

From Structure to Function: Visualizing Supramolecular Assemblies

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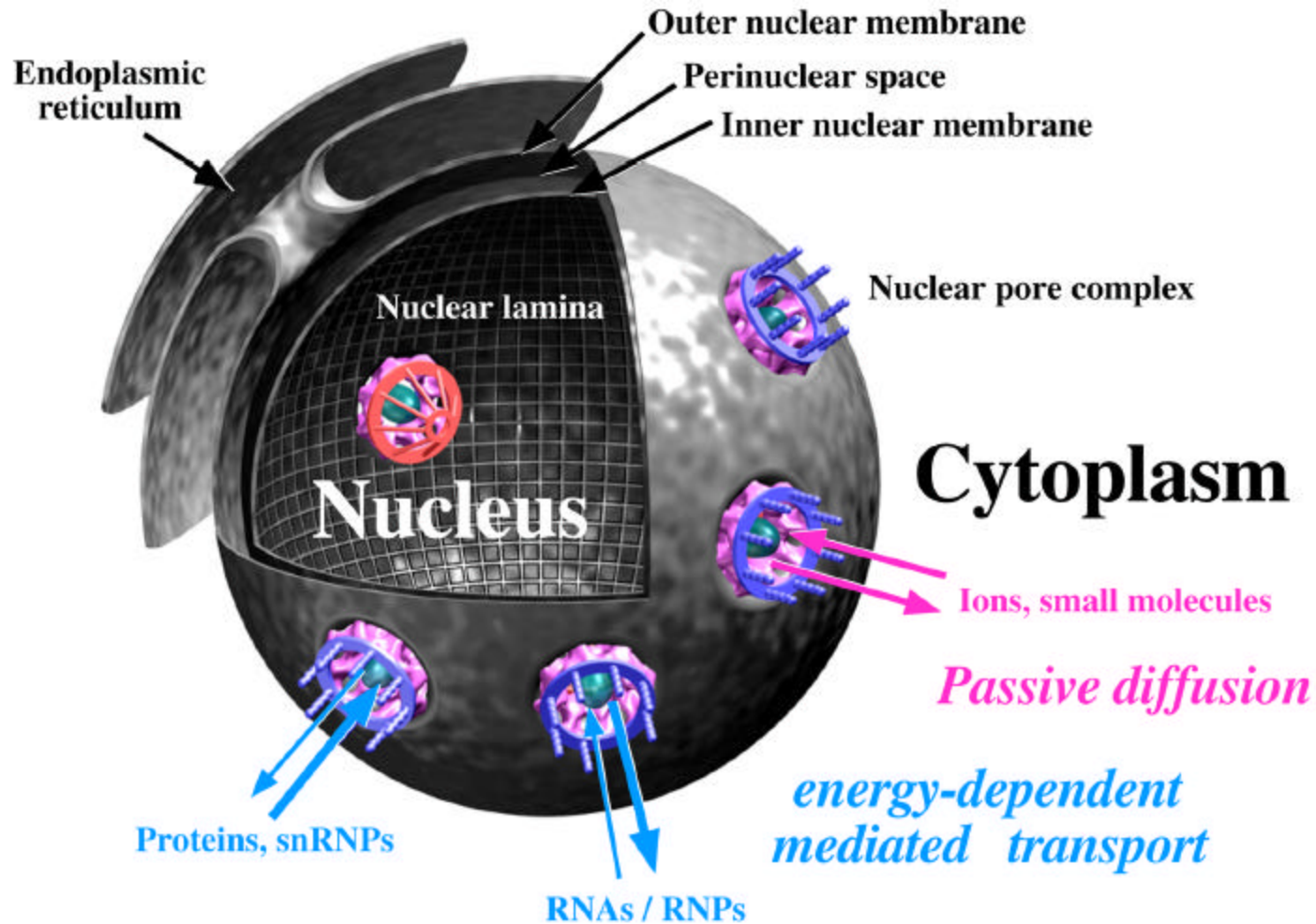
The Molecular Graphics Laboratory

