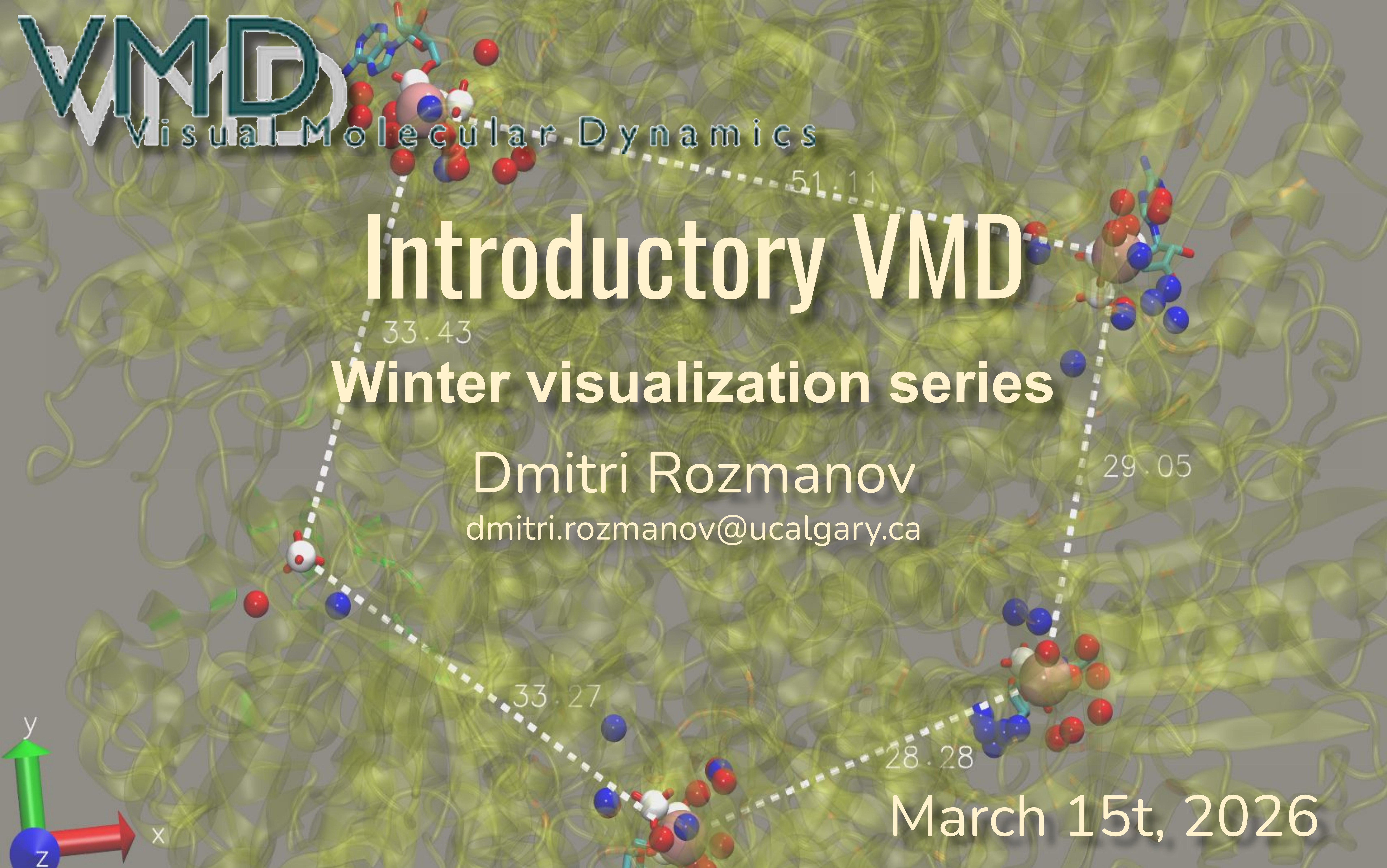
VMD
Visual Molecular Dynamics



Introductory VMD

Winter visualization series

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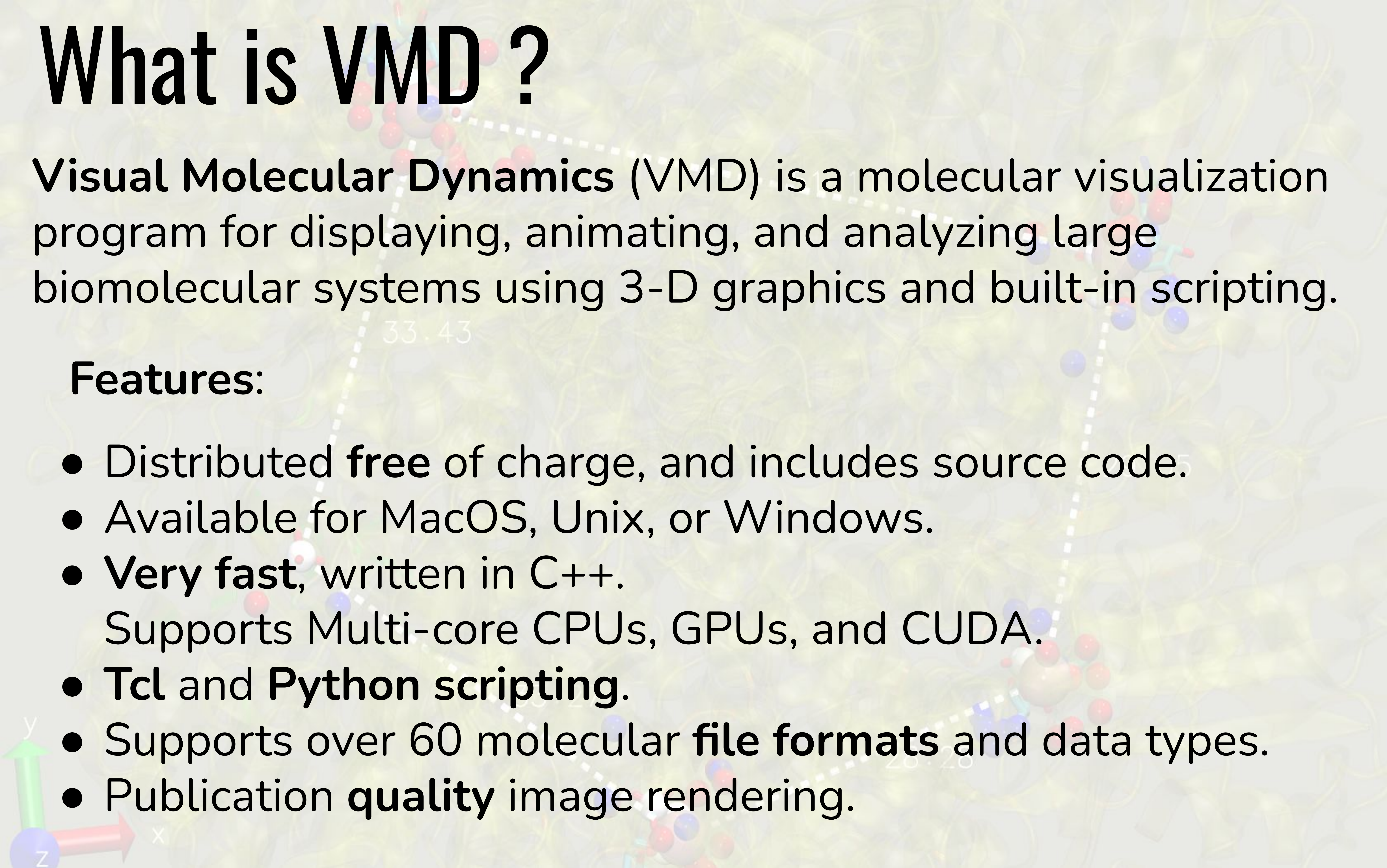
dmitri.rozmanov@ucalgary.ca

March 15t, 2026

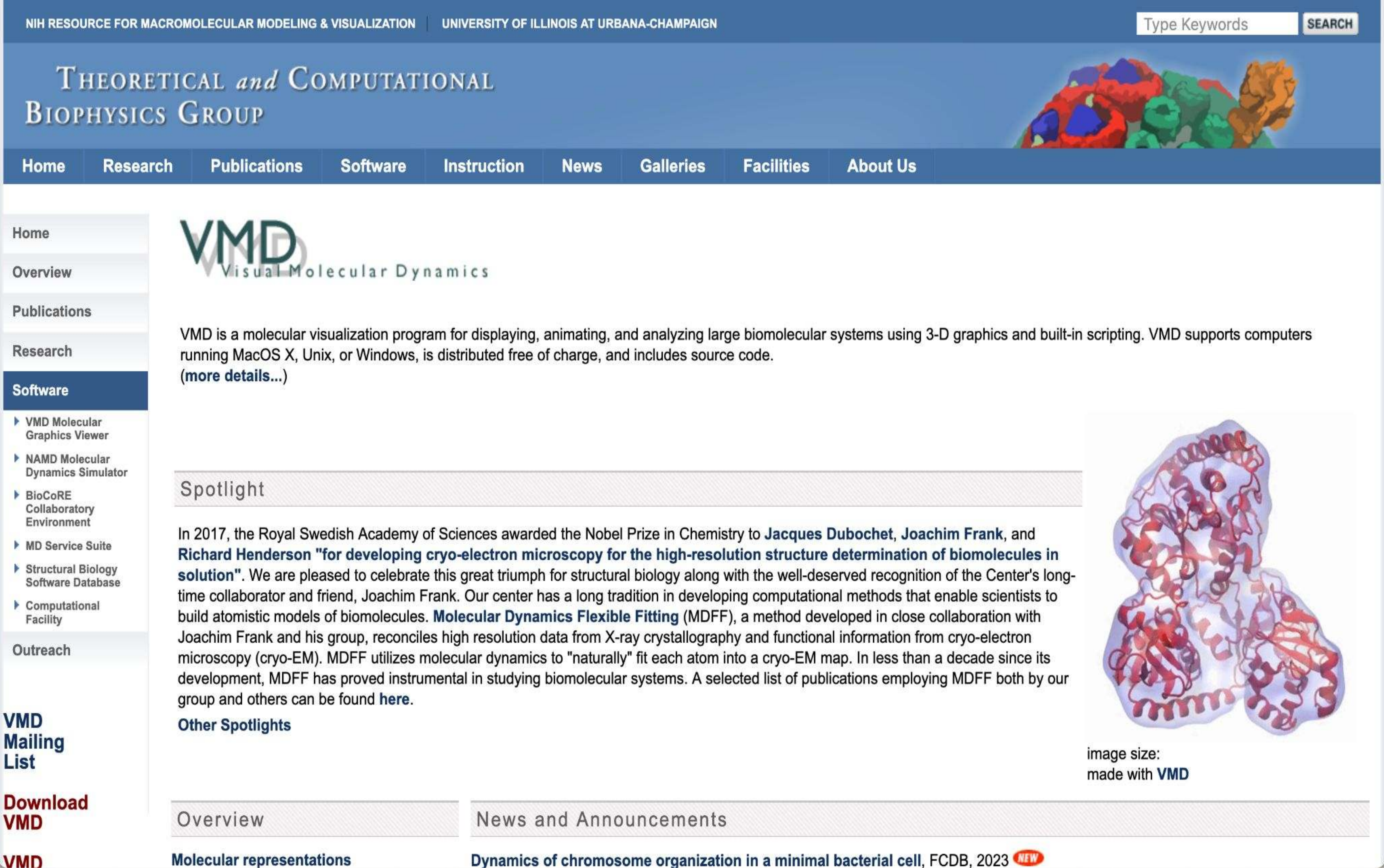
What is VMD ?



Visual Molecular Dynamics (VMD) is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting.

Features:

- Distributed **free** of charge, and includes source code.
- Available for MacOS, Unix, or Windows.
- **Very fast**, written in C++.
  Supports Multi-core CPUs, GPUs, and CUDA.
- **Tcl** and **Python scripting**.
- Supports over 60 molecular **file formats** and data types.
- Publication **quality** image rendering.



VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. VMD supports computers running MacOS X, Unix, or Windows, is distributed free of charge, and includes source code.
(**more details...**)

Spotlight

In 2017, the Royal Swedish Academy of Sciences awarded the Nobel Prize in Chemistry to **Jacques Dubochet**, **Joachim Frank**, and **Richard Henderson "for developing cryo-electron microscopy for the high-resolution structure determination of biomolecules in solution"**. We are pleased to celebrate this great triumph for structural biology along with the well-deserved recognition of the Center's long-time collaborator and friend, Joachim Frank. Our center has a long tradition in developing computational methods that enable scientists to build atomistic models of biomolecules. **Molecular Dynamics Flexible Fitting** (MDFF), a method developed in close collaboration with Joachim Frank and his group, reconciles high resolution data from X-ray crystallography and functional information from cryo-electron microscopy (cryo-EM). MDFF utilizes molecular dynamics to "naturally" fit each atom into a cryo-EM map. In less than a decade since its development, MDFF has proved instrumental in studying biomolecular systems. A selected list of publications employing MDFF both by our group and others can be found **here**.

Other Spotlights

image size:
made with **VMD**

Overview

Molecular representations

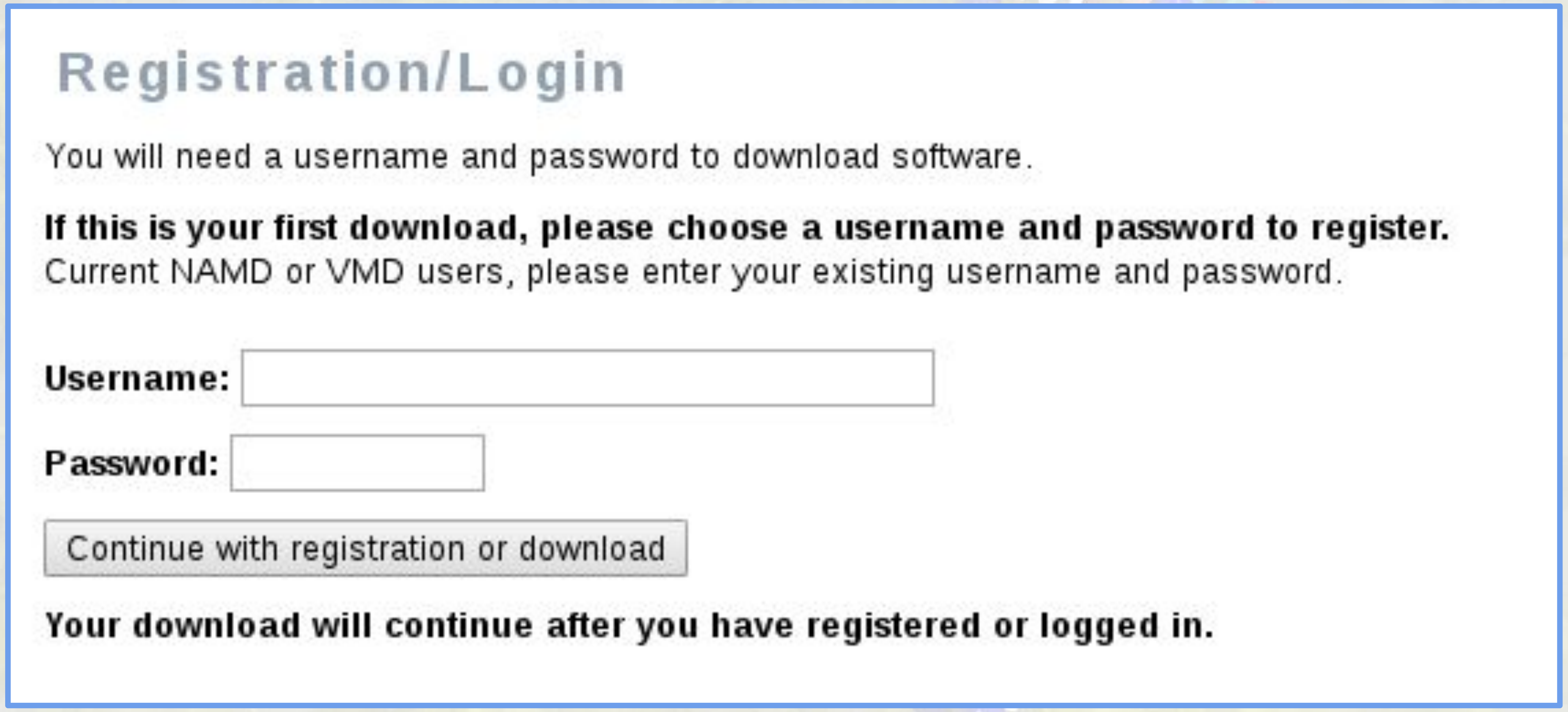
News and Announcements

Dynamics of chromosome organization in a minimal bacterial cell, FCDB, 2023 NEW

Getting VMD

Download:
https://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=VMD

VMD is Copyright © 1995-2016 **Theoretical and Computational Biophysics Group** and at the **University of Illinois** at Urbana-Champaign.



Registration/Login

You will need a username and password to download software.

If this is your first download, please choose a username and password to register.
Current NAMD or VMD users, please enter your existing username and password.

Username:

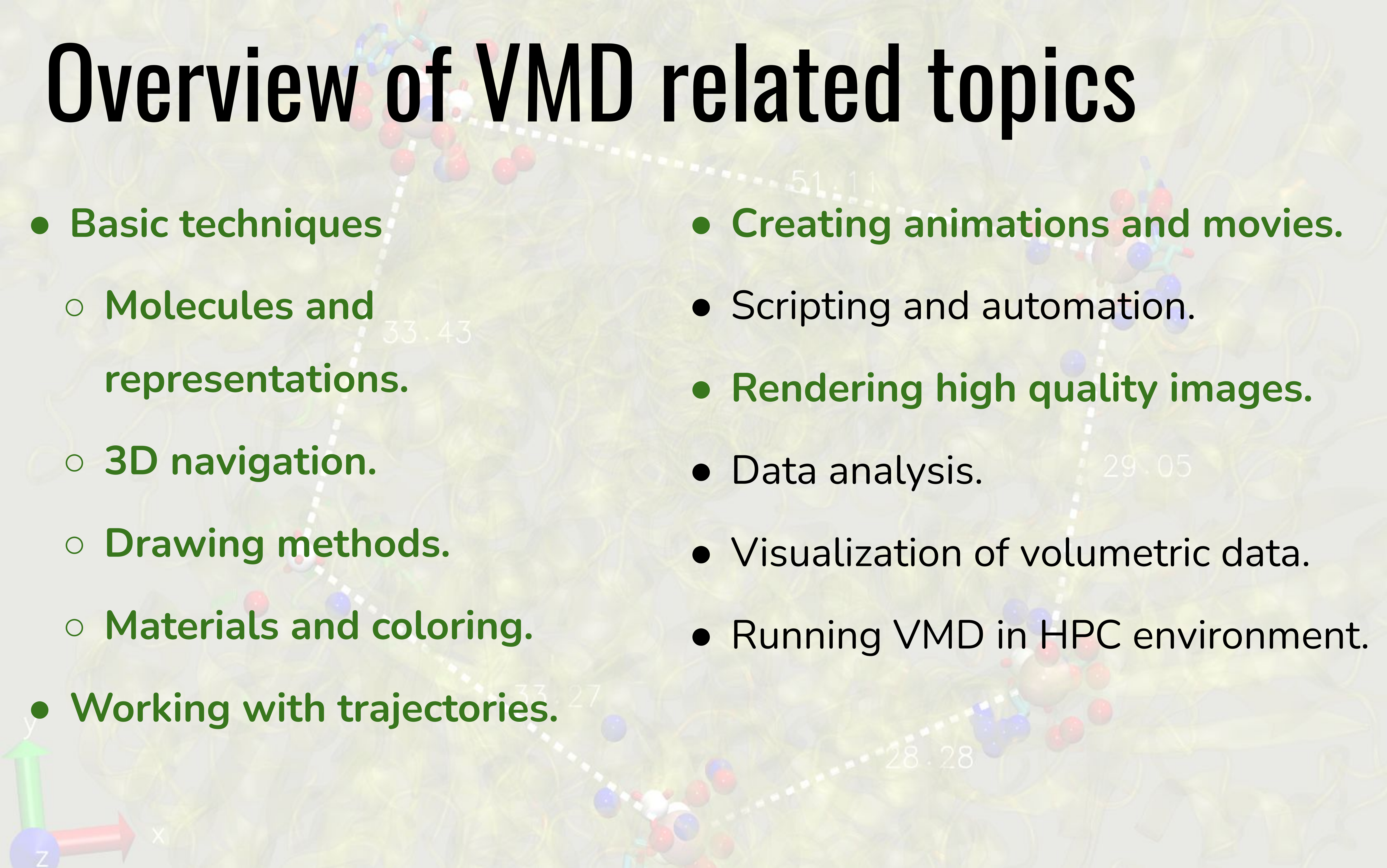
Password:

Your download will continue after you have registered or logged in.

Citing VMD
Humphrey, W., Dalke, A. and Schulten, K., ”VMD - Visual Molecular Dynamics”, J. Molec. Graphics, 1996, vol. 14, pp. 33-38.

Also see: http://www.ks.uiuc.edu/Research/vmd/allversions/cite.html

Overview of VMD related topics



- **Basic techniques**
  - **Molecules and representations.**
  - **3D navigation.**
  - **Drawing methods.**
  - **Materials and coloring.**
- **Working with trajectories.**
- **Creating animations and movies.**
- Scripting and automation.
- **Rendering high quality images.**
- Data analysis.
- Visualization of volumetric data.
- Running VMD in HPC environment.

Starting VMD

Theoretical and Computational Biophysics Group
NIH Resource for Macromolecular Modeling and Bioinformatics
University of Illinois at Urbana-Champaign
R. Brunner, E. Caddigan, J. Cohen, A. Dalke, P. Grayson,
J. Gullingsrud, D. Hardy, W. Humphrey, B. Isralewitz, S. Izrailev,
A. Kohlmeyer, D. Norris, J. Saam, J. Stone, J. Ulrich, K. Vandivort

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Dalke, A. and Schulten, K., `VMD - Visual
mics', J. Molec. Graphics 1996, 14.1, 33-38.
------------------------------------------------
ailable, 8 CPUs detected.
NVIDIA GeForce GT 750M OpenGL Engine
IL MDE CVA MTX NPOT PP PS GLSL(OVF)
ring mode is available.
16384x16384), 3-D (2048x2048x2048), Multitexture (8)
d 2 plugins in directory:
 1.9.3.app/Contents/vmd/plugins/MACOSXX86/molfile

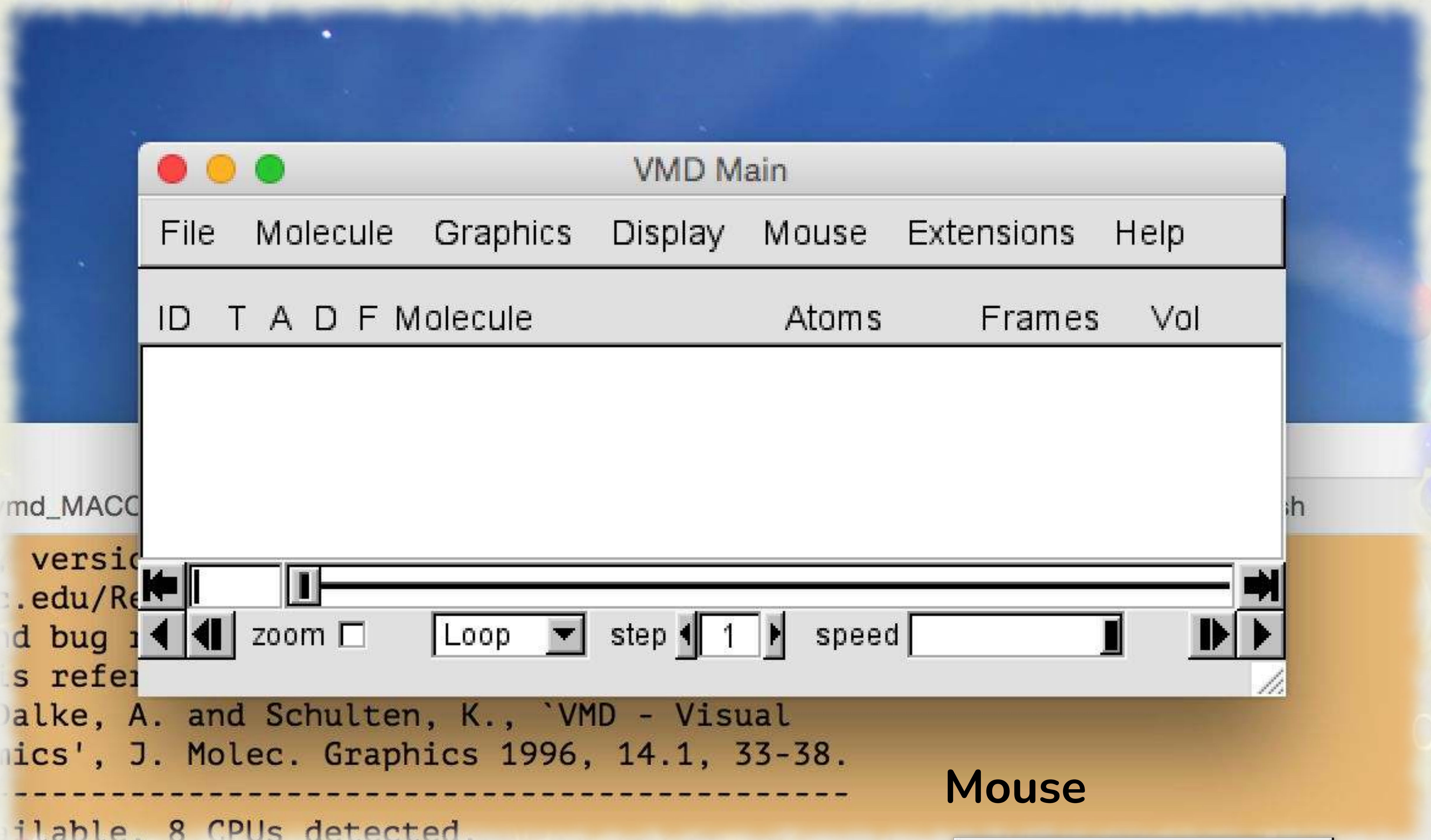
, version 1.9.3 (November 30, 2016)
Info) Exiting normally.
Dmitris-MacBook-Pro:~ rozmanov$ vmd
Info) VMD for MACOSXX86, version 1.9.3 (November 30, 2016)
Info) http://www.ks.uiuc.edu/Research/vmd/
Info) Email questions and bug reports to vmd@ks.uiuc.edu
Info) Please include this reference in published work using VMD:
Info)    Humphrey, W., Dalke, A. and Schulten, K., `VMD - Visual
Info)    Molecular Dynamics', J. Molec. Graphics 1996, 14.1, 33-38.
Info) -------------------------------------------------------------
Info) Multithreading available, 8 CPUs detected.
Info) OpenGL renderer: NVIDIA GeForce GT 750M OpenGL Engine
Info)   Features: STENCIL MDE CVA MTX NPOT PP PS GLSL(OVF)
Info)   Full GLSL rendering mode is available.
Info)   Textures: 2-D (16384x16384), 3-D (2048x2048x2048), Multitexture (8)
Info) Dynamically loaded 2 plugins in directory:
Info) /Applications/VMD 1.9.3.app/Contents/vmd/plugins/MACOSXX86/molfile
vmd > 
```

Main control window

Terminal window

OpenGL graphics window

Main control



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alke, A. and Schulten, K., `VMD - Visual
ics', J. Molec. Graphics 1996, 14.1, 33-38.
---------------------------------------------
ilable, 8 CPUs detected.
```
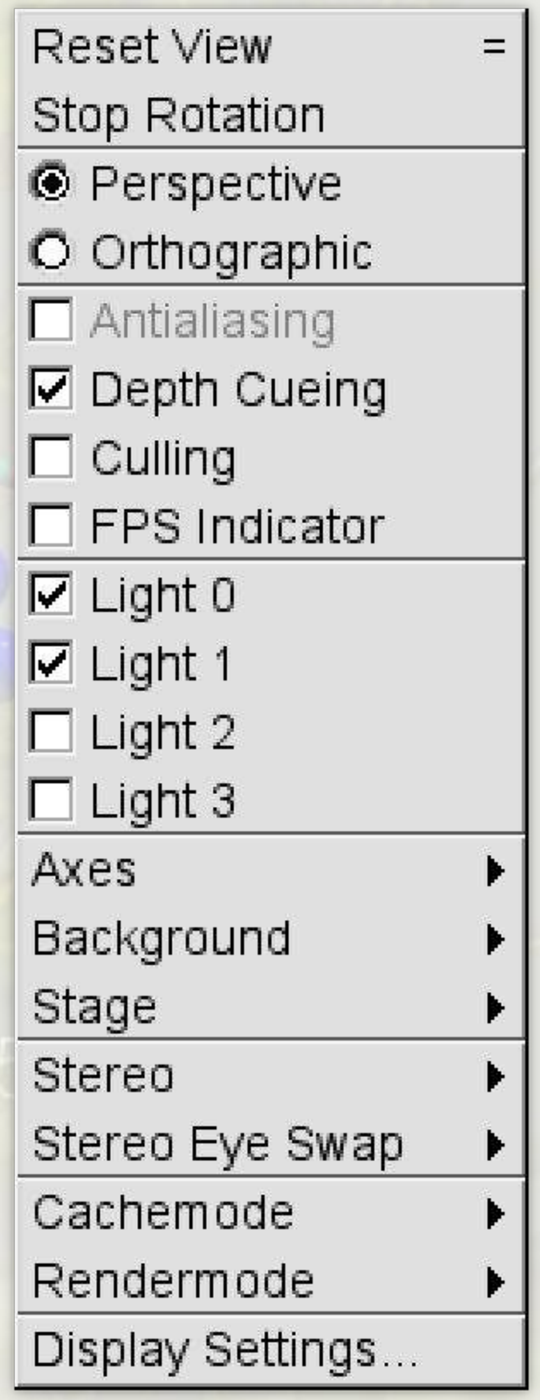
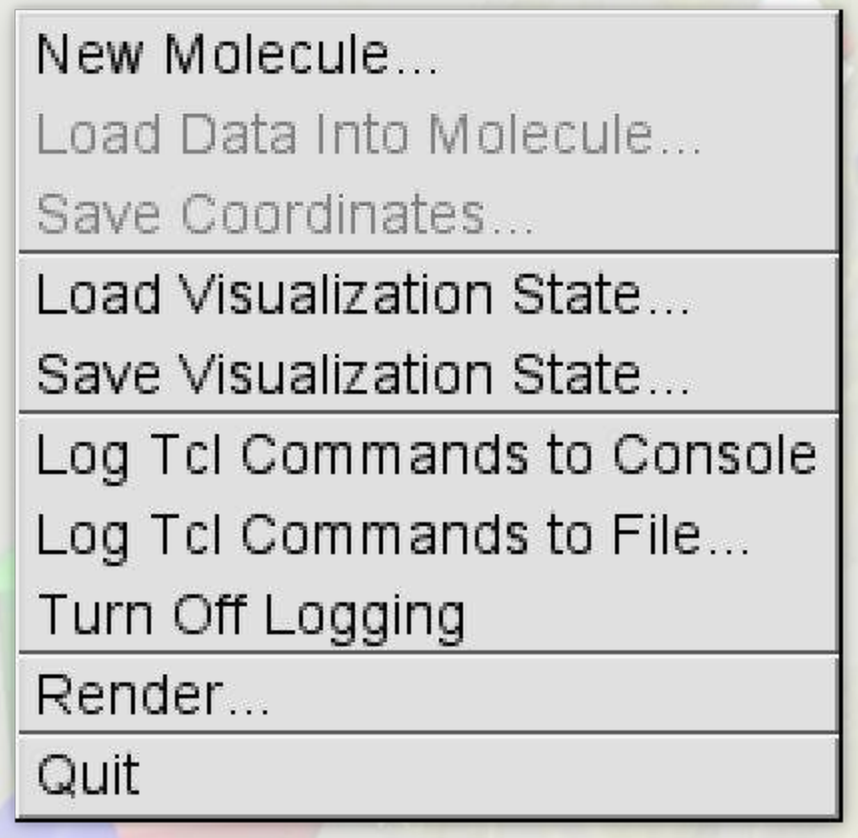

Display



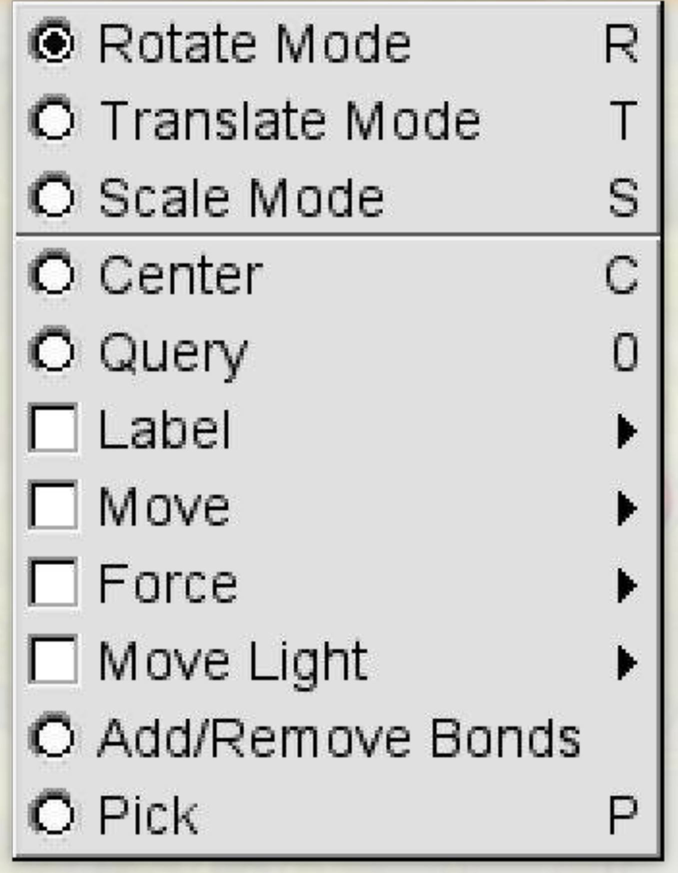
File



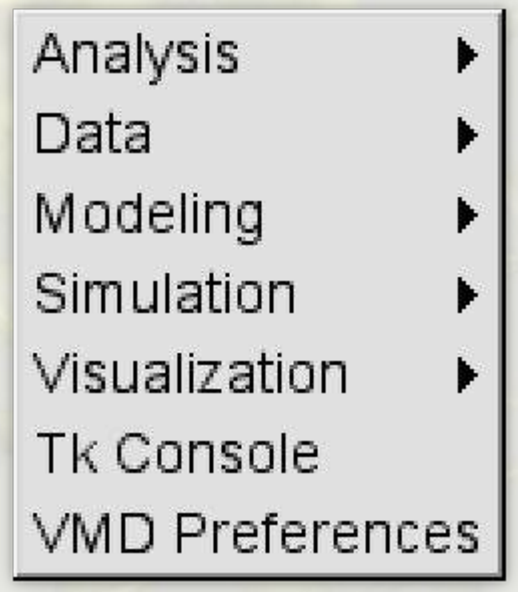
Molecule

Graphics

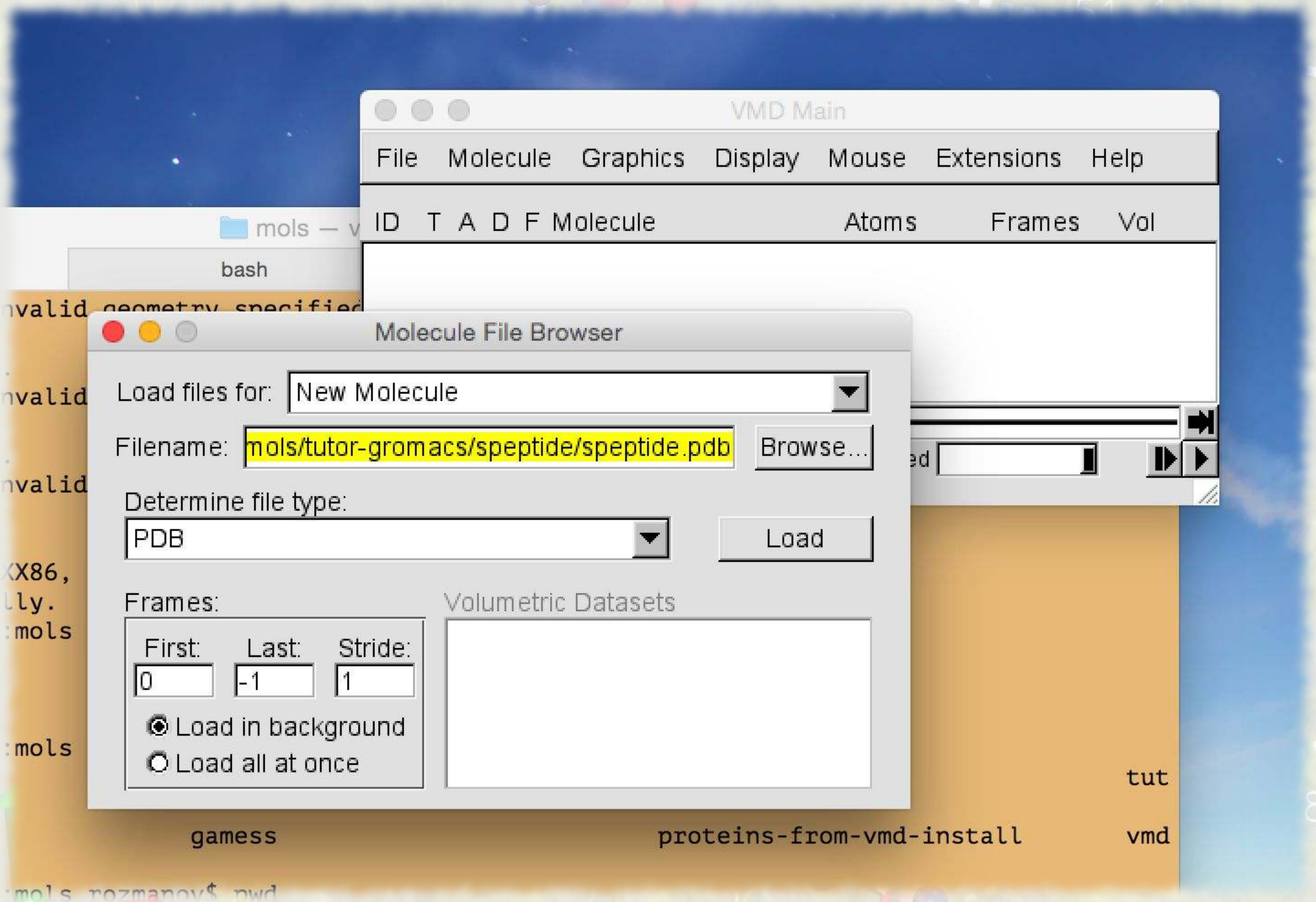
Mouse



Extensions



Loading a new molecule



Load files for: New Molecule

Filename: mols/tutor-gromacs/speptide/speptide.pdb

Determine file type: PDB

Frames:

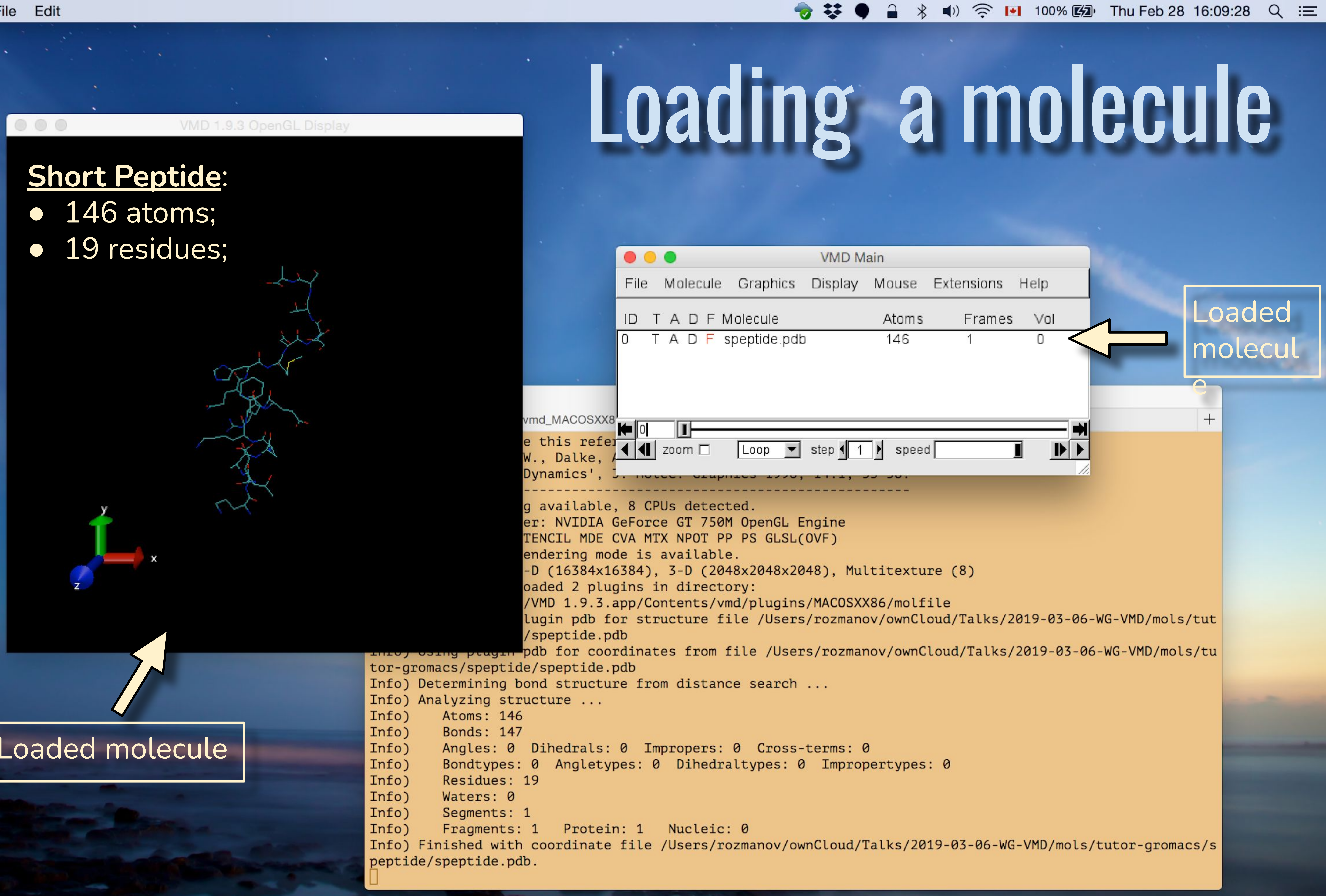
First: 0 Last: -1 Stride: 1

● Load in background

○ Load all at once

1. Load for a **New Molecule**.
2. Determine type **Automatically**.
3. Select file **speptide.pdb**
4. Click **Load**.
5. Close the **dialog**.

Loading a molecule



Short Peptide:
- 146 atoms;
- 19 residues;

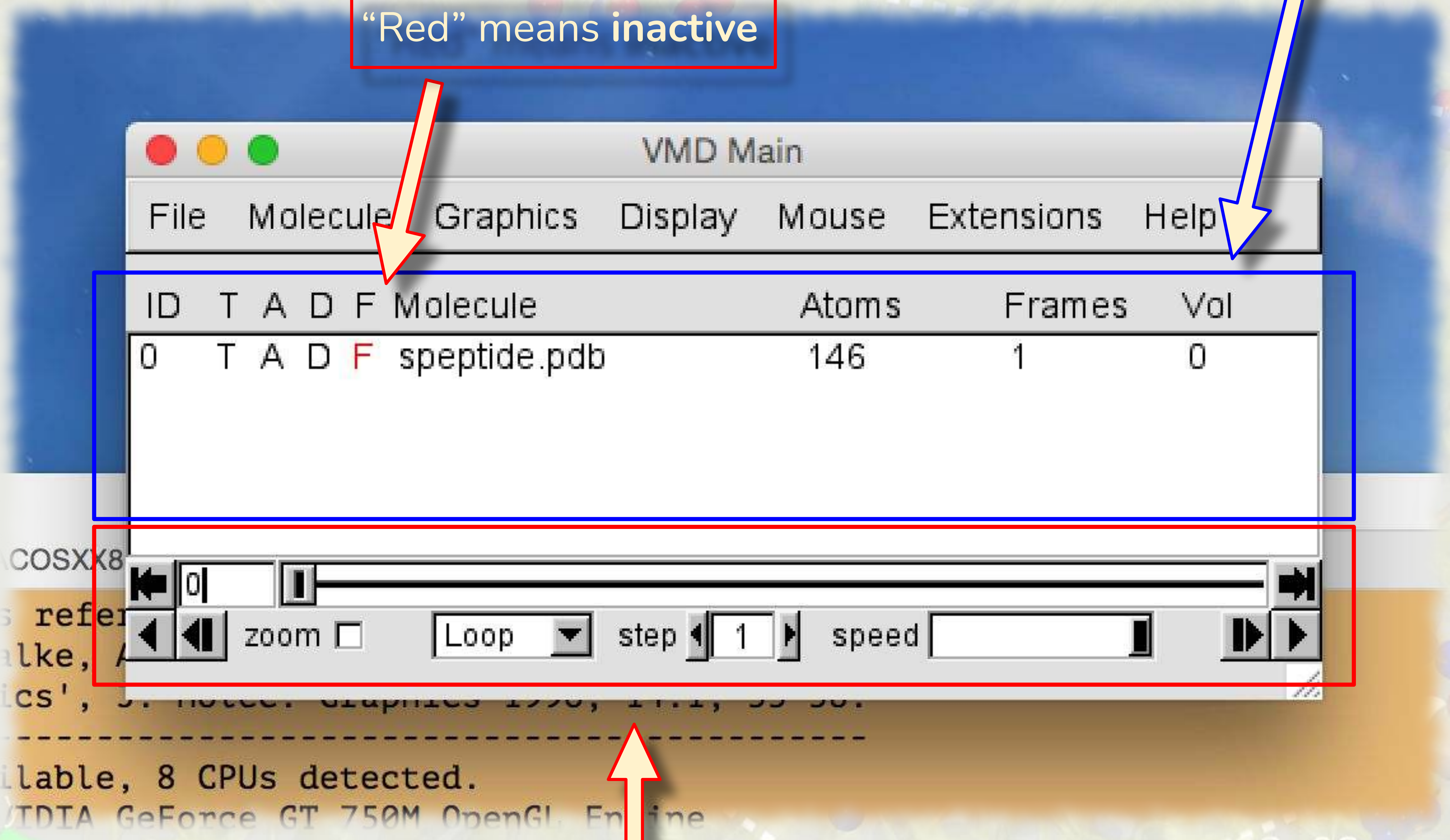
ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

Loaded molecule

Loaded molecule

```
e this refer
W., Dalke,
Dynamics',
-----------------------------------------------------
g available, 8 CPUs detected.
er: NVIDIA GeForce GT 750M OpenGL Engine
TENCIL MDE CVA MTX NPOT PP PS GLSL(OVF)
endering mode is available.
-D (16384x16384), 3-D (2048x2048x2048), Multitexture (8)
oaded 2 plugins in directory:
/VMD 1.9.3.app/Contents/vmd/plugins/MACOSXX86/molfile
lugin pdb for structure file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tut
/speptide.pdb
pdb for coordinates from file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tu
tor-gromacs/speptide/speptide.pdb
Info) Determining bond structure from distance search ...
Info) Analyzing structure ...
Info)    Atoms: 146
Info)    Bonds: 147
Info)    Angles: 0  Dihedrals: 0  Impropers: 0  Cross-terms: 0
Info)    Bondtypes: 0  Angletypes: 0  Dihedraltypes: 0  Impropertypes: 0
Info)    Residues: 19
Info)    Waters: 0
Info)    Segments: 1
Info)    Fragments: 1   Protein: 1   Nucleic: 0
Info) Finished with coordinate file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tutor-gromacs/s
peptide/speptide.pdb.
```

Main control window



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

List of molecules

“Red” means **inactive**

Trajectory animation controls

ID - molecule number.

T - “Top” stat.

A - Active.

D - Drawn.

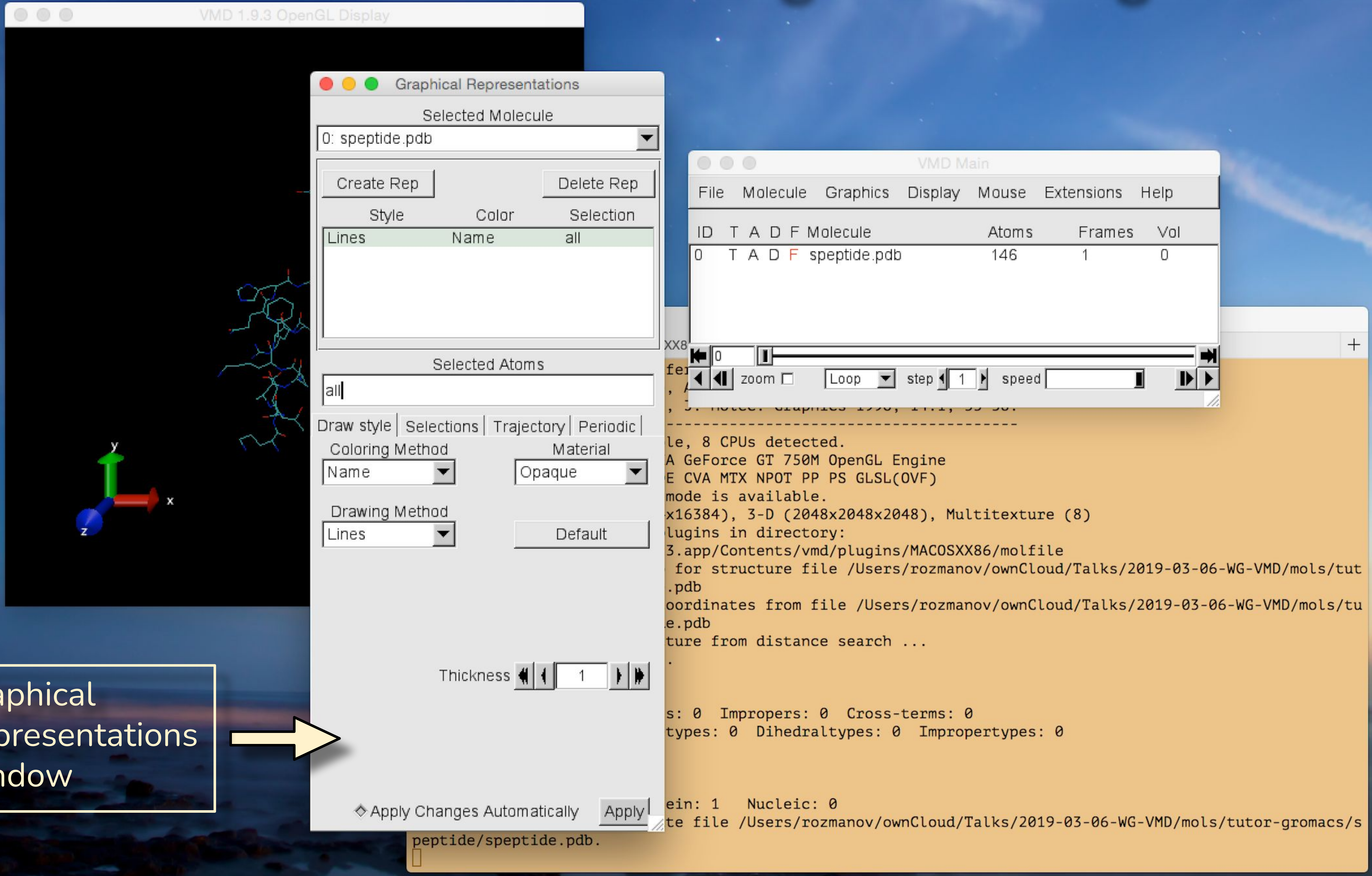
F - Fixed.

of **Atoms**.

of **Frames**.

Volumetric data.

Working with a single molecule



Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness: 1

◇ Apply Changes Automatically

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

```
------------------------------------
le, 8 CPUs detected.
A GeForce GT 750M OpenGL Engine
E CVA MTX NPOT PP PS GLSL(OVF)
mode is available.
x16384), 3-D (2048x2048x2048), Multitexture (8)
lugins in directory:
3.app/Contents/vmd/plugins/MACOSXX86/molfile
 for structure file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tut
.pdb
oordinates from file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tu
e.pdb
ture from distance search ...
.



s: 0  Impropers: 0  Cross-terms: 0
types: 0  Dihedraltypes: 0  Impropertypes: 0



ein: 1   Nucleic: 0
te file /Users/rozmanov/ownCloud/Talks/2019-03-06-WG-VMD/mols/tutor-gromacs/s
peptide/speptide.pdb.
```

Graphical Representations window

Representations

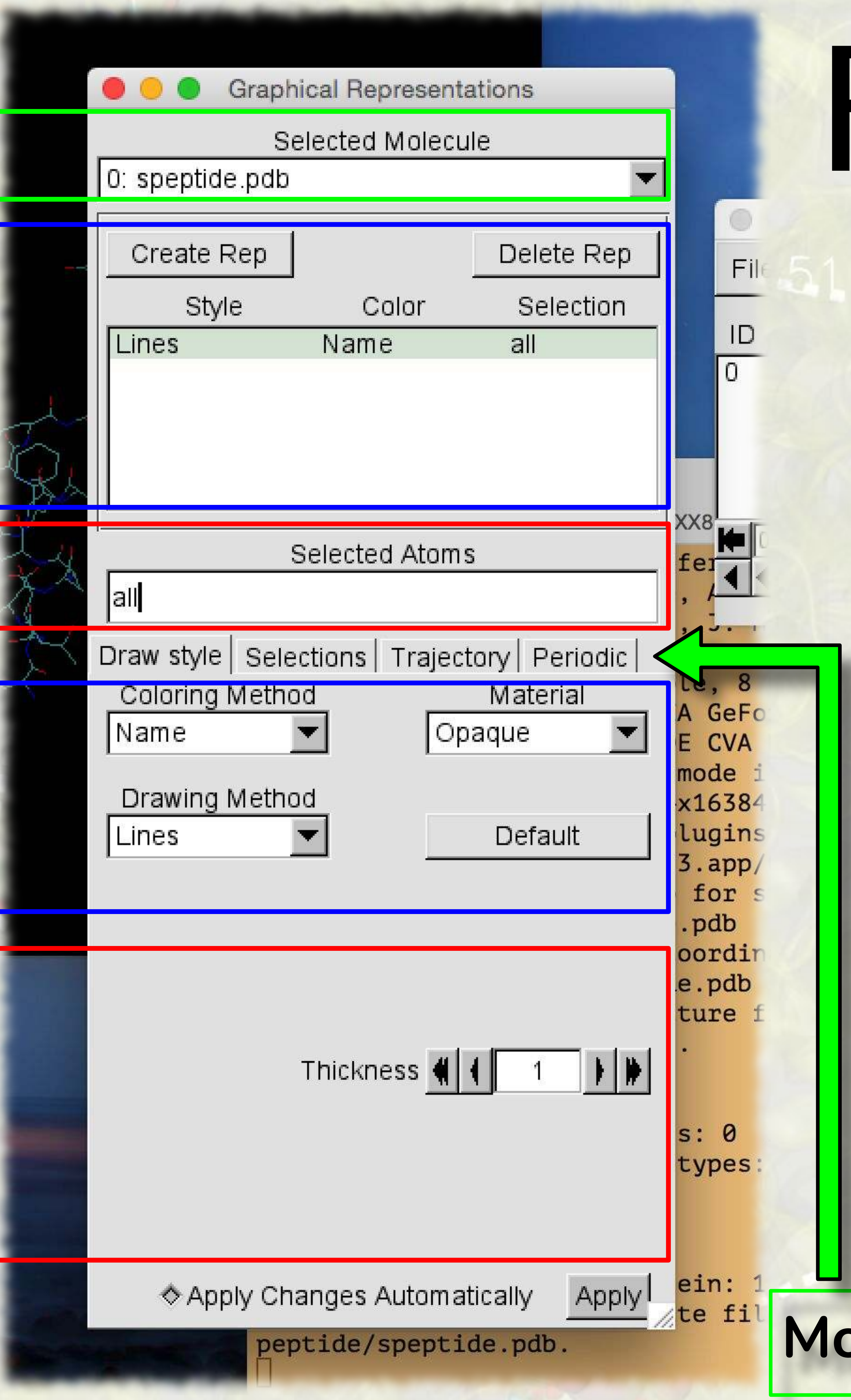
Molecule selector.

List of Representations.

Atom selection.

Drawing method, Coloring scheme, Material controls.

Drawing method parameters.



Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

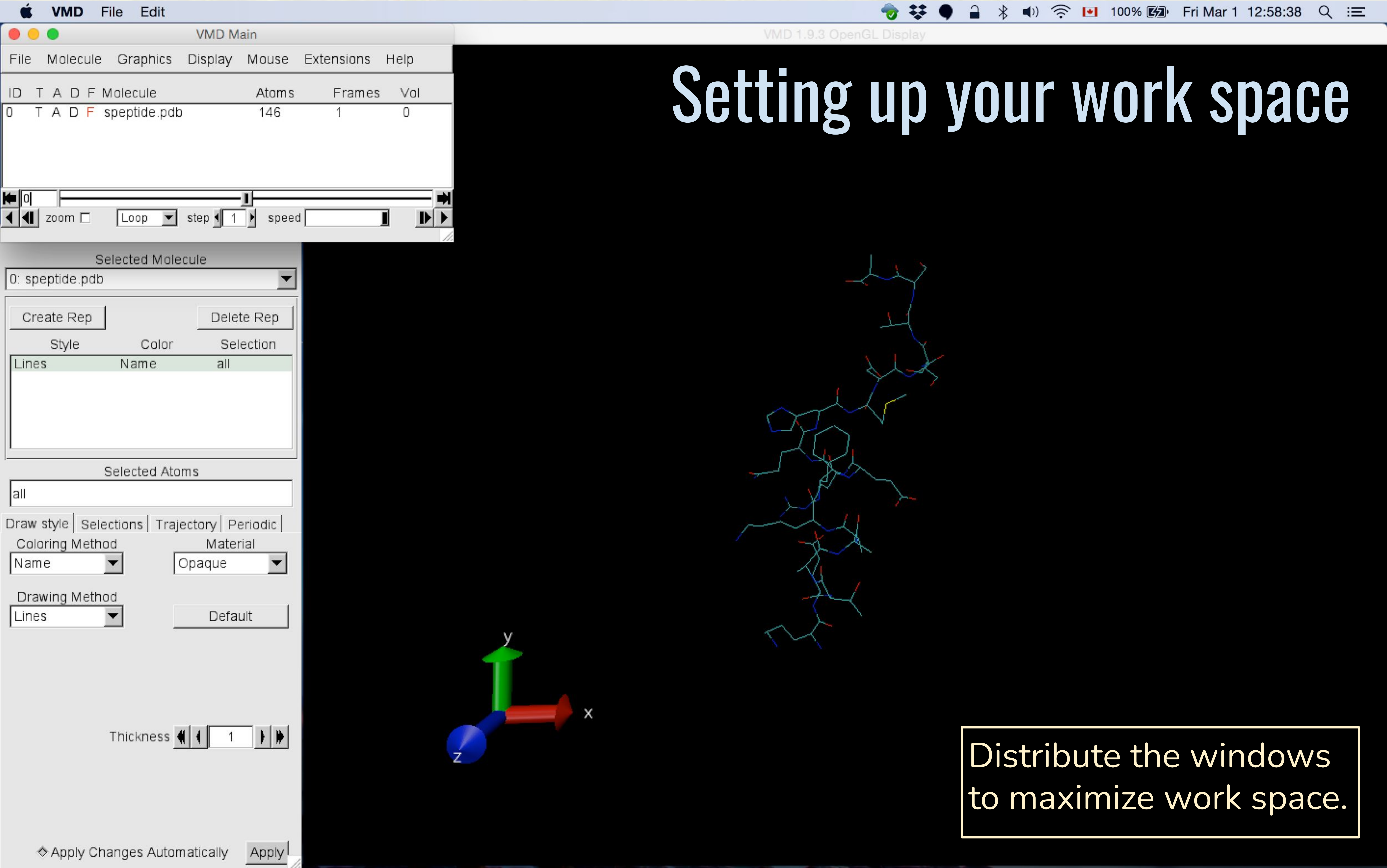
Thickness: 1

More options

- Atom selection
- Drawing method
- Coloring method
- Material

A molecule can have multiple representations.

Setting up your work space



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

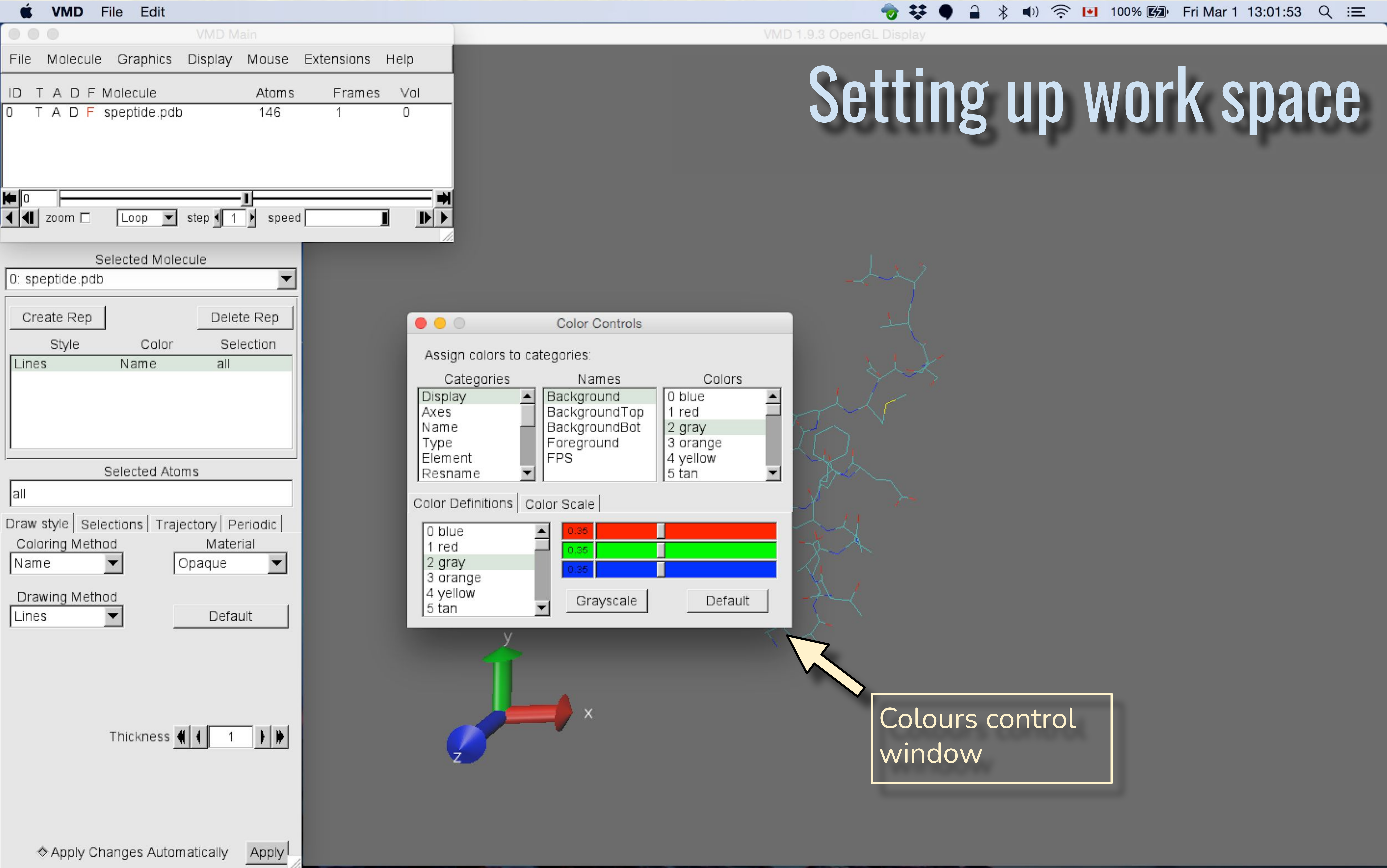
Material: Opaque

Drawing Method: Lines

Thickness: 1

Distribute the windows to maximize work space.

Setting up work space



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness: 1

Assign colors to categories:

Categories	Names	Colors
Display	Background	0 blue
Axes	BackgroundTop	1 red
Name	BackgroundBot	2 gray
Type	Foreground	3 orange
Element	FPS	4 yellow
Resname		5 tan

Color Definitions: 0 blue, 1 red, 2 gray, 3 orange, 4 yellow, 5 tan

0.35
0.35
0.35

Colours control window

Colour control

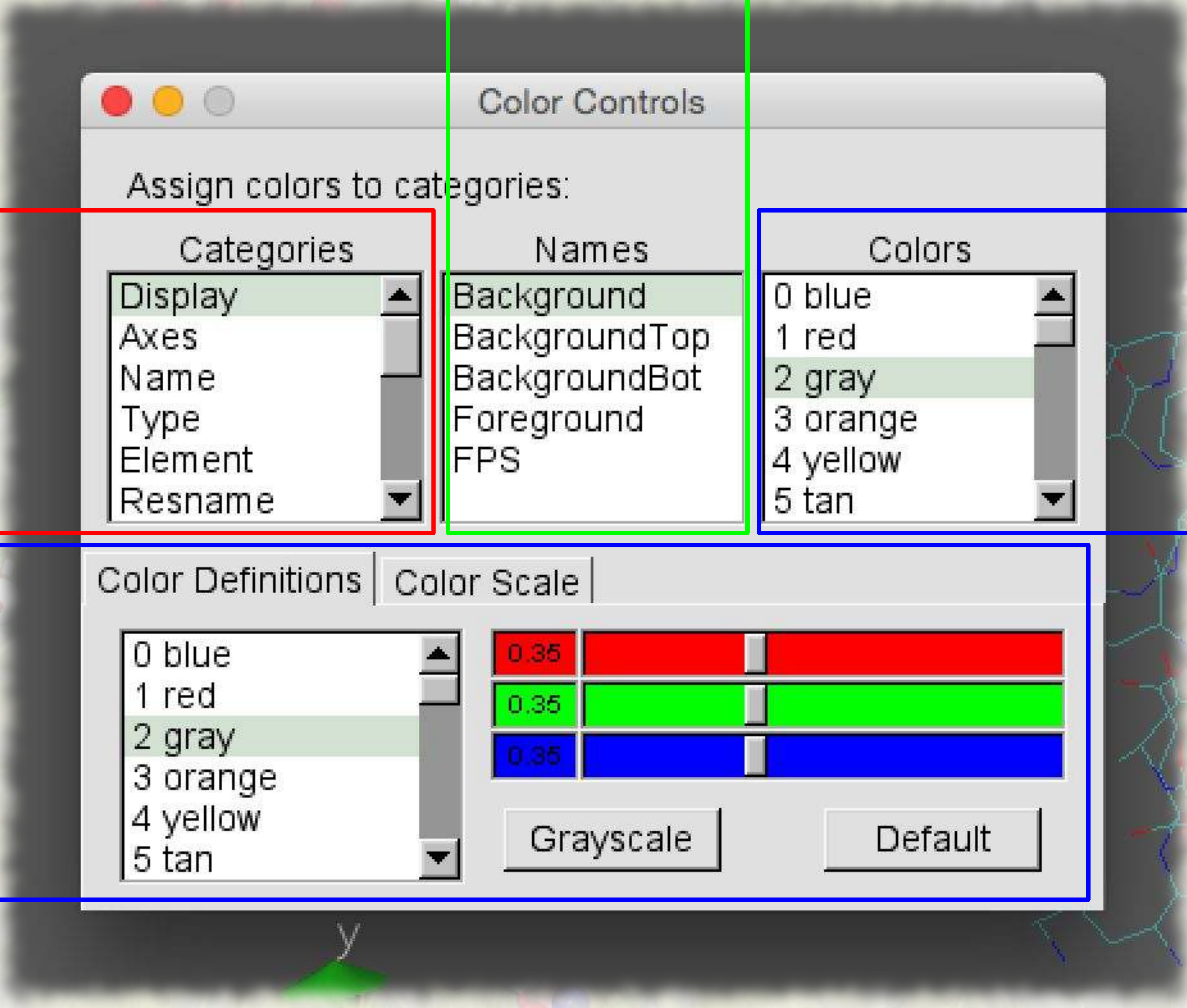
Floating dialog.
Stays until closed.

Items and Objects

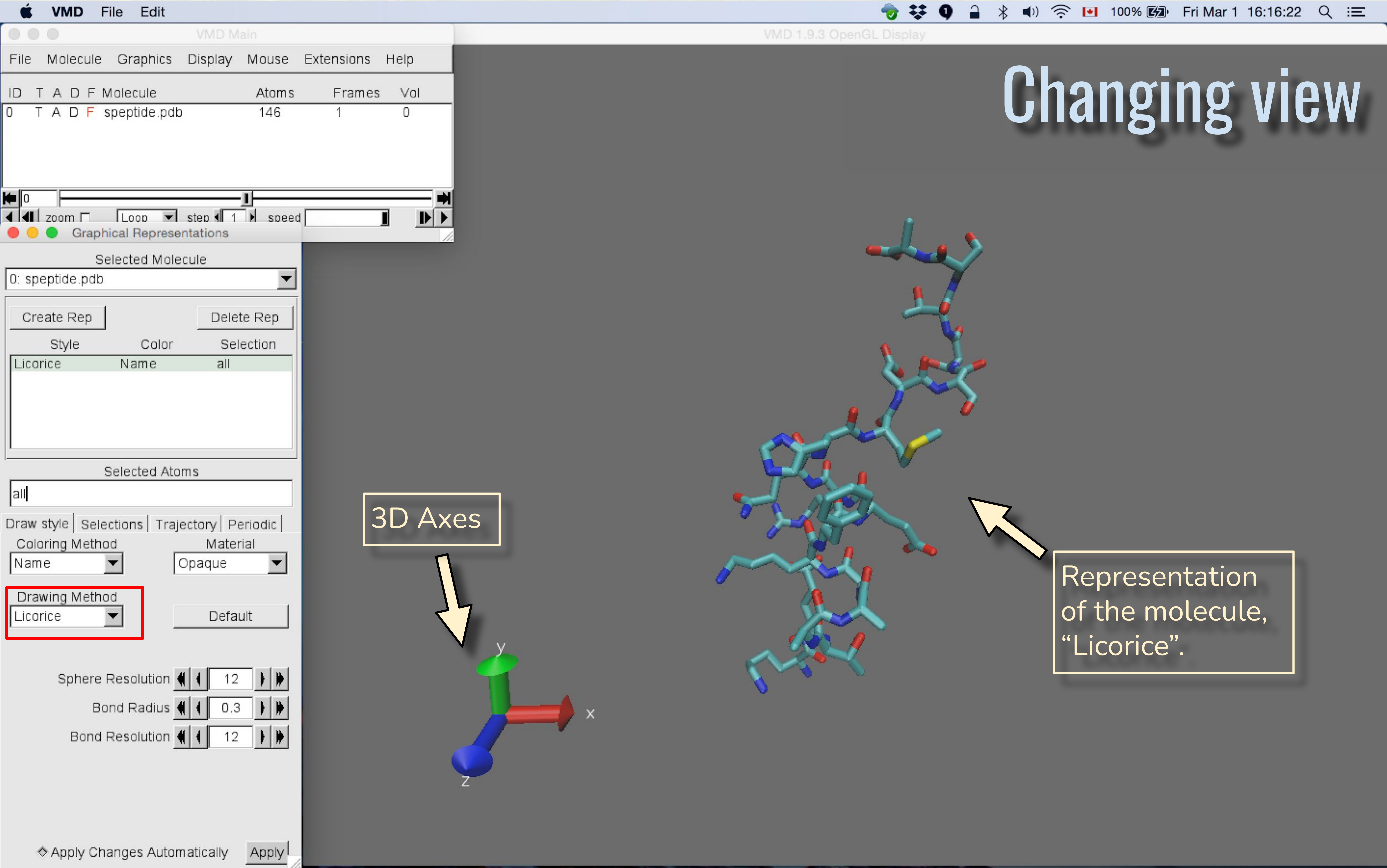
Categories

Colour Selector

Colour Editor



Changing view



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
0	T	A	D	F	speptide.pdb	146	1	0

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Licorice	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

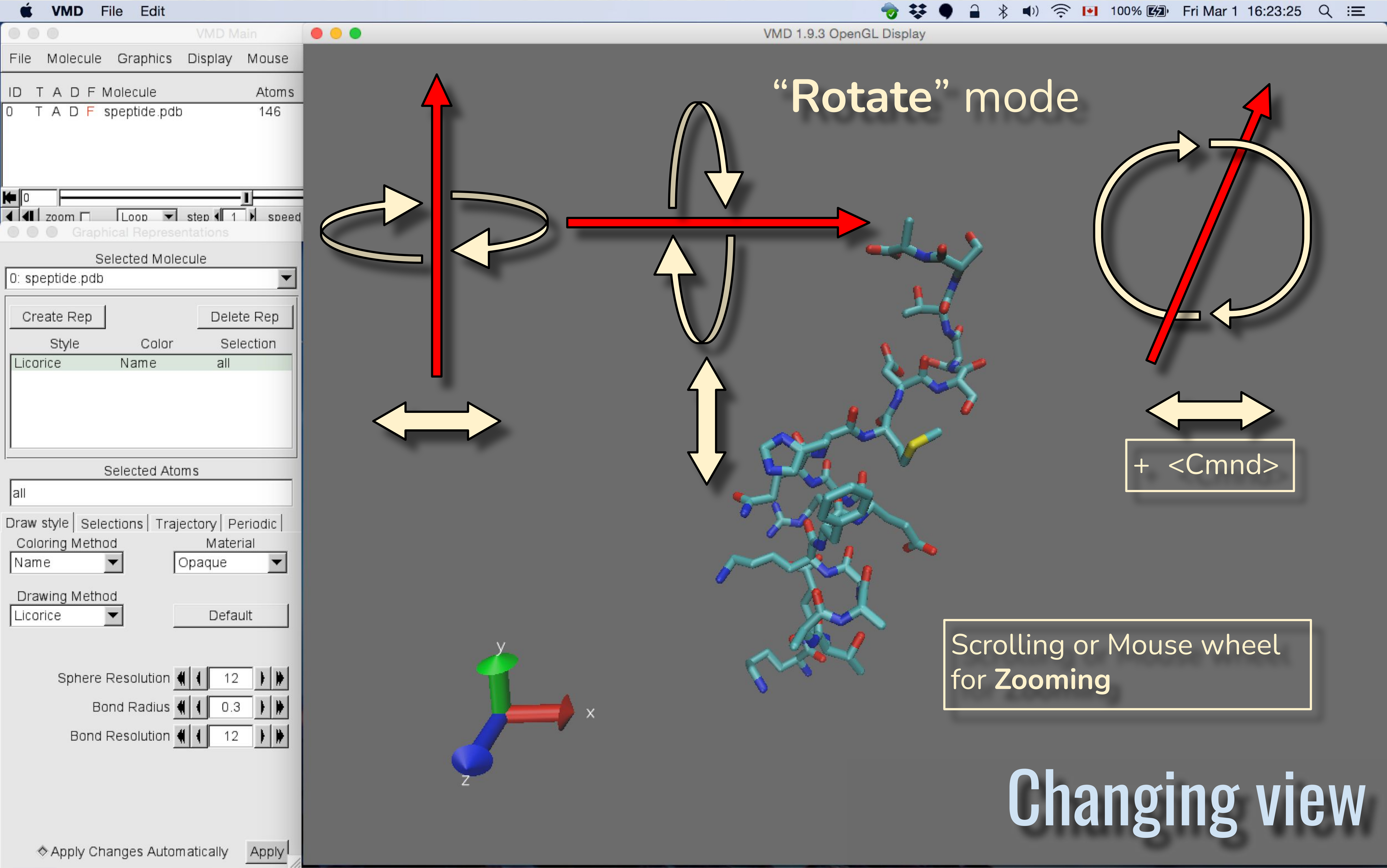
Sphere Resolution: 12

Bond Radius: 0.3

Bond Resolution: 12

3D Axes

Representation of the molecule, “Licorice”.



Changing view

“Rotate” mode

+ <Cmnd>

Scrolling or Mouse wheel for **Zooming**

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Licorice	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

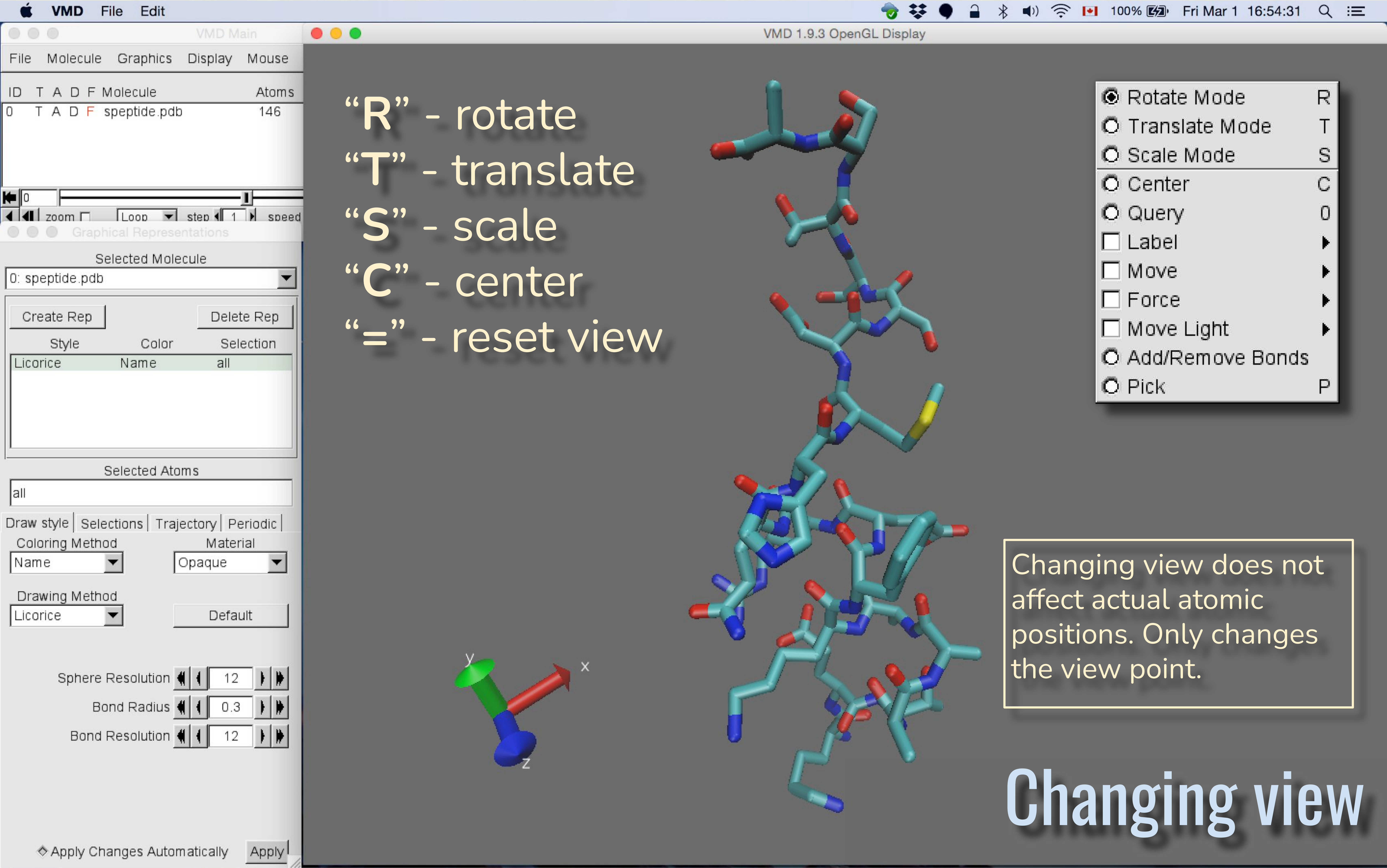
Sphere Resolution: 12

Bond Radius: 0.3

Bond Resolution: 12

◇ Apply Changes Automatically

Changing view



“R” - rotate
“T” - translate
“S” - scale
“C” - center
“=” - reset view

Changing view does not affect actual atomic positions. Only changes the view point.

ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

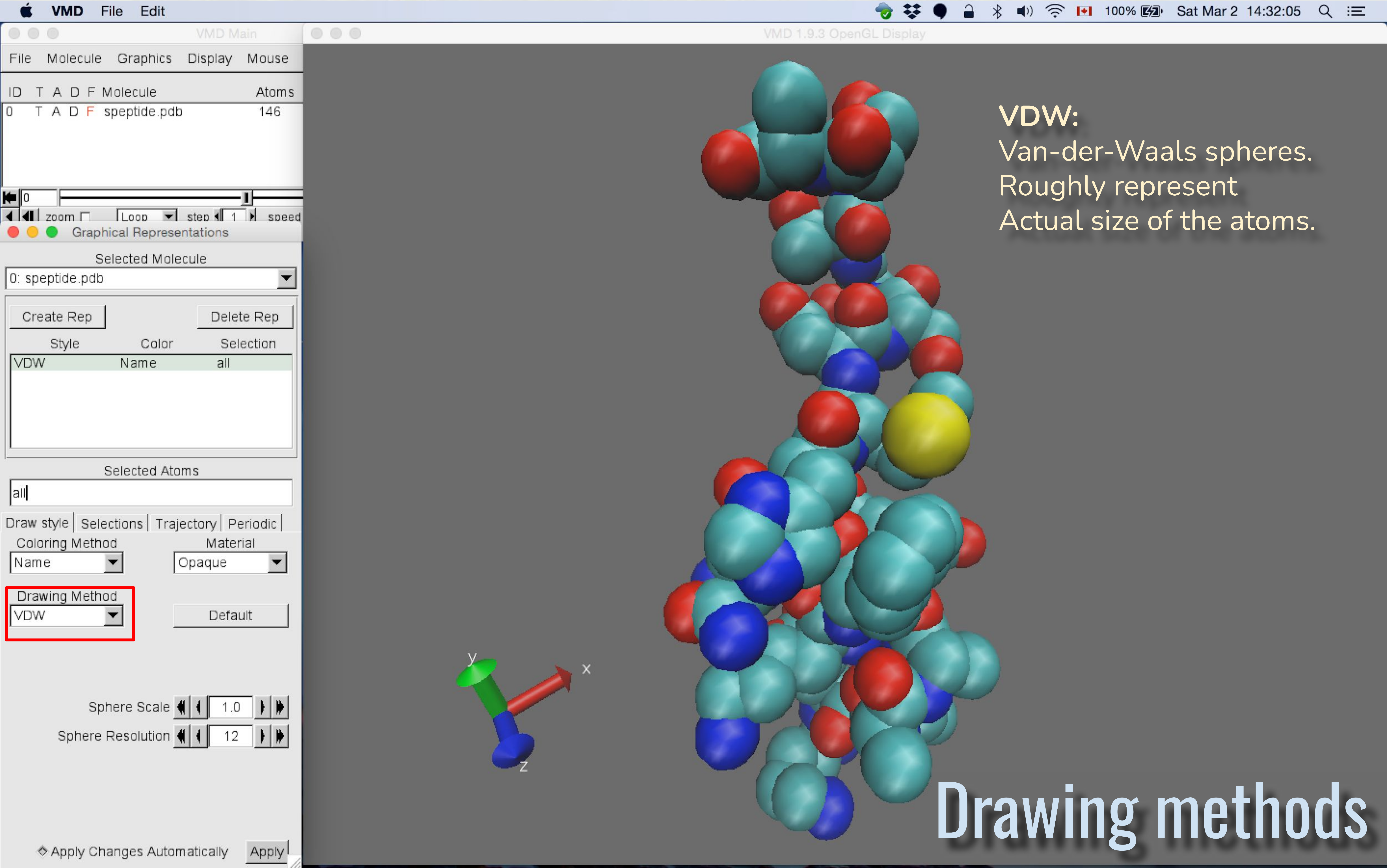
Selected Molecule: 0: speptide.pdb

Style	Color	Selection
Licorice	Name	all

Selected Atoms: all

Coloring Method: Name
Material: Opaque
Drawing Method: Licorice
Sphere Resolution: 12
Bond Radius: 0.3
Bond Resolution: 12

Drawing methods



ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
VDW	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

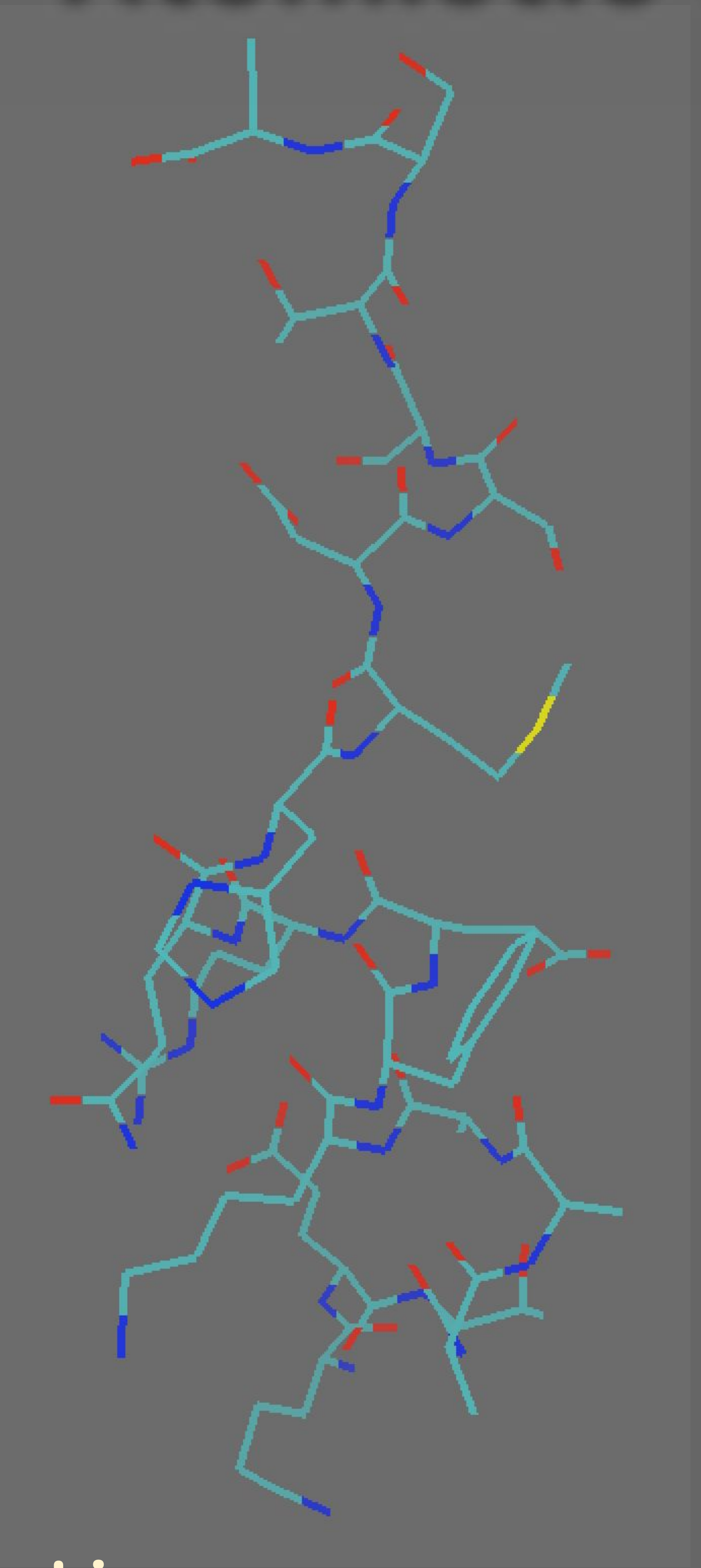
Drawing Method: VDW

Sphere Scale: 1.0

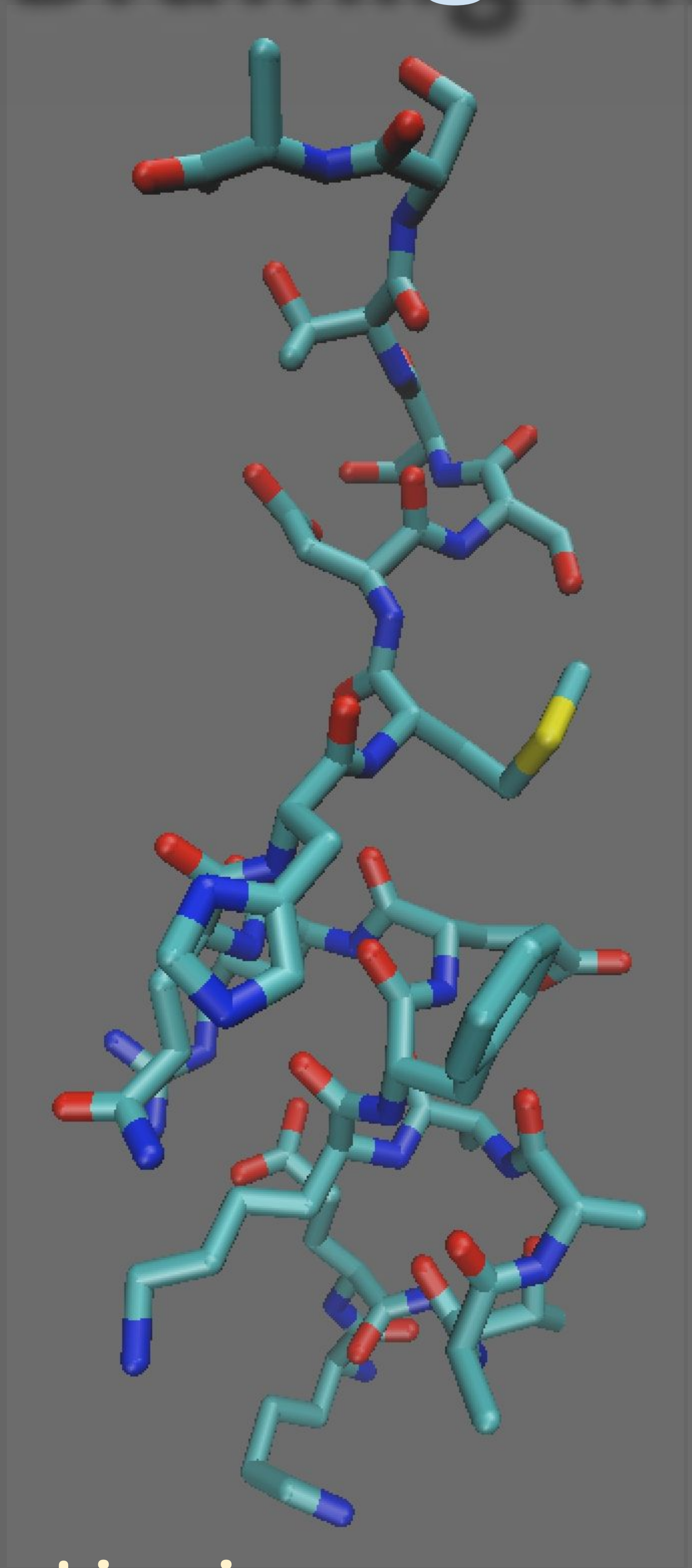
Sphere Resolution: 12

VDW:
Van-der-Waals spheres.
Roughly represent
Actual size of the atoms.

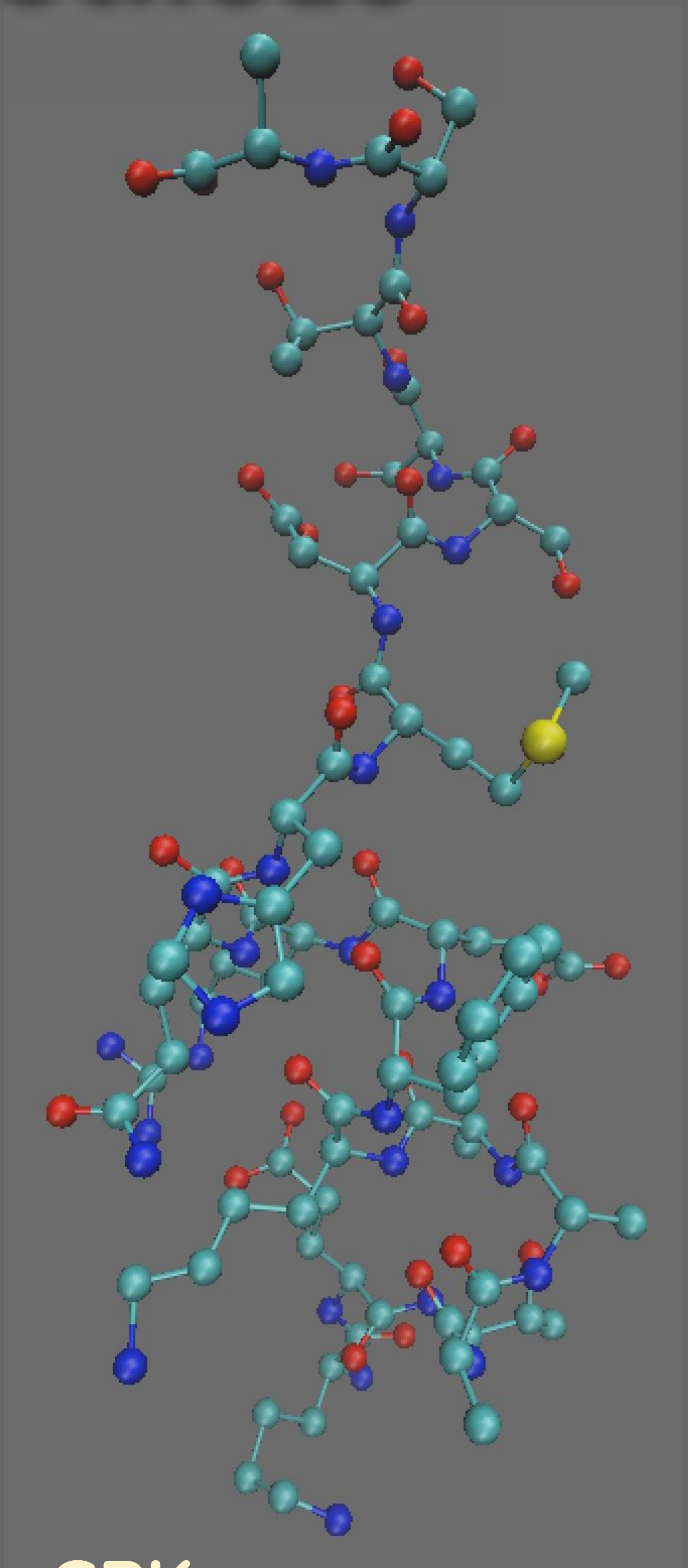
Atomistic Drawing Methods



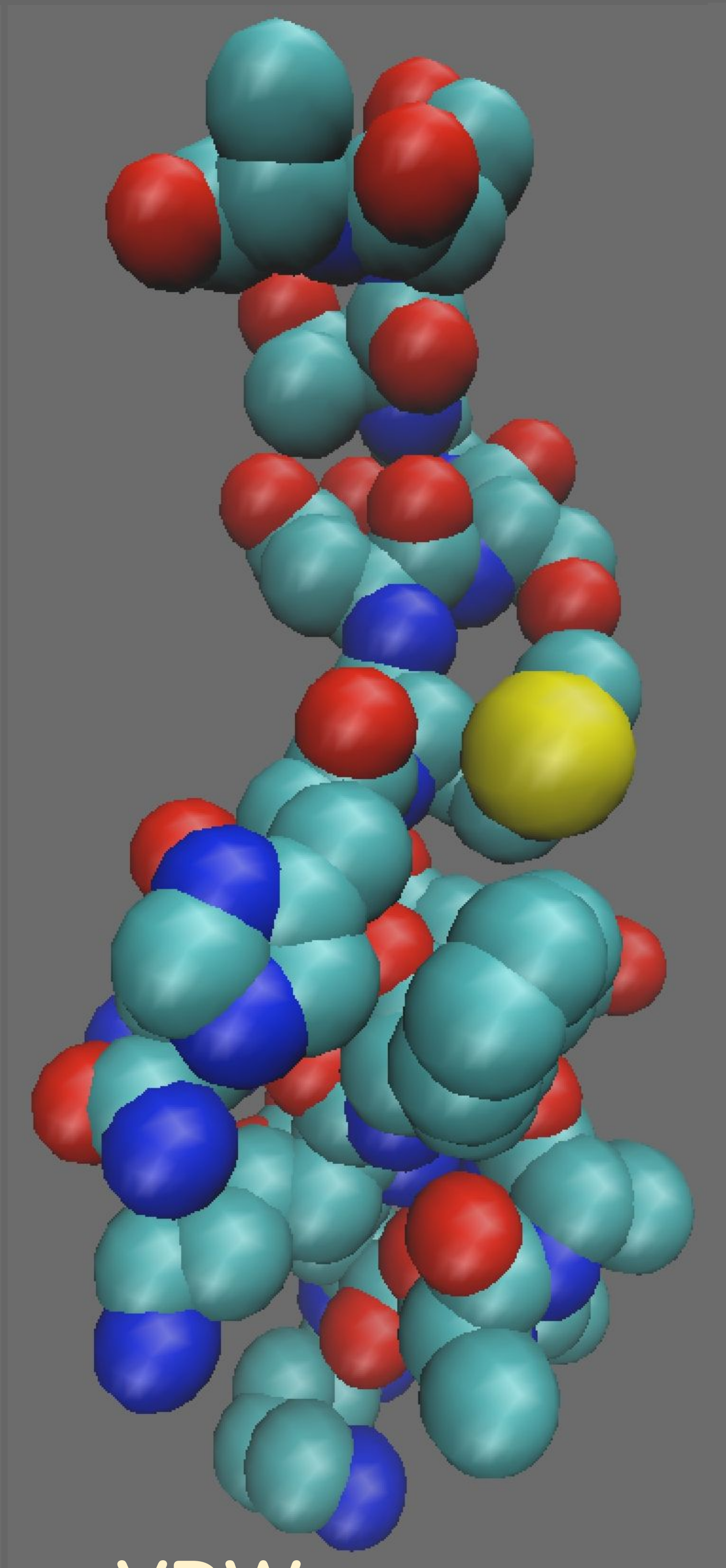
Lines:
Structure, atoms.
Very lightweight.
Default.



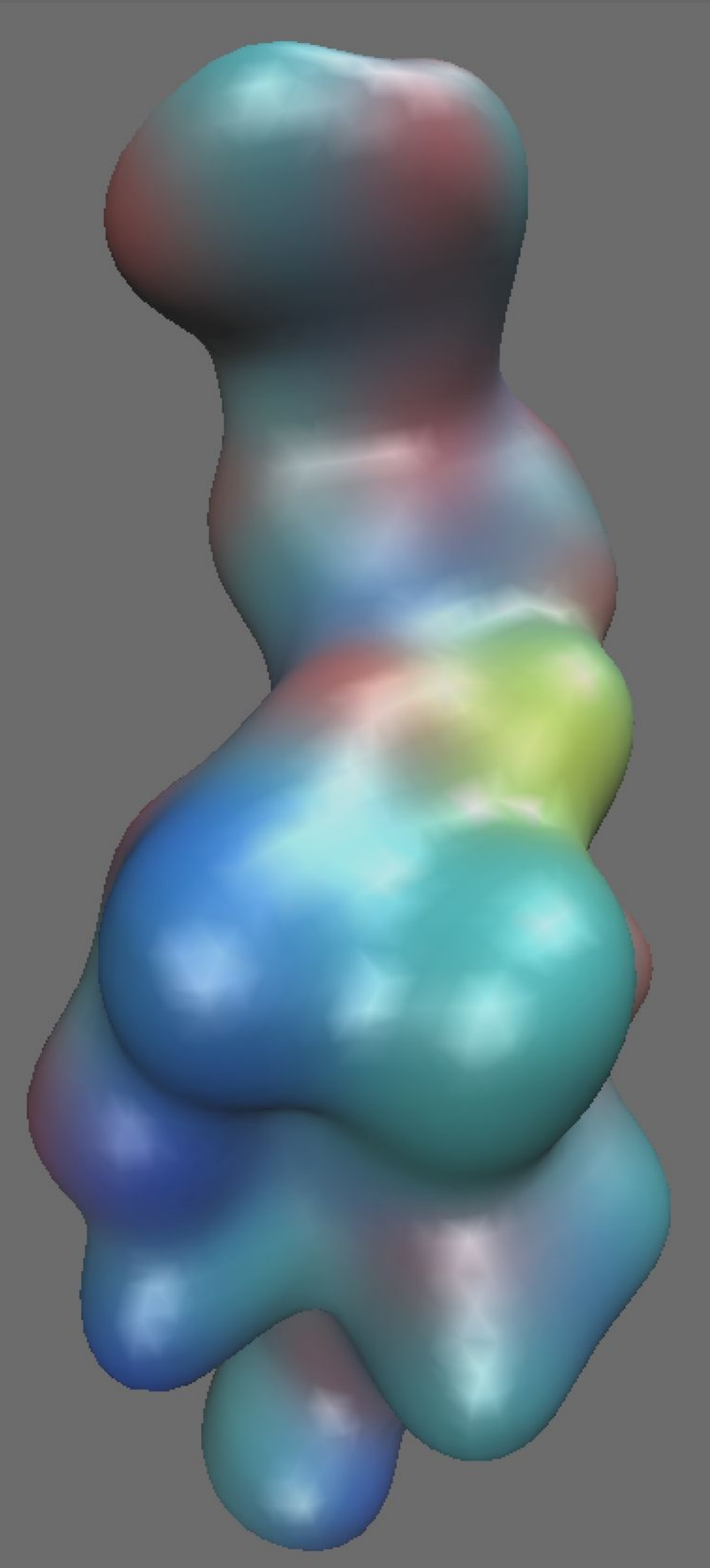
Licorice:
Structure, atoms.
Minimalistic.
Looks better.



CPK:
Structure, atoms.
Relative atom sizes.
Demanding.
Often too cluttered.

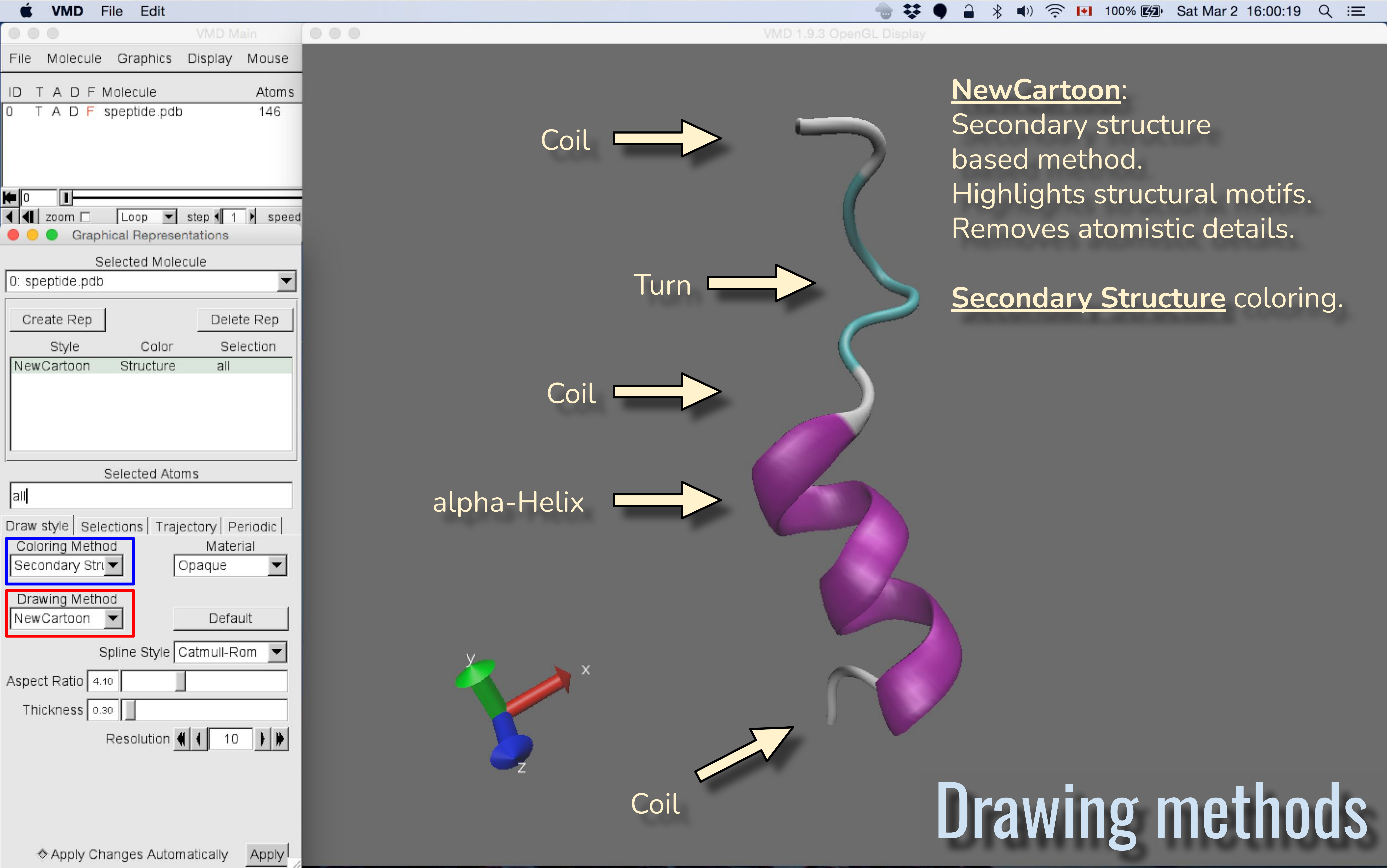


VDW:
Structure, atoms.
Realistic volume.
Too ugly.
Cluttered.



Quick Surf:
Volume.
Clean.

Drawing methods



ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
NewCartoon	Structure	all

Selected Atoms: all

Coloring Method: Secondary Stru

Material: Opaque

Drawing Method: NewCartoon

Spline Style: Catmull-Rom

Aspect Ratio: 4.10

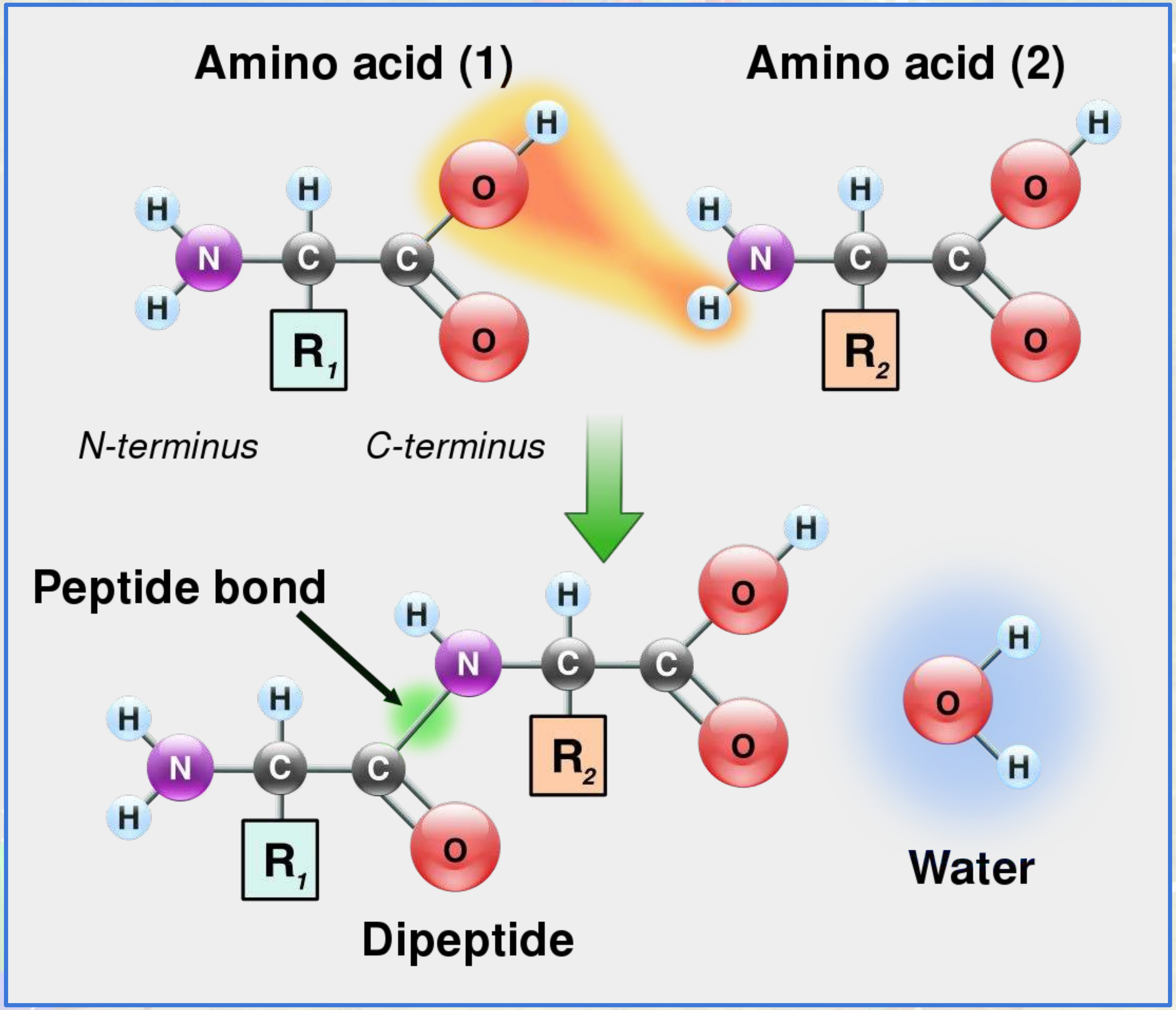
Thickness: 0.30

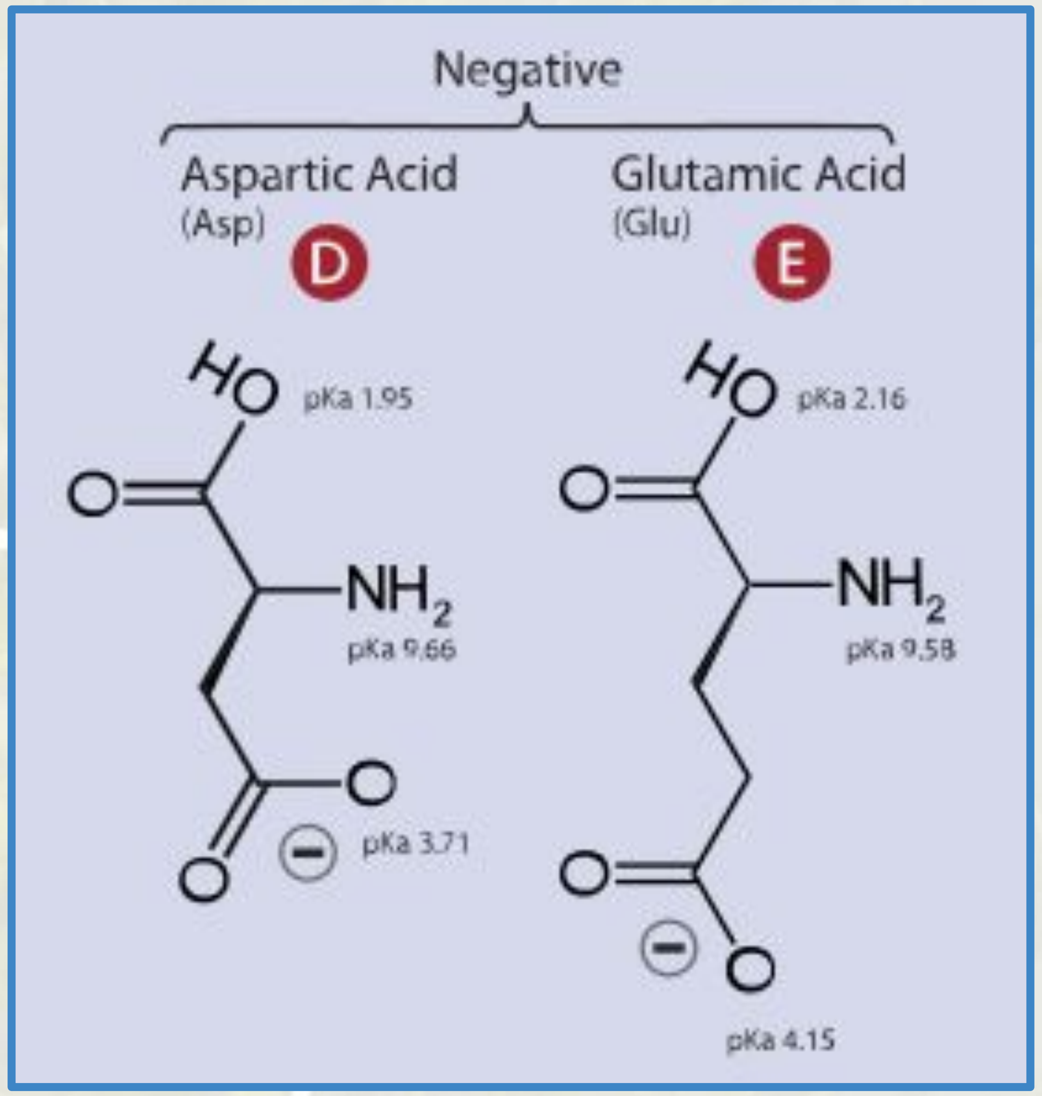
Resolution: 10

NewCartoon:
Secondary structure
based method.
Highlights structural motifs.
Removes atomistic details.

