National Institute of Allergy and Infectious Diseases

Health Innovations Conference

Walking Through Proteins-
applying Virtual Reality to Structural Biology

March 19, 2019

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Computational Structural Biologist
Office of Cyber Infrastructure and Computational Biology

An Abbreviated History of Computational Structural Biology-

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UCSF Mida

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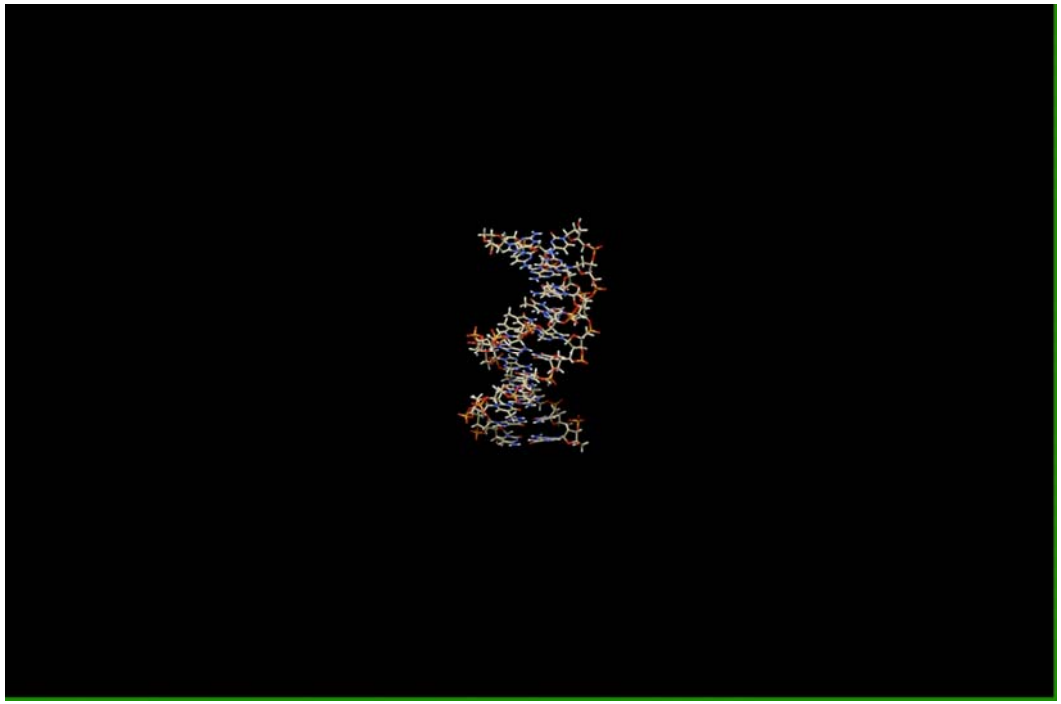
UCSF Midas

- Required specialized hardware on which to run
  - Evans and Sutherland Picture System
  - ~ $100,000

UCSF Chimera (2004)