The Scripps Research Institute
La Jolla, California

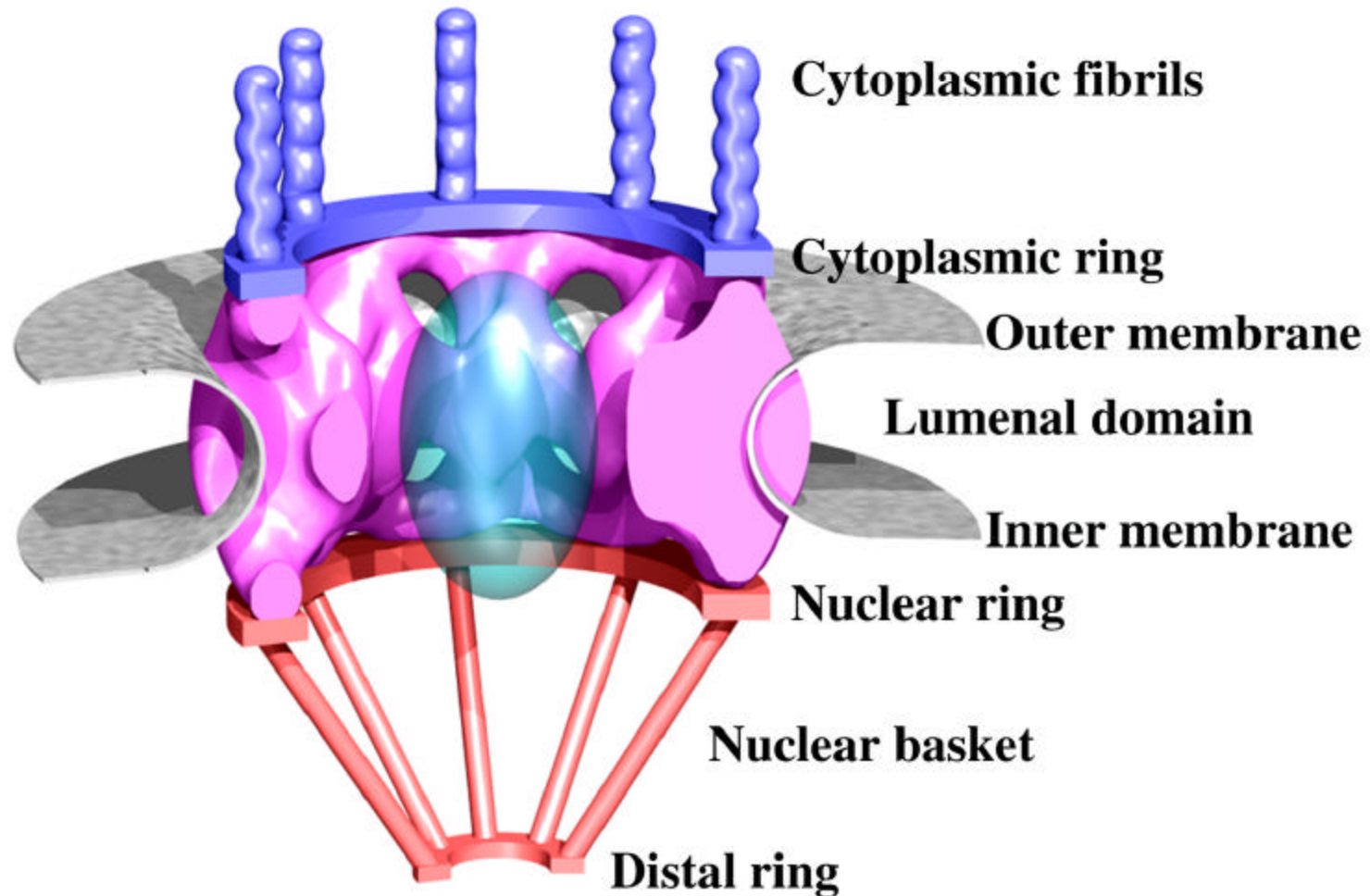


SciPy 2002 CALTECH, Ca

The Nuclear Pore Complex

