Advanced VMD:
Trajectories, movies, scripting

WestGrid webinar

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Downloadable material

- All examples shown during the webinar use downloadable files.
  - Structures
  - Trajectories
  - Scripts
- Address
  - *https://nextcloud.computecanada.ca/index.php/s/kcHgbbEgwS3GkHM/download*
  - With *wget*, add *-O advanced_vmd.tar*
- Extract the files from the archive.

  tar -xf advanced_vmd.tar

Contents

In the previous webinar

- Basics
  - Loading structures
  - Representations
  - Atom selections
  - 3D navigation
- Drawing methods
- Materials and colouring
- Image rendering

New topics

- Trajectories
  - Troubleshooting
  - Post-processing
- Movies
  - Using the “Movie Maker”
- Scripting
  - Tk Console
  - Tcl scripts
  - *vmdrc*
- Combining trajectories, movies, and scripting

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- **Combining trajectories, movies, and scripting**

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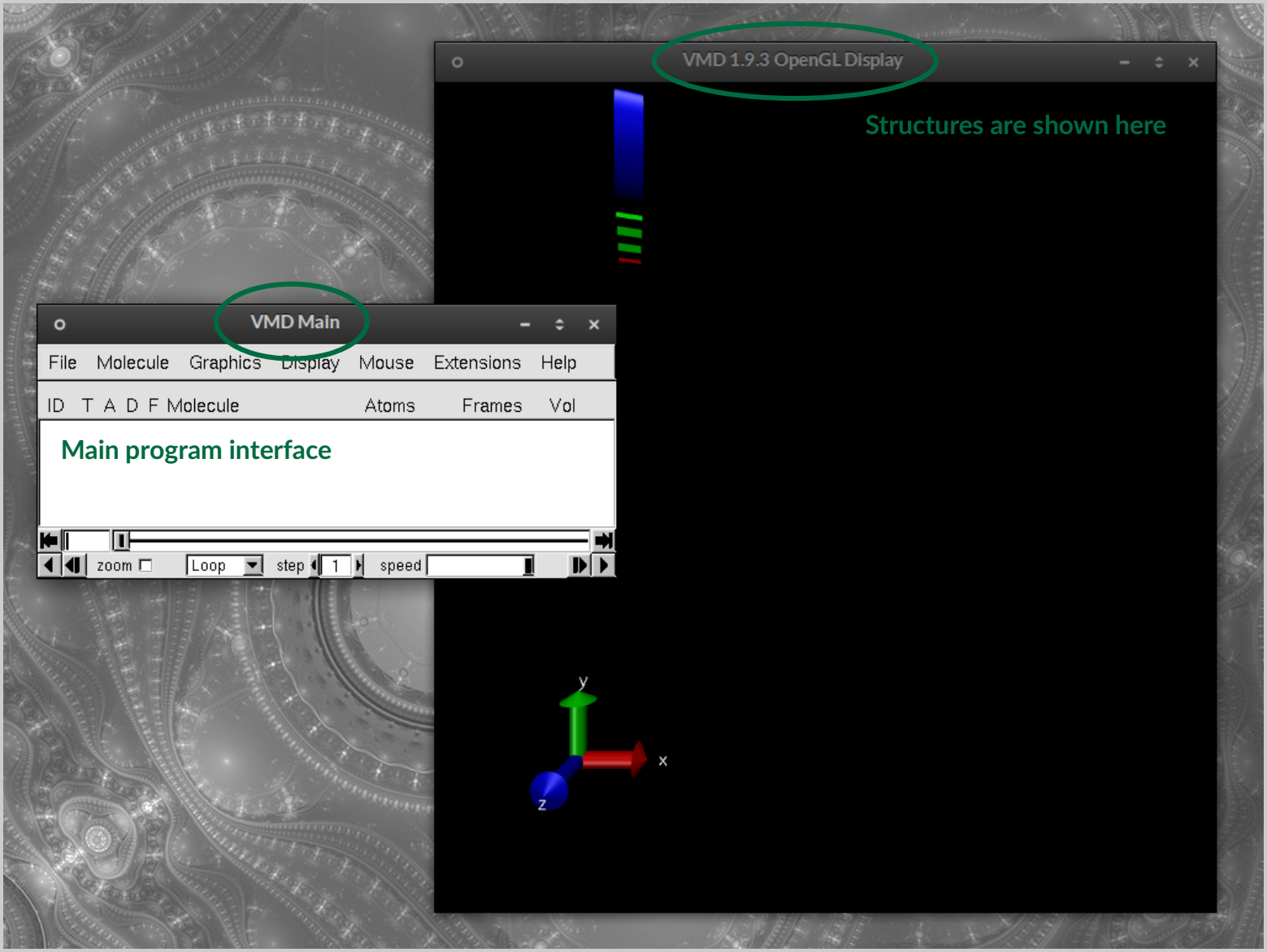
VMD Windows


VMD 1.9.3 OpenGL Display
Structures are shown here
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
Main program interface
zoom
Loop
step
1
speed
y
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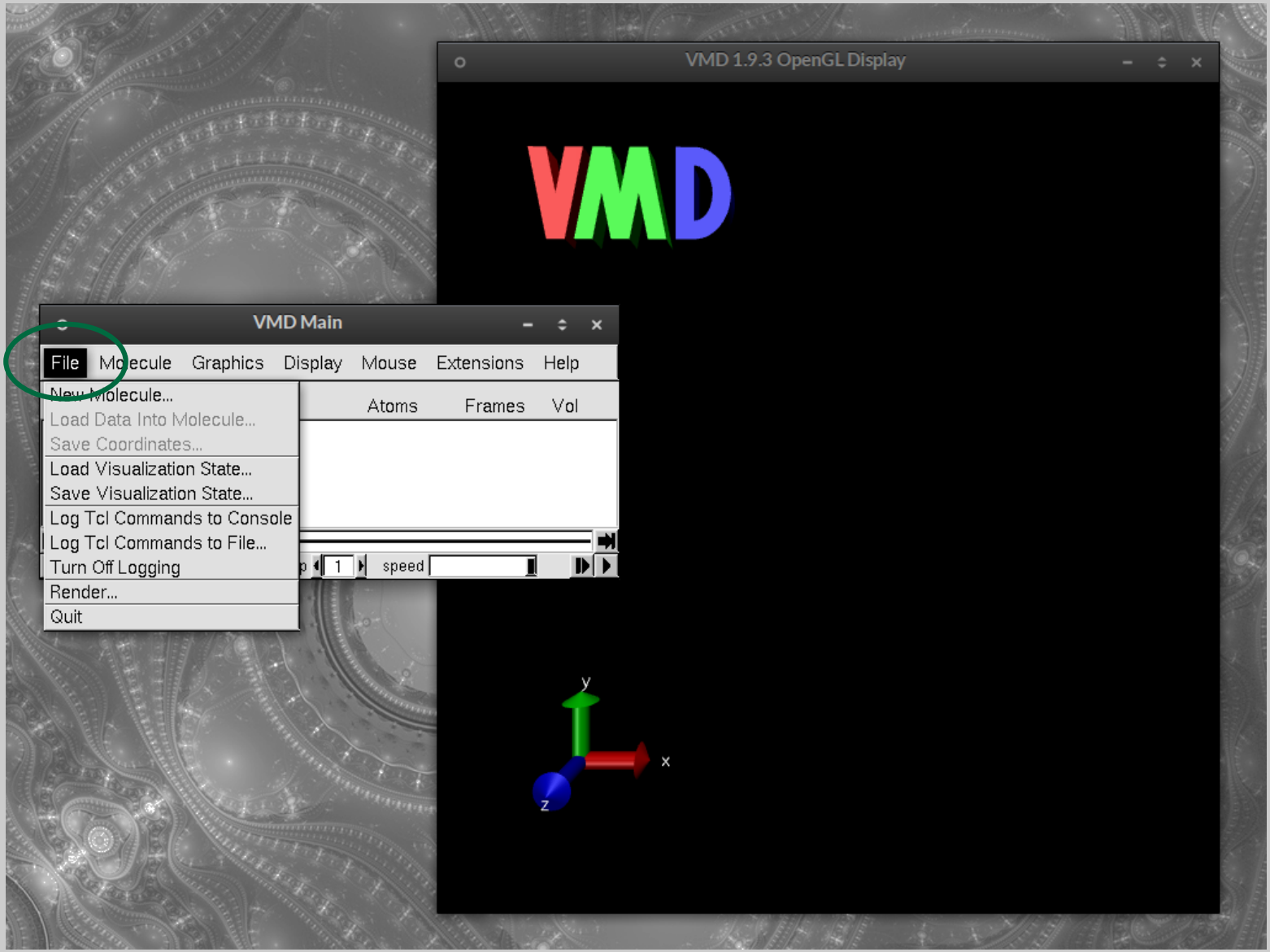
Loading a structure



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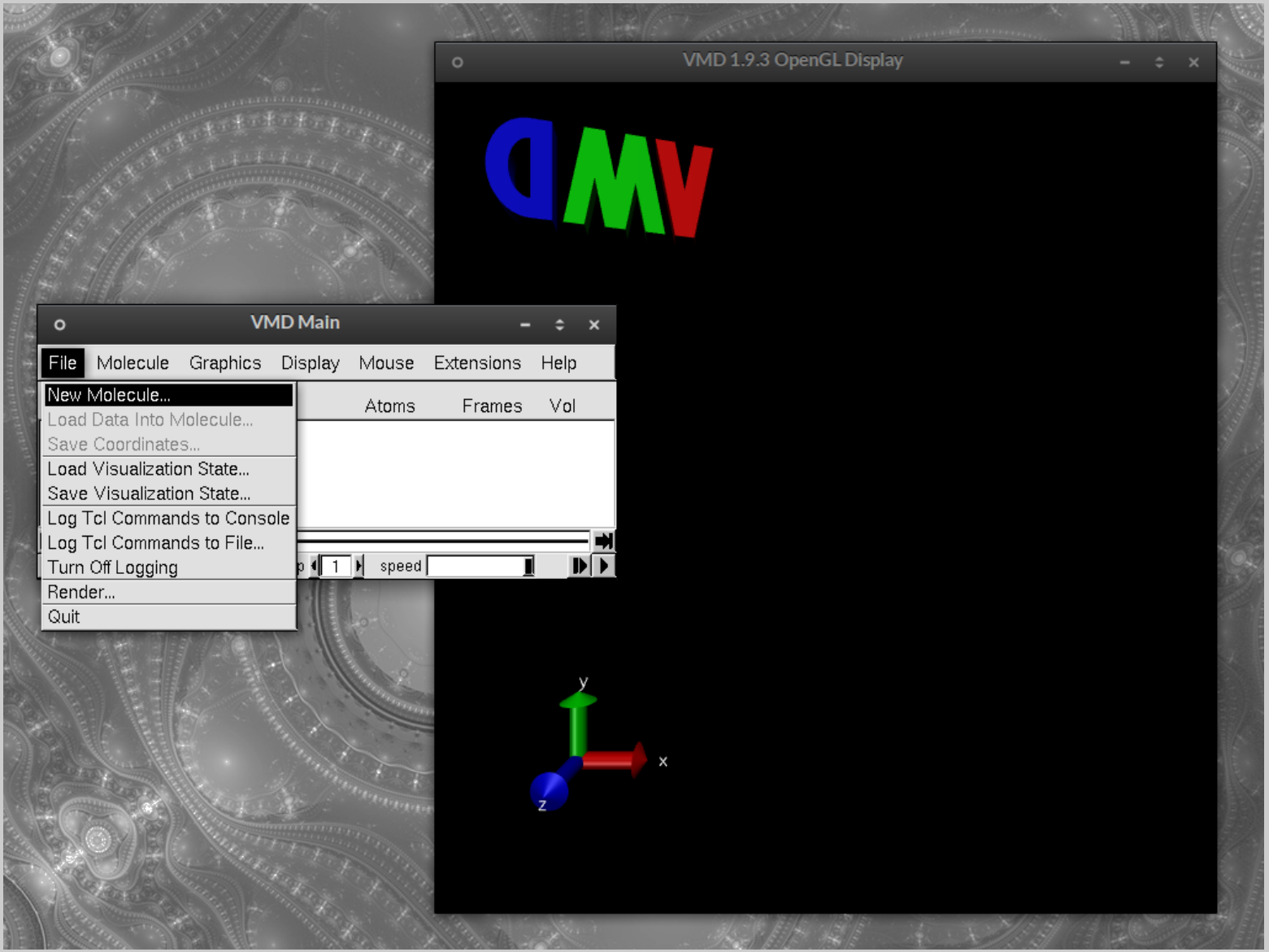

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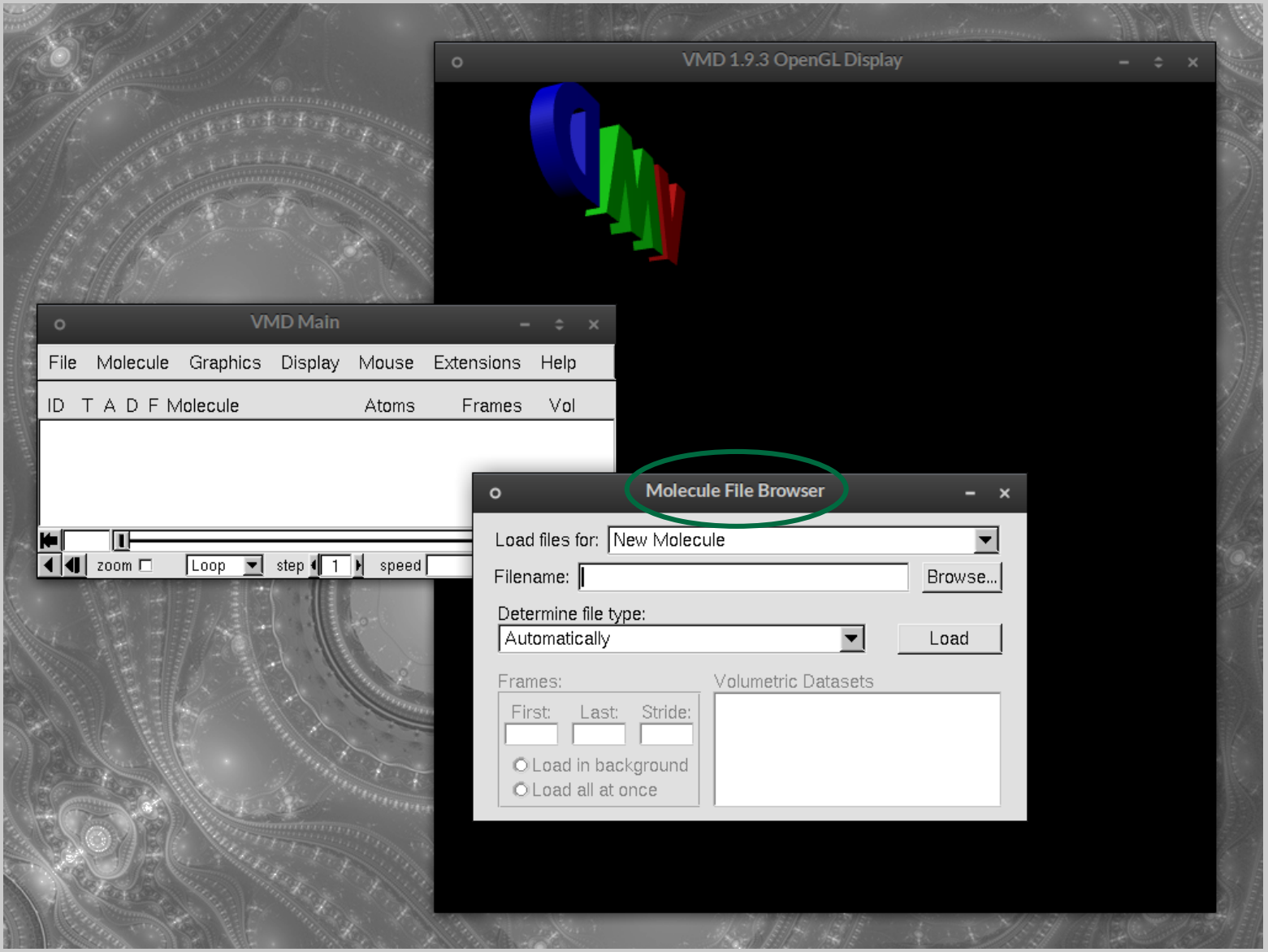

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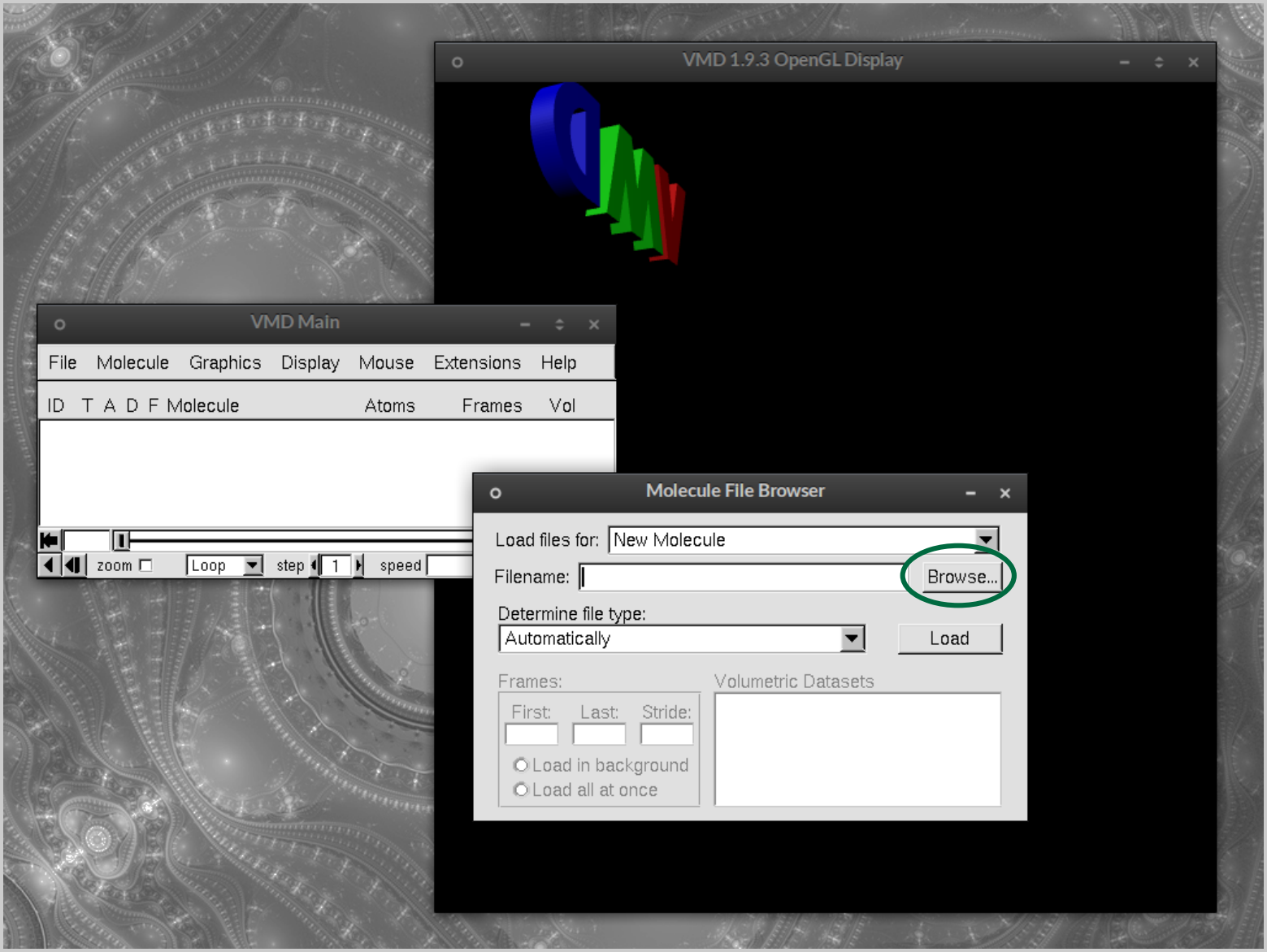

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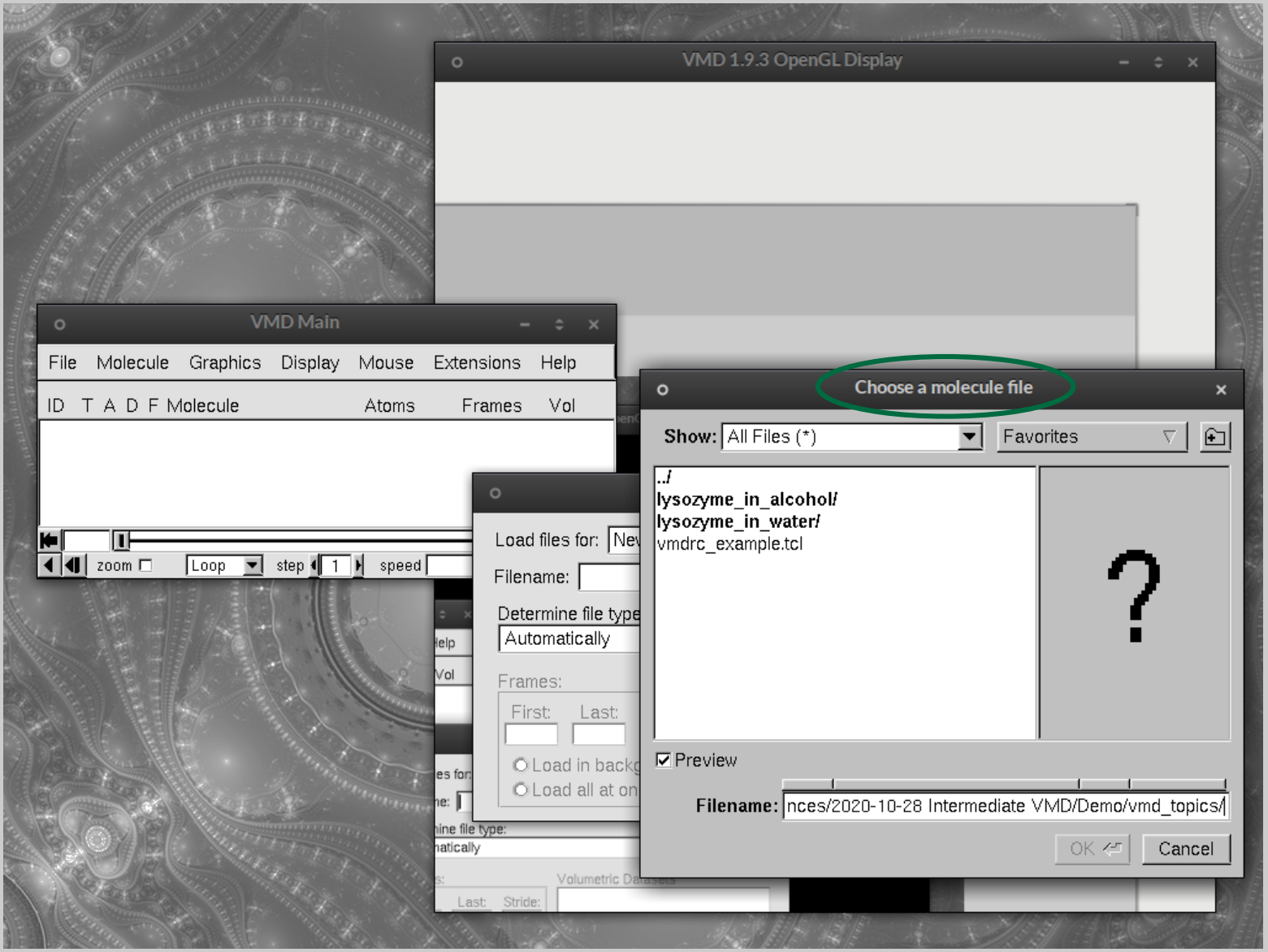

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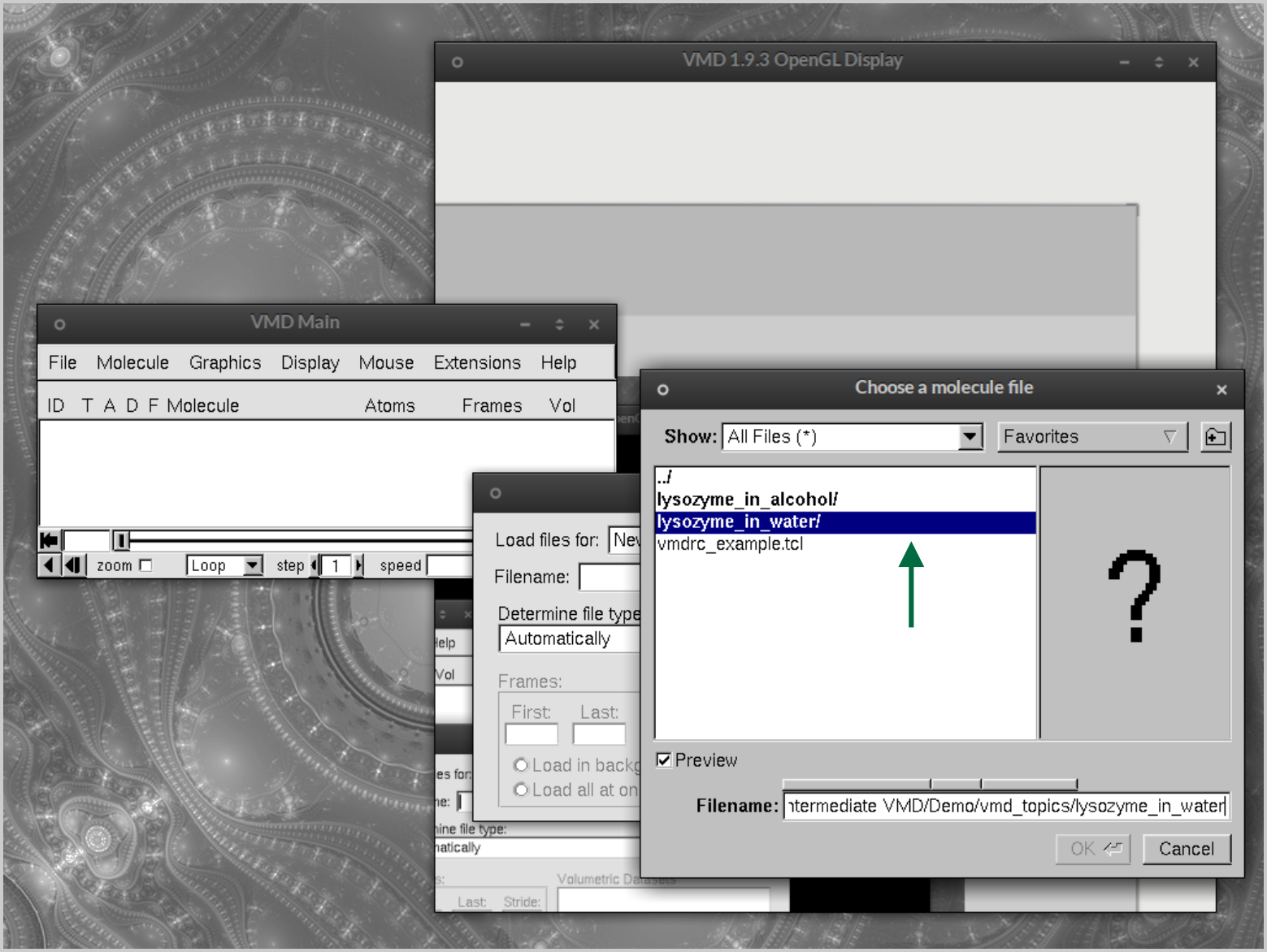

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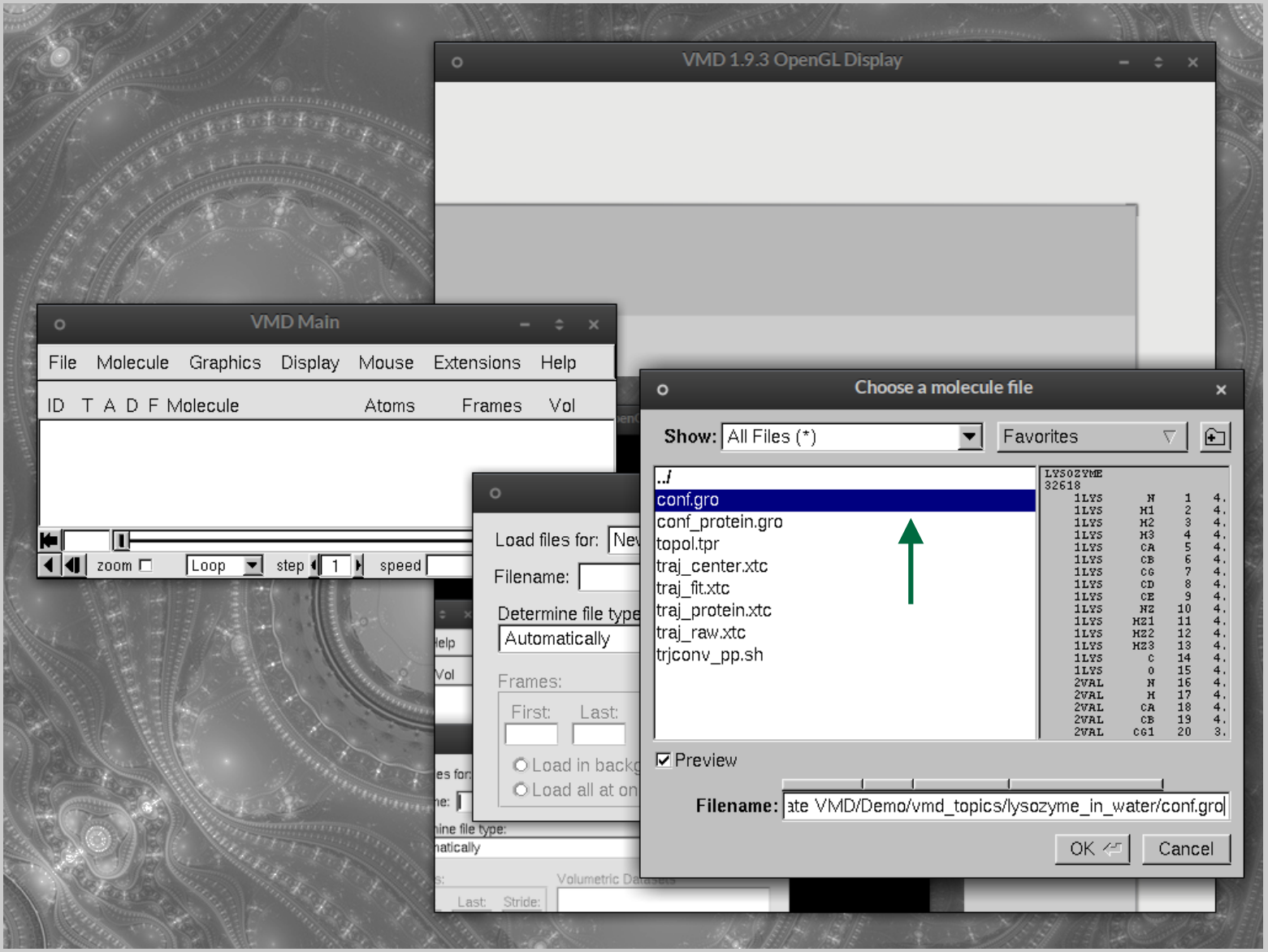

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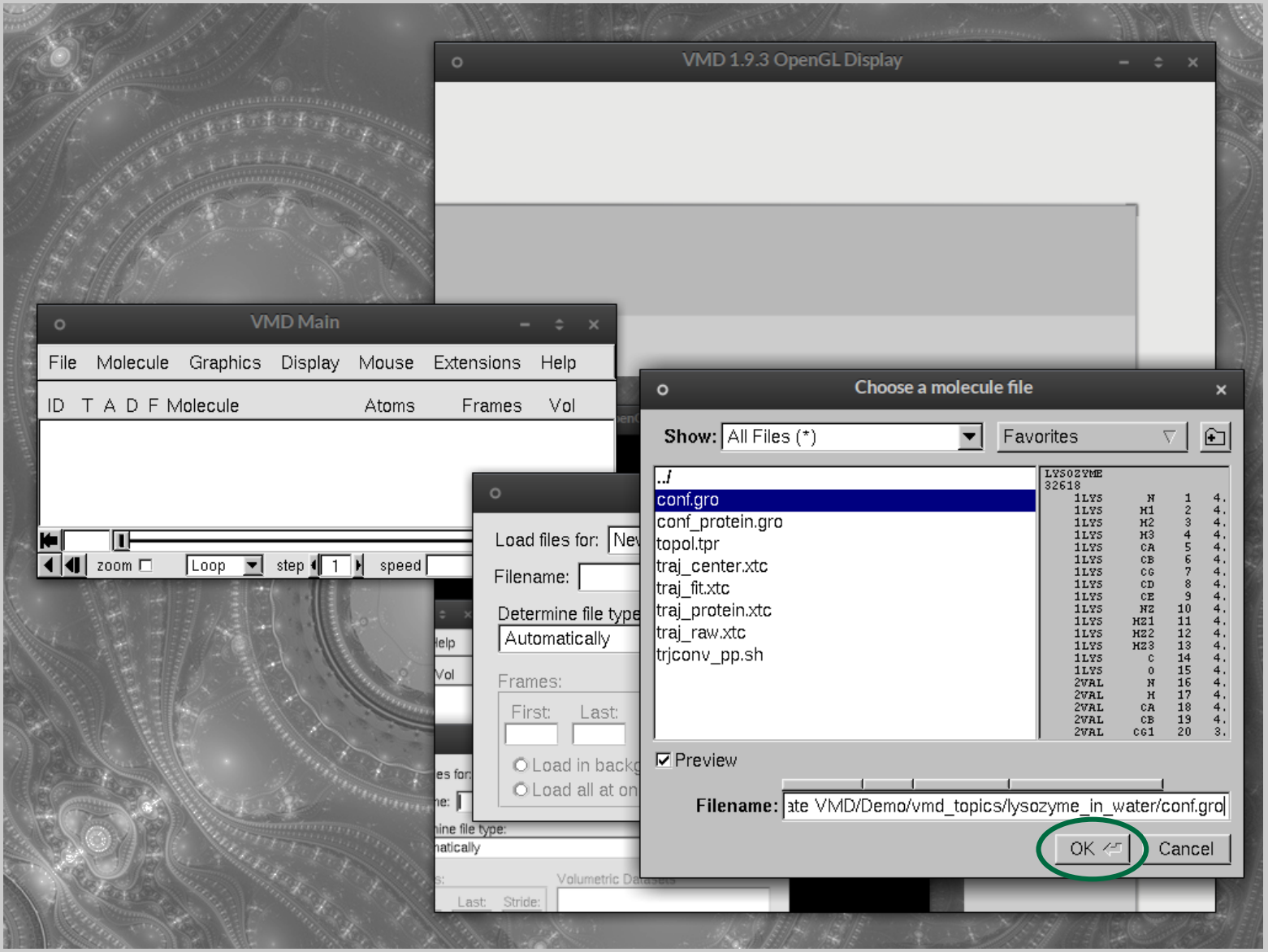

