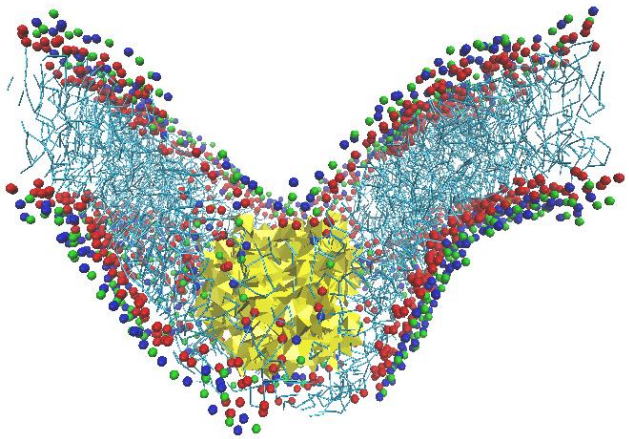
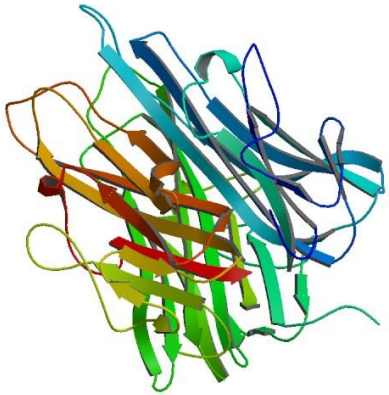
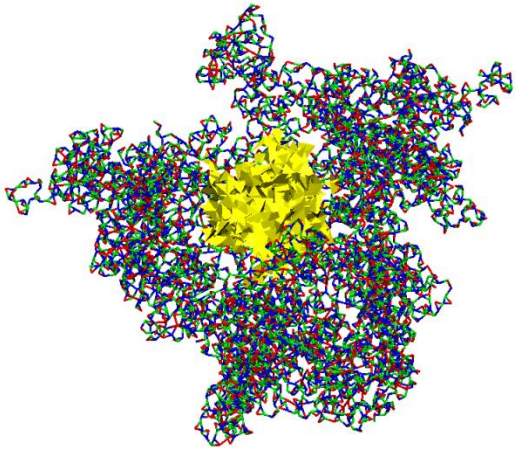
# VMD

# Visual Molecular Dynamics

SETS Workshop at Syracuse University – July 10, 2012







http://www.rcsb.org/pdb/images/1tnf_bio_r_500.jpg

# Installation Instructions

- Open your preferred Internet browser, and navigate to http://www.ks.uiuc.edu/.
- From the Software tab, highlight VMD and select Download.
- Select Windows OpenGL, CUDA under the latest version.

# Installation Instructions

- Enter the username and password you would like to create, and click Continue.
- A new user registration page will appear. Please fill this information in, and click Register.
- On the next page, agree to the license agreement.

# Installation Instructions

- Click “Save and Run” from the dialog box that appears at the bottom of the next page.


- If your computer gives a warning message, simply click Actions → Run Anyway.

- On the next page, agree to the license agreement.

# Installation Instructions

- Click Next when the installation wizard appears.
- Choose a preferable location. For most users, the default location will be acceptable.
- On the next screen, click Install, then press Finish.

# What is VMD?

- A software tool for visualizing molecular dynamics.
- Free / Open Source
- Interactive manipulation of molecules

# Why do we use VMD?

- Visualize molecular dynamics simulations
- Analyze trajectories
- Visualize system configurations
- Imaging of biological molecules