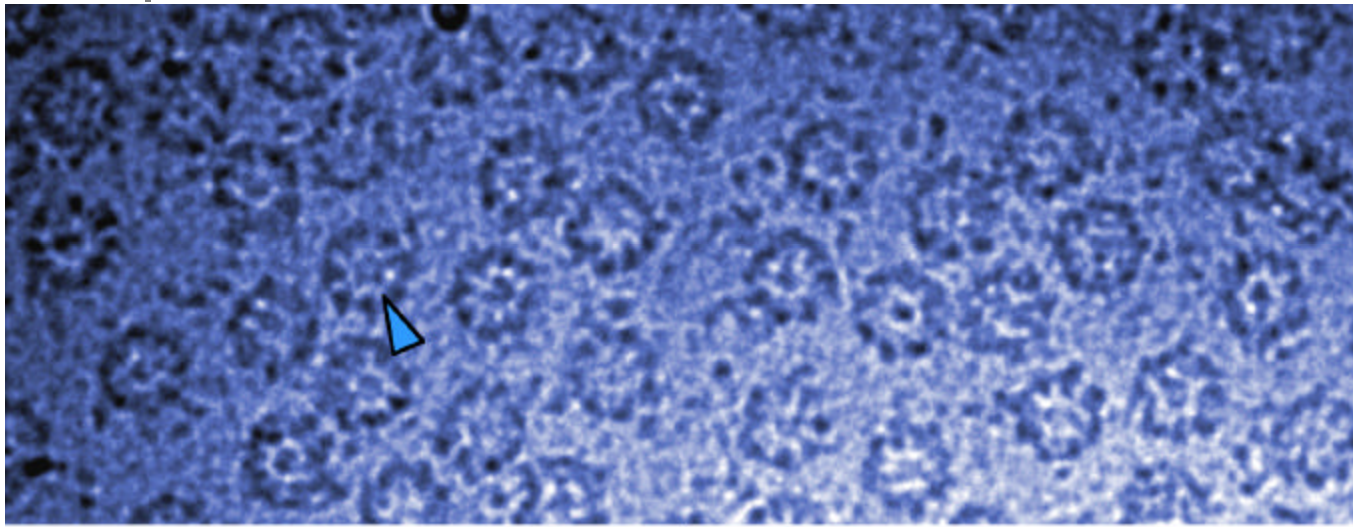


The Nuclear Pore Complex

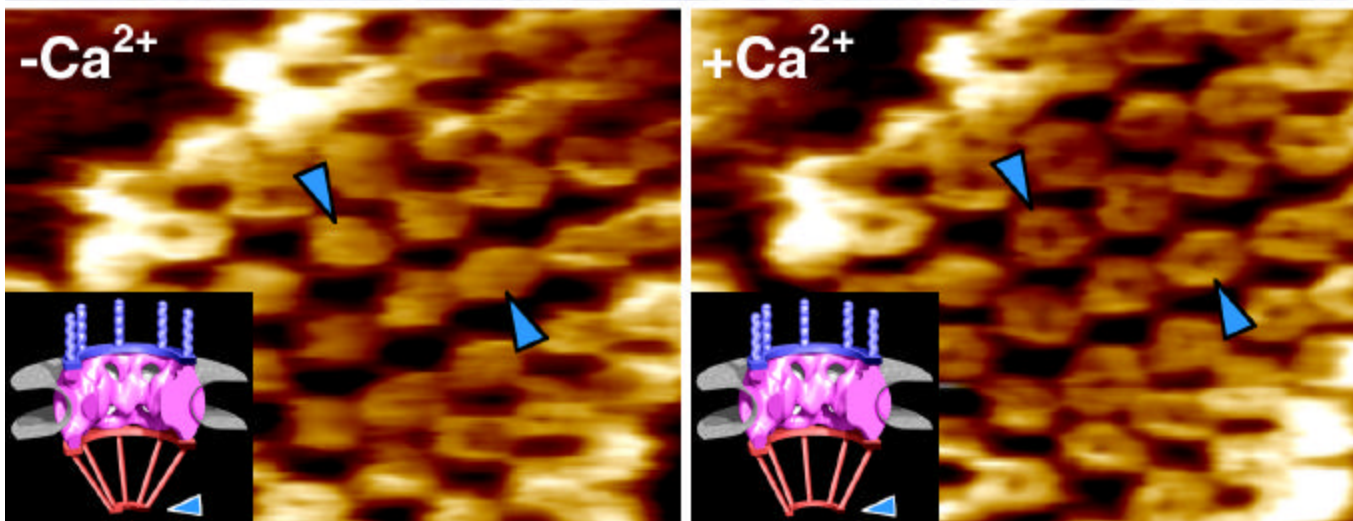


The Nuclear Pore Complex:

Acquiring data from various sources



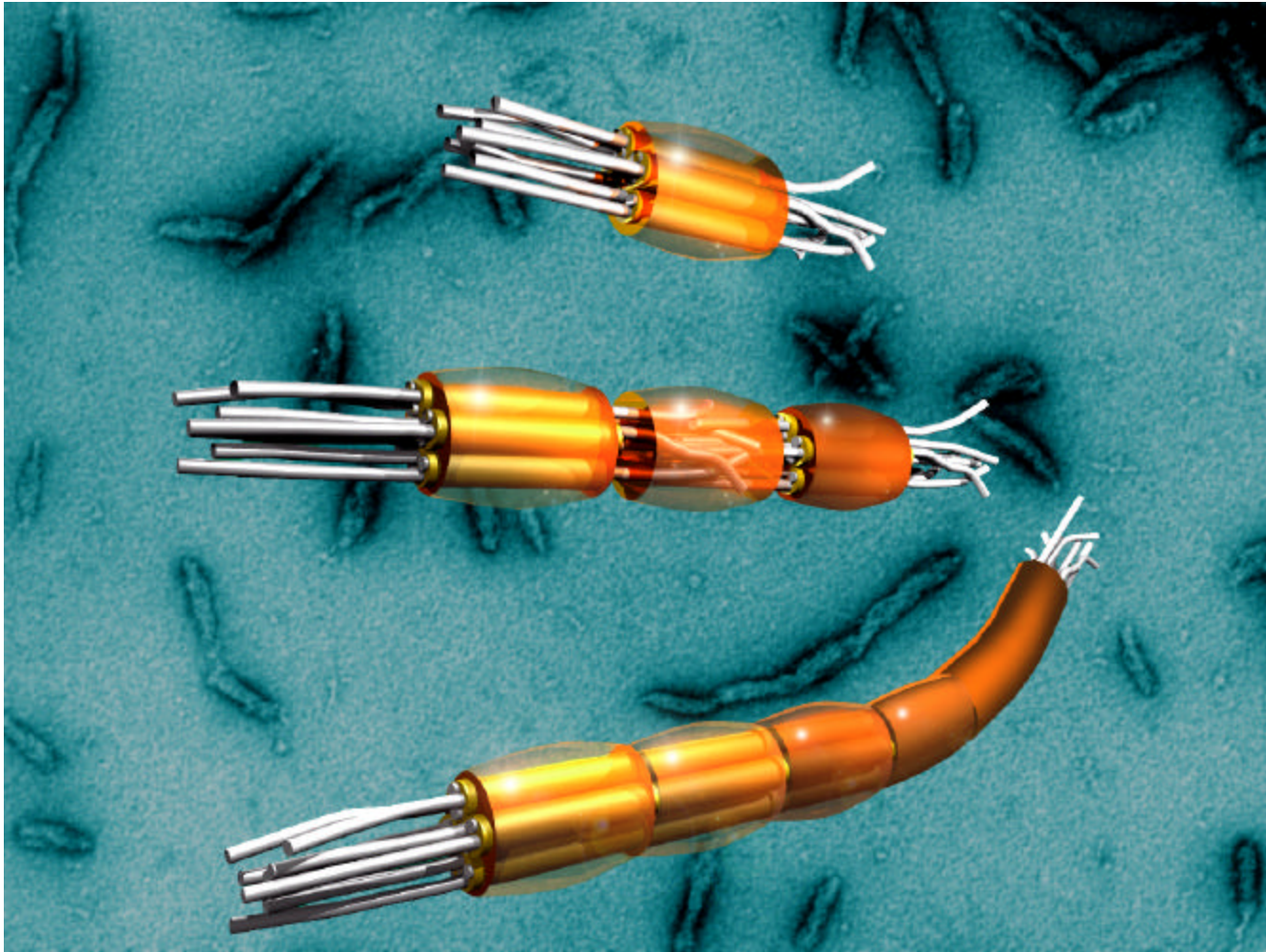
cryo-electron
microscopy:
high resolution