Secondary Structure coloring.

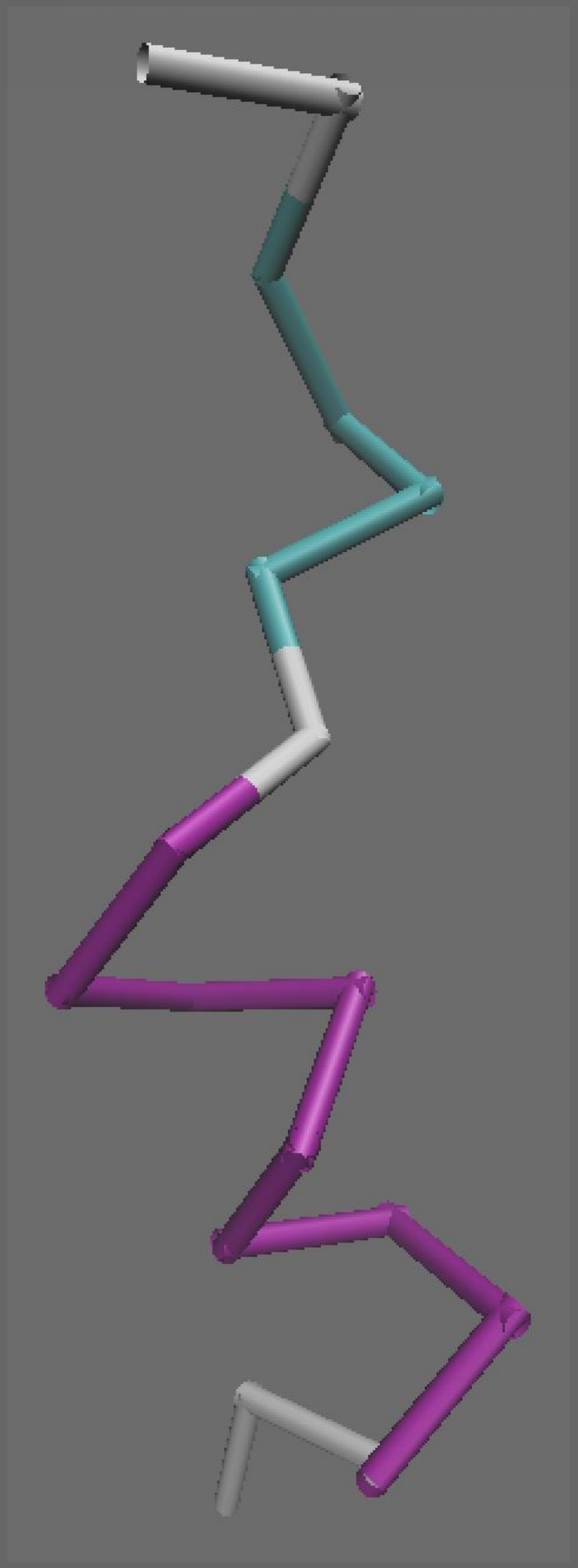
Peptide bonds and peptides



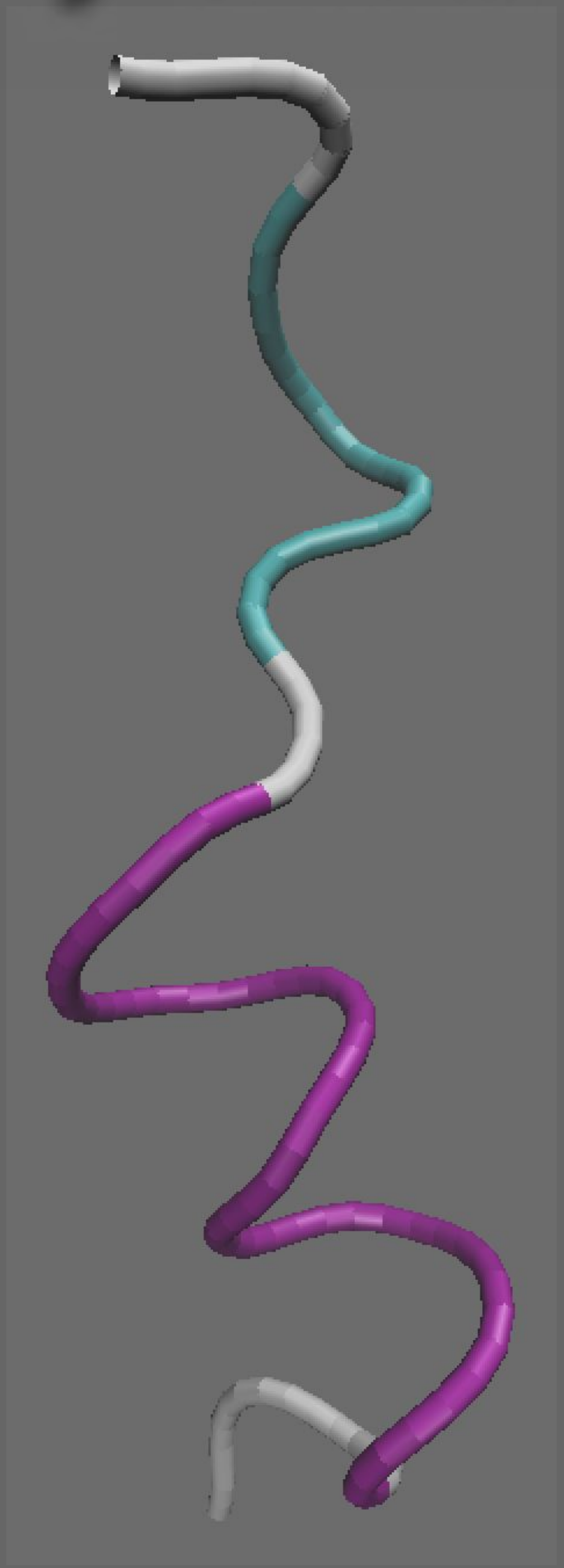


- **21 amino acids** for proteins;
- **Peptide**: **2 to 50** amino acids.
- **Protein**: **> 50** amino acids in the chain.
- Long chains form 3D motifs, called **secondary structure**.
- **Backbone**: $[C\text{-}C\text{-}N]_n$.
- Most common: **alpha-helices** and **beta-sheets**.

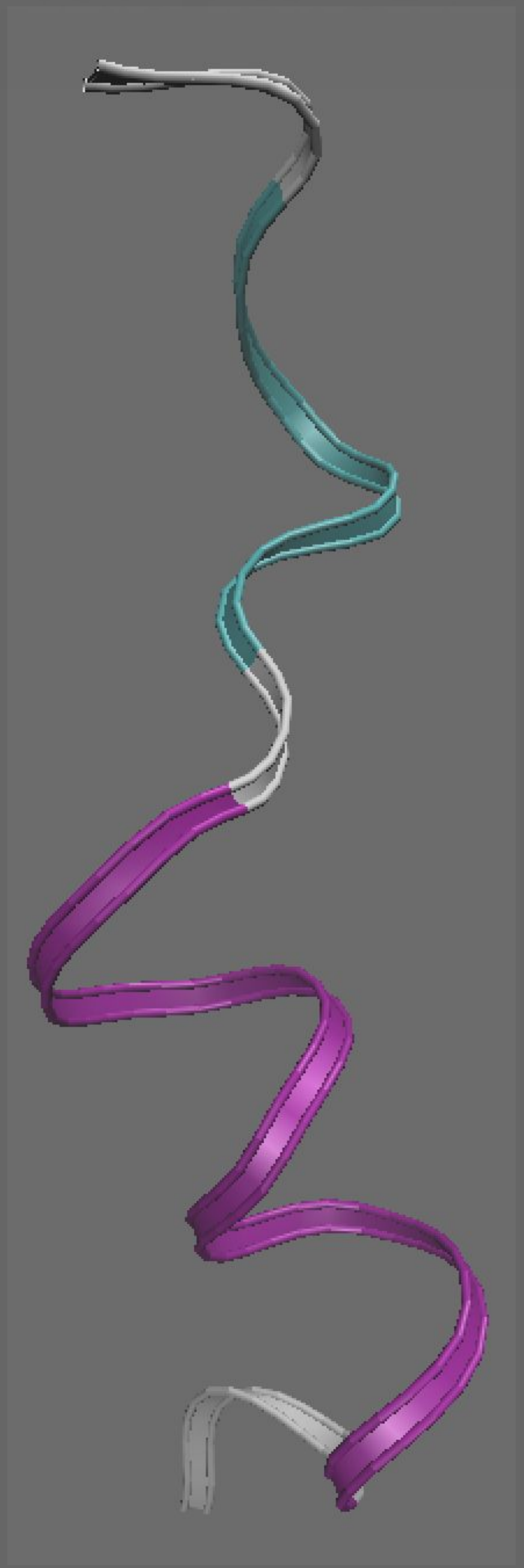
Secondary Structure based Drawing Methods



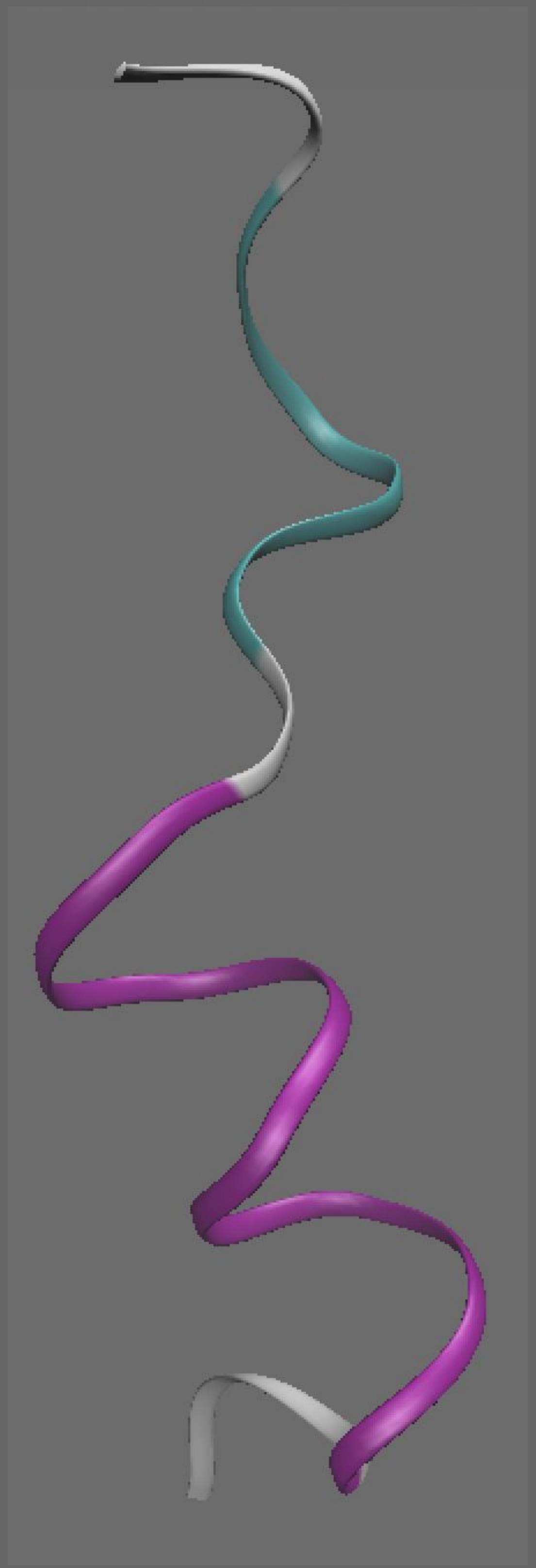
Trace:
Peptide backbone information.



Tube:
Smoothed backbone. Looks much cleaner.

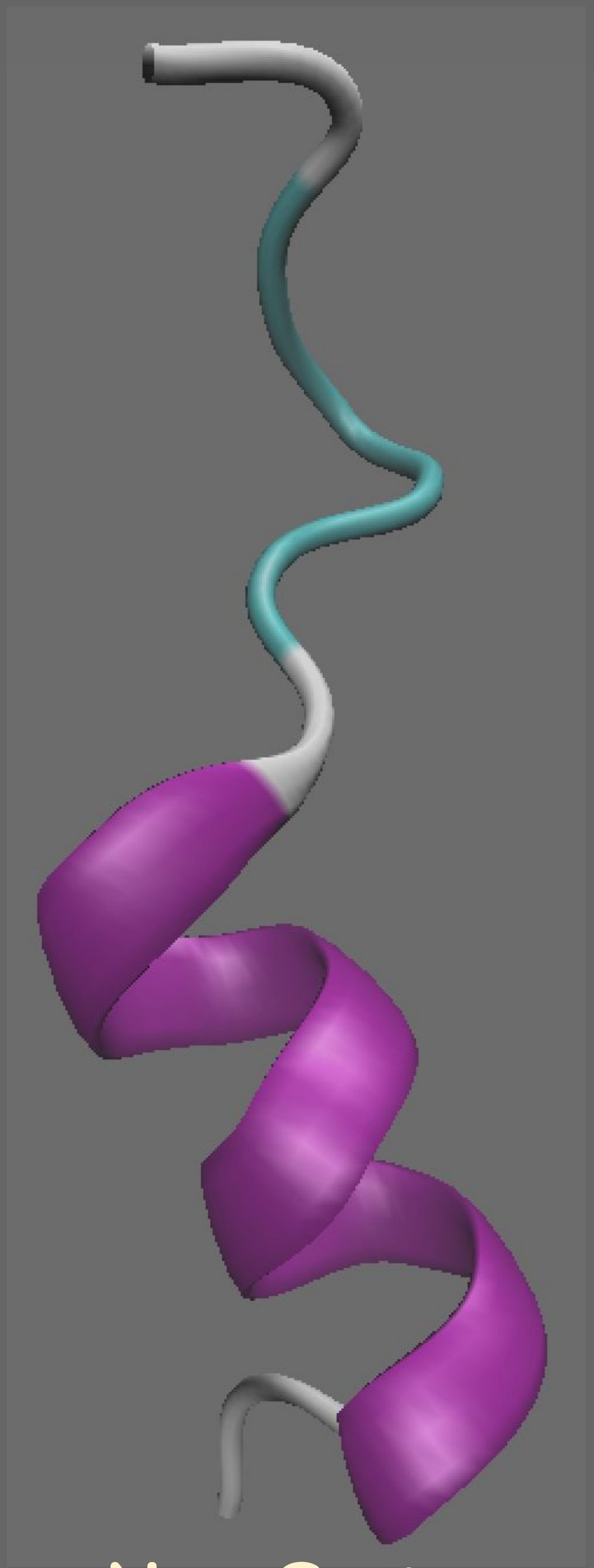


Ribbons:
Backbone orientation information



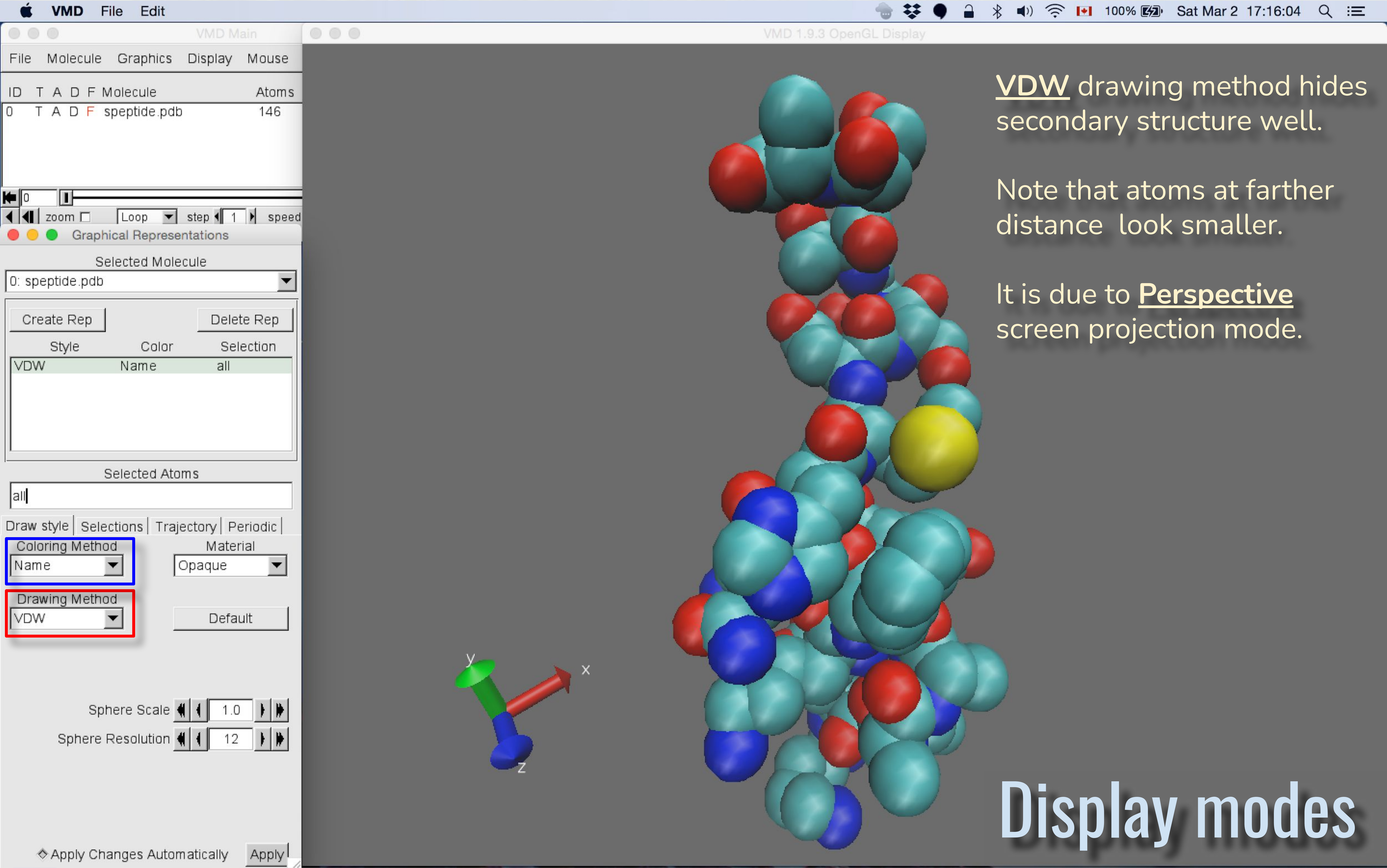
NewRibbons:
Cleaner new version.

Cartoon:
Backbone with Secondary motif assignments.



NewCartoon:
Cleaner new version.

Display modes



ID	T	A	D	F	Molecule	Atoms
0	T	A	D	F	speptide.pdb	146

zoom ☐ Loop step 1 speed

Selected Molecule: 0: speptide.pdb

Style	Color	Selection
VDW	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: VDW

Sphere Scale: 1.0

Sphere Resolution: 12

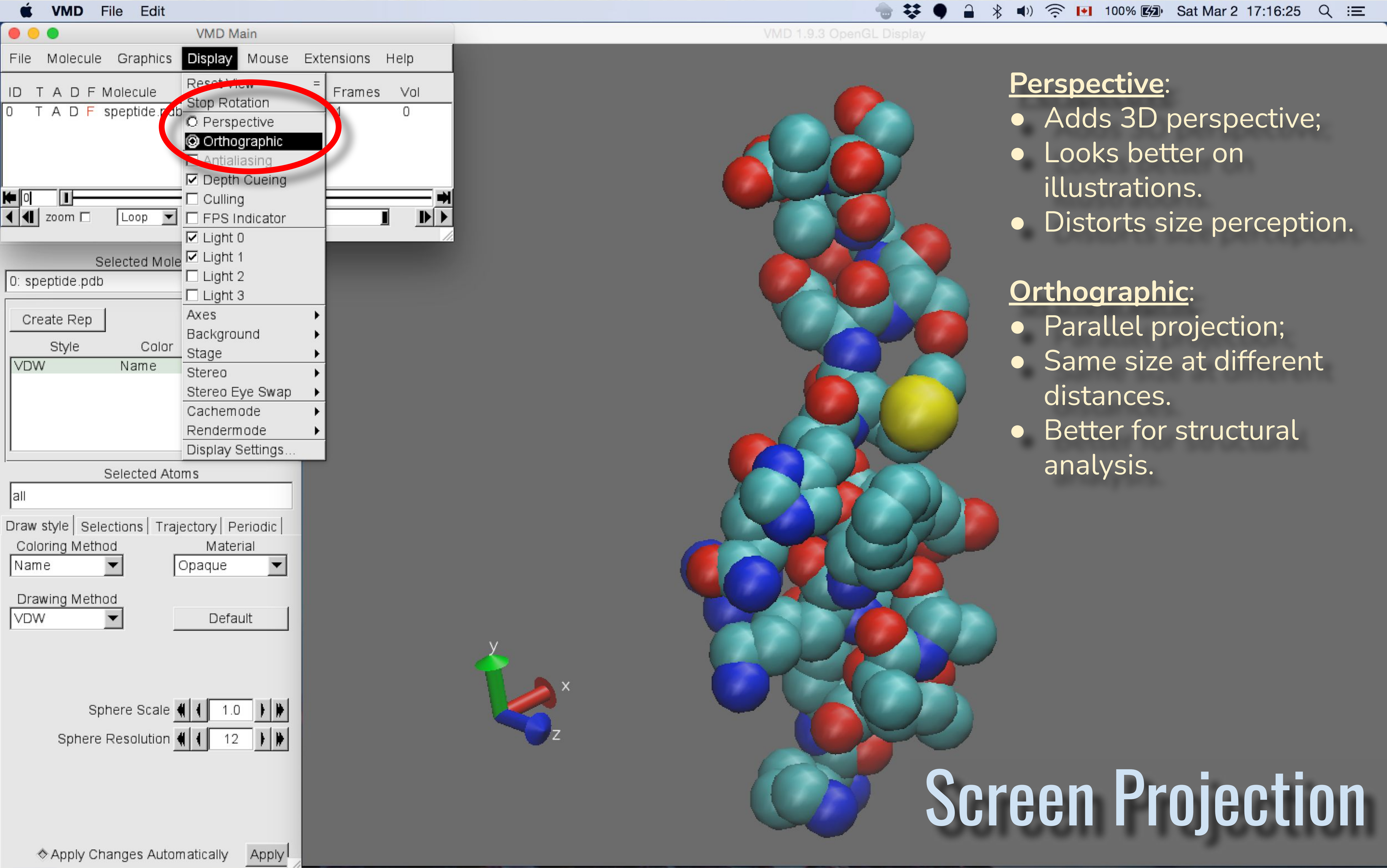
◇ Apply Changes Automatically

VDW drawing method hides secondary structure well.

Note that atoms at farther distance look smaller.

It is due to **Perspective** screen projection mode.

Screen Projection

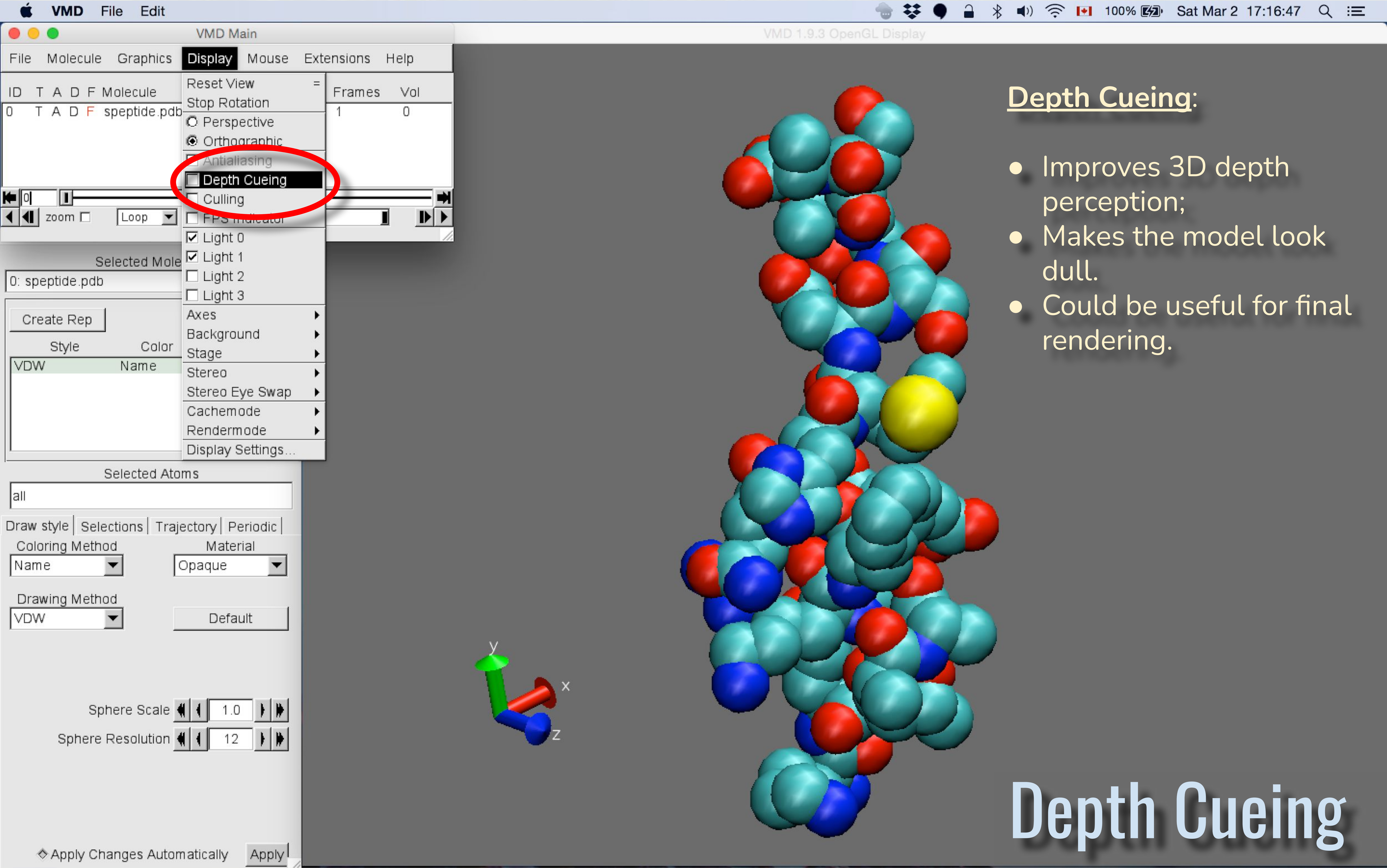


Perspective:

- Adds 3D perspective;
- Looks better on illustrations.
- Distorts size perception.

Orthographic:

- Parallel projection;
- Same size at different distances.
- Better for structural analysis.

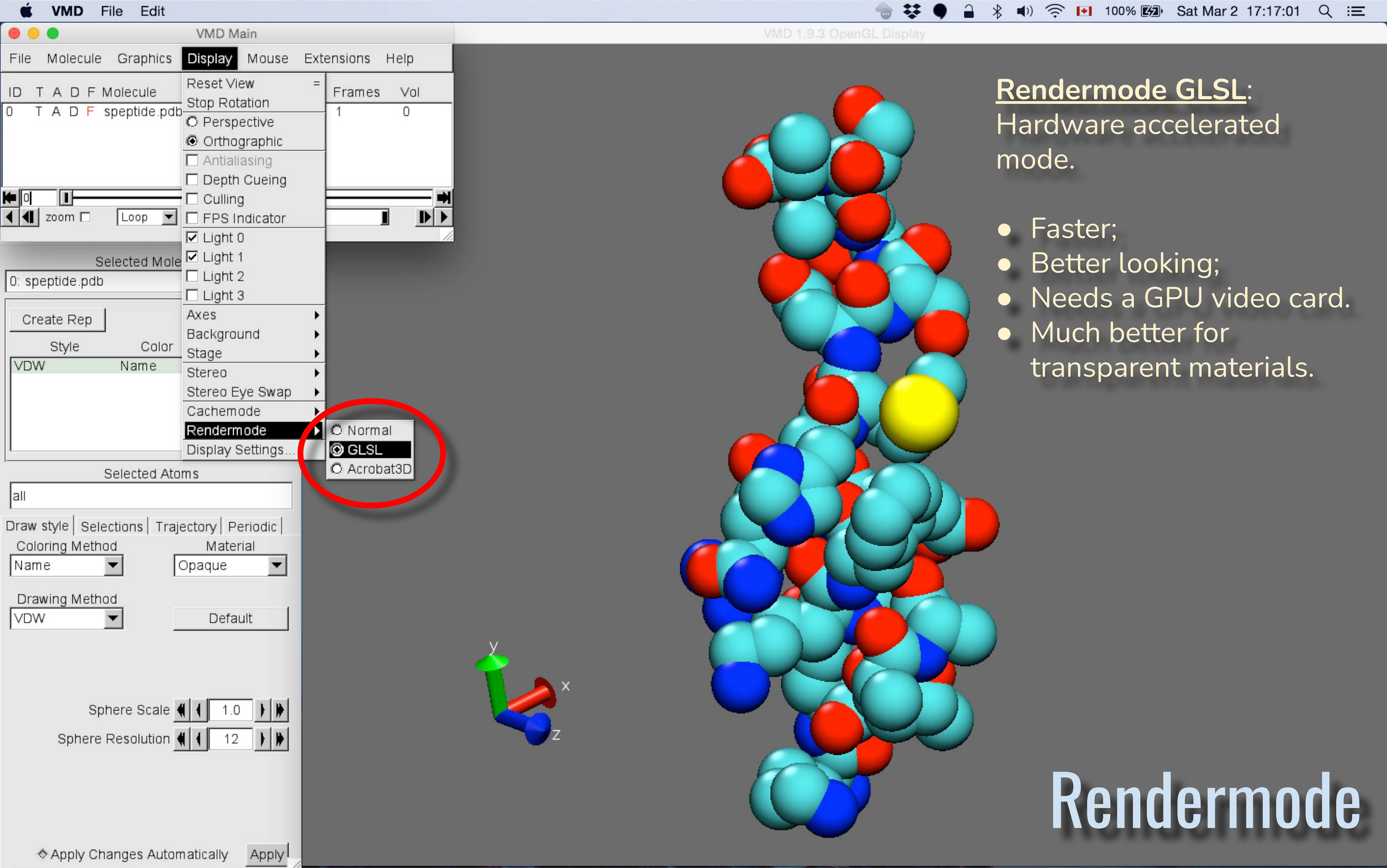


Depth Cueing:

- Improves 3D depth perception;
- Makes the model look dull.
- Could be useful for final rendering.

Depth Cueing

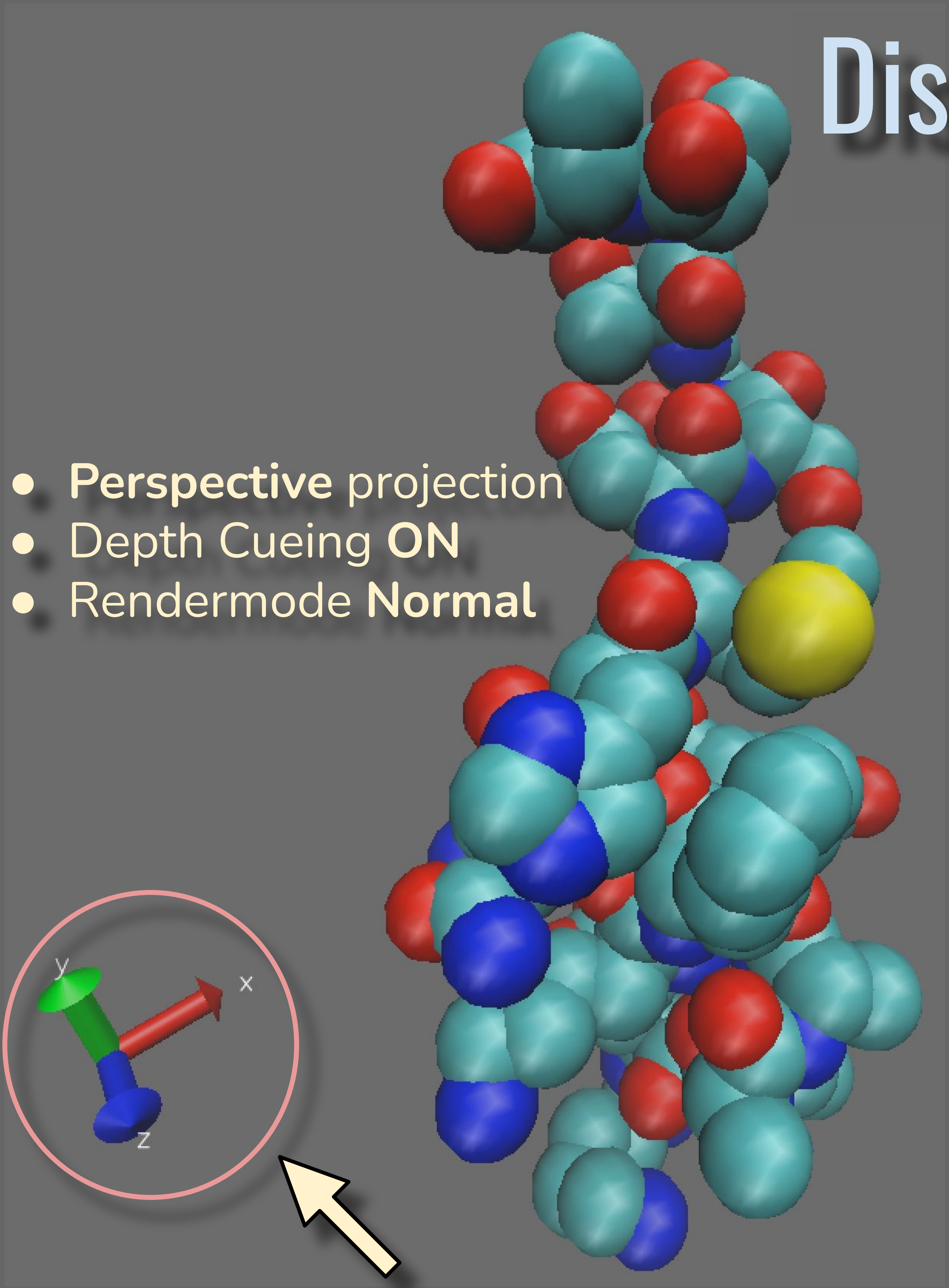
Rendermode



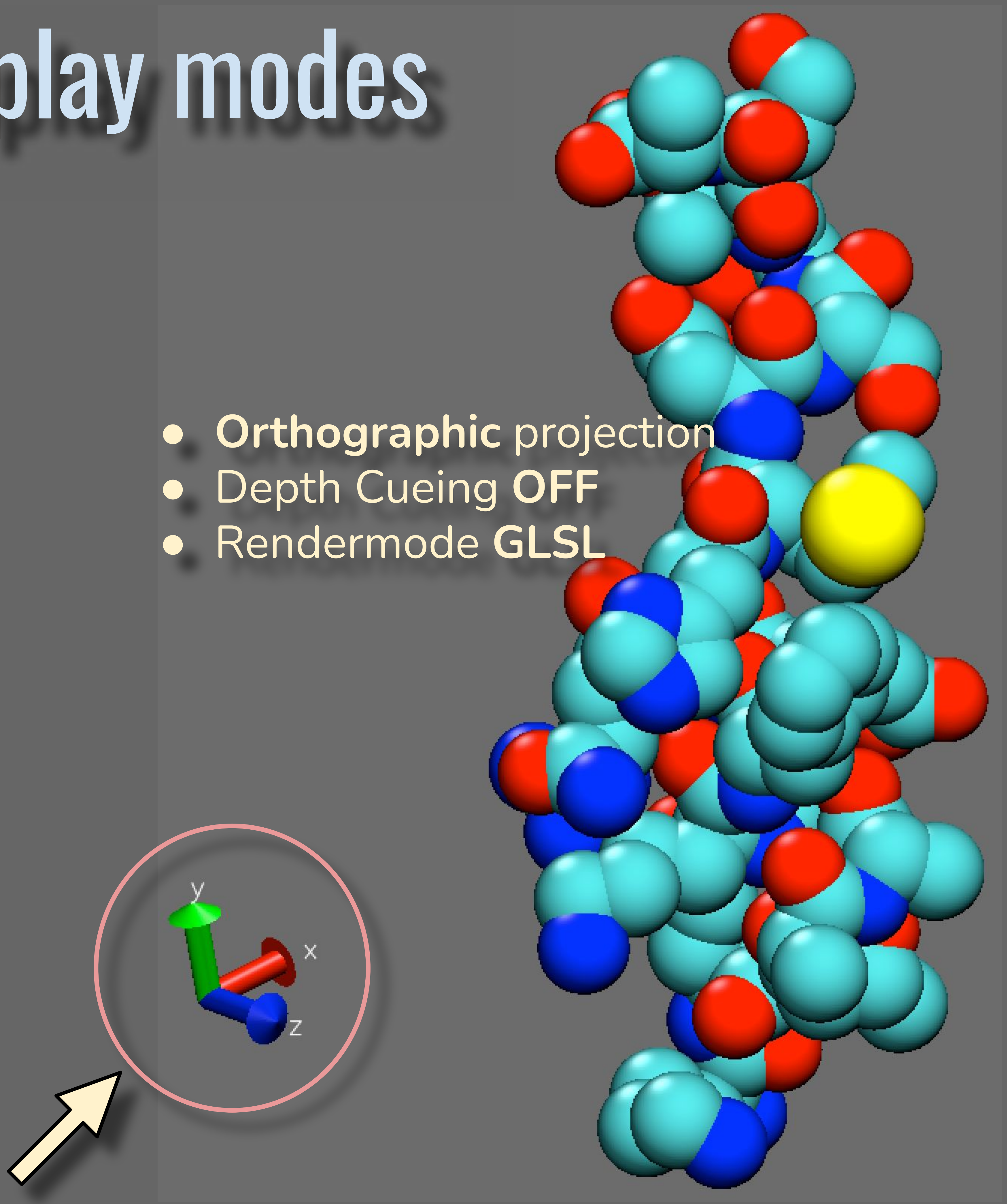
Rendermode GLSL: Hardware accelerated mode.

- Faster;
- Better looking;
- Needs a GPU video card.
- Much better for transparent materials.

Display modes



- **Perspective** projection
- Depth Cueing **ON**
- Rendermode **Normal**



- **Orthographic** projection
- Depth Cueing **OFF**
- Rendermode **GLSL**

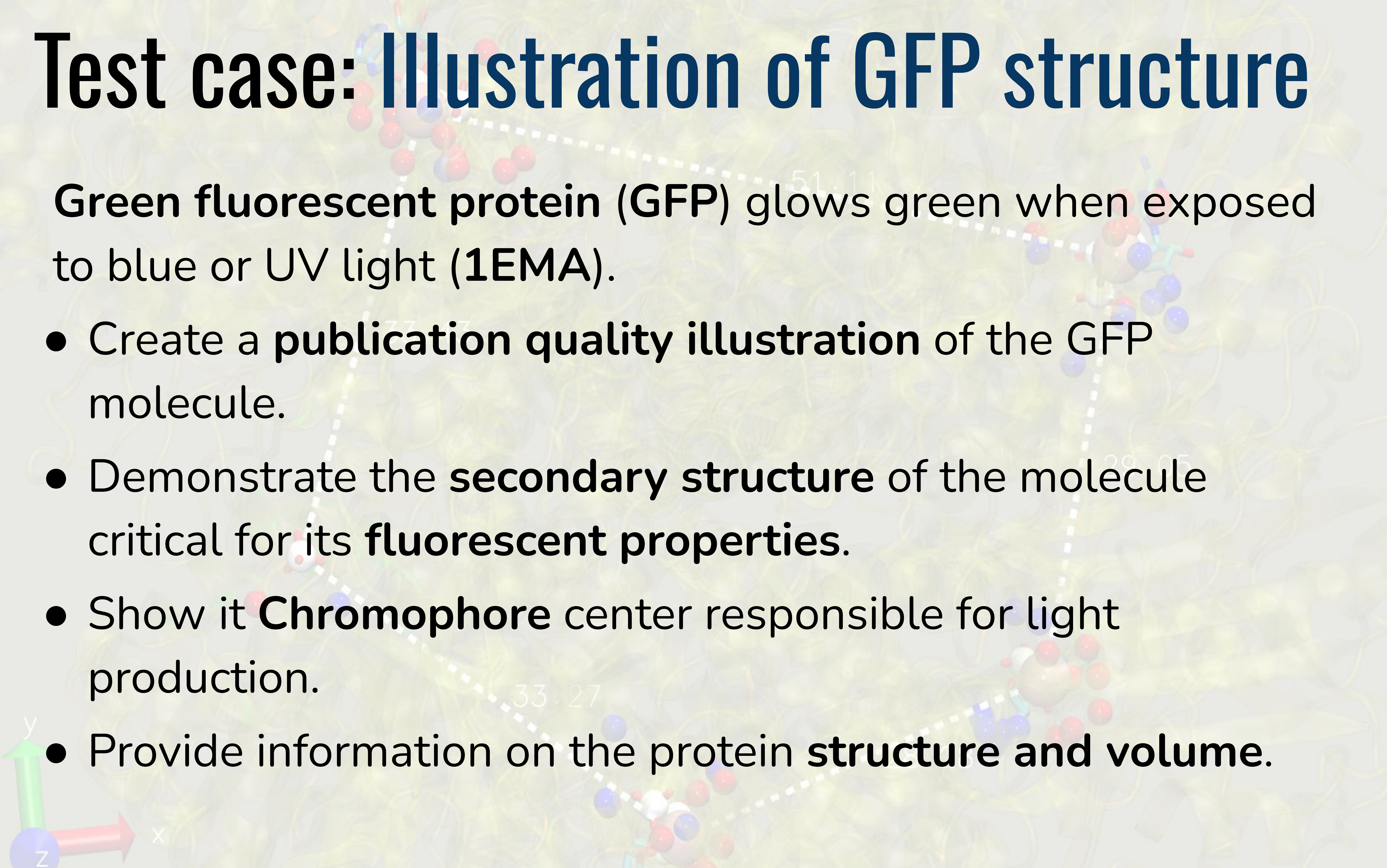
Same point of view, but axes look very different.

VMD image workflow

- Start with a **Molecule** – molecular data from the input file.
- Create **Graphical Representations** of the molecule.
- **Representations** are defined by:
  - **Selection** of the atoms – logical expression.
  - **Drawing method** – determines the way atoms are shown.
  - **Material** – determines the appearance of the drawing.
- **Combination** of the visual output of all these **Graphical Representations** forms the **final result**.

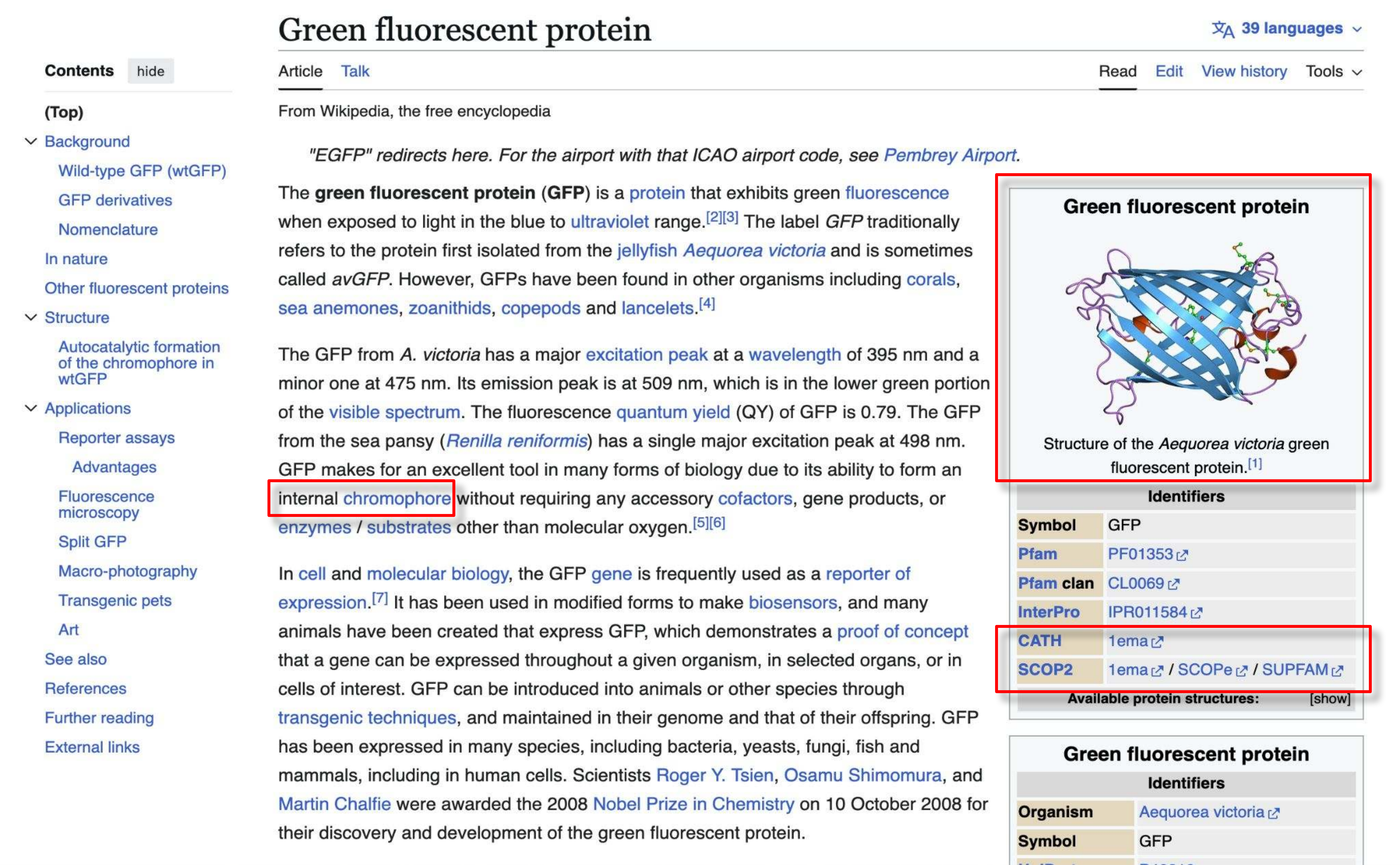
- **Multiple molecules** can be used in one scene, if needed.

Test case: Illustration of GFP structure



Green fluorescent protein (**GFP**) glows green when exposed to blue or UV light (**1EMA**).

- Create a **publication quality illustration** of the GFP molecule.
- Demonstrate the **secondary structure** of the molecule critical for its **fluorescent properties**.
- Show it **Chromophore** center responsible for light production.
- Provide information on the protein **structure and volume**.



Green fluorescent protein

From Wikipedia, the free encyclopedia

"EGFP" redirects here. For the airport with that ICAO airport code, see Pembrey Airport.

The **green fluorescent protein** (**GFP**) is a protein that exhibits green fluorescence when exposed to light in the blue to ultraviolet range.[2][3] The label *GFP* traditionally refers to the protein first isolated from the jellyfish *Aequorea victoria* and is sometimes called *avGFP*. However, GFPs have been found in other organisms including corals, sea anemones, zoanithids, copepods and lancelets.[4]

The GFP from *A. victoria* has a major excitation peak at a wavelength of 395 nm and a minor one at 475 nm. Its emission peak is at 509 nm, which is in the lower green portion of the visible spectrum. The fluorescence quantum yield (QY) of GFP is 0.79. The GFP from the sea pansy (*Renilla reniformis*) has a single major excitation peak at 498 nm. GFP makes for an excellent tool in many forms of biology due to its ability to form an internal chromophore without requiring any accessory cofactors, gene products, or enzymes / substrates other than molecular oxygen.[5][6]

In cell and molecular biology, the GFP gene is frequently used as a reporter of expression.[7] It has been used in modified forms to make biosensors, and many animals have been created that express GFP, which demonstrates a proof of concept that a gene can be expressed throughout a given organism, in selected organs, or in cells of interest. GFP can be introduced into animals or other species through transgenic techniques, and maintained in their genome and that of their offspring. GFP has been expressed in many species, including bacteria, yeasts, fungi, fish and mammals, including in human cells. Scientists Roger Y. Tsien, Osamu Shimomura, and Martin Chalfie were awarded the 2008 Nobel Prize in Chemistry on 10 October 2008 for their discovery and development of the green fluorescent protein.

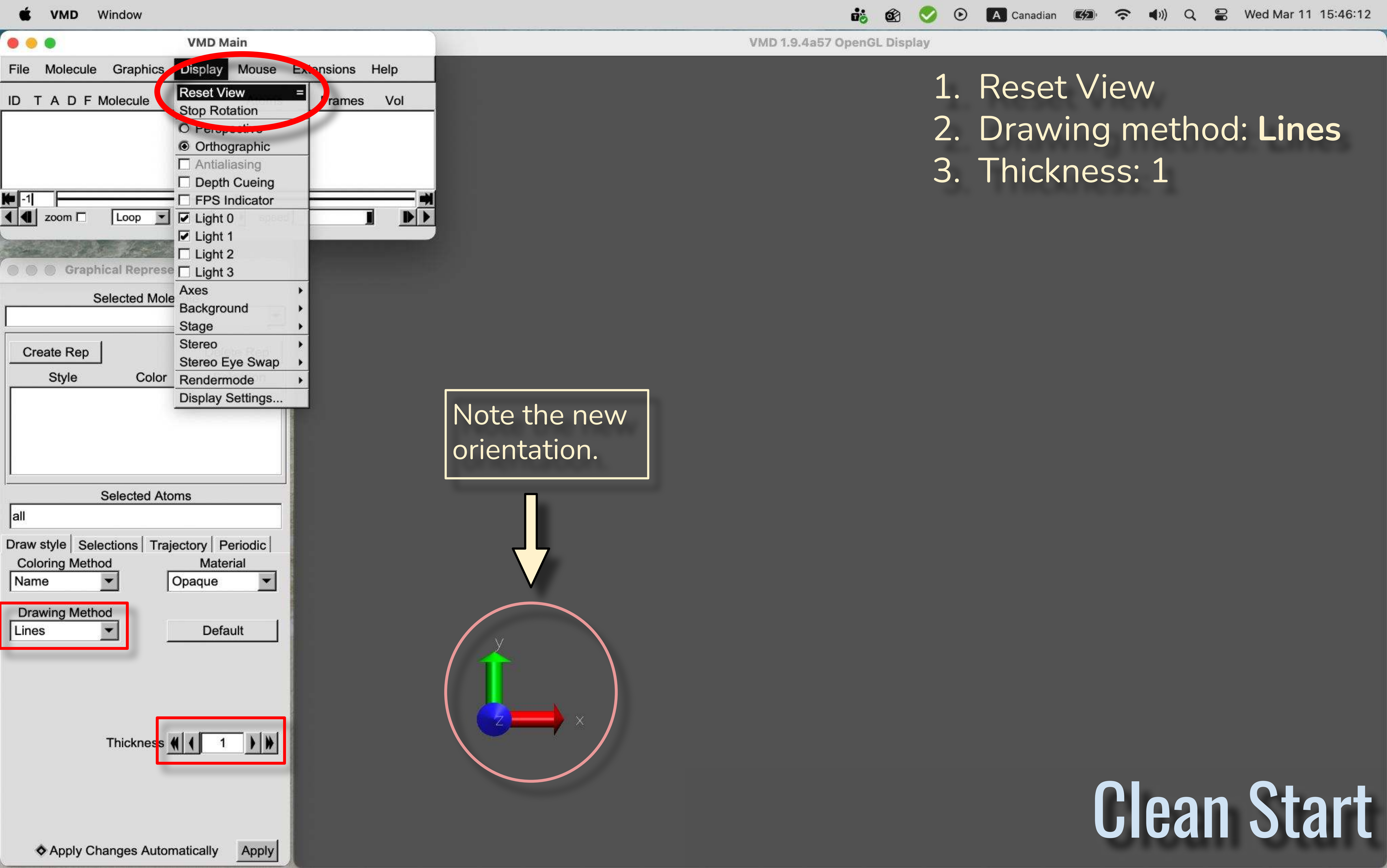
Green fluorescent protein

Structure of the *Aequorea victoria* green fluorescent protein.[1]

Identifiers	
Symbol	GFP
Pfam	PF01353
Pfam clan	CL0069
InterPro	IPR011584
CATH	1ema
SCOP2	1ema / SCOPe / SUPFAM
Available protein structures:	[show]

Green fluorescent protein

Identifiers	
Organism	Aequorea victoria
Symbol	GFP



Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

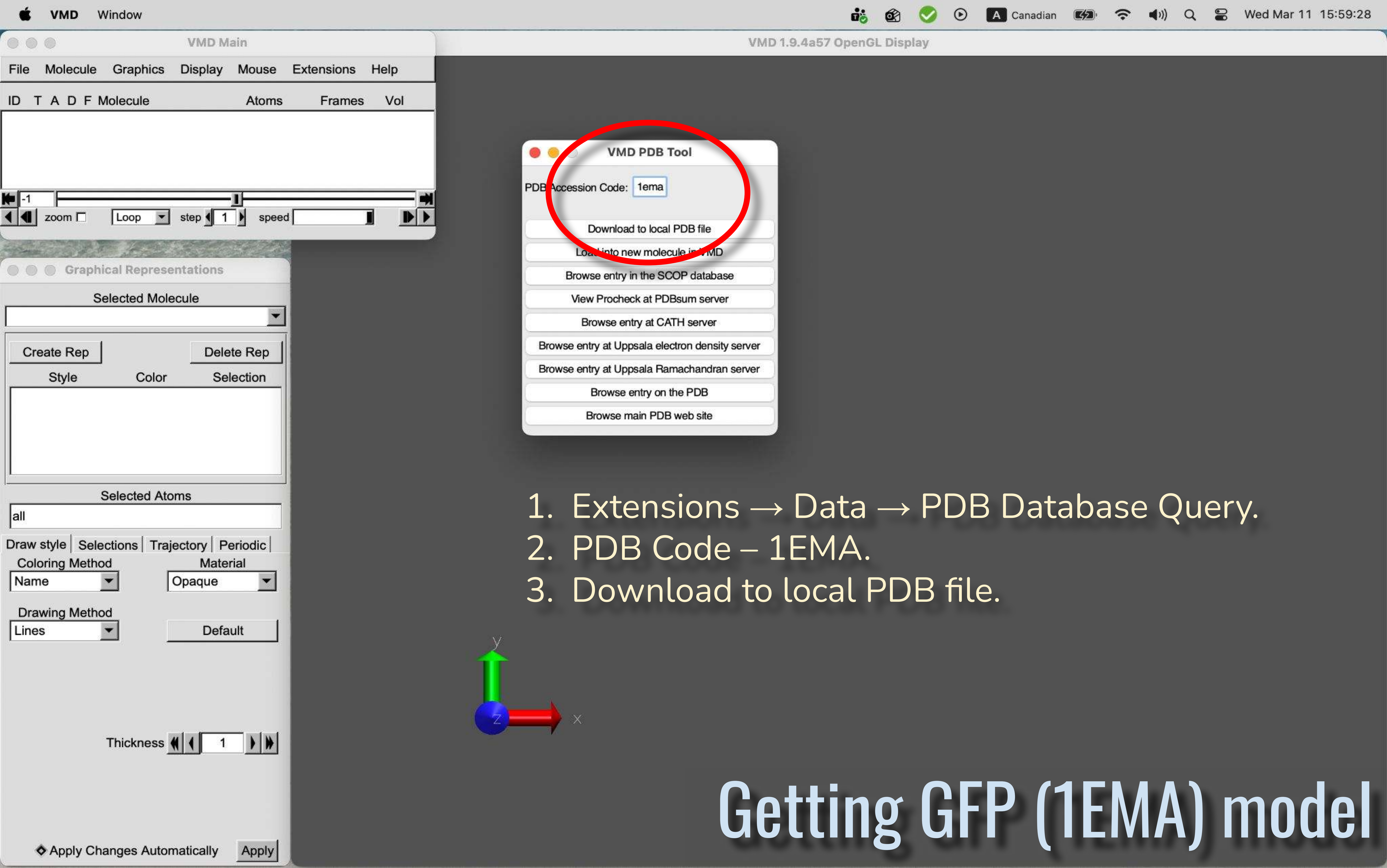
Thickness: 1

1. Reset View
2. Drawing method: **Lines**
3. Thickness: 1

Note the new orientation.

