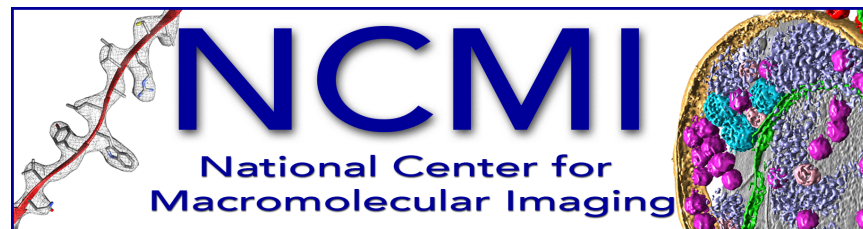


# Chimera, Segmentation, Rigid Fitting of Structures into Maps

Greg Pintilie, NCMi, BCM, Houston

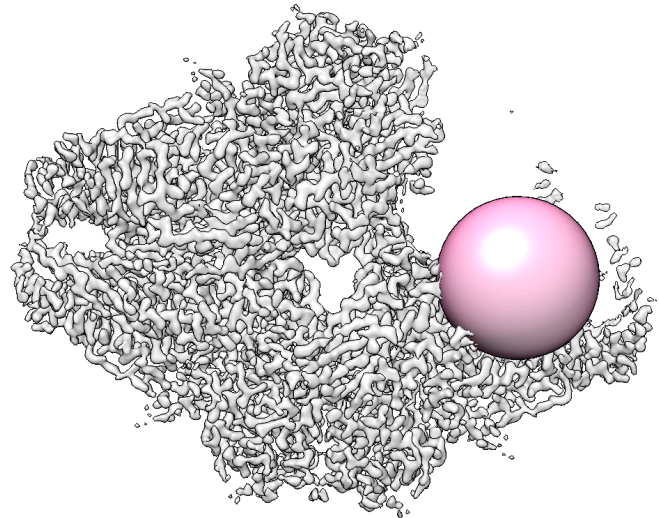


# Overview

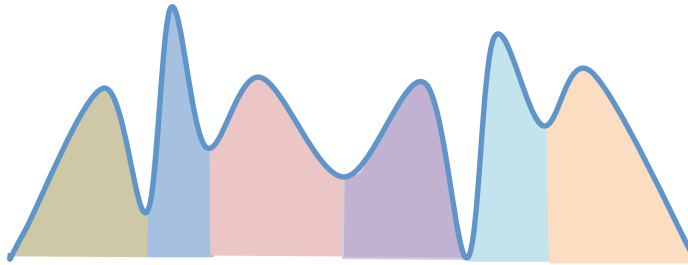
- Segmentation
- Fitting structures into maps
- Validation of fitting results
- Demo/Tutorial

# Segmentation of Density Maps

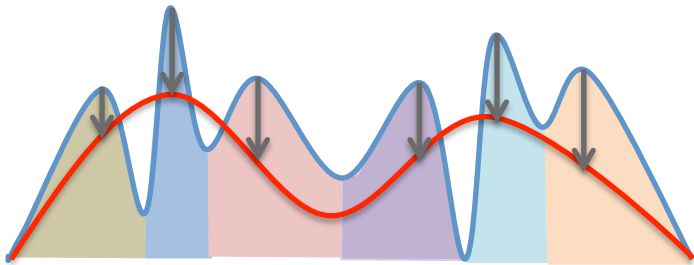
- Tools
  - Chimera
    - Volume Eraser
    - Zone Tool
  - Amira
  - Segger (Chimera)