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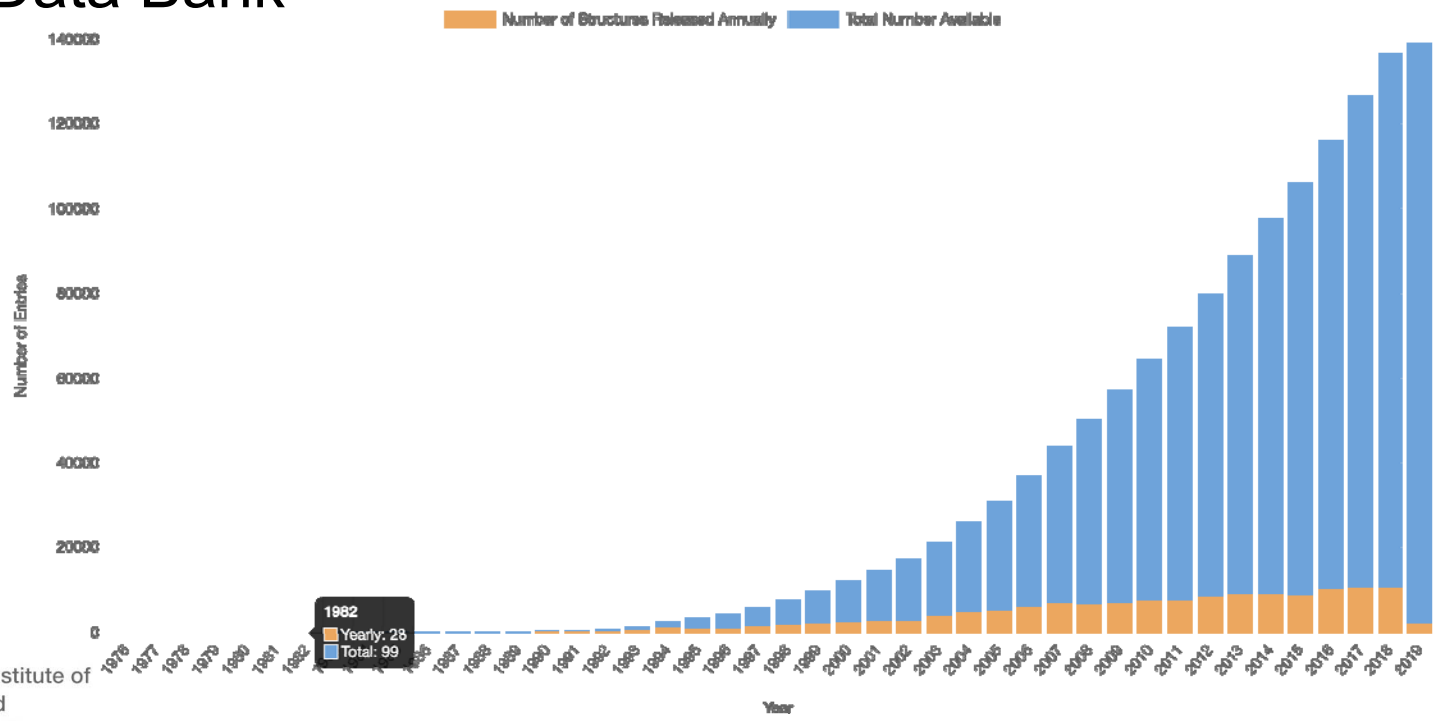
UCSF Chimera

- Runs on generic Windows and Mac computers with graphics cards

Revolution in amount of protein structure data

Protein Data Bank



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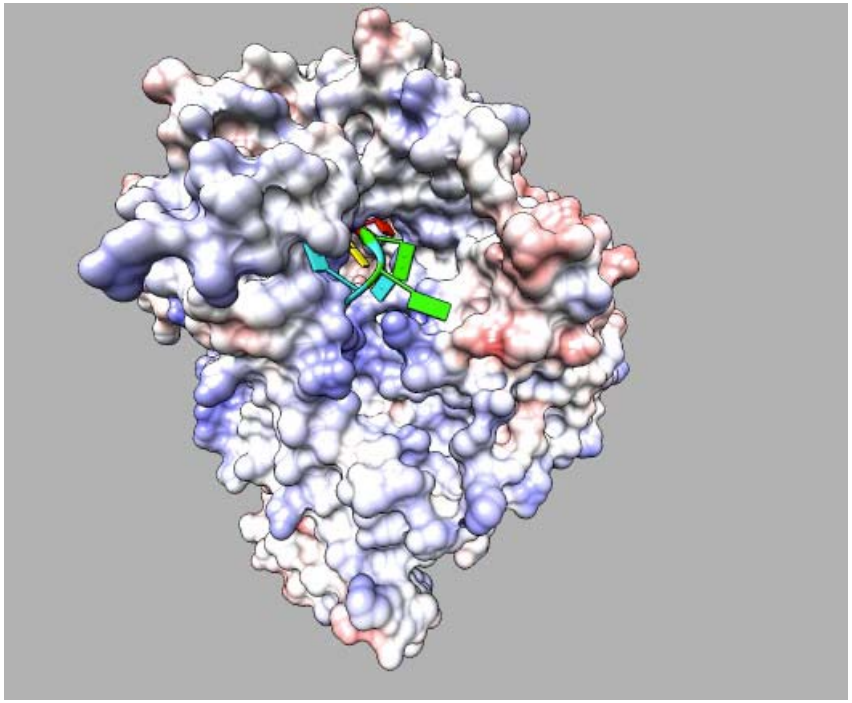

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UCSF ChimeraX and Virtual Reality (2019)

Requires VR hardware and High End Graphics Card

- Either HTC Vive or Oculus Rift
  - ~$500 for headset, two controllers, two base stations
- NVIDIA RTX 2080 Ti graphics card (in new VR Lab in Uganda)
  - ~$800
- Windows PC (Mac ??)