Clean Start

Getting GFP (1EMA) model



PDB Accession Code: 1ema

Selected Atoms: all

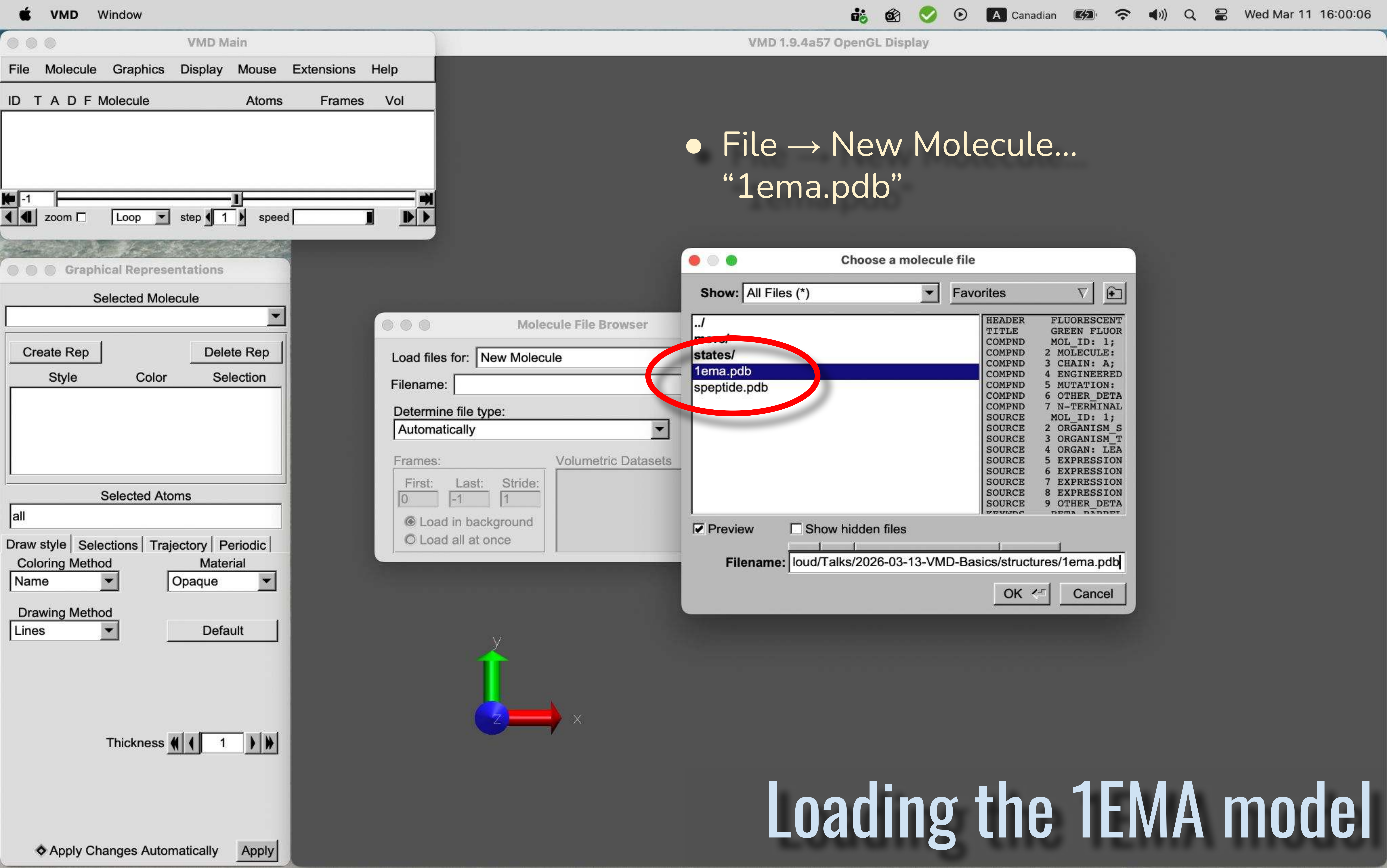
Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness: 1

1. Extensions → Data → PDB Database Query.
2. PDB Code – 1EMA.
3. Download to local PDB file.



- File → New Molecule… "1ema.pdb"

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness: 1

Load files for: New Molecule

Determine file type: Automatically

First: 0 Last: -1 Stride: 1

◉ Load in background
○ Load all at once

Show: All Files (*)

```
../
more/
states/
1ema.pdb
speptide.pdb
```

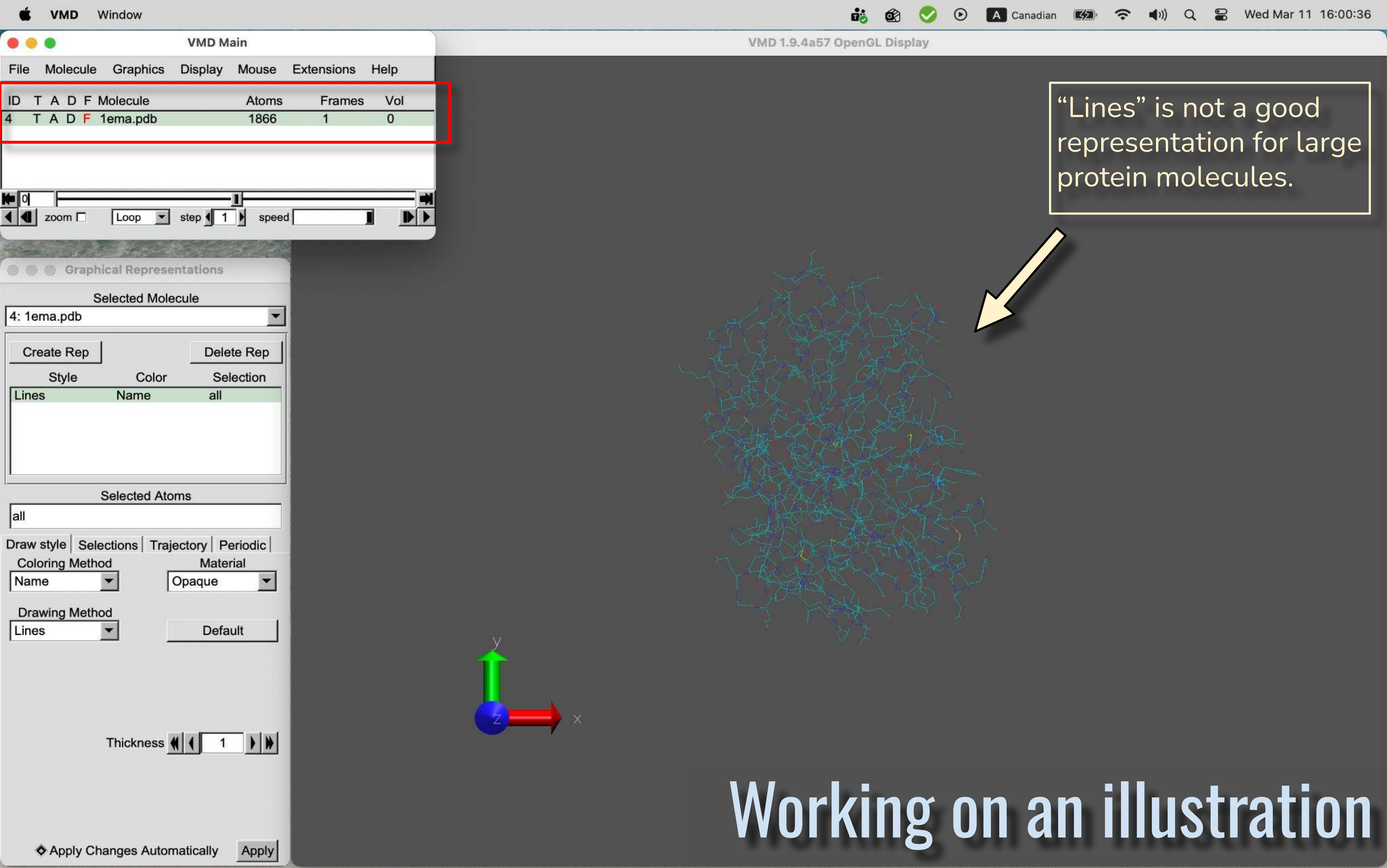
```
HEADER    FLUORESCENT
TITLE     GREEN FLUOR
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE:
COMPND   3 CHAIN: A;
COMPND   4 ENGINEERED
COMPND   5 MUTATION:
COMPND   6 OTHER_DETA
COMPND   7 N-TERMINAL
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_S
SOURCE   3 ORGANISM_T
SOURCE   4 ORGAN: LEA
SOURCE   5 EXPRESSION
SOURCE   6 EXPRESSION
SOURCE   7 EXPRESSION
SOURCE   8 EXPRESSION
SOURCE   9 OTHER_DETA
```

☑ Preview ☐ Show hidden files

Filename: loud/Talks/2026-03-13-VMD-Basics/structures/1ema.pdb

Loading the 1EMA model

Working on an illustration



“Lines” is not a good representation for large protein molecules.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
4	T	A	D	F	1ema.pdb	1866	1	0

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

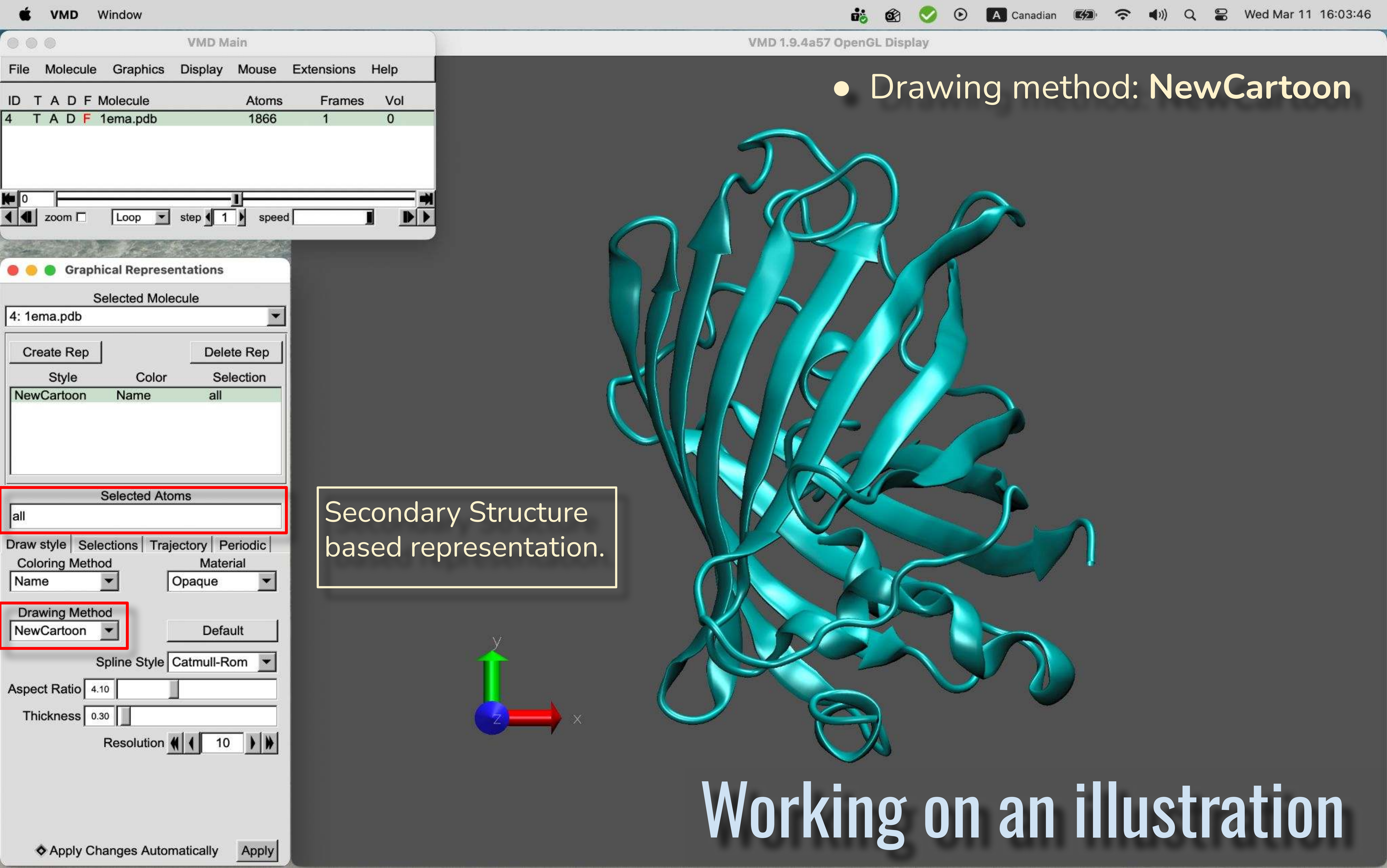
Drawing Method: Lines

Thickness: 1

Working on an illustration

- Drawing method: **NewCartoon**

Secondary Structure based representation.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
4	T	A	D	F	1ema.pdb	1866	1	0

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: NewCartoon

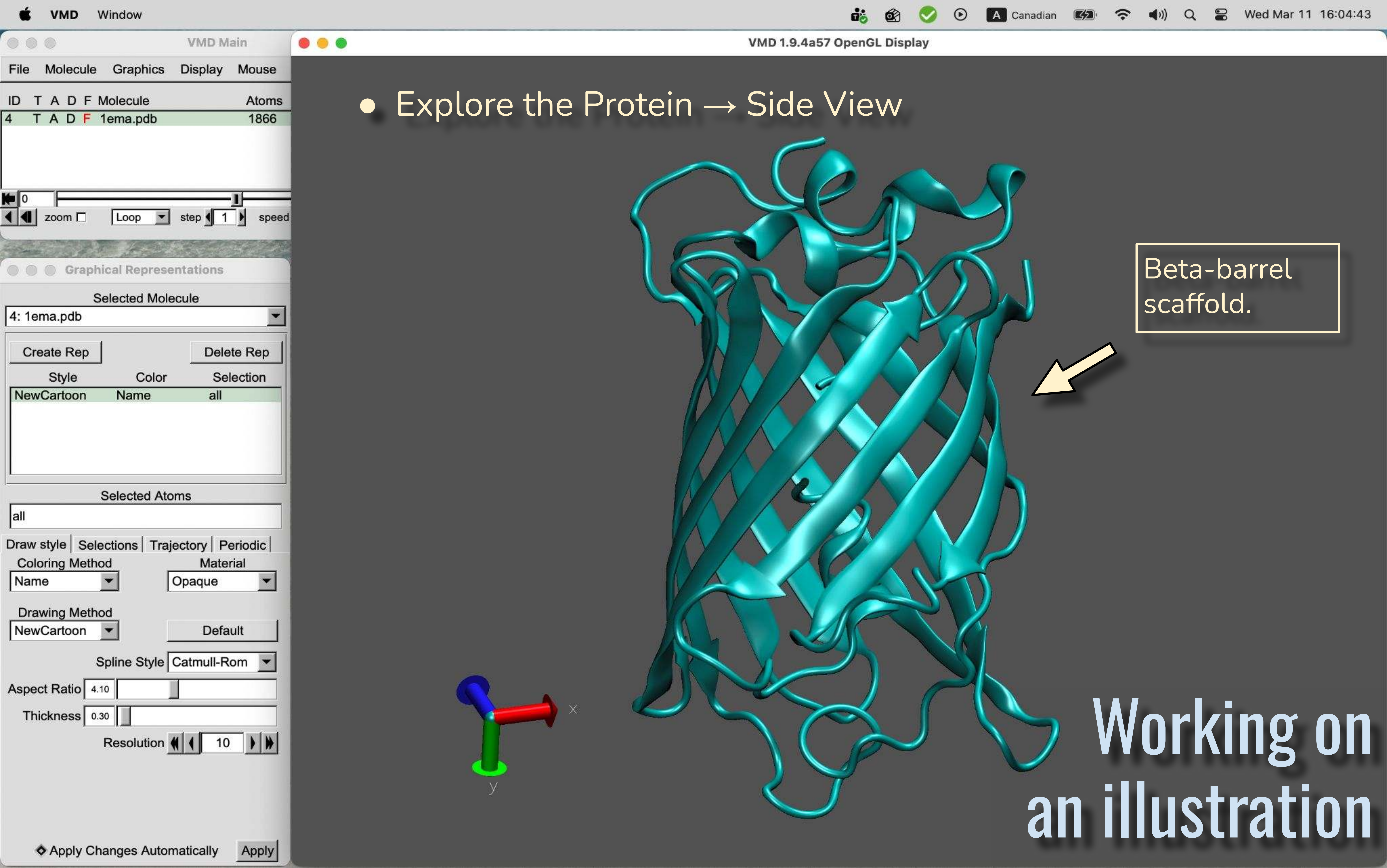
Spline Style: Catmull-Rom

Aspect Ratio: 4.10

Thickness: 0.30

Resolution: 10

- Explore the Protein → Side View



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all

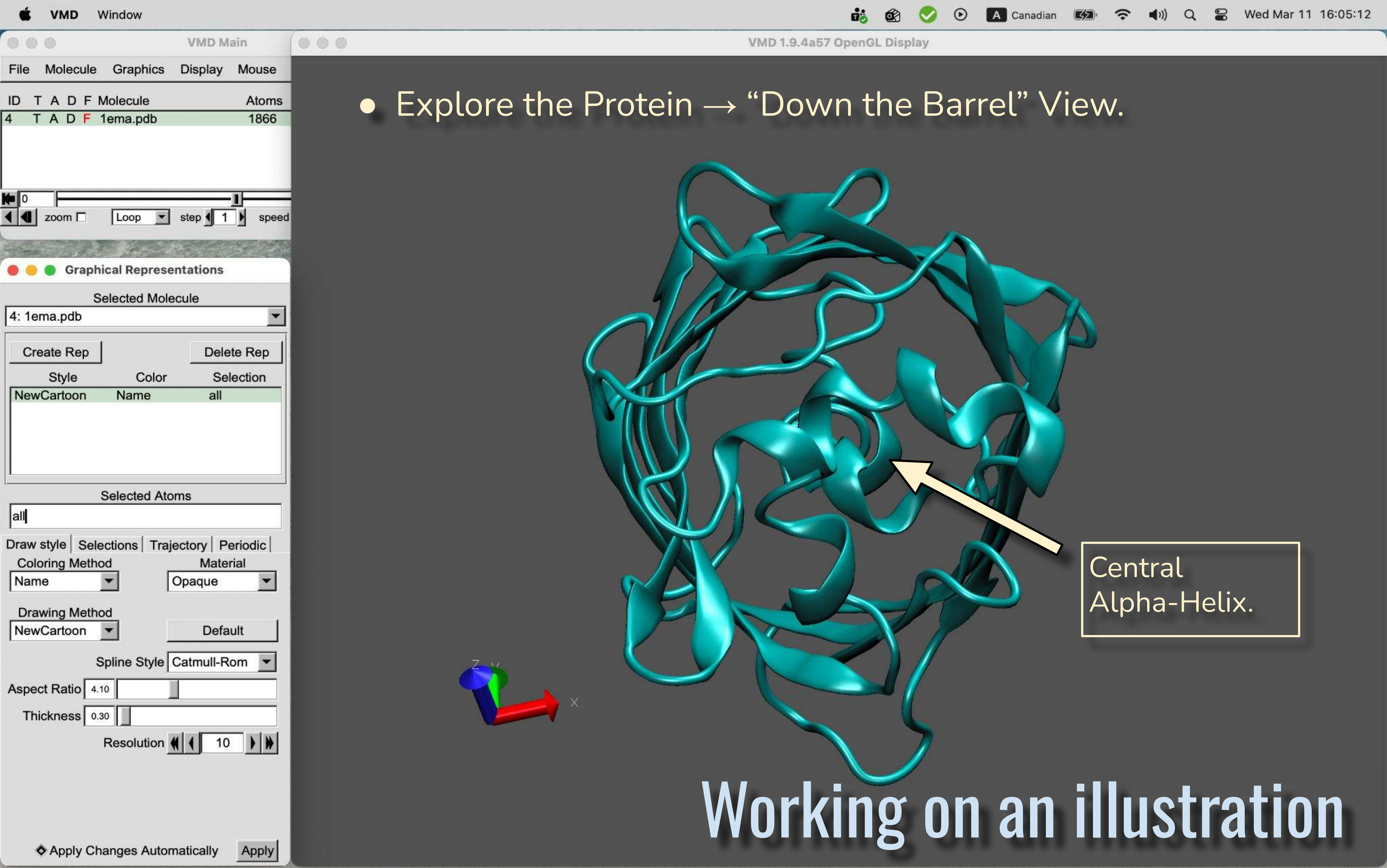
Selected Atoms: all

Coloring Method: Name
Material: Opaque
Drawing Method: NewCartoon
Spline Style: Catmull-Rom
Aspect Ratio: 4.10
Thickness: 0.30
Resolution: 10

Beta-barrel scaffold.

Working on an illustration

- Explore the Protein → “Down the Barrel” View.



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all

Selected Atoms: all

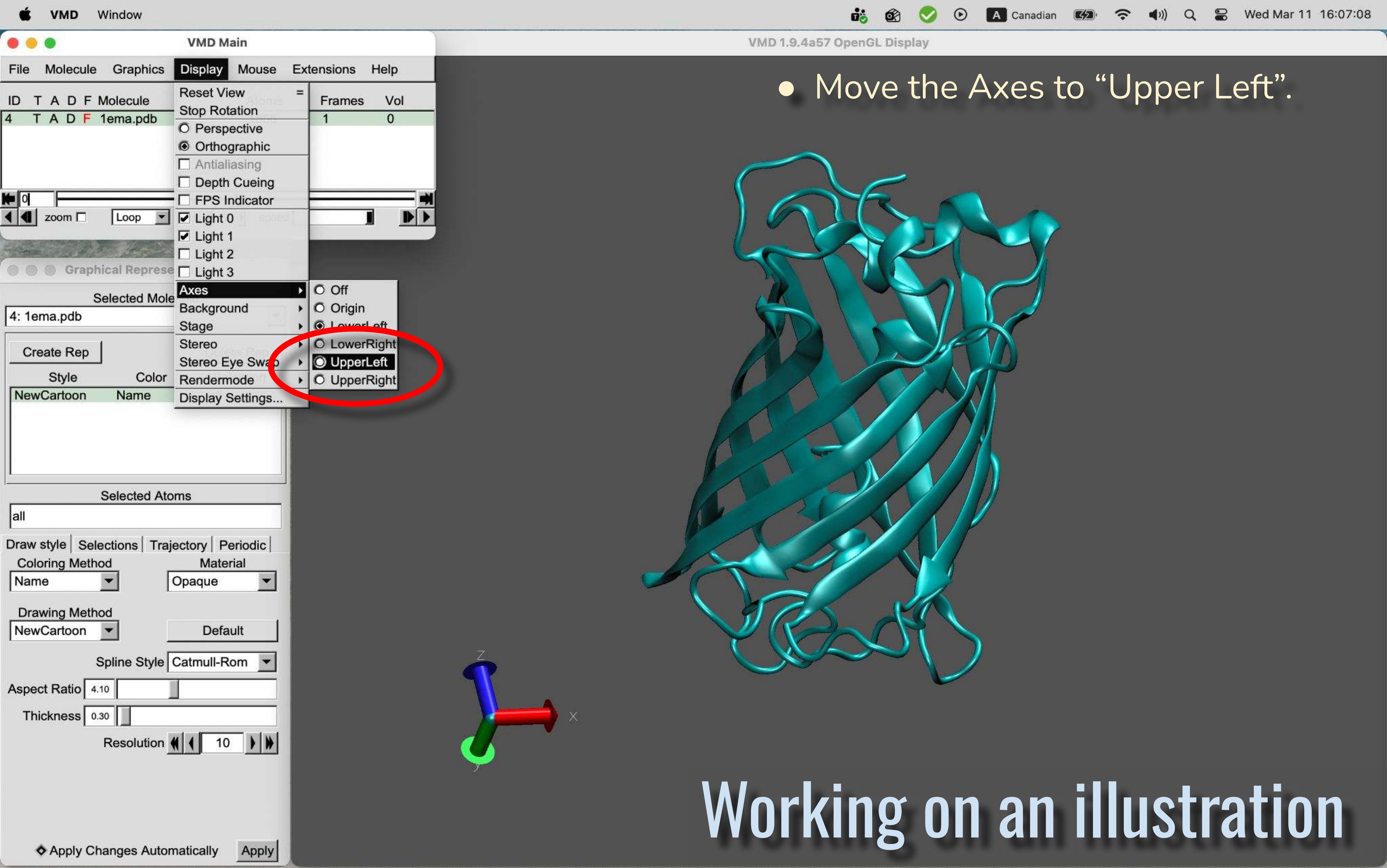
Coloring Method: Name
Material: Opaque
Drawing Method: NewCartoon
Spline Style: Catmull-Rom
Aspect Ratio: 4.10
Thickness: 0.30
Resolution: 10

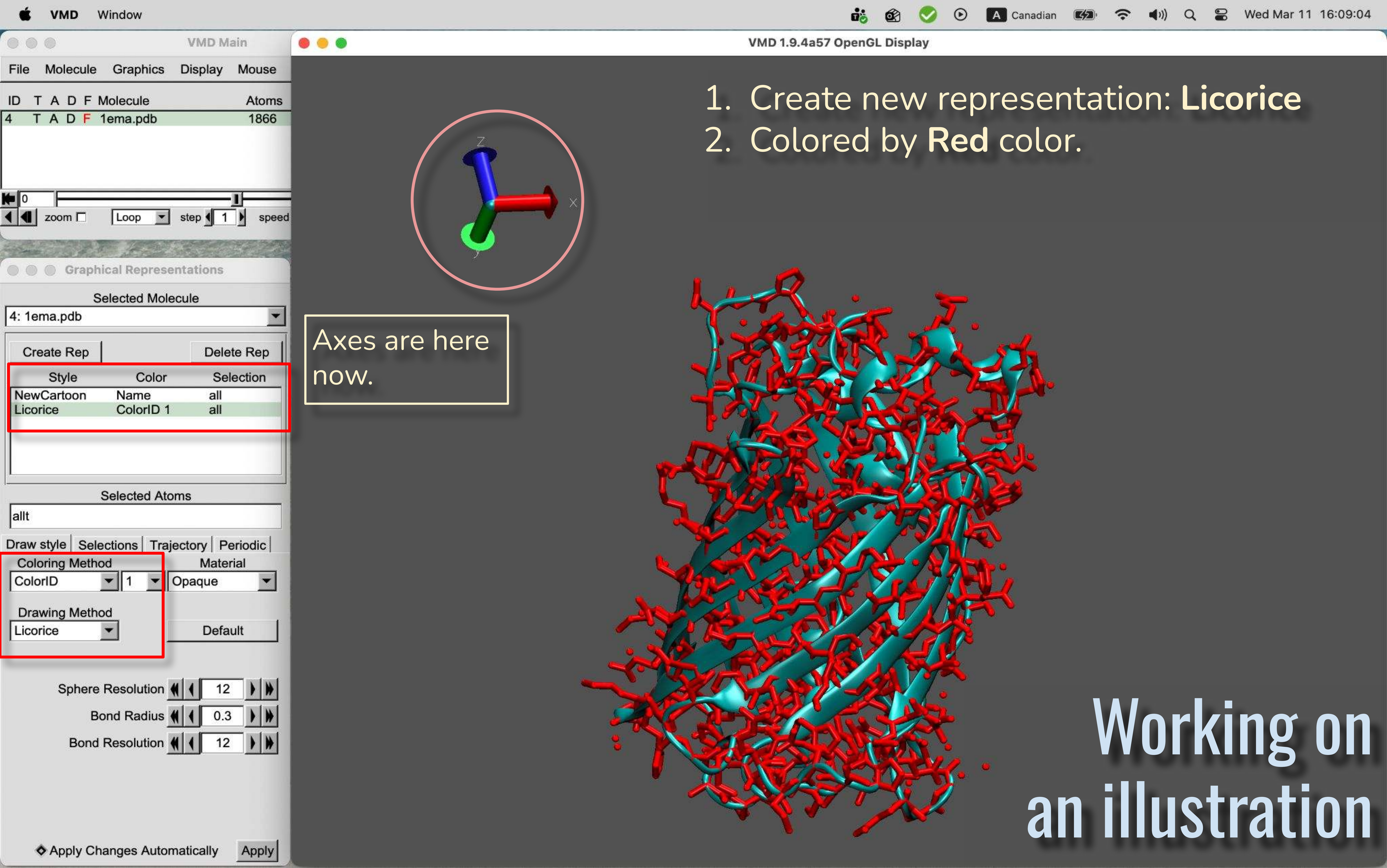
Central Alpha-Helix.

Working on an illustration

Working on an illustration

- Move the Axes to “Upper Left”.





1. Create new representation: **Licorice**
2. Colored by **Red** color.

Axes are here now.

ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	all

Selected Atoms: allt

Coloring Method: ColorID 1

Material: Opaque

Drawing Method: Licorice

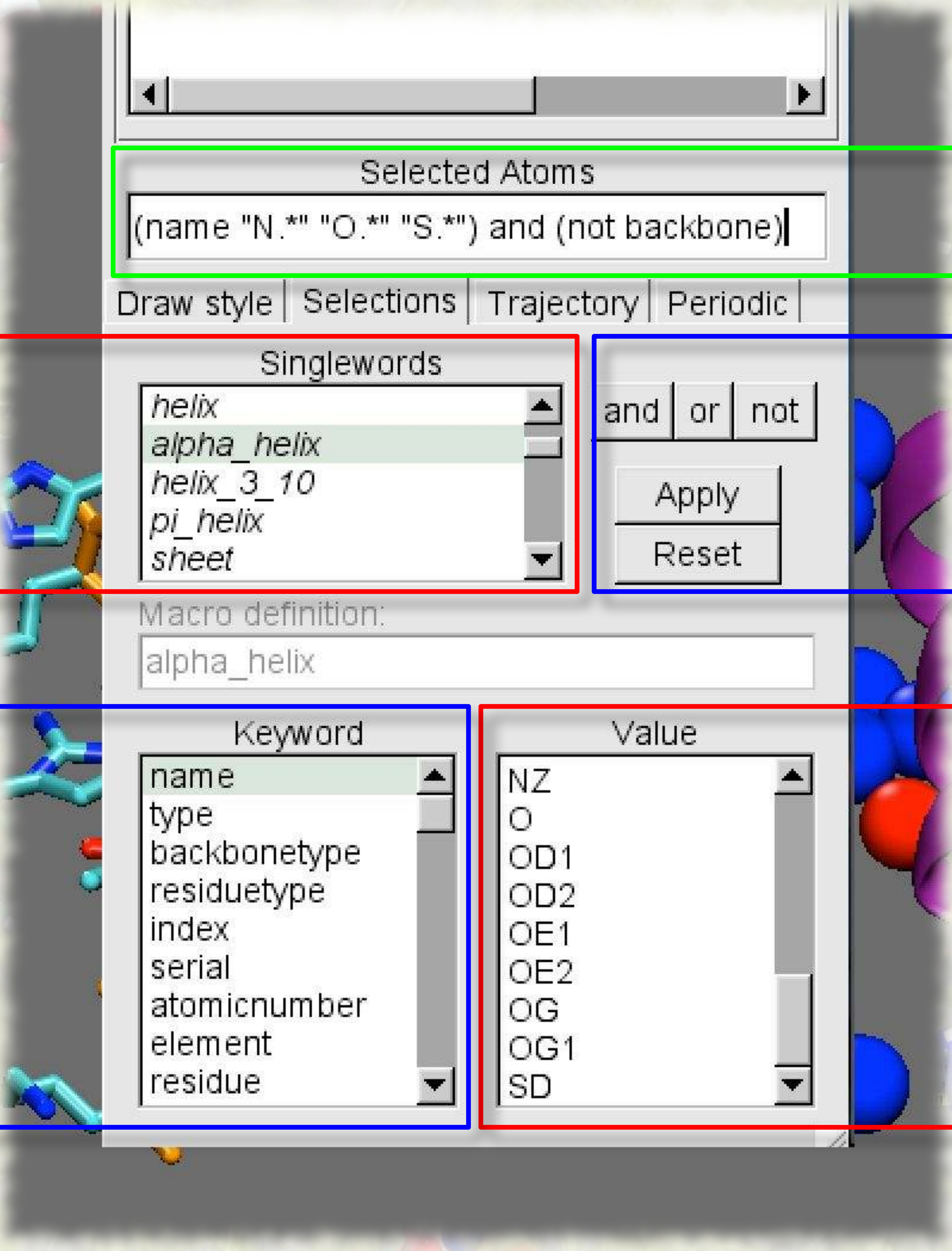
Sphere Resolution 12

Bond Radius 0.3

Bond Resolution 12

Working on an illustration

Selections Tab



Selected Atoms: (name "N.*" "O.*" "S.*") and (not backbone)

Macro definition: alpha_helix

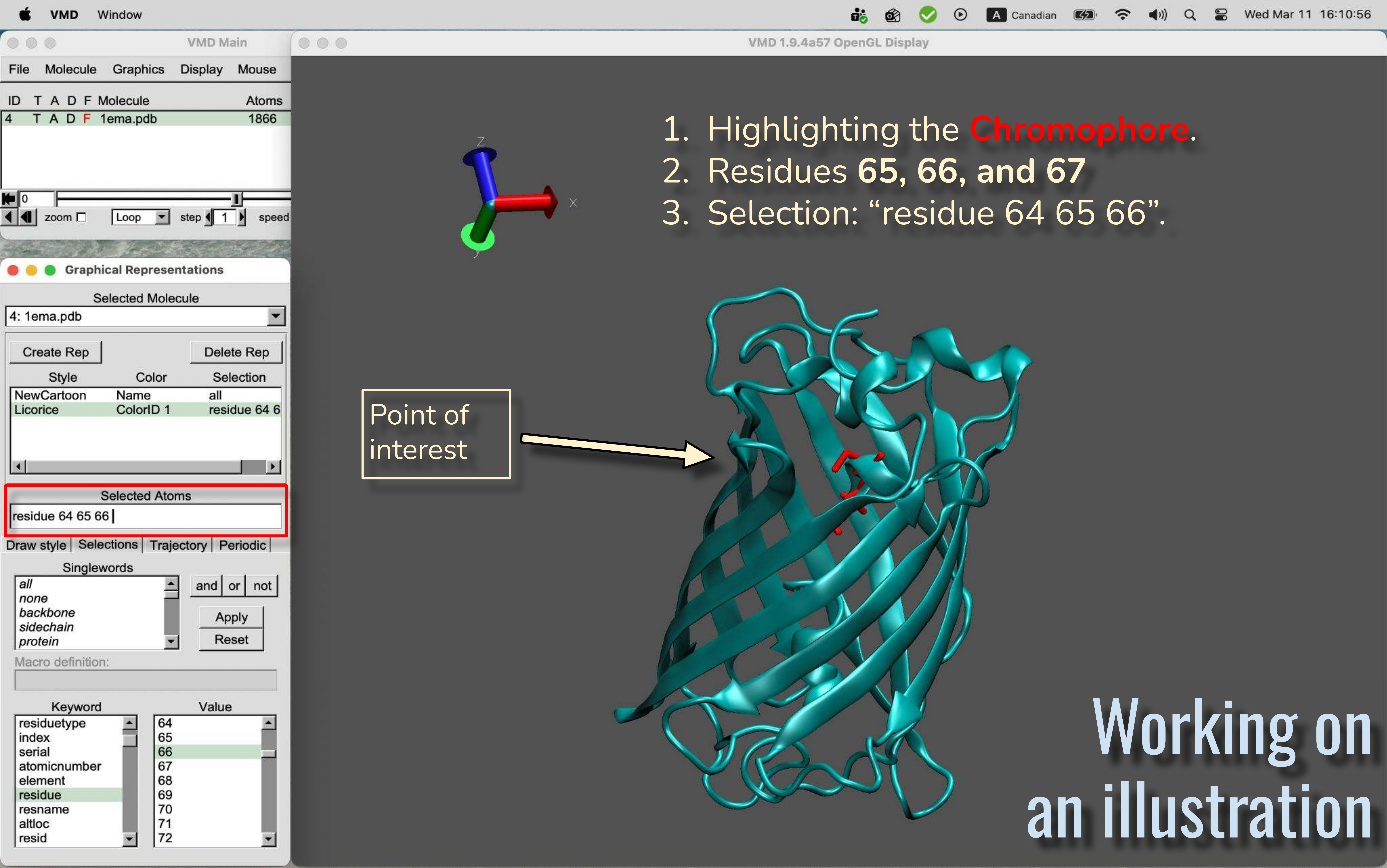
Current selection

Single word **predefined** selections

Input buttons

List of data fields, **keywords**

List of **values** for a selected **keyword**



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	residue 64 6

Selected Atoms: residue 64 65 66

Singlewords: all, none, backbone, sidechain, protein

Macro definition:

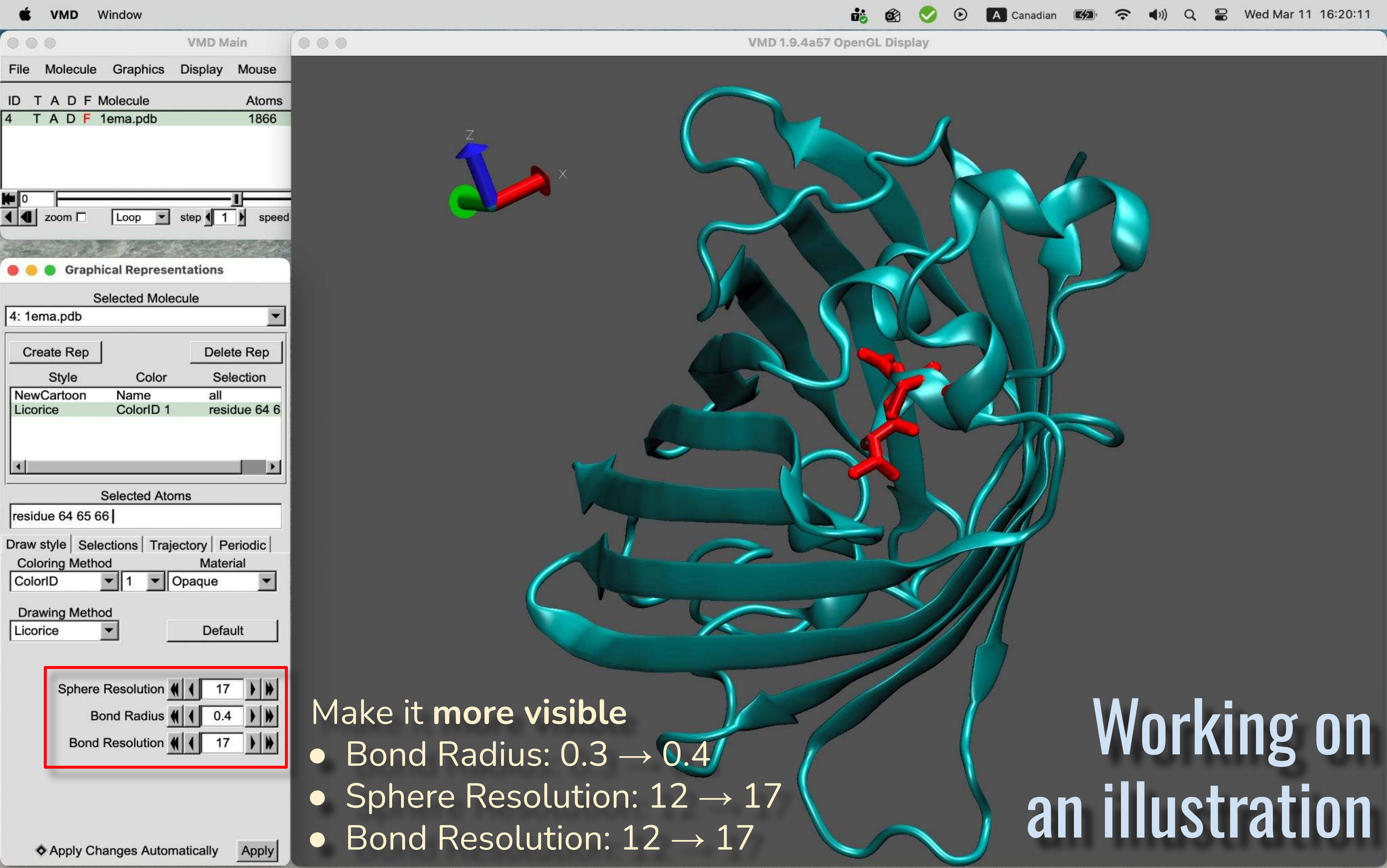
Keyword	Value
residuetype	64
index	65
serial	66
atomicnumber	67
element	68
residue	69
resname	70
altloc	71
resid	72

1. Highlighting the Chromophore.
2. Residues **65, 66, and 67**
3. Selection: “residue 64 65 66”.

Point of interest

Working on an illustration

Working on an illustration



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	residue 64 6

Selected Atoms: residue 64 65 66

Coloring Method: ColorID 1

Material: Opaque

Drawing Method: Licorice

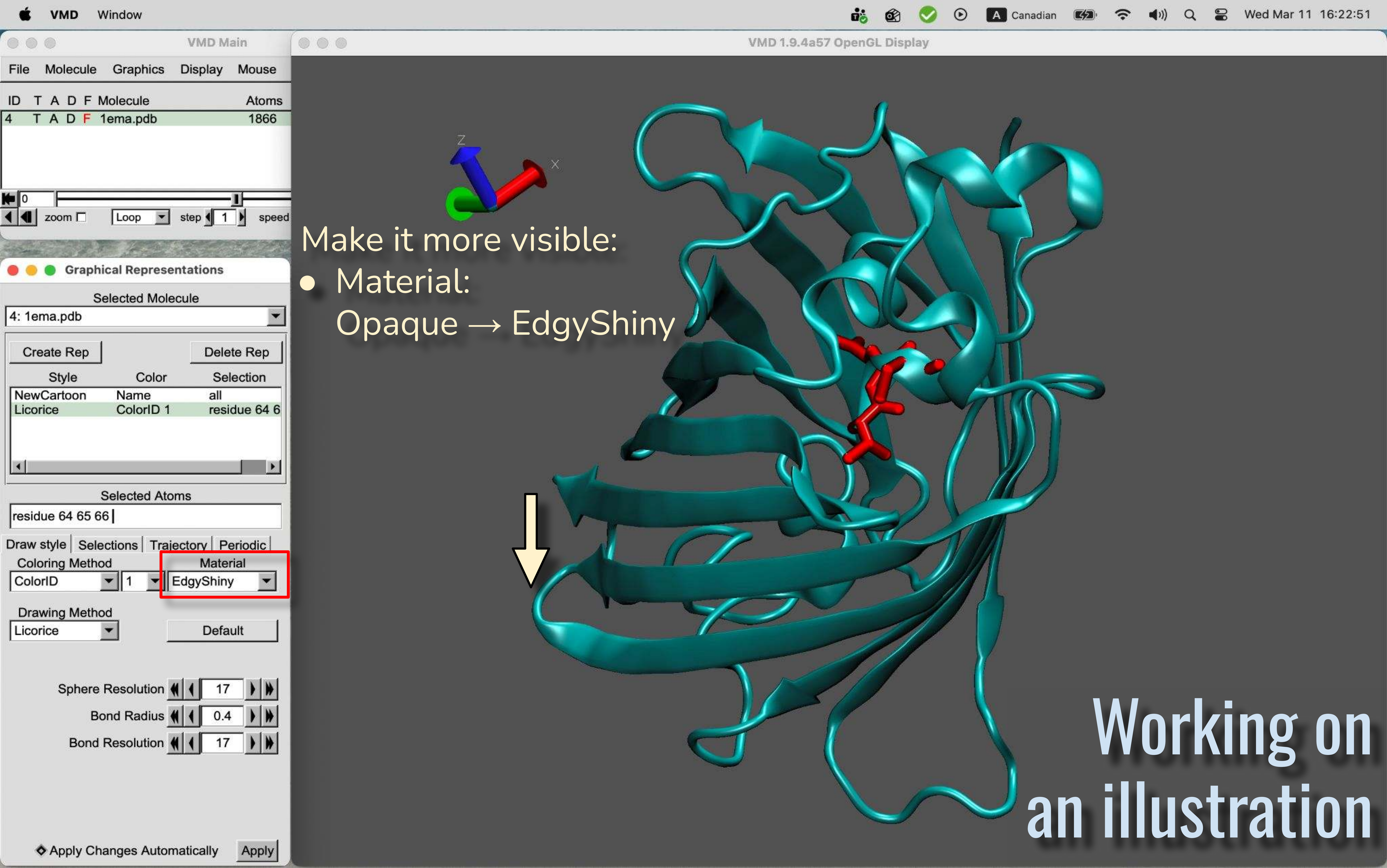
Sphere Resolution: 17

Bond Radius: 0.4

Bond Resolution: 17

Make it **more visible**

- Bond Radius: 0.3 → 0.4
- Sphere Resolution: 12 → 17
- Bond Resolution: 12 → 17



Working on an illustration

Make it more visible:

- Material: Opaque → EdgyShiny

ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	residue 64 6

Selected Atoms: residue 64 65 66

Coloring Method: ColorID 1

Material: EdgyShiny

Drawing Method: Licorice

Sphere Resolution: 17

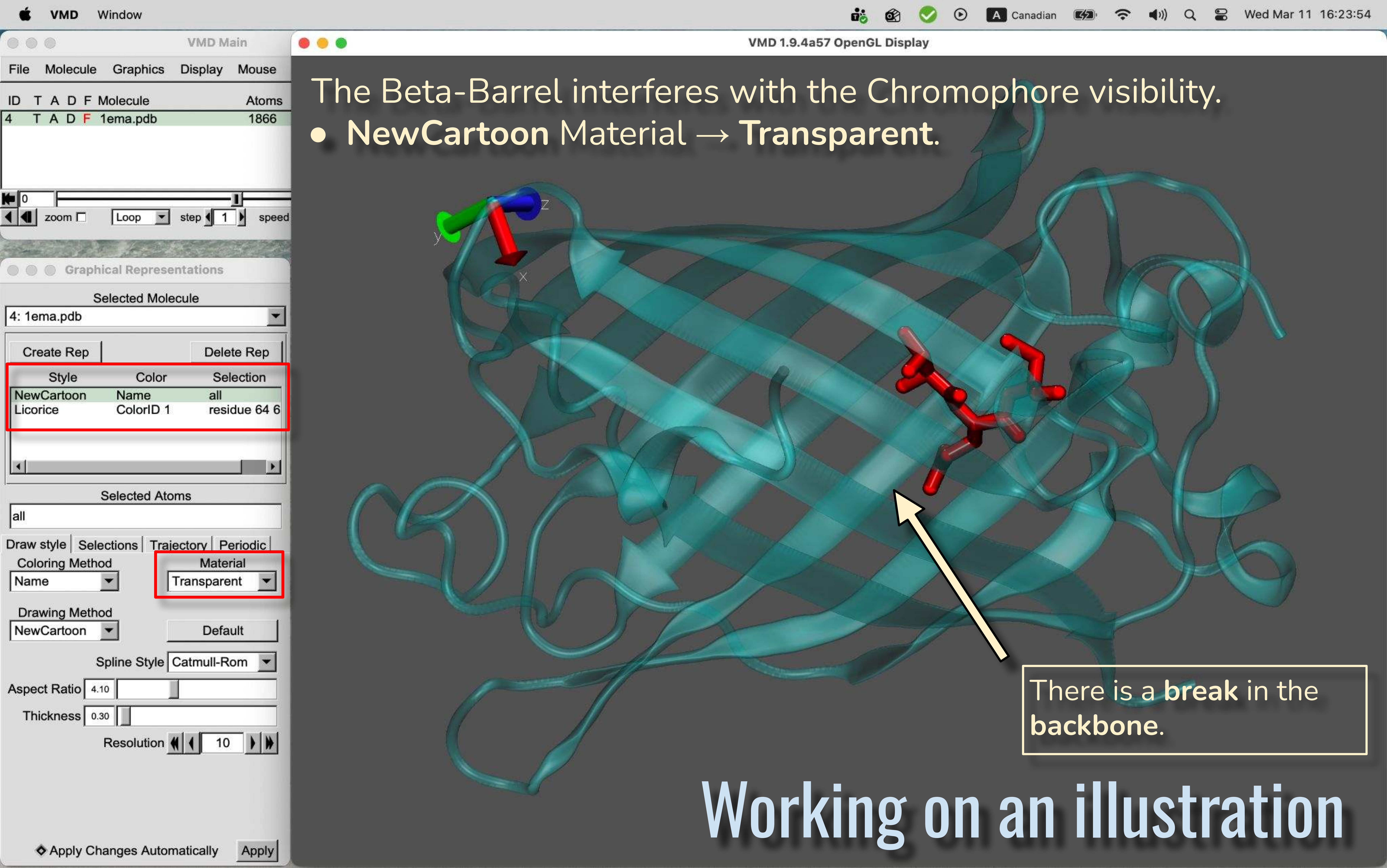
Bond Radius: 0.4

Bond Resolution: 17

Working on an illustration

The Beta-Barrel interferes with the Chromophore visibility.

- **NewCartoon** Material → **Transparent**.



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	residue 64 6

Selected Atoms: all

Coloring Method: Name

Material: Transparent

Drawing Method: NewCartoon

Spline Style: Catmull-Rom

Aspect Ratio: 4.10

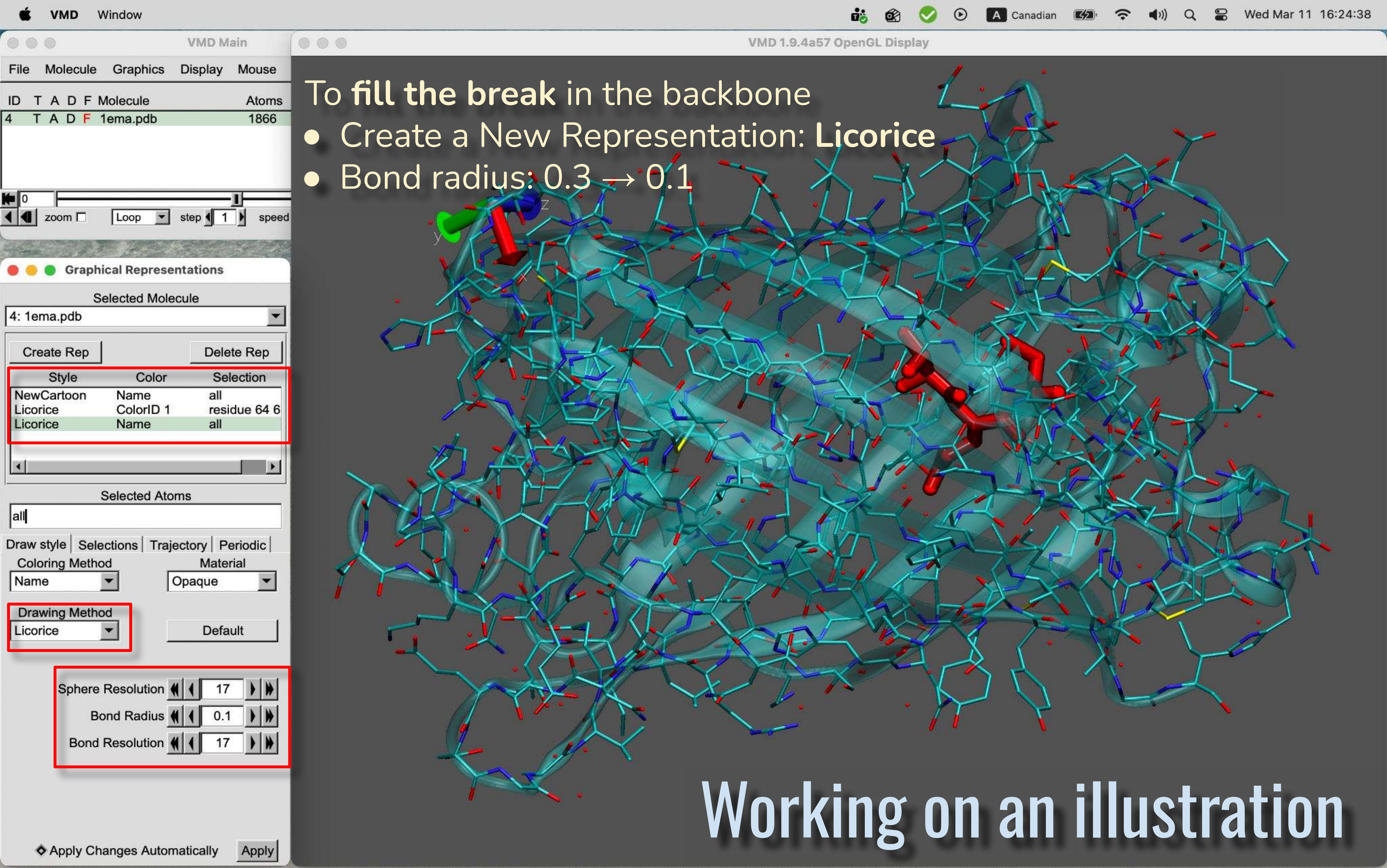
Thickness: 0.30

Resolution: 10

There is a **break** in the **backbone**.

To **fill the break** in the backbone

- Create a New Representation: **Licorice**
- Bond radius: 0.3 → 0.1



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Sphere Resolution: 17

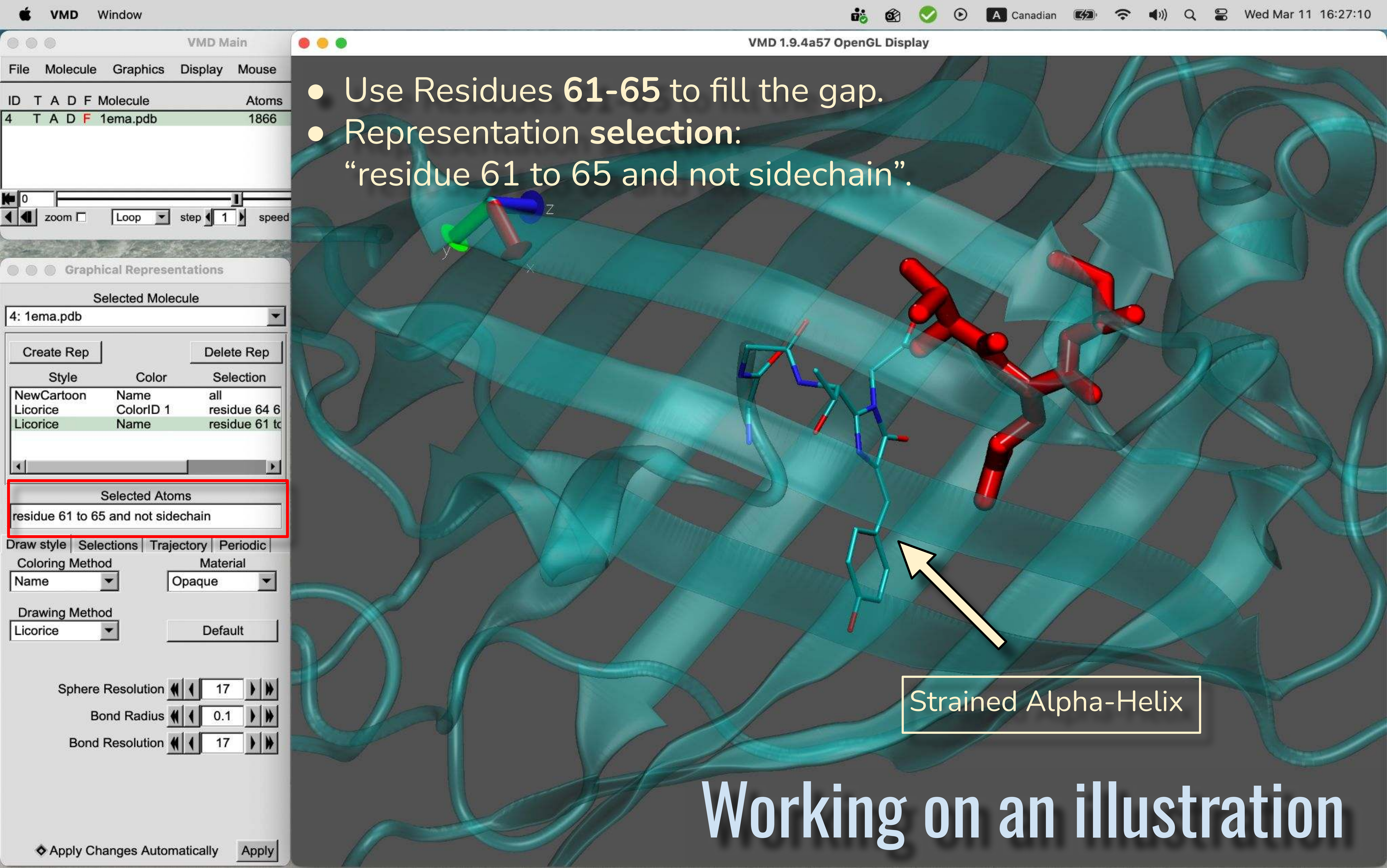
Bond Radius: 0.1

Bond Resolution: 17

Working on an illustration

Working on an illustration

- Use Residues **61-65** to fill the gap.
- Representation **selection**:
  “residue 61 to 65 and not sidechain”.