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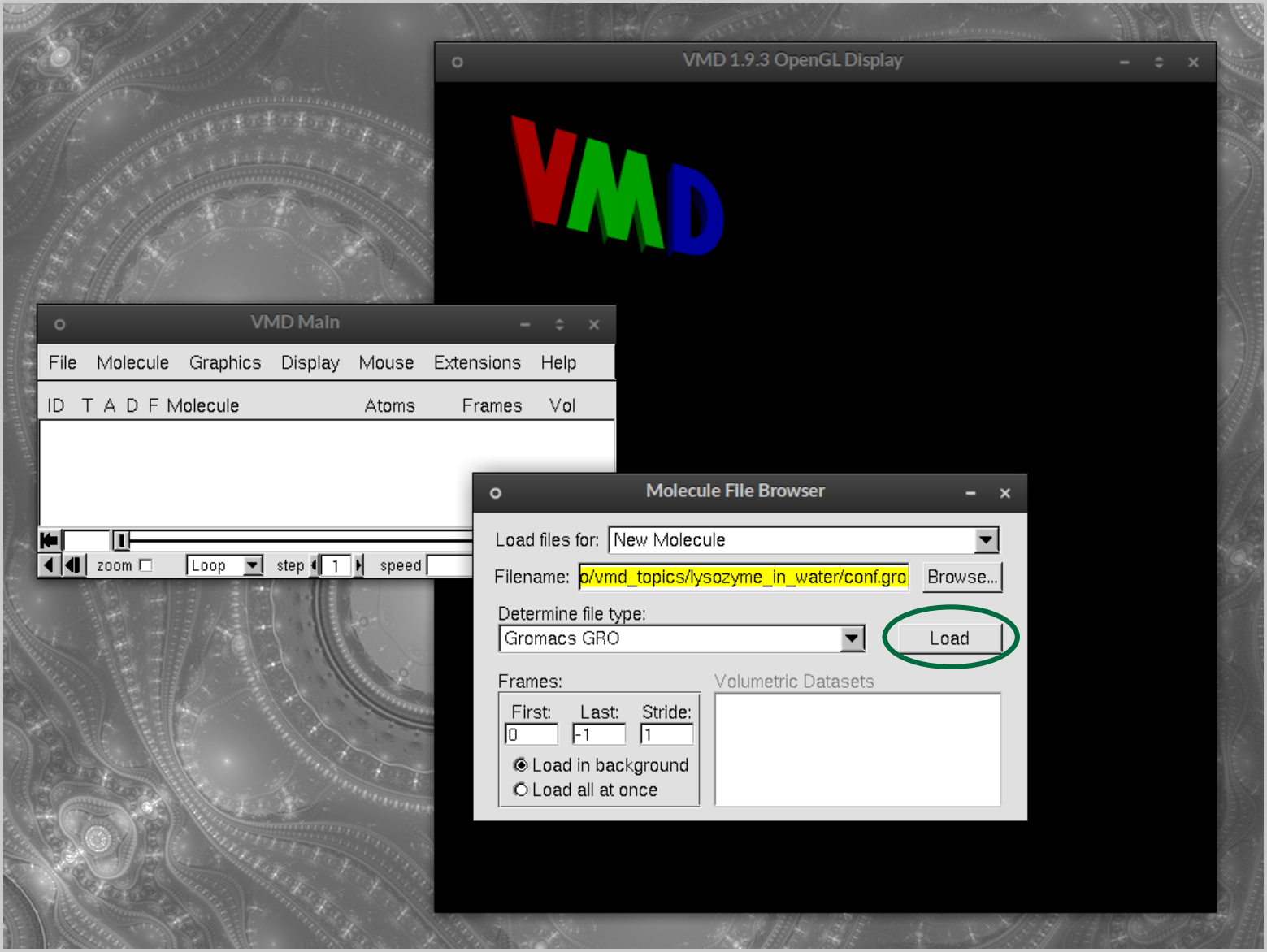

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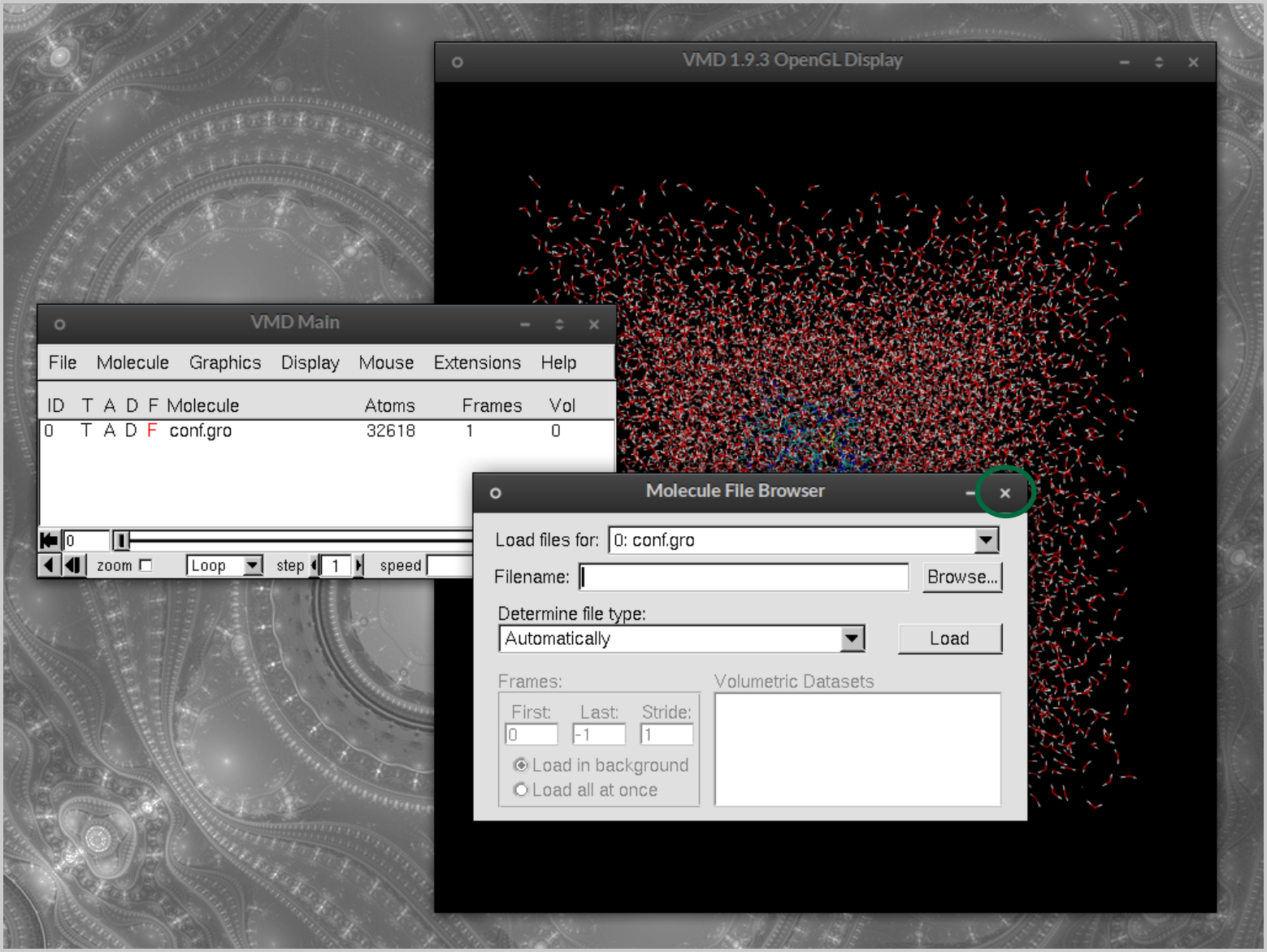

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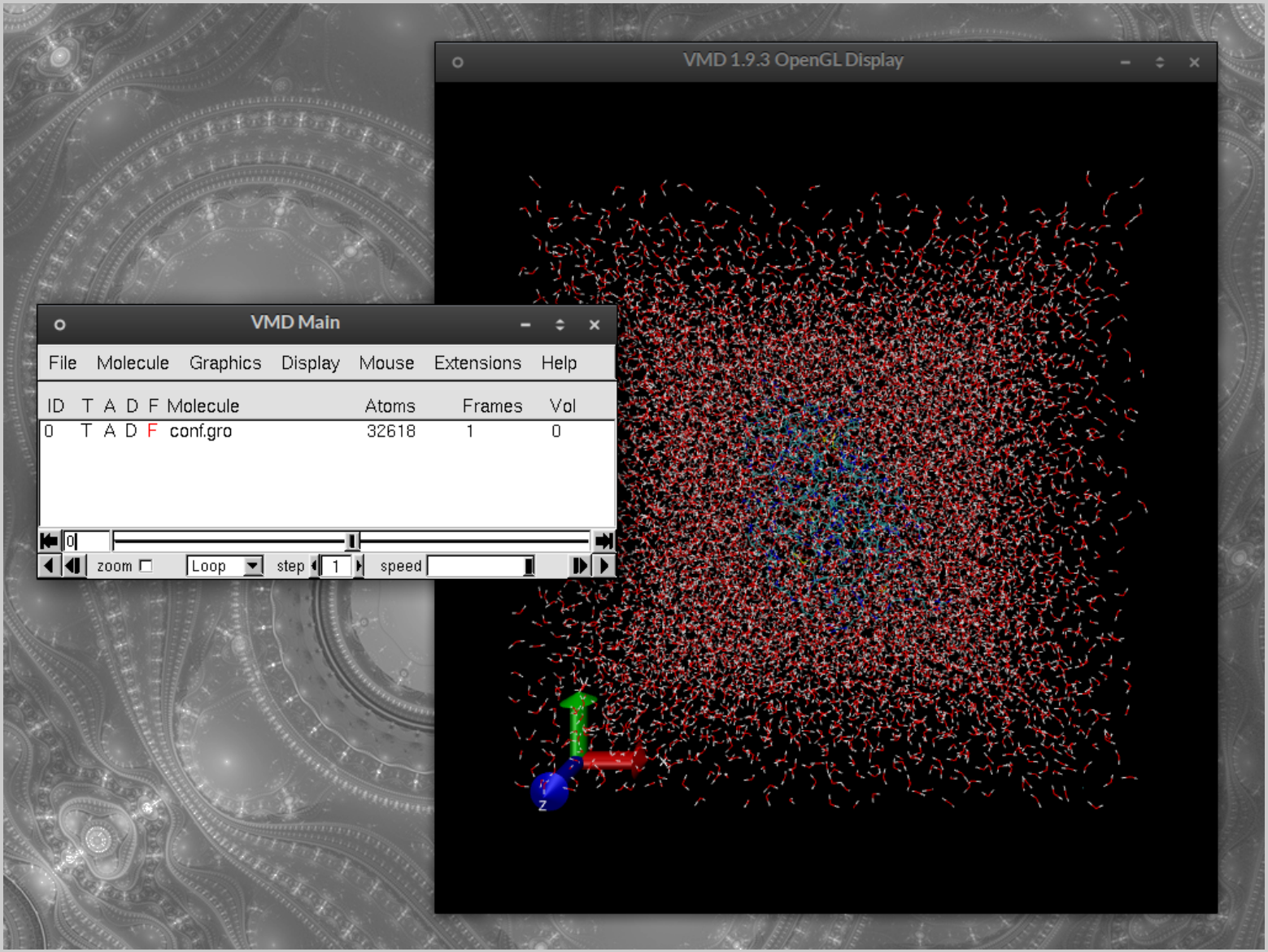
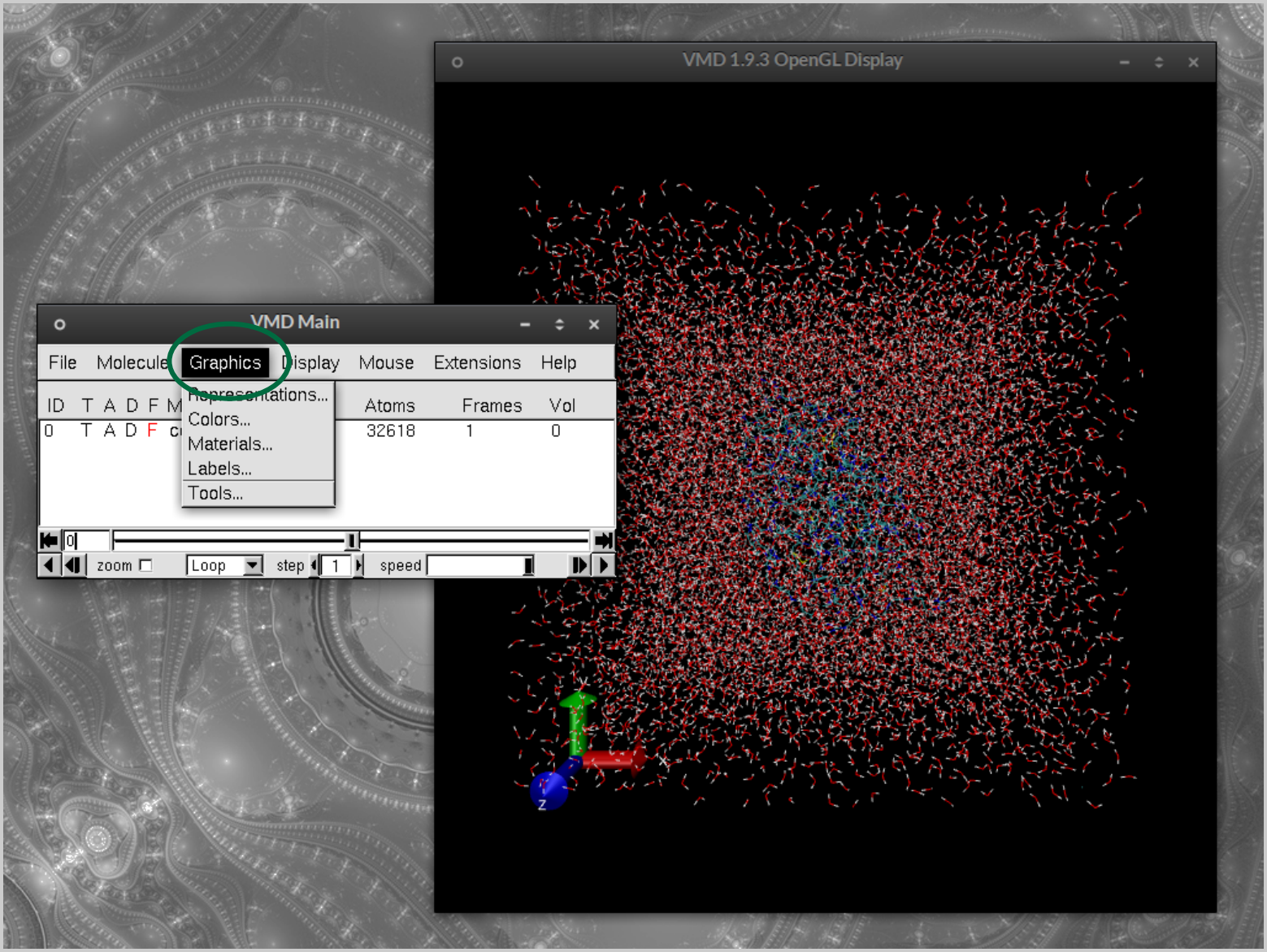


Loading a structure

- The VMD interface uses many windows.
  - The “Main” window gives access to all controls and other windows.
  - A single “OpenGL Display” window shows all structures.
- File formats are automatically detected.
- A wide variety of formats (60+) are supported.

Graphical representations



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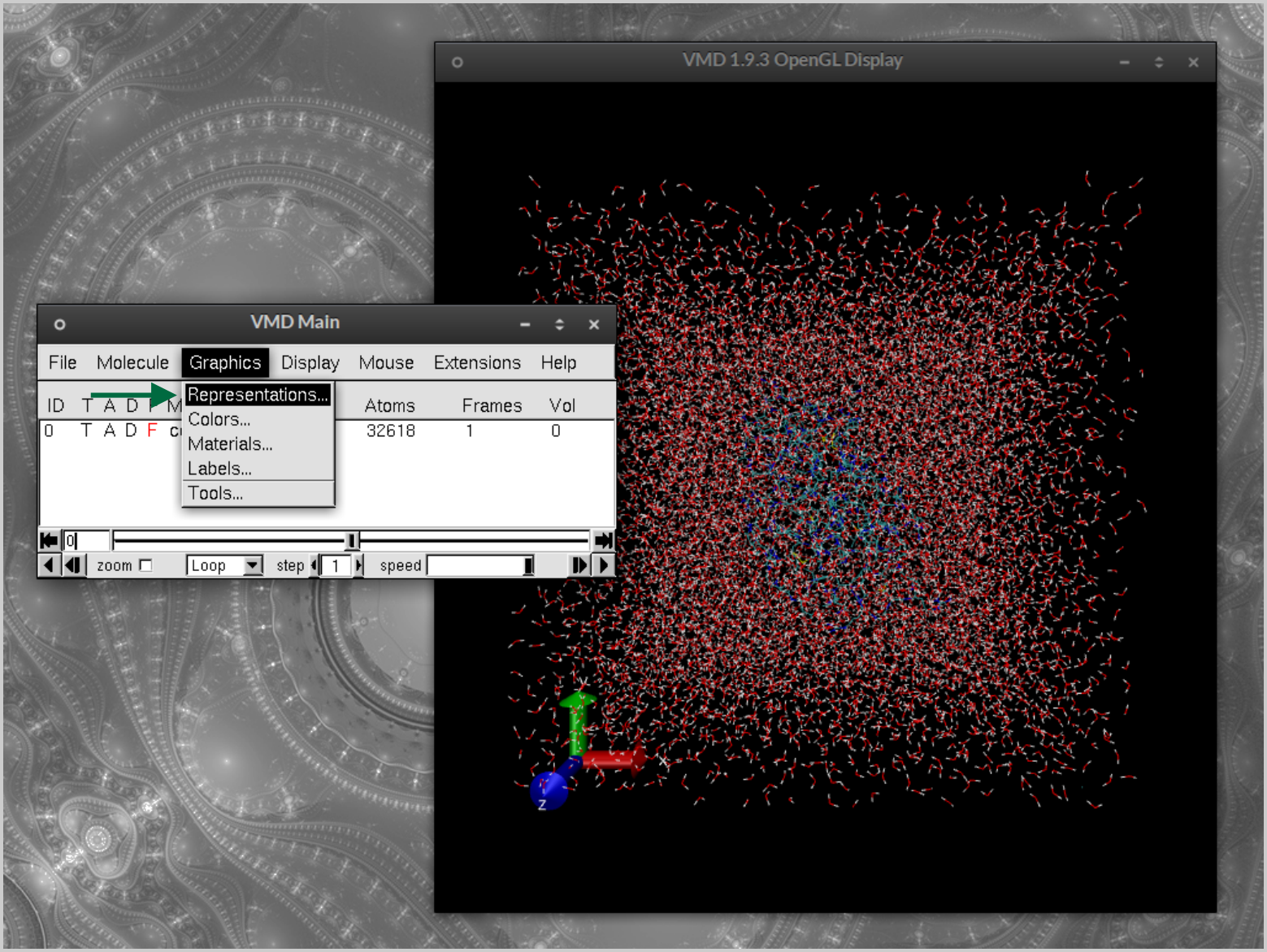

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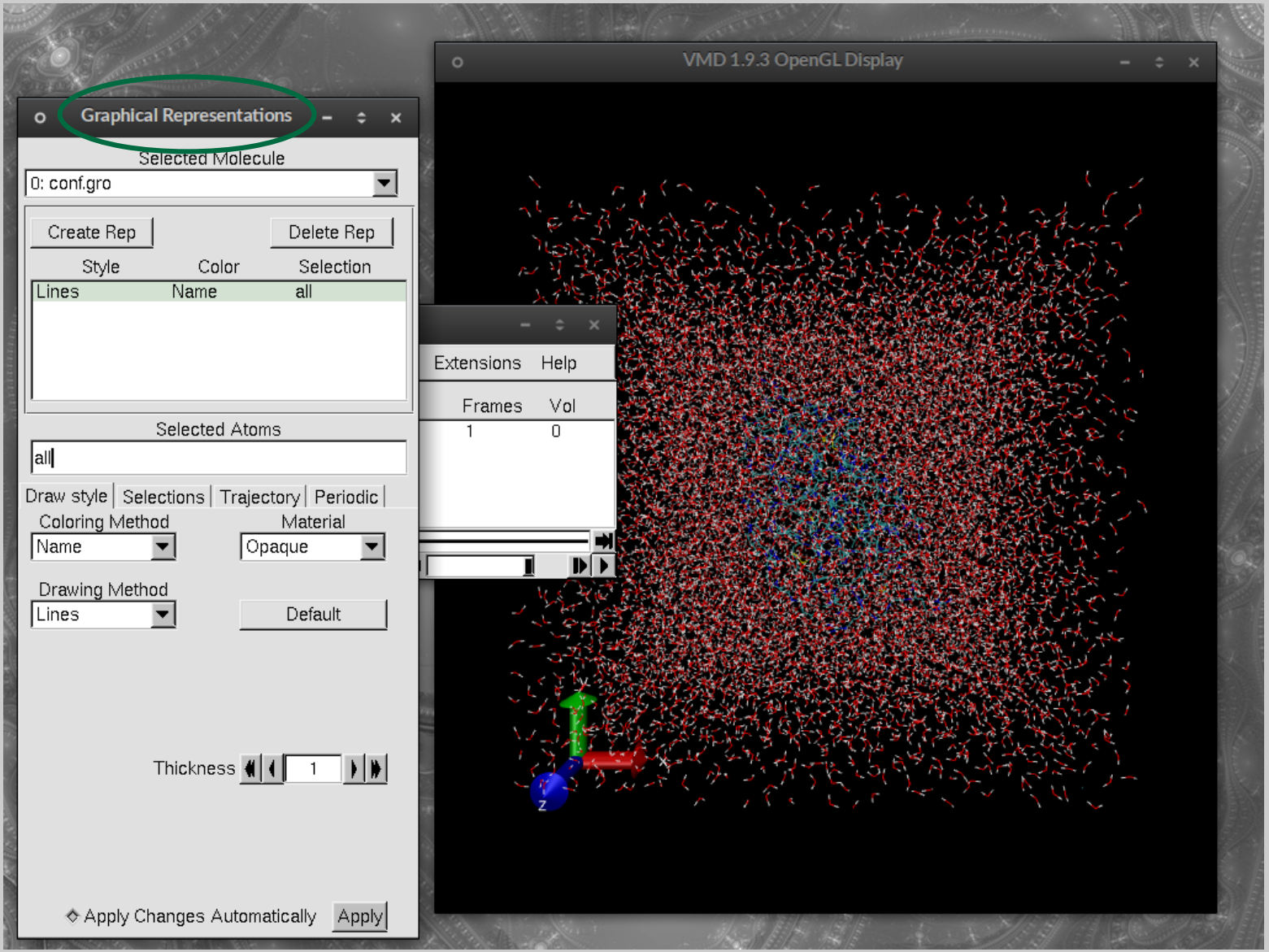

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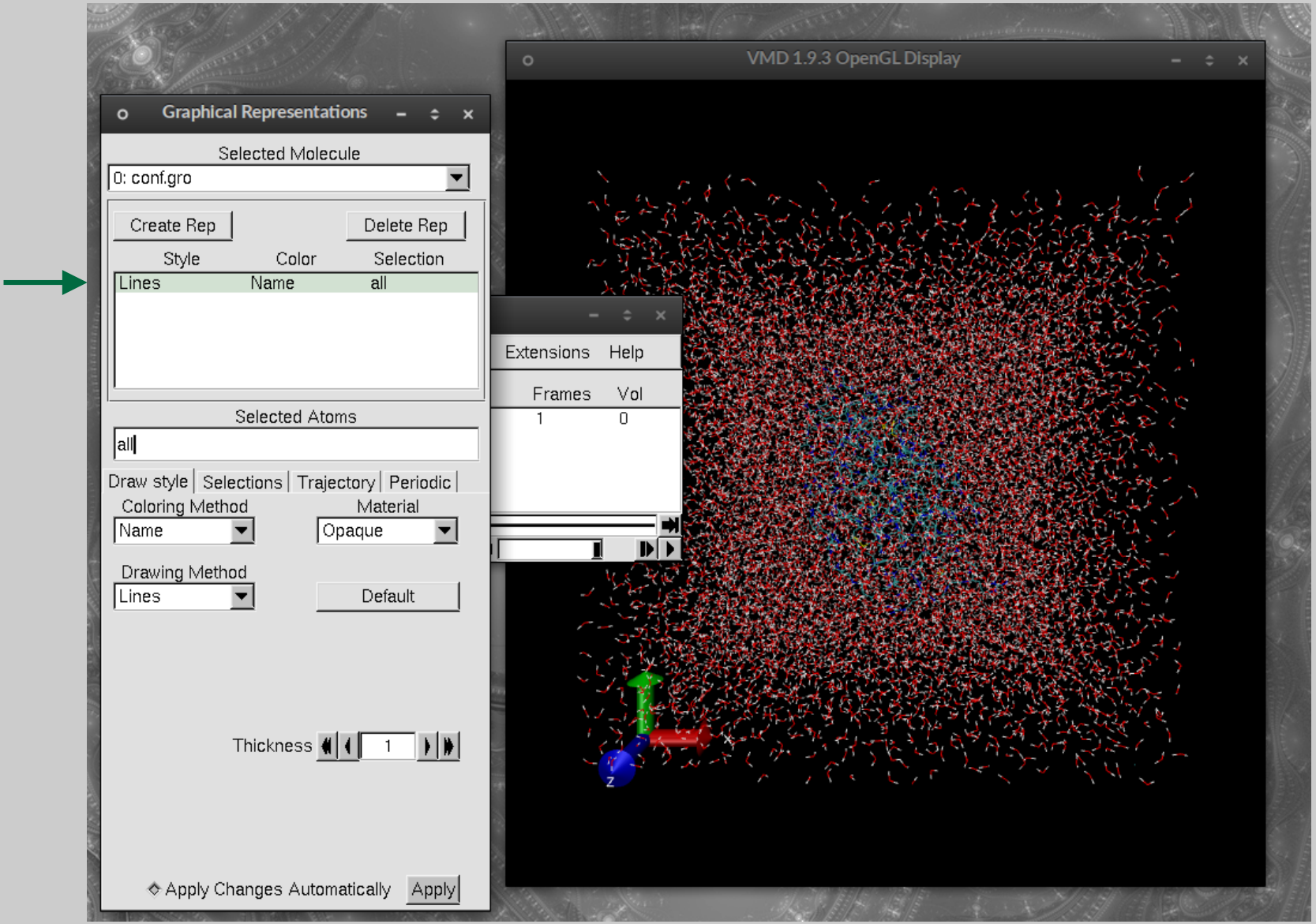

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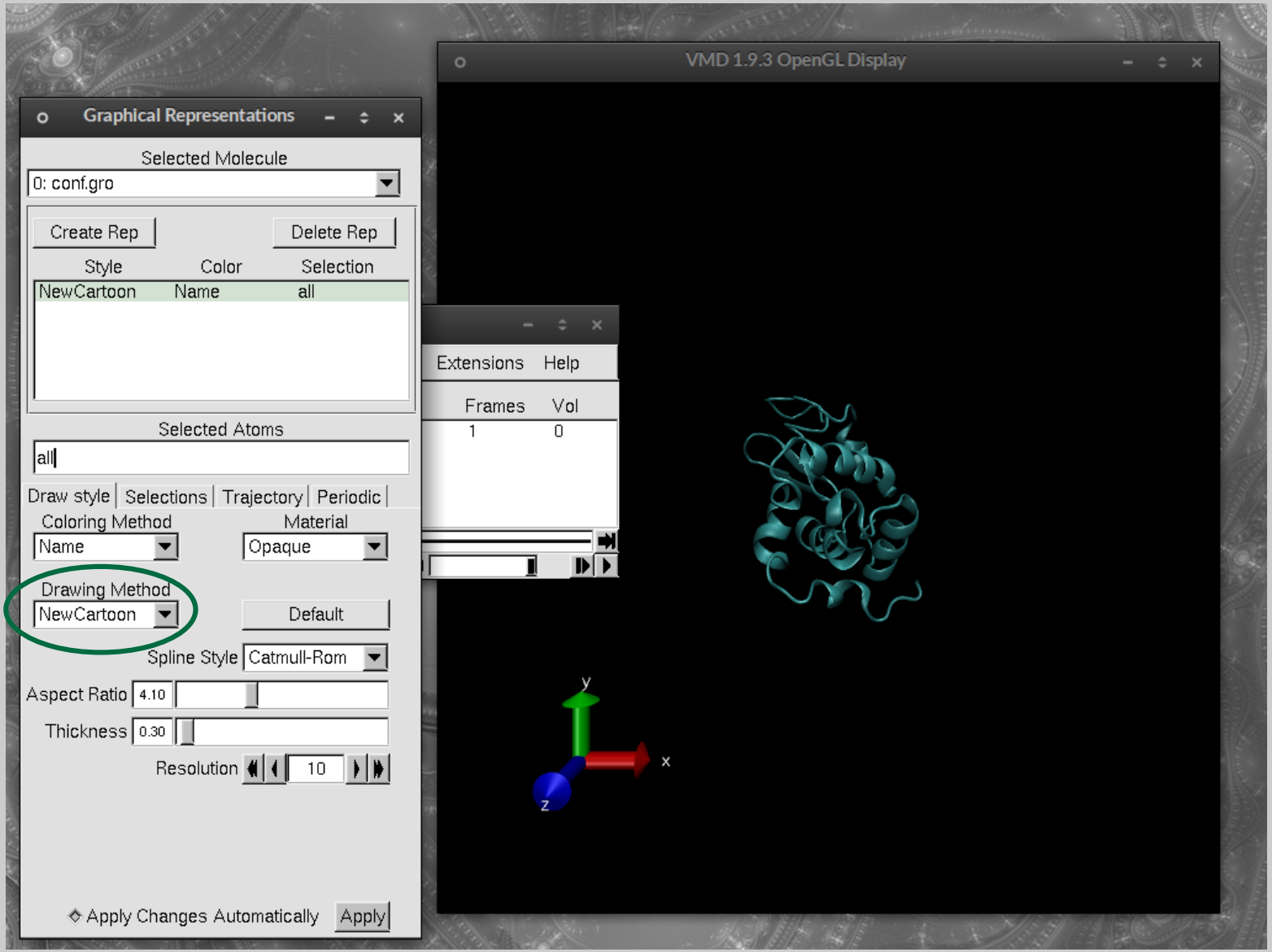