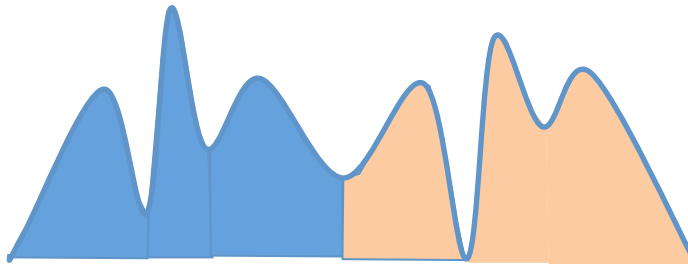
# Segger – 1D Example



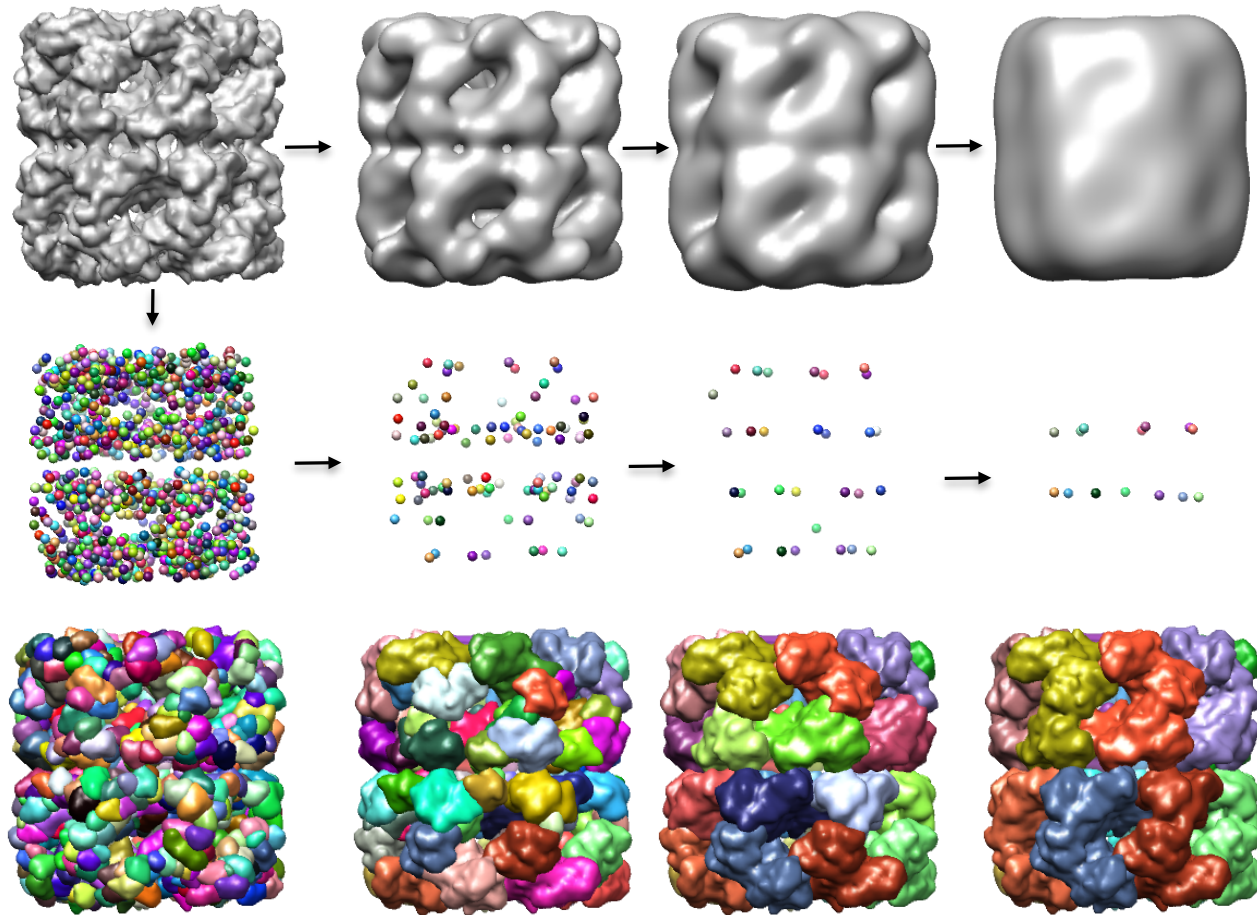
Topological/Watershed  
Segmentation  
(Non-parameteric clustering)