Portable solutions

Cray XMP Supercomputer

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iPhone 7

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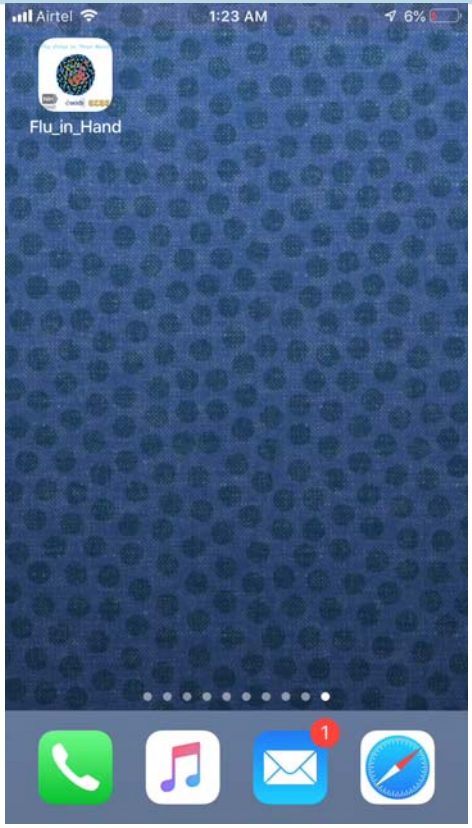
Portable Augmented Reality- Merge Cube

NIAID App- Flu in Hand



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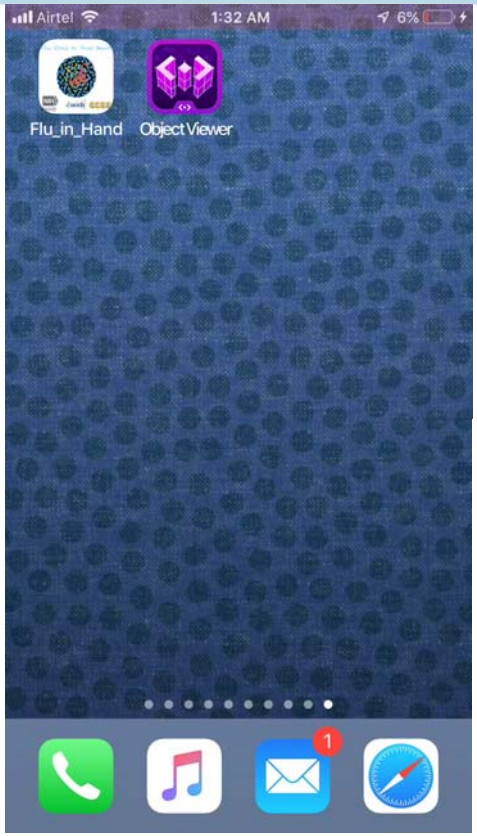
Object Viewer for Merge Cube