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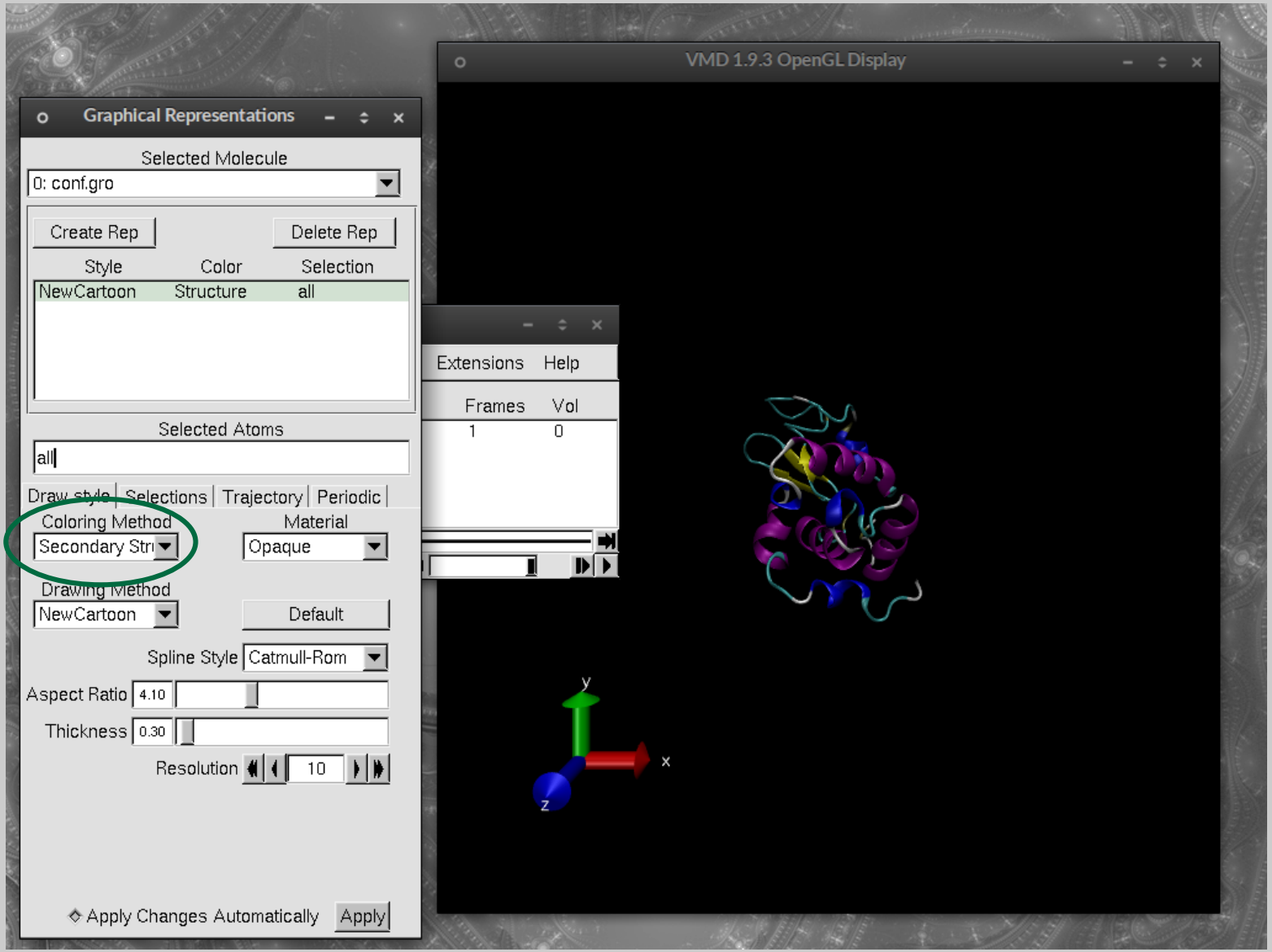

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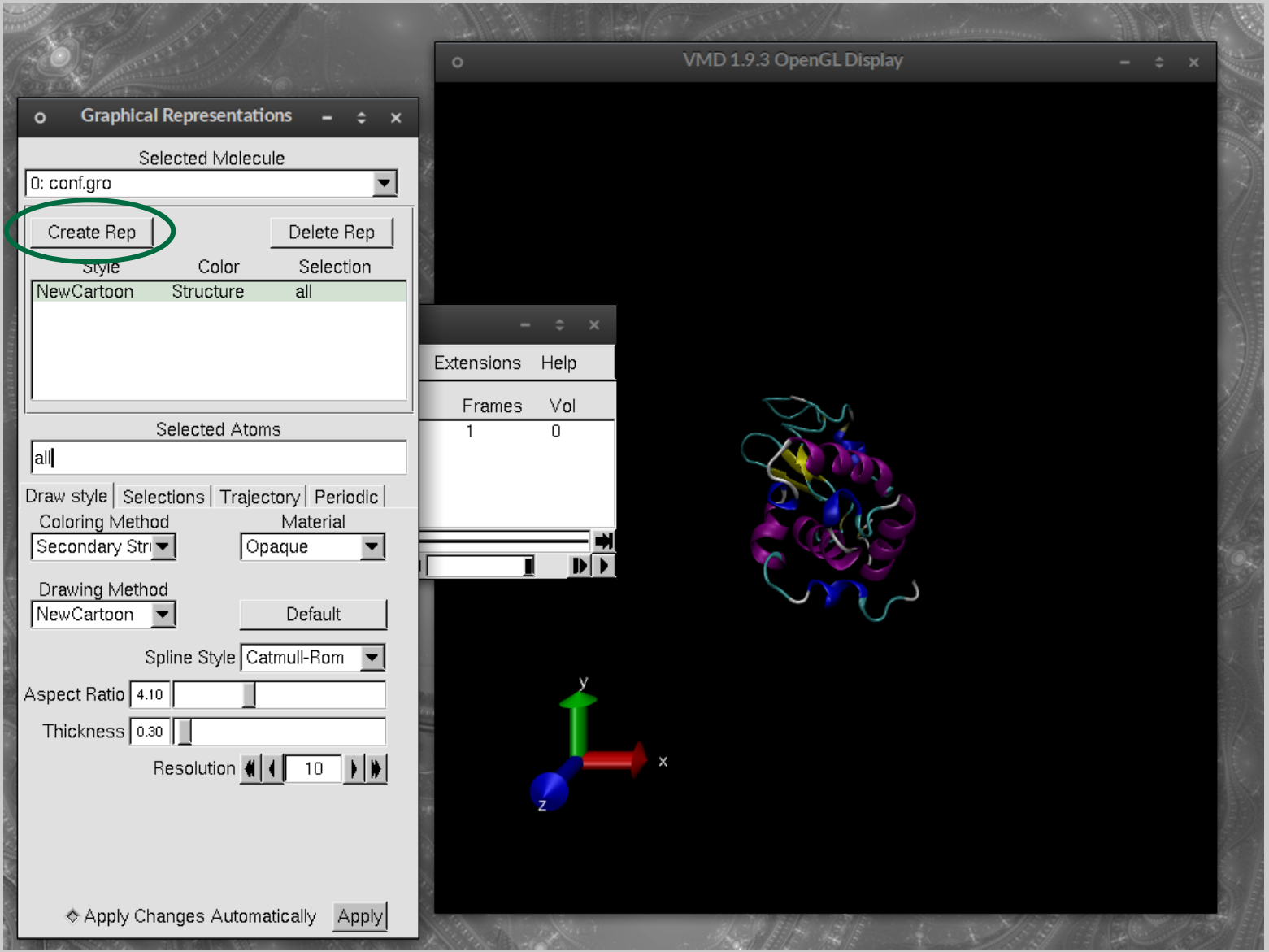

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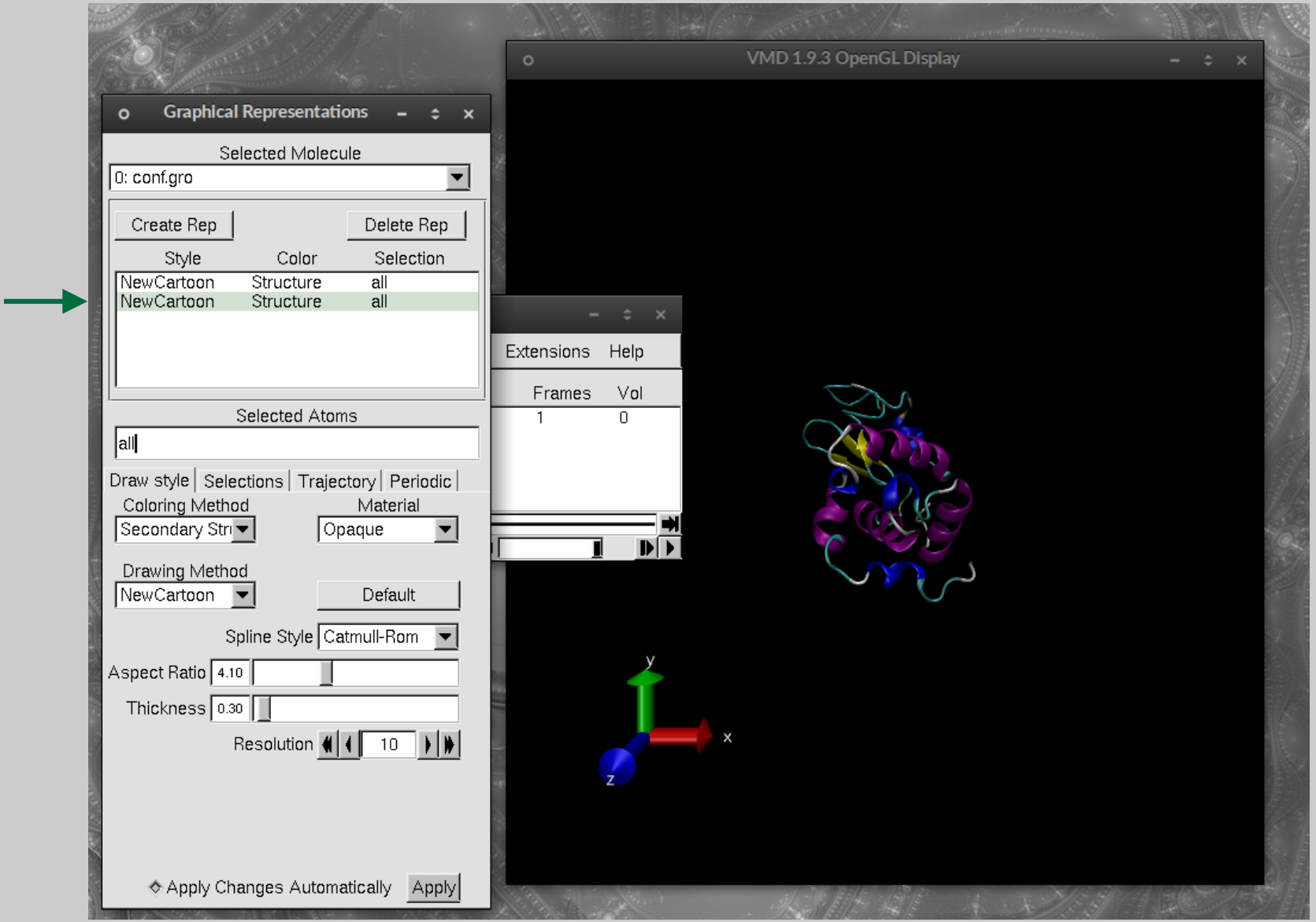

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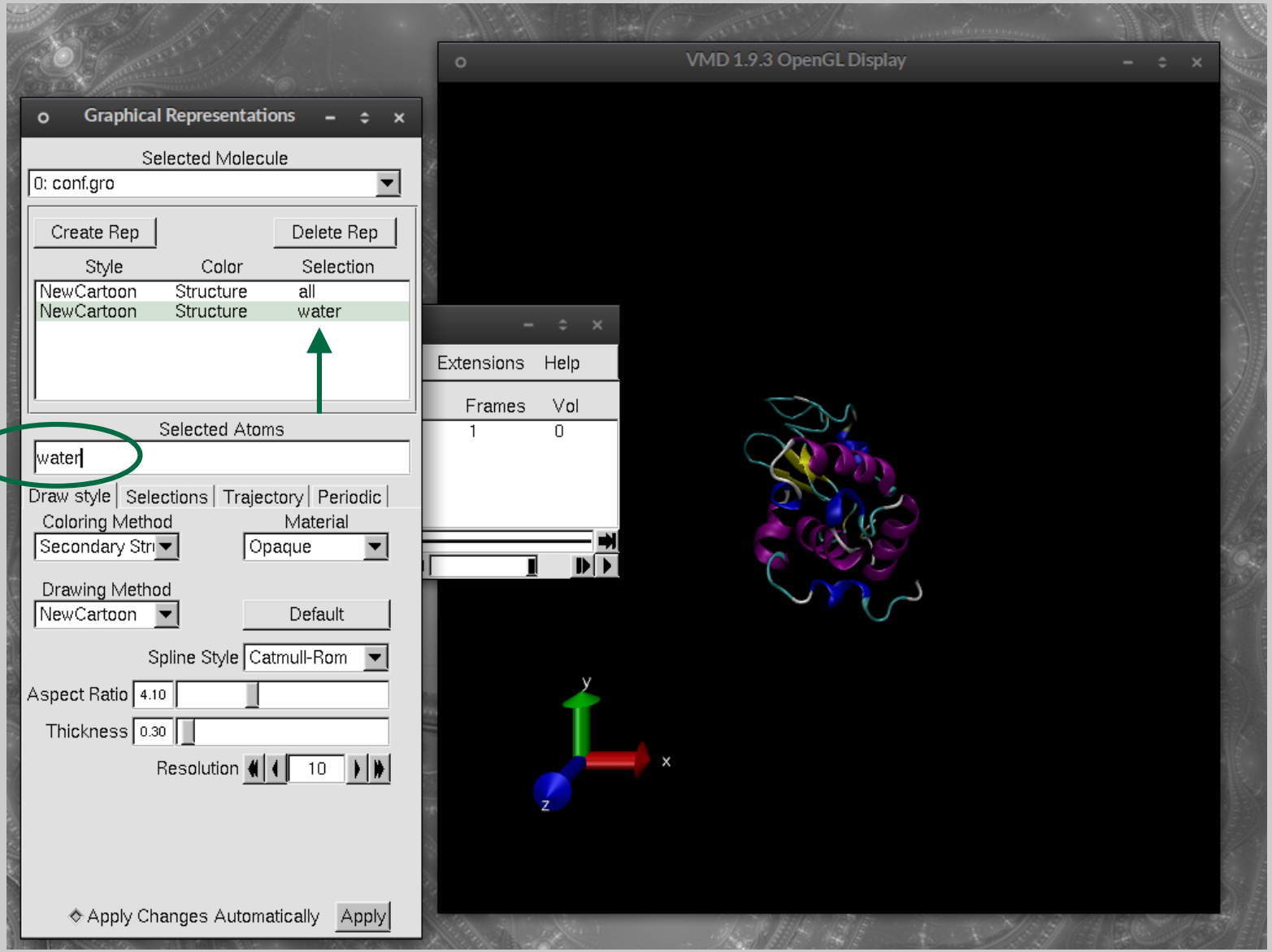

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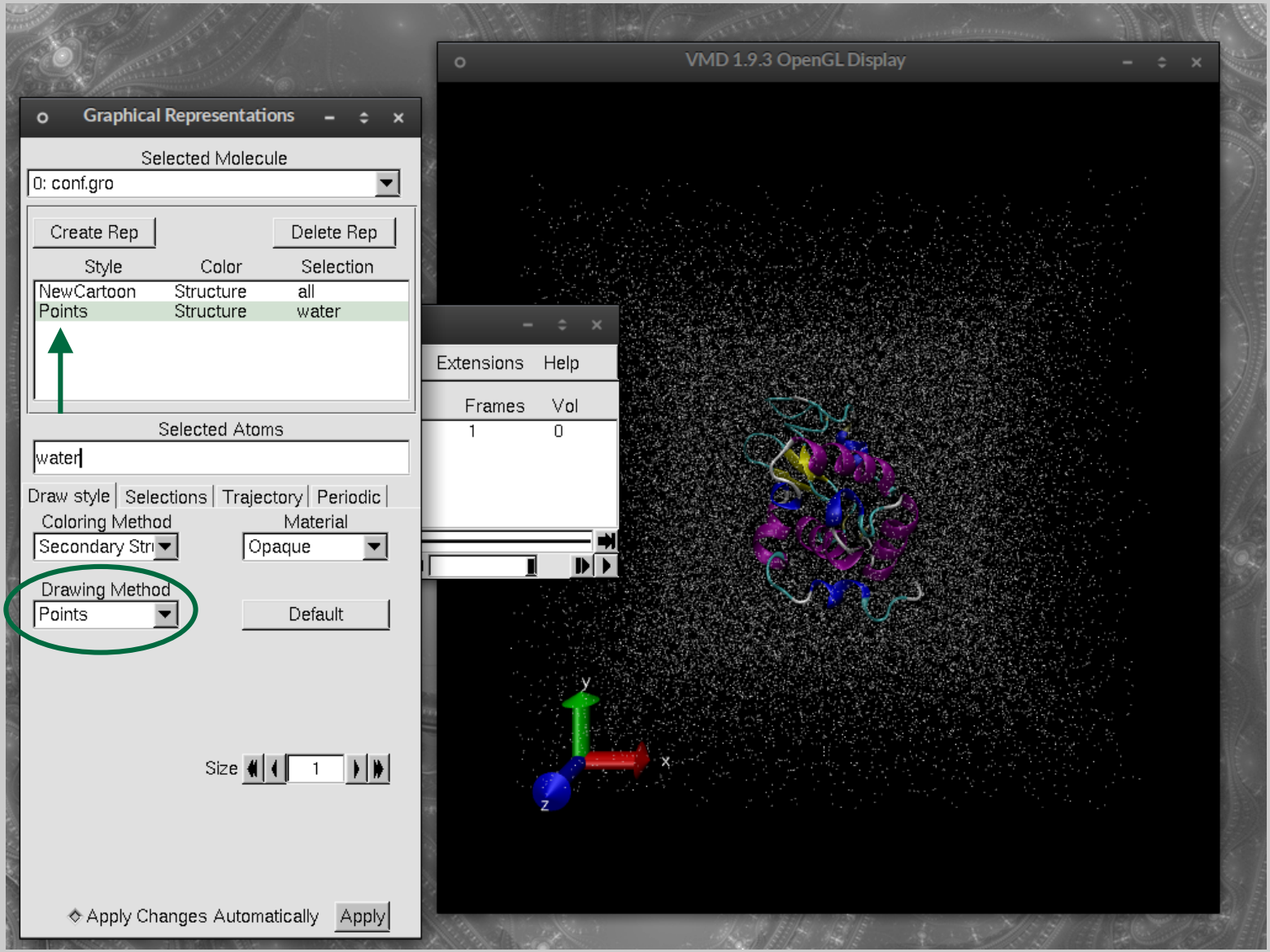

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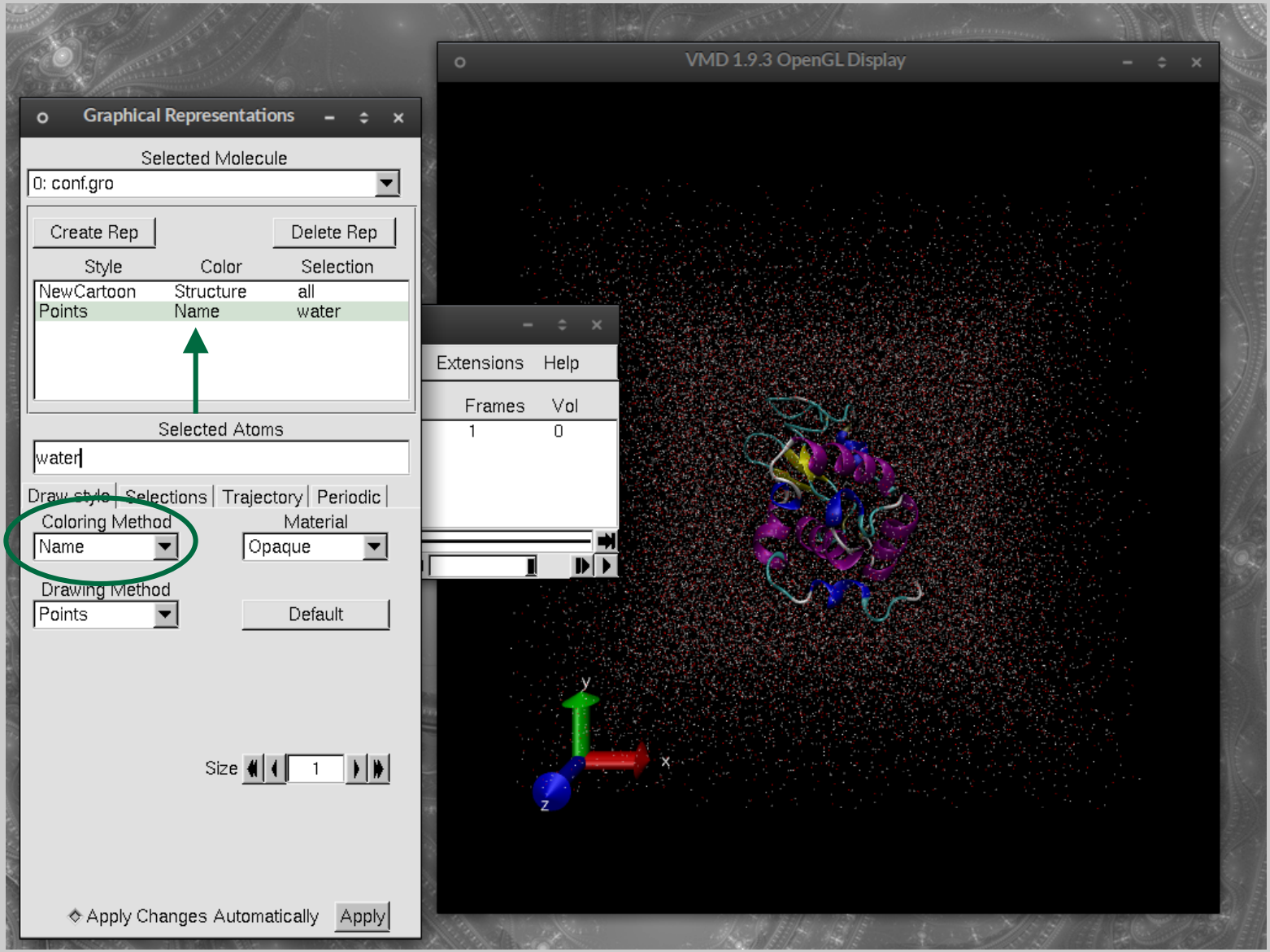

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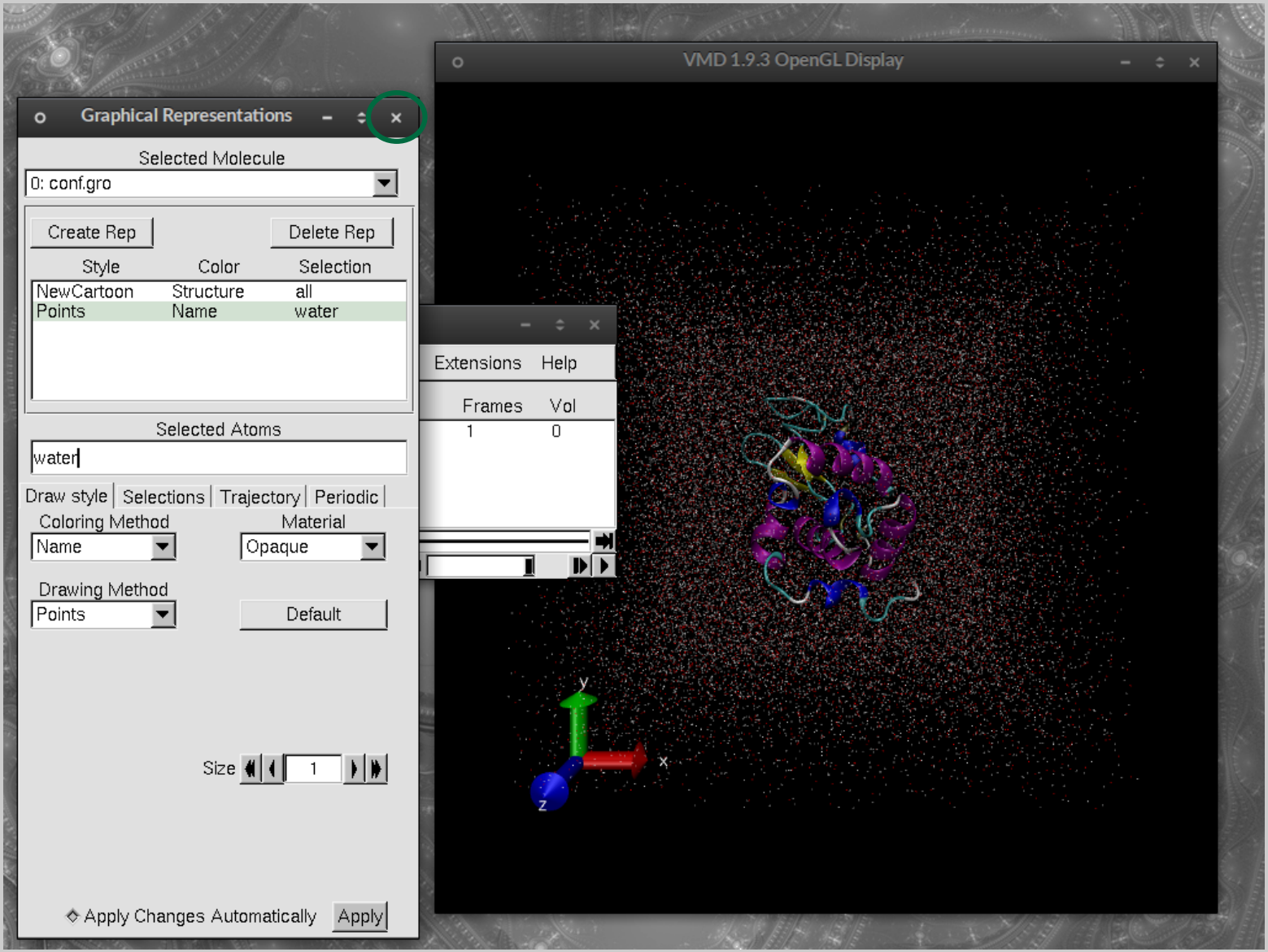

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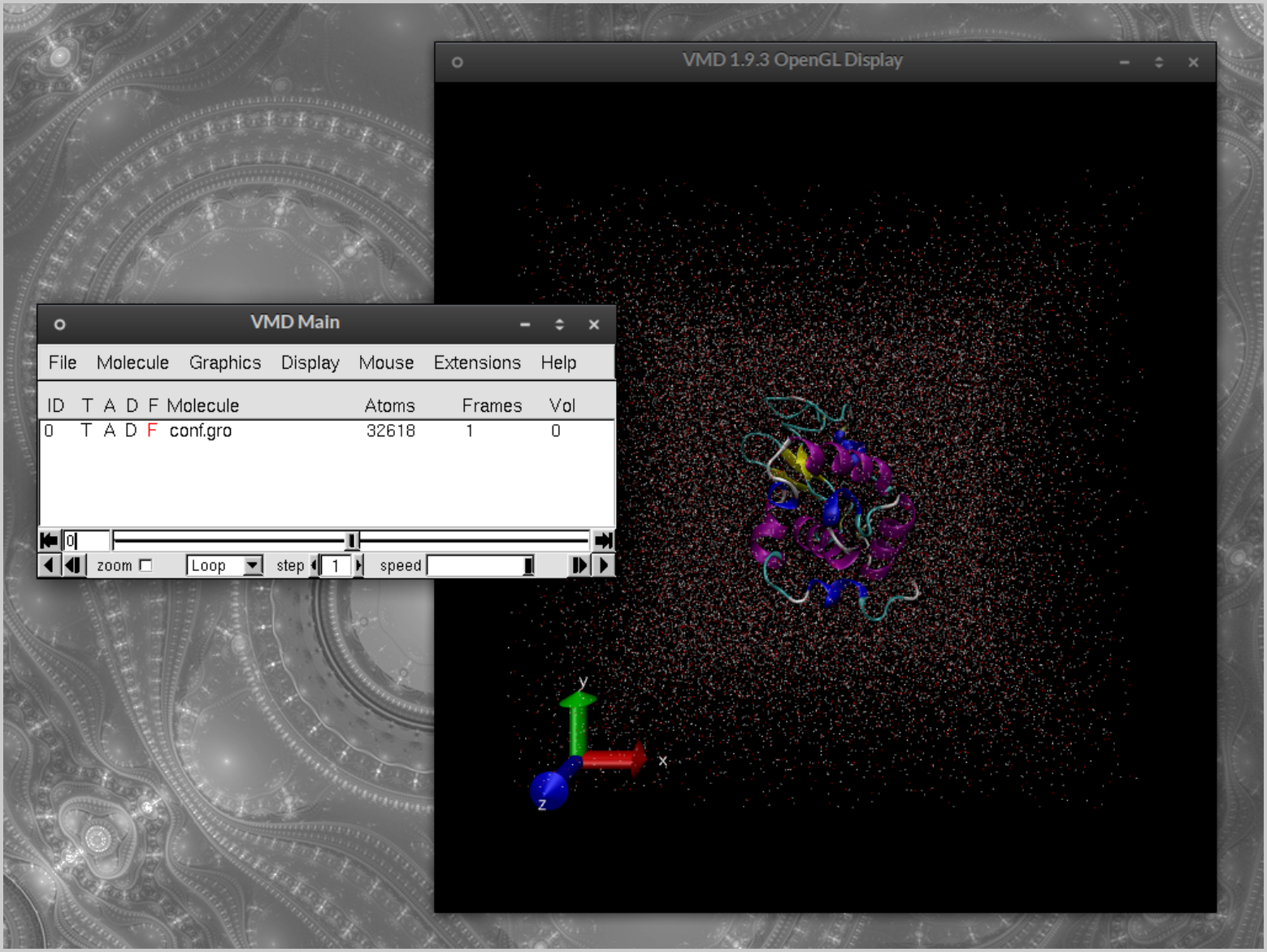


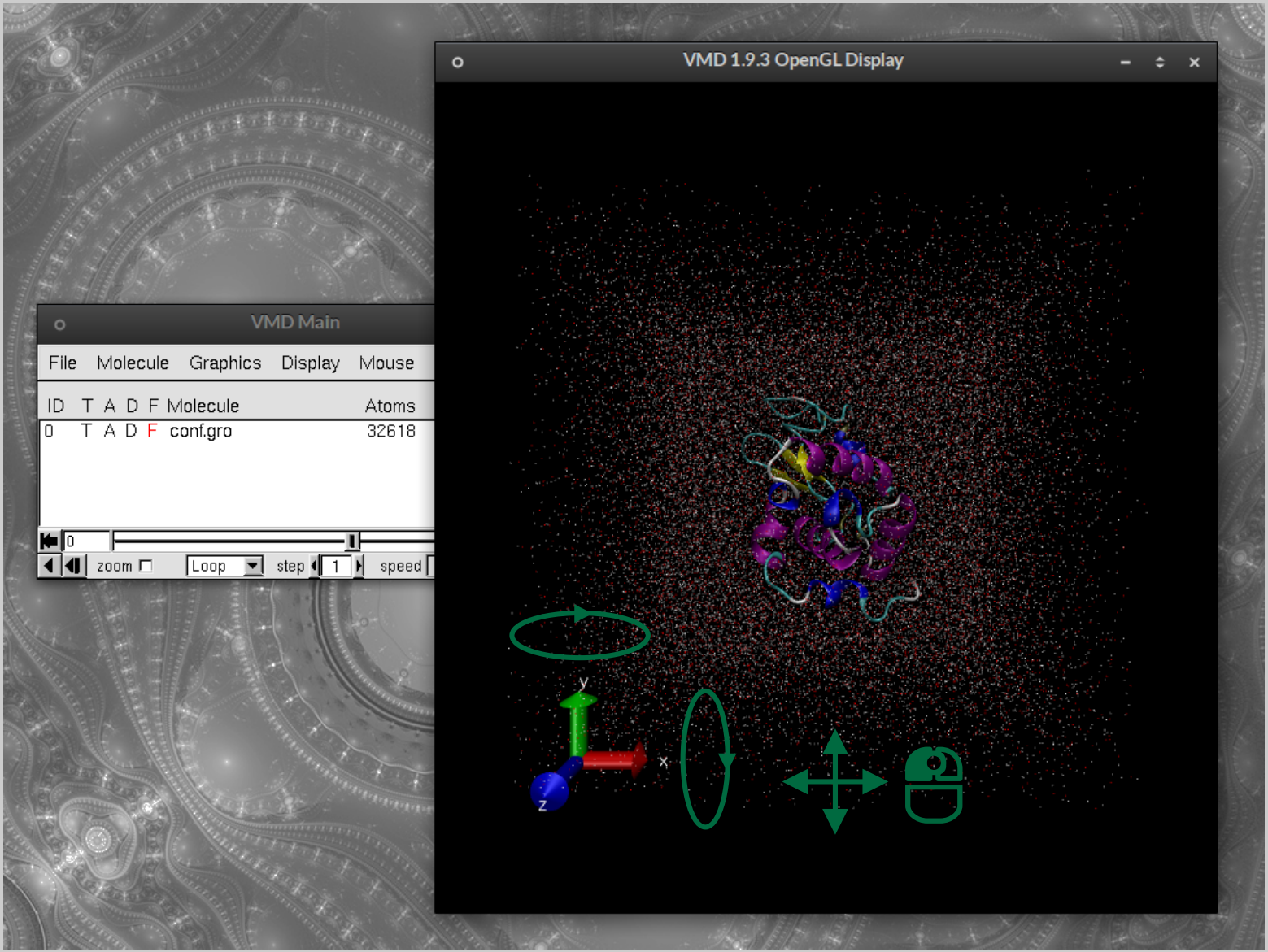
Graphical representations

- Each structure (VMD calls it a “Molecule”) can have one or more graphical representations.
- There is a wide array of drawing styles.
  - Lines, licorice, VdW spheres, surface, balls and sticks, cartoons, etc.
- Representations can be coloured.
  - By atom name, chain, residue type (hydrophobic, polar, acid, basic), rainbow chain (ResID), secondary structure, B-factor (Beta)
- Atom selections can be used to display only part of a structure.
  - A selection applies to a single representation.
  - Powerful “Atom Selection Language”