'Smoothing and grouping'  
Scale space analysis

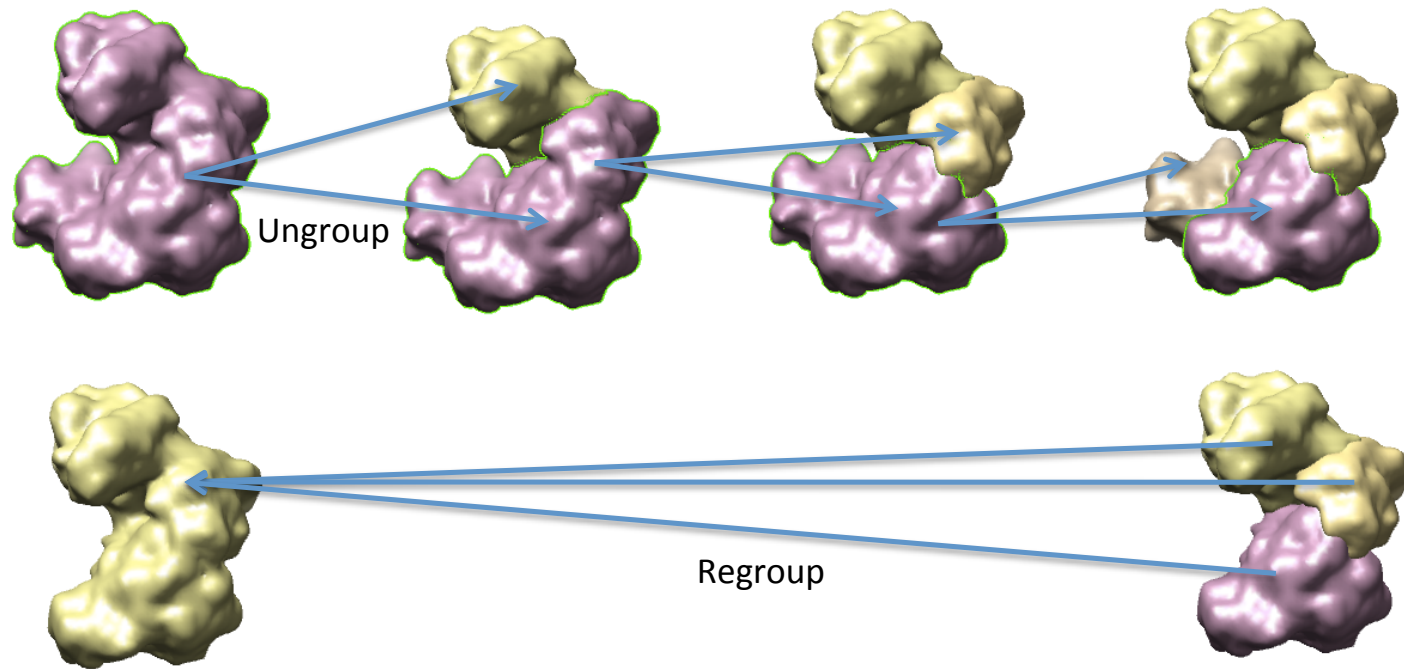


# Segger Segmentation – 3D



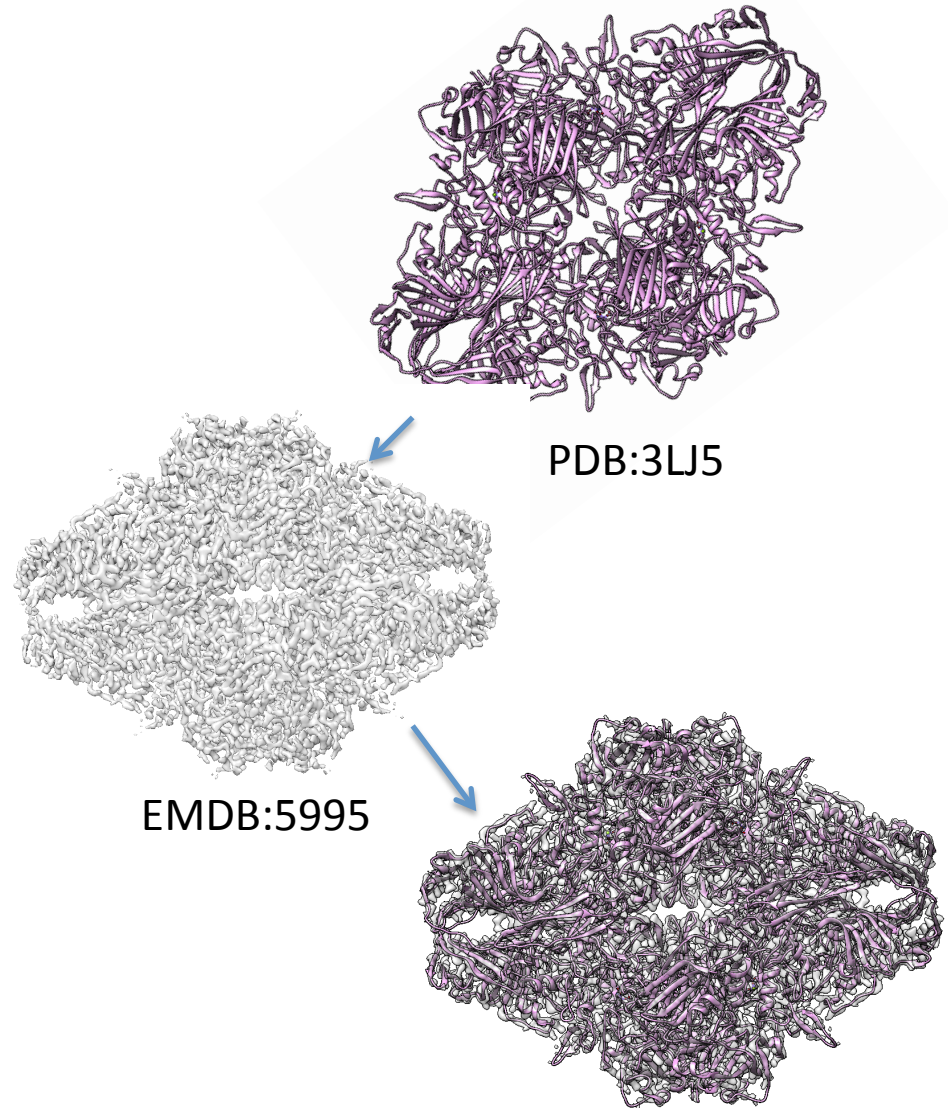
“Smoothing and grouping”

# Segger - Interactive Regrouping