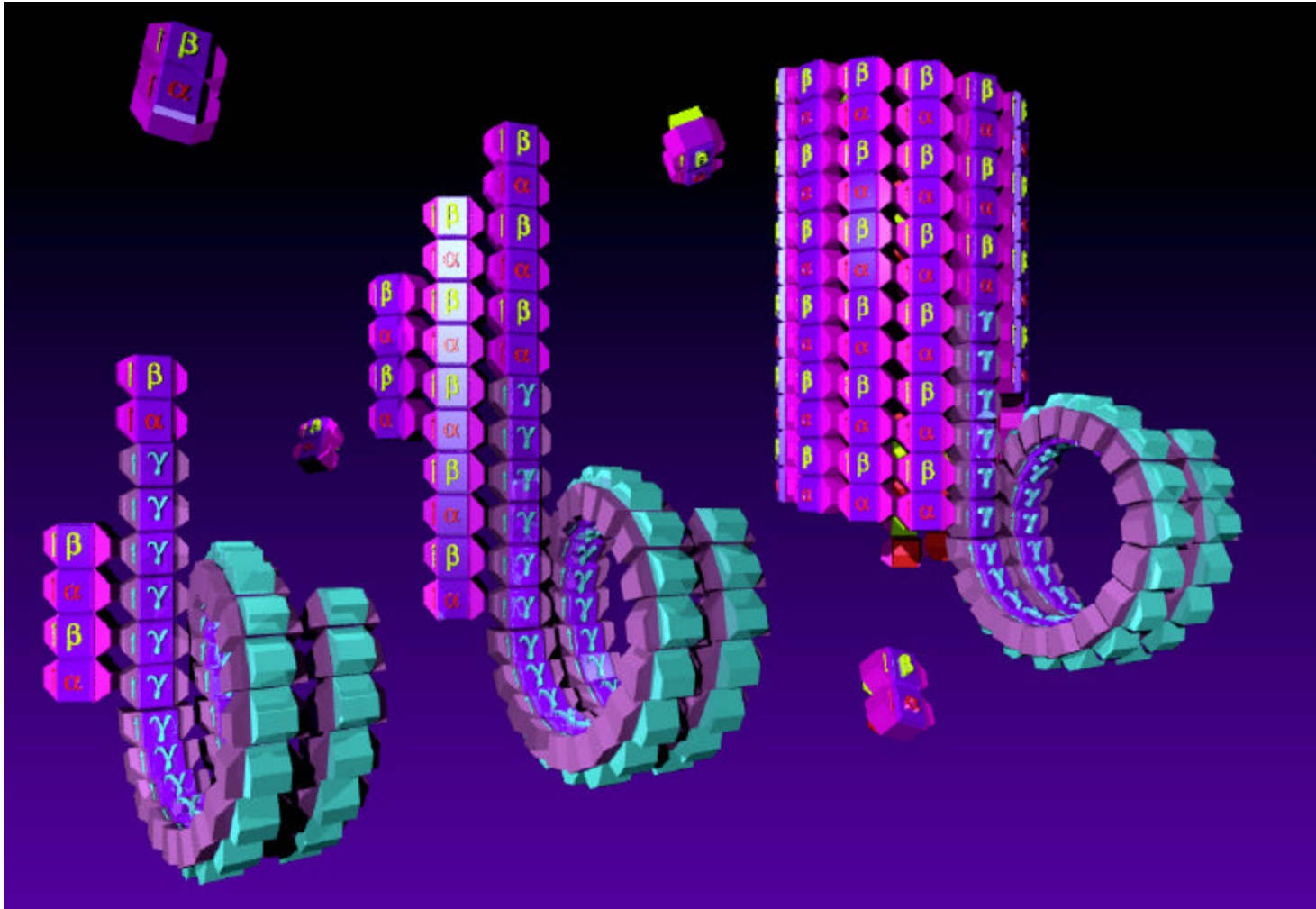
atomic force
microscopy:
lower resolution
native environm.
time-lapse