Atom selection examples

name CA	Alpha carbons
resid 35	Residue 35
resid 35 to 40	Residues 35–40
name CA and resname ALA	Alanine alpha carbons
backbone	Protein backbone atoms
not protein	Any atom not in a protein
name "C.*"	Carbon atoms
mass < 5	Atoms heavier than 5 a.u.
numbonds = 2	Atoms bonded to 2 other atoms
abs(charge) > 1	Atoms with a large net charge
z < 6 and z > 3	Atoms between 3 and 6 Å in z
within 5 of name FE	Atoms within 5 Å of iron atoms
protein within 5 of nucleic	Protein atoms close to nucleic acids
water within 3 of protein	Water close to proteins

3D navigation



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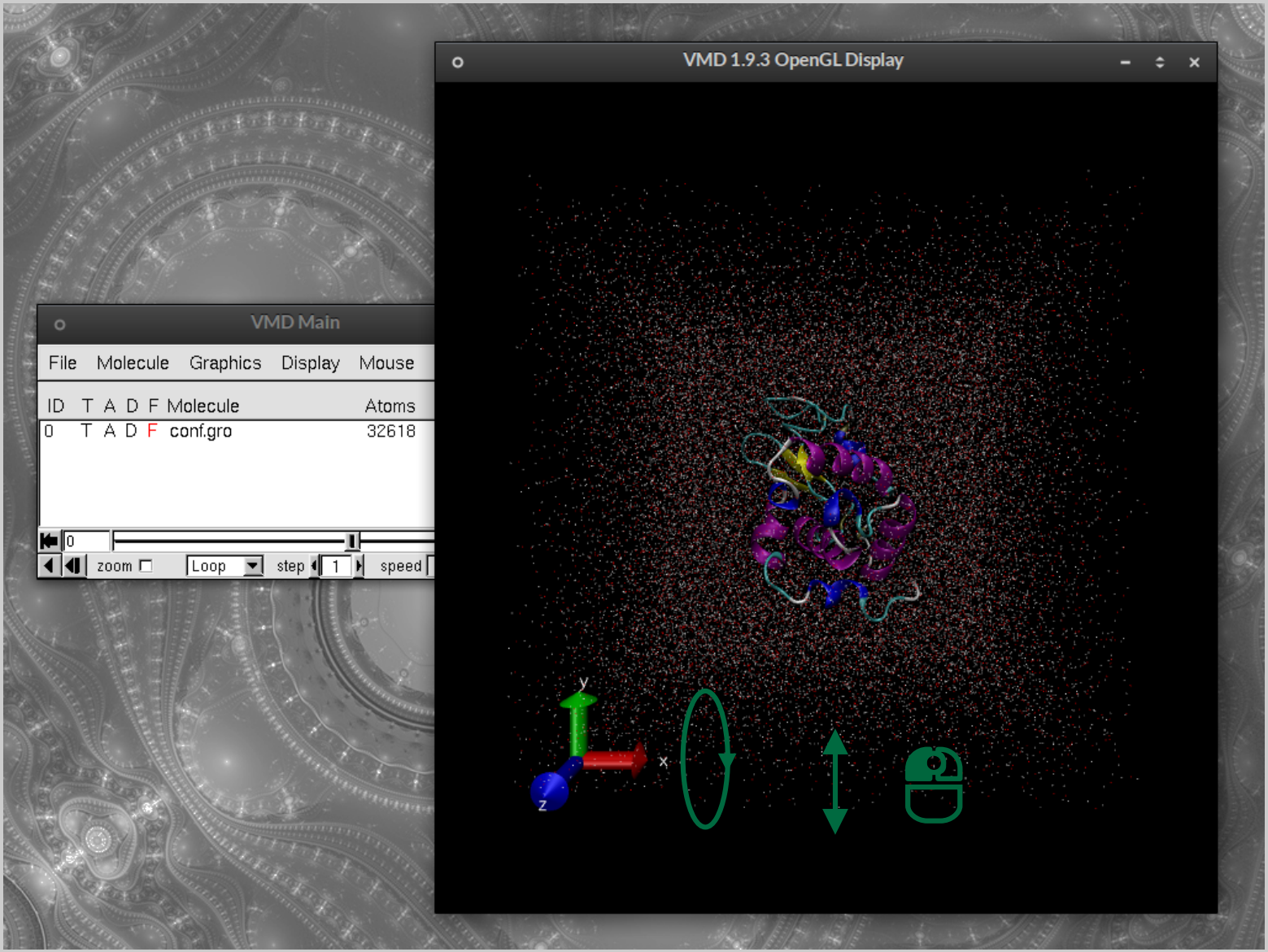
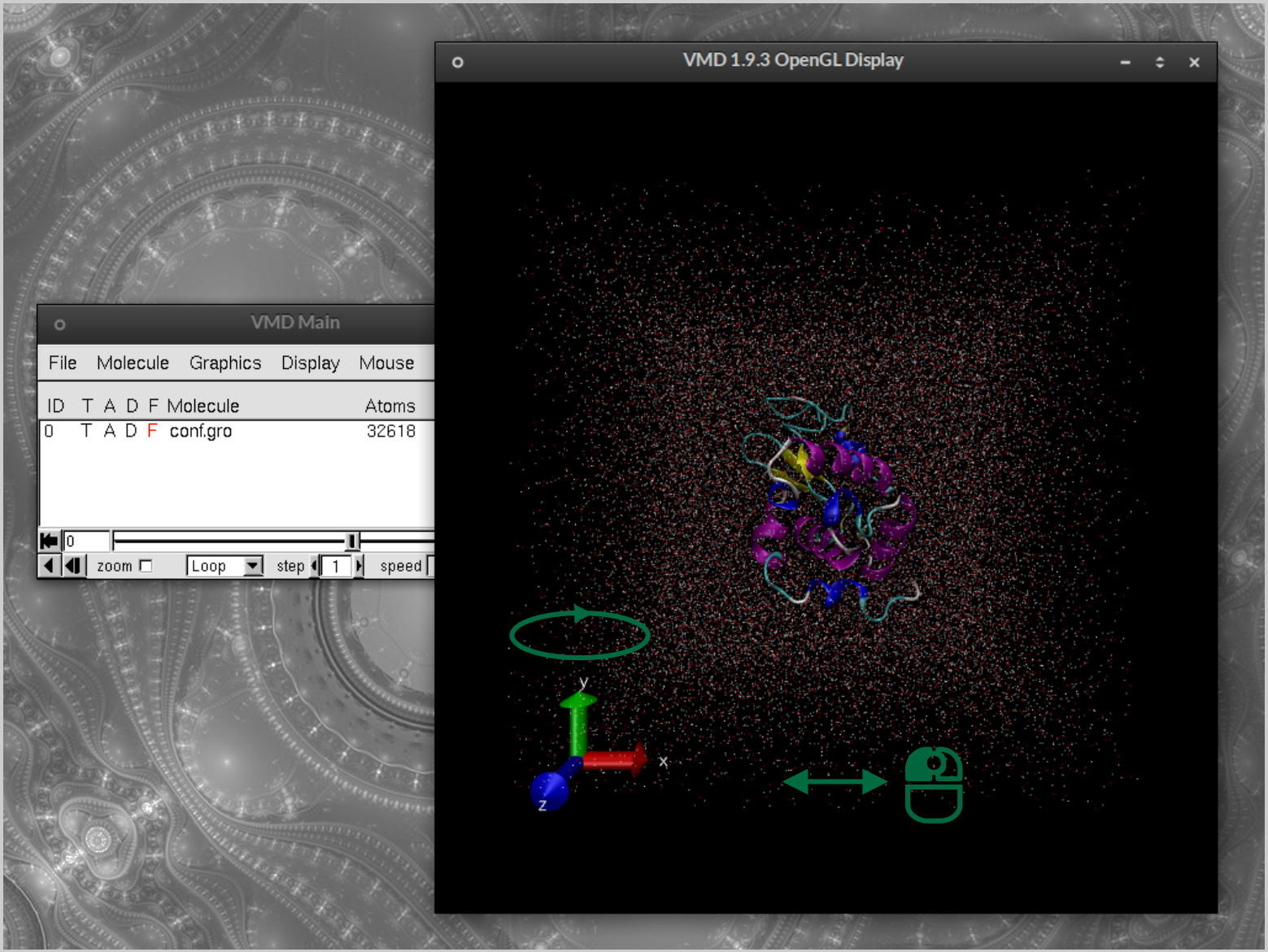
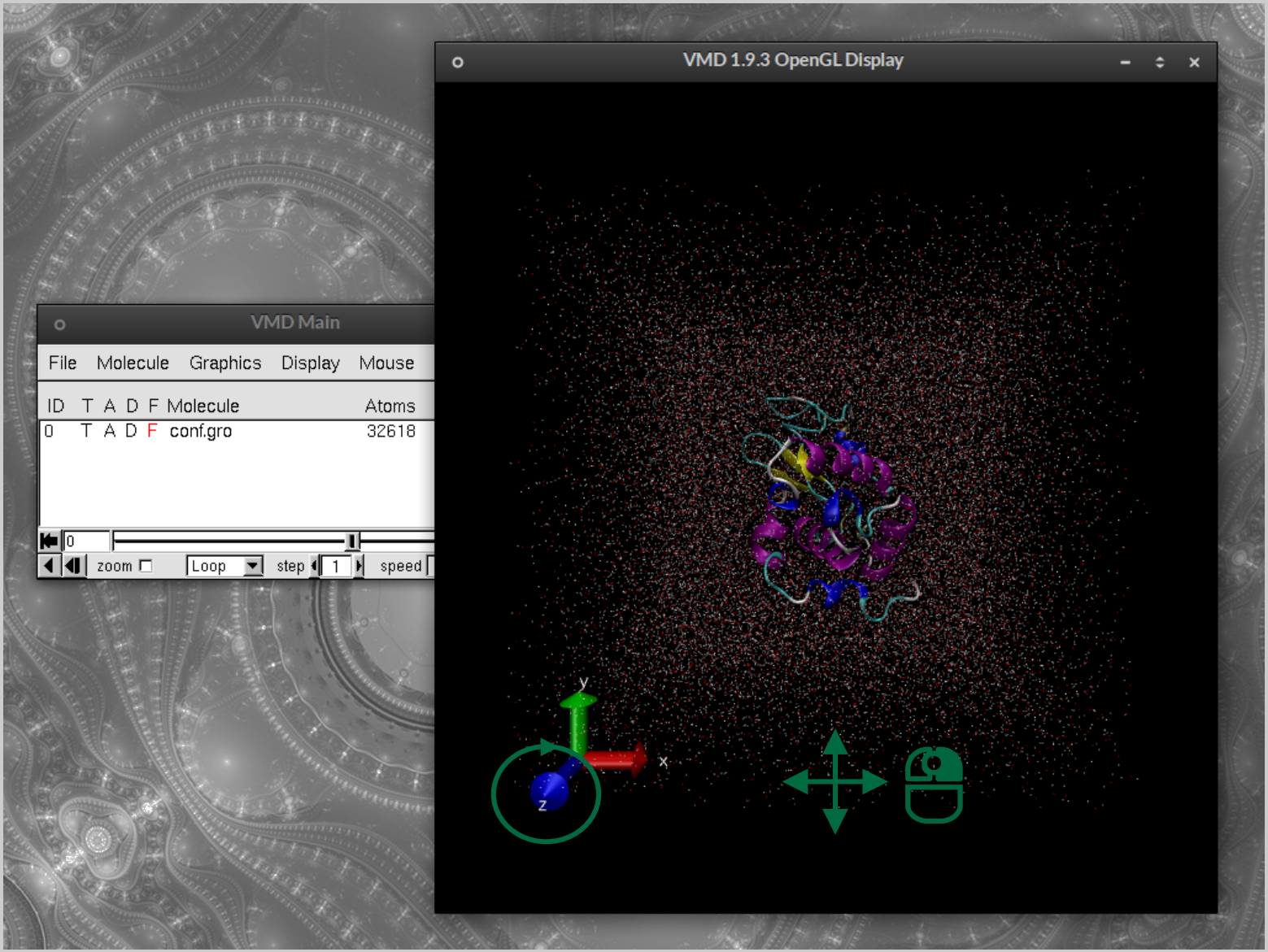


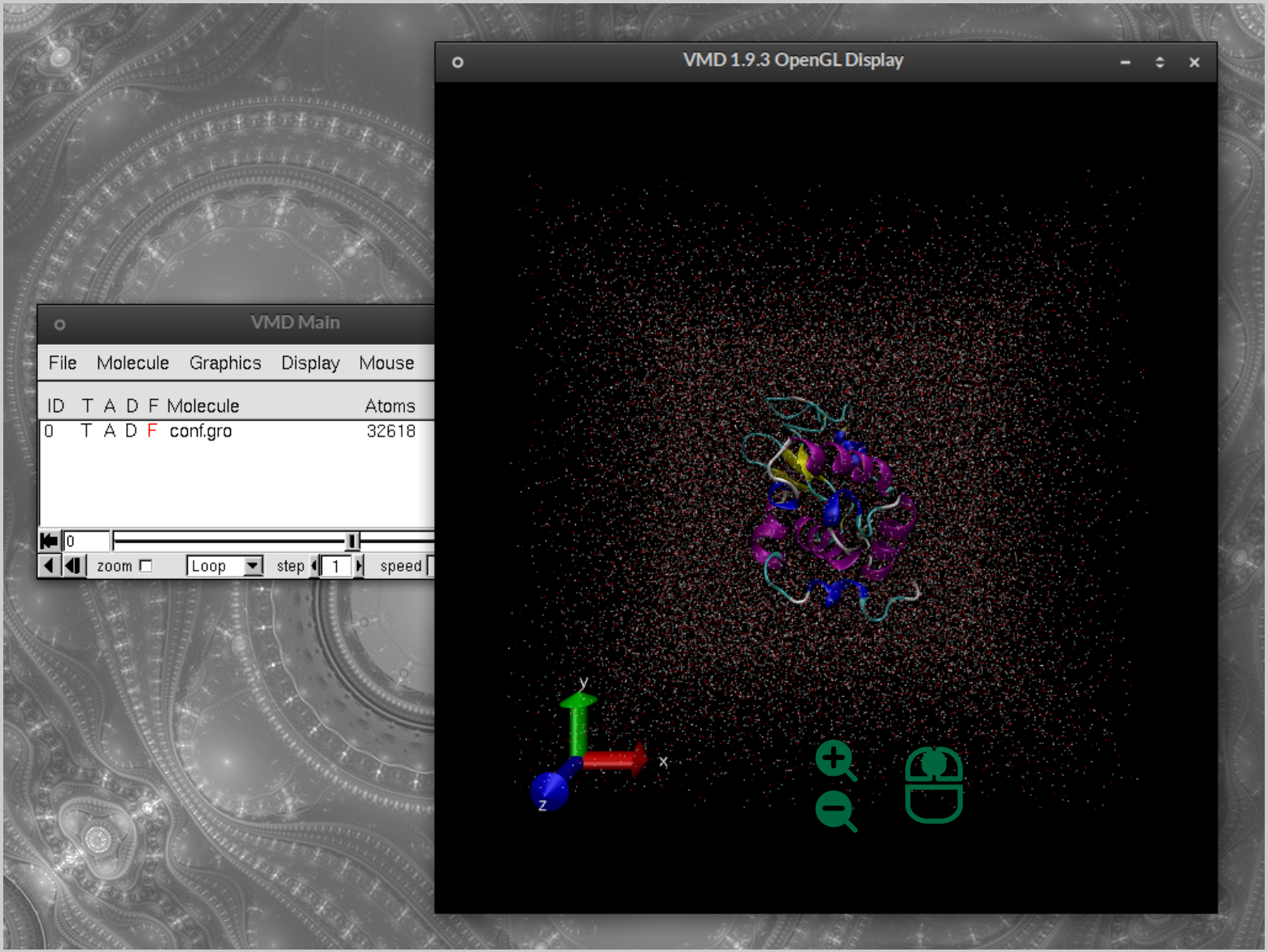
3D navigation



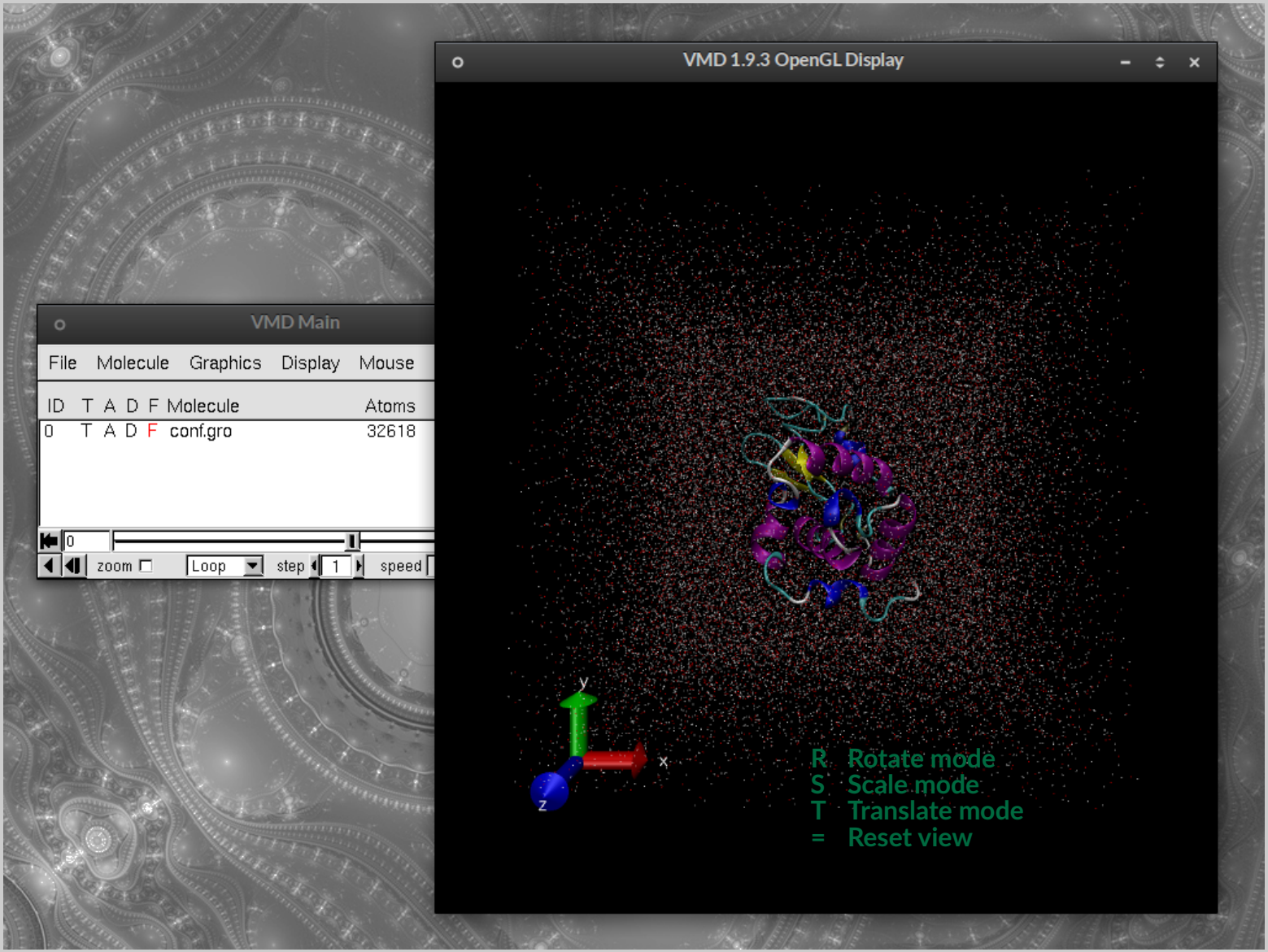
3D navigation



3D navigation



3D navigation



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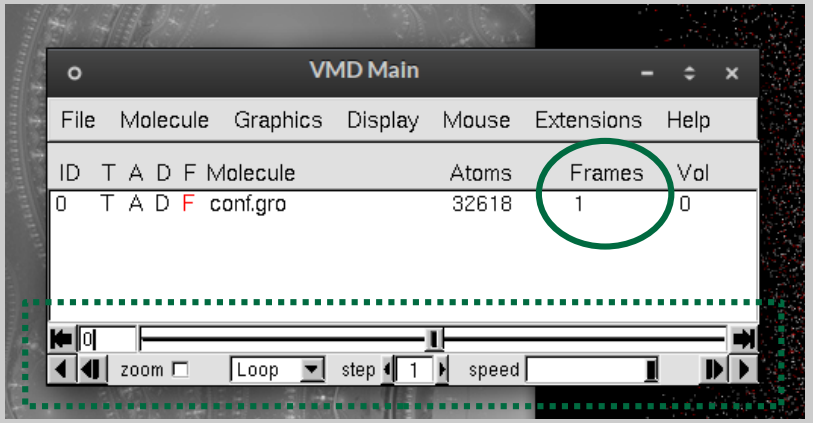
Trajectory basics

- VMD can read molecular trajectories in a variety of formats:
  - DCD (NAMD, CHARMM)
  - XTC, TRR (Gromacs)
  - CRD (Amber)
- For interactive visualisation, analysis, and making movies
- Most trajectory controls are available from the “Main” window.
- Loading trajectories is done through the “Molecule File Browser” (as for structures).



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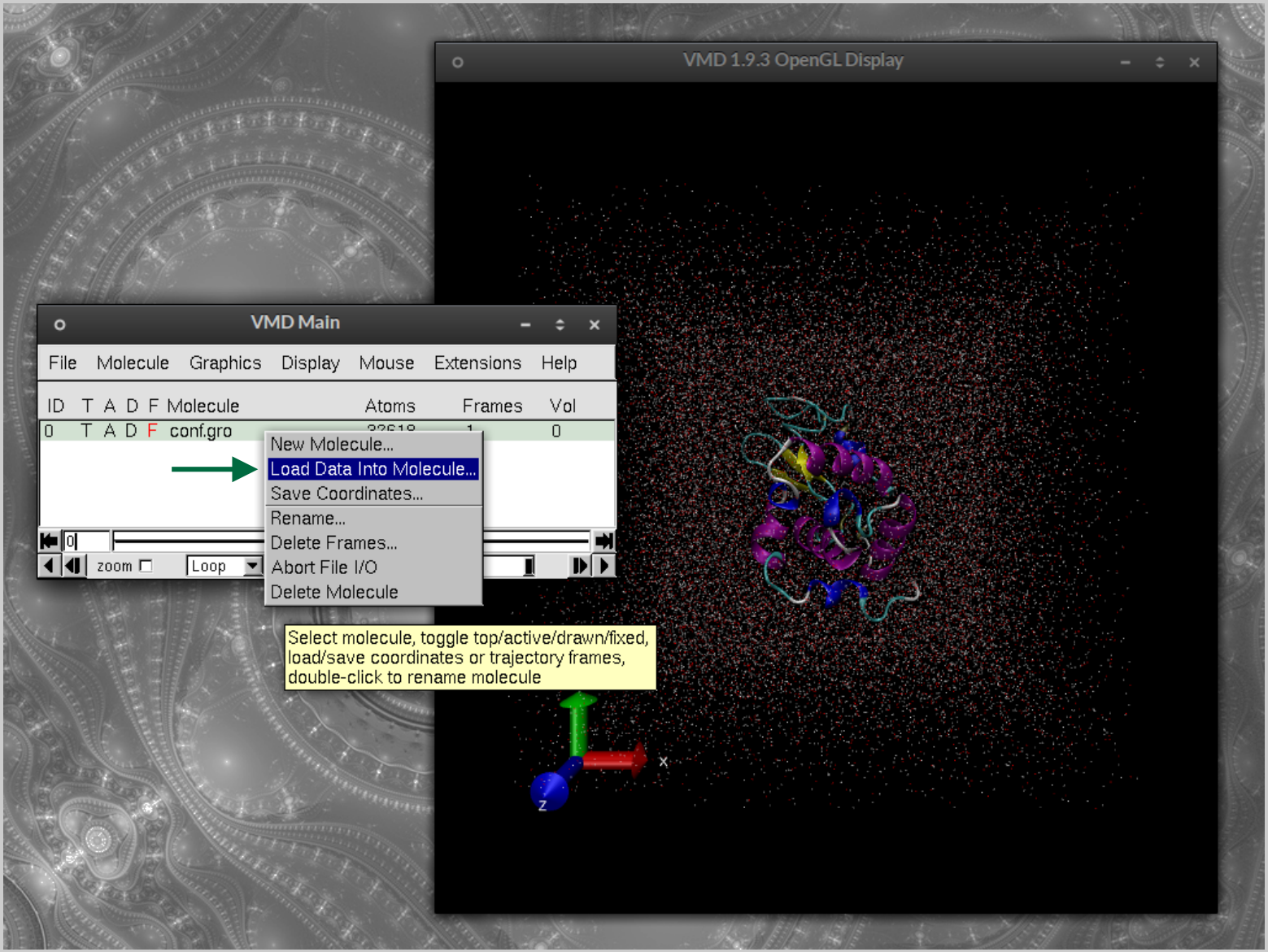

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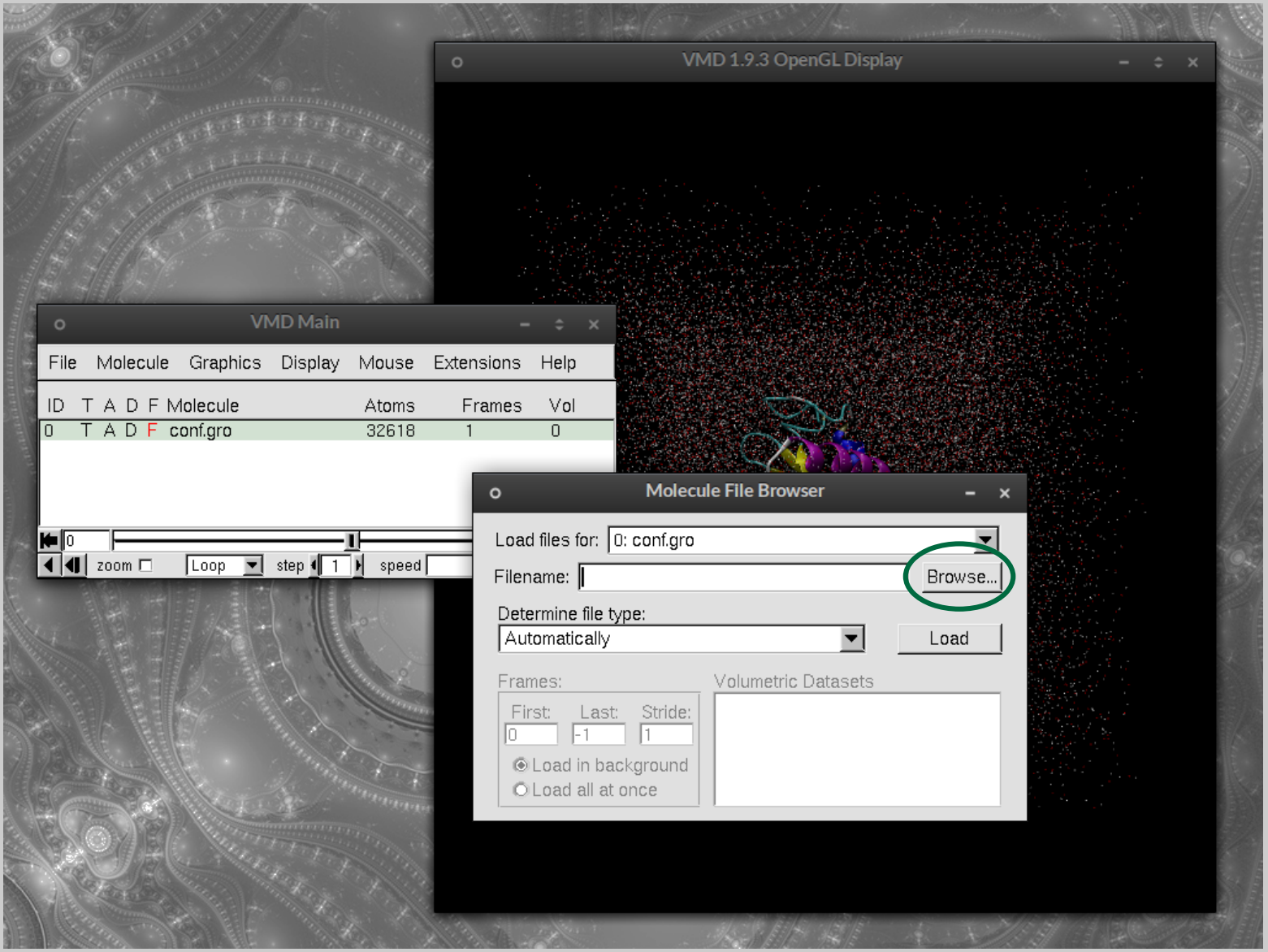

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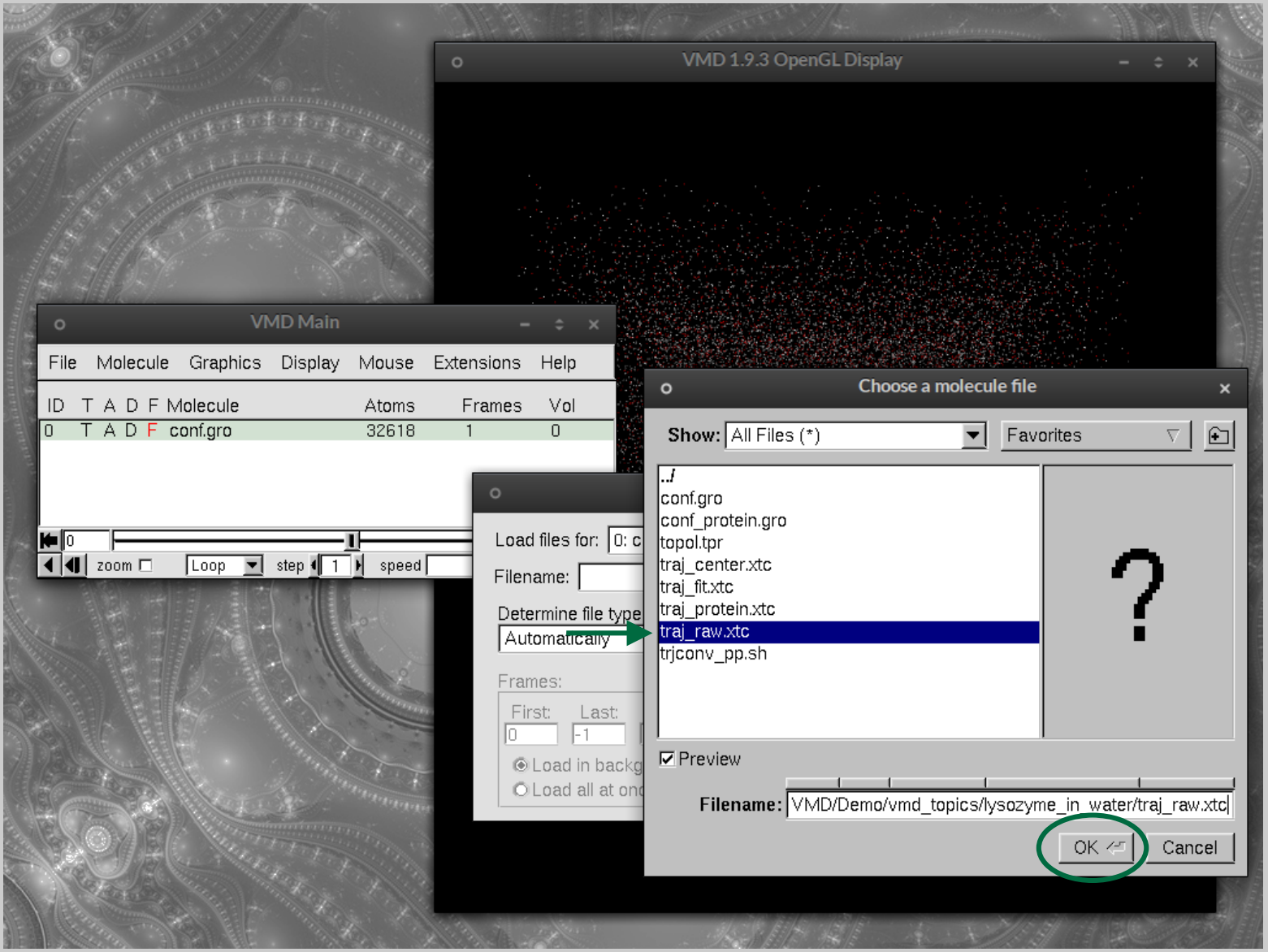