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Name	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 tc

Selected Atoms: residue 61 to 65 and not sidechain

Coloring Method: Name

Material: Opaque

Drawing Method: Licorice

Sphere Resolution: 17

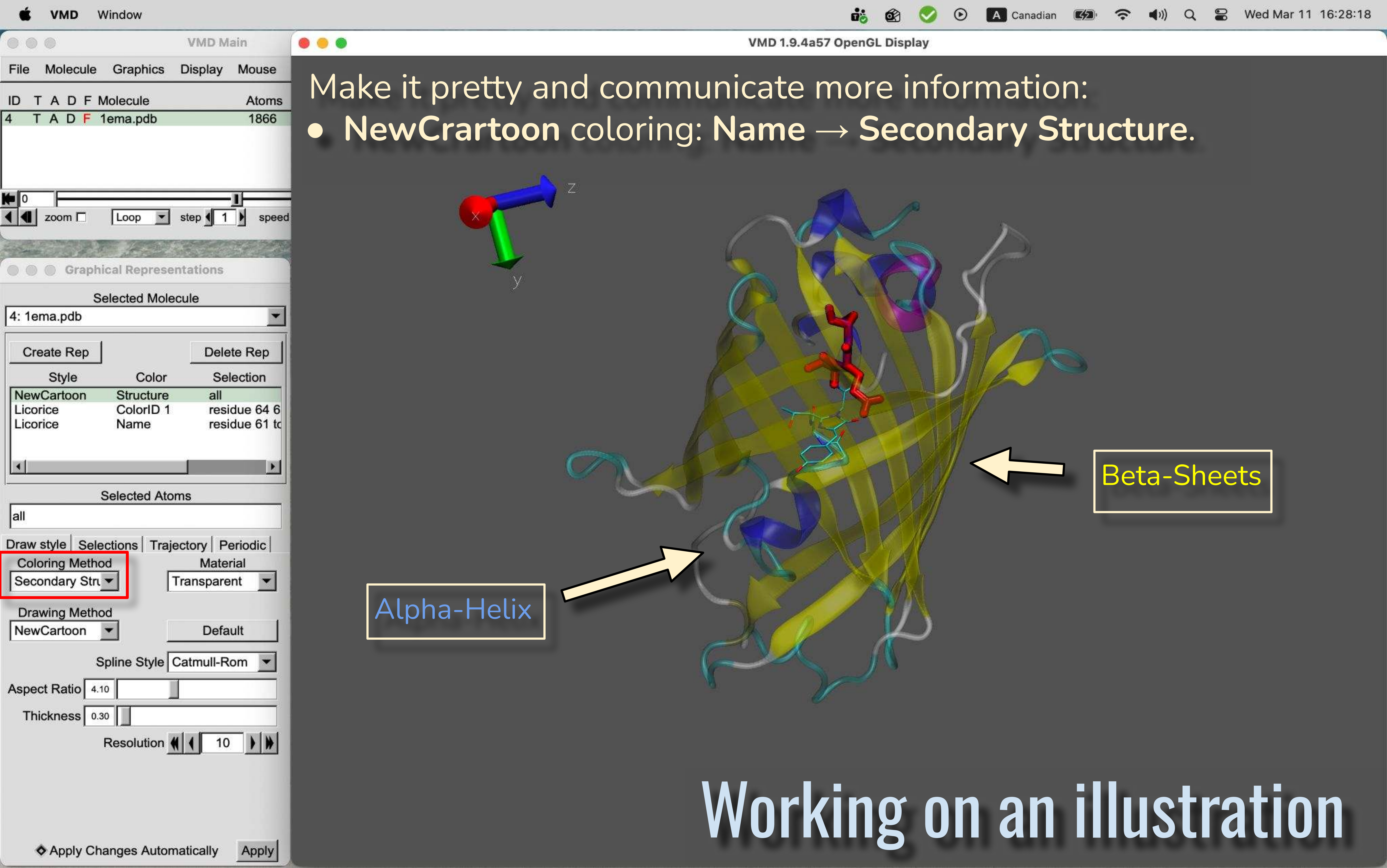
Bond Radius: 0.1

Bond Resolution: 17

Strained Alpha-Helix

Make it pretty and communicate more information:

- **NewCrartoon** coloring: **Name** → **Secondary Structure**.



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Structure	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 tc

Selected Atoms: all

Coloring Method: Secondary Stru

Material: Transparent

Drawing Method: NewCartoon

Spline Style: Catmull-Rom

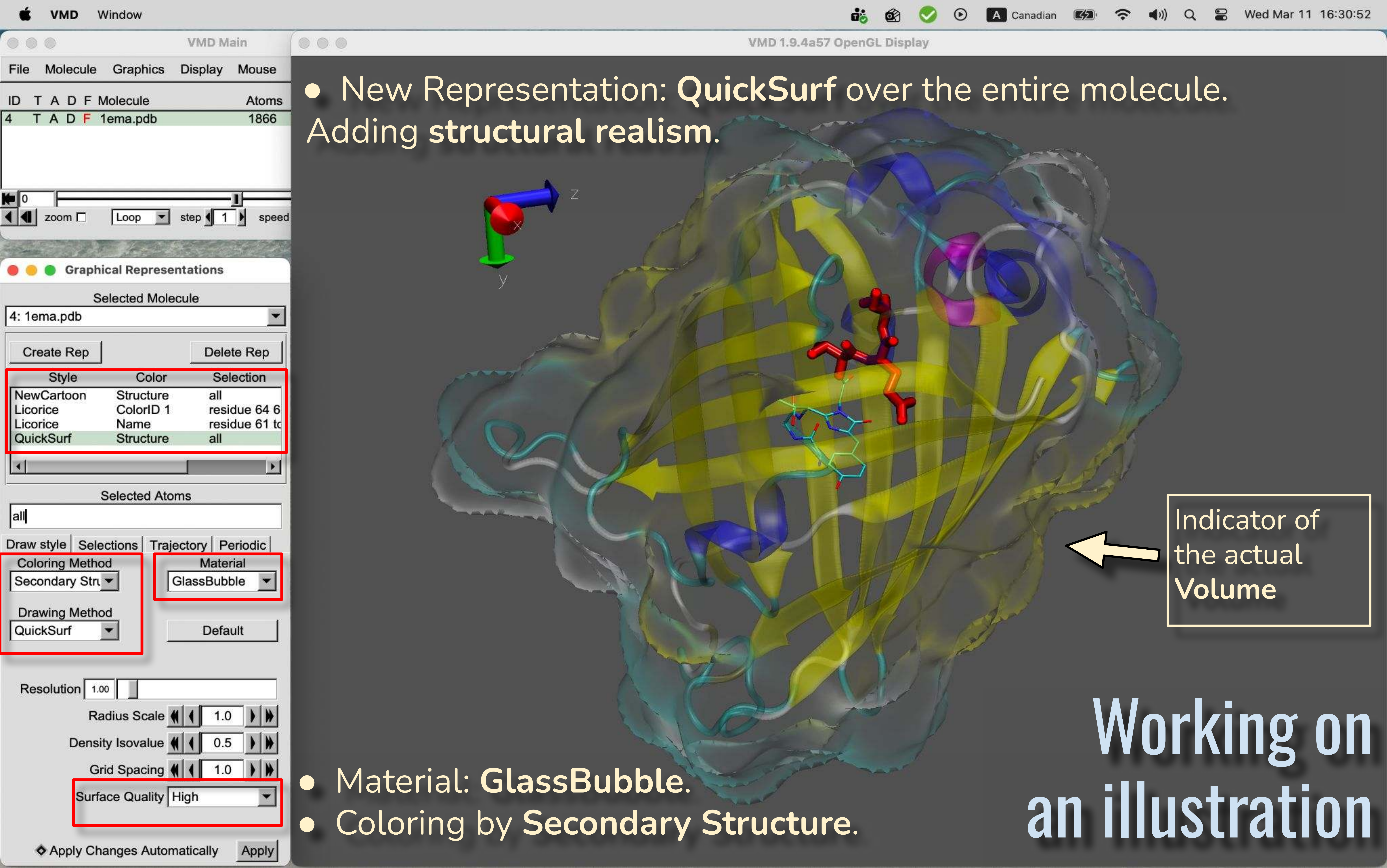
Aspect Ratio: 4.10

Thickness: 0.30

Resolution: 10

◆ Apply Changes Automatically

Working on an illustration



- New Representation: **QuickSurf** over the entire molecule.

Adding **structural realism**.

Indicator of the actual **Volume**

- Material: **GlassBubble**.
- Coloring by **Secondary Structure**.

Working on an illustration

ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Structure	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 tc
QuickSurf	Structure	all

Selected Atoms: all

Coloring Method: Secondary Stru

Material: GlassBubble

Drawing Method: QuickSurf

Resolution: 1.00

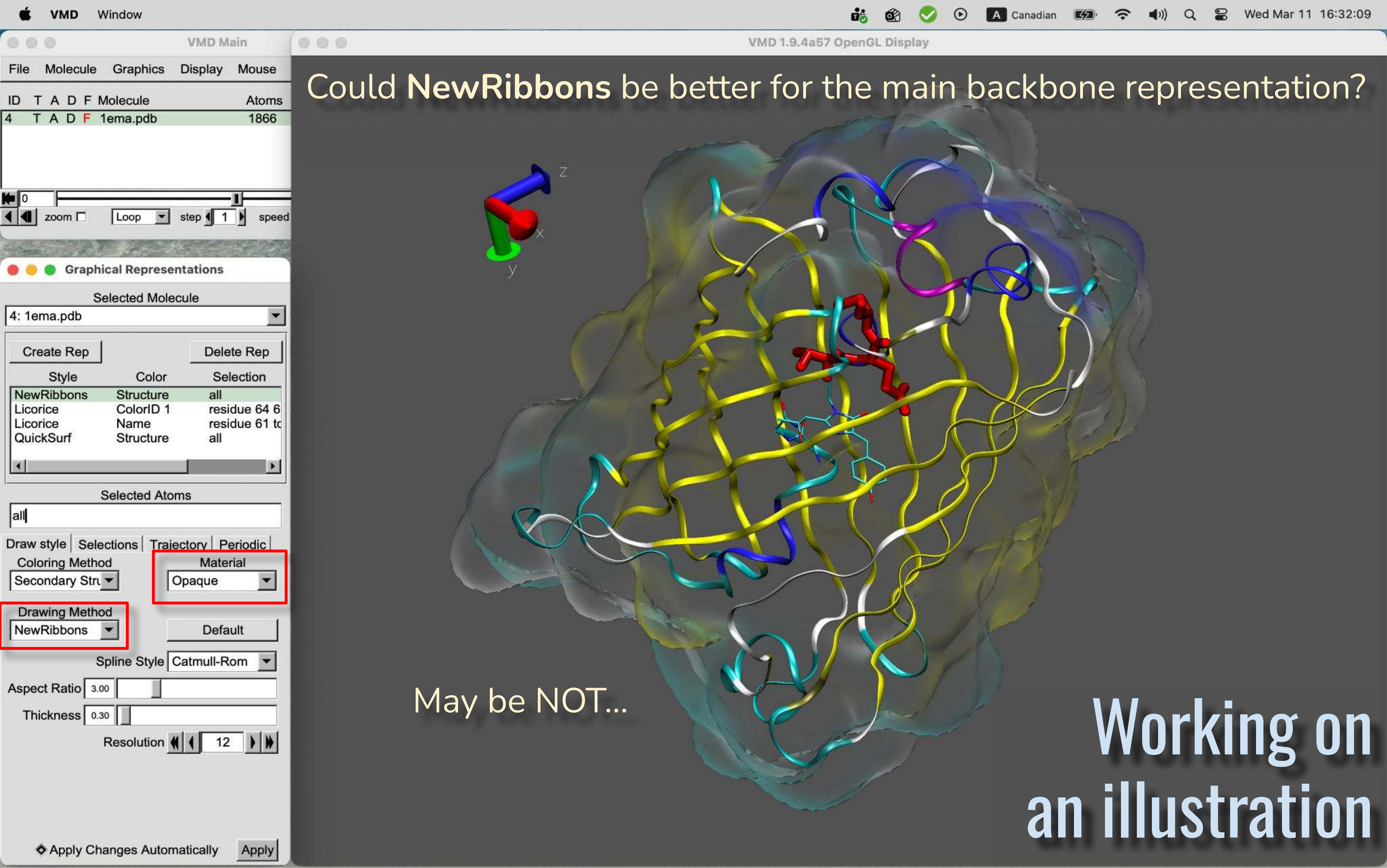
Radius Scale: 1.0

Density Isovalue: 0.5

Grid Spacing: 1.0

Surface Quality: High

Could **NewRibbons** be better for the main backbone representation?



ID	T	A	D	F	Molecule	Atoms
4	T	A	D	F	1ema.pdb	1866

0 zoom ☐ Loop step 1 speed

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewRibbons	Structure	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 tc
QuickSurf	Structure	all

Selected Atoms: all

Coloring Method: Secondary Stru

Material: Opaque

Drawing Method: NewRibbons

Spline Style: Catmull-Rom

Aspect Ratio: 3.00

Thickness: 0.30

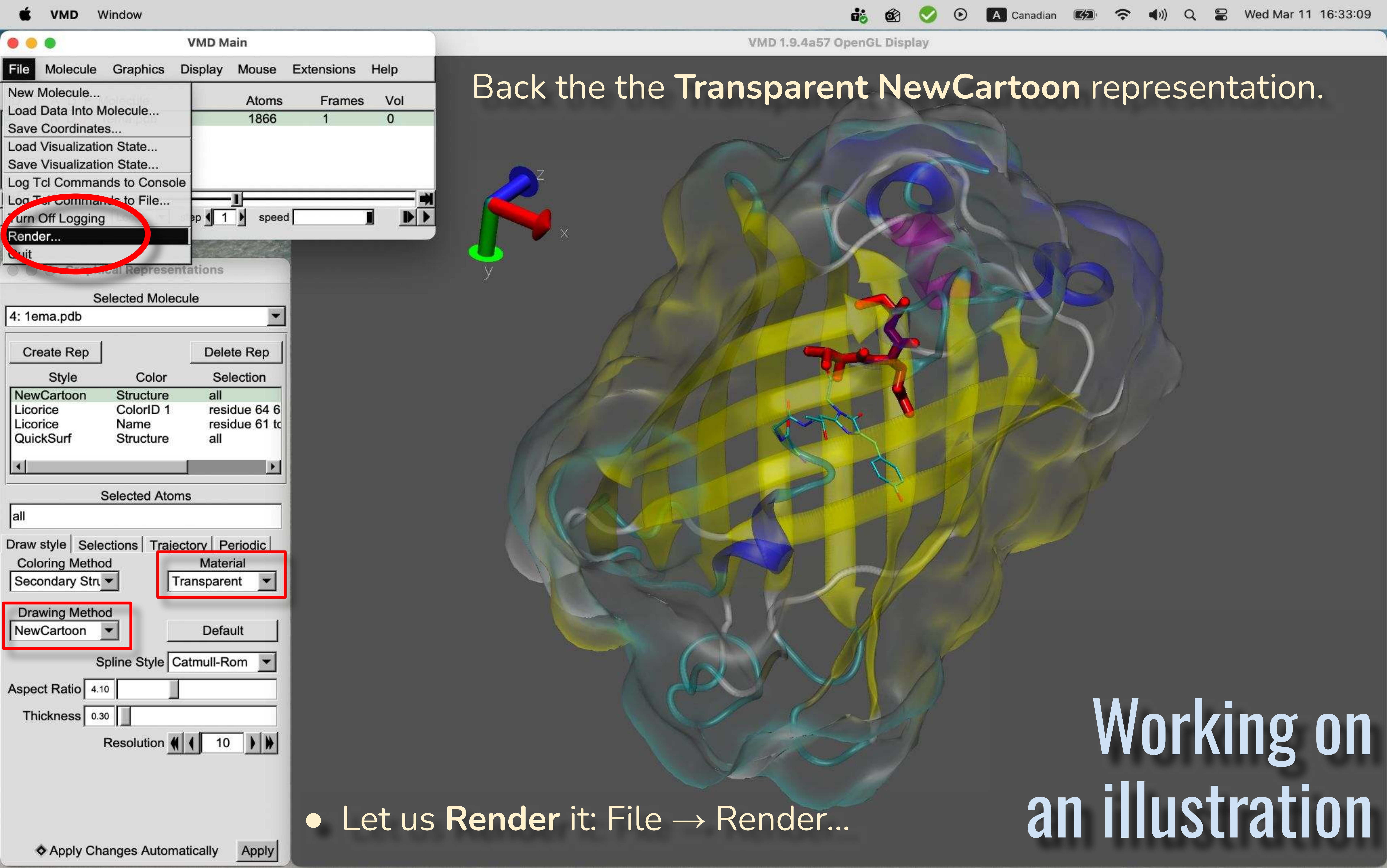
Resolution: 12

◇ Apply Changes Automatically

May be NOT...

Working on
an illustration

Back the the **Transparent NewCartoon** representation.



Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Structure	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 to
QuickSurf	Structure	all

Selected Atoms: all

Coloring Method: Secondary Stru

Material: Transparent

Drawing Method: NewCartoon

Spline Style: Catmull-Rom

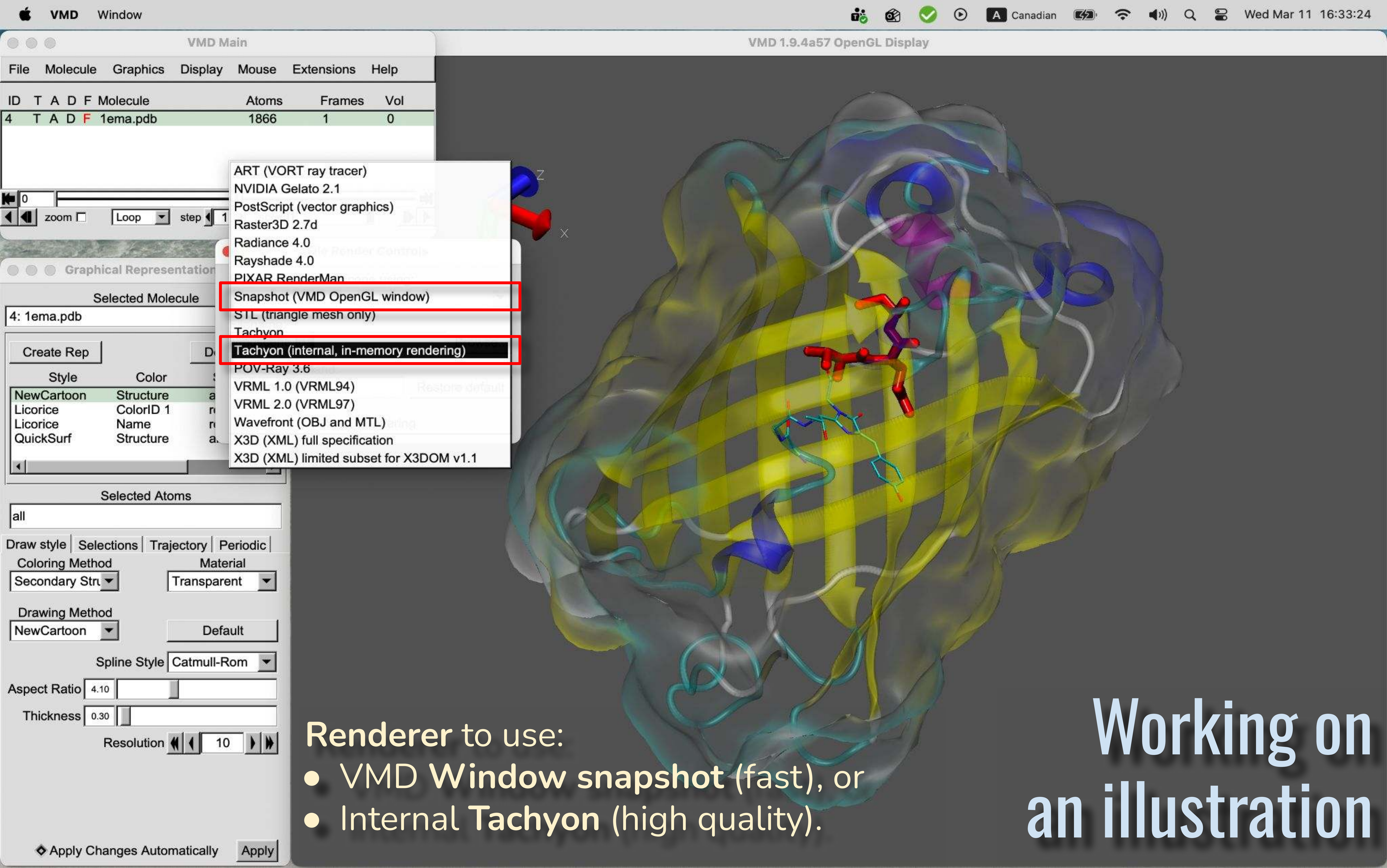
Aspect Ratio: 4.10

Thickness: 0.30

Resolution: 10

- Let us **Render** it: File → Render...

Working on an illustration



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
4	T	A	D	F	1ema.pdb	1866	1	0

Selected Molecule: 4: 1ema.pdb

Style	Color
NewCartoon	Structure
Licorice	ColorID 1
Licorice	Name
QuickSurf	Structure

Selected Atoms: all

Coloring Method: Secondary Stru

Material: Transparent

Drawing Method: NewCartoon

Spline Style: Catmull-Rom

Aspect Ratio: 4.10

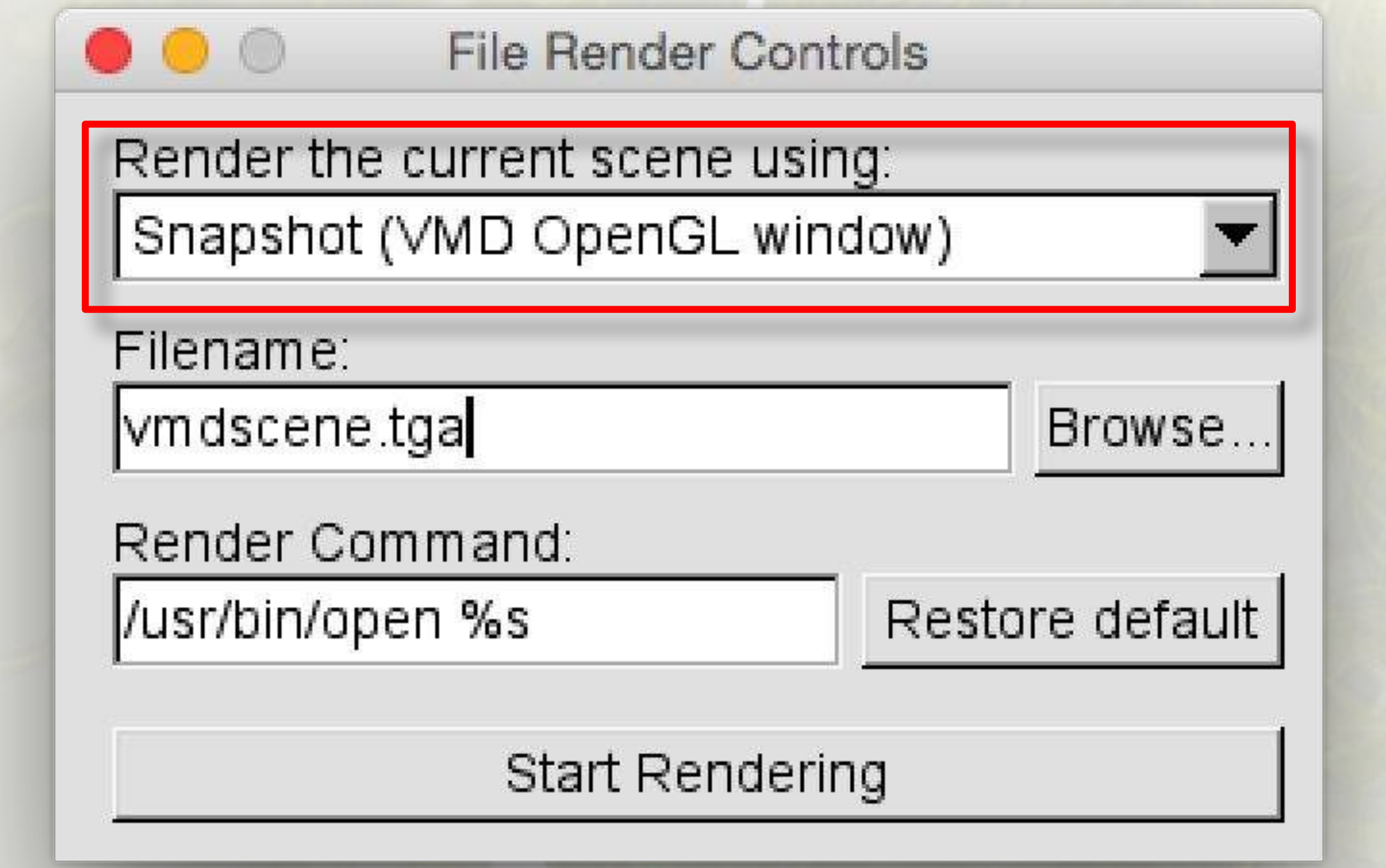
Thickness: 0.30

Resolution: 10

Renderer to use:

- VMD **Window snapshot** (fast), or
- Internal **Tachyon** (high quality).

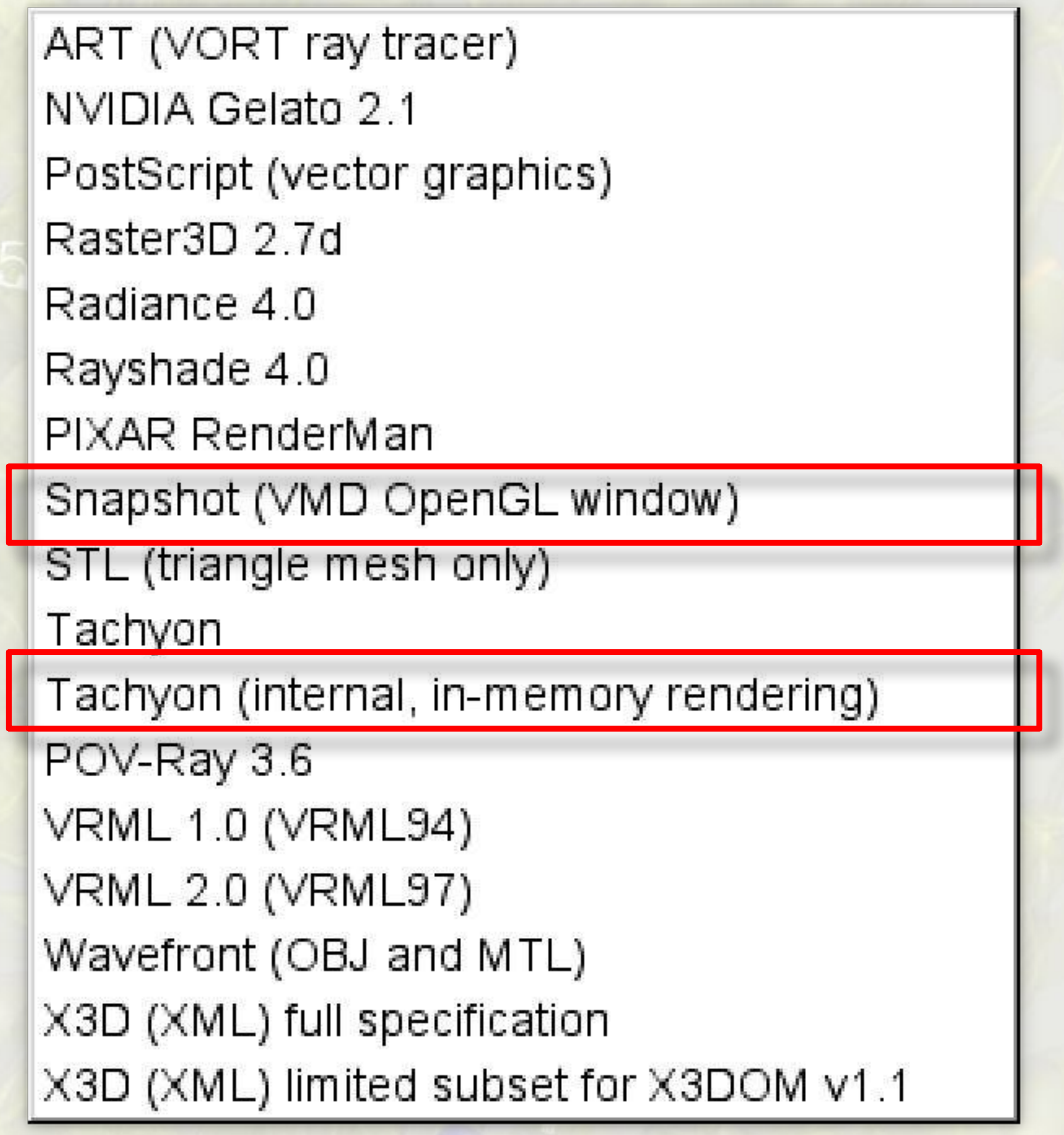
Render dialog



Render the current scene using: Snapshot (VMD OpenGL window)

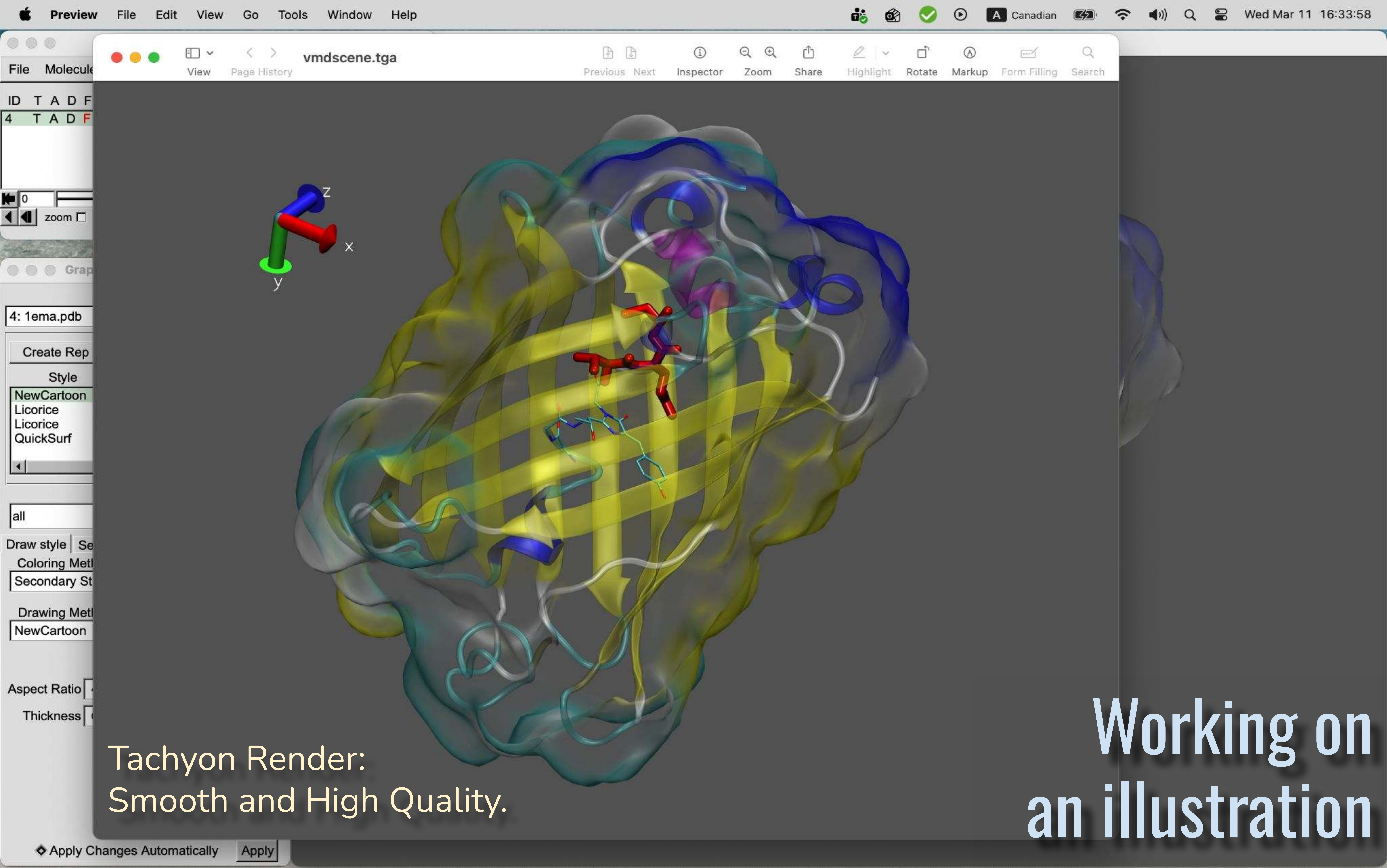
Filename: vmdscene.tga

Render Command: /usr/bin/open %s



ART (VORT ray tracer)
NVIDIA Gelato 2.1
PostScript (vector graphics)
Raster3D 2.7d
Radiance 4.0
Rayshade 4.0
PIXAR RenderMan
Snapshot (VMD OpenGL window)
STL (triangle mesh only)
Tachyon
Tachyon (internal, in-memory rendering)
POV-Ray 3.6
VRML 1.0 (VRML94)
VRML 2.0 (VRML97)
Wavefront (OBJ and MTL)
X3D (XML) full specification
X3D (XML) limited subset for X3DOM v1.1

- Internal and External renderers.
- External renderers require additional software.
- Internal (included) options are normally enough.



4: 1ema.pdb

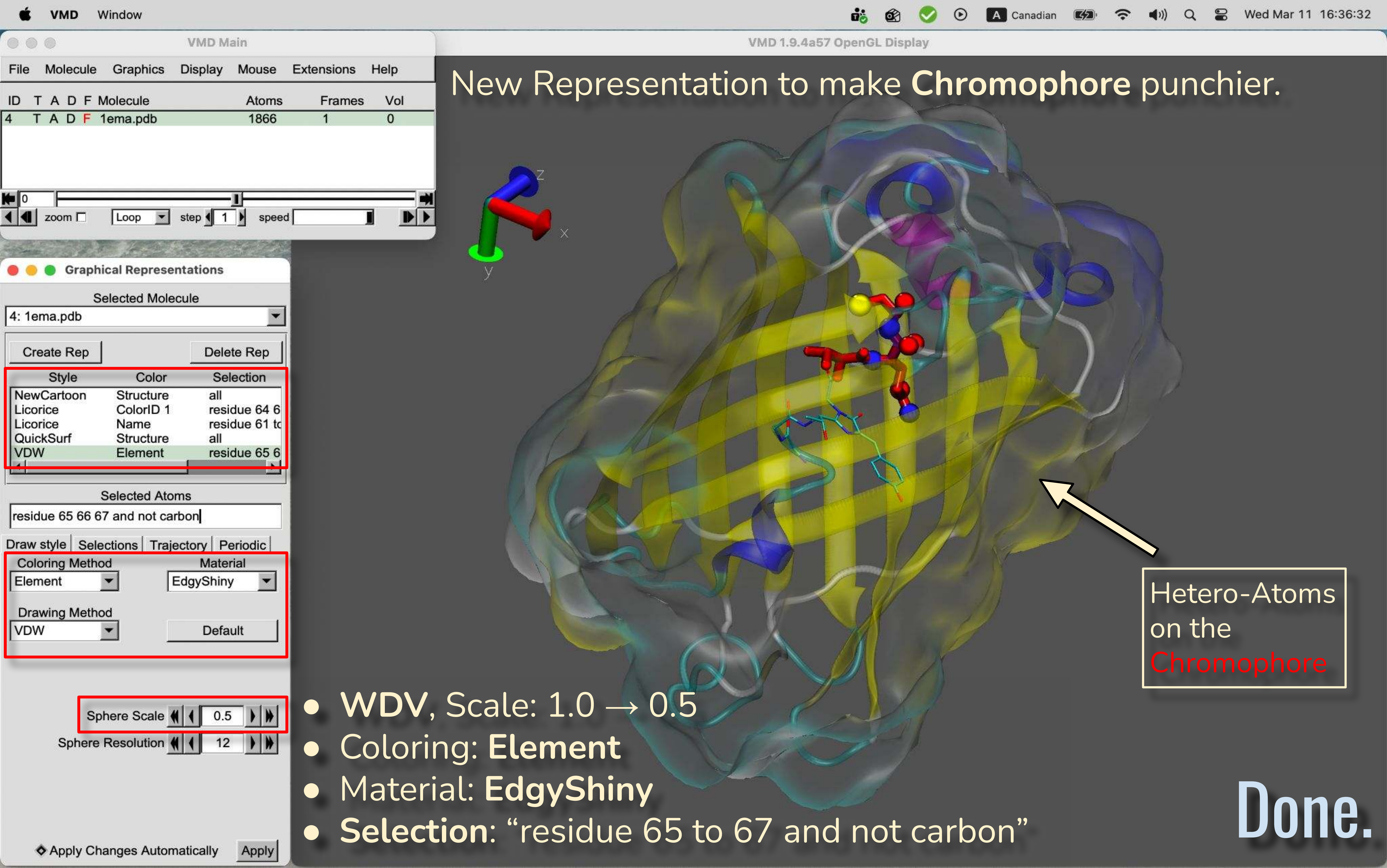
all

Coloring Metl
Secondary St

Drawing Metl
NewCartoon

Working on an illustration

Tachyon Render:
Smooth and High Quality.



New Representation to make **Chromophore** punchier.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
4	T	A	D	F	1ema.pdb	1866	1	0

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Structure	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 tc
QuickSurf	Structure	all
VDW	Element	residue 65 6

Selected Atoms: residue 65 66 67 and not carbon

Coloring Method: Element

Material: EdgyShiny

Drawing Method: VDW

Sphere Scale: 0.5

Sphere Resolution: 12

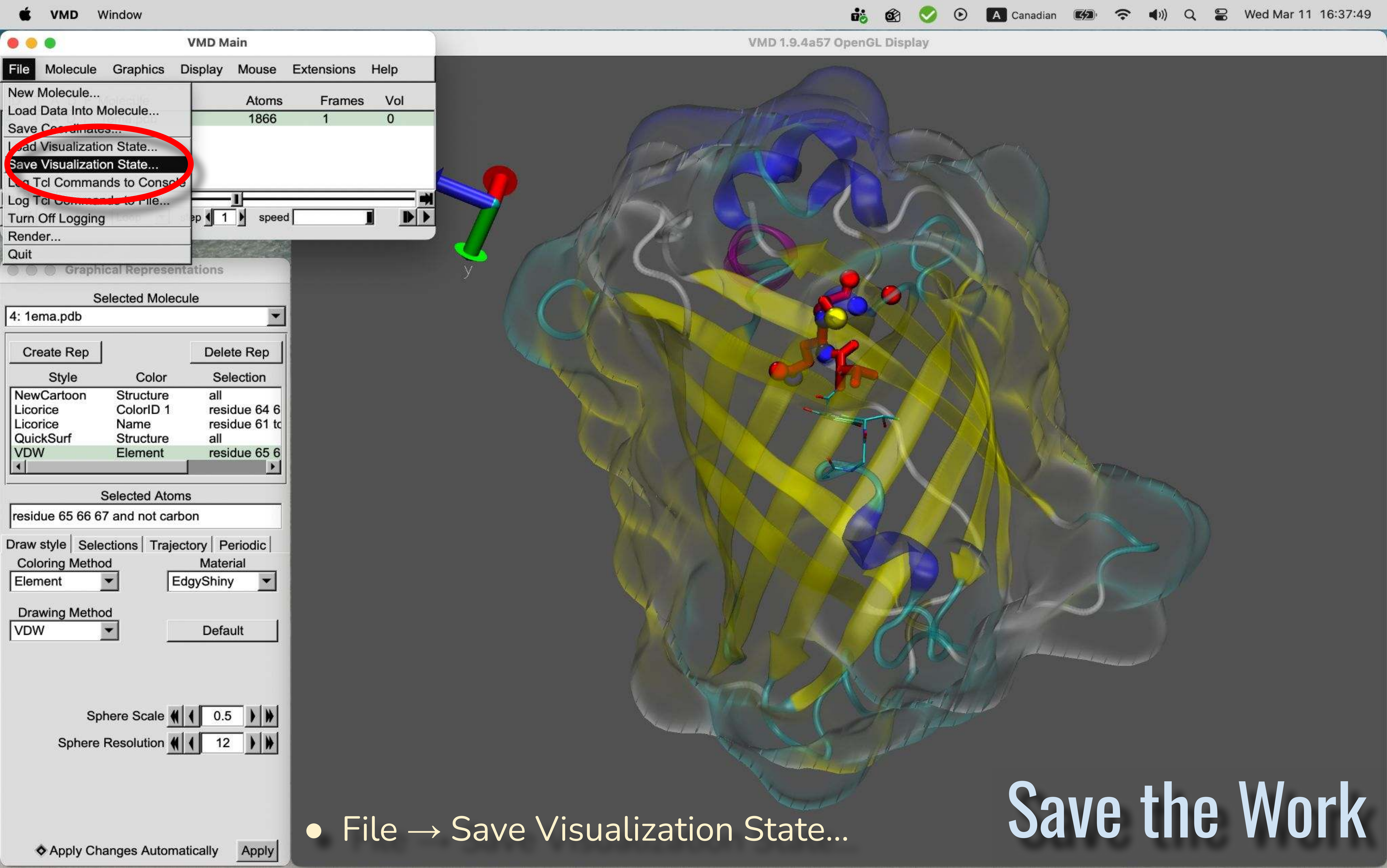
Hetero-Atoms on the Chromophore

- **WDV**, Scale: 1.0 → 0.5
- Coloring: **Element**
- Material: **EdgyShiny**
- **Selection**: “residue 65 to 67 and not carbon”

Done.

Save the Work

- File → Save Visualization State…



Atoms: 1866, Frames: 1, Vol: 0

Selected Molecule: 4: 1ema.pdb

Style	Color	Selection
NewCartoon	Structure	all
Licorice	ColorID 1	residue 64 6
Licorice	Name	residue 61 tc
QuickSurf	Structure	all
VDW	Element	residue 65 6

Selected Atoms: residue 65 66 67 and not carbon

Coloring Method: Element

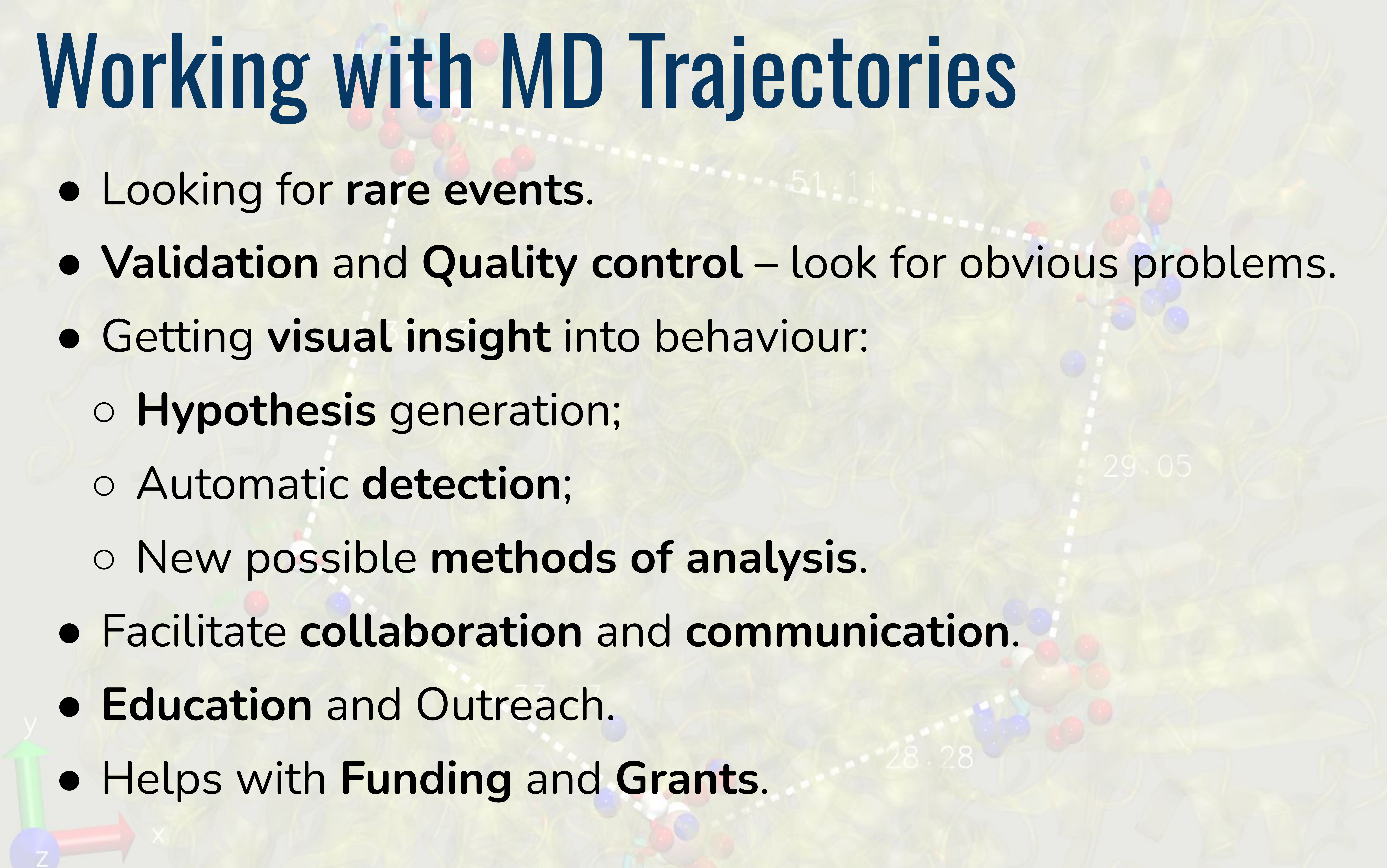
Material: EdgyShiny

Drawing Method: VDW

Sphere Scale: 0.5

Sphere Resolution: 12

Working with MD Trajectories



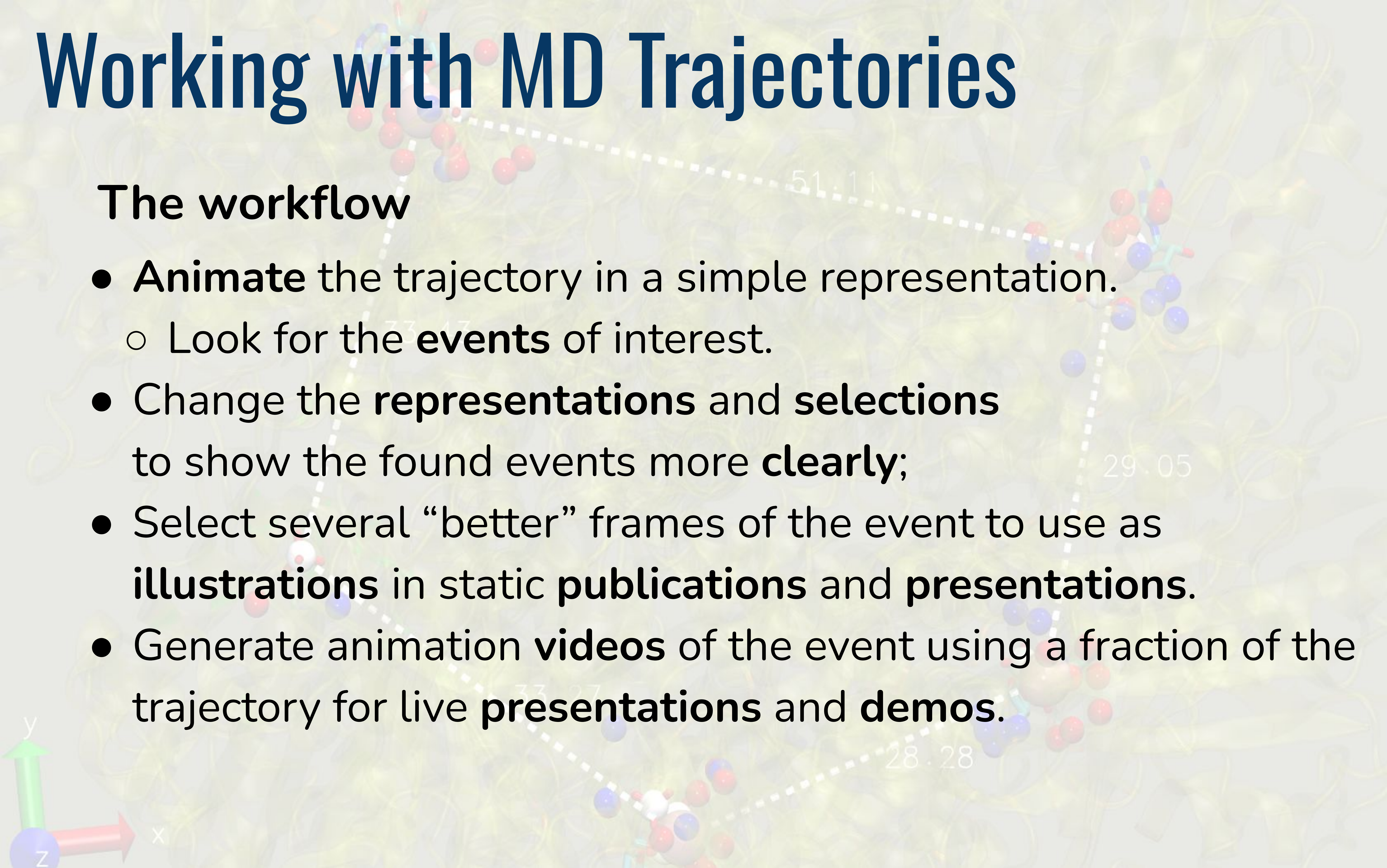
- Looking for **rare events**.
- **Validation** and **Quality control** – look for obvious problems.
- Getting **visual insight** into behaviour:
  - **Hypothesis** generation;
  - Automatic **detection**;
  - New possible **methods of analysis**.
- Facilitate **collaboration** and **communication**.
- **Education** and Outreach.
- Helps with **Funding** and **Grants**.

Working with MD Trajectories

- MD **Trajectories** are typically have two parts
  - **Topology** – constant part
    - Atom types, bonds, force field, etc.
  - **Configurations** – atomic coordinates at time steps
    - AKA frames, snapshots.
    - 100-1000s more per trajectory (many).

- **Gromacs**: GRO + XTC
- **NAMD / CHARMM**: PSF + DCD
- Multi-frame PDB or XYZ files are also possible (contain both).

Working with MD Trajectories

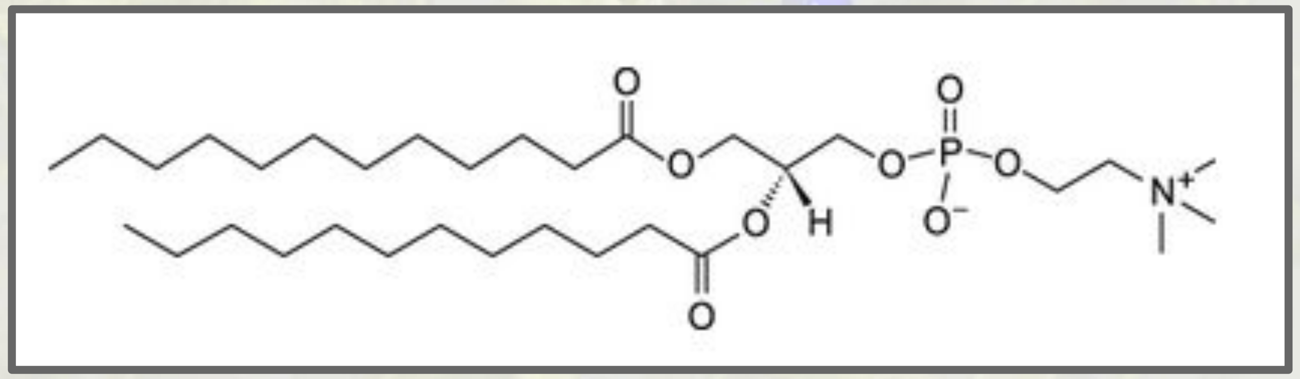


The workflow

- **Animate** the trajectory in a simple representation.
  - Look for the **events** of interest.
- Change the **representations** and **selections** to show the found events more **clearly**;
- Select several “better” frames of the event to use as **illustrations** in static **publications** and **presentations**.
- Generate animation **videos** of the event using a fraction of the trajectory for live **presentations** and **demos**.

Working with MD Trajectories

Case Study: **DLPC lipid bilayer simulation**

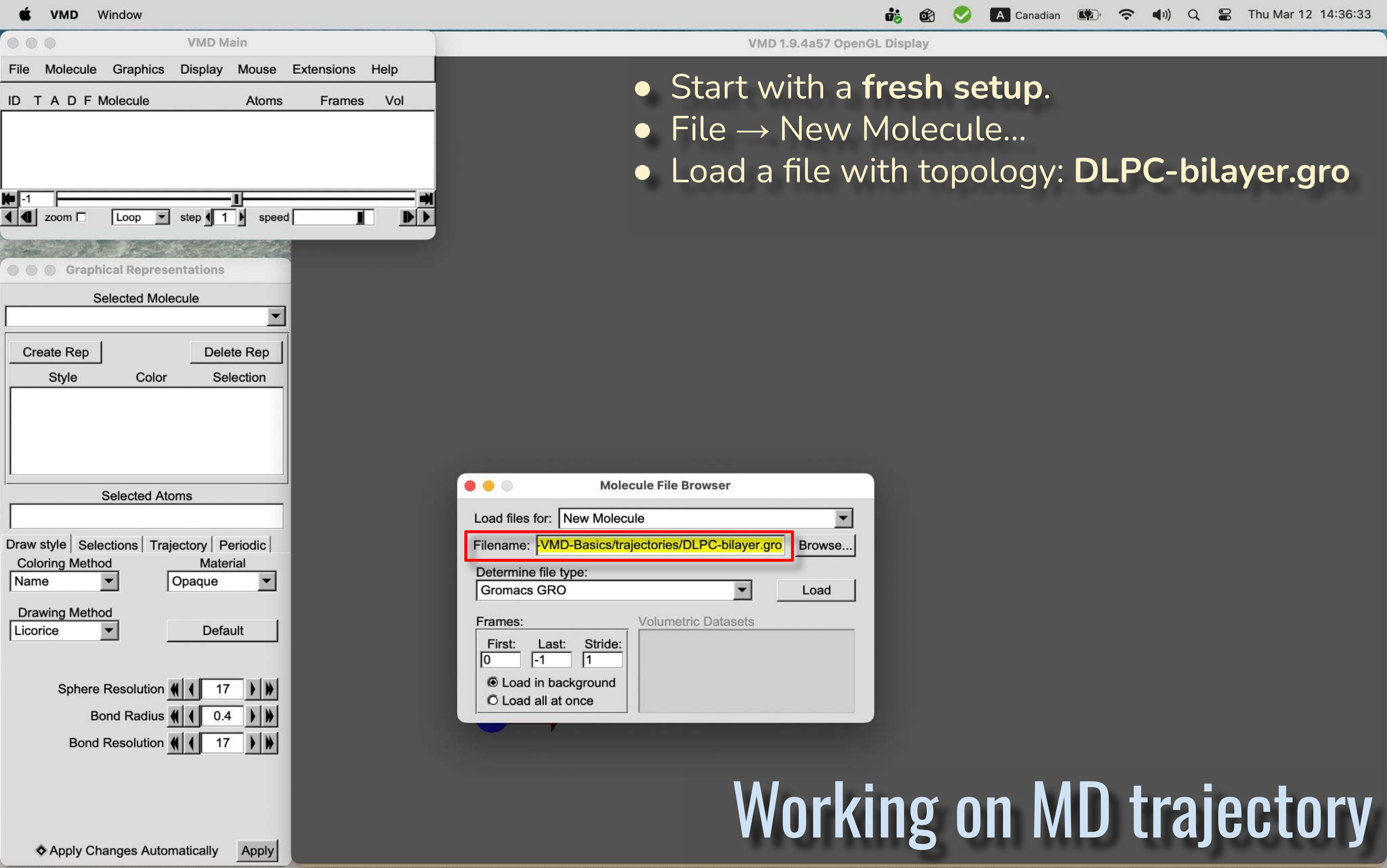


- System contains
  - **2369** DLPC lipid molecules.
  - **2305** water molecules.
  - 9603 atoms total.
- The trajectory contains about **1000 snapshots**.
- The simulation demonstrates a **pore formation event**.