Intermediate Filaments: a model for vimentin filament assembly



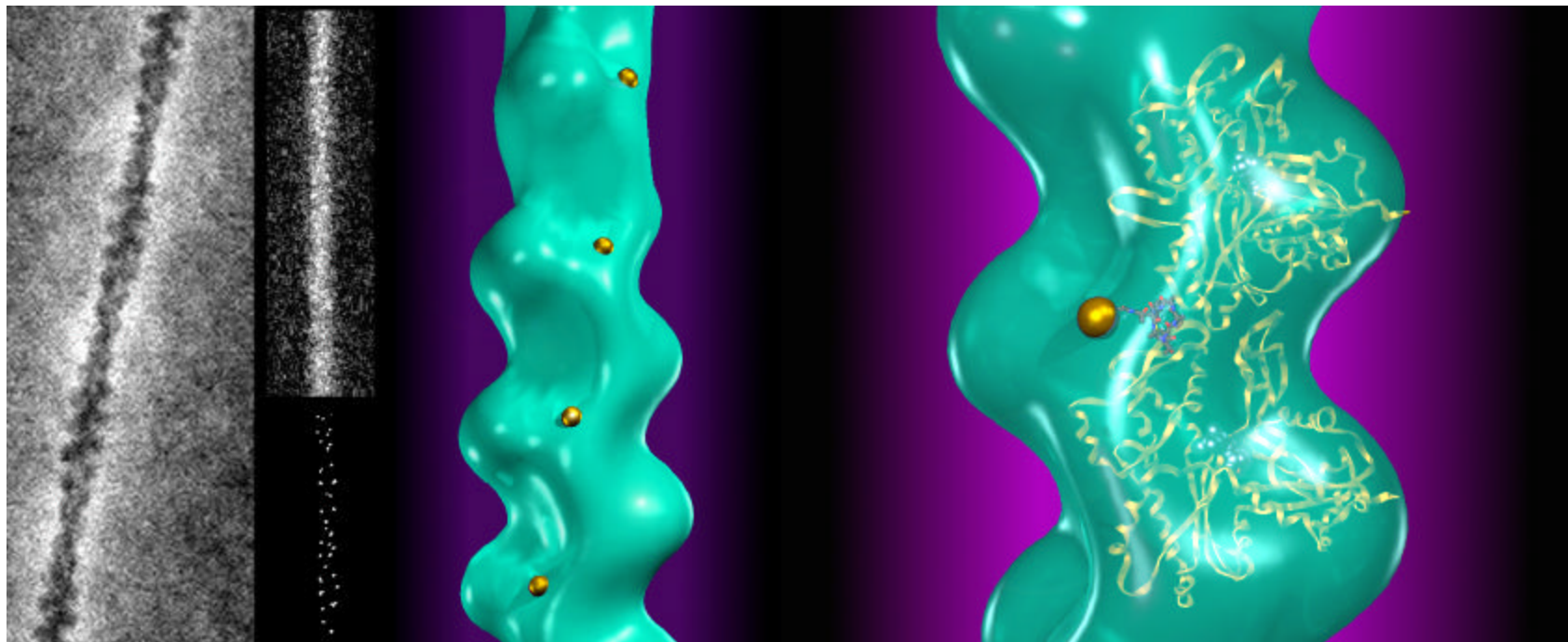
Microtubules: a model for growth and dynamics



Actin Filaments: refining the atomic model

electron microscopy
(EM) data

correlating EM and X-ray data



3-D reconstruction
of EM data

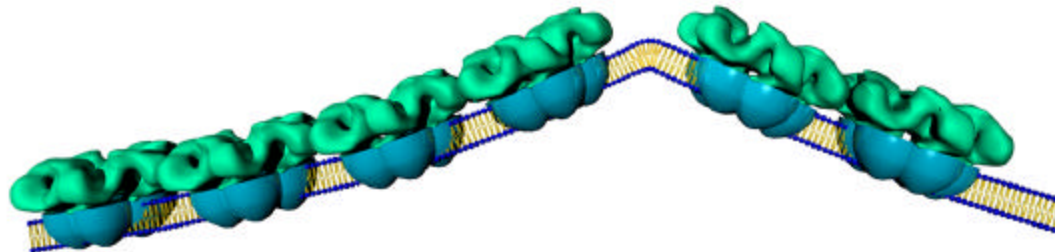
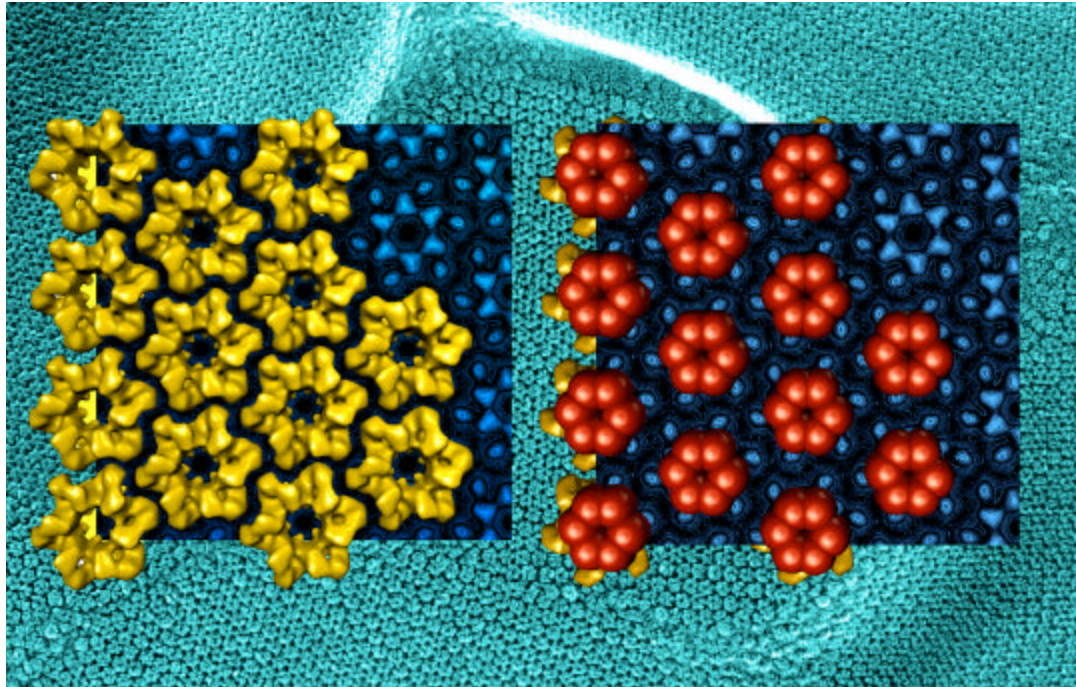