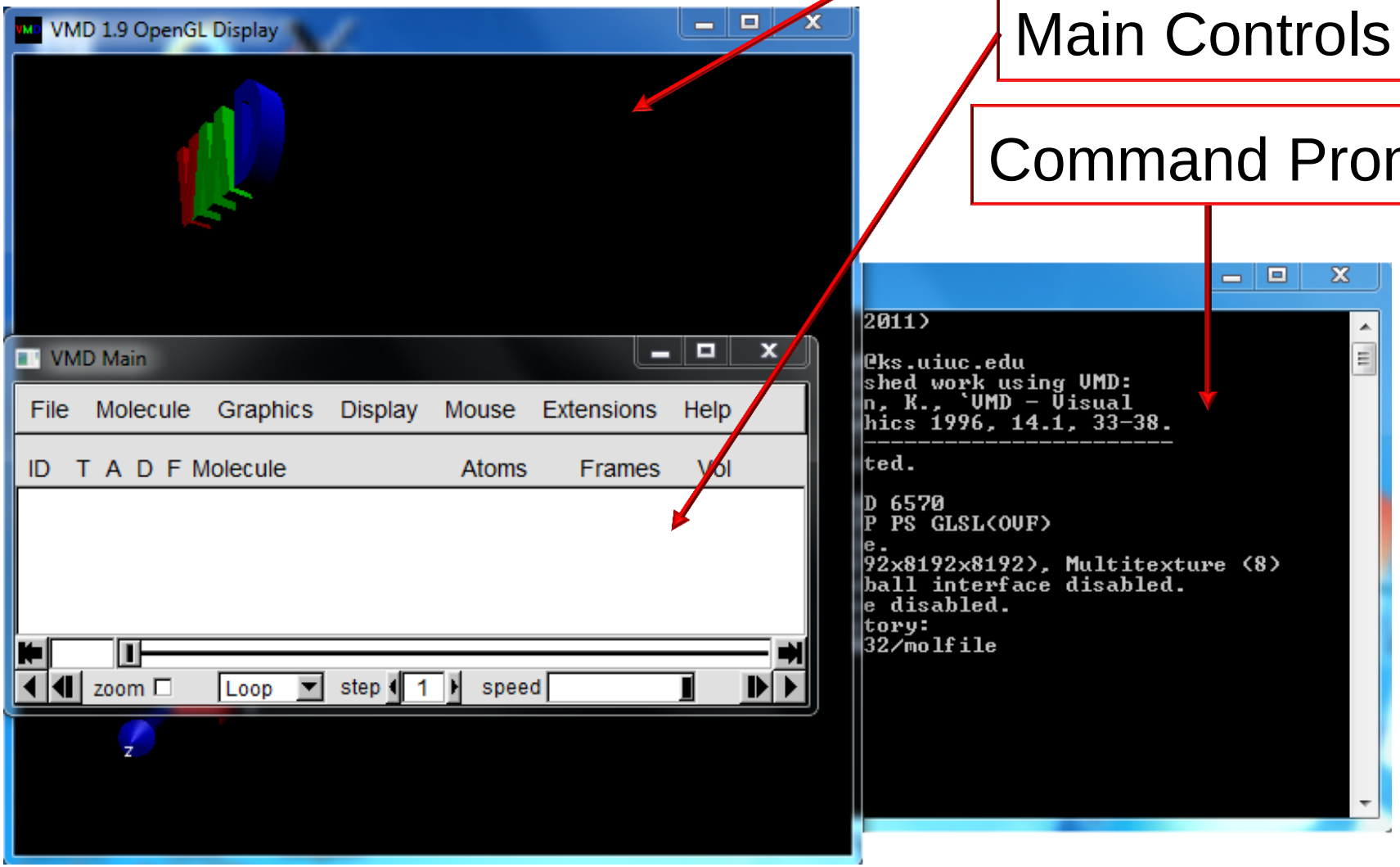
# Features and Options

- Load PDB and GRO files
- Load XTC and TRR trajectories
- Rotate, translate and scale molecular systems
- Play trajectories at variable speeds

# Features and Options

- Create images of molecules and systems
- Create movies of trajectories
- Change 3D visual representations of molecules
  - Style: Ribbons, van der Waals, Dynamic Bonds, etc.
  - Coloring: Residue, Molecule Type, Element, etc.
  - Lighting: Depth Cueing, Stage Lighting, Shiny, etc.

# Using the VMD Interface



# Loading Data into VMD

http://www.rcsb.org/ Molecule 2O61

# Loading Data into VMD

- Choose a new molecule, or load additional data into an existing molecule.
- Extensive list of file types available
- Load multiple molecules at the same time

# Visual Representations

http://www.rcsb.org/ Molecule 2O61

# Visual Representations

- Alter lighting of the display
- Different shapes and geometrical representations
  - Ribbons, van der Waals, dynamic bonds, etc.
- Various coloring schemes
  - Atom type, residue name, element, etc.

# Trajectories and Complex Systems

# Trajectories and Complex Systems

- Can begin editing display while trajectory is loading
- Rotate, scale or translate the complex system or molecule while the trajectory is running
- Alter speed and steps of the visualization
- Show only specific components of a complex system

# Test Your Knowledge

True or False: VMD allows a user to view their molecular dynamics simulations and systems.


True


False

# Test Your Knowledge

True or False: VMD allows a user to view their molecular dynamics simulations and systems.


True

# Test Your Knowledge

True or False: A user can only rotate a molecule or system in VMD.


True


False

# Test Your Knowledge

True or False: A user can only rotate a molecule or system in VMD.


False

# Test Your Knowledge

How do you load a trajectory into VMD for visualization?

**A** File → New
Molecule → Select
Trajectory File

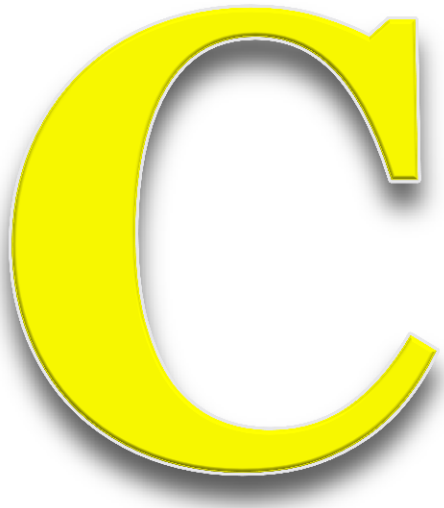
**B** Molecule → Load
Molecule → Select
Trajectory File

**C** File → New
Molecule → Select
Structure → Load
Trajectory File

**D** Molecule → New
Molecule → Select
Structure → Load
Trajectory File

# Test Your Knowledge

How do you load a trajectory into VMD for visualization?




File → New Molecule → Select Structure → Load Trajectory File