Paper Talks 2 – Visualizing Cellular and Molecular Data

Primer Talk

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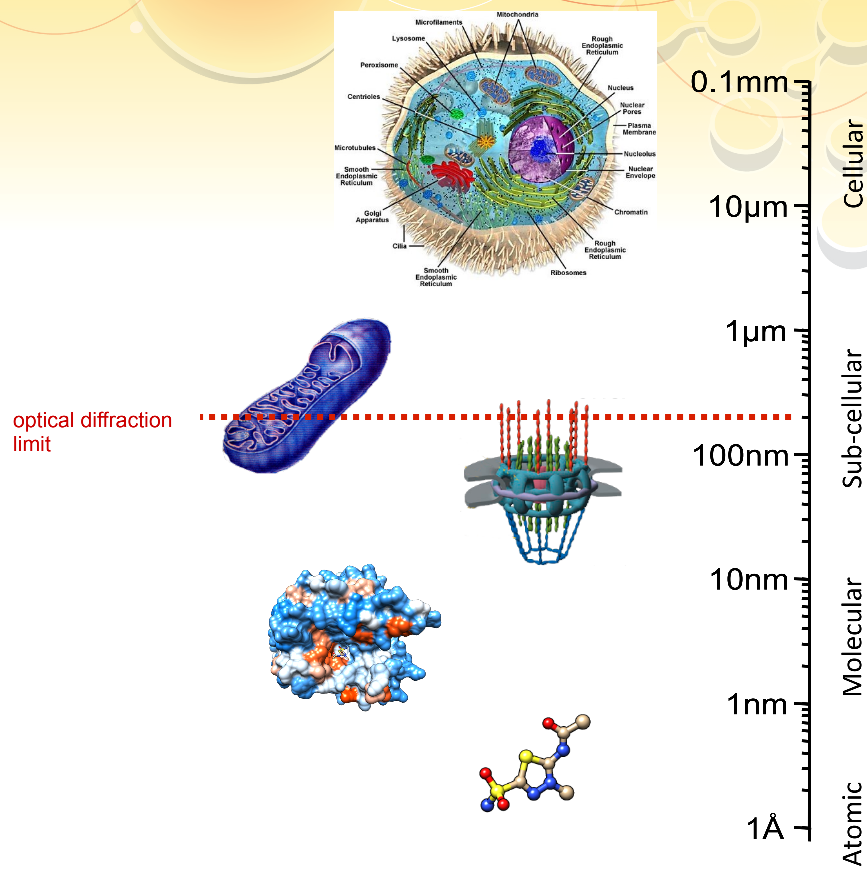
Fundamental Principle of Biology

- Sequence ➔ Structure ➔ Function

“If you want to understand function, study structure!” Francis Crick, 1988

Challenges in Understanding Biology

- Size scale for molecular function spans at least six orders of magnitude
- Time scale of important dynamical cellular processes ranges from picoseconds to hours/days
- Recent thinking has emphasized a systems-level approach ("systems biology") rather than considering individual components in isolation