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AUM: Asymmetric Unit Membrane

a model to explain urinal tract infection ?





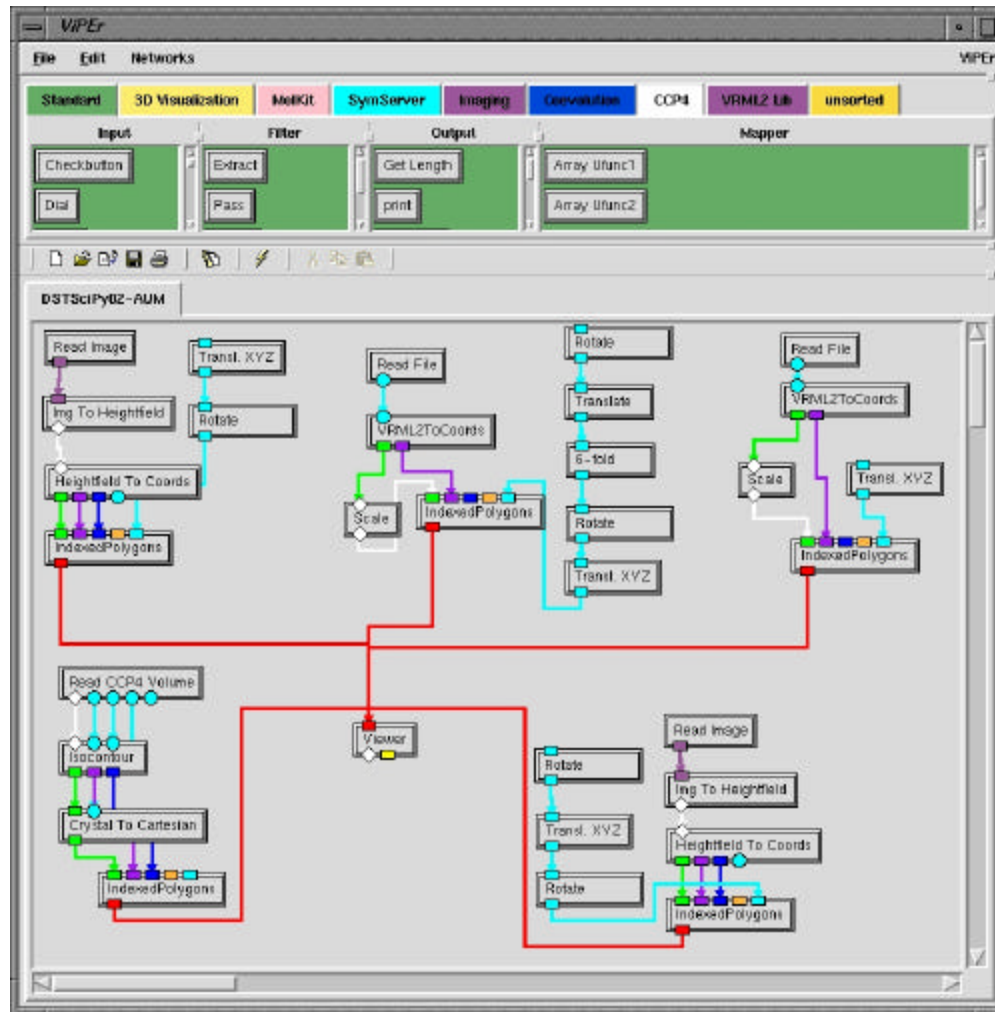
The Challenges

- Data acquisition from various sources:
 - electron microscopy
 - atomic force microscopy
 - X-ray crystallography
 - other emerging technologies
- Visualization of data
- Correlation and combination in 3-D
 - Refinement and validation



Solution: ViPEr – a visual programming environment for Python

an extensive overview of ViPEr will be given on Friday !

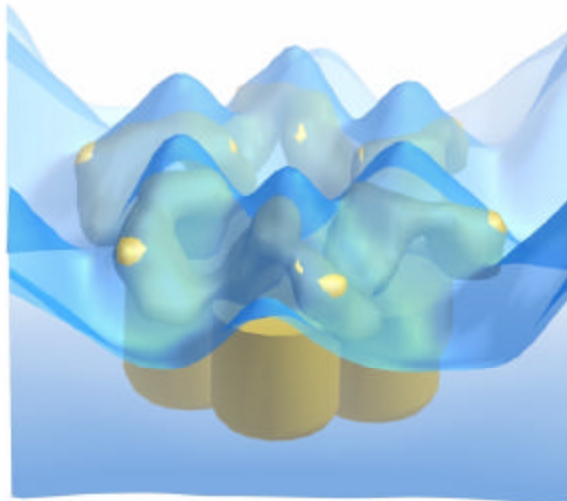
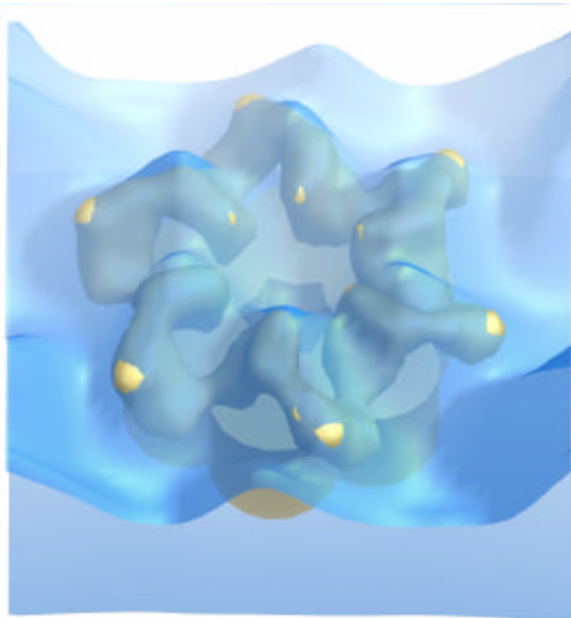


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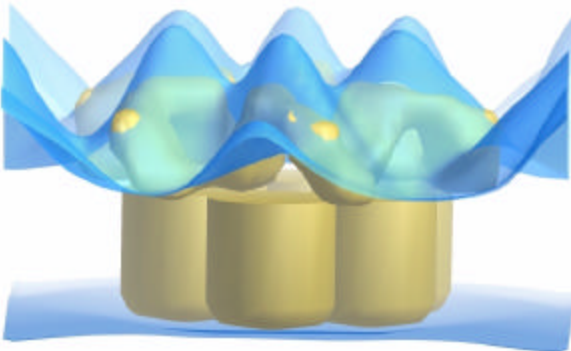


Refining the AUM model

by correlating EM and AFM data in 3-D



blue: AFM
surface scan
under native
conditions (in
physiol. buffer)



yellow: EM 3-D
reconstruction of
negatively stained
particles





Tangible Models

- o Intuitive access to complex shapes and relationships of molecules and their interactions
- o Tactile interface to the process of molecular design
- o Teaching principle, developing new scientific hypotheses





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- o Michel Sanner
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