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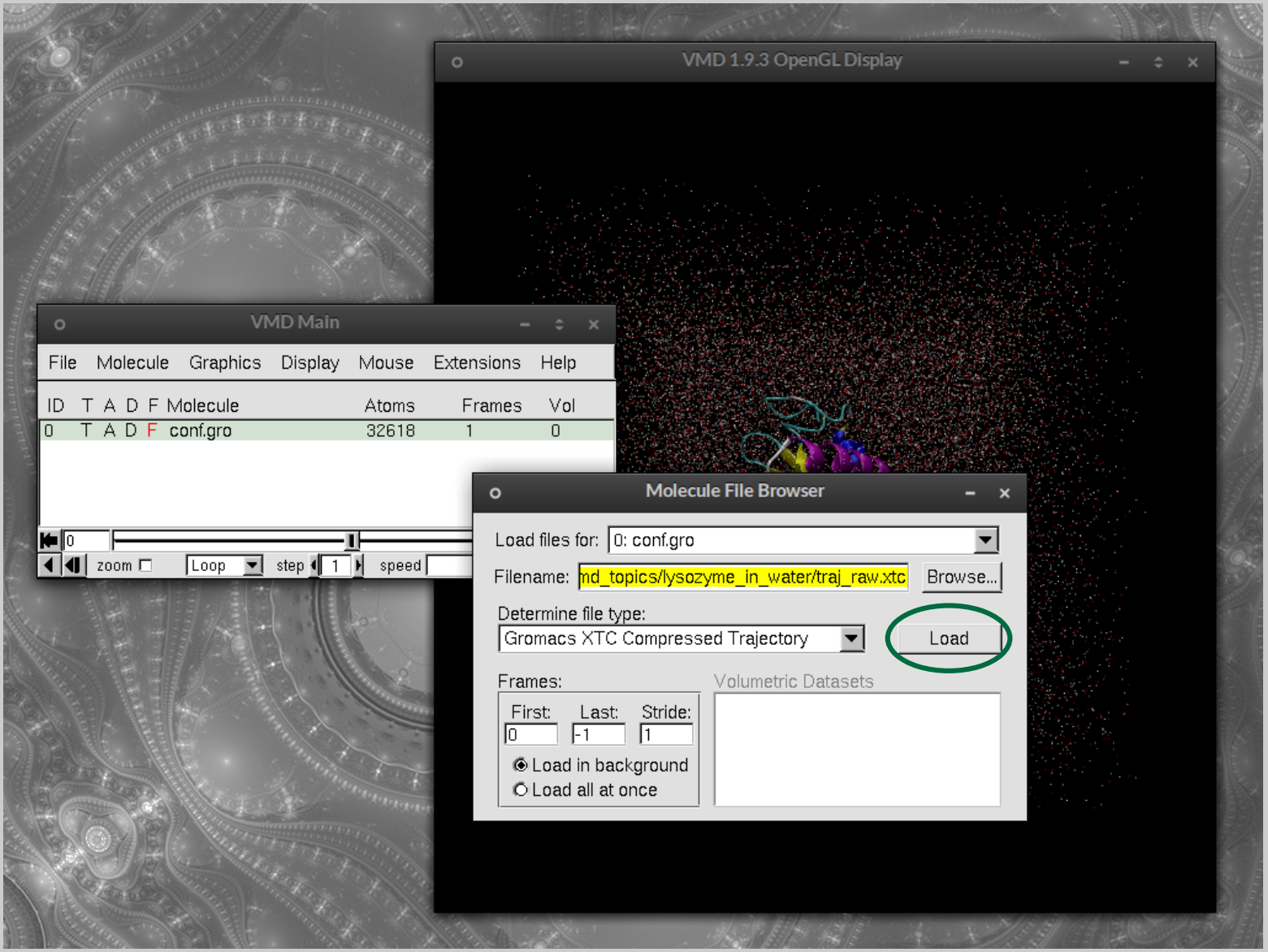

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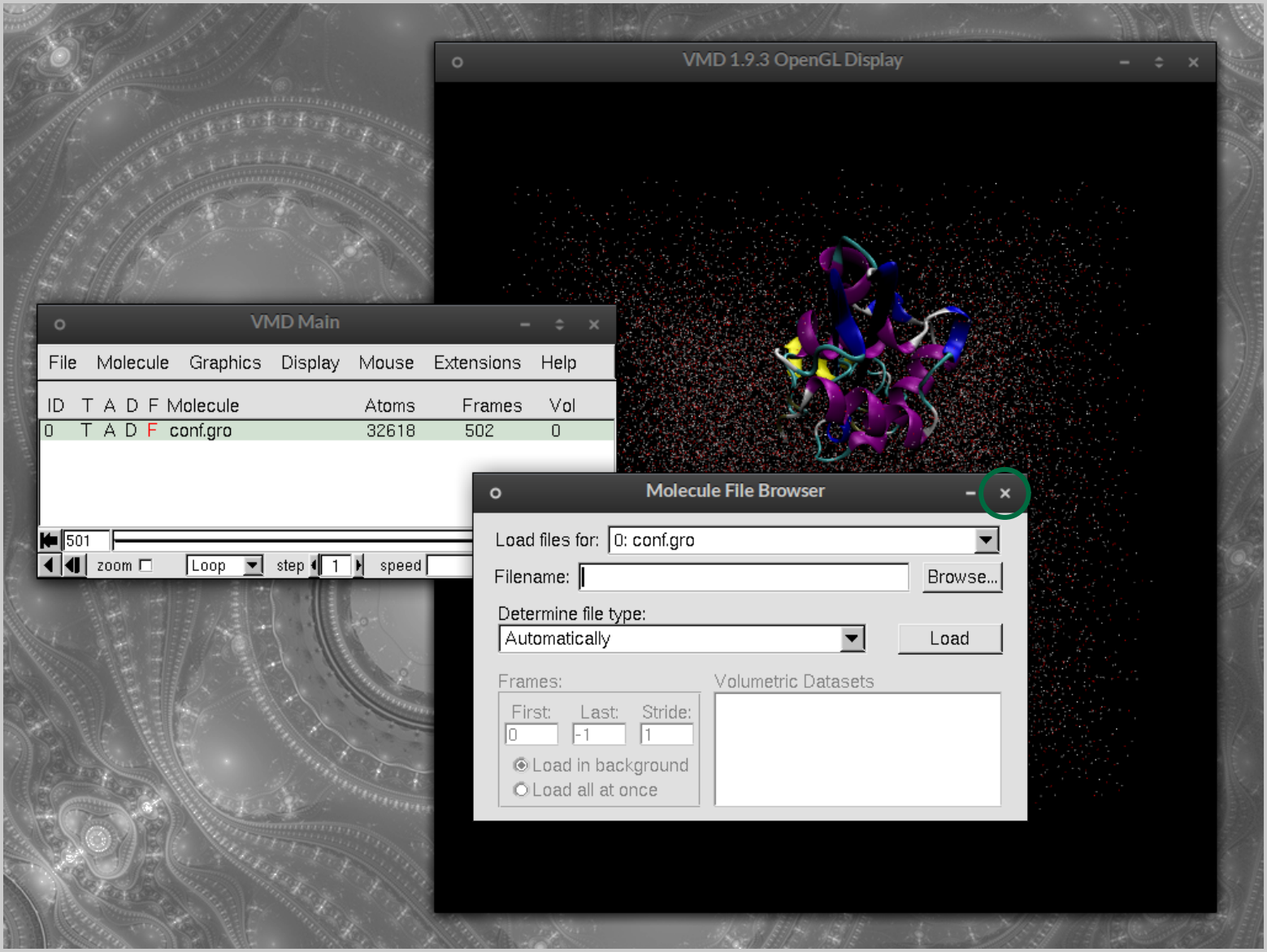

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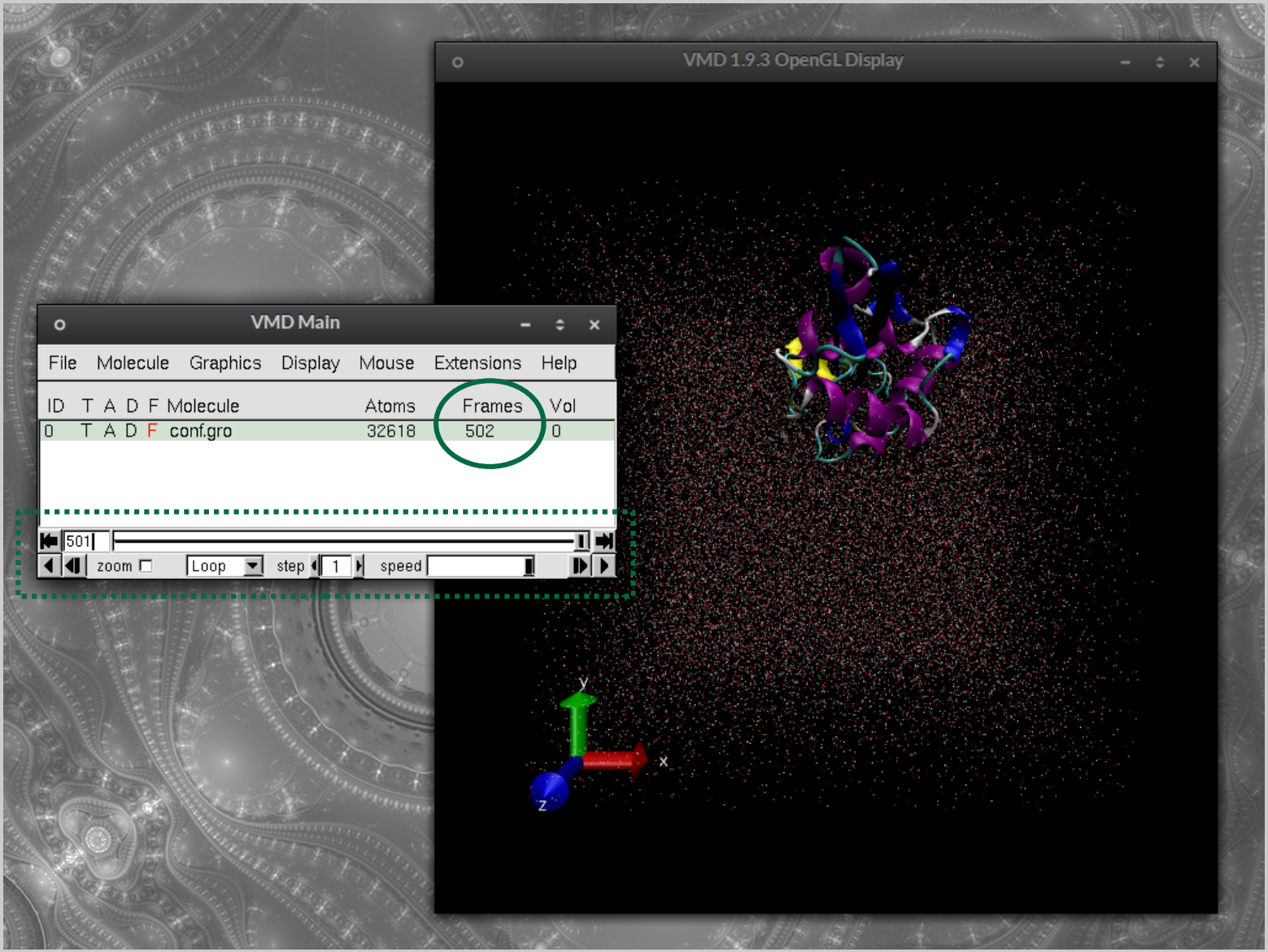

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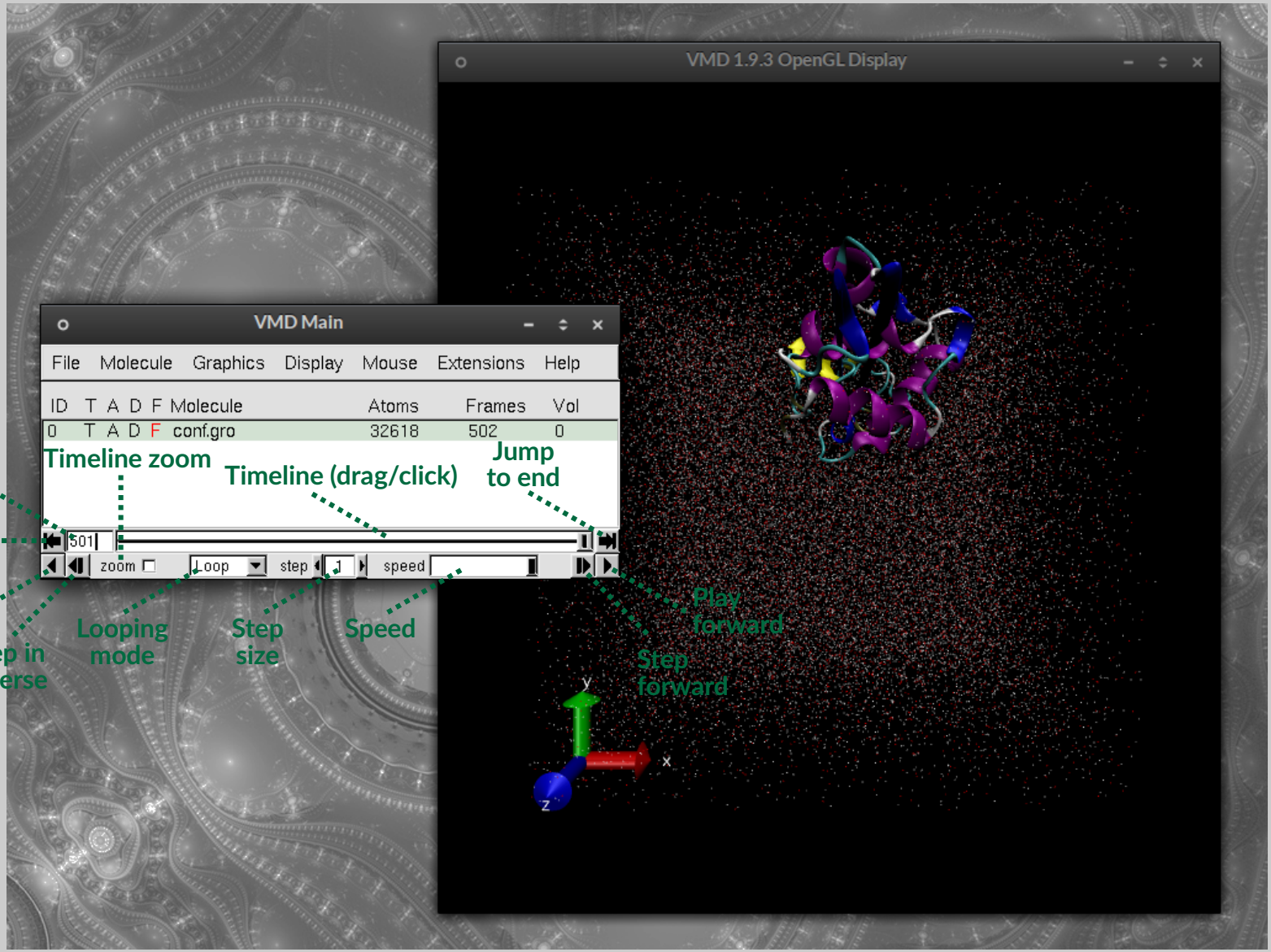
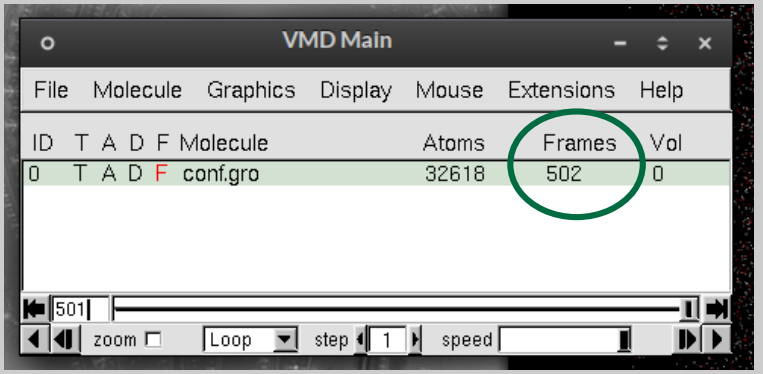


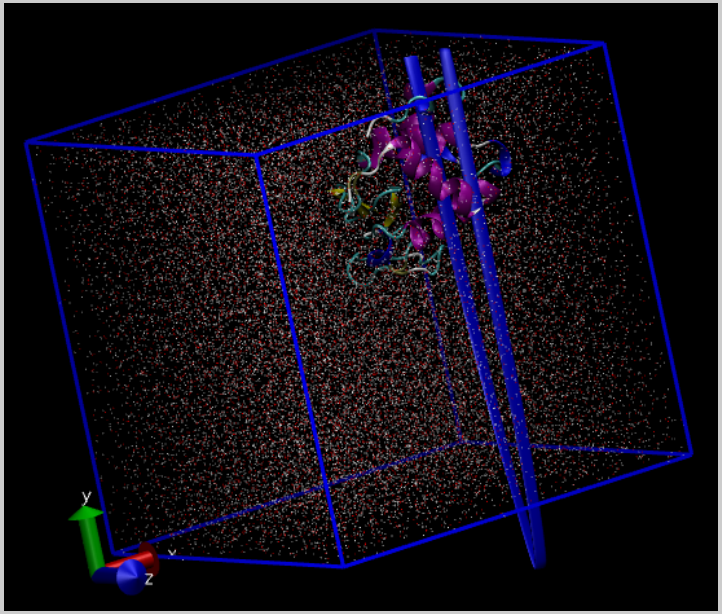
Trajectory troubleshooting

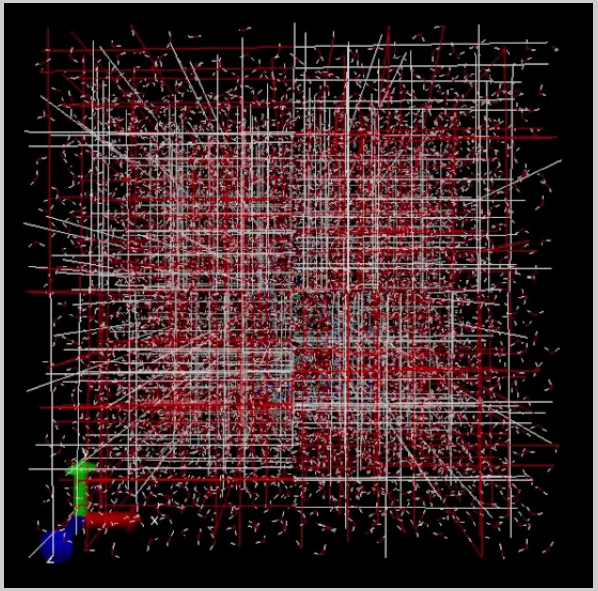
- Unexpected number of frames
  - VMD has no separate “topology” vs “trajectory” concepts.
  - The first frame is the original “topology”.
  - Trajectories typically store initial coordinates as a frame.
  - 2 more frames than expected



Trajectory troubleshooting

- Lines/bonds all over the place
  - Atoms are bonded across periodic boundary conditions (PBC).
  - Trajectory post-processing is required to make molecules whole.





Trajectory troubleshooting

- Number of atom mismatch between topology and trajectory
  - The files must match exactly.
  - If atoms are removed from the trajectory by post-processing, a corresponding topology must also be created.
- Out of memory errors or crash
  - VMD loads all trajectory frames in memory.
  - Compressed trajectories require more memory than file size.
    - The compressed XTC in this demo is 60M but requires 250M of memory, or about 4 times the file size.
  - Post-processing can be used to reduce file size.
    - Removing atoms outside of a selection
    - Removing frames outside of a time range
    - Skipping frames

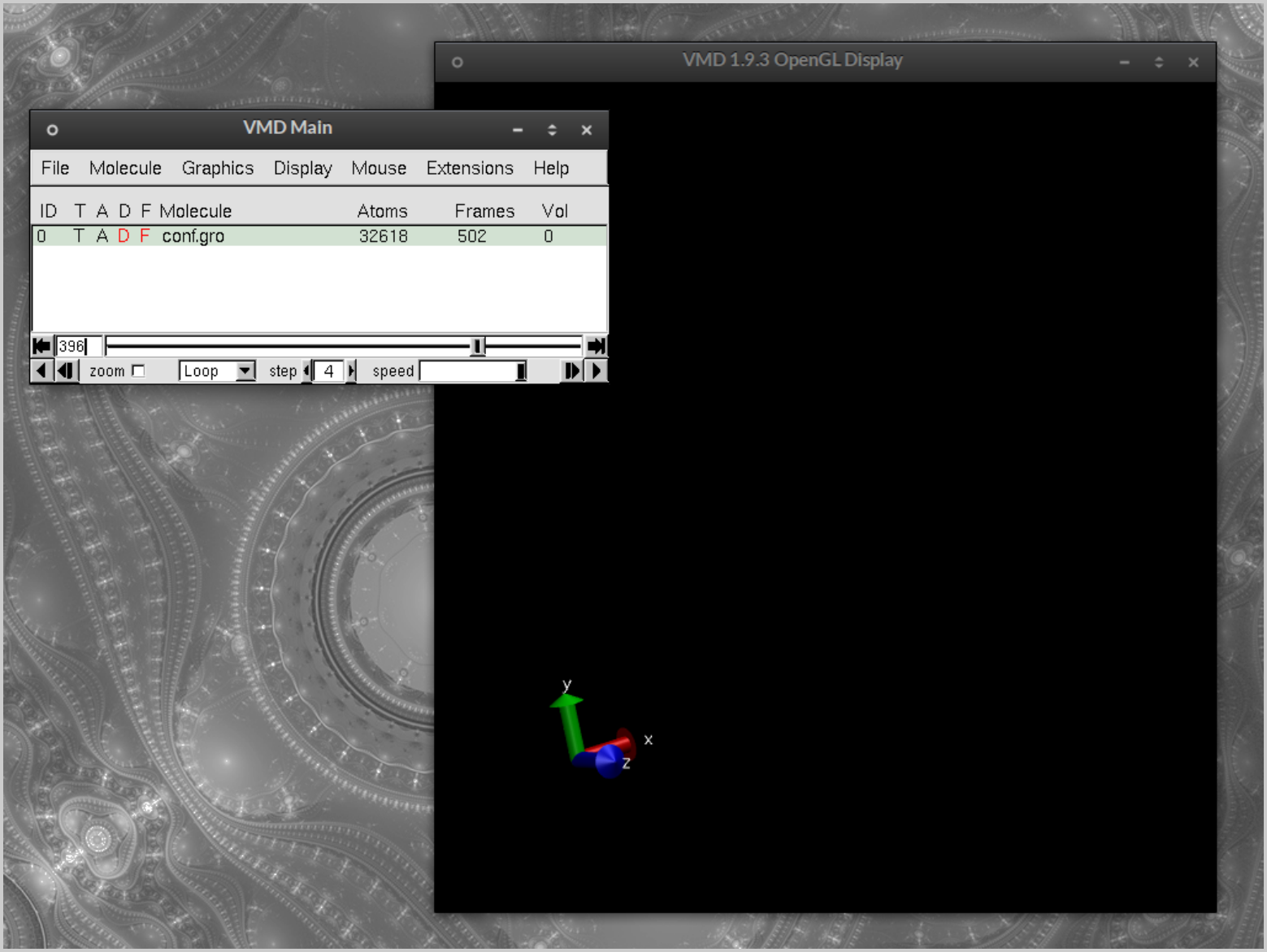
Trajectory post-processing

- Transforming raw MD trajectories through operations
  - Making molecules whole (PBC treatement)
  - Centering a selection
  - Fitting (RMSD minimisation) a selection
  - Removing atoms outside of a selection
  - Removing frames outside of a time range
  - Skipping frames
- Makes certain analyses easier
- Makes visualisation easier

Trajectory post-processing

```
#!/usr/bin/env bash

# trjconv_pp.sh - Post-process raw GROMACS trajectory

# Center protein, and make molecules whole
gmx trjconv -s "topol.tpr" -f "traj_raw.xtc" -center -pbc mol \
            -o "traj_center.xtc" <<-eof
    Protein
    System
eof

# Apply RMSD-minimising fit to protein
gmx trjconv -s "topol.tpr" -f "traj_center.xtc" -fit progressive \
            -o "traj_fit.xtc" <<-eof
    Protein
    System
eof

# Remove non-protein atoms
gmx trjconv -s "topol.tpr" -f "traj_fit.xtc" \
            -o "traj_protein.xtc" <<-eof
    Protein
eof

# Create topology for protein-only trajectory
gmx trjconv -s "topol.tpr" -f "conf.gro" \
            -o "conf_protein.gro" <<-eof
    Protein
eof
                                                    29,3          Tout
```

Trajectory post-processing



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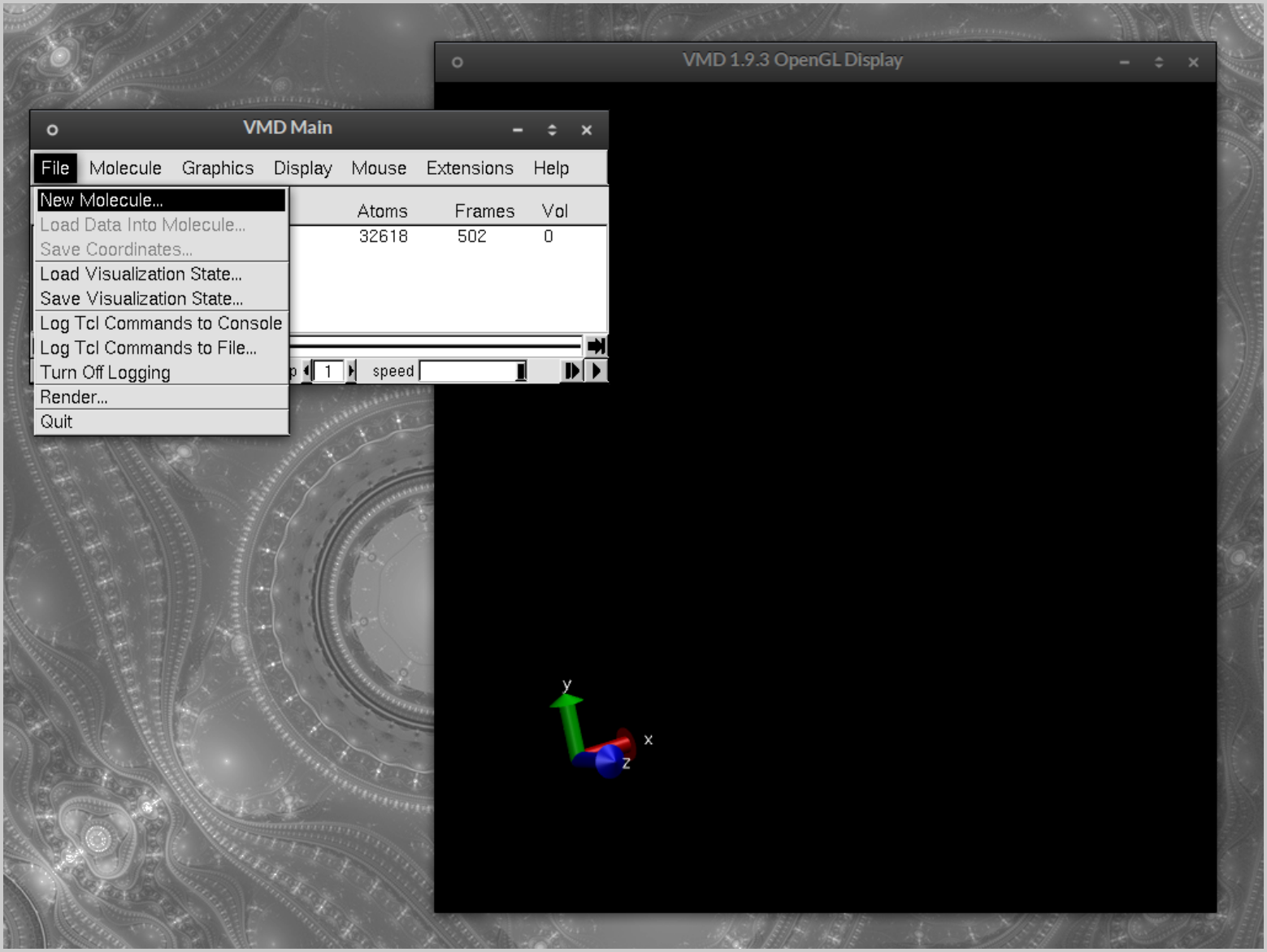
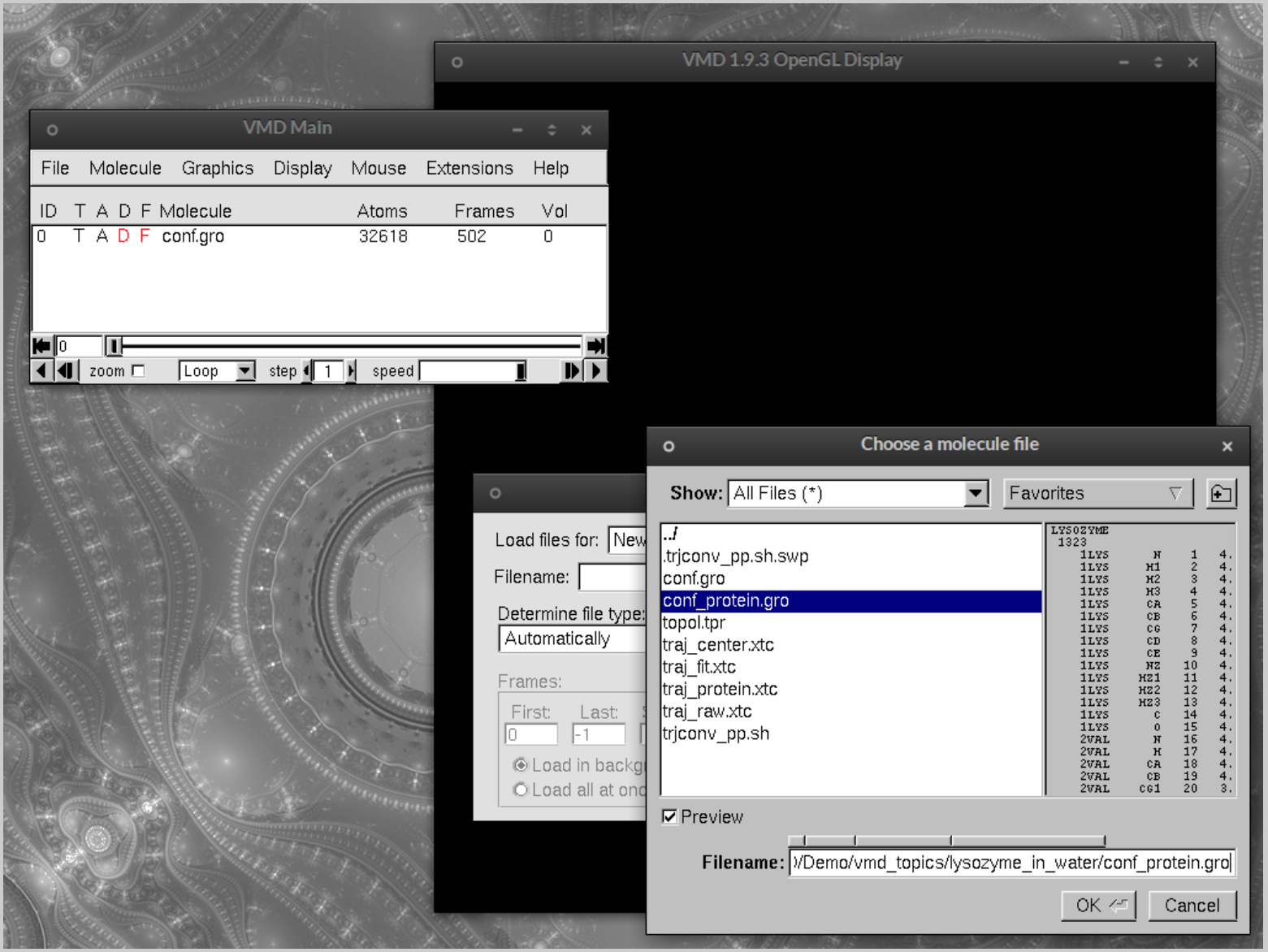
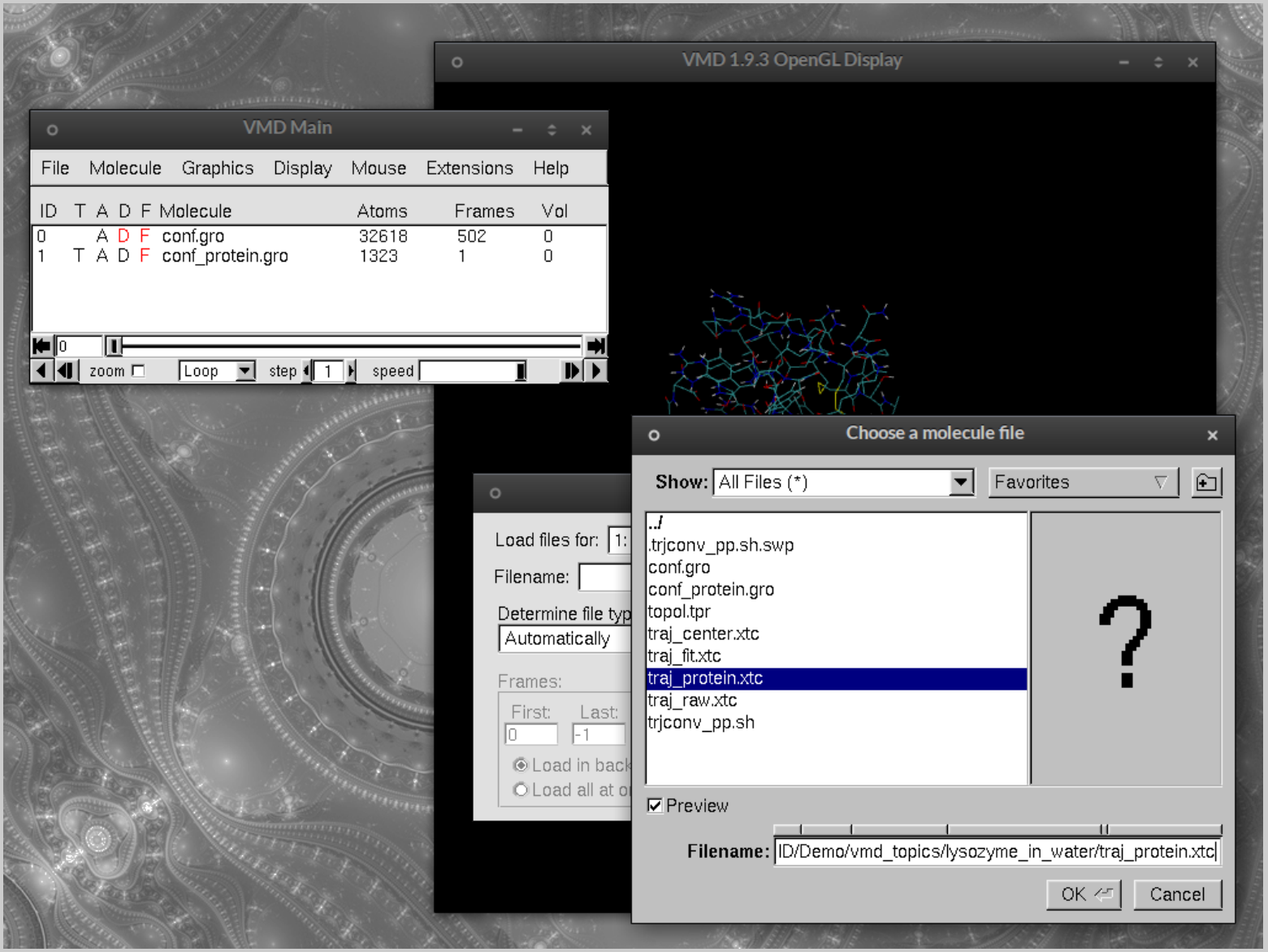