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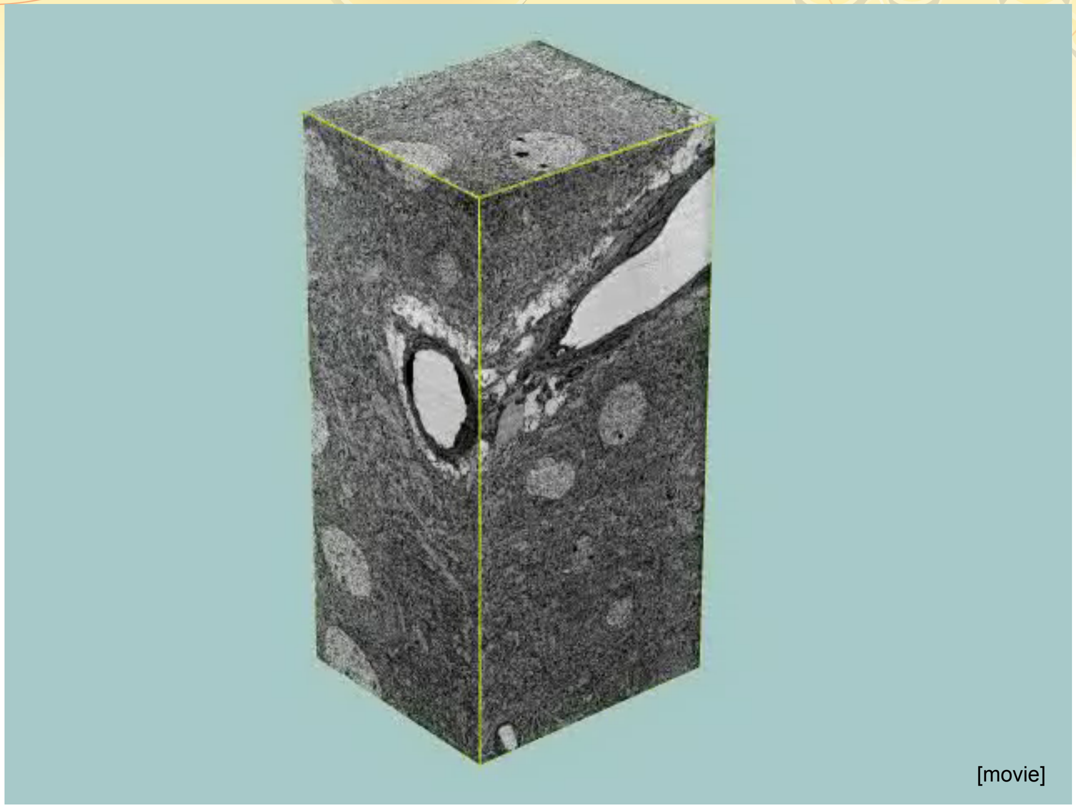
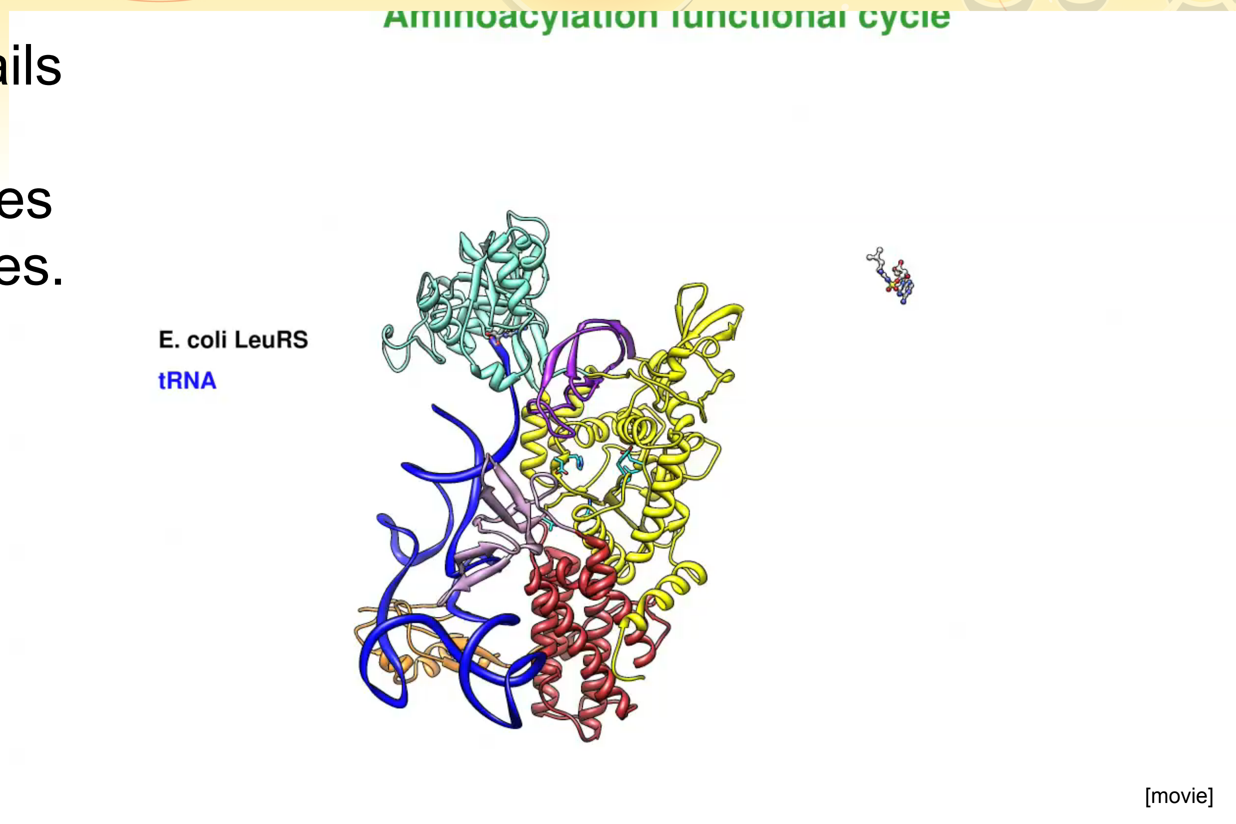
Example: Rat Brain Electron Microscopy

