

Overview of UCSF Chimera

Spoken Tutorial Project

<http://spoken-tutorial.org>

National Mission on Education through ICT

<http://sakshat.ac.in>

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Learning Objectives



Learning Objectives

► About UCSF Chimera



Learning Objectives

- ▶ **About UCSF Chimera**
- ▶ **Download and installation on Ubuntu Linux OS**



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- ▶ **Uses and Advantages**



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- ▶ **Play video clippings of Chimera available on our website**



System Requirement



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- ▶ **Ubuntu Linux OS version 14.04**



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- ▶ **UCSF Chimera version 1.13**



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- ▶ **UCSF Chimera version 1.13**
- ▶ **Mozilla Firefox browser version 54.0**



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- ▶ **Ubuntu Linux OS version 14.04**
- ▶ **UCSF Chimera version 1.13**
- ▶ **Mozilla Firefox browser version 54.0**
- ▶ **Working internet connection**



About UCSF Chimera



About UCSF Chimera

- ▶ It is a software for 3D visualization and analysis of molecular structures



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- ▶ It is a software for 3D visualization and analysis of molecular structures
- ▶ Developed by the Resource for Biocomputing, Visualization, and Informatics (RBVI), University of California, San Francisco (UCSF)



About UCSF Chimera



About UCSF Chimera

- ▶ It can be downloaded free of charge for academic, government, nonprofit and personal use



About UCSF Chimera

- ▶ It can be downloaded free of charge for academic, government, nonprofit and personal use
- ▶ Runs on Windows, Mac OSX and Linux OS



About UCSF Chimera



About UCSF Chimera

- ▶ **Used by academic and industry researchers, educators, and students**



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- ▶ Used by academic and industry researchers, educators, and students
- ▶ <http://www.cgl.ucsf.edu/chimera/>



Advantages of Chimera



Advantages of Chimera

- ▶ It has set of features accessible through both commands and graphical interface



Advantages of Chimera

- ▶ It has set of features accessible through both commands and graphical interface
- ▶ Visualize molecular data on all scales, including large molecular assemblies



Advantages of Chimera



Advantages of Chimera

- **Production of high quality images and movies for publication and presentation**



Advantages of Chimera

- ▶ **Production of high quality images and movies for publication and presentation**
- ▶ **Designed to accommodate outside development of software extensions**



Video Clippings



Video Clippings

- ▶ **UCSF Chimera Spoken Tutorials**



Spoken Tutorial: Structure Manipulation



Spoken Tutorial: Structure Manipulation

- ▶ **Open a structure on the Chimera window**
- ▶ **Move, rotate and zoom the structure**
- ▶ **Scale and clip**
- ▶ **Change the display**



Spoken Tutorial: Picking and Selection



Spoken Tutorial: Picking and Selection

- ▶ Show labels for atoms and residues
- ▶ Select atoms and residues using **Select** menu or by Picking
- ▶ Change the color and display of the residues
- ▶ Add, delete or change atoms, rotate bonds



Spoken Tutorial: Writing commands



Spoken Tutorial: Writing commands

- ▶ **Change the display to atoms**
- ▶ **Show and hide ribbons**
- ▶ **Change the color of the amino acid residues**
- ▶ **Label individual residues**



Spoken Tutorial: Surface Properties



Spoken Tutorial: Surface Properties

- ▶ Show surfaces for protein and DNA structures.
- ▶ Create images of protein surface colored by:

Amino acid hydrophobicity

Electrostatic Potential



Spoken Tutorial: Build Structures



Spoken Tutorial: Build Structures

- ▶ **Create structures of small molecules, peptides and DNA fragments**
- ▶ **Modify structure, minimize energy and join models**



Spoken Tutorial: Structure Analysis



Spoken Tutorial: Structure Analysis

- ▶ **Measure distance between atoms in the structure**
- ▶ **Show Hydrogen bonds**
- ▶ **Identify non-polar interactions**
- ▶ **Rotate bonds in the residues to get different rotamers**



Spoken Tutorial: Superimposing and Morphing



Spoken Tutorial: Superimposing and Morphing

- ▶ **Superimpose and compare different structures of the same protein**
- ▶ **Morph conformations and create a trajectory**



Spoken Tutorial: Attributes



Spoken Tutorial: Attributes

- ▶ **Change attributes of atoms, residues and models**
- ▶ **Color atoms in a protein according to B-factor values**
- ▶ **Color residues according to kdHydrophobicity values**



Spoken Tutorial: Animation



Spoken Tutorial: Animation

- ▶ **Adjust background lighting and effects**
- ▶ **Create scenes for animation**
- ▶ **Place scenes along a timeline**
- ▶ **Record a movie of the resulting animation**



Axes and Planes



Axes and Planes

- ▶ **Show Axes, Planes and Centroids for structure of Green Fluorescent Protein**
- ▶ **Show 2D-Labels**
- ▶ **Draw Arrows**
- ▶ **Clip a model of Myoglobin using Per-Model clipping tool**



Summary



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Assignment



Assignment

- ▶ **Install Chimera on your PC**
- ▶ **Explore Chimera interface**



About the Spoken Tutorial Project

- ▶ Watch the video available at http://spoken-tutorial.org/What_is_a_Spoken_Tutorial
- ▶ It summarises the Spoken Tutorial project



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- ▶ If you do not have good bandwidth, you can download and watch it



Spoken Tutorial Workshops

The Spoken Tutorial Project Team

- ▶ Conducts workshops using spoken tutorials
- ▶ Gives certificates to those who pass an online test
- ▶ For more details, please write to contact@spoken-tutorial.org



Forum for specific questions

- ▶ Do you have questions in **THIS Spoken Tutorial?**
- ▶ Please visit
<http://forums.spoken-tutorial.org>
- ▶ Choose the minute and second where you have the question
- ▶ Explain your question briefly
- ▶ Someone from our team will answer them



Forum for specific questions

- ▶ The Spoken Tutorial forum is for specific questions on this tutorial
- ▶ Please do not post unrelated and general questions on them
- ▶ This will help reduce the clutter
- ▶ With less clutter, we can use this discussion as instructional material



Acknowledgements

- ▶ Spoken Tutorial Project is a part of the Talk to a Teacher project
- ▶ It is supported by the National Mission on Education through ICT, MHRD, Government of India
- ▶ More information on this Mission is available at

<http://spoken-tutorial.org/NMEICT-Intro>

