UCSF ChimeraX - II - Overview EM

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Contents

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## Warning: package 'knitr' was built under R version 3.5.2
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1 Workshop goal

In this second section we'll explore briefly electron density maps. This is usefulf for CryoEM data but also X-ray crystallography.

1.1 Learning objectives

- Open a density map
- display density
- color etc.
- Close and quit

1.2 NOTES on format

Embedded movies only appear within the HTML version of this document. For PDF and DOCX version refer to the foot notes for URL.

Figure 1: *"Verify mouse settings in System Preferences."*

Note: If you are left-handed inverting Left and Right assignments might work better for you.

Note:

`TASK`

This button will invite you to act on **suggested actions** as we go along the workshop.

2 Introduction

Some of the material presented here is inspired by a demonstration of **ChimeraX** by **Tom Goddard** (Programmer/Analyst, UCSF Resource for Biocomputing, Visualization, and Informatics) who develops the software. *YouTube* "Movie Making for cryoEM using ChimeraX."[1] (The movie is 49 min long.)

[1] https://youtu.be/yOMKwCbXl0g

(Credit: SBGrid Consortium. Published on Apr 20, 2017)

2.1 Background

The "*Guide to Unterstanding PDB data*"[2] provides important information on the methods used for the determination of atomic structures, biological assemblies, resolution, etc.

[2] https://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/methods-for-determining-structure

3 Density maps

In previous workshops we have only worked with atomic coordinates. Density maps are the primary result of experimental analysis of CryoEM and X-Ray crystallography that scientists use to build atomic coordinates if the *resolution* is adequate. (For a comparison between CryoEM and X-Ray crystallography density maps see *e.g.* Wlodawer, Li, and Dauter (2017).)

> A definition of *resolution*, in structure determinations, is the distance corresponding to the smallest observable feature: if two objects are closer than this distance, they appear as one combined blob rather than two separate objects[3] (see also embedded movie[4].)

[3] http://proteopedia.org/wiki/index.php/Resolution

(Credit: movie by James Holton[^CX23]) [^CX23]:http://bl831.als.lbl.gov/~jamesh/movies/

[4] https://youtu.be/omFOLG5Z5w4

3.1 What is a density map?

Electron density maps are obtained:

- in X-Ray crystallography: by diffraction
- in cryoelectron microscopy: by averaging 2D images in different orientations

In both cases complex mathematical formulae are used *via* computer software (including Fast Fourrier Transforms.) The final result is a series of *grid points* in space assigned with an electron density value: this is where *matter* is located.

3.1.1 Cryo EM Maps

The video "*A 3 minute introduction to CryoEM*"[5] provides a good visual summary of the process:

[5] https://youtu.be/BJKkC0W-6Qk

(Credit: Gabe Lander Thesis defense, 2009. Published on Aug 17, 2011)

3.2 X-Ray maps

The video "*What is Cryo-Electron Microscopy (Cryo-EM)*"[6] highlights both methods. The X-Ray method is summarized in 20 seconds (starting at 20 seconds in the movie and ending at 40 seconds.)

(Credit: GUC San Francisco (UCSF) - Published on May 28, 2015)

[6] https://youtu.be/Qq8DO-4BnIY?t=20s

3.3 Density map databases

Density maps may be deposited at **The Electron Microscopy Data Bank (EMDB)** that contain the same data but with different user interface or web functionality:

- Americas: http://www.emdatabank.org/
- Europe: https://www.ebi.ac.uk/pdbe/emdb/
- Japan: https://pdbj.org/emnavi/

3.3.1 Search PDB and EMDB

Structural entries may be combined with PDB entries from which there exists an atomic structure: http://emdatabank.org/search.html

3.3.1.1 Search EMDB

Browse/search:

- Simple search (RCSB): http://emsearch.rutgers.edu
- Advanced search (PDBe): http://pdbe.org/emsearch

Resources:

Searching, Visualizing and Analysing EMDB Data–PDBe Webinar Recording (July 8, 2013)[7]

[7] https://bit.ly/2HwOITT

3.3.1.2 Search PDB

Browse PDB entries determined using 3DEM methods:

- RCSB PDB[8]
- PDBe[9]
- PDBj[10]

[8] https://bit.ly/2HwOITT

[9] https://bit.ly/2r291Ns

[10] https://pdbj.org/emnavi/

4 Exercise in ChimeraX

Follow the **ChimeraX** menu cascade below to bring the "Quick Start Guide"

`Help` > `Quick Start Guide`

This will open a page within the internal web browser of **ChimeraX**. The page is LOCAL on your computer and part of the software installation.

SCROLL DOWN to the portion titled: **"Example Density-Map Commands"**

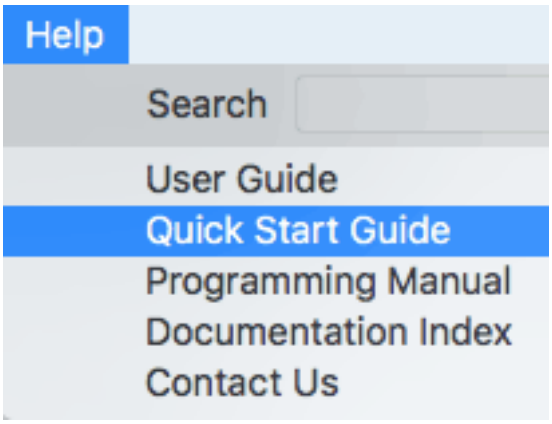

Figure 2: *"Open Quick Start Guide."*

On THIS PAGE the commands are clickable and will be immediately applied within **ChimeraX**.

Note: it is also possible to open a version on the web (ChimeraX Quick Start Guide)[11], however the commands are not click-and-execute as in the local verison.

[11] https://www.cgl.ucsf.edu/chimerax/docs/quickstart/index.html

You can then click on the pre-written commands and see the results within the graphical window.

REFERENCES

Wlodawer, A., M. Li, and Z. Dauter. 2017. "High-Resolution Cryo-EM Maps and Models: A Crystallographer's Perspective." *Structure* 25 (10): 1589–97. https://doi.org/10.1016/j.str.2017.07.012.