A 50 x 50 x 100 micron volume of rat cortex imaged by serial block-face scanning EM is shown. Datasets can be very large – a Drosophila brain at 10nm voxel size is ~100TB. Long range goal is to determine the neural connection network for an entire fly, rat, or human brain.



Example: leucine binding transfer RNA

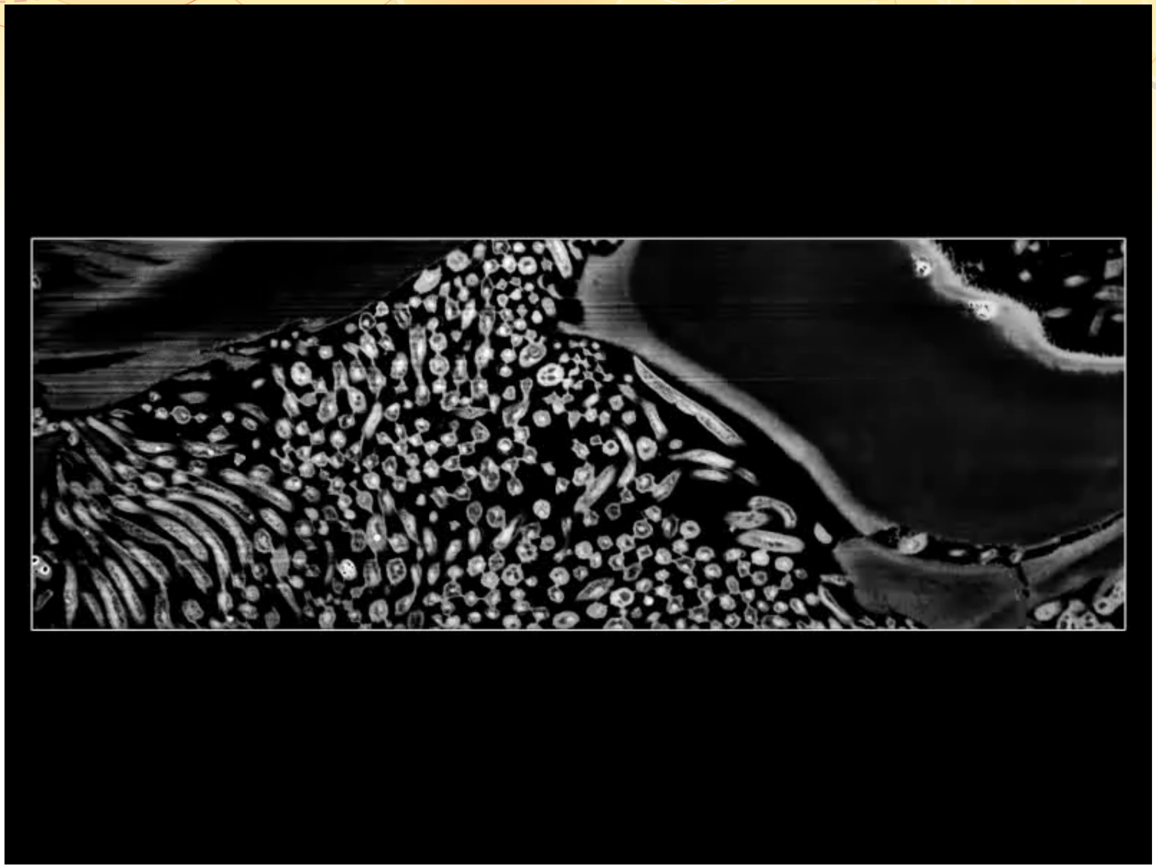
Understanding of the details of molecular interactions requires atomic coordinates of co-crystallized molecules.