Trajectory post-processing



Trajectory post-processing



Contents

- Basics
  - Loading structures
  - Representations
  - Atom selections
  - 3D navigation
- Drawing methods
- Materials and colouring
- Image rendering
- Trajectories
  - Troubleshooting
  - Post-processing
- **Movies**
  - **Using the “Movie Maker”**
- Scripting
  - Tk Console
  - Tcl scripts
  - *vmdrc*
- Combining trajectories, movies, and scripting

Movie-making strategies

- Three-step process
  - Animating a trajectory or structure
  - Rendering movie frames
  - Encoding the movie from the separate frames
- Animation and rendering
  - Movie Maker
  - Scripting
- Encoding
  - Movie Maker
  - External tools

Animating

- Movie Maker
  - Molecular trajectory
  - Single structure with changing viewpoint (XY 8-loop or Y rotation)
  - Easy
  - Limited
- Movie Maker and scripting
  - User-defined procedure to step through a trajectory, change the viewpoint, etc.
  - More flexible
- Pure scripting
  - Total control

Rendering

- Movie Maker
  - No need to deal explicitly with rendering
    - Frames are created in a working directory, then deleted
    - For internal encoding
  - Individual frames in JPEG, TARGA
    - For encoding with external tools
    - Additional step, but better quality
- Scripting
  - Create frames using commands
  - Encoding through external tools

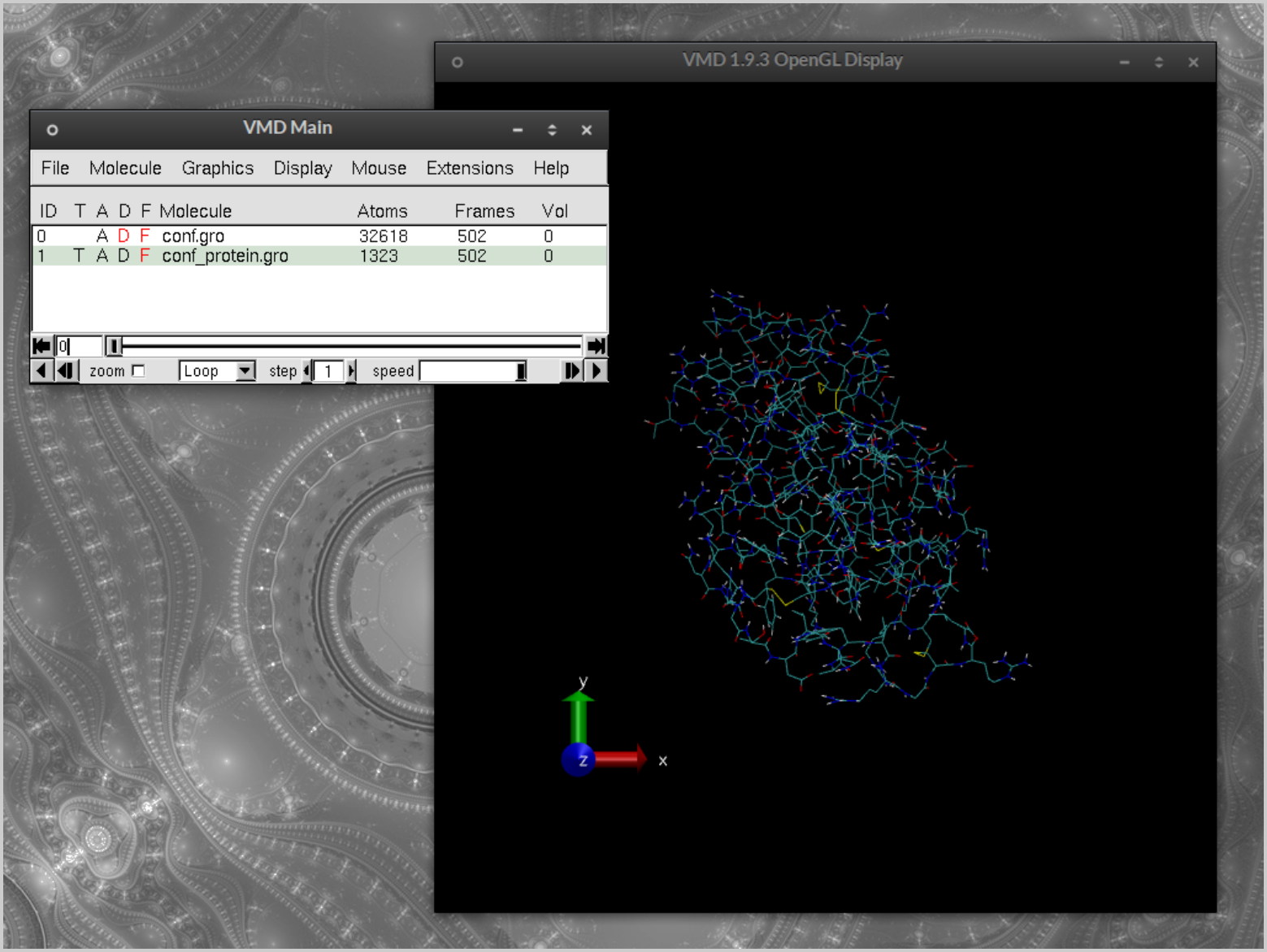
Encoding

- Movie Maker
  - Movies in MPEG-1, MPEG-2, animated GIF
  - Using external *ppmtompeg*, *mencoder*, *ffmpeg*
  - Somewhat low-quality movies
  - Old codecs…
- External tools
  - Encoding (*ffmpeg* to produce MP4 with H.265 codec)
  - Post-processing frames (ImageMagick to add text, graphs…)
  - Add audio (Audacity)

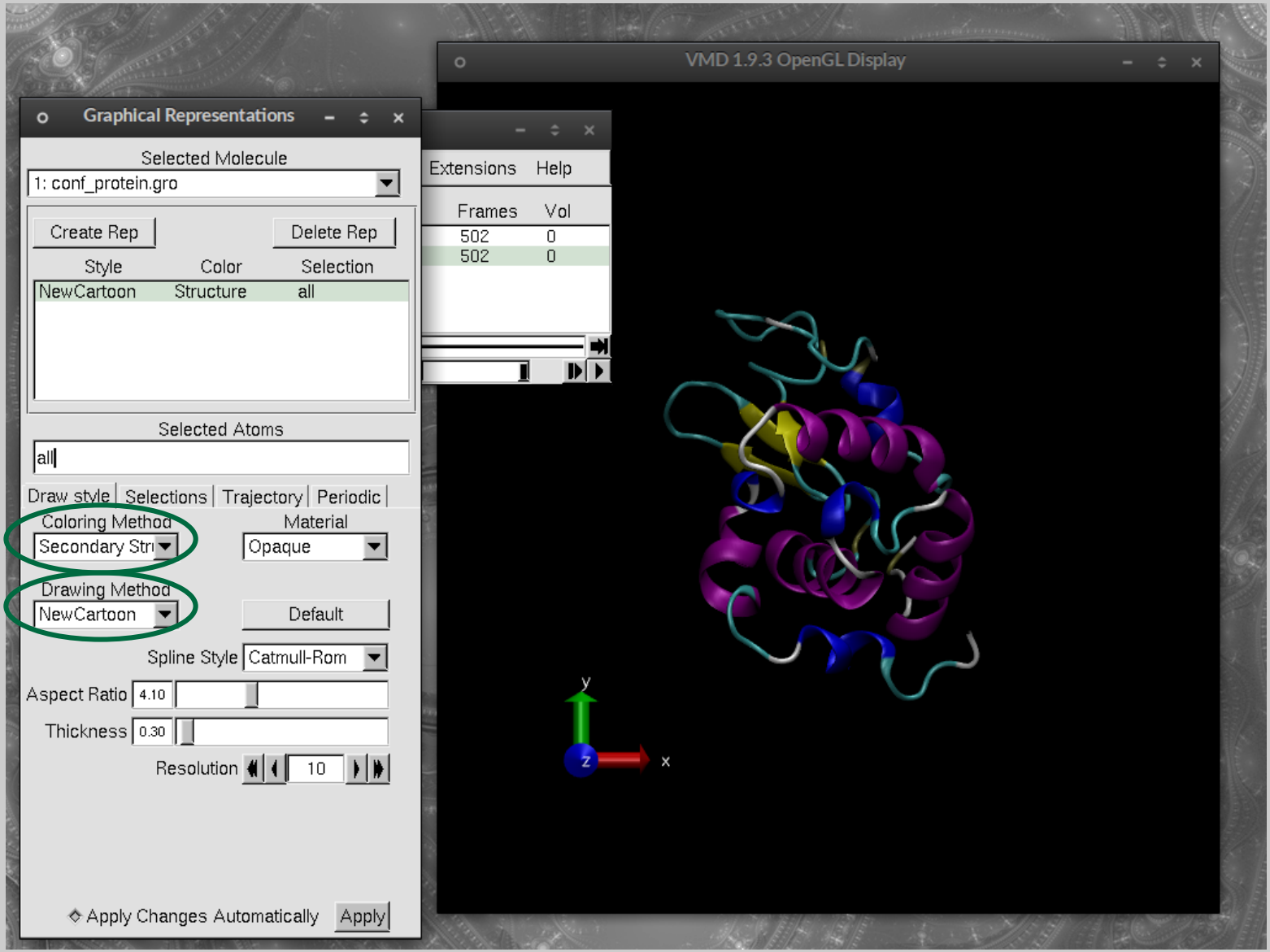
Movie Maker

- Load your trajectory/structure
- Set graphical representations
  - Trajectory smoothing
- Movie Maker
  - Set animation options
  - Choose rendering and encoding options
  - Make tea (it can take a while…)

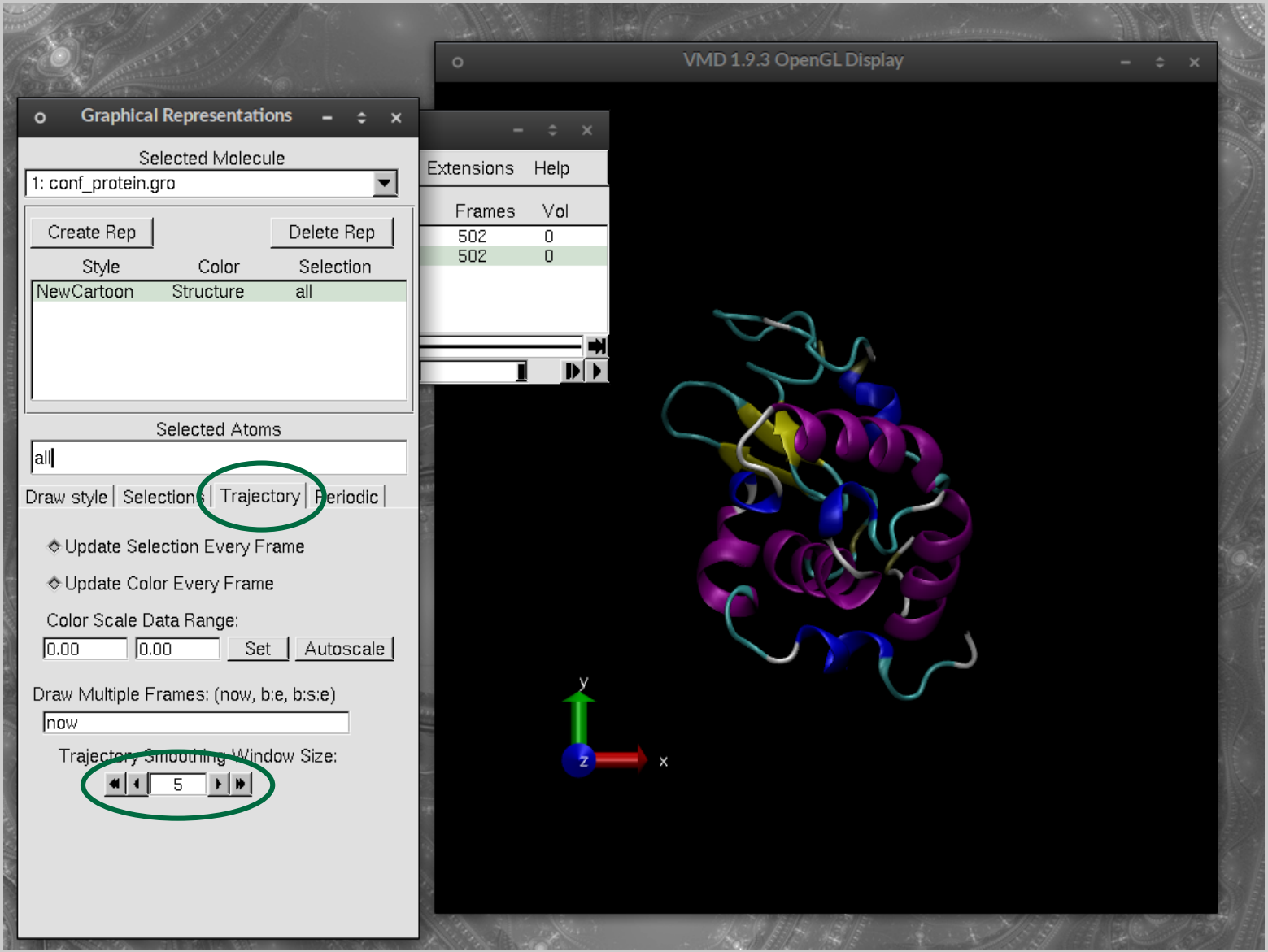
Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom
Loop
step 1
speed
y
z
x

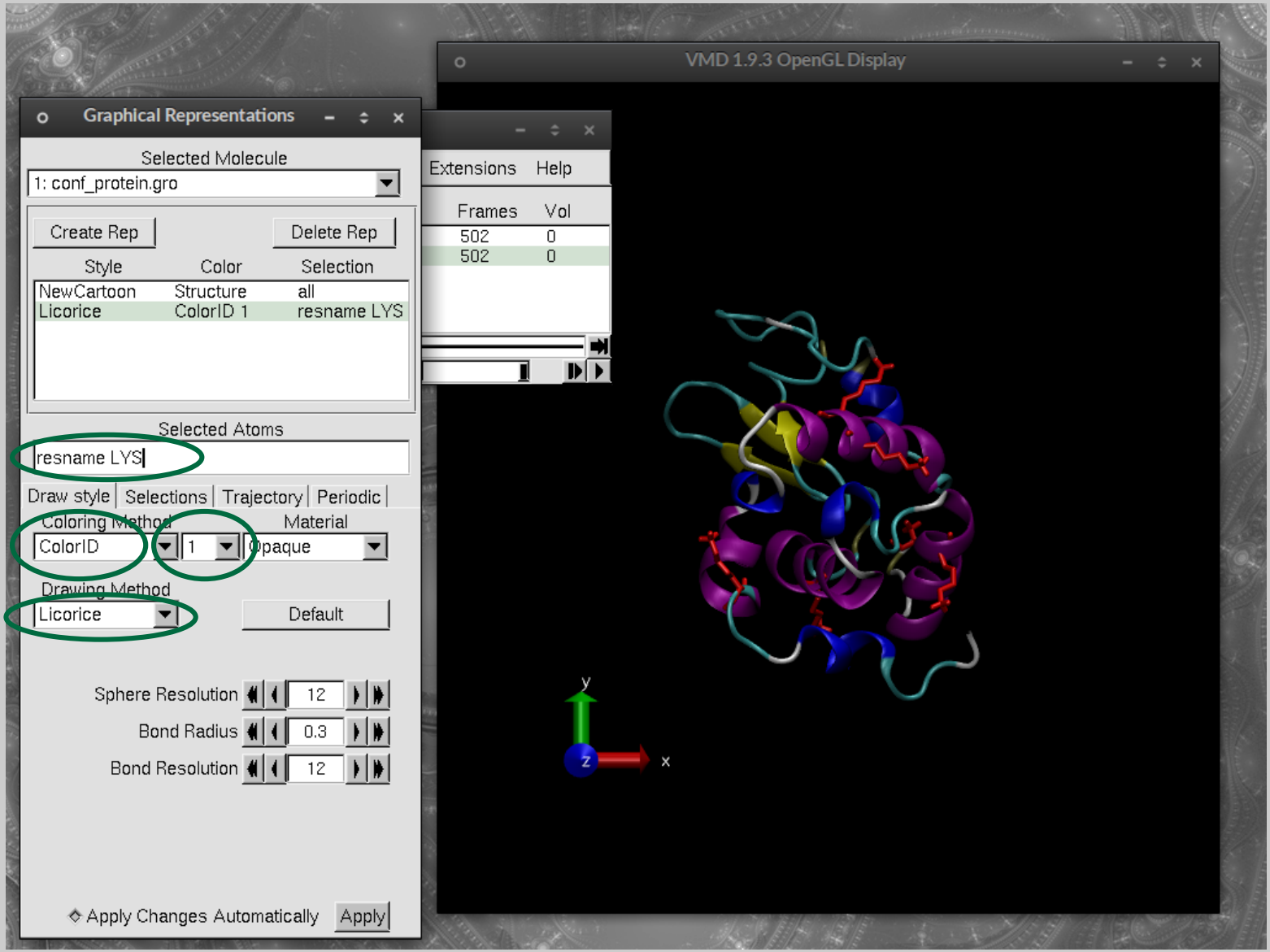
Movie Maker


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
1: conf_protein.gro
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Selected Atoms
all
Draw style
Selections
Trajectory
Periodic
Coloring Method
Secondary Str
Material
Opaque
Drawing Method
NewCartoon
Default
Spline Style
Catmull-Rom
Aspect Ratio
4.10
Thickness
0.30
Resolution
10
Apply Changes Automatically
Apply
Extensions
Help
Frames
Vol
502
0
502
0
y
z
x

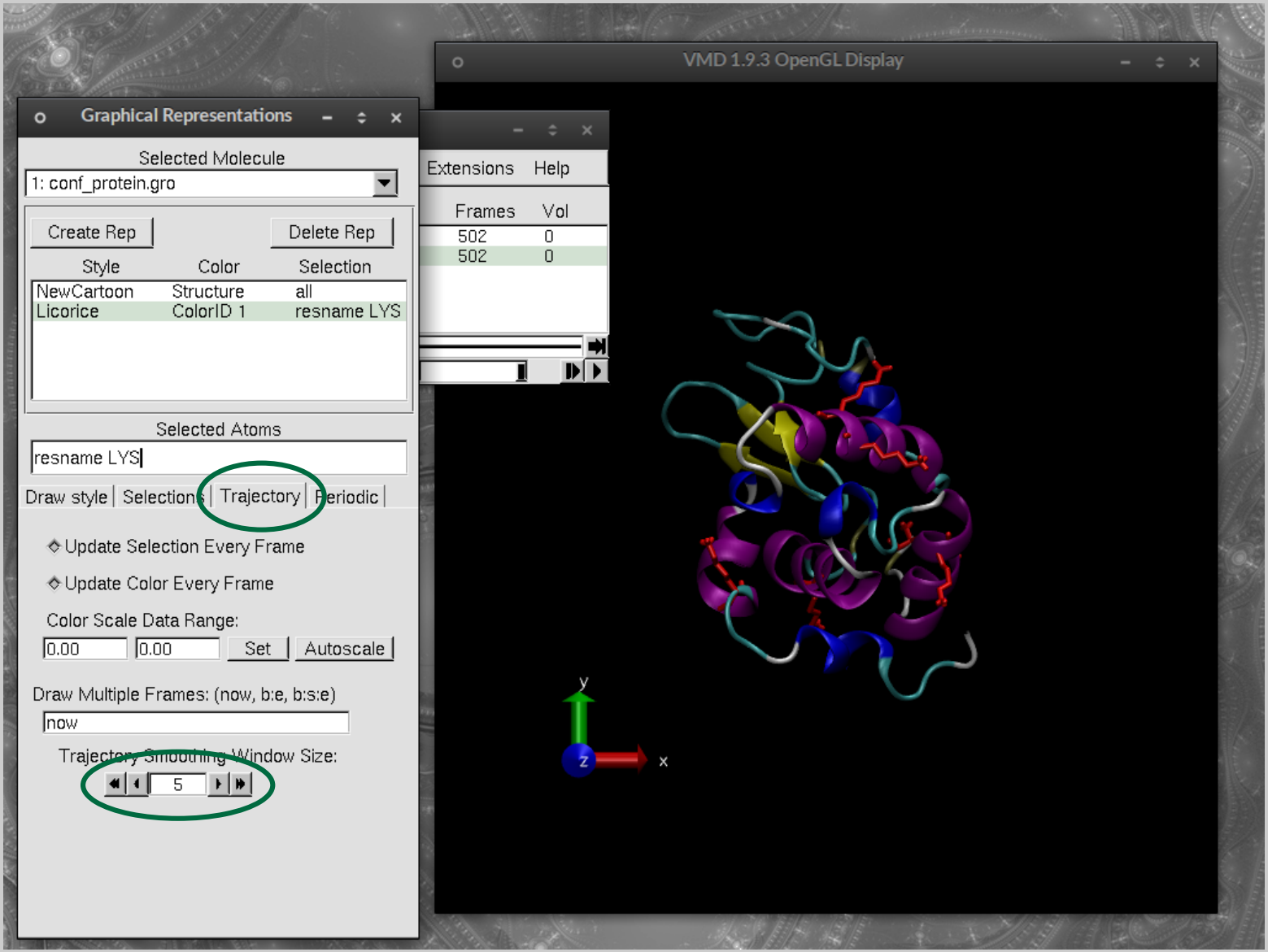
Movie Maker


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
1: conf_protein.gro
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Selected Atoms
all
Draw style
Selections
Trajectory
Periodic
Update Selection Every Frame
Update Color Every Frame
Color Scale Data Range:
0.00
0.00
Set
Autoscale
Draw Multiple Frames: (now, b:e, b:s:e)
now
Trajectory Smoothing Window Size:
5
Extensions
Help
Frames
Vol
502
0
502
0
y
z
x

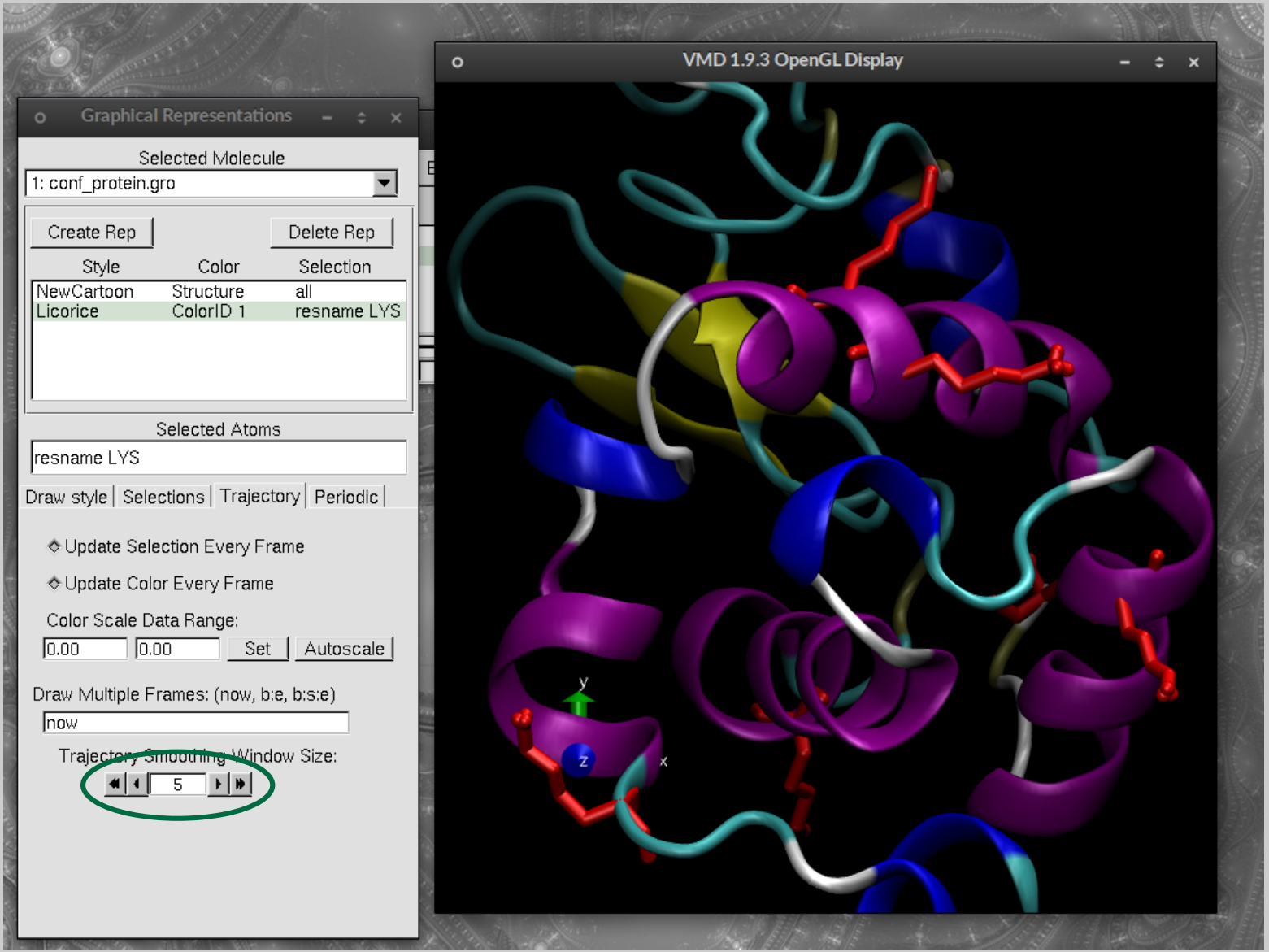
Movie Maker


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
1: conf_protein.gro
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Licorice
ColorID 1
resname LYS
Selected Atoms
resname LYS
Draw style
Selections
Trajectory
Periodic
Coloring Method
Material
ColorID
1
Opaque
Drawing Method
Licorice
Default
Sphere Resolution
12
Bond Radius
0.3
Bond Resolution
12
Apply Changes Automatically
Apply
Extensions
Help
Frames
Vol
502
0
502
0
y
z
x

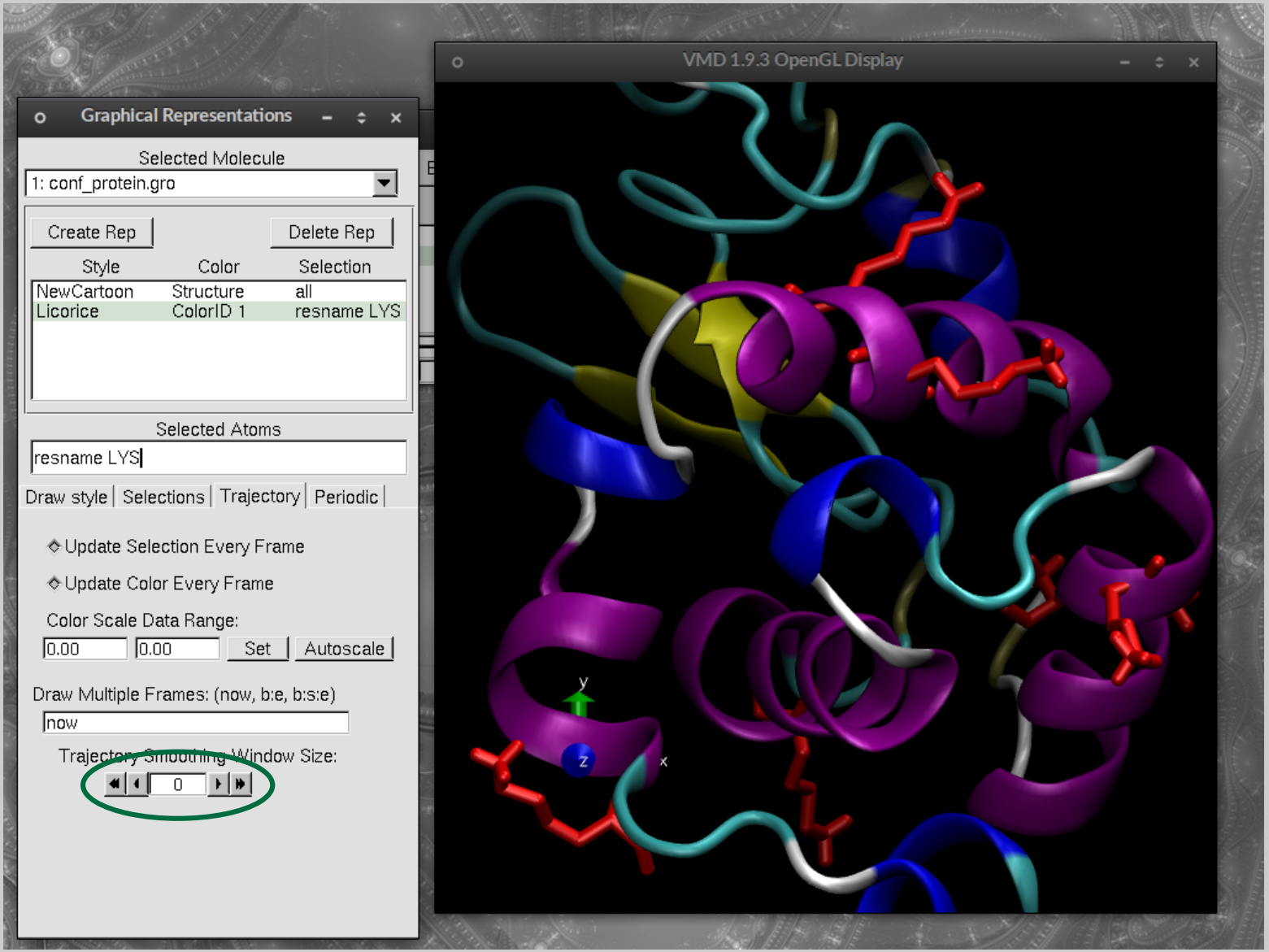
Movie Maker


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
1: conf_protein.gro
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Licorice
ColorID 1
resname LYS
Selected Atoms
resname LYS
Draw style
Selections
Trajectory
Periodic
Update Selection Every Frame
Update Color Every Frame
Color Scale Data Range:
0.00
0.00
Set
Autoscale
Draw Multiple Frames: (now, b:e, b:s:e)
now
Trajectory Smoothing Window Size:
5
Extensions
Help
Frames
Vol
502
0
502
0
y
z
x