Bennett et al. 2014, Atomistic Simulations of Pore Formation and Closure in Lipid Bilayers. *Biophys J.* 106(1) 210-219.

Working on MD trajectory

- Start with a **fresh setup**.
- File → New Molecule…
- Load a file with topology: **DLPC-bilayer.gro**



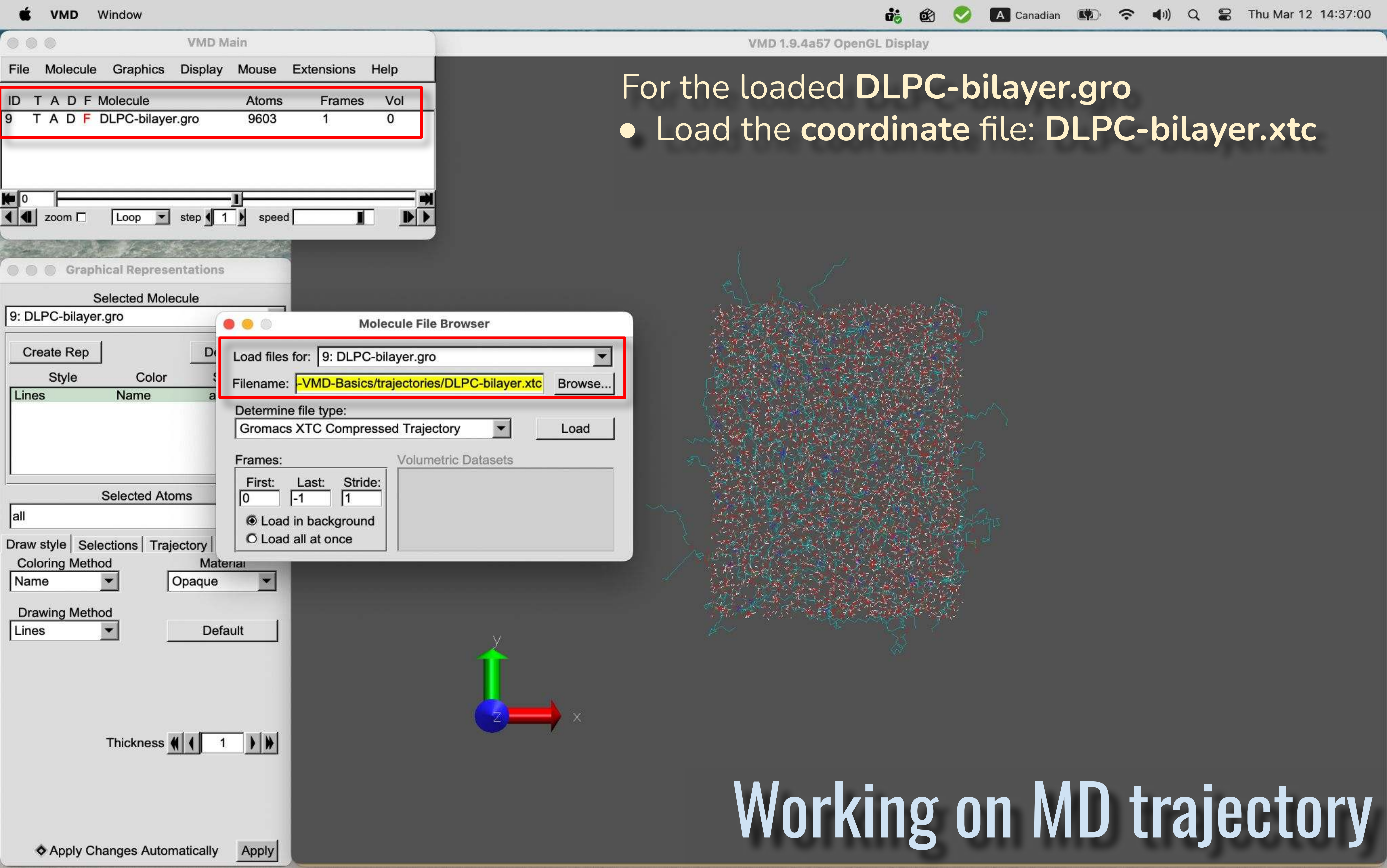
Coloring Method: Name
Material: Opaque
Drawing Method: Licorice
Sphere Resolution: 17
Bond Radius: 0.4
Bond Resolution: 17

Load files for: New Molecule
Filename: -VMD-Basics/trajectories/DLPC-bilayer.gro
Determine file type: Gromacs GRO
Frames: First: 0 Last: -1 Stride: 1
● Load in background
○ Load all at once

Working on MD trajectory

For the loaded **DLPC-bilayer.gro**

- Load the **coordinate** file: **DLPC-bilayer.xtc**



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1	0

Molecule File Browser

Load files for: 9: DLPC-bilayer.gro

Filename: -VMD-Basics/trajectories/DLPC-bilayer.xtc

Determine file type: Gromacs XTC Compressed Trajectory

Frames:

First: 0 Last: -1 Stride: 1

◉ Load in background
○ Load all at once

Graphical Representations

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color
Lines	Name

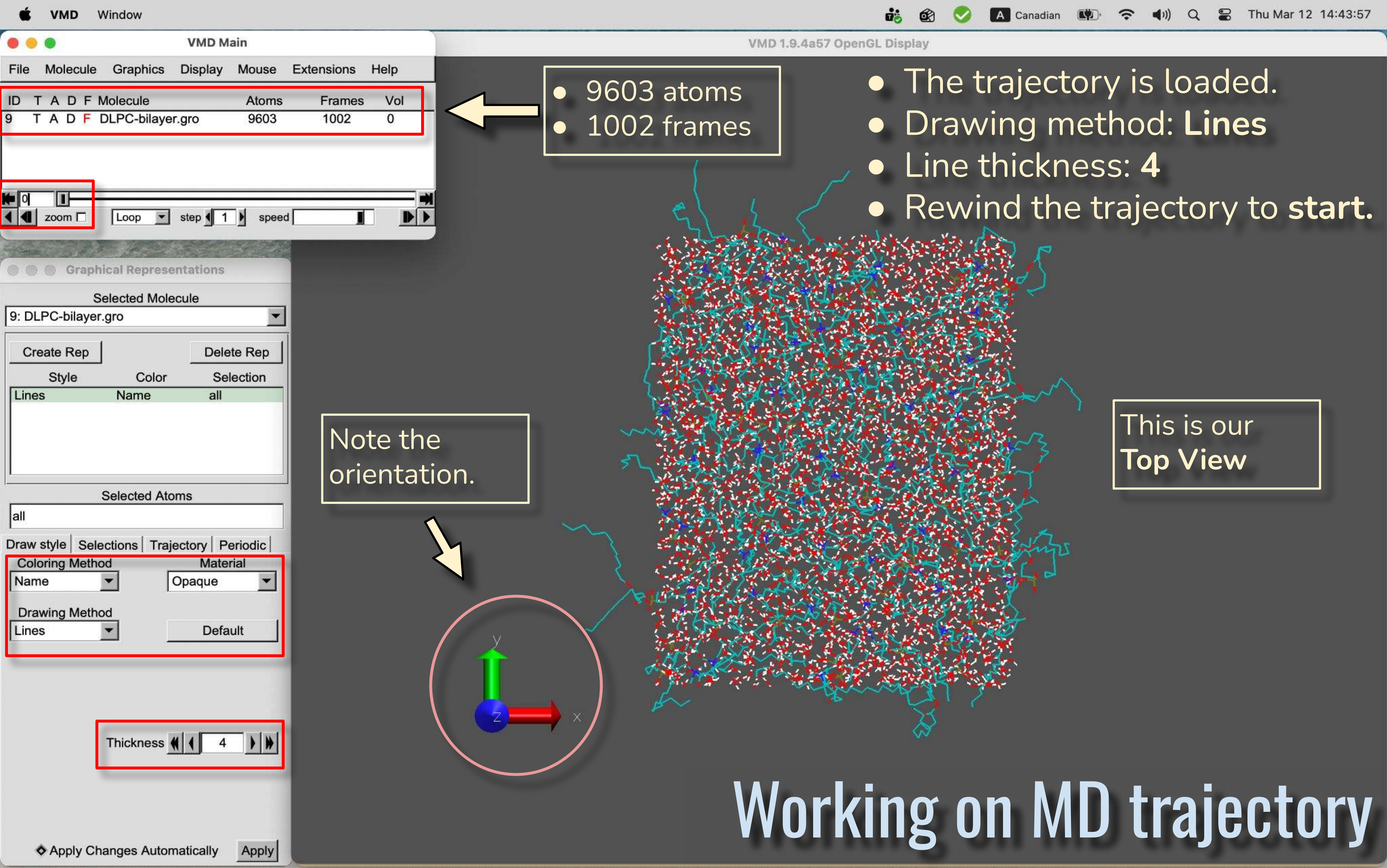
Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness 1



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 0

Step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness: 4

- 9603 atoms
- 1002 frames

- The trajectory is loaded.
- Drawing method: **Lines**
- Line thickness: **4**
- Rewind the trajectory to **start.**

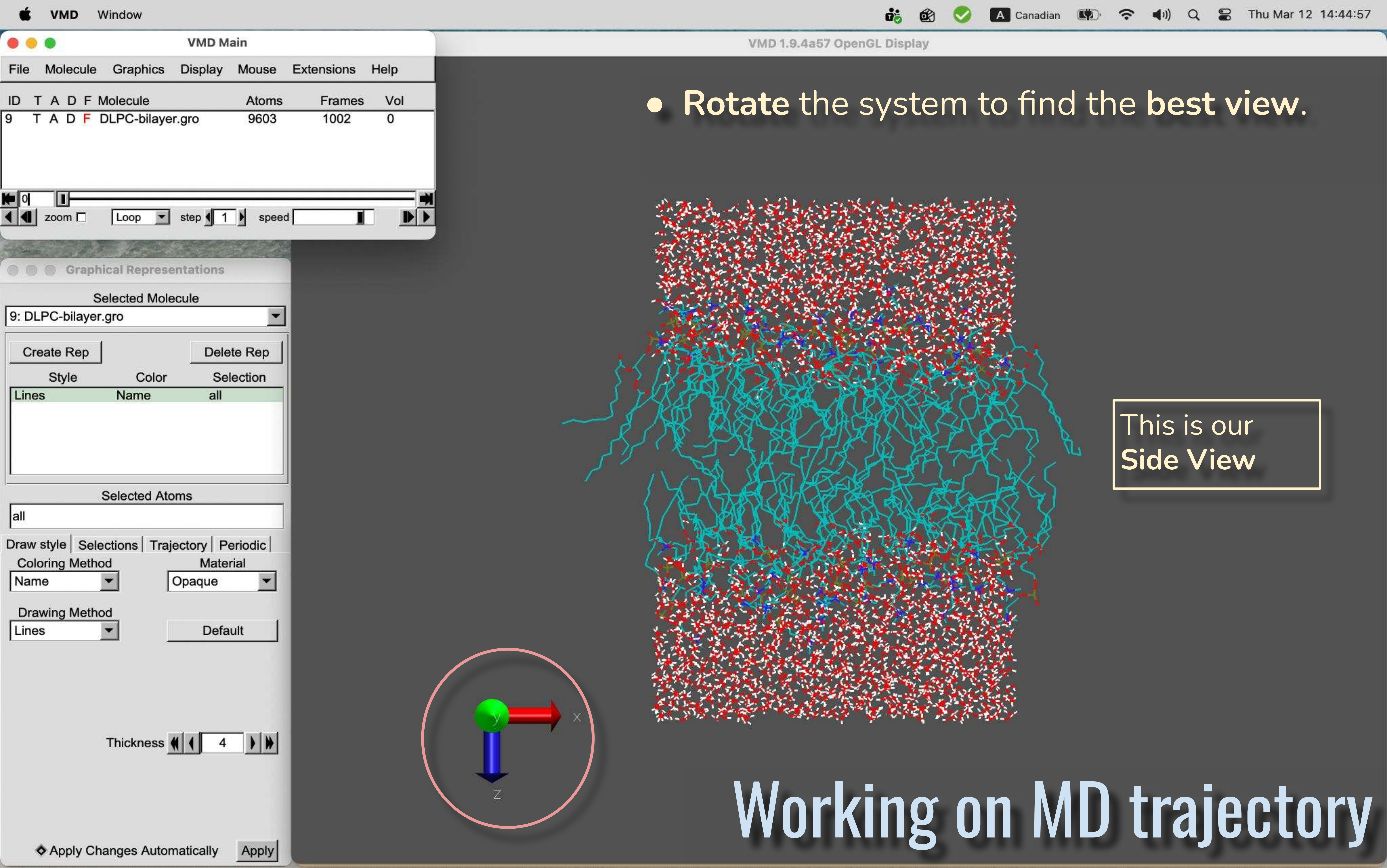
Note the orientation.

This is our **Top View**

Working on MD trajectory

Working on MD trajectory

- **Rotate** the system to find the **best view**.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 0, step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name

Material: Opaque

Drawing Method: Lines

Thickness: 4

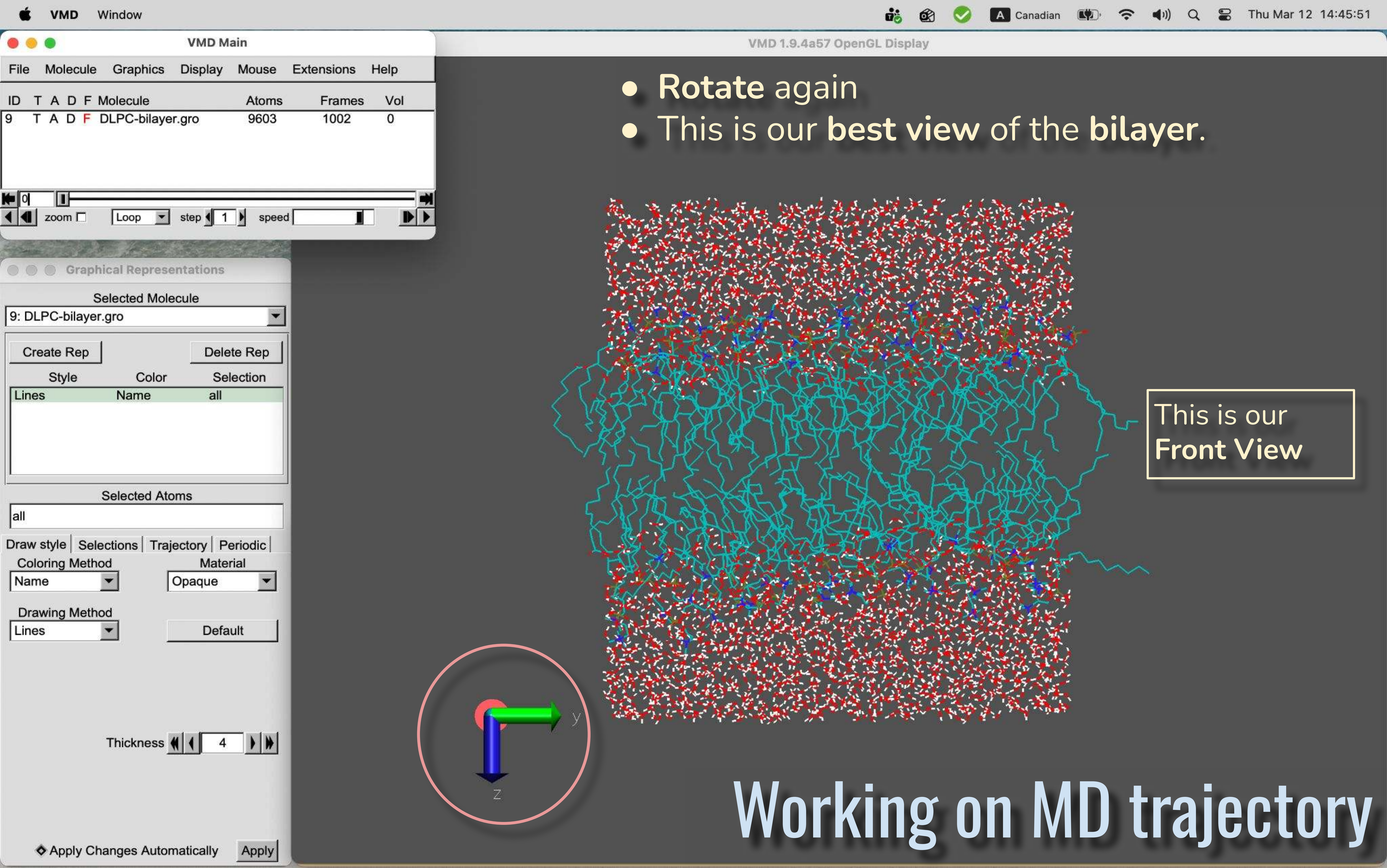
◇ Apply Changes Automatically

This is our
Side View

Working on MD trajectory

- **Rotate** again
- This is our **best view** of the **bilayer**.

This is our
Front View



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Selected Molecule: 9: DLPC-bilayer.gro

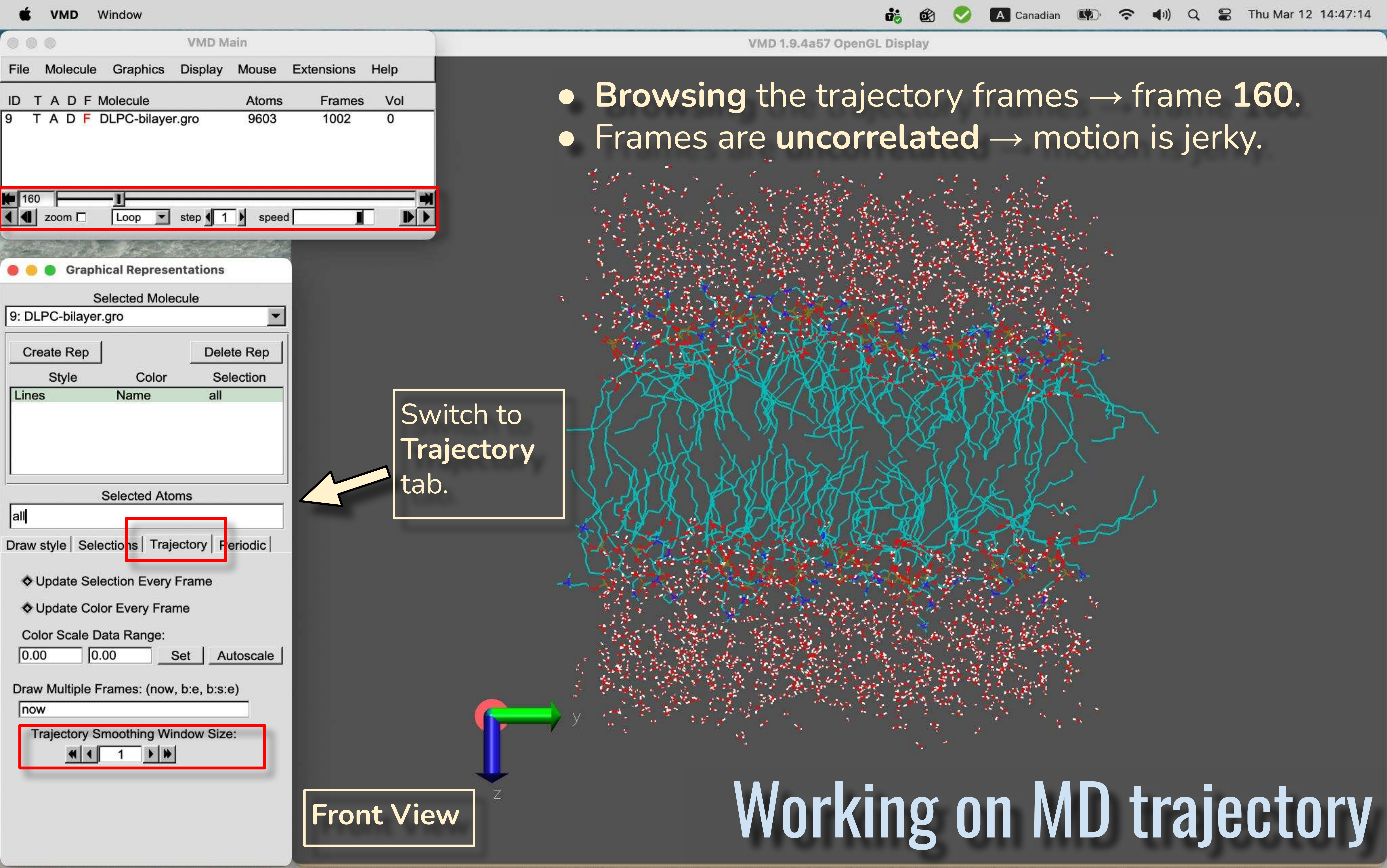
Style	Color	Selection
Lines	Name	all

Selected Atoms: all

Coloring Method: Name
Material: Opaque
Drawing Method: Lines
Thickness: 4

Working on MD trajectory

- **Browsing** the trajectory frames → frame **160**.
- Frames are **uncorrelated** → motion is jerky.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

160

zoom ☐

Loop

step 1

speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

◆ Update Selection Every Frame

◆ Update Color Every Frame

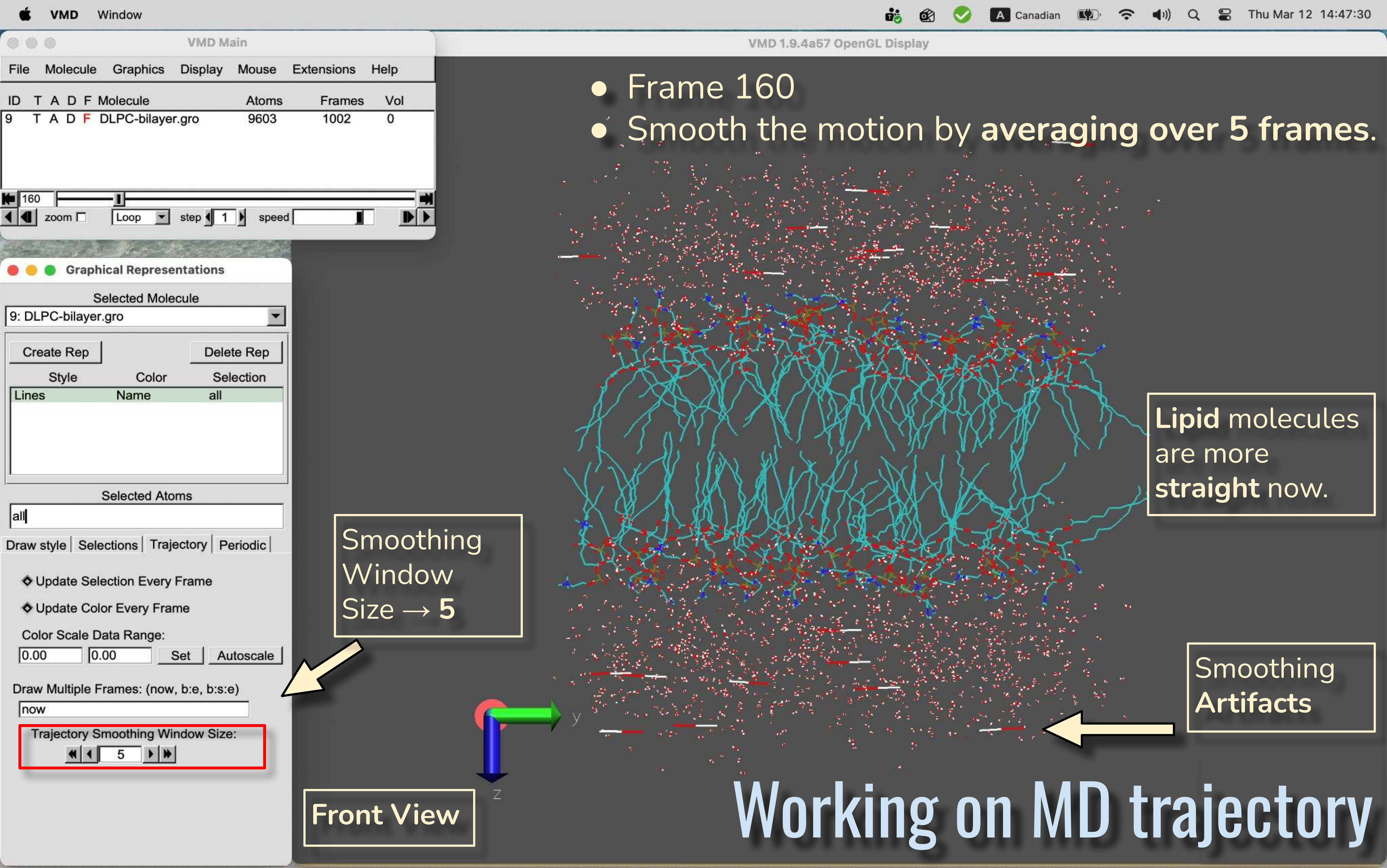
Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e) now

Trajectory Smoothing Window Size: 1

Switch to **Trajectory** tab.

Front View



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

160 zoom ☐ Loop step 1 speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	all

Selected Atoms: all

◆ Update Selection Every Frame

◆ Update Color Every Frame

Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e)

now

Trajectory Smoothing Window Size: 5

- Frame 160
- Smooth the motion by **averaging over 5 frames.**

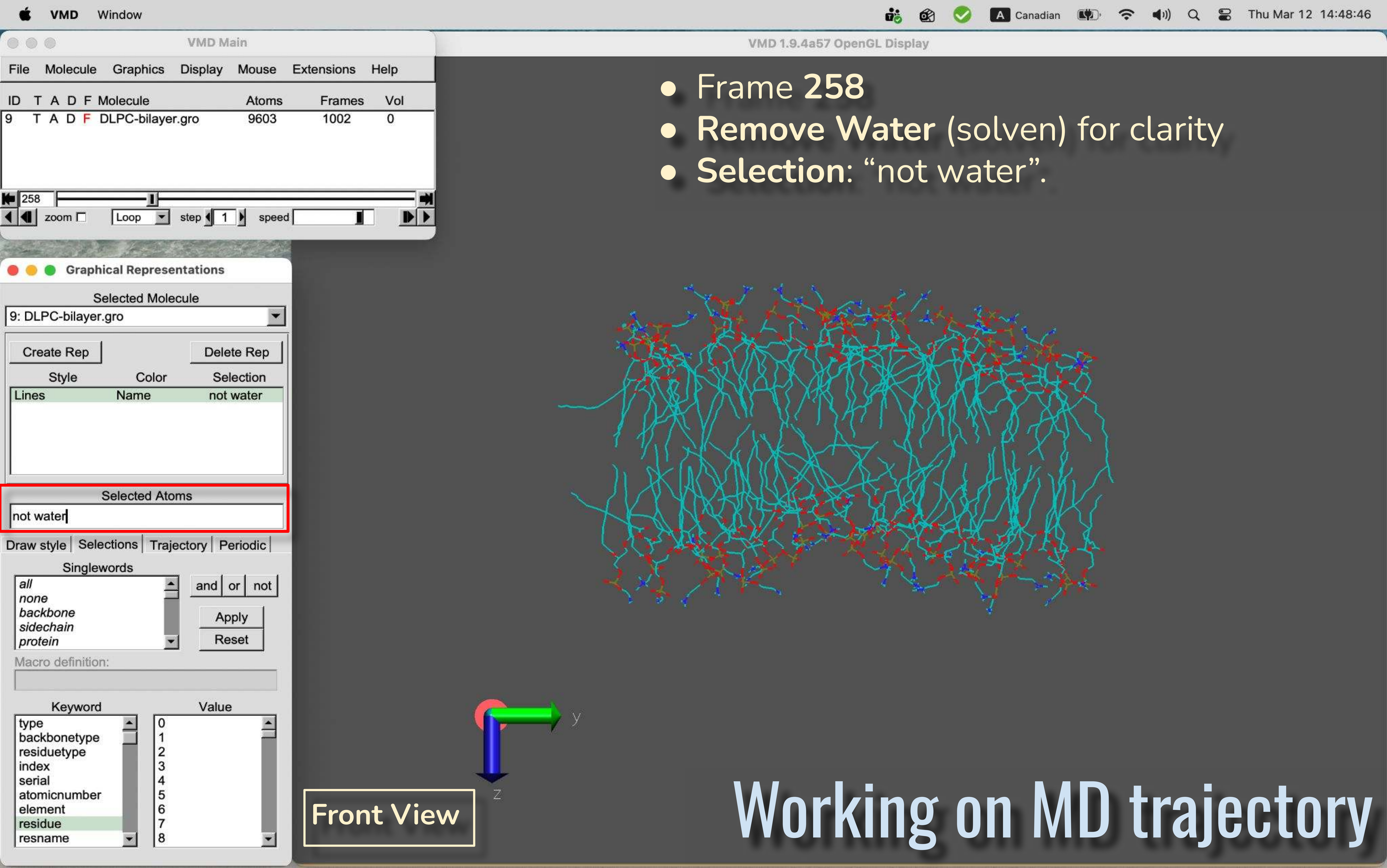
Lipid molecules are more **straight** now.

Smoothing Window Size → **5**

Smoothing **Artifacts**

Front View

Working on MD trajectory



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 258

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water

Selected Atoms: not water

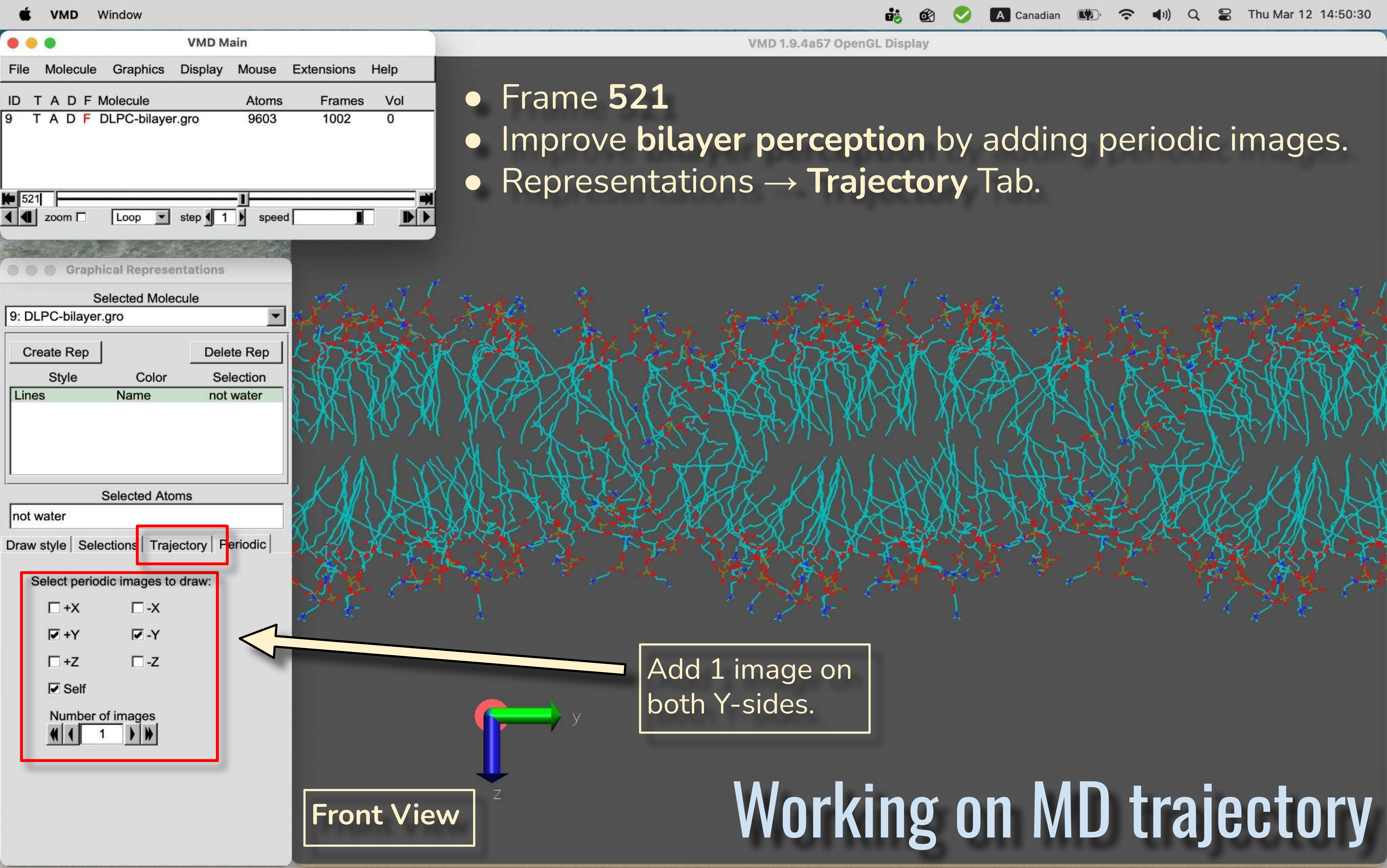
- Frame **258**
- **Remove Water** (solven) for clarity
- **Selection**: “not water”.

Front View

Working on MD trajectory

Working on MD trajectory

- Frame **521**
- Improve **bilayer perception** by adding periodic images.
- Representations → **Trajectory** Tab.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

521 zoom ☐ Loop step 1 speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water

Selected Atoms: not water

Select periodic images to draw:

☐ +X ☐ -X
☑ +Y ☑ -Y
☐ +Z ☐ -Z
☑ Self

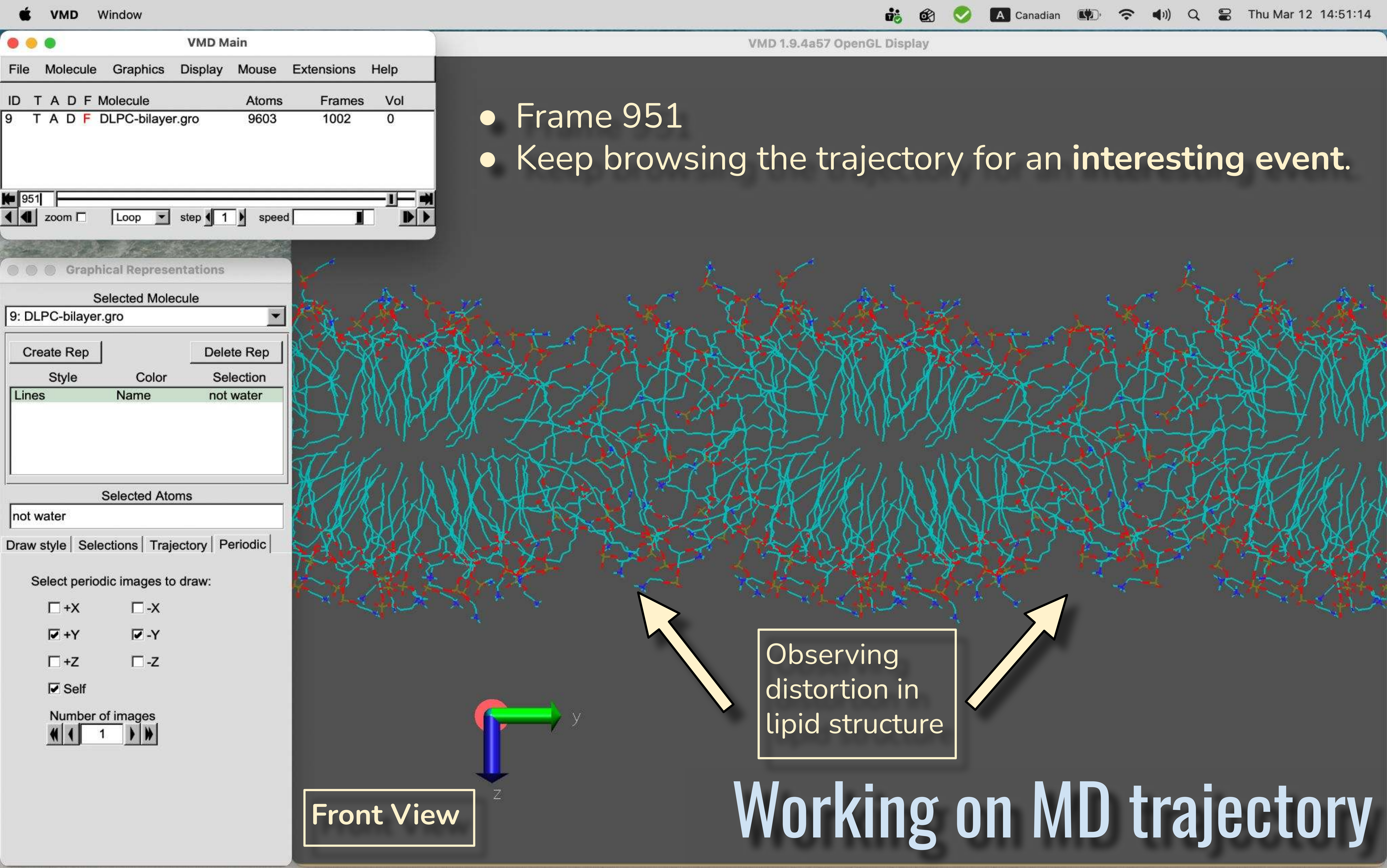
Number of images: 1

Add 1 image on both Y-sides.

Front View

Working on MD trajectory

- Frame 951
- Keep browsing the trajectory for an **interesting event**.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

951

zoom ☐ Loop step 1 speed

Selected Molecule

9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water

Selected Atoms

not water

Select periodic images to draw:

☐ +X ☐ -X

☑ +Y ☑ -Y

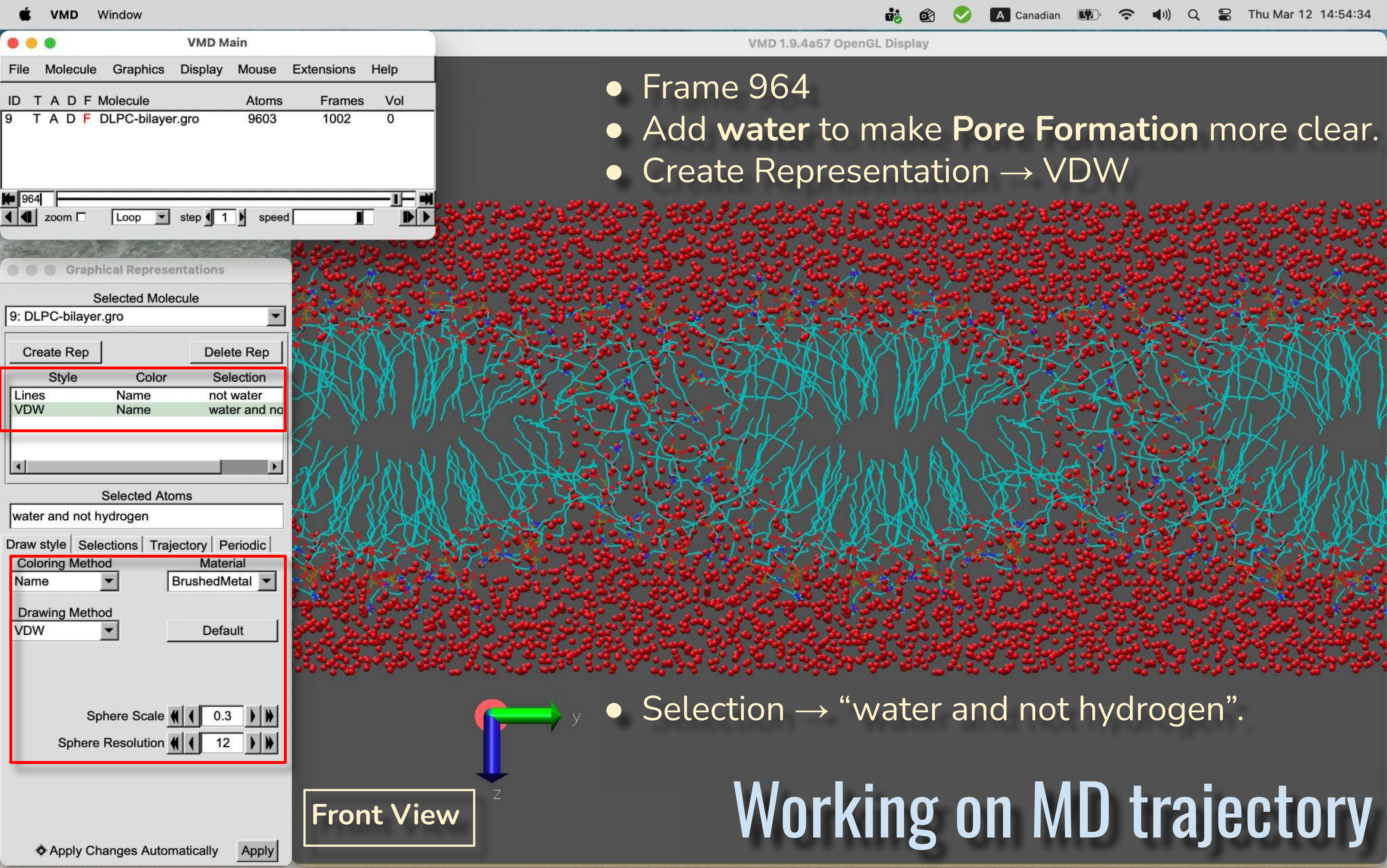
☐ +Z ☐ -Z

☑ Self

Number of images 1

Observing distortion in lipid structure

Front View



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

964

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: water and not hydrogen

Coloring Method: Name

Material: BrushedMetal

Drawing Method: VDW

Sphere Scale: 0.3

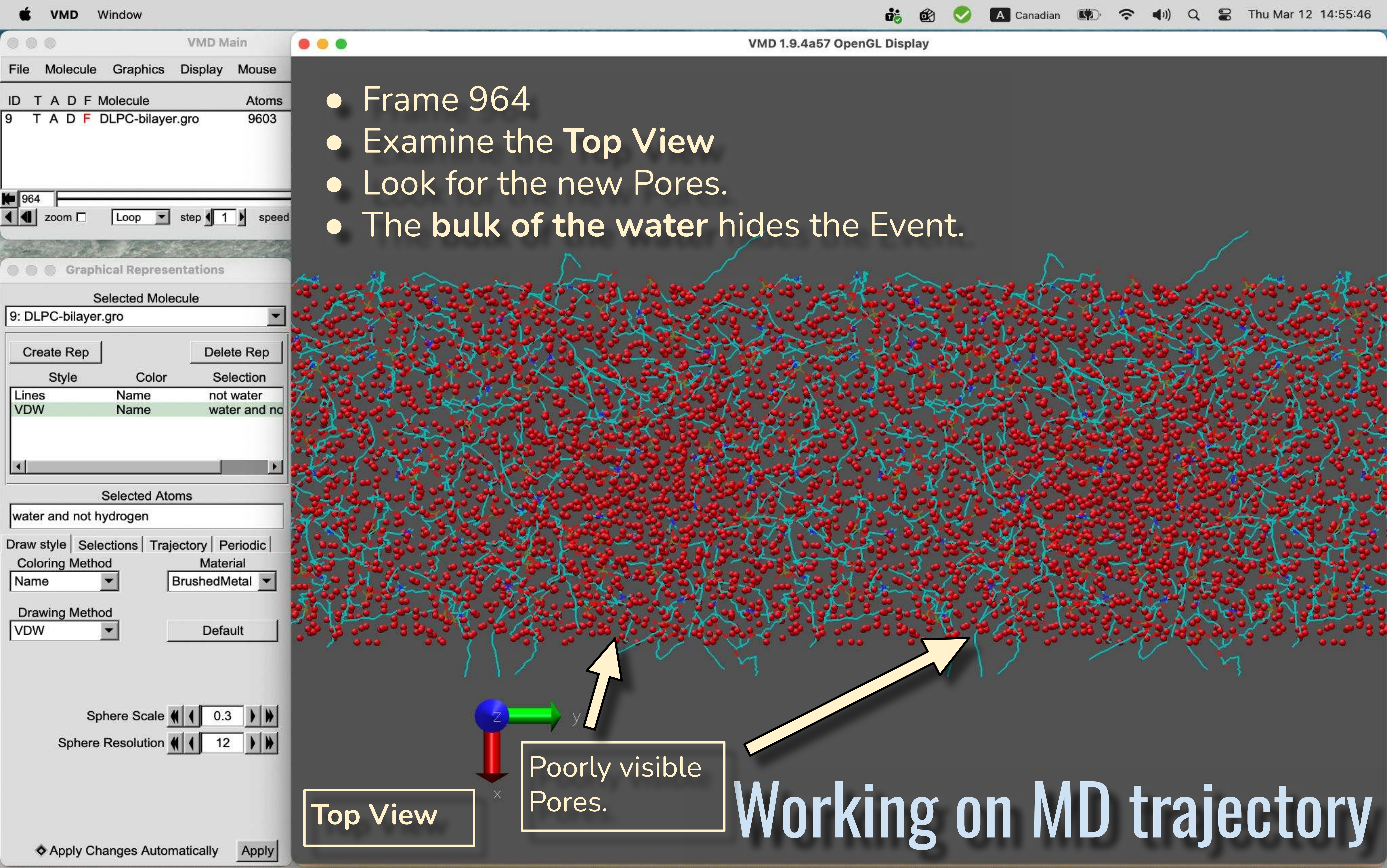
Sphere Resolution: 12

- Frame 964
- Add **water** to make **Pore Formation** more clear.
- Create Representation → VDW

- Selection → “water and not hydrogen”.

Front View

Working on MD trajectory



ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

Frame: 964

step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: water and not hydrogen

Coloring Method: Name

Material: BrushedMetal

Drawing Method: VDW

Sphere Scale: 0.3

Sphere Resolution: 12

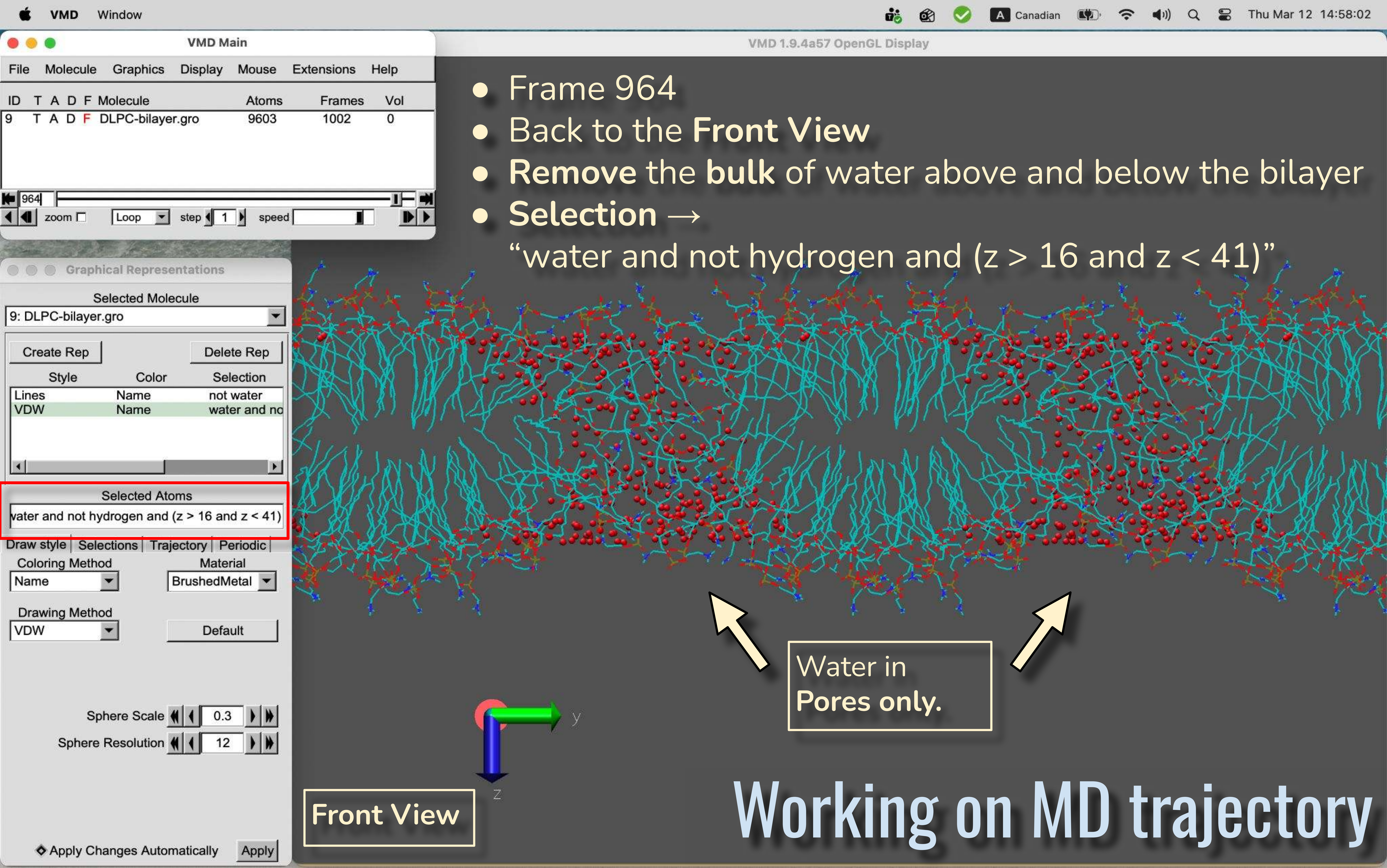
- Frame 964
- Examine the **Top View**
- Look for the new Pores.
- The **bulk of the water** hides the Event.

Top View

Poorly visible Pores.

Working on MD trajectory

Working on MD trajectory



- Frame 964
- Back to the **Front View**
- **Remove** the **bulk** of water above and below the bilayer
- **Selection** →
  “water and not hydrogen and (z > 16 and z < 41)”

Water in
Pores only.

Front View

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and nc

Selected Atoms: vater and not hydrogen and (z > 16 and z < 41)

Coloring Method: Name

Material: BrushedMetal

Drawing Method: VDW

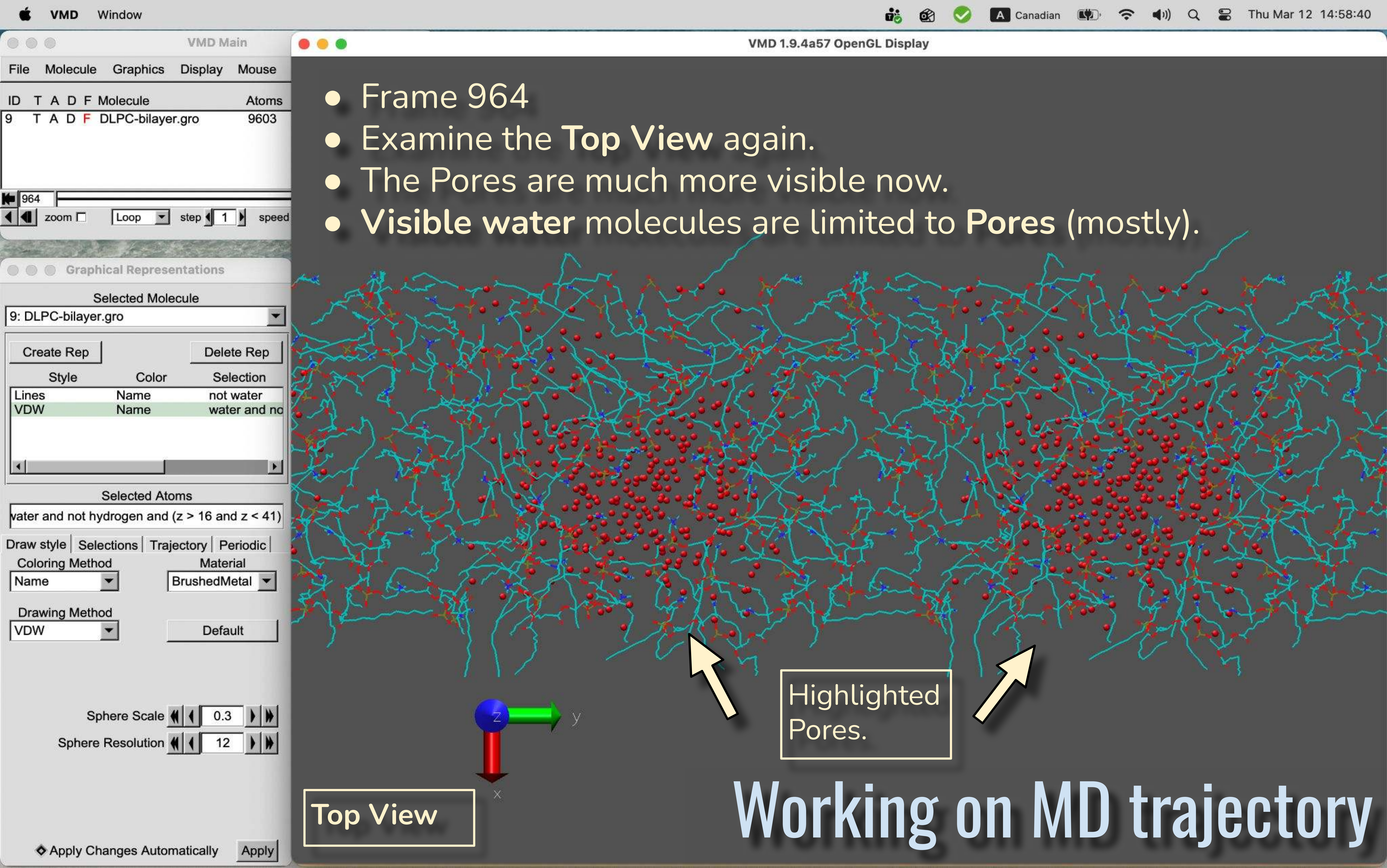
Sphere Scale: 0.3

Sphere Resolution: 12

Frame: 964

Loop

step: 1



ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

964

zoom ☐ Loop step 1 speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 16 and z < 41)

Coloring Method: Name

Material: BrushedMetal

Drawing Method: VDW

Sphere Scale: 0.3

Sphere Resolution: 12

- Frame 964
- Examine the **Top View** again.
- The Pores are much more visible now.
- **Visible water** molecules are limited to **Pores** (mostly).

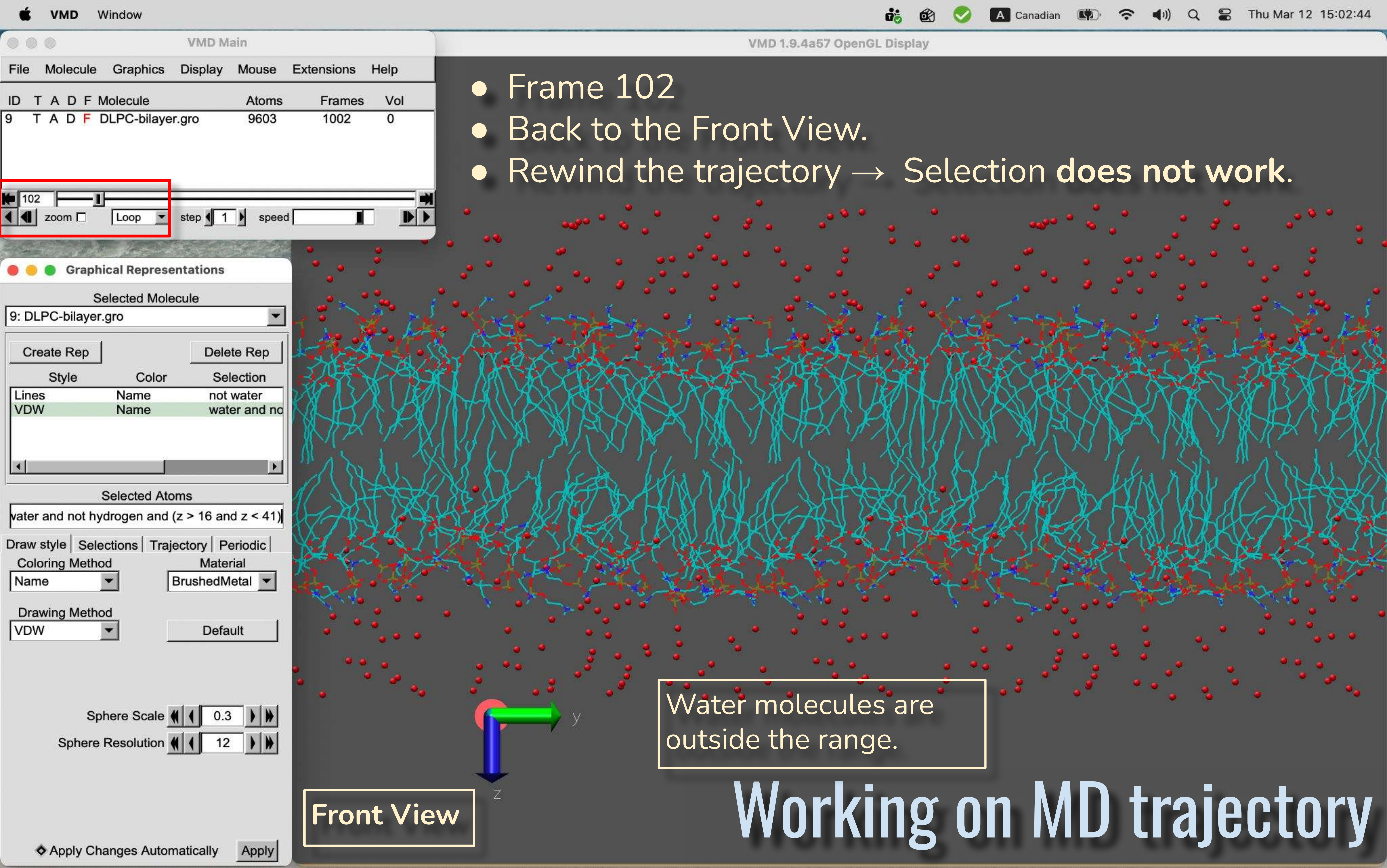
Highlighted Pores.