[movie]

Example: Termite Gut via Scanning EM

Highlights bacteria in termite hind gut that degrade lignocellulose. Layers 15 nm thick were shaved off by a focused ion beam to produce the stack of images. Structures were then segmented by hand and colored using UCSF Chimera.



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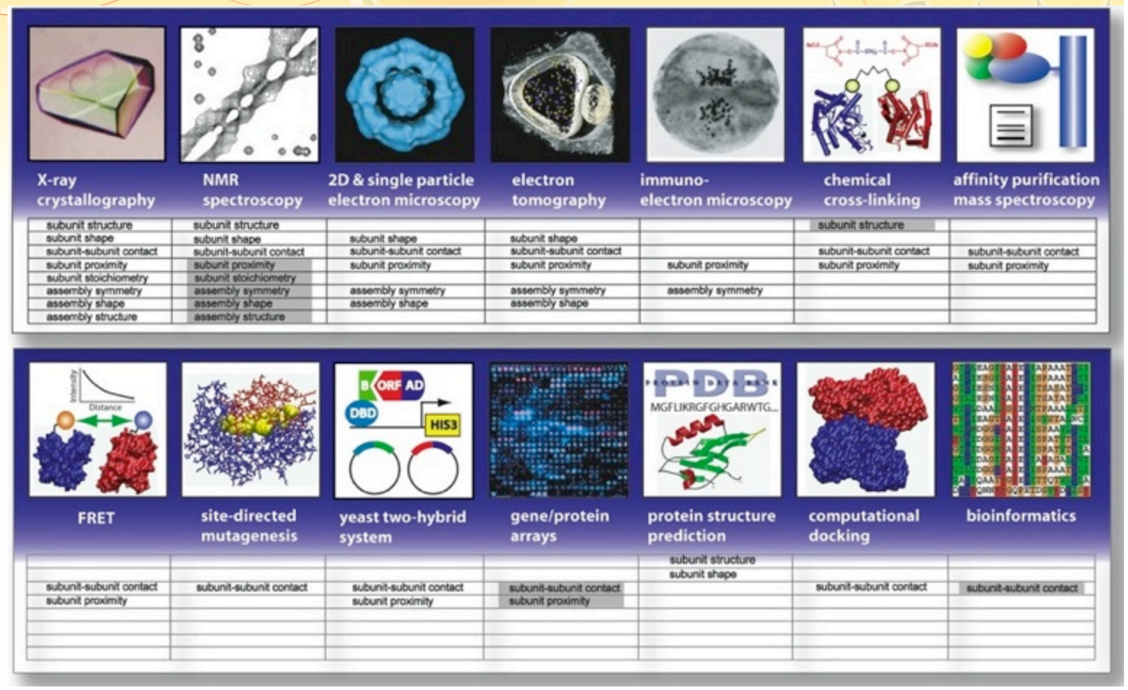
Challenges for Software Developers

