Phenix

Python-based Hierarchical ENvironment for Integrated Xtallography

Cryo_fit FAQ

Contents

- [At my last step (8_cryo_fit), I see "step 0 correlation coefficient: nan" in my md.log file](#)
- [How long does it take to run cryo_fit?](#)

At my last step (8_cryo_fit), I see "step 0 correlation coefficient: nan" in my md.log file

This message often indicates when the initial atomic model is not placed into a cryo-EM map.

Try [dock_in_map](#)

## 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)

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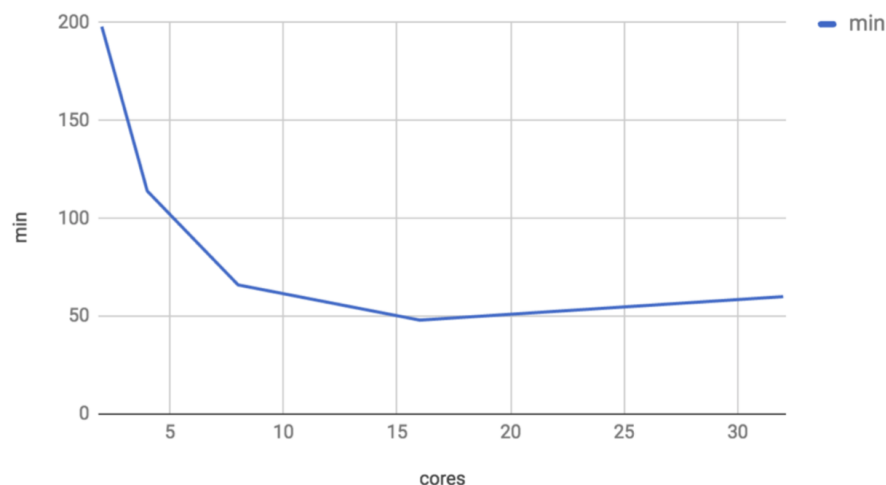
- Based on this result, number of cores is recommended up to 16