Top View

Working on MD trajectory

Working on MD trajectory

- Frame 102
- Back to the Front View.
- Rewind the trajectory → Selection **does not work**.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 102
zoom ☐
Loop
step 1
speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

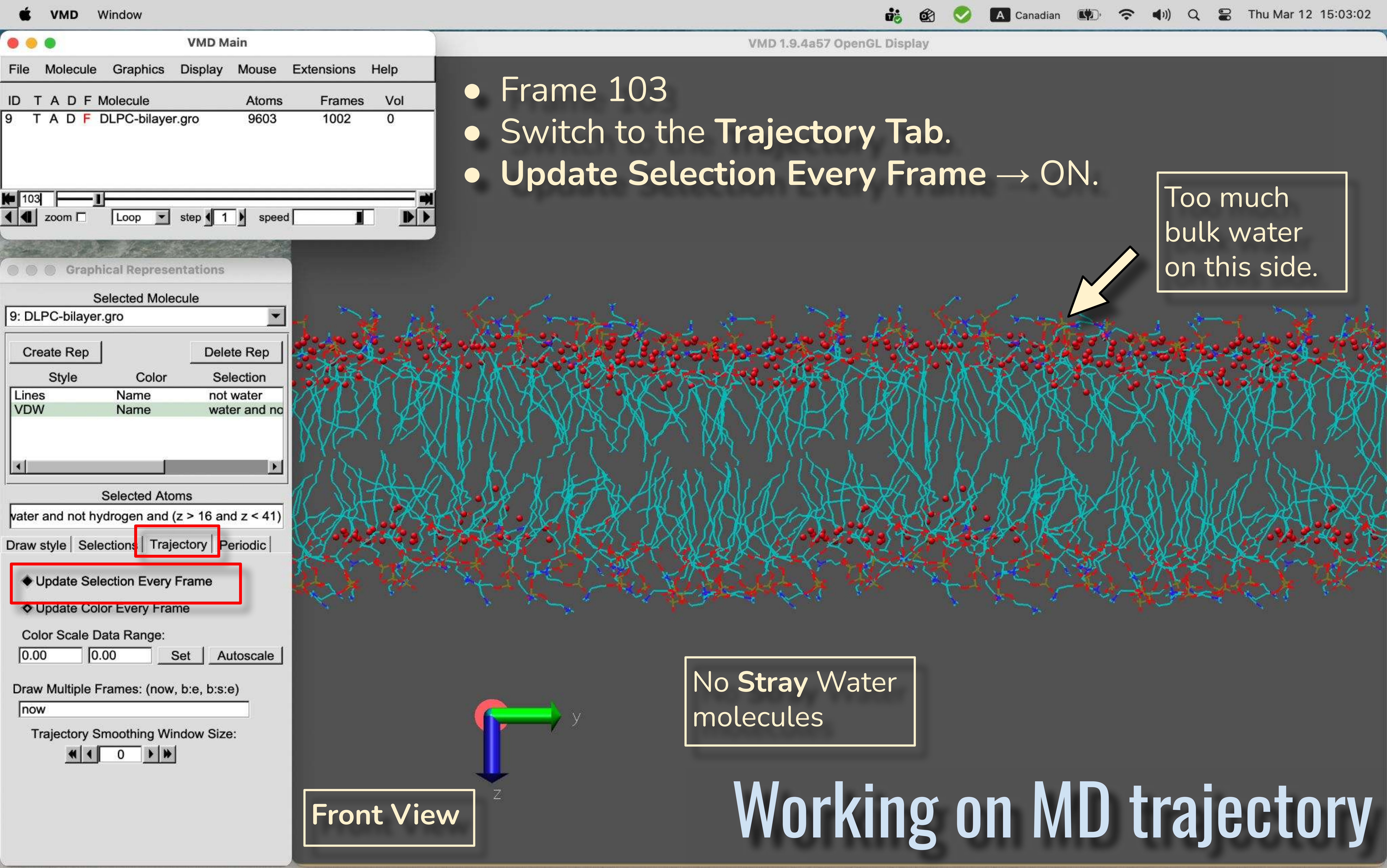
Selected Atoms: vater and not hydrogen and (z > 16 and z < 41)

Coloring Method: Name
Material: BrushedMetal
Drawing Method: VDW
Sphere Scale: 0.3
Sphere Resolution: 12

Water molecules are outside the range.

Front View

Working on MD trajectory



- Frame 103
- Switch to the **Trajectory Tab**.
- **Update Selection Every Frame** → ON.

Too much bulk water on this side.

No **Stray** Water molecules

Front View

VMD Main

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 103 — Loop — step 1

Graphical Representations

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 16 and z < 41)

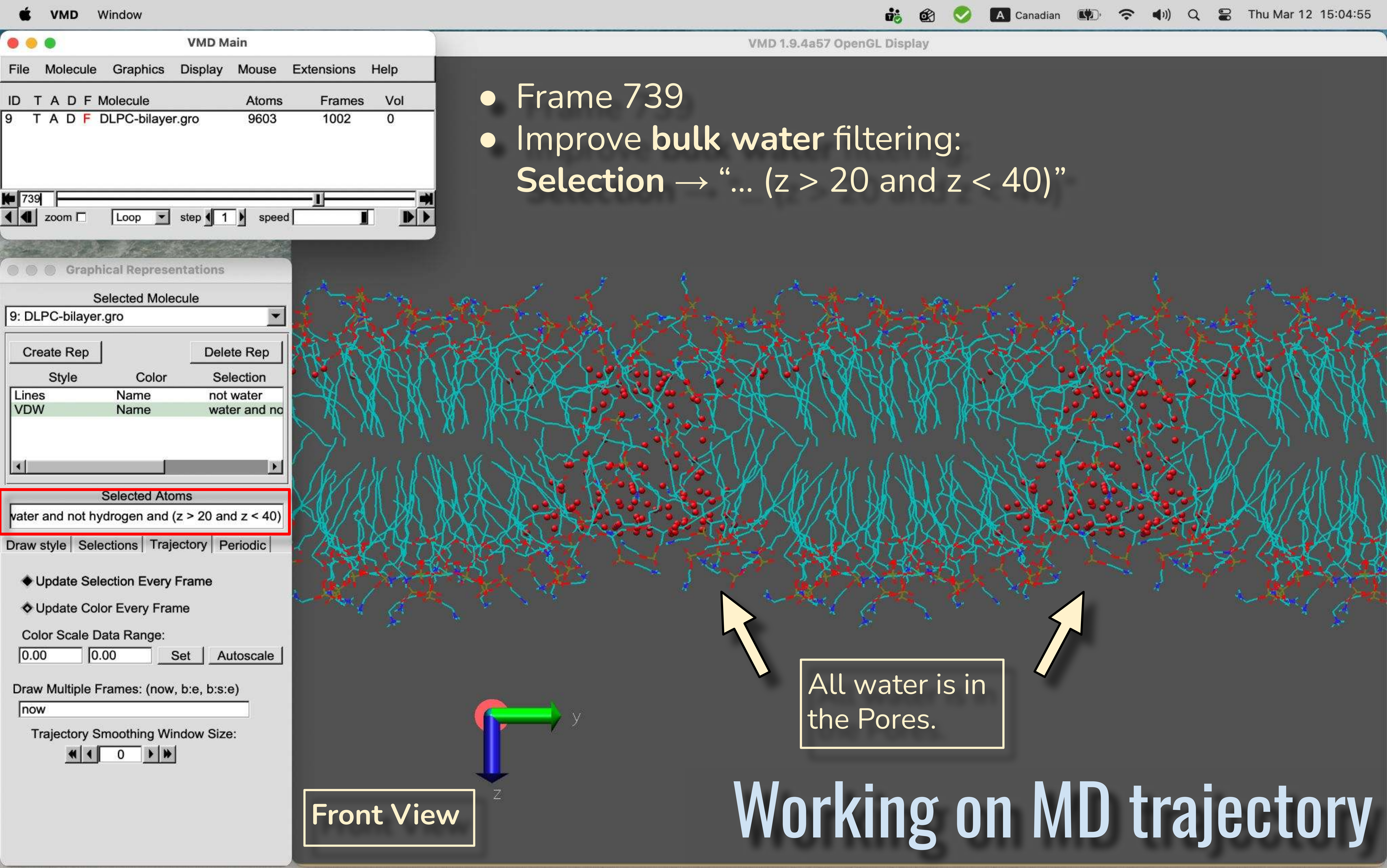
◆ Update Selection Every Frame

◇ Update Color Every Frame

Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e): now

Trajectory Smoothing Window Size: 0



- Frame 739
- Improve **bulk water** filtering:
  Selection → "... (z > 20 and z < 40)"

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

739 zoom ☐ Loop step 1 speed

Selected Molecule
9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms
vater and not hydrogen and (z > 20 and z < 40)

◆ Update Selection Every Frame

◇ Update Color Every Frame

Color Scale Data Range:
0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e)
now

Trajectory Smoothing Window Size:
0

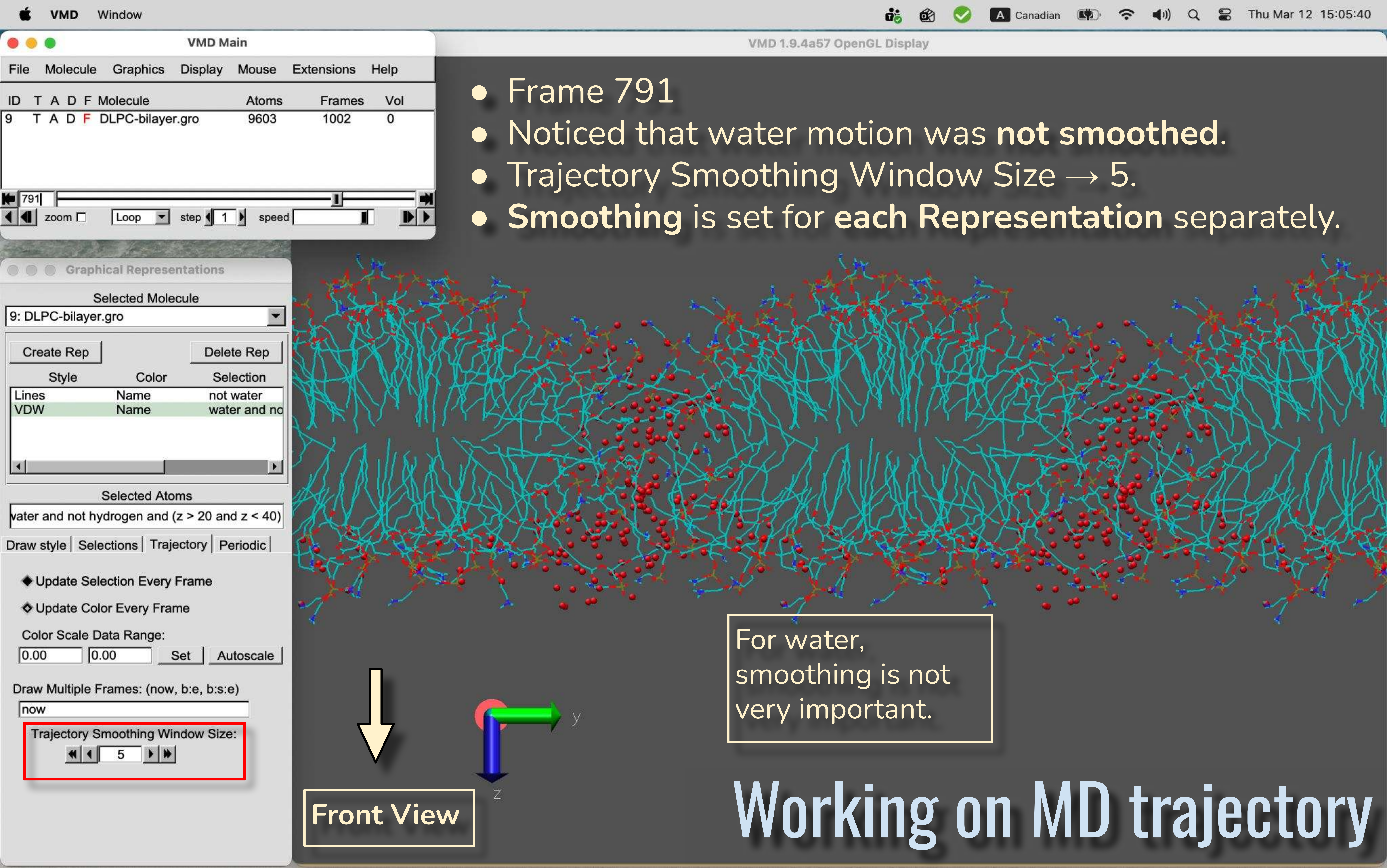
All water is in the Pores.

Front View

Working on MD trajectory

Working on MD trajectory

- Frame 791
- Noticed that water motion was **not smoothed**.
- Trajectory Smoothing Window Size → 5.
- **Smoothing** is set for **each Representation** separately.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

791

Loop

step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

◆ Update Selection Every Frame

◇ Update Color Every Frame

Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e) now

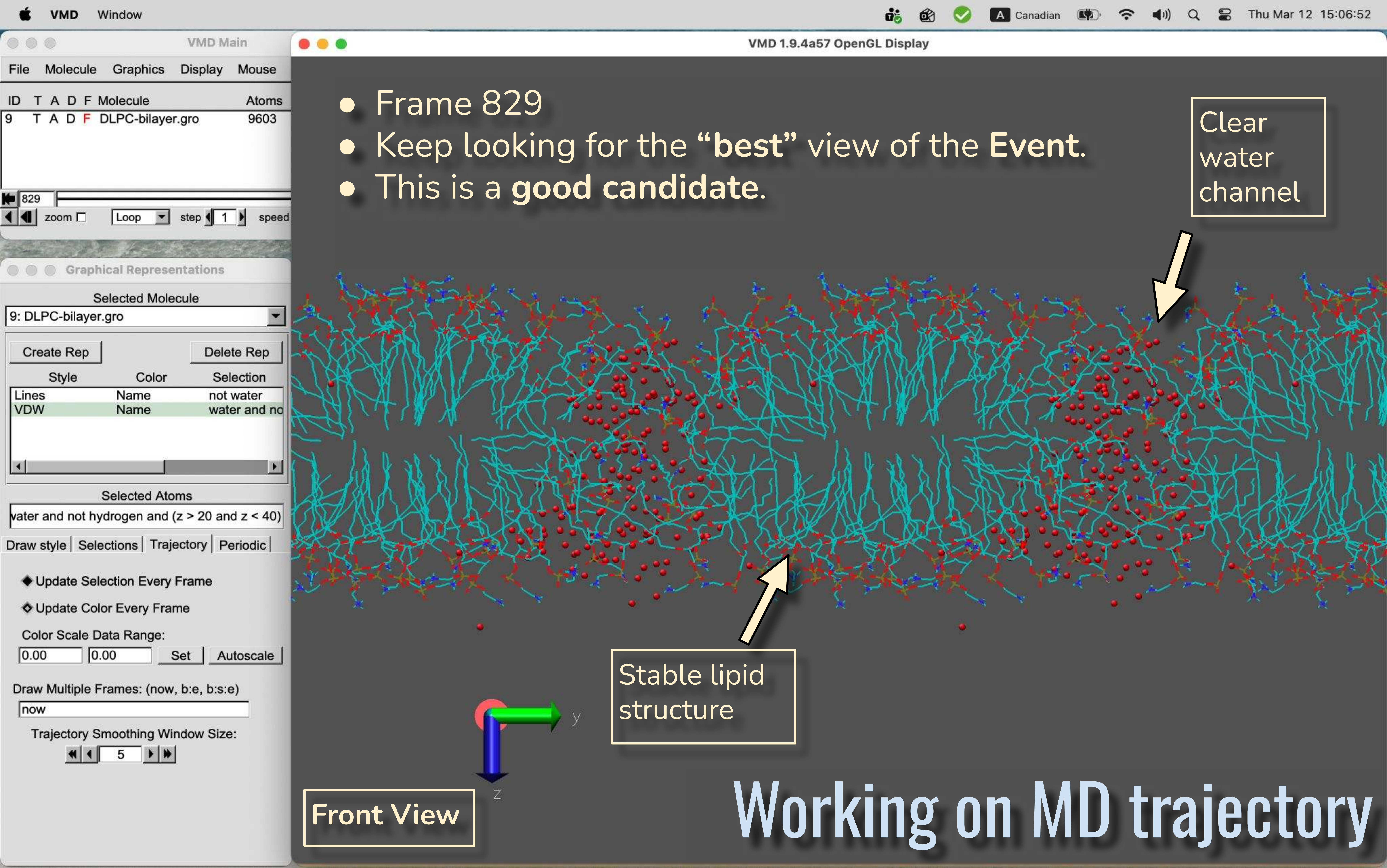
Trajectory Smoothing Window Size: 5

Front View

For water,
smoothing is not
very important.

Working on MD trajectory

- Frame 829
- Keep looking for the “**best**” view of the **Event**.
- This is a **good candidate**.



Clear water channel

Stable lipid structure

Front View

ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

829

zoom ☐ Loop step 1 speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

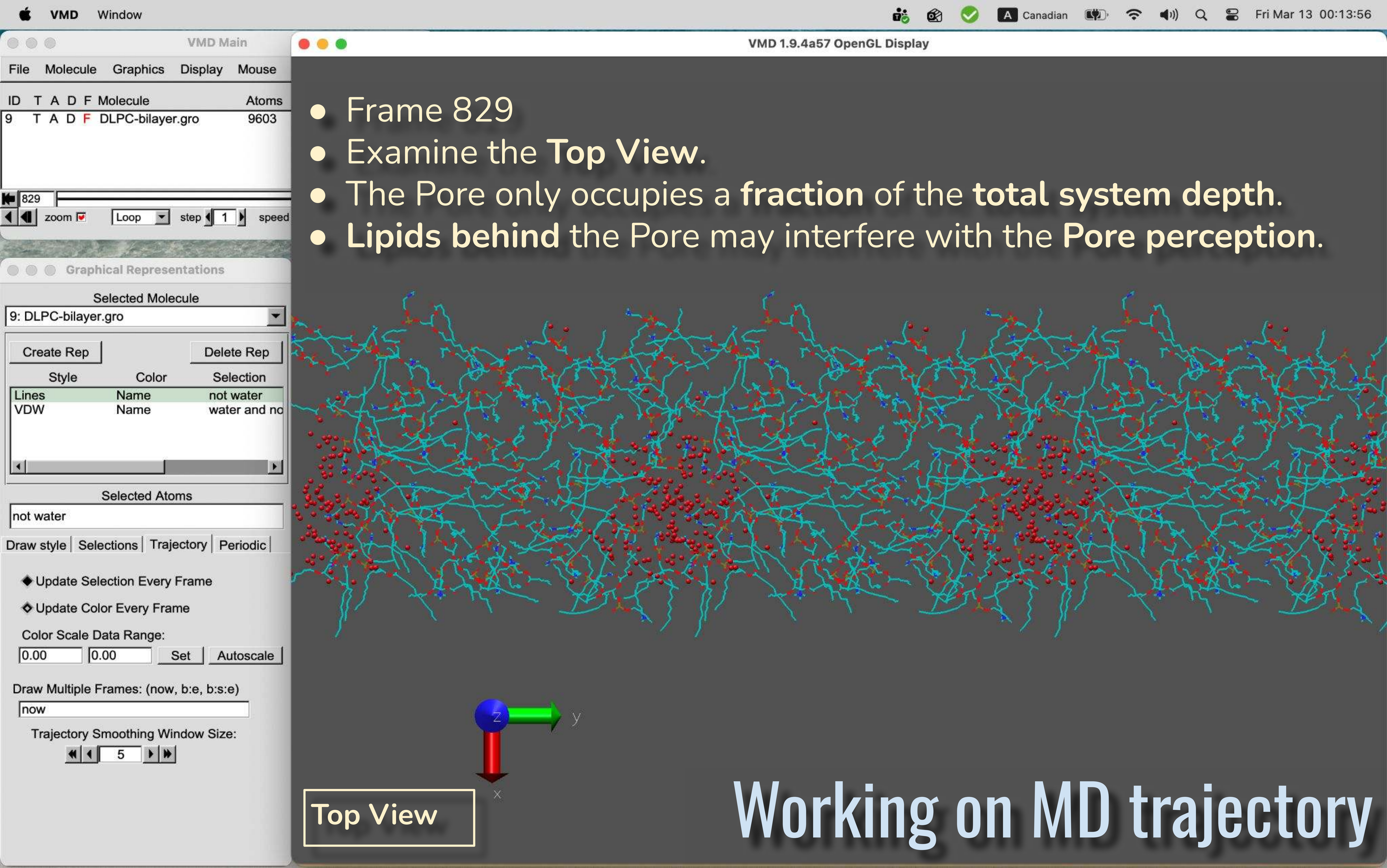
◆ Update Selection Every Frame

◇ Update Color Every Frame

Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e) now

Trajectory Smoothing Window Size: 5



- Frame 829
- Examine the **Top View**.
- The Pore only occupies a **fraction** of the **total system depth**.
- **Lipids behind** the Pore may interfere with the **Pore perception**.

Top View

Working on MD trajectory

ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

Frame: 829 · step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water
VDW	Name	water and no

Selected Atoms: not water

◆ Update Selection Every Frame

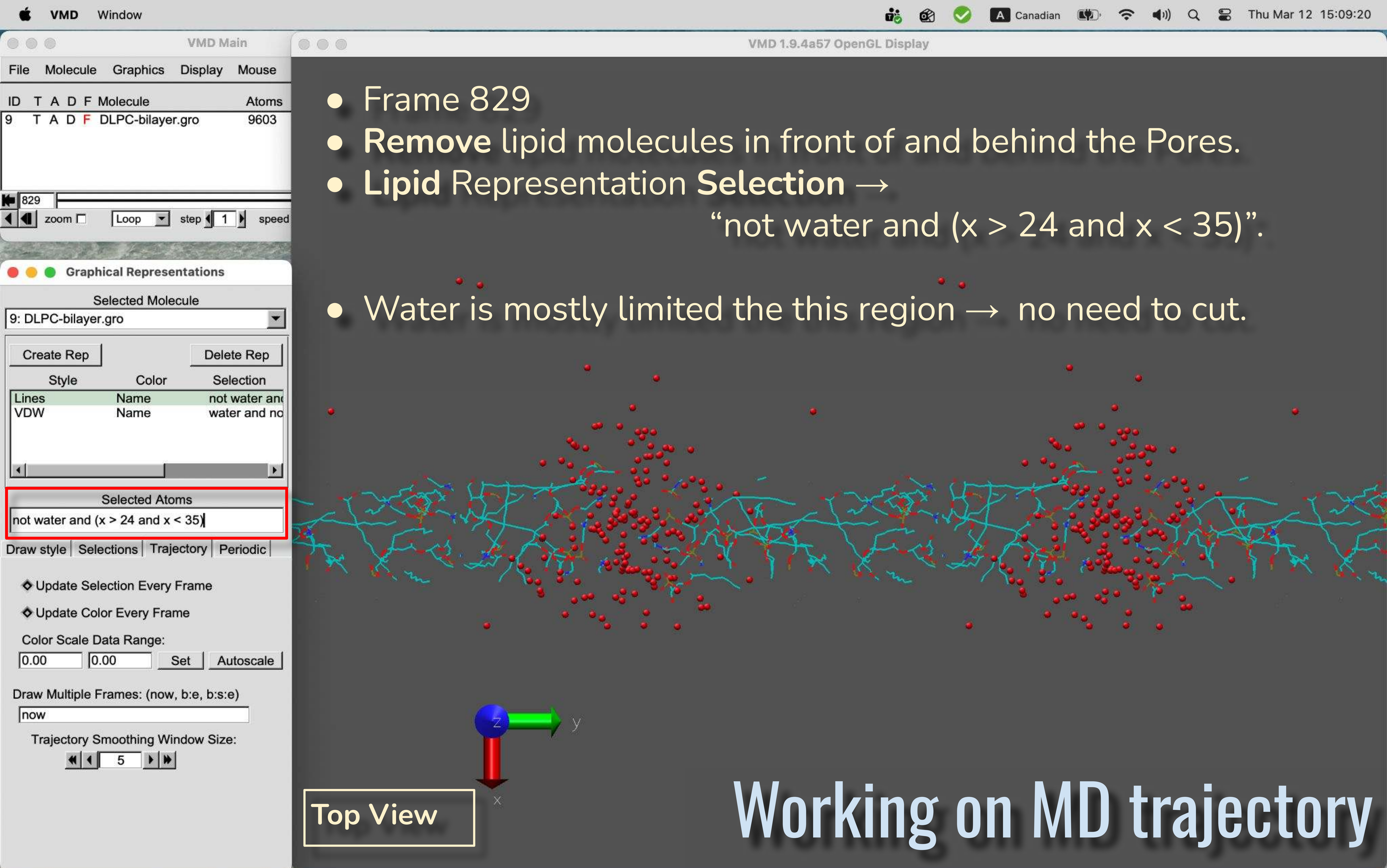
◇ Update Color Every Frame

Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e) now

Trajectory Smoothing Window Size: 5

Working on MD trajectory



- Frame 829
- **Remove** lipid molecules in front of and behind the Pores.
- **Lipid** Representation **Selection** →
  “not water and (x > 24 and x < 35)”.
- Water is mostly limited the this region → no need to cut.

ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

Frame: 829, step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water anc
VDW	Name	water and no

Selected Atoms: not water and (x > 24 and x < 35)

◆ Update Selection Every Frame

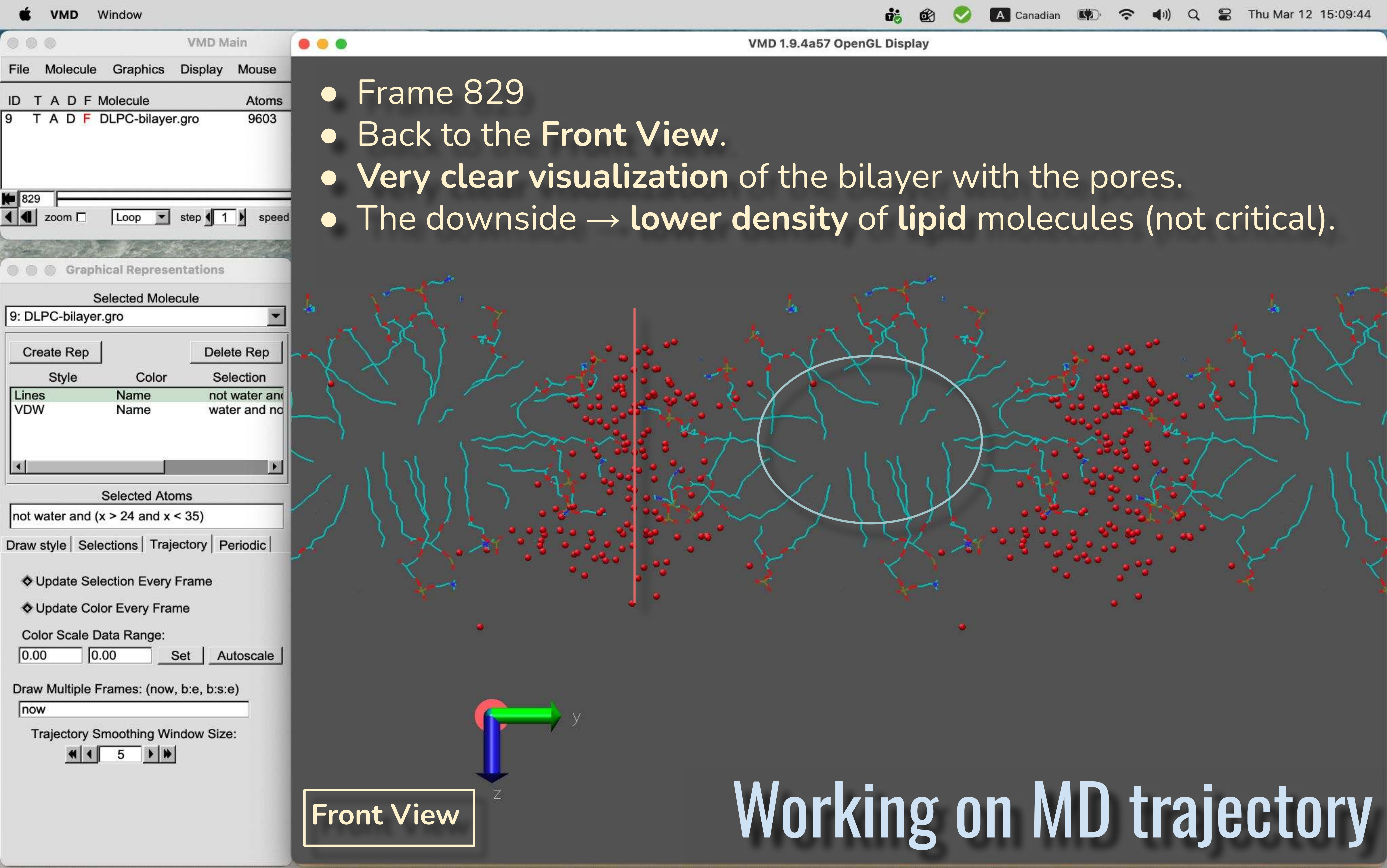
◆ Update Color Every Frame

Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e) now

Trajectory Smoothing Window Size: 5

Top View



- Frame 829
- Back to the **Front View**.
- **Very clear visualization** of the bilayer with the pores.
- The downside → **lower density** of **lipid** molecules (not critical).

ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

Frame: 829
step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Lines	Name	not water and
VDW	Name	water and no

Selected Atoms: not water and (x > 24 and x < 35)

◆ Update Selection Every Frame
◆ Update Color Every Frame

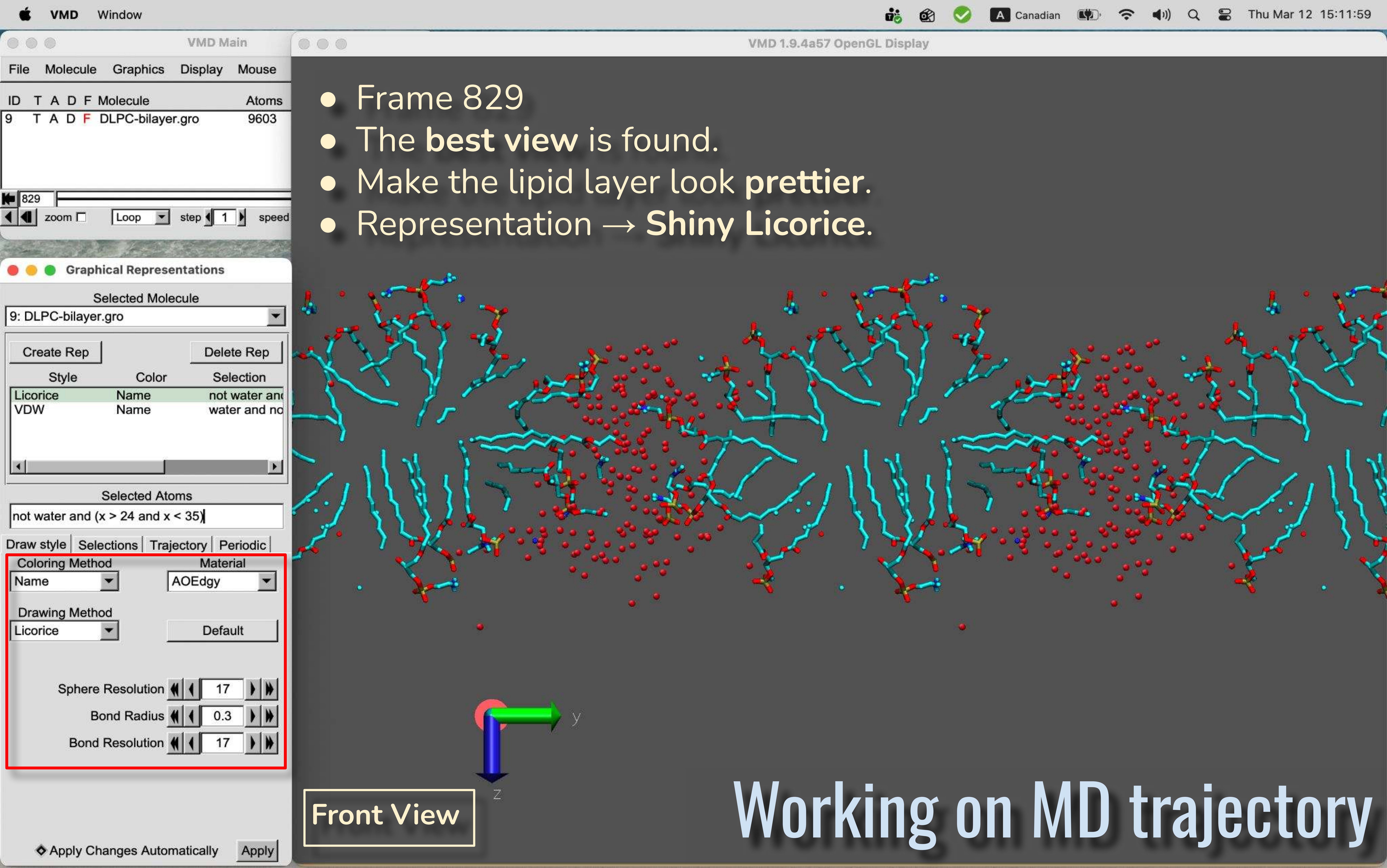
Color Scale Data Range: 0.00 0.00

Draw Multiple Frames: (now, b:e, b:s:e) now

Trajectory Smoothing Window Size: 5

Front View

Working on MD trajectory



- Frame 829
- The **best view** is found.
- Make the lipid layer look **prettier**.
- Representation → **Shiny Licorice**.

Front View

Working on MD trajectory

ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

Frame: 829

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

Selected Atoms: not water and (x > 24 and x < 35)

Coloring Method: Name

Material: AOEdgy

Drawing Method: Licorice

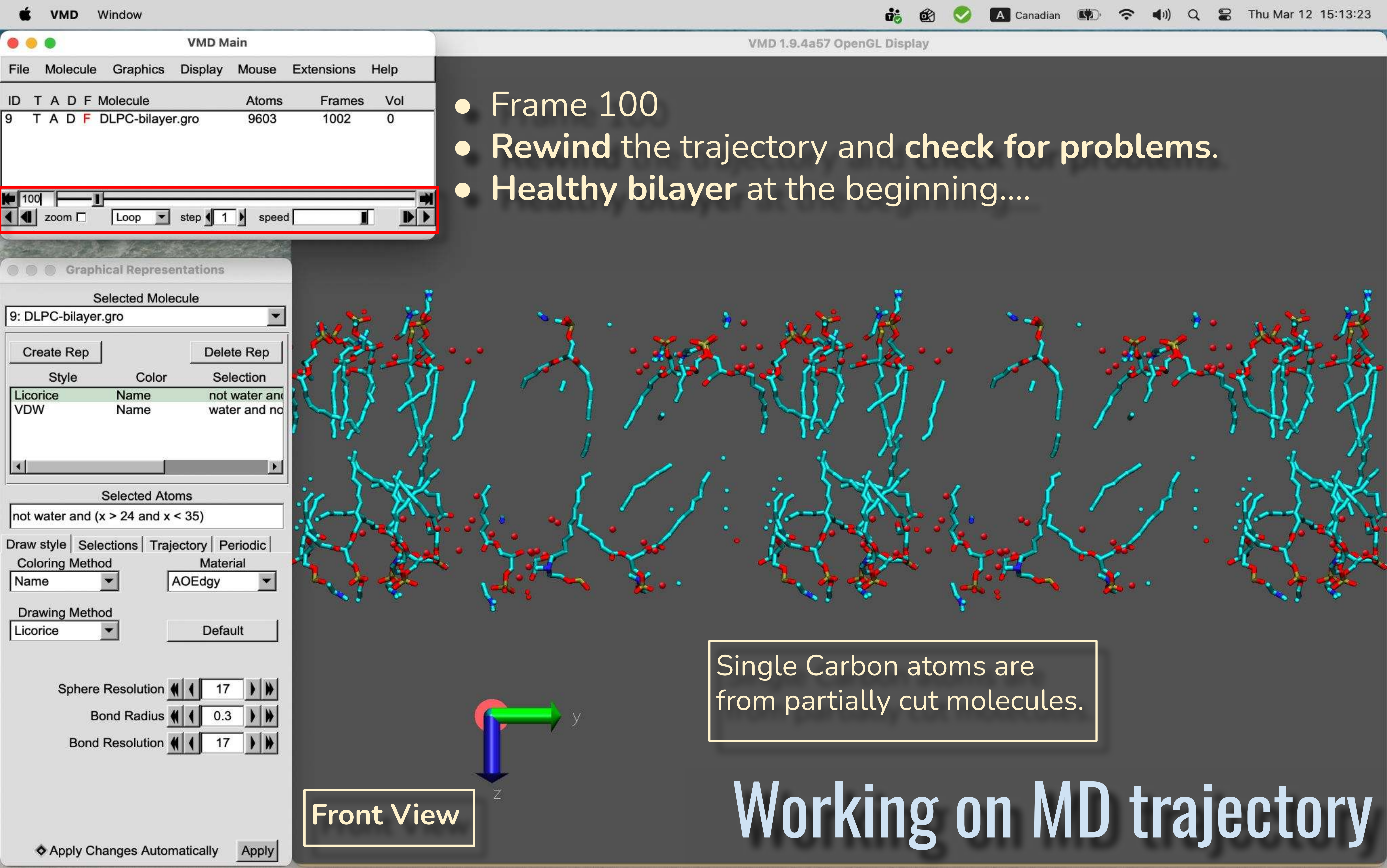
Sphere Resolution: 17

Bond Radius: 0.3

Bond Resolution: 17

Working on MD trajectory

- Frame 100
- **Rewind** the trajectory and **check for problems**.
- **Healthy bilayer** at the beginning….



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 100 step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

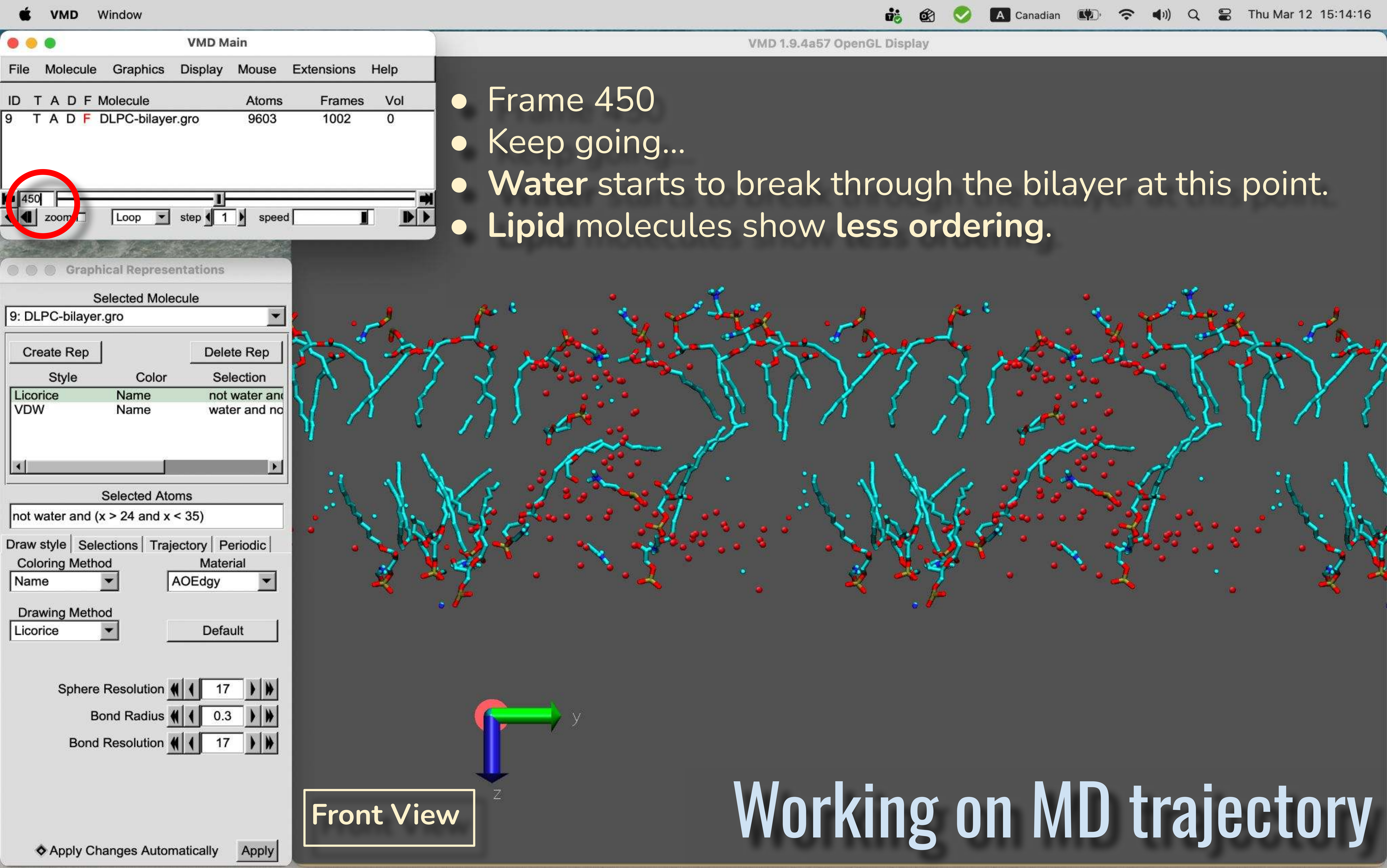
Selected Atoms: not water and (x > 24 and x < 35)

Coloring Method: Name
Material: AOEdgy
Drawing Method: Licorice
Sphere Resolution: 17
Bond Radius: 0.3
Bond Resolution: 17

Single Carbon atoms are from partially cut molecules.

Front View

Working on MD trajectory



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 450 · Loop · step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

Selected Atoms: not water and (x > 24 and x < 35)

Coloring Method: Name

Material: AOEdgy

Drawing Method: Licorice

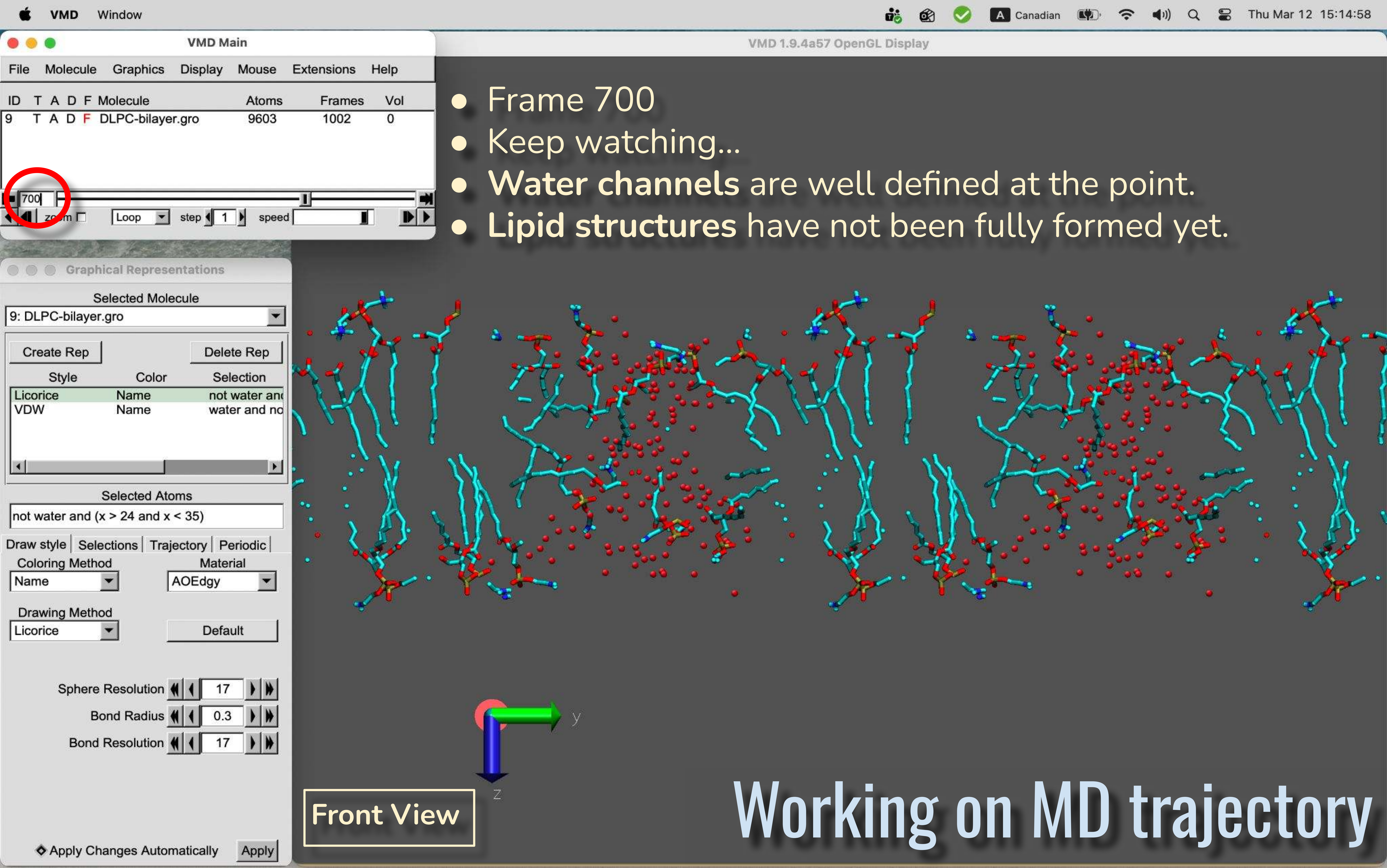
Sphere Resolution: 17

Bond Radius: 0.3

Bond Resolution: 17

- Frame 450
- Keep going…
- **Water** starts to break through the bilayer at this point.
- **Lipid** molecules show **less ordering**.

Front View



- Frame 700
- Keep watching…
- **Water channels** are well defined at the point.
- **Lipid structures** have not been fully formed yet.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 700

step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

Selected Atoms: not water and (x > 24 and x < 35)

Coloring Method: Name

Material: AOEdgy

Drawing Method: Licorice

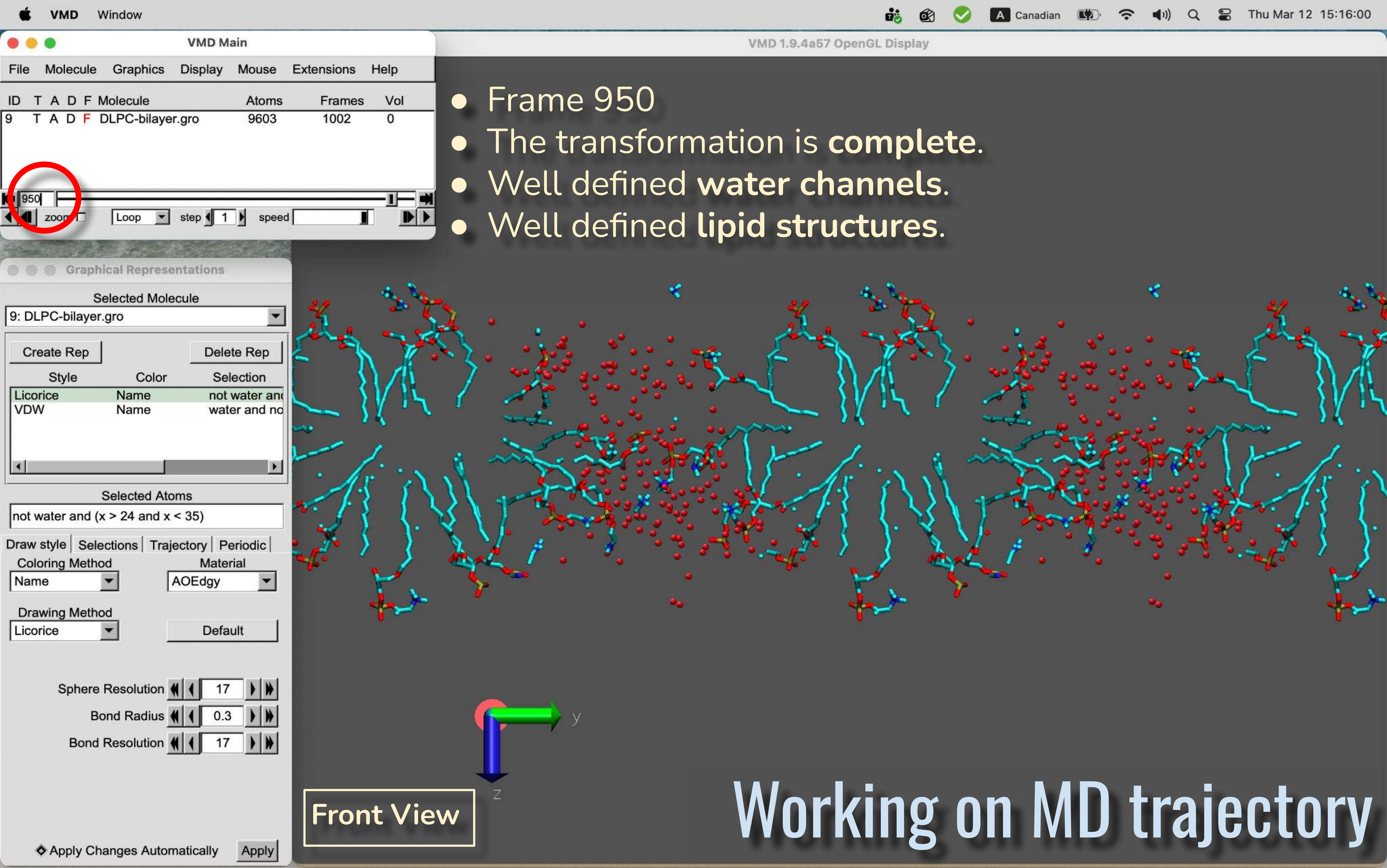
Sphere Resolution: 17

Bond Radius: 0.3

Bond Resolution: 17

Front View

Working on MD trajectory



- Frame 950
- The transformation is **complete**.
- Well defined **water channels**.
- Well defined **lipid structures**.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 950
Loop
step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

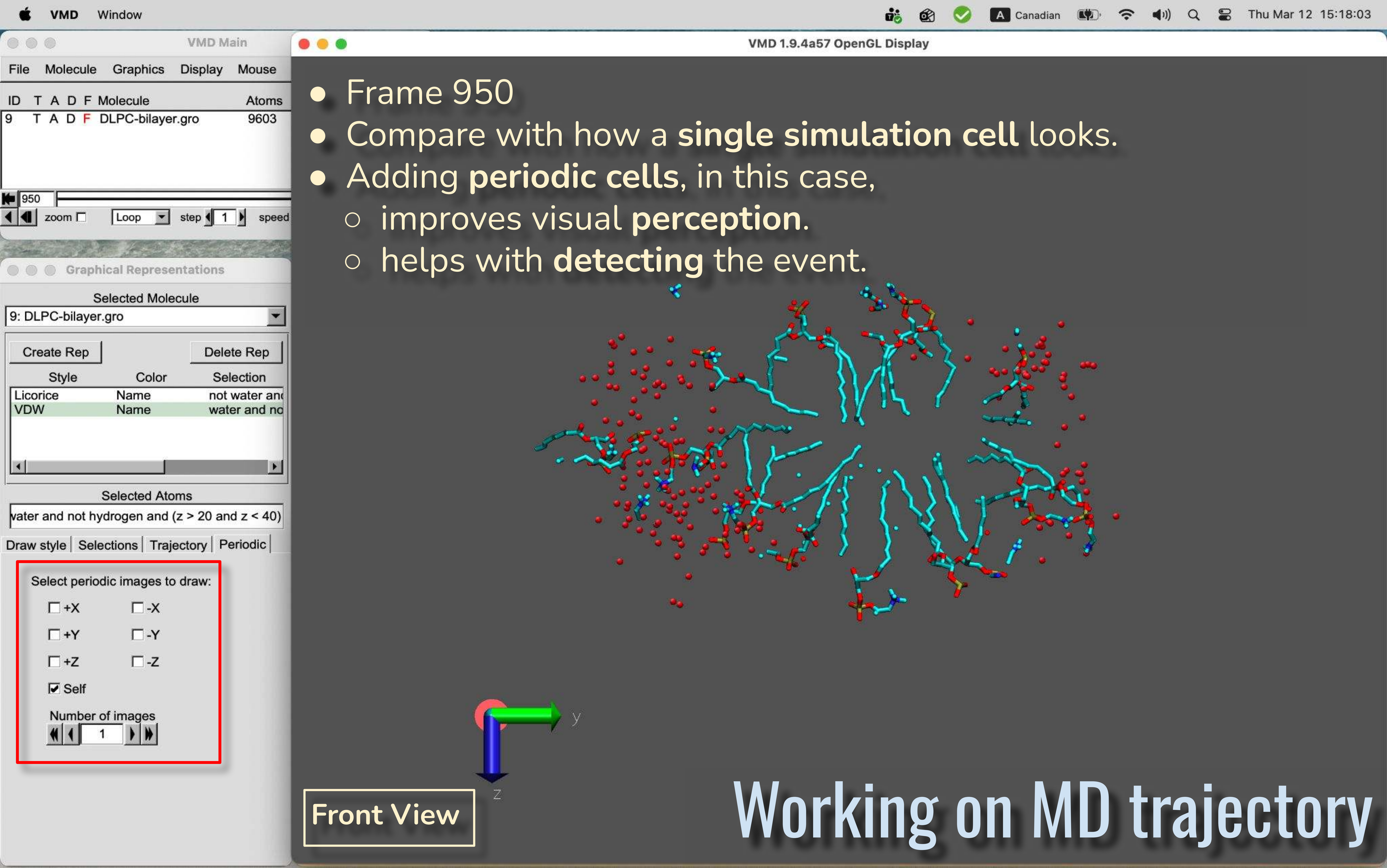
Selected Atoms: not water and (x > 24 and x < 35)

Coloring Method: Name
Material: AOEdgy
Drawing Method: Licorice
Sphere Resolution: 17
Bond Radius: 0.3
Bond Resolution: 17

◇ Apply Changes Automatically

Front View

Working on MD trajectory



- Frame 950
- Compare with how a **single simulation cell** looks.
- Adding **periodic cells**, in this case,
  - improves visual **perception**.
  - helps with **detecting** the event.

