at my 8 cryo_fit step.](#)
- [I see "step 0 correlation coefficient: nan" at my 8 cryo_fit step.](#)
- [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.](#)

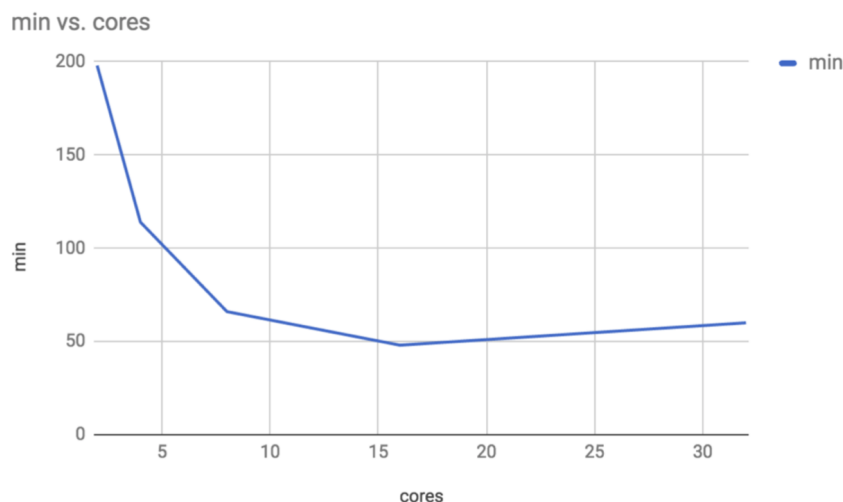
How long does it take to run cryo_fit?

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_space_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.

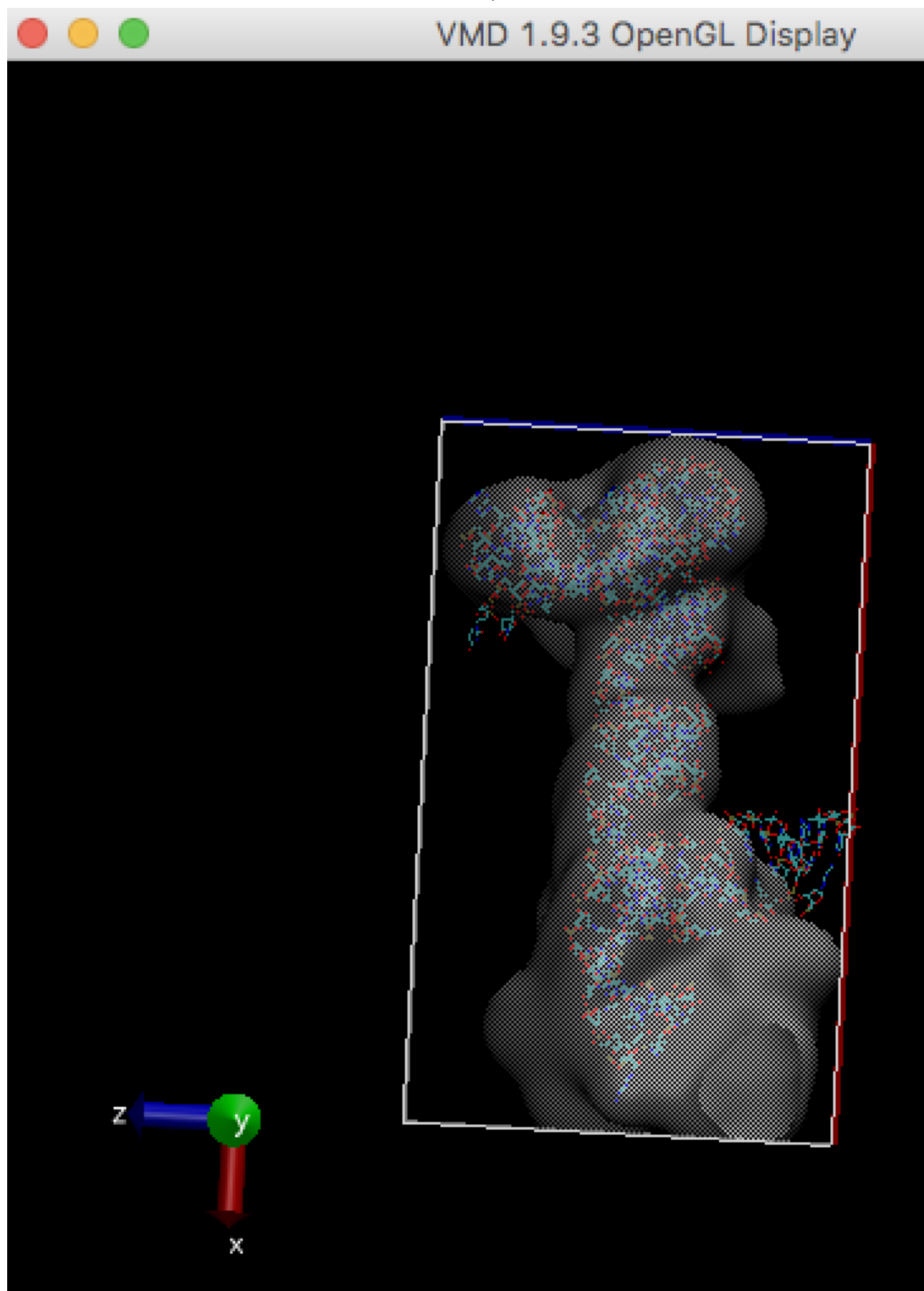
- `step_8` may be full of `stepxb_nx.pdb`.
- Most likely, this means that initial cc is too low for MD simulation.
- When Doonam ran `real_space_refine` first, then run `real_space_refined` atomic model in `cryo_fit`, it was solved.
- Alternatively, UCSF Chimera's 'fit in map' or UCSF ChimeraX's `isolve` 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.