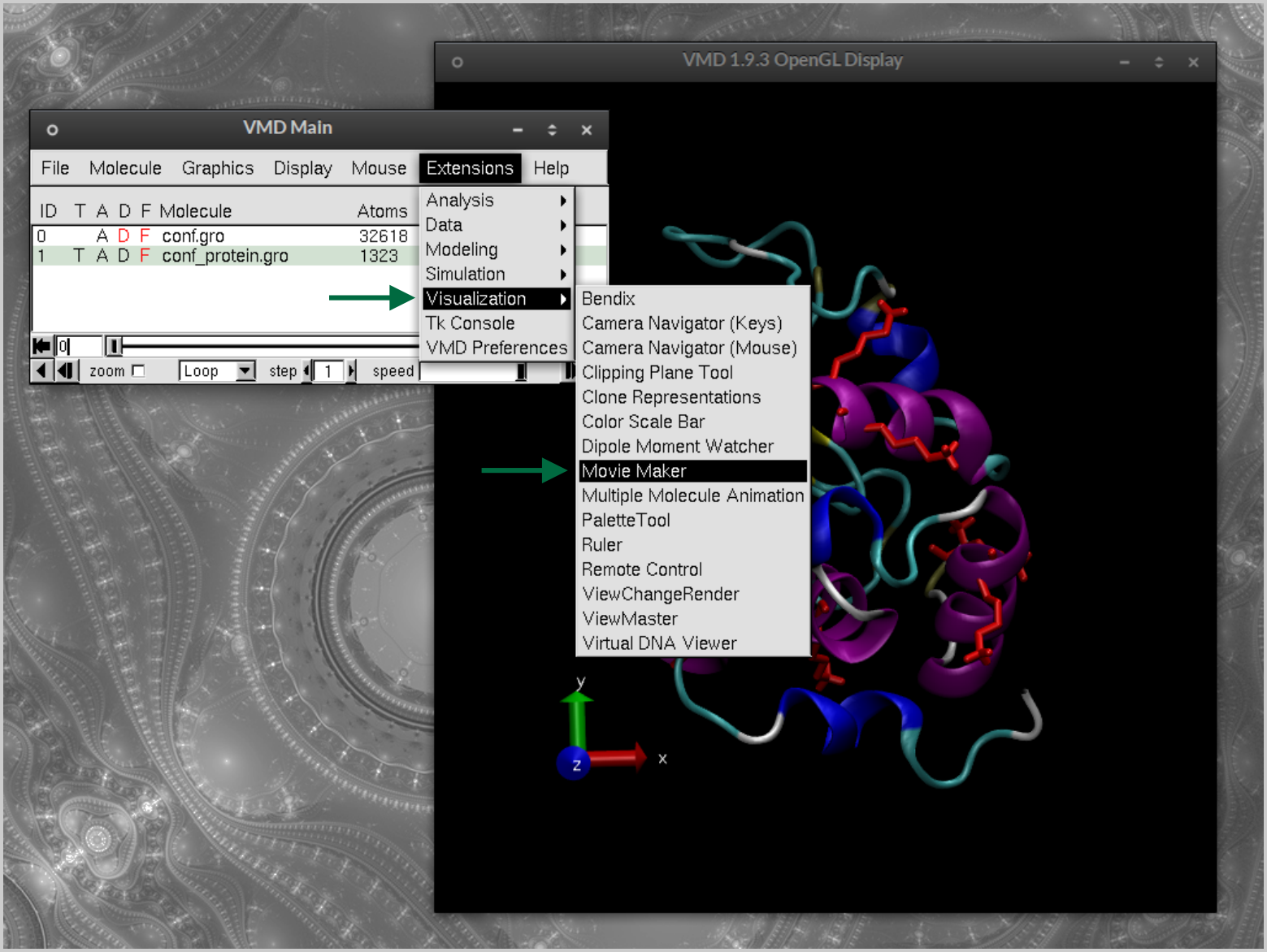
Movie Maker


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
1: conf_protein.gro
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Licorice
ColorID 1
resname LYS
Selected Atoms
resname LYS
Draw style
Selections
Trajectory
Periodic
Update Selection Every Frame
Update Color Every Frame
Color Scale Data Range:
0.00
0.00
Set
Autoscale
Draw Multiple Frames: (now, b:e, b:s:e)
now
Trajectory Smoothing Window Size:
5
y
z
x

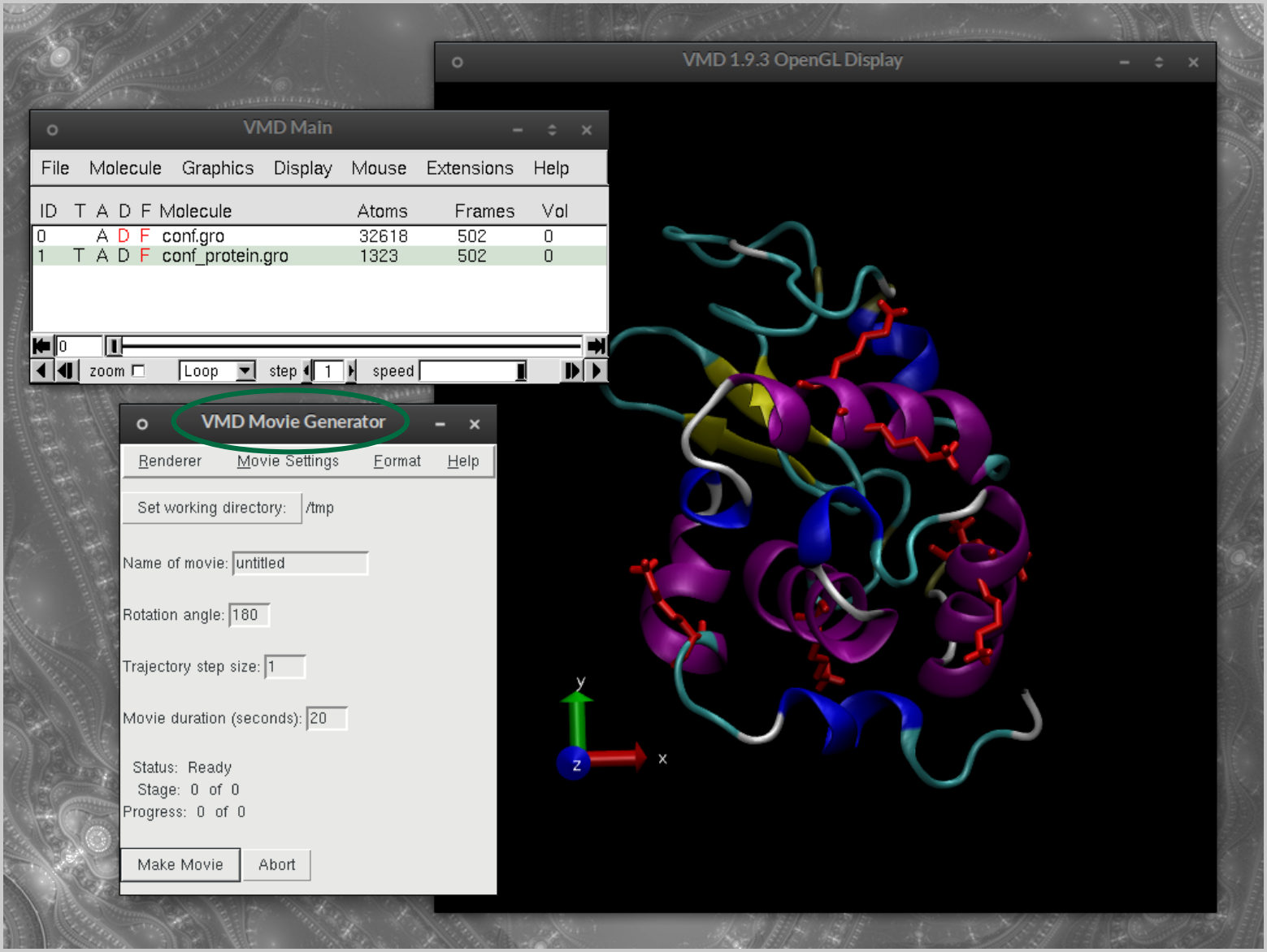
Movie Maker


VMD 1.9.3 OpenGL Display
Graphical Representations
Selected Molecule
1: conf_protein.gro
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
all
Licorice
ColorID 1
resname LYS
Selected Atoms
resname LYS
Draw style
Selections
Trajectory
Periodic
Update Selection Every Frame
Update Color Every Frame
Color Scale Data Range:
0.00
0.00
Set
Autoscale
Draw Multiple Frames: (now, b:e, b:s:e)
now
Trajectory Smoothing Window Size:
0
y
z
x

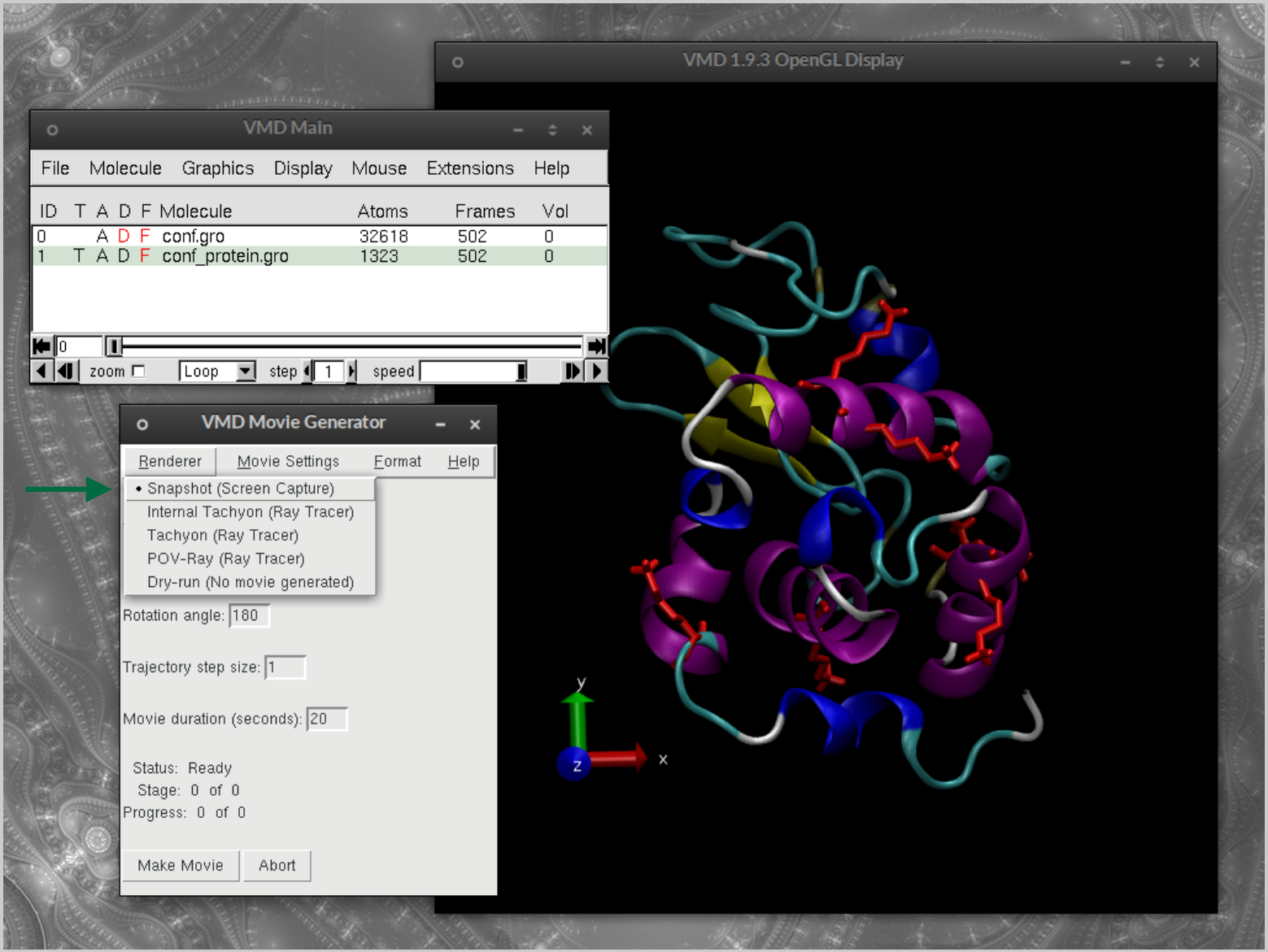
Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule Atoms
0 A D F conf.gro 32618
1 T A D F conf_protein.gro 1323
zoom
Loop
step
1
speed
Analysis
Data
Modeling
Simulation
Visualization
Tk Console
VMD Preferences
Bendix
Camera Navigator (Keys)
Camera Navigator (Mouse)
Clipping Plane Tool
Clone Representations
Color Scale Bar
Dipole Moment Watcher
Movie Maker
Multiple Molecule Animation
PaletteTool
Ruler
Remote Control
ViewChangeRender
ViewMaster
Virtual DNA Viewer
y
z
x

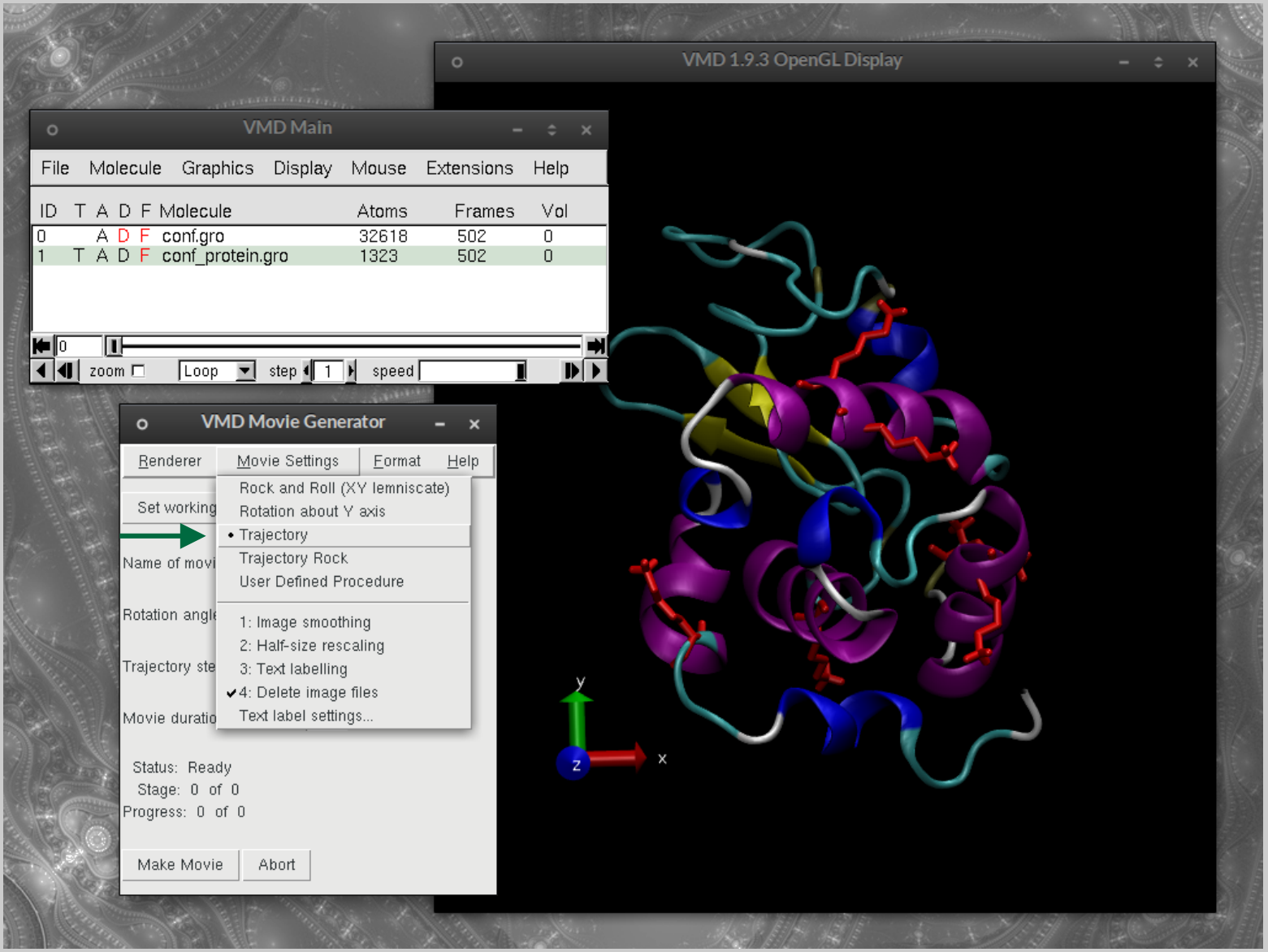
Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom Loop step 1 speed
VMD Movie Generator
Renderer Movie Settings Format Help
Set working directory: /tmp
Name of movie: untitled
Rotation angle: 180
Trajectory step size: 1
Movie duration (seconds): 20
Status: Ready
Stage: 0 of 0
Progress: 0 of 0
Make Movie Abort
y
z
x

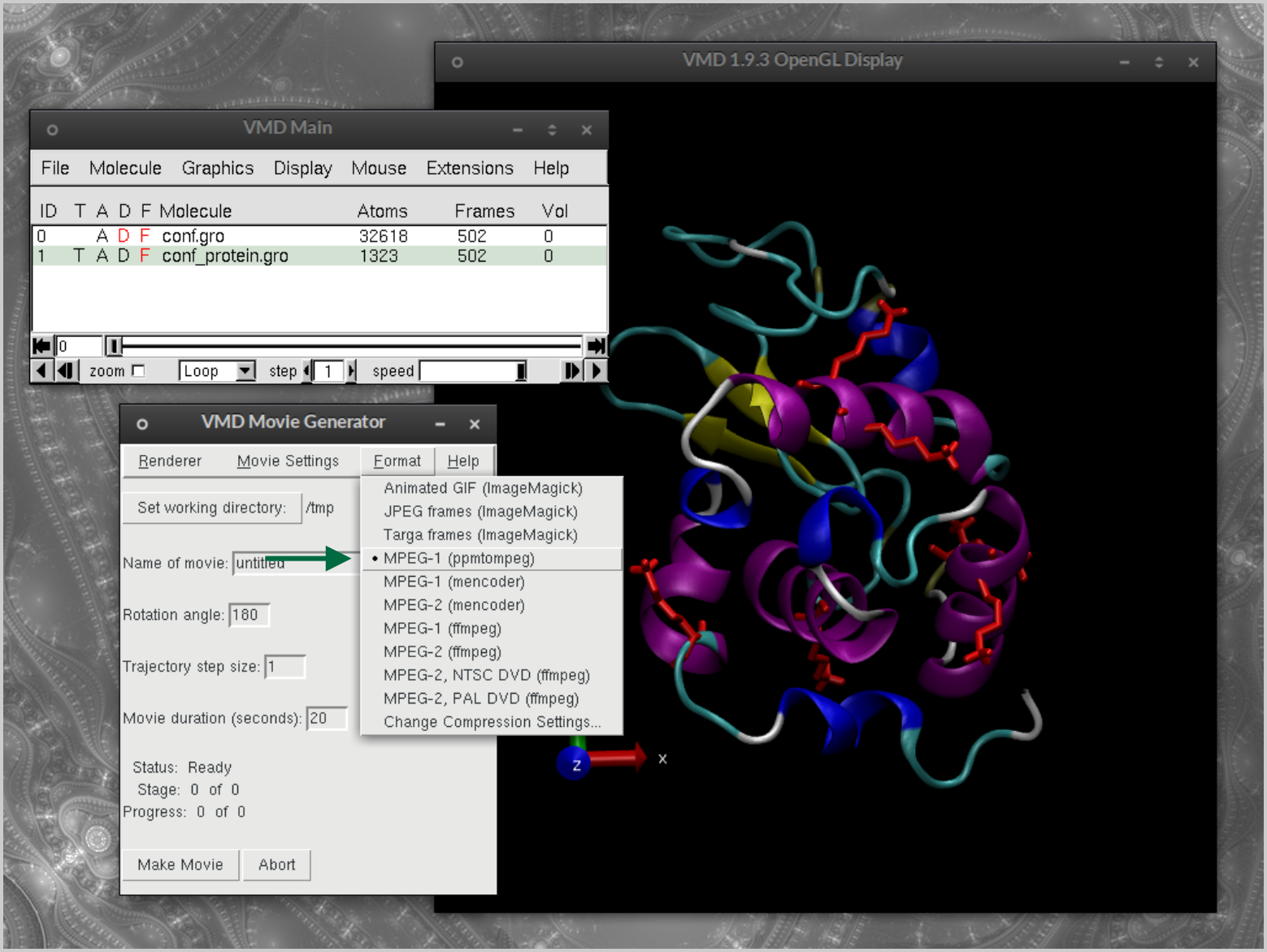
Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom Loop step 1 speed
VMD Movie Generator
Renderer Movie Settings Format Help
• Snapshot (Screen Capture)
Internal Tachyon (Ray Tracer)
Tachyon (Ray Tracer)
POV-Ray (Ray Tracer)
Dry-run (No movie generated)
Rotation angle: 180
Trajectory step size: 1
Movie duration (seconds): 20
Status: Ready
Stage: 0 of 0
Progress: 0 of 0
Make Movie
Abort
y
x
z

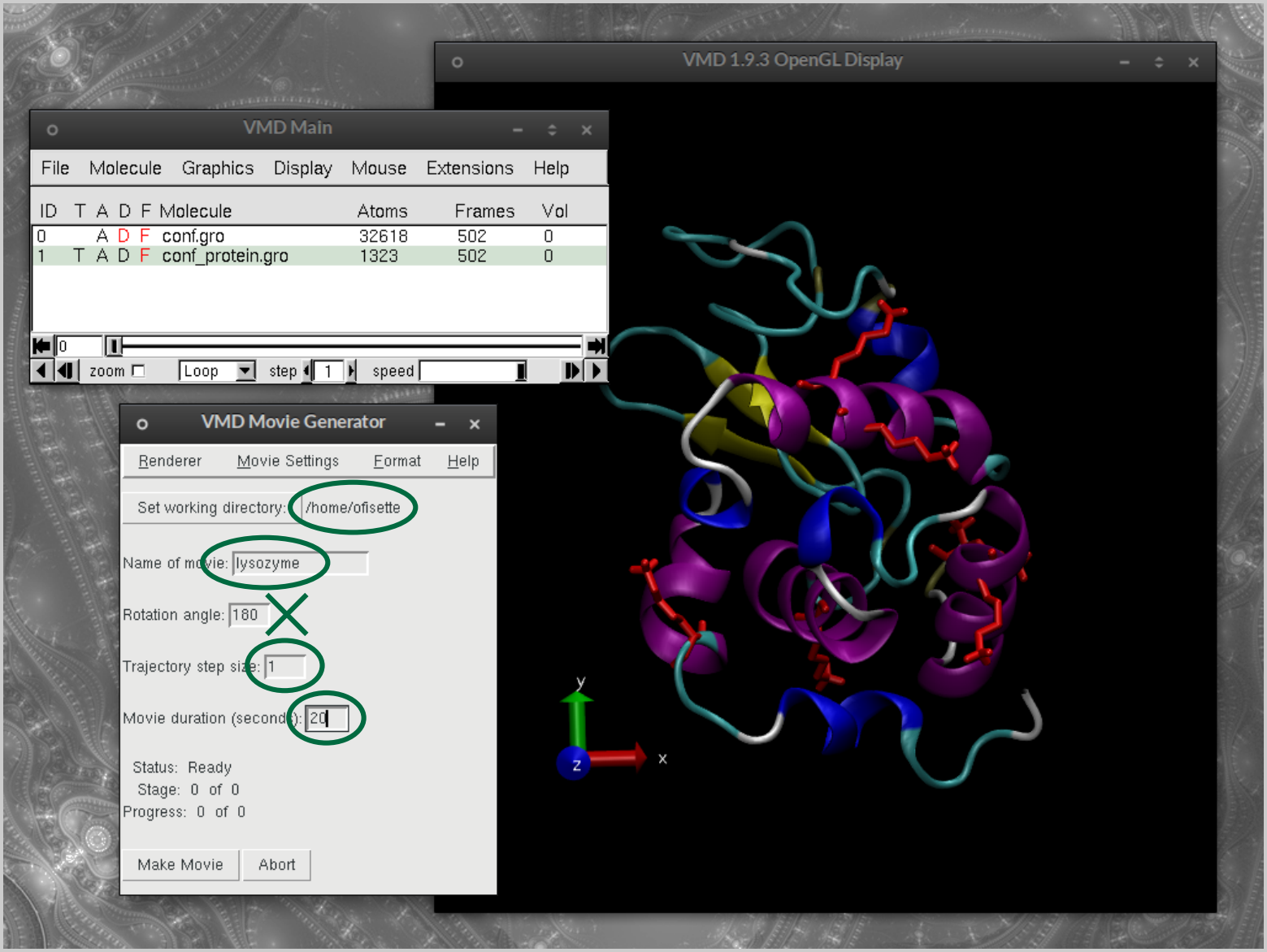
Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom Loop step 1 speed
VMD Movie Generator
Renderer Movie Settings Format Help
Set working
Name of movi
Rotation angl
Trajectory ste
Movie duratio
Rock and Roll (XY lemniscate)
Rotation about Y axis
• Trajectory
Trajectory Rock
User Defined Procedure
1: Image smoothing
2: Half-size rescaling
3: Text labelling
✔4: Delete image files
Text label settings...
Status: Ready
Stage: 0 of 0
Progress: 0 of 0
Make Movie
Abort
y
z
x

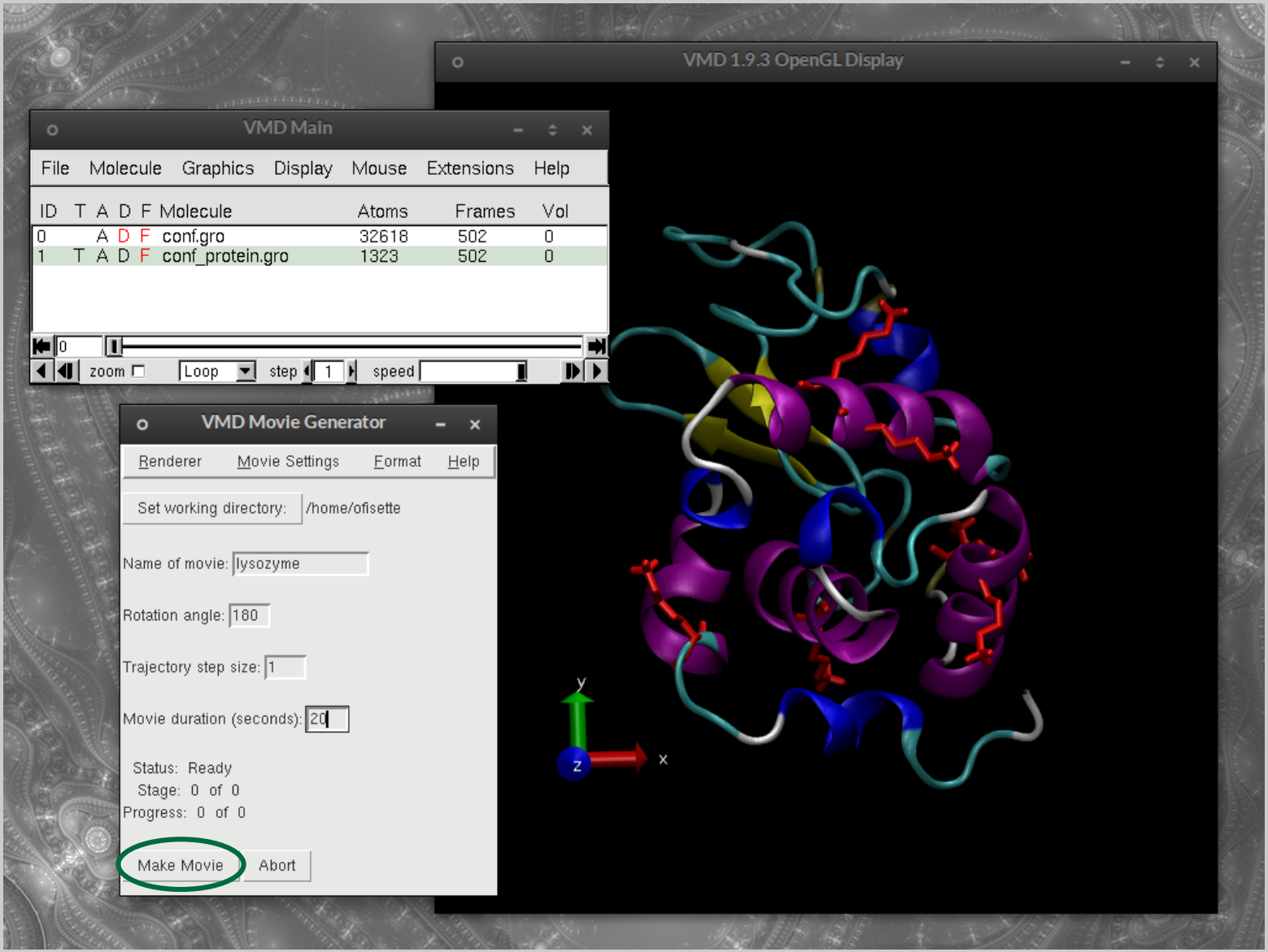
Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom Loop step 1 speed
VMD Movie Generator
Renderer Movie Settings Format Help
Set working directory: /tmp
Name of movie: untitled
Rotation angle: 180
Trajectory step size: 1
Movie duration (seconds): 20
Status: Ready
Stage: 0 of 0
Progress: 0 of 0
Make Movie Abort
Animated GIF (ImageMagick)
JPEG frames (ImageMagick)
Targa frames (ImageMagick)
• MPEG-1 (ppmtompeg)
MPEG-1 (mencoder)
MPEG-2 (mencoder)
MPEG-1 (ffmpeg)
MPEG-2 (ffmpeg)
MPEG-2, NTSC DVD (ffmpeg)
MPEG-2, PAL DVD (ffmpeg)
Change Compression Settings...
z
x

Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom Loop step 1 speed
VMD Movie Generator
Renderer Movie Settings Format Help
Set working directory: /home/ofisette
Name of movie: lysozyme
Rotation angle: 180
Trajectory step size: 1
Movie duration (seconds): 20
Status: Ready
Stage: 0 of 0
Progress: 0 of 0
Make Movie Abort
y
x
z

Movie Maker


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 A D F conf.gro 32618 502 0
1 T A D F conf_protein.gro 1323 502 0
zoom Loop step 1 speed
VMD Movie Generator
Renderer Movie Settings Format Help
Set working directory: /home/ofisette
Name of movie: lysozyme
Rotation angle: 180
Trajectory step size: 1
Movie duration (seconds): 20
Status: Ready
Stage: 0 of 0
Progress: 0 of 0
Make Movie
Abort
y
z
x

Contents

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- Image rendering
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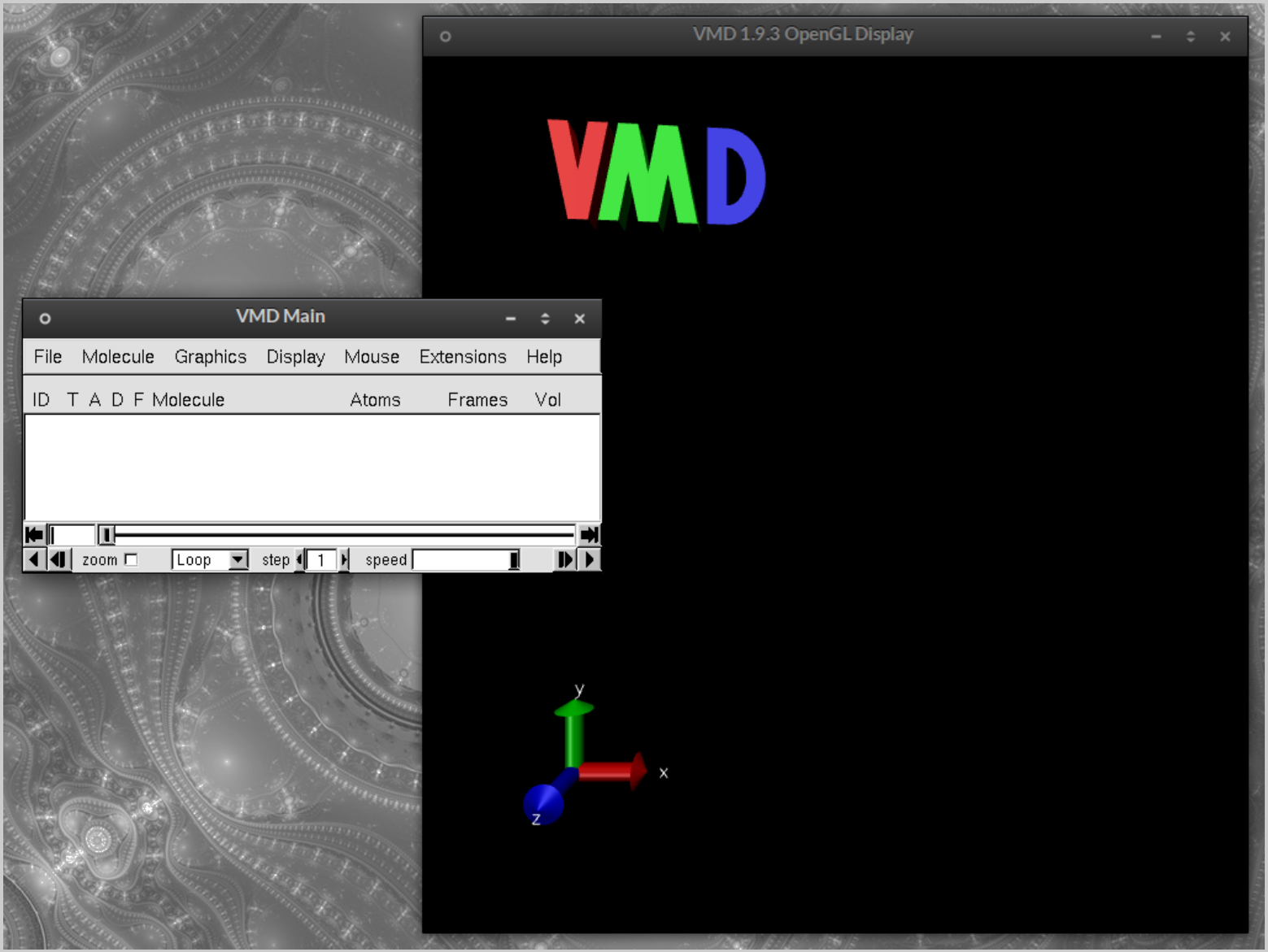
  - Troubleshooting
  - Post-processing
- Movies
  - Using the “Movie Maker”
- **Scripting**
  - **Tk Console**
  - **Tcl scripts**
  - ***vmdrc***
- Combining trajectories, movies, and scripting