ID	T	A	D	F	Molecule	Atoms
9	T	A	D	F	DLPC-bilayer.gro	9603

Frame: 950

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

Select periodic images to draw:

☐ +X ☐ -X

☐ +Y ☐ -Y

☐ +Z ☐ -Z

☑ Self

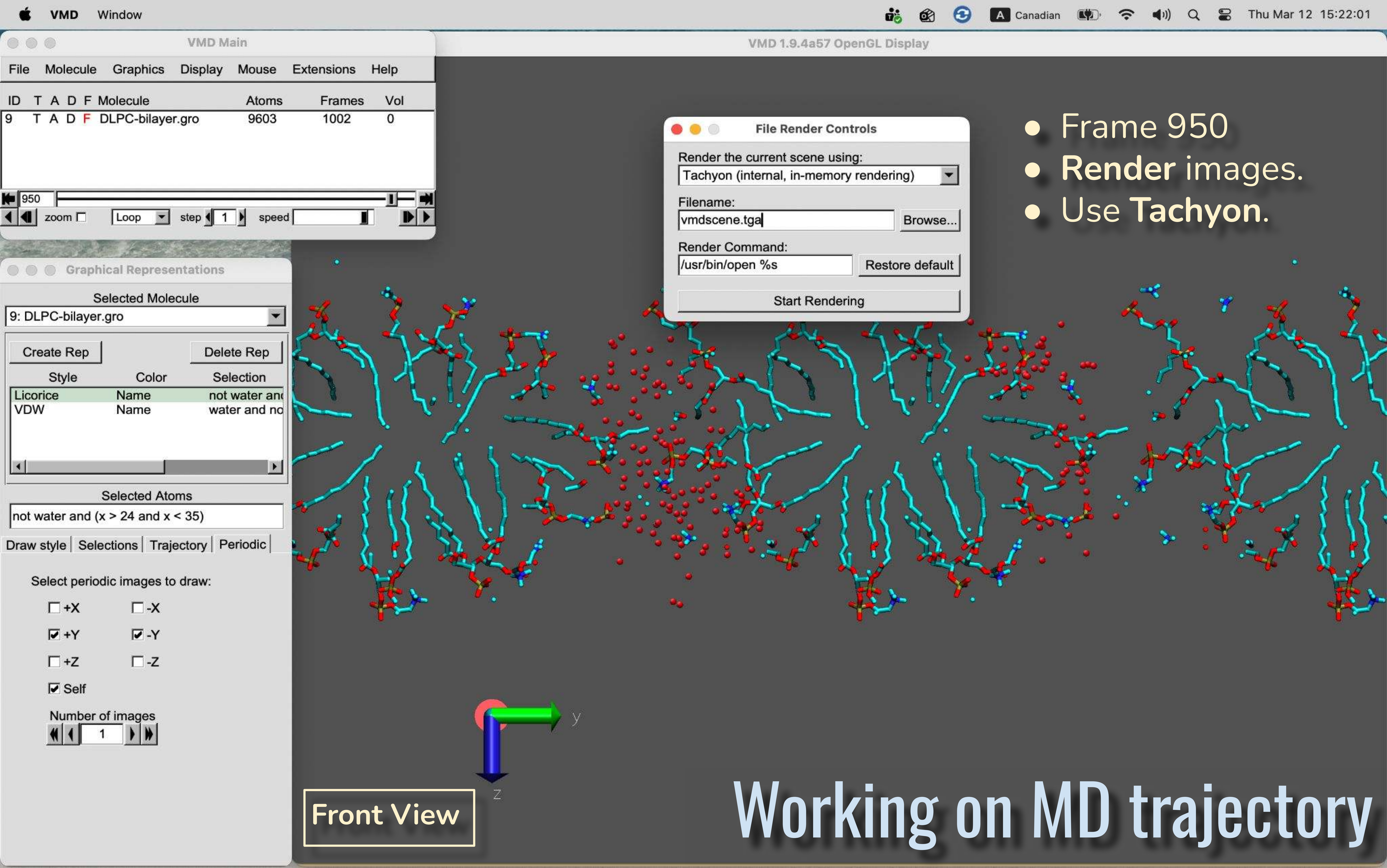
Number of images: 1

Front View

Working on MD trajectory

Working on MD trajectory

- Frame 950
- **Render** images.
- Use **Tachyon**.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 950

step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
Licorice	Name	not water and
VDW	Name	water and no

Selected Atoms: not water and (x > 24 and x < 35)

Select periodic images to draw:

☐ +X ☐ -X
☑ +Y ☑ -Y
☐ +Z ☐ -Z
☑ Self

Number of images: 1

Render the current scene using: Tachyon (internal, in-memory rendering)

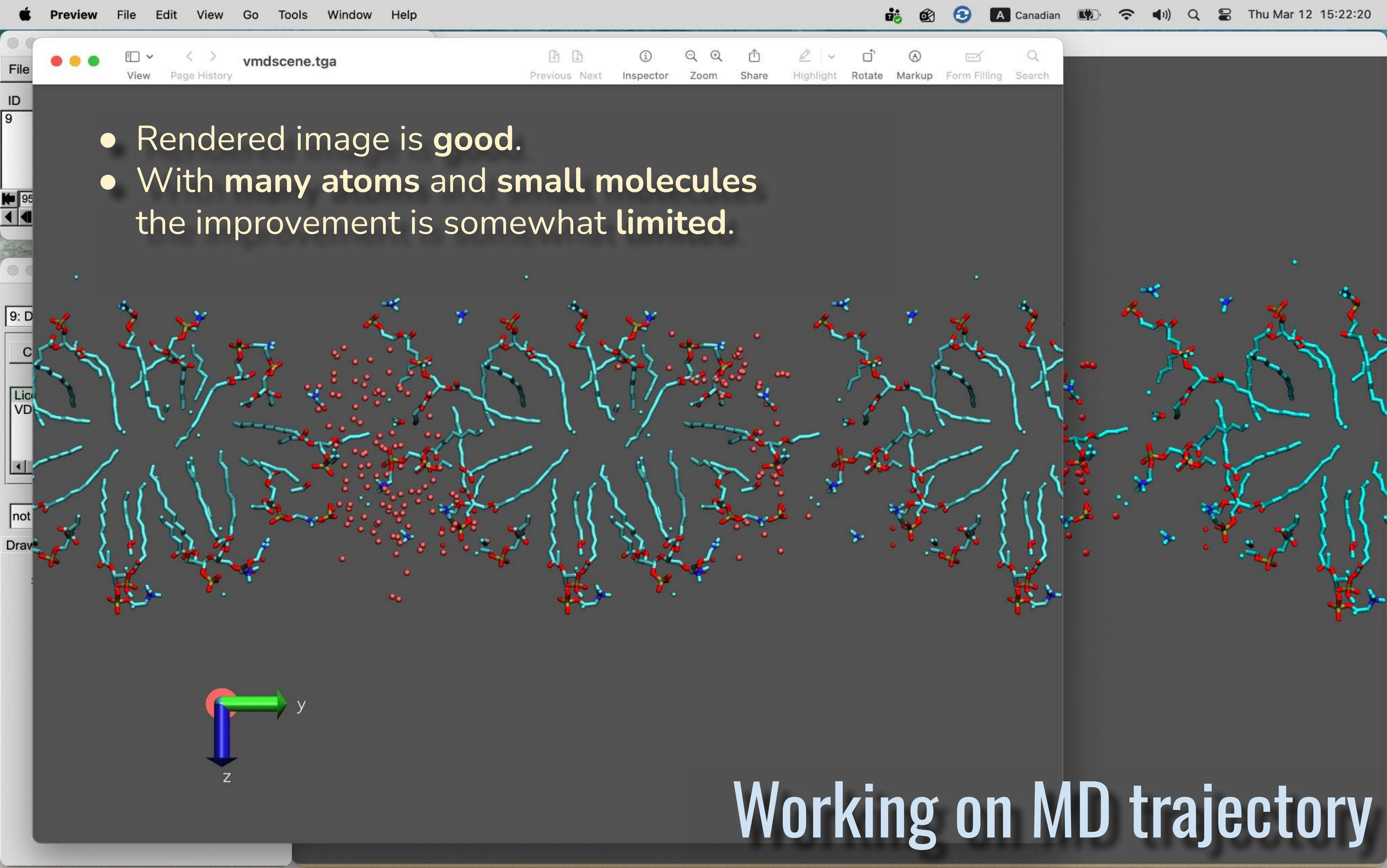
Filename: vmdscene.tga

Render Command: /usr/bin/open %s

Front View

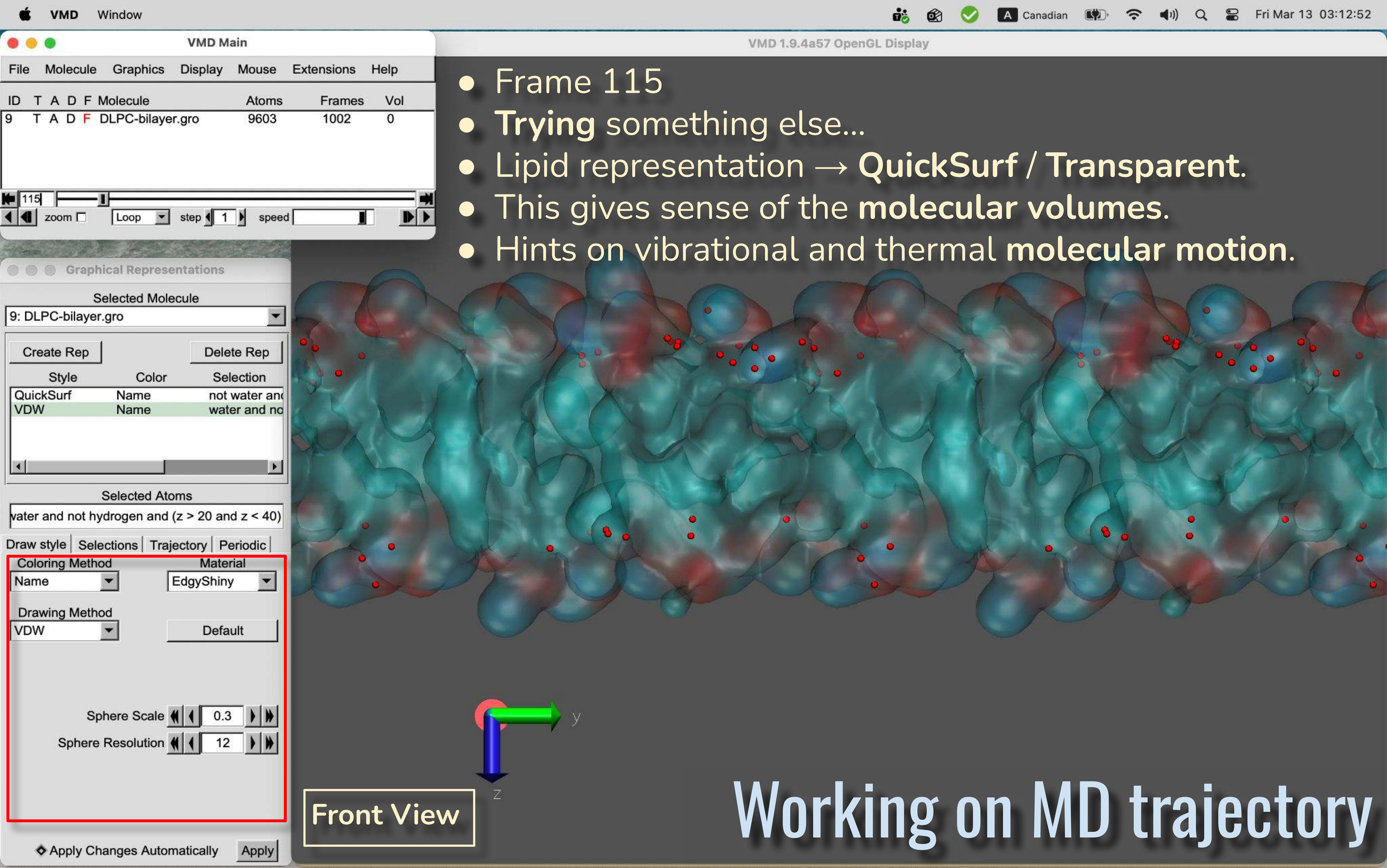
Working on MD trajectory

- Rendered image is **good**.
- With **many atoms** and **small molecules** the improvement is somewhat **limited**.



Working on MD trajectory

- Frame 115
- **Trying** something else…
- Lipid representation → **QuickSurf** / **Transparent**.
- This gives sense of the **molecular volumes**.
- Hints on vibrational and thermal **molecular motion**.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 115
step: 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
QuickSurf	Name	not water and
VDW	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

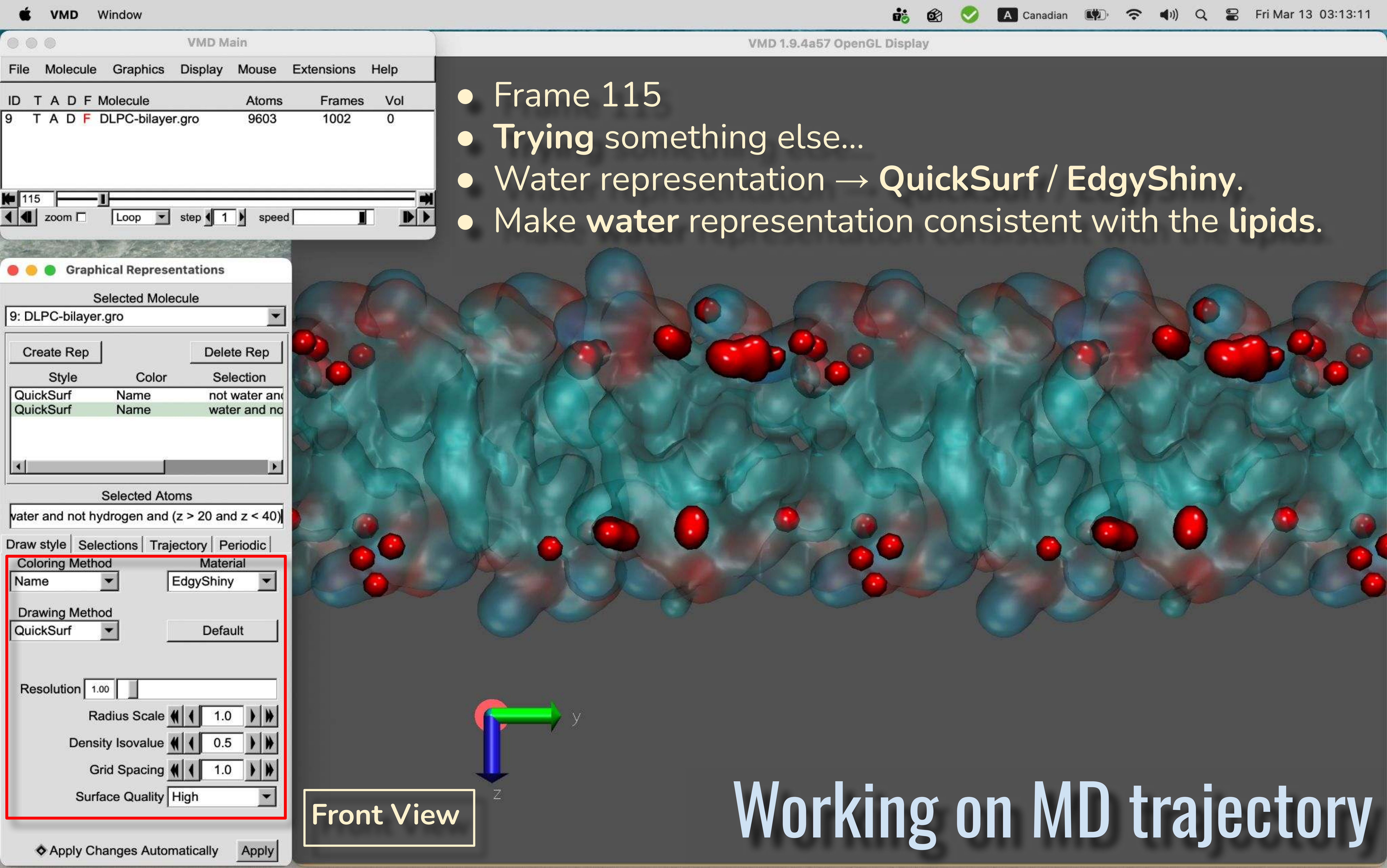
Coloring Method: Name

Material: EdgyShiny

Drawing Method: VDW

Sphere Scale: 0.3

Sphere Resolution: 12



- Frame 115
- **Trying** something else...
- Water representation → **QuickSurf** / **EdgyShiny**.
- Make **water** representation consistent with the **lipids**.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

115 zoom ☐ Loop step 1 speed

Selected Molecule: 9: DLPC-bilayer.gro

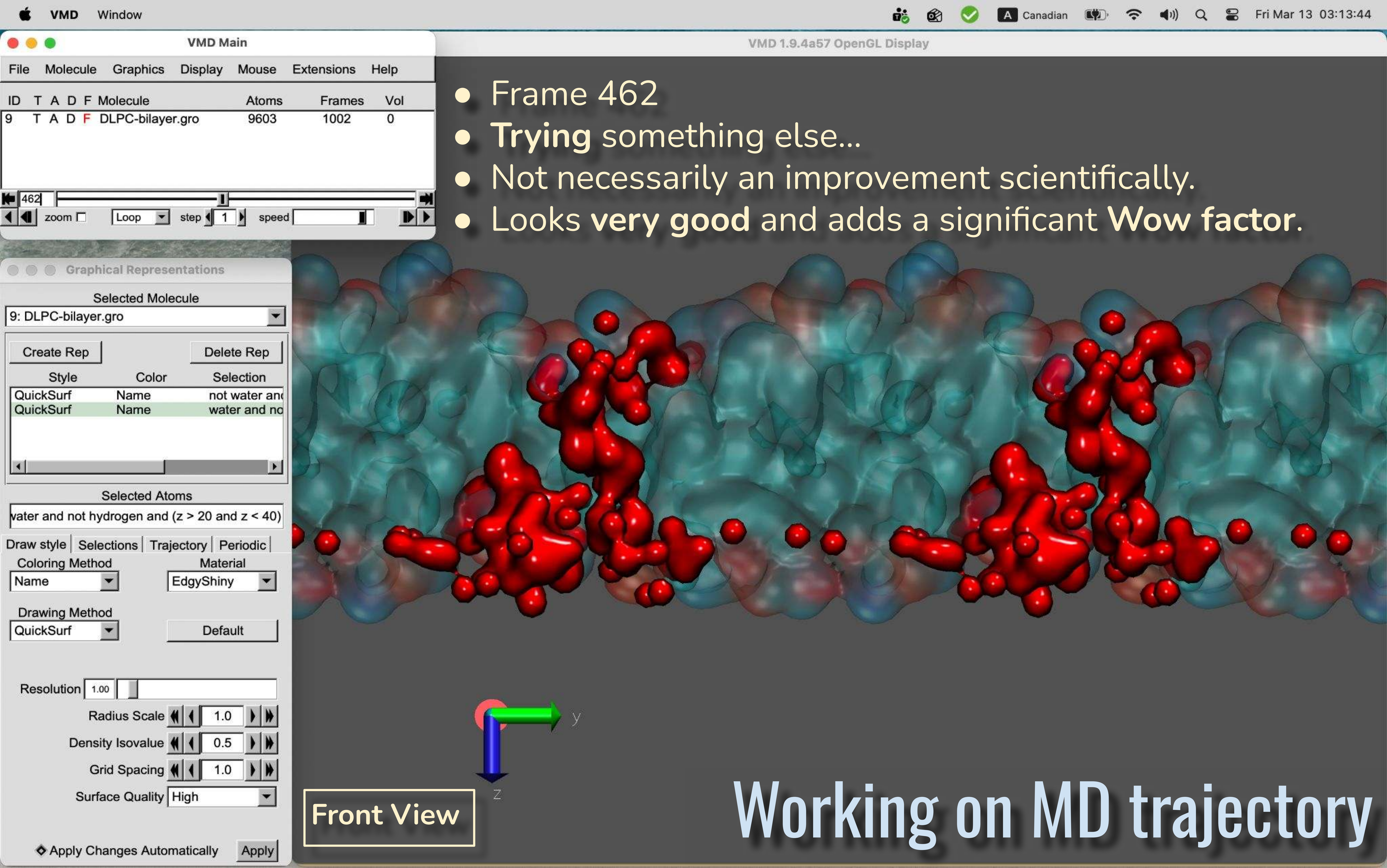
Style	Color	Selection
QuickSurf	Name	not water and
QuickSurf	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

Coloring Method: Name
Material: EdgyShiny
Drawing Method: QuickSurf
Resolution: 1.00
Radius Scale: 1.0
Density Isovalue: 0.5
Grid Spacing: 1.0
Surface Quality: High

Front View

Working on MD trajectory



- Frame 462
- **Trying** something else...
- Not necessarily an improvement scientifically.
- Looks **very good** and adds a significant **Wow factor**.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 462

zoom ☐ Loop step 1 speed

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
QuickSurf	Name	not water and
QuickSurf	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

Coloring Method: Name

Material: EdgyShiny

Drawing Method: QuickSurf

Resolution: 1.00

Radius Scale: 1.0

Density Isovalue: 0.5

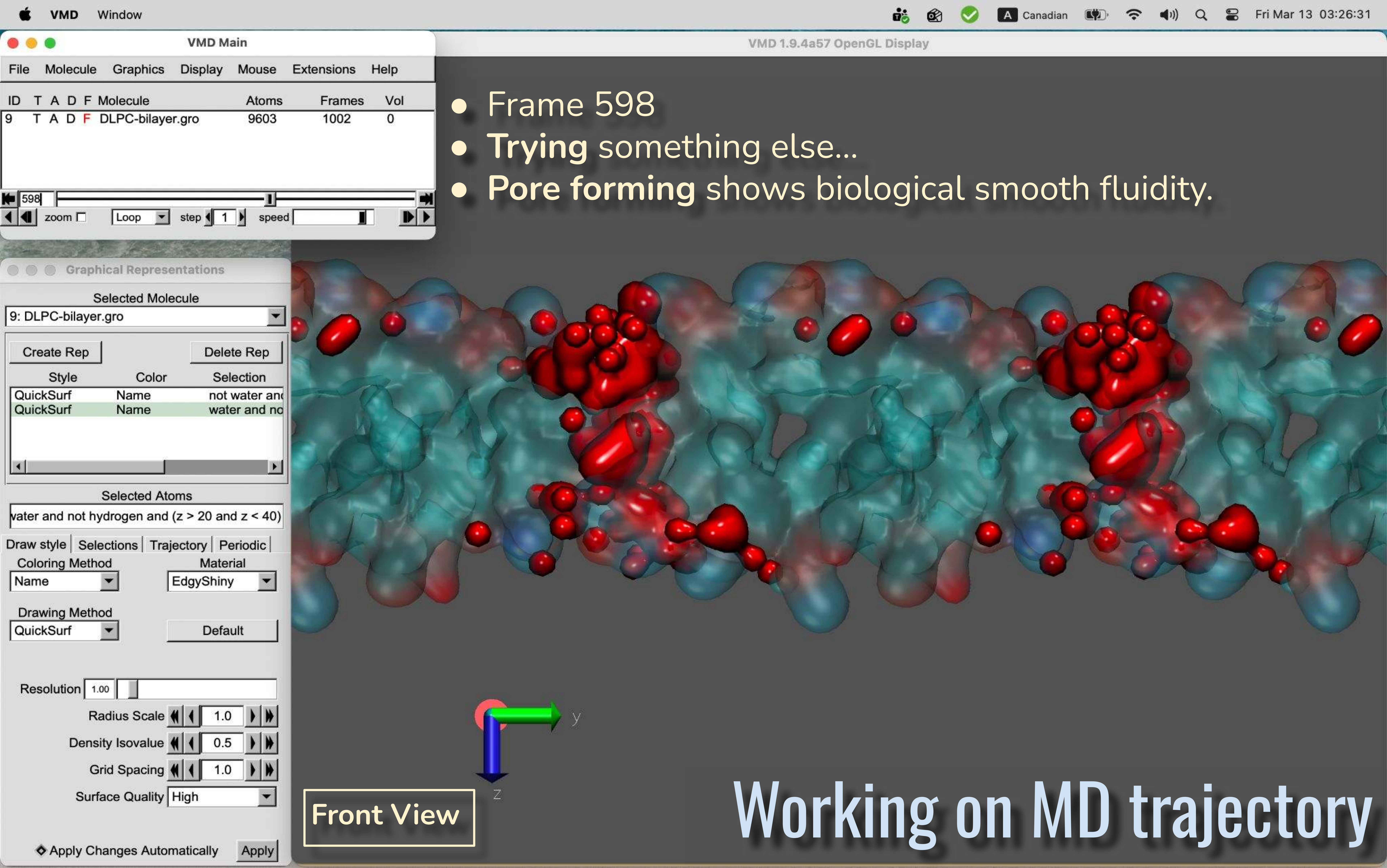
Grid Spacing: 1.0

Surface Quality: High

◇ Apply Changes Automatically

Front View

Working on MD trajectory



- Frame 598
- **Trying** something else...
- **Pore forming** shows biological smooth fluidity.

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

598 zoom ☐ Loop step 1 speed

Selected Molecule
9: DLPC-bilayer.gro

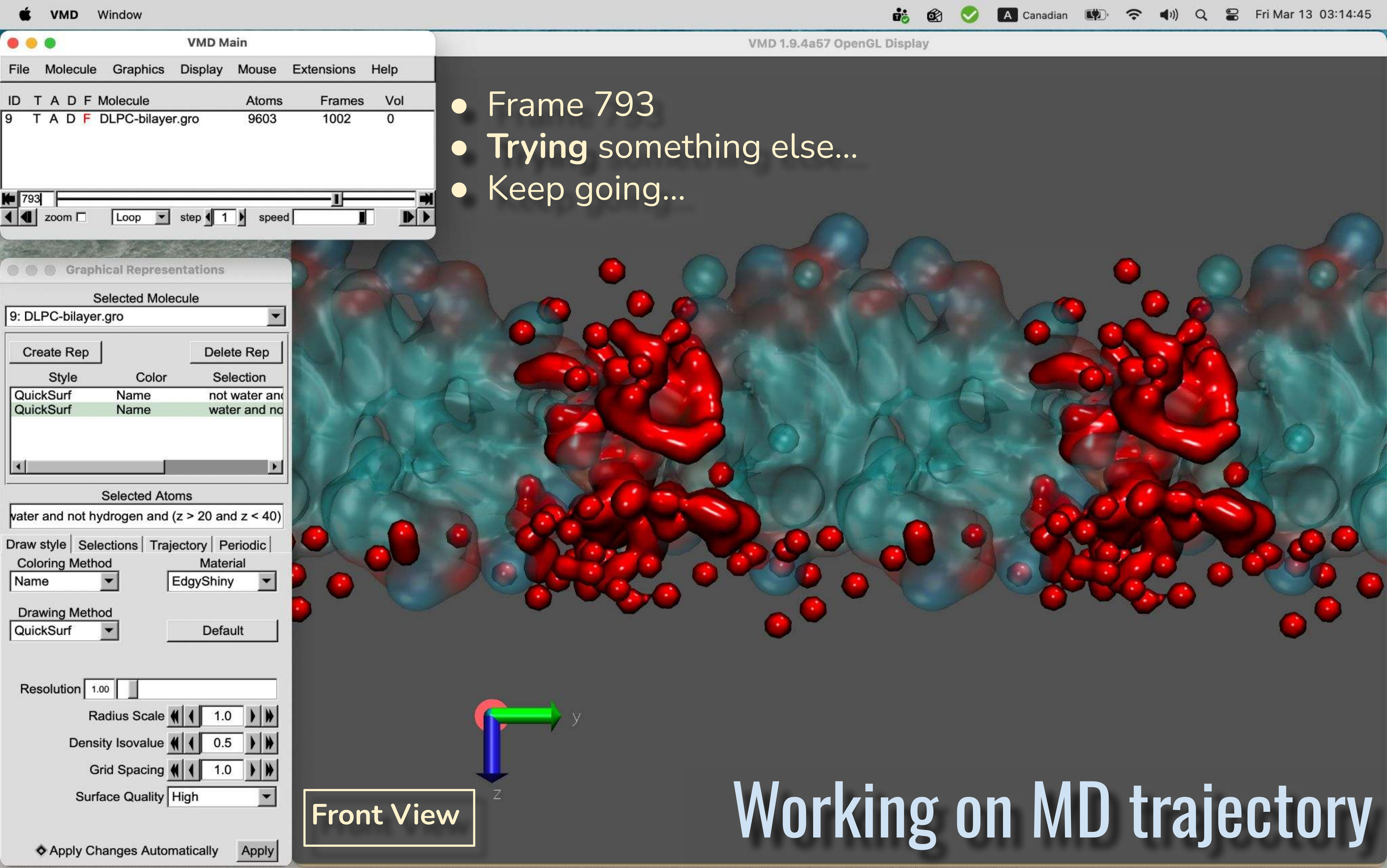
Style	Color	Selection
QuickSurf	Name	not water and
QuickSurf	Name	water and no

Selected Atoms
vater and not hydrogen and (z > 20 and z < 40)

Coloring Method: Name
Material: EdgyShiny
Drawing Method: QuickSurf
Resolution: 1.00
Radius Scale: 1.0
Density Isovalue: 0.5
Grid Spacing: 1.0
Surface Quality: High
◆ Apply Changes Automatically

Front View

Working on MD trajectory



- Frame 793
- **Trying** something else...
- Keep going...

Front View

Working on MD trajectory

ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

793

step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
QuickSurf	Name	not water an
QuickSurf	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

Coloring Method: Name

Material: EdgyShiny

Drawing Method: QuickSurf

Resolution 1.00

Radius Scale 1.0

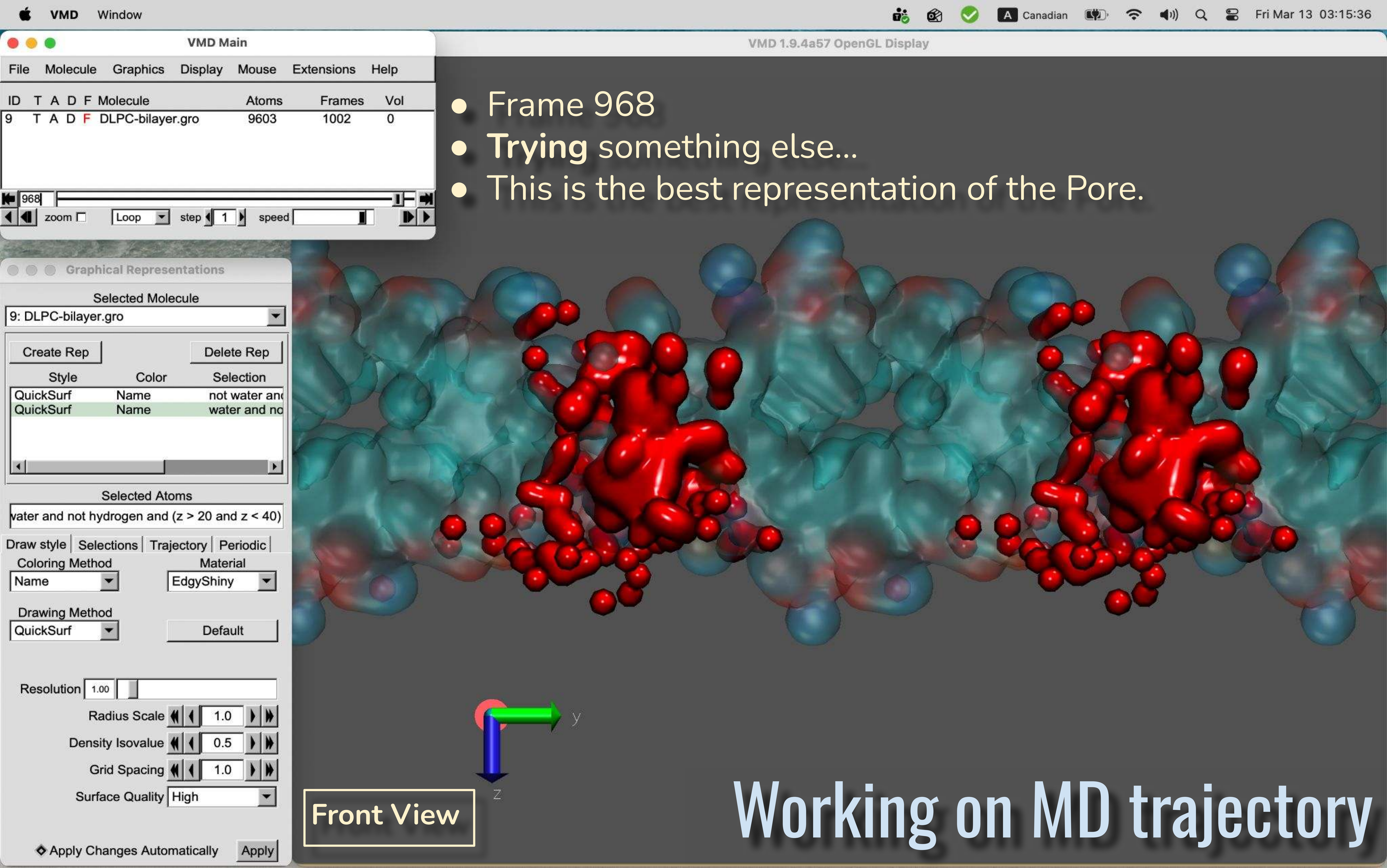
Density Isovalue 0.5

Grid Spacing 1.0

Surface Quality High

Working on MD trajectory

- Frame 968
- **Trying** something else…
- This is the best representation of the Pore.



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Frame: 968 · step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Color	Selection
QuickSurf	Name	not water anc
QuickSurf	Name	water and no

Selected Atoms: vater and not hydrogen and (z > 20 and z < 40)

Coloring Method: Name

Material: EdgyShiny

Drawing Method: QuickSurf

Resolution: 1.00

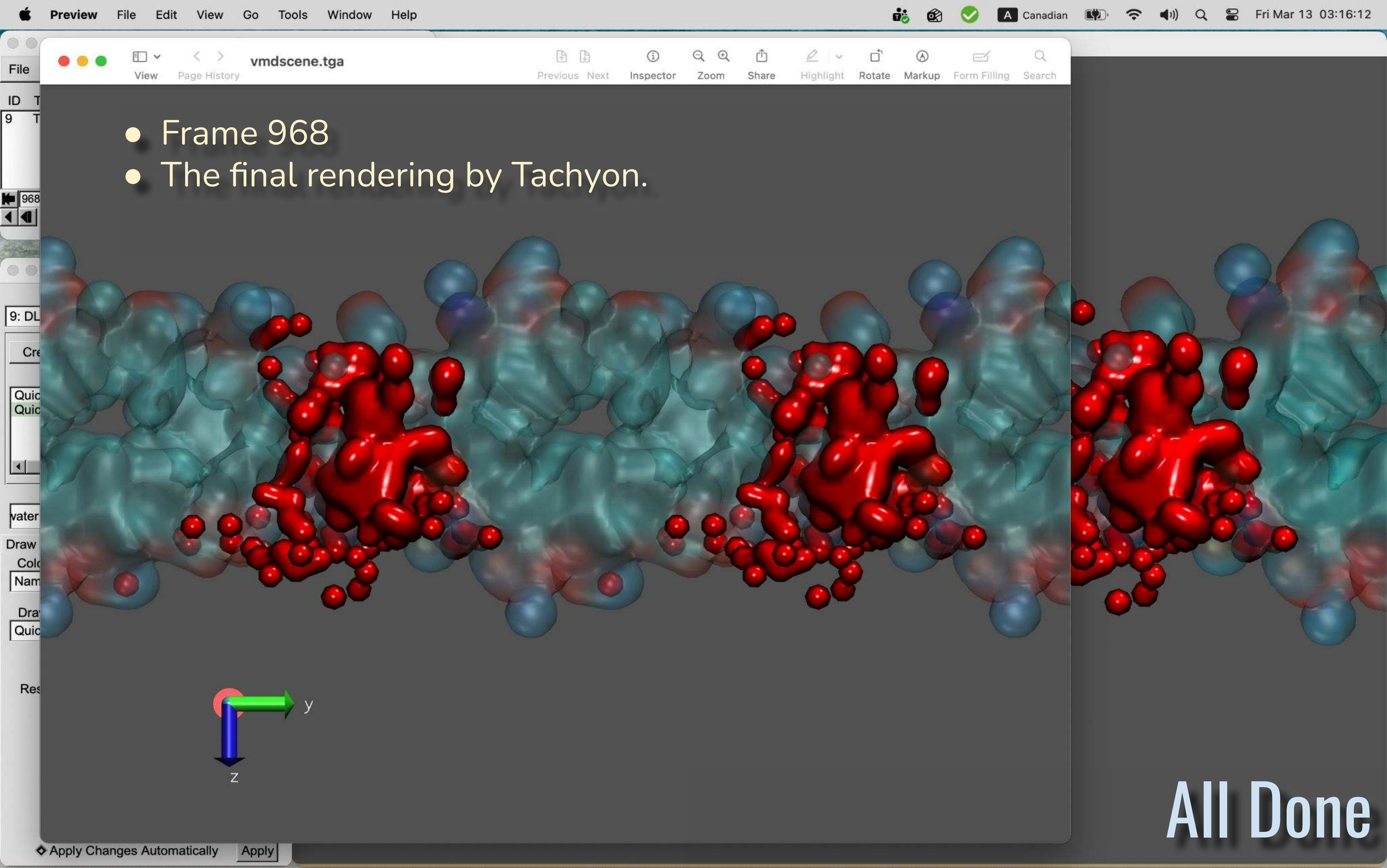
Radius Scale: 1.0

Density Isovalue: 0.5

Grid Spacing: 1.0

Surface Quality: High

Front View

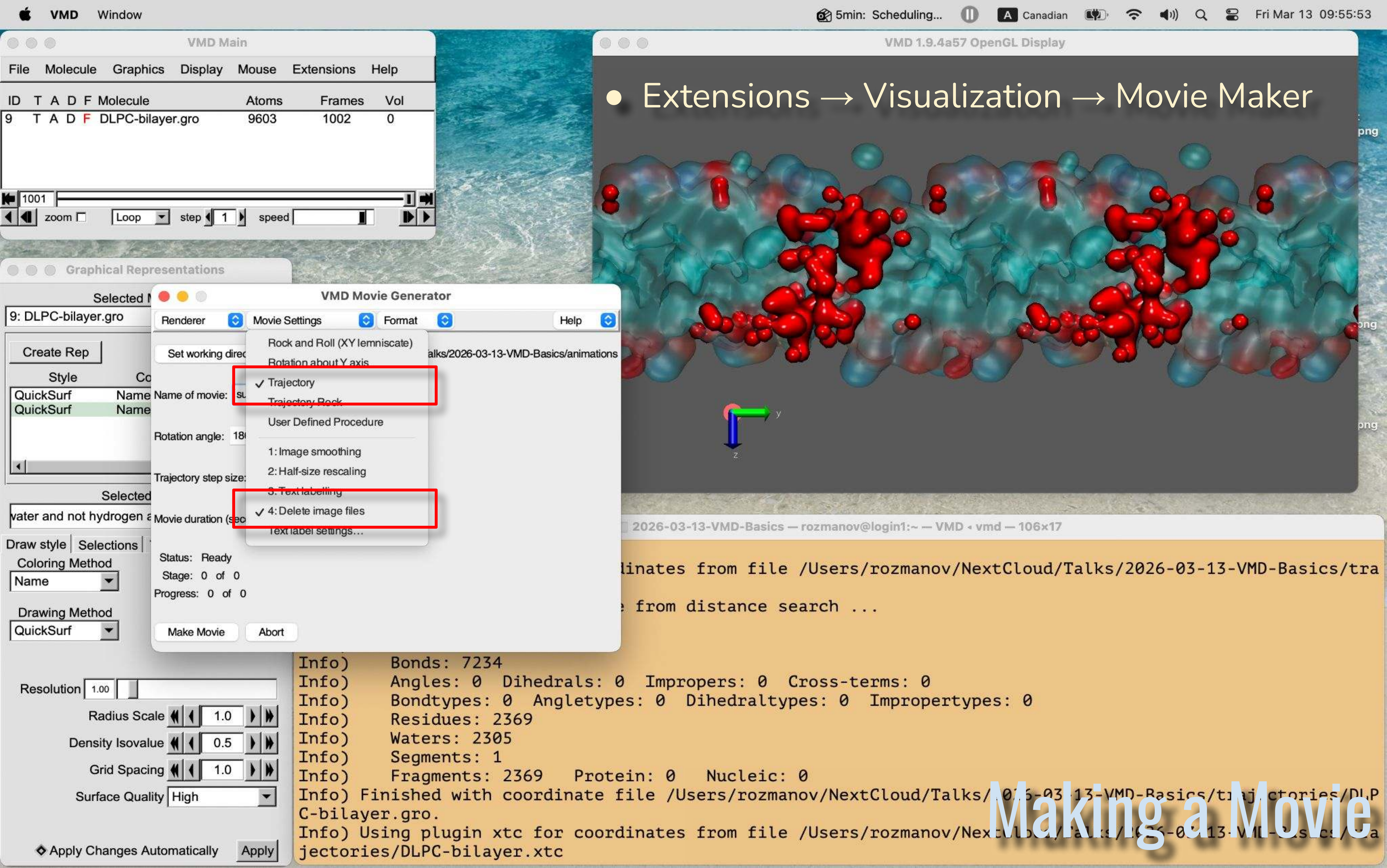


- Frame 968
- The final rendering by Tachyon.

All Done

Making a Movie

- Extensions → Visualization → Movie Maker



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

1001

Loop

step 1

Selected Molecule: 9: DLPC-bilayer.gro

Style	Co
QuickSurf	Name
QuickSurf	Name

Selected: vater and not hydrogen a

Coloring Method: Name

Drawing Method: QuickSurf

Resolution: 1.00

Radius Scale: 1.0

Density Isovalue: 0.5

Grid Spacing: 1.0

Surface Quality: High

◇ Apply Changes Automatically

Apply

alks/2026-03-13-VMD-Basics/animations

Name of movie: su

Rotation angle: 18

Status: Ready

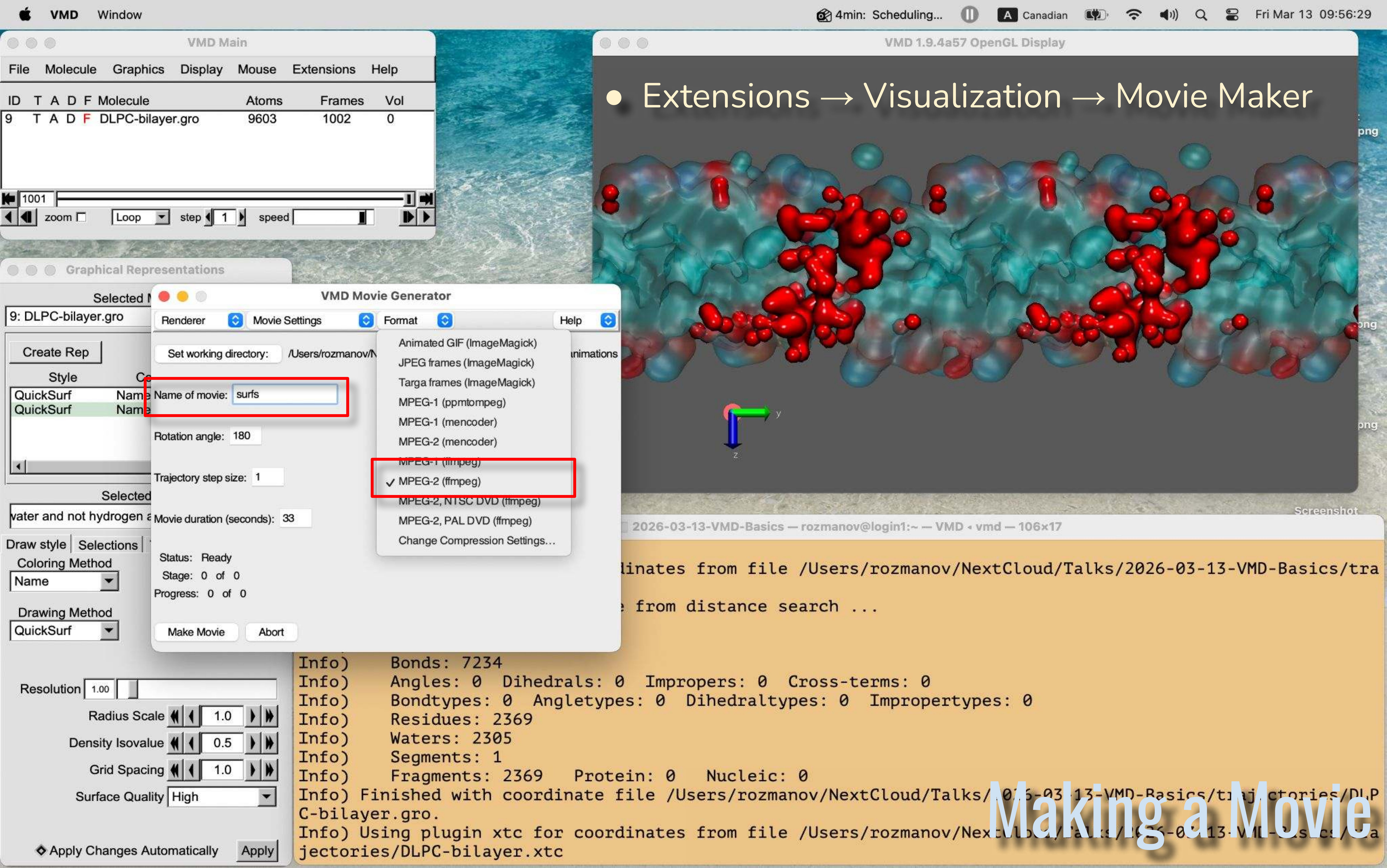
Stage: 0 of 0

Progress: 0 of 0

```
inates from file /Users/rozmanov/NextCloud/Talks/2026-03-13-VMD-Basics/tra

 from distance search ...

Info)    Bonds: 7234
Info)    Angles: 0  Dihedrals: 0  Impropers: 0  Cross-terms: 0
Info)    Bondtypes: 0  Angletypes: 0  Dihedraltypes: 0  Impropertypes: 0
Info)    Residues: 2369
Info)    Waters: 2305
Info)    Segments: 1
Info)    Fragments: 2369   Protein: 0   Nucleic: 0
Info) Finished with coordinate file /Users/rozmanov/NextCloud/Talks/2026-03-13-VMD-Basics/trajectories/DLP
C-bilayer.gro.
Info) Using plugin xtc for coordinates from file /Users/rozmanov/NextCloud/Talks/2026-03-13-VMD-Basics/tra
jectories/DLPC-bilayer.xtc
```

Making a Movie

- Extensions → Visualization → Movie Maker



ID	T	A	D	F	Molecule	Atoms	Frames	Vol
9	T	A	D	F	DLPC-bilayer.gro	9603	1002	0

Selected Molecule: 9: DLPC-bilayer.gro

Style	Coloring
QuickSurf	Name
QuickSurf	Name

Selected Atoms: water and not hydrogen

Coloring Method: Name

Drawing Method: QuickSurf

Resolution: 1.00

Radius Scale: 1.0

Density Isovalue: 0.5

Grid Spacing: 1.0

Surface Quality: High

Set working directory: /Users/rozmanov/N animations

Name of movie: surfs

Rotation angle: 180

Trajectory step size: 1

Movie duration (seconds): 33

Status: Ready

Stage: 0 of 0

Progress: 0 of 0

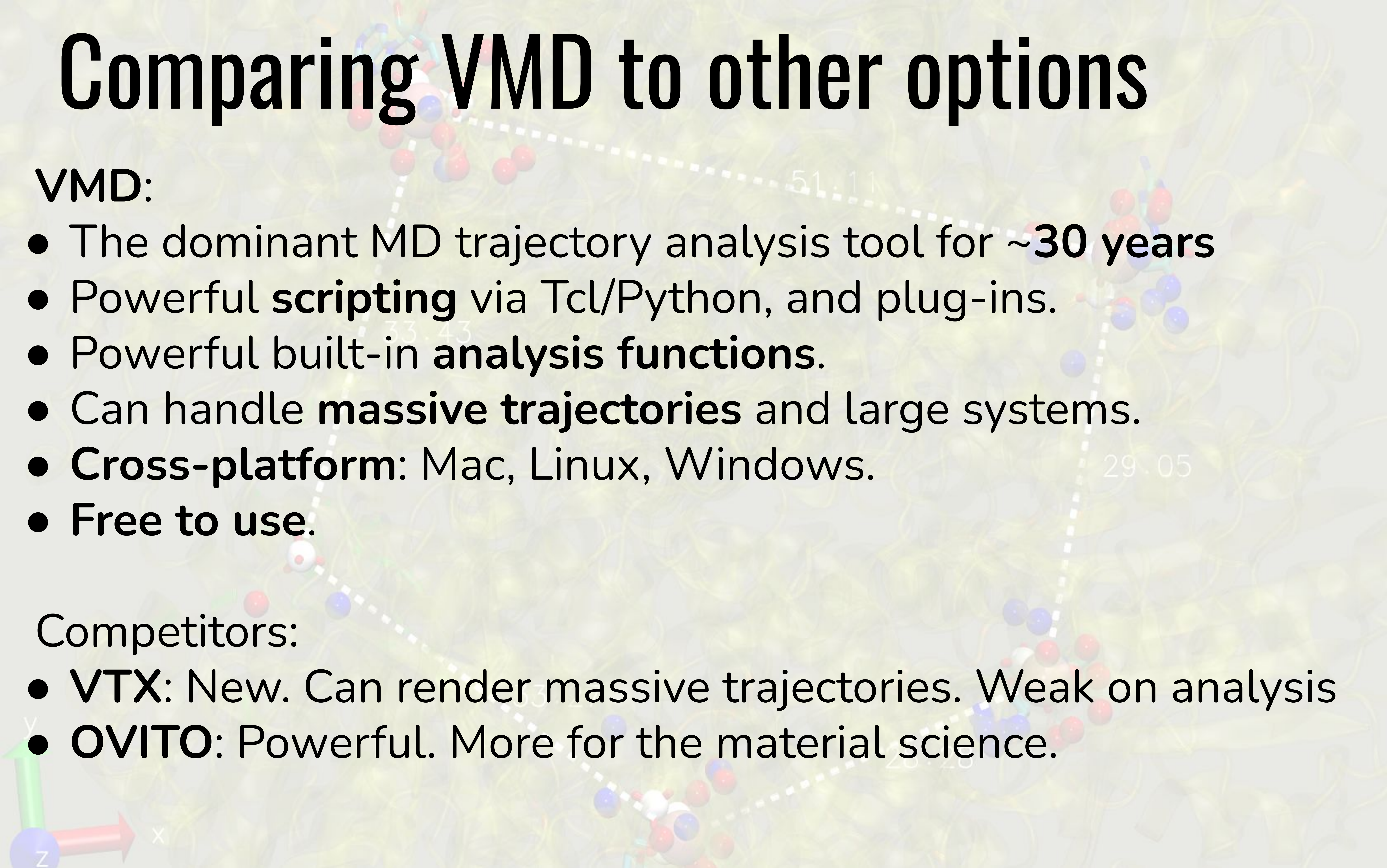
Format: MPEG-2 (ffmpeg)

```
dinates from file /Users/rozmanov/NextCloud/Talks/2026-03-13-VMD-Basics/tra

e from distance search ...

Info)    Bonds: 7234
Info)    Angles: 0  Dihedrals: 0  Impropers: 0  Cross-terms: 0
Info)    Bondtypes: 0  Angletypes: 0  Dihedraltypes: 0  Impropertypes: 0
Info)    Residues: 2369
Info)    Waters: 2305
Info)    Segments: 1
Info)    Fragments: 2369   Protein: 0   Nucleic: 0
Info) Finished with coordinate file /Users/rozmanov/NextCloud/Talks/2026-03-13-VMD-Basics/trajectories/DLP
C-bilayer.gro.
Info) Using plugin xtc for coordinates from file /Users/rozmanov/NextCloud/Talks/2026-03-13-VMD-Basics/tra
jectories/DLPC-bilayer.xtc
```

Comparing VMD to other options

Tool	Single Structre	MD Trajectory	QC Orbitals	Molecular Builder	High Performance	Open source
VMD	Yes	Yes	No	No	Yes	No
ChimeraX	Yes	Limited	No	No	Limited	No
PyMOL	Yes	Limited	No	No	No	Yes/No
VTX	Yes	Yes	No	No	Yes	Yes
Avogadro	Yes	No	No	Yes	No	Yes
Gabedit	Yes	No	Yes	Yes	No	Yes
Molekel	Yes	No	Yes	No	No	Mixed
Jmol	Yes	No	Limited	No	No	Yes

Comparing VMD to other options

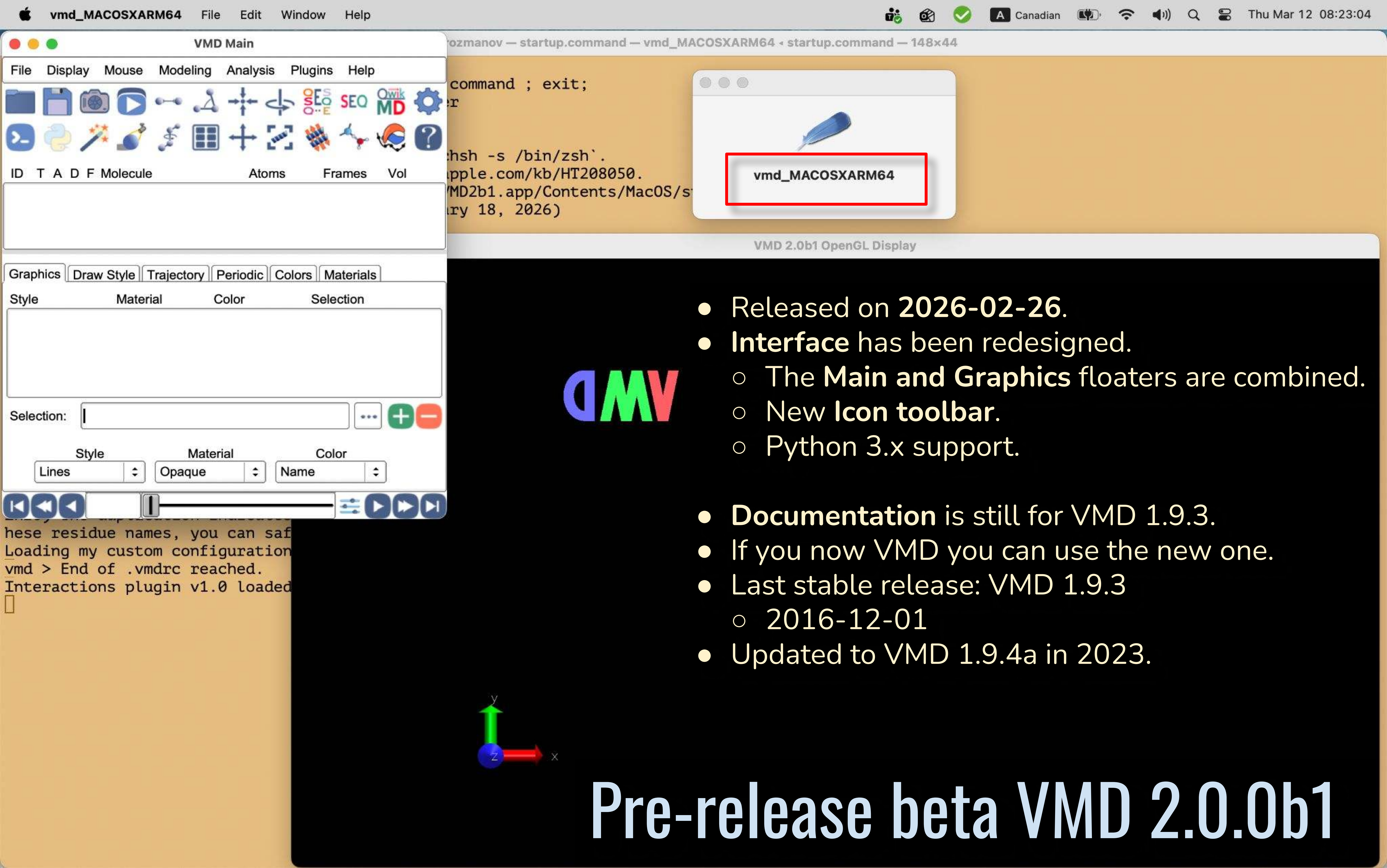


VMD:

- The dominant MD trajectory analysis tool for ~**30 years**
- Powerful **scripting** via Tcl/Python, and plug-ins.
- Powerful built-in **analysis functions**.
- Can handle **massive trajectories** and large systems.
- **Cross-platform**: Mac, Linux, Windows.
- **Free to use**.

Competitors:

- **VTX**: New. Can render massive trajectories. Weak on analysis
- **OVITO**: Powerful. More for the material science.



```
command ; exit;
er

chsh -s /bin/zsh`.
apple.com/kb/HT208050.
VMD2b1.app/Contents/MacOS/s
ary 18, 2026)
```

```
hese residue names, you can saf
Loading my custom configuration
vmd > End of .vmdrc reached.
Interactions plugin v1.0 loaded
```

- Released on **2026-02-26**.
- **Interface** has been redesigned.
  - The **Main and Graphics** floaters are combined.
  - New **Icon toolbar**.
  - Python 3.x support.

- **Documentation** is still for VMD 1.9.3.
- If you now VMD you can use the new one.
- Last stable release: VMD 1.9.3
  - 2016-12-01
- Updated to VMD 1.9.4a in 2023.

Pre-release beta VMD 2.0.0b1

VMD resources

- VMD Home: http://www.ks.uiuc.edu/Research/vmd/
- FAQ: http://www.ks.uiuc.edu/Research/vmd/allversions/vmd_faq.html
- VMD Documentation: https://www.ks.uiuc.edu/Research/vmd/current/docs.html

- VMD on Compute Canada: https://docs.computecanada.ca/wiki/VMD

Data sources:

- PDB Data Bank: https://www.wwpdb.org
- Nucleic Acids Data Bank: http://ndbserver.rutgers.edu

Thank you!