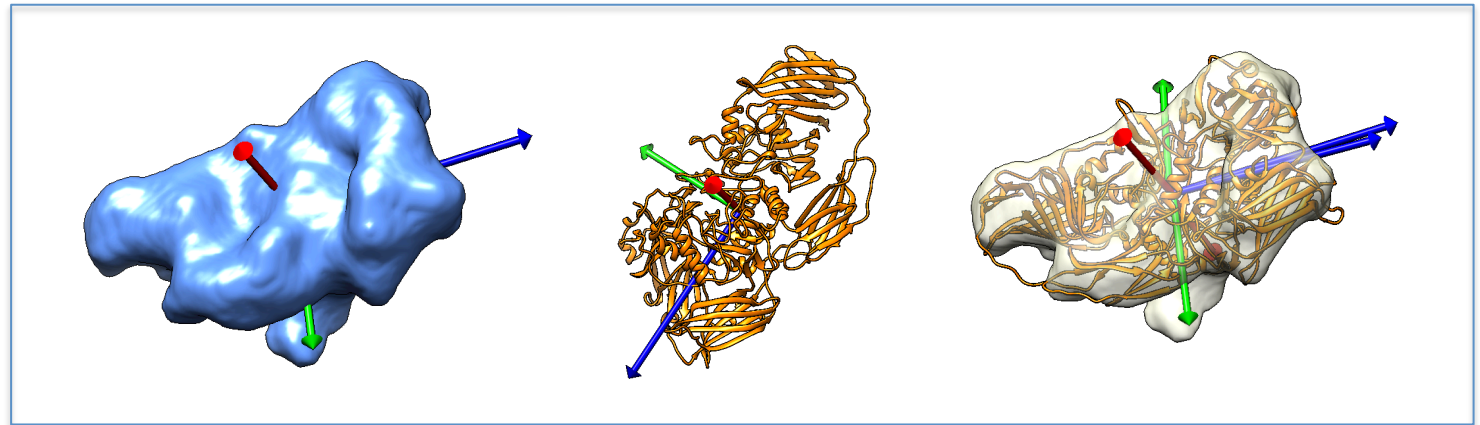


# Rigidly Fitting Structures Into Maps

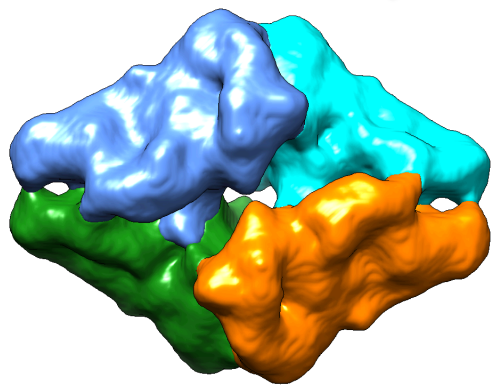
- Tools
  - Chimera
    - Fit in Map
  - Situs
  - ADP-EM
  - EMfit
  - Segger (Chimera)
    - Fit to Segments