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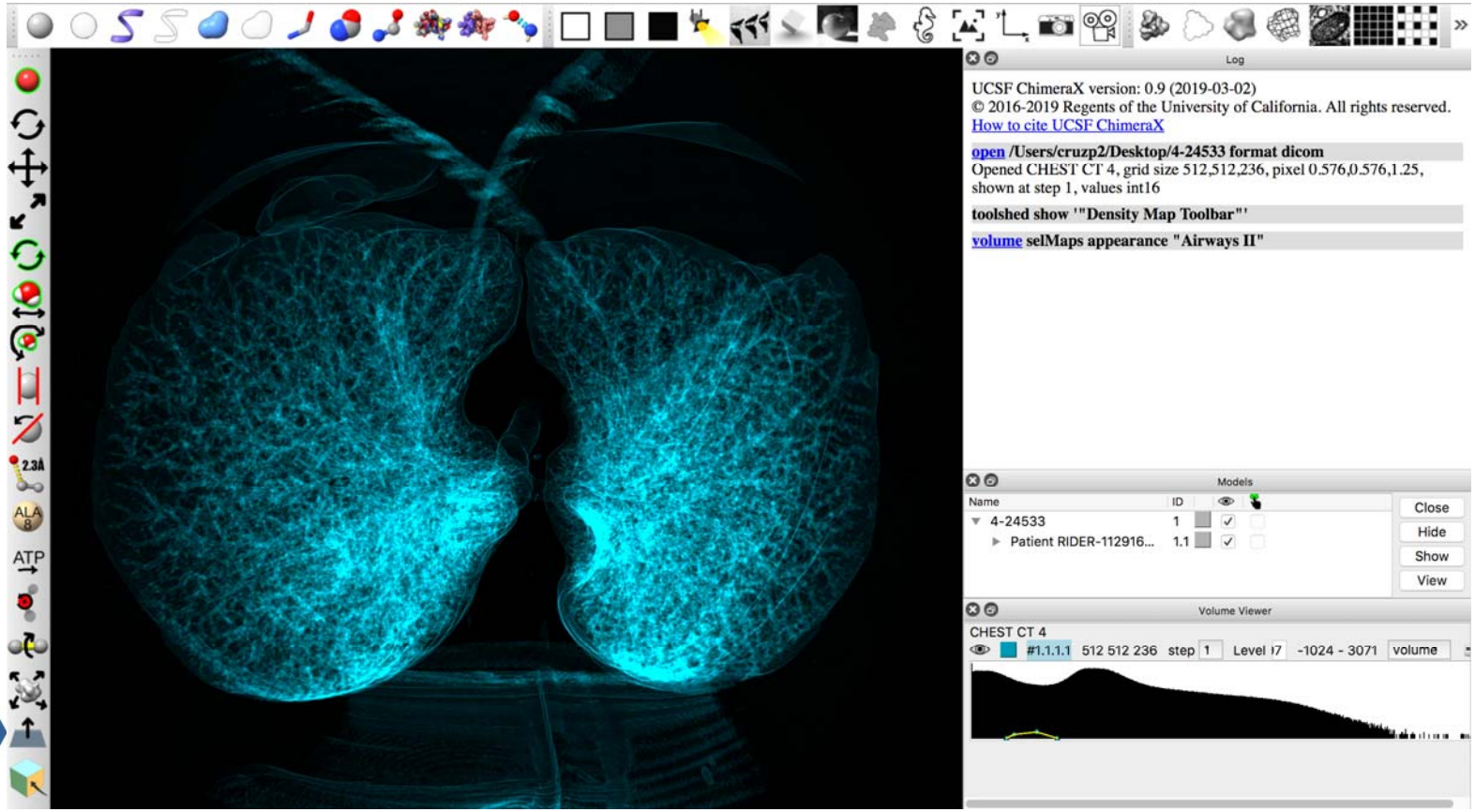
Other types of structures- CoMFA Fields

- Comparative Molecular Field Analysis (CoMFA)
  - Drug Discovery statistical method
  - Predicts activity of small molecules in a binding site
  - Shows regions around molecules where changes affect activity

ChimeraX Medical Image- Lung CT Scan



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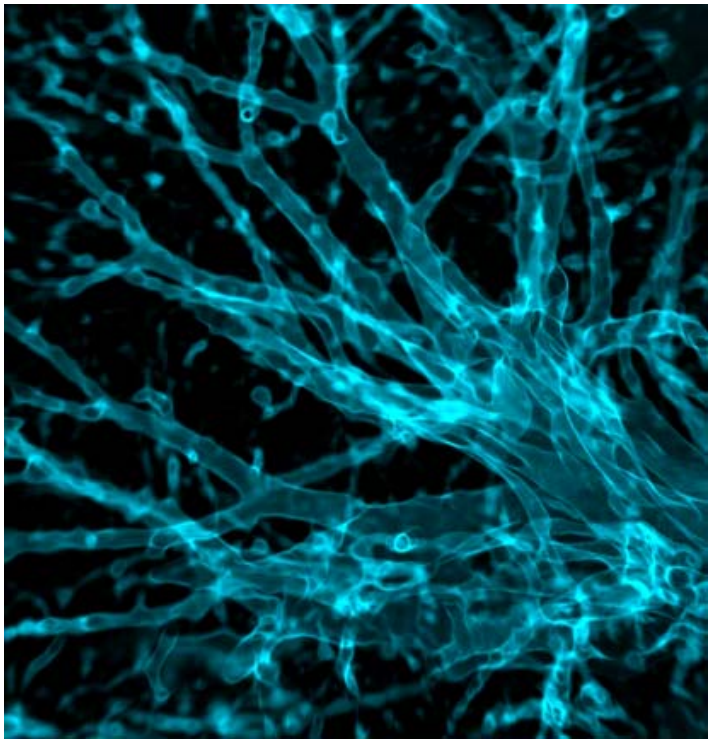
Close up of lung CT scan



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Conclusions

- New perspectives of 3D relationships
- Viewpoint inside structures
- View ligand binding and binding sites in unprecedented detail
- Used for medical imaging
- Relatively inexpensive hardware