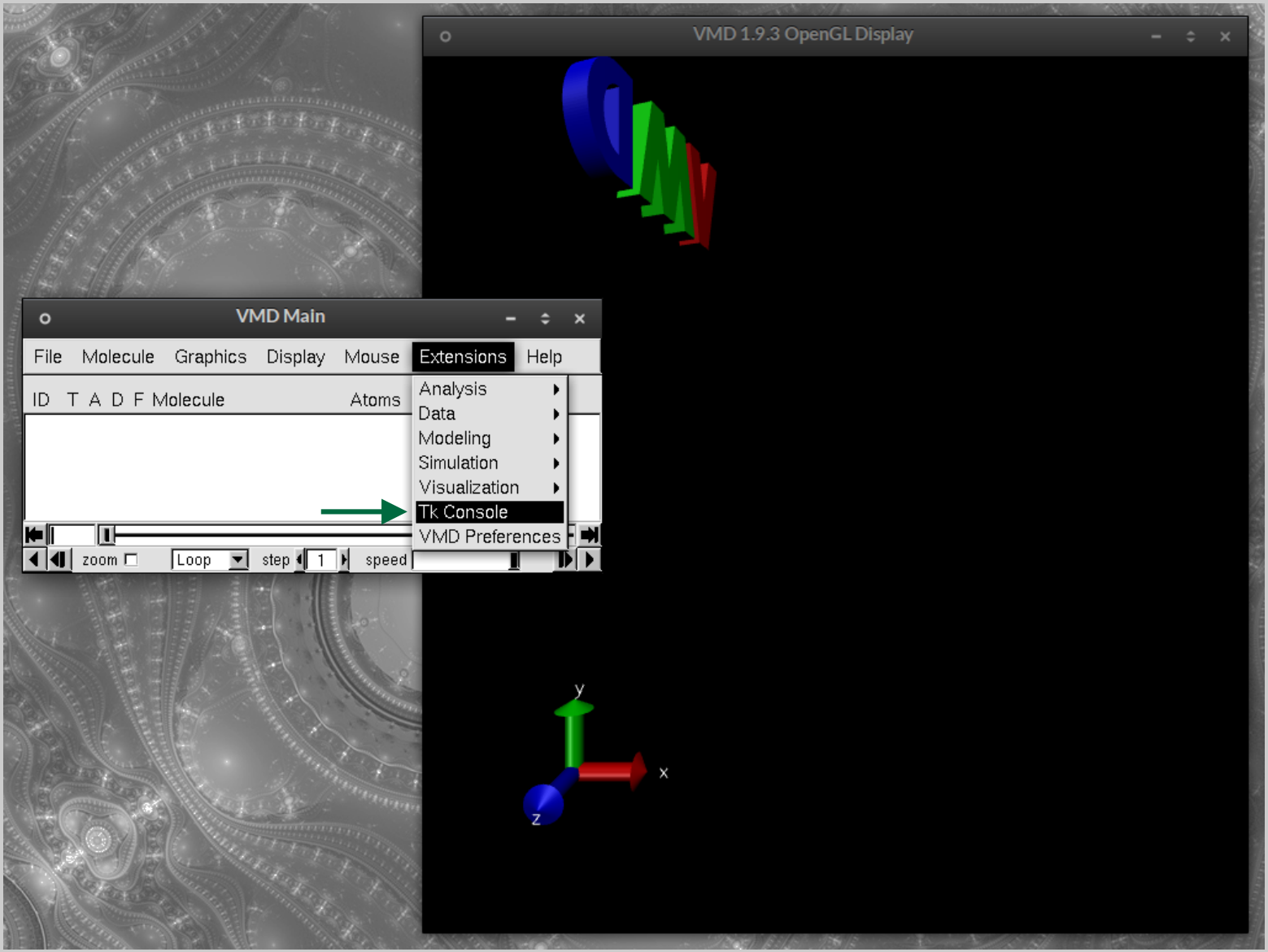
Scripting

- VMD can be controlled through text commands.
- This has advantages over the graphical interface.
  - Easier (avoid convoluted menus and windows)
  - Faster (automated command repetition)
  - Reproducible (commands stored in a script)
- There are many ways to control VMD through text commands.
  - Typing in the “Tk Console”
  - Loading scripts (*play* command) from the “Tk Console”
  - Creating a *vmdrc* file

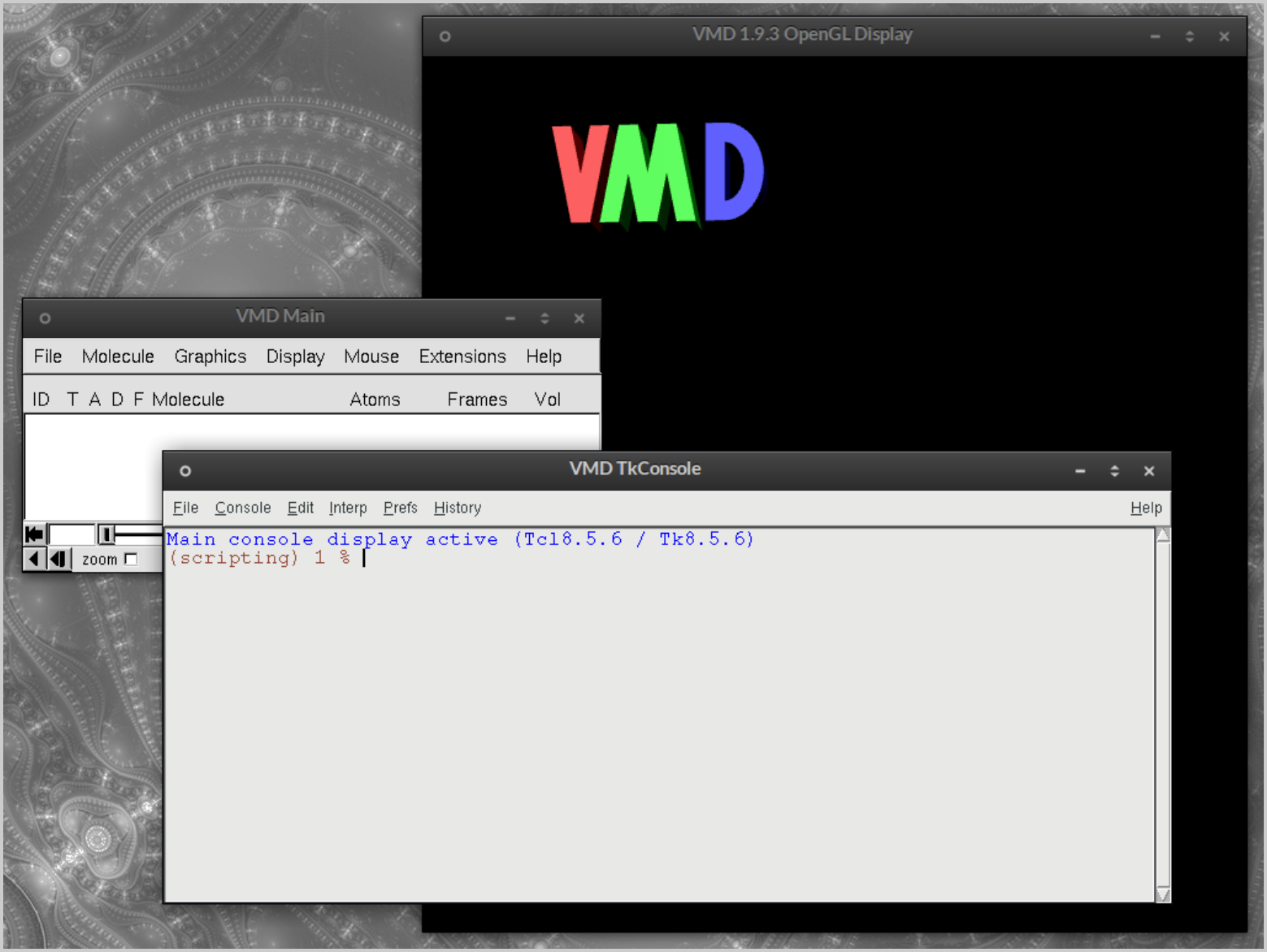
Tk Console


VMD 1.9.3 OpenGL Display
VMD
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
zoom
Loop
step 1
speed
y
x
z

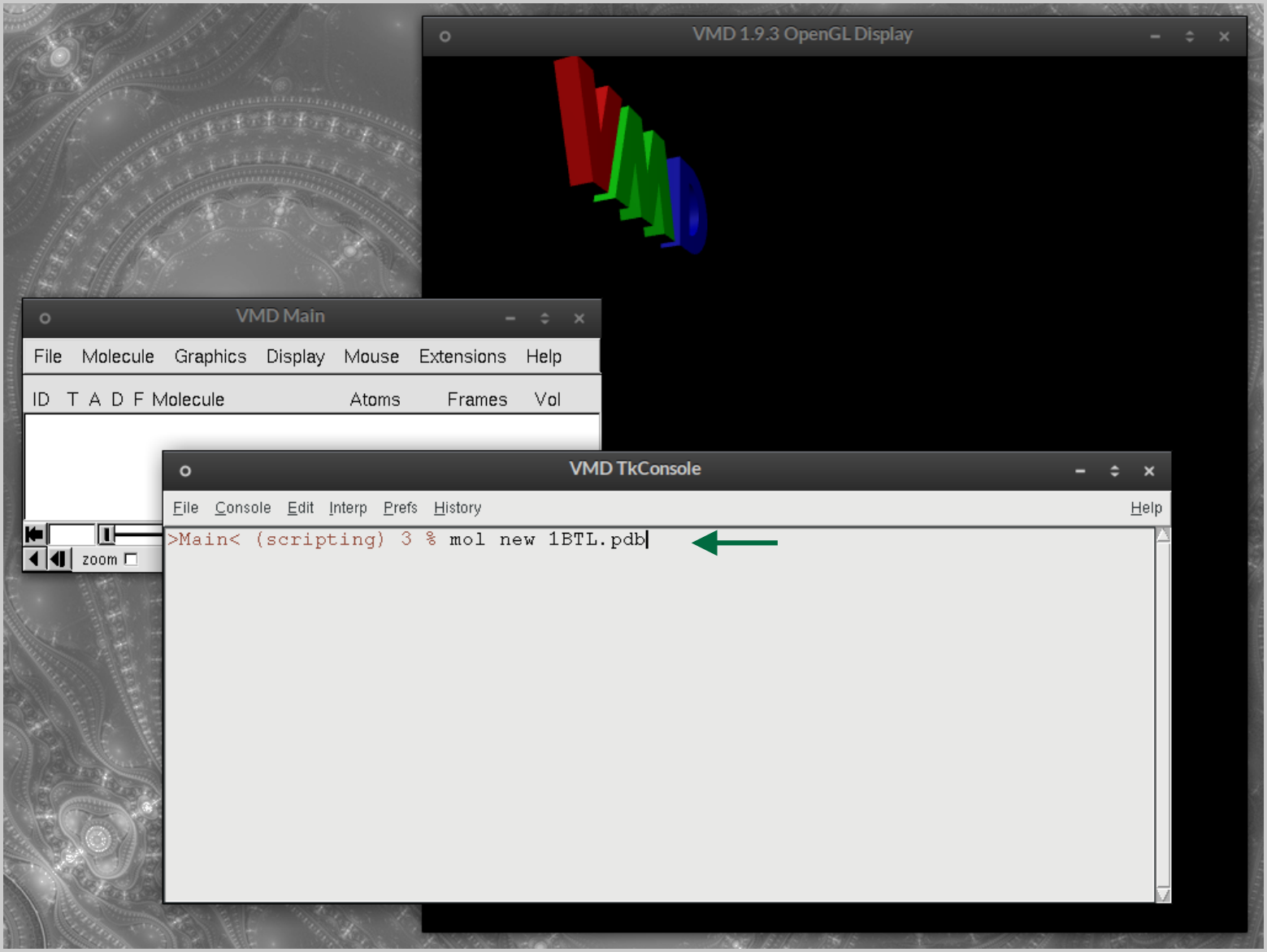
Tk Console


VMD 1.9.3 OpenGL Display
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Analysis
Data
Modeling
Simulation
Visualization
Tk Console
VMD Preferences
zoom
Loop
step
1
speed
y
x
z

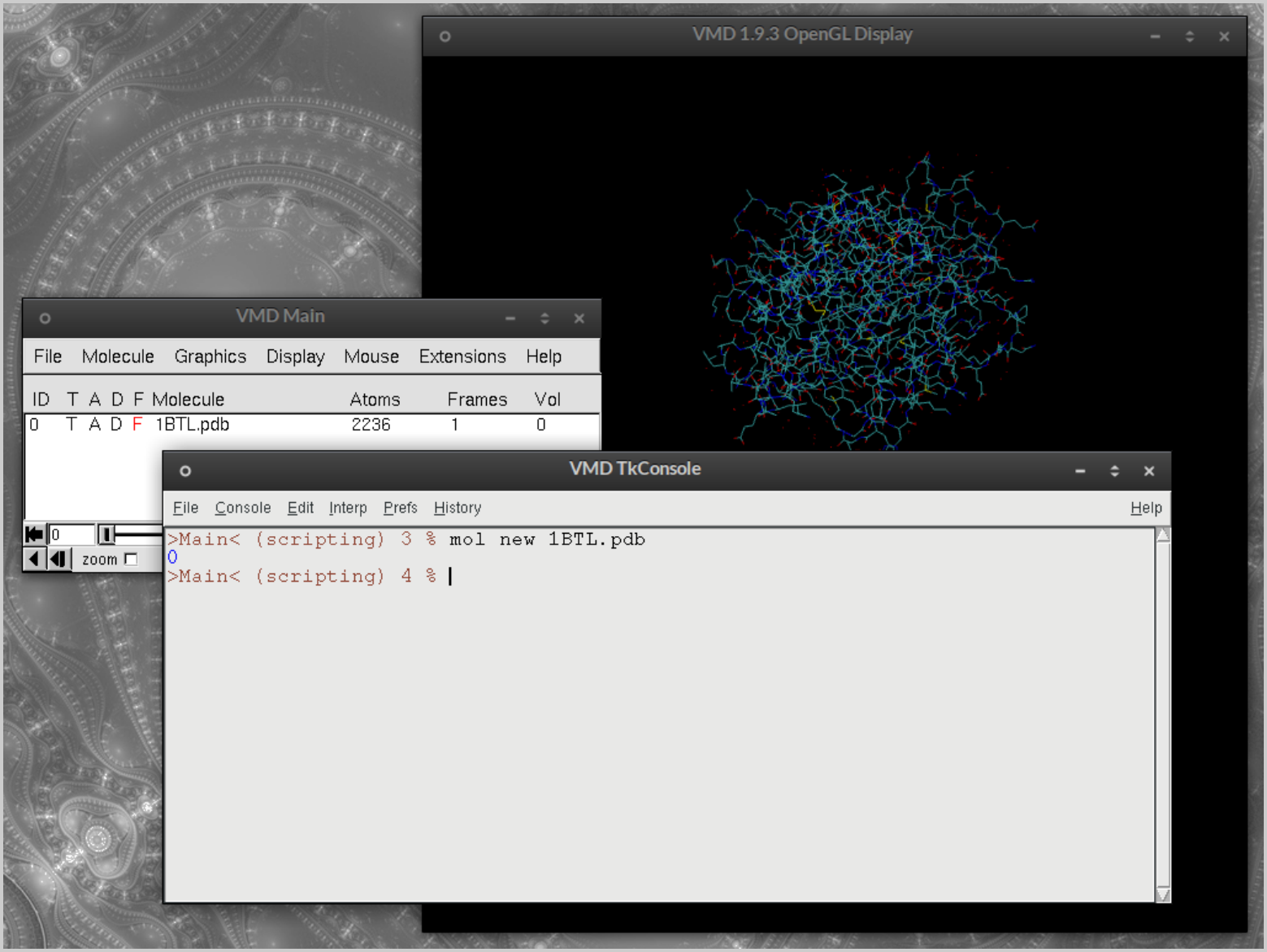
Tk Console


VMD 1.9.3 OpenGL Display
VMD
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
zoom
VMD TkConsole
File Console Edit Interp Prefs History Help
Main console display active (Tcl8.5.6 / Tk8.5.6)
(scripting) 1 %

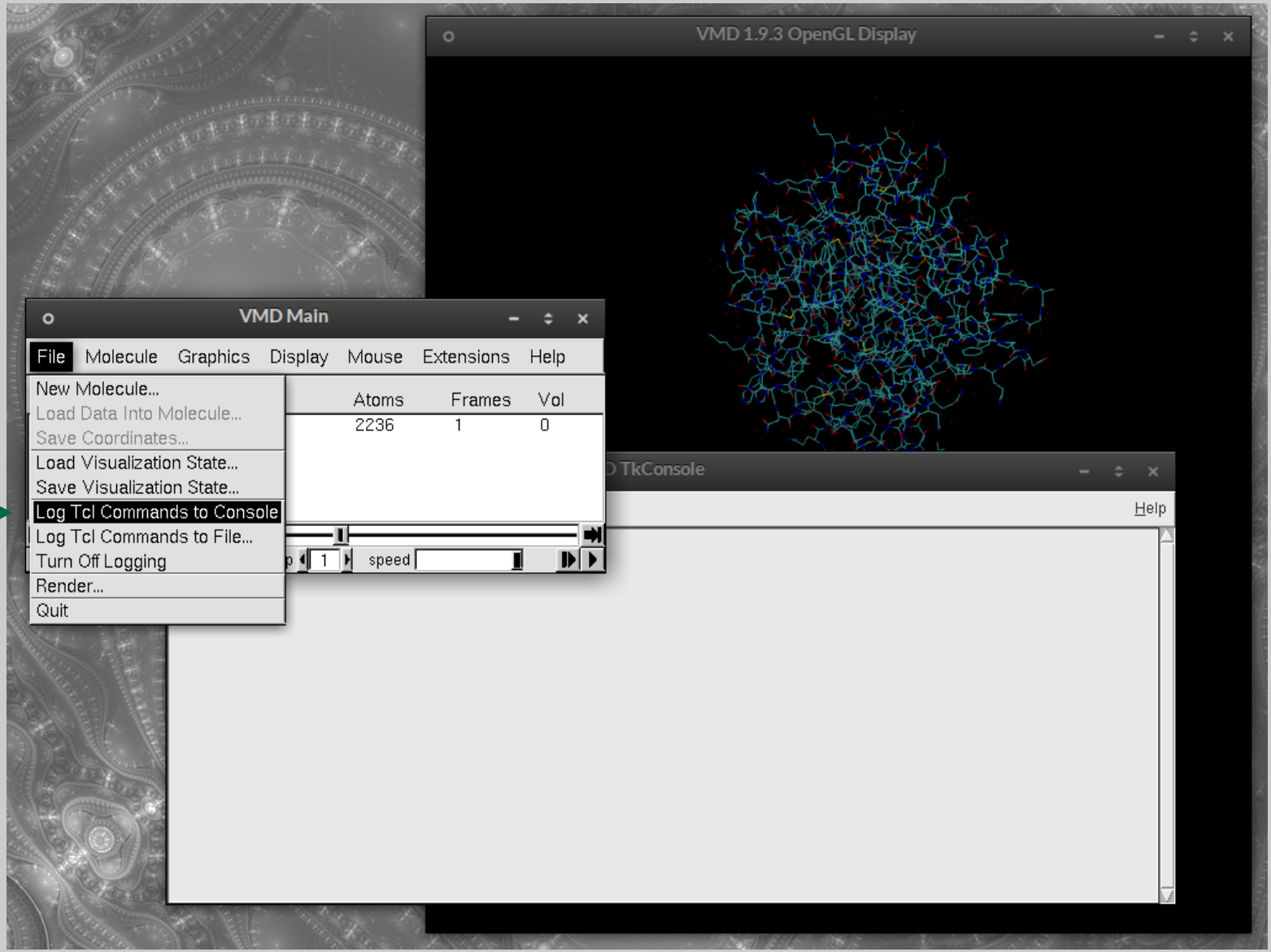
Tk Console


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
zoom
VMD TkConsole
File Console Edit Interp Prefs History Help
>Main< (scripting) 3 % mol new 1BTL.pdb

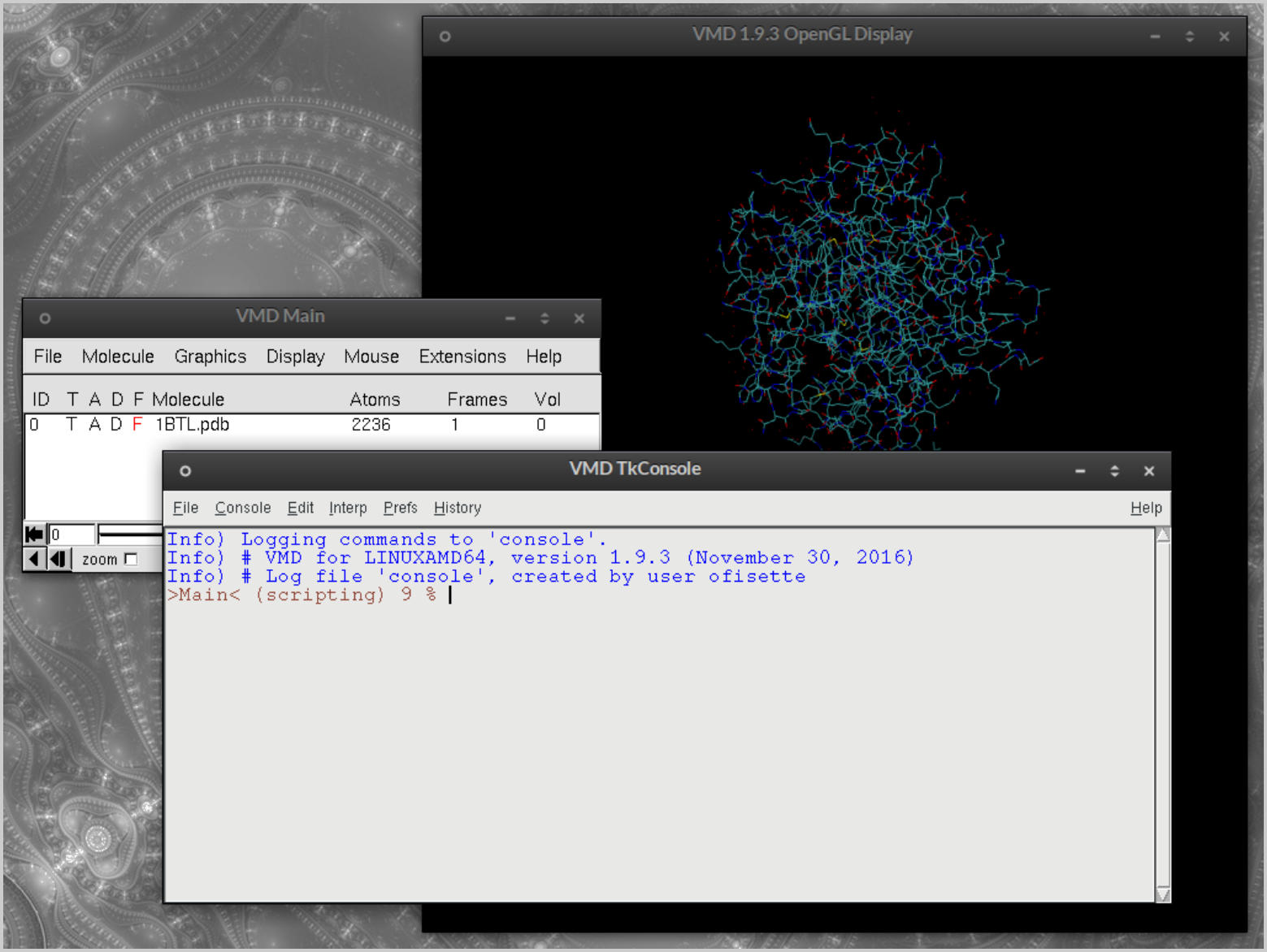
Tk Console


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 T A D F 1BTL.pdb 2236 1 0
zoom
VMD TkConsole
File Console Edit Interp Prefs History Help
>Main< (scripting) 3 % mol new 1BTL.pdb
0
>Main< (scripting) 4 %

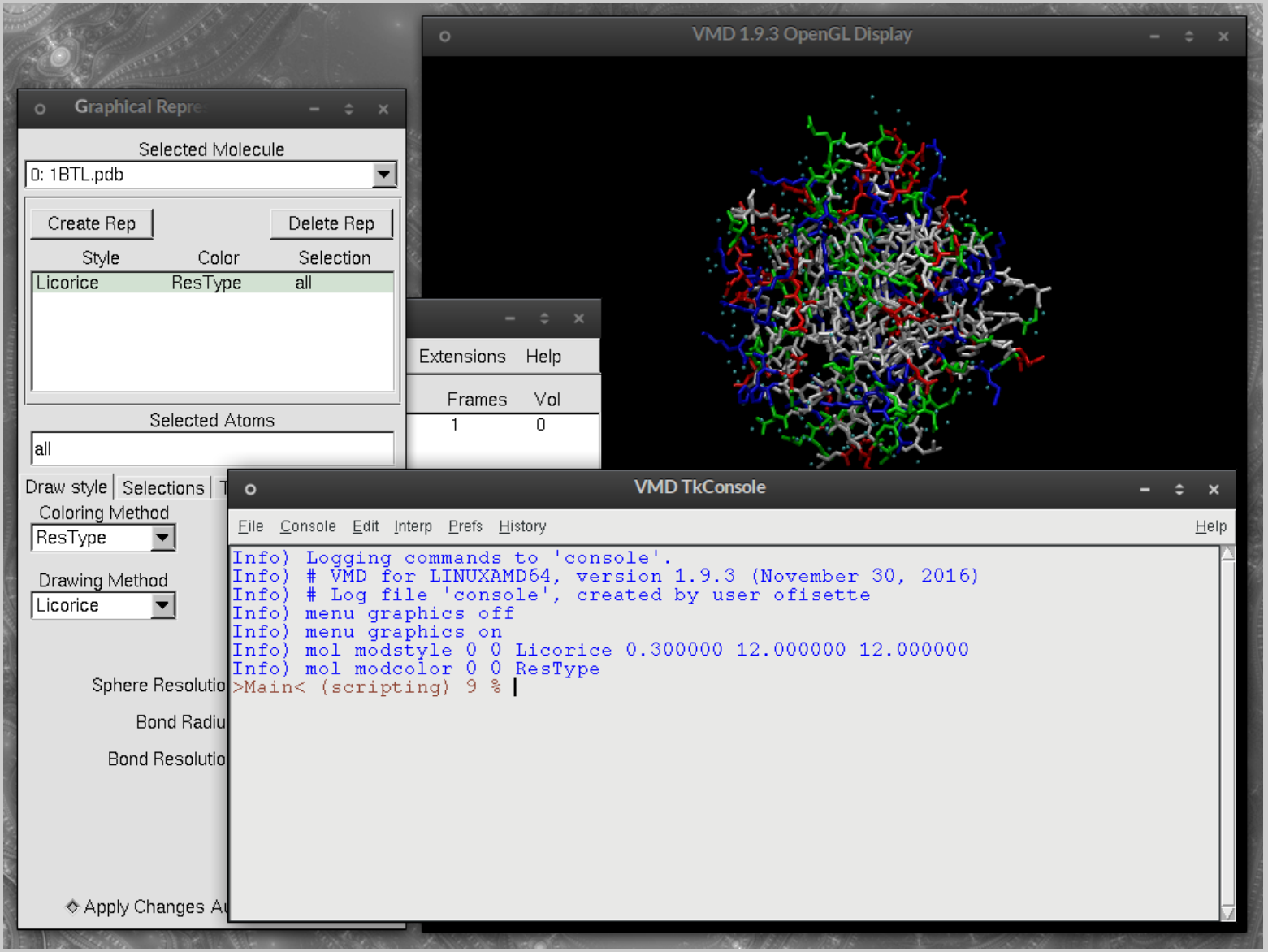
Tk Console


VMD 1.9.3 OpenGL Display
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
New Molecule...
Load Data Into Molecule...
Save Coordinates...
Load Visualization State...
Save Visualization State...
Log Tcl Commands to Console
Log Tcl Commands to File...
Turn Off Logging
Render...
Quit
Atoms
Frames
Vol
2236
1
0
speed
TkConsole
Help

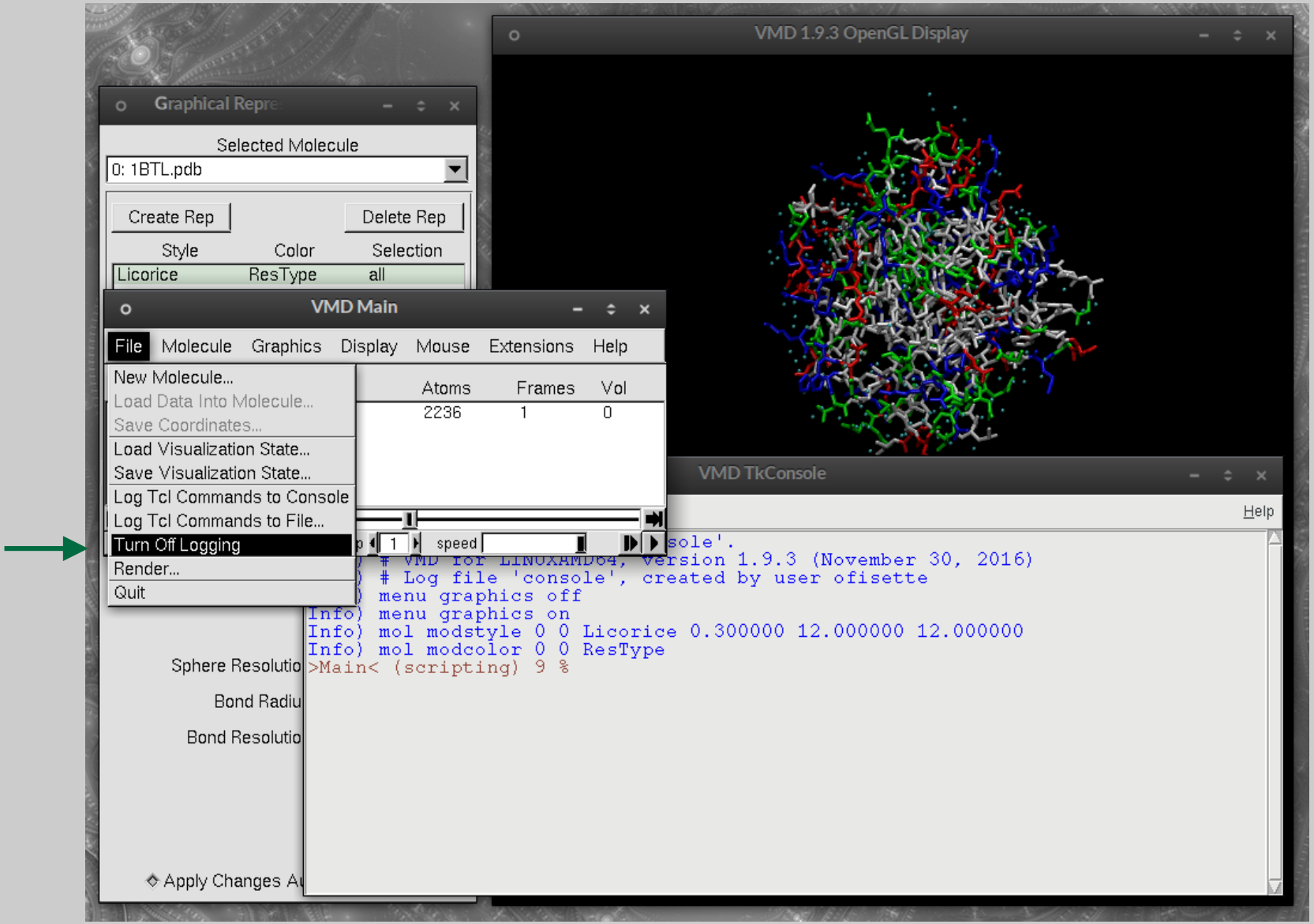
Tk Console


VMD 1.9.3 OpenGL Display
VMD Main
File Molecule Graphics Display Mouse Extensions Help
ID T A D F Molecule Atoms Frames Vol
0 T A D F 1BTL.pdb 2236 1 0
zoom
VMD TkConsole
File Console Edit Interp Prefs History Help
Info) Logging commands to 'console'.
Info) # VMD for LINUXAMD64, version 1.9.3 (November 30, 2016)
Info) # Log file 'console', created by user ofisette
>Main< (scripting) 9 %