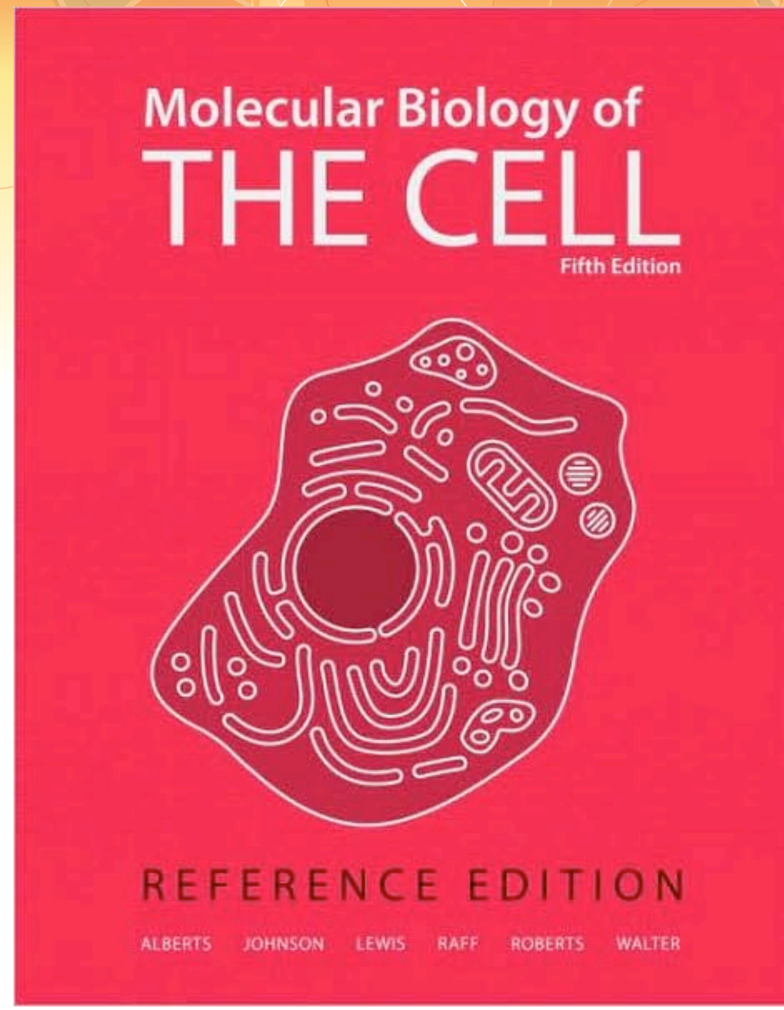
- There's a plethora of experimental data from numerous functional elements determined using different technologies at different resolutions at different time scales and in different data formats



Sali A, Earnest T, Glaeser R, Baumeister W. From words to literature in structural proteomics. *Nature* 422, 216-225, 2003. Ward A, Sali A, Wilson I. Integrative structural biology. *Science* 339, 913-915, 2013.

Recommended Reference Text

Molecular Biology of the Cell
5th Edition
by Alberts, Johnson, Lewis, Raff, Roberts and Walter
published by Garland Science



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Papers in This Session

- 1. Robust Detection and Visualization of Cytoskeletal Structures in Fibrillar Scaffolds
  - Problem: segmentation of structures from multi-channel fluorescence microscopy
  - Challenge: segmentation is a hard problem, especially when structures are dynamic
- 2. PresentaBALL – a Powerful Package for Presentations and Lessons in Structural Biology
  - Problem: understanding the details of molecular structure requires considerable expertise
  - Challenge: provide easy-to-use learning tools that can still convey complex structures

- 3. From Biochemical Reaction Networks to 3D Dynamics in the Cell: The ZigCell3D Modeling, Simulation, and Visualization Framework
  - Problem: the many interacting biochemical pathways within a cell make it difficult to understand the relationships and dependencies at play
  - Challenge: provide a tool assist with navigating the interaction network and simulating the detailed molecular interactions
- 4. The Molecular Control Toolkit: Controlling 3D Molecular Graphics via Gesture and Voice
  - Problem: molecular models are inherently three dimensional
  - Challenge: develop easy-to-use user interfaces that permit facile contol of models