Phenix workshop
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Tom Terwilliger
Los Alamos National Laboratory
New Mexico Consortium
Complete set of cryo-EM tools in Phenix

Starting map → Map improvement → Segmentation

Map manipulation → Map symmetry

Validation

Refinement → Docking, model-building
New Phenix cryo-EM tools

- Display map properties
- Find symmetry
- Combine maps
- Unique part of map
- Docking

- Show-map-info
- Map-symmetry
- Combine-focused-maps
- Map-box (extract-unique)
- Dock-in-map
Displaying map properties with show_map_info

**Typical cryo-EM map:**

- Center: (0,0,0)
- Origin: (-128, -128, -128)
- Extent (map size): 256, 256, 256
- Unit cell grid: 256 x 256 x 256
- Unit cell: 300 Å x 300 Å x 300 Å

Origin at (-128, -128, -128)

Shift origin to place corner at (0,0,0)

Unit cell grid: (256 x 256 x 256)

Unit cell: 300 Å x 300 Å x 300 Å
Map with origin at (0, 0, 0)

Origin at (0,0,0)

Unit cell grid: (256 x 256 x 256)
Unit cell: 300 Å x 300 Å x 300 Å

Center: (128, 128, 128)
Origin: (0, 0, 0)
Extent (map size): 256, 256, 256
Unit cell grid: 256 x 256 x 256
Unit cell: 300 Å x 300 Å x 300 Å
Cutting out part of a map with \texttt{map\_box}

\textbf{Boxed map}

Box cut from 100 – 256 in each direction

\textit{Unit cell grid: (256 x 256 x 256)}

\textit{Unit cell: 300 Å x 300 Å x 300 Å}

Origin at (0,0,0)
**Displaying map properties with show_map_info**

- **Origin** at (100, 100, 100)
- **Extent (map size)**: 156, 156, 156
- **Box map cell**: 183 Å x 183 Å x 183 Å
- **Unit cell grid**: 256 x 256 x 256
- **Unit cell**: 300 Å x 300 Å x 300 Å
Procedure for finding symmetry:

- Test point group symmetries (e.g., C7, D2, I, O, T)
- Helical symmetry
- Principal rotation axes along z, x, y
- Score based on map correlation for symmetry-related points and number of operators
Extracting unique part of map with `map_box` (extract_unique option)

**Procedure:**

- Use symmetry of map
- Contour map at level that yields regions about 50 residues in size
- Group symmetry-related regions
- Choose one member of each group
- Optimize compactness and connectivity of unique part of map
Combining maps with combine_focused_maps

Procedure for combining maps:

- Superimpose density
- Rotation/translation from refined models
- Average target and focused map density
- Weight using map-model correlations
Combining maps with combine_focused_maps

Features

- Averaging of entire chains or local regions
- Application of symmetry to focused map (e.g., superimpose chain B of focused map on chains EFGH of target map)
Combining maps with combine_focused_maps

Target map

Focused map (chain B)

Composite map
Docking models with dock-in-map

EMD_8750

1ss8 chain A

**Search procedure:**

Pure translation
- low-res
- high-res

Rotation / translation
- low-res
- high-res

Score based on rigid-body refinement map-model correlation
Docking models with dock-in-map

EMD_8750

Features

- Multiple chains
- Density search
- Symmetry
- Multiprocessing

1ss8 chain A
Docking models with dock-in-map

EMD_8750

1ss8 chain A docked in map

1ss8 chain A
Phenix cryo-EM structure determination tools

Map improvement

Auto-sharpen
Combine-focused-maps

Segmentation

Map-box (extract-unique)
Segment-and-split-map

Docking

Dock-in-map
Map-to-model
Cryo-fit

Auto-building

Real-space-refine

Flexible fitting

Refinement

Segment-and-split-map
Phenix cryo-EM utilities

- Display map properties ➔ Show-map-info
- Map manipulation ➔ Map-box ➔ Map-to-structure-factors
- Find symmetry ➔ Map-symmetry
- Guess sequence ➔ Sequence-from-map
- Validate structure ➔ Mtriage ➔ EMringer ➔ Validation-cryoEM

MEQASFSLSG
The Phenix Project

Lawrence Berkeley Laboratory
Paul Adams, Pavel Afonine, Nigel Moriarty, Billy Poon, Oleg Sobolev, Dorothee Liebschner

Los Alamos National Laboratory
Tom Terwilliger, Li-Wei Hung

Duke University
Jane & David Richardson, Chris Williams, Bradley Hintze, Vincent Chen

Cambridge University
Randy Read, Airlie McCoy, Tristan Croll, Rob Oeffner, Kaushik Hatti, Massimo Sammito

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