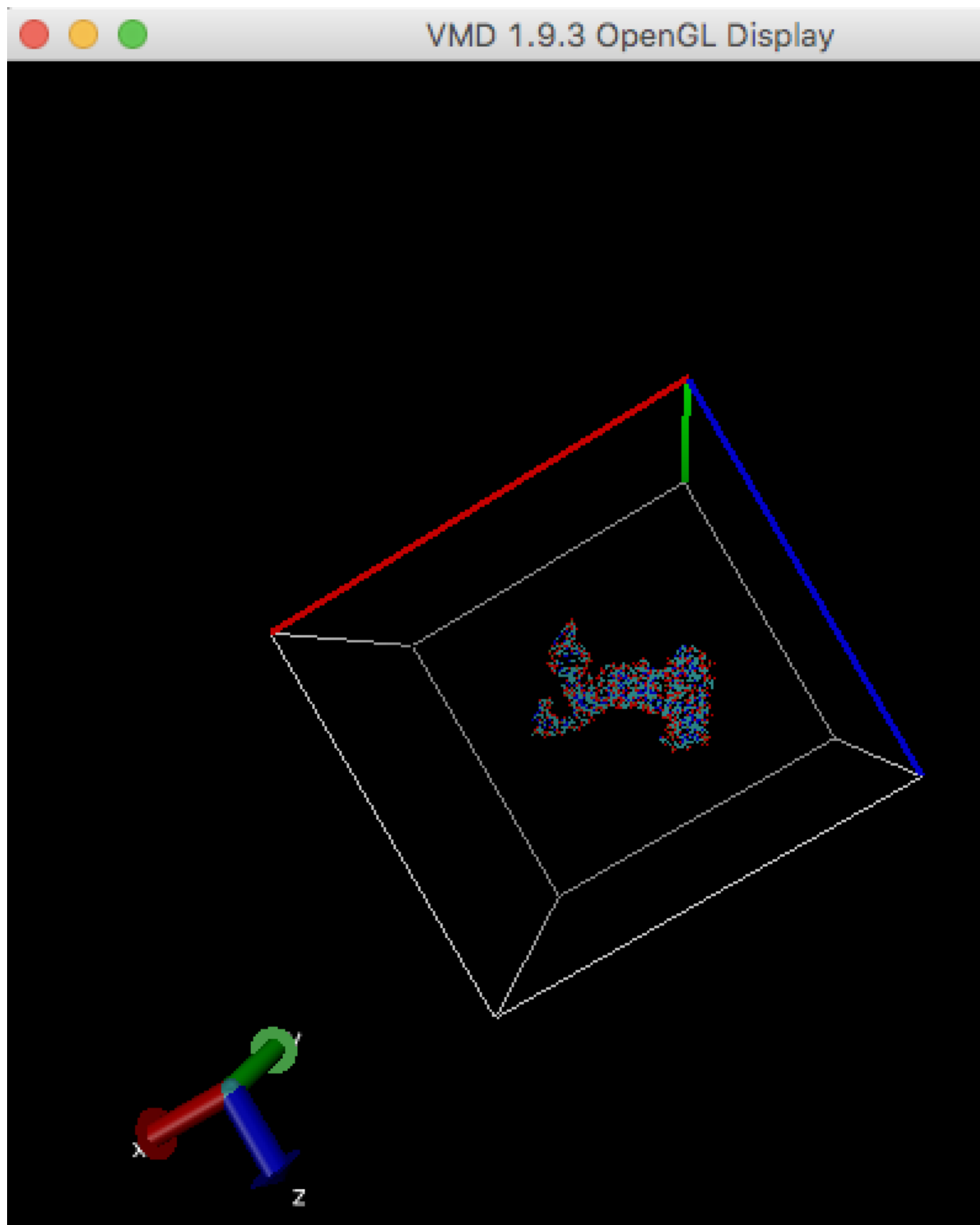
- This often indicates that the initial atomic model is not placed into a cryo-EM map.
- Try [dock in map](#) or UCSF Chimera's fit in map, and provide refitted atomic model to `cryo_fit`

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.

- 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.



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- 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.
- It is rare, but when you used a partial 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 [phenix.map_box](#), cryo_fit's automatic mrc to sit map format conversion may not work properly.

- 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.