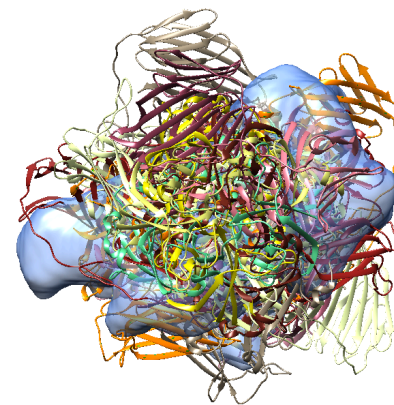
# Segger – Fit to Segments



Align centers and principal axes



Segmented Map

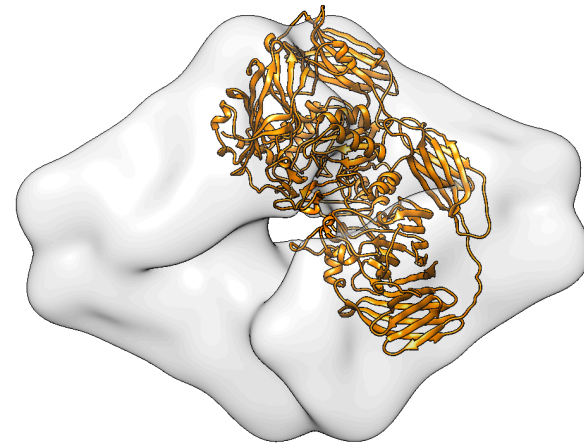
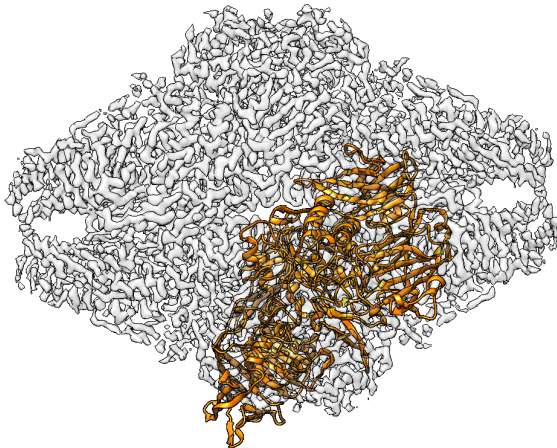
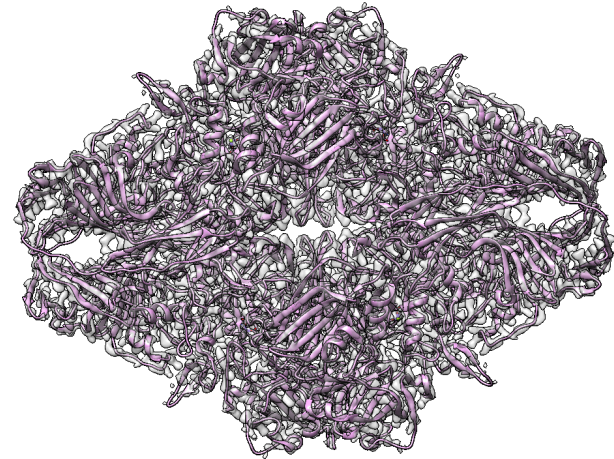


Align centers and do rotational search



# Validation of Rigidly Fitted Models

- How do we know a model is fitted correctly into the density map?
  - Do features align?
  - What are cross-correlation and other scores?



# Validation of Rigidly Fitted Models

- Z-score
  - Sort scores from highest to lowest
  - Is top score the correct fit?
    - How many standard deviations above the mean is the top score

$$Z = \frac{S_1 - Avg(S_{2..N})}{StDev(S_{2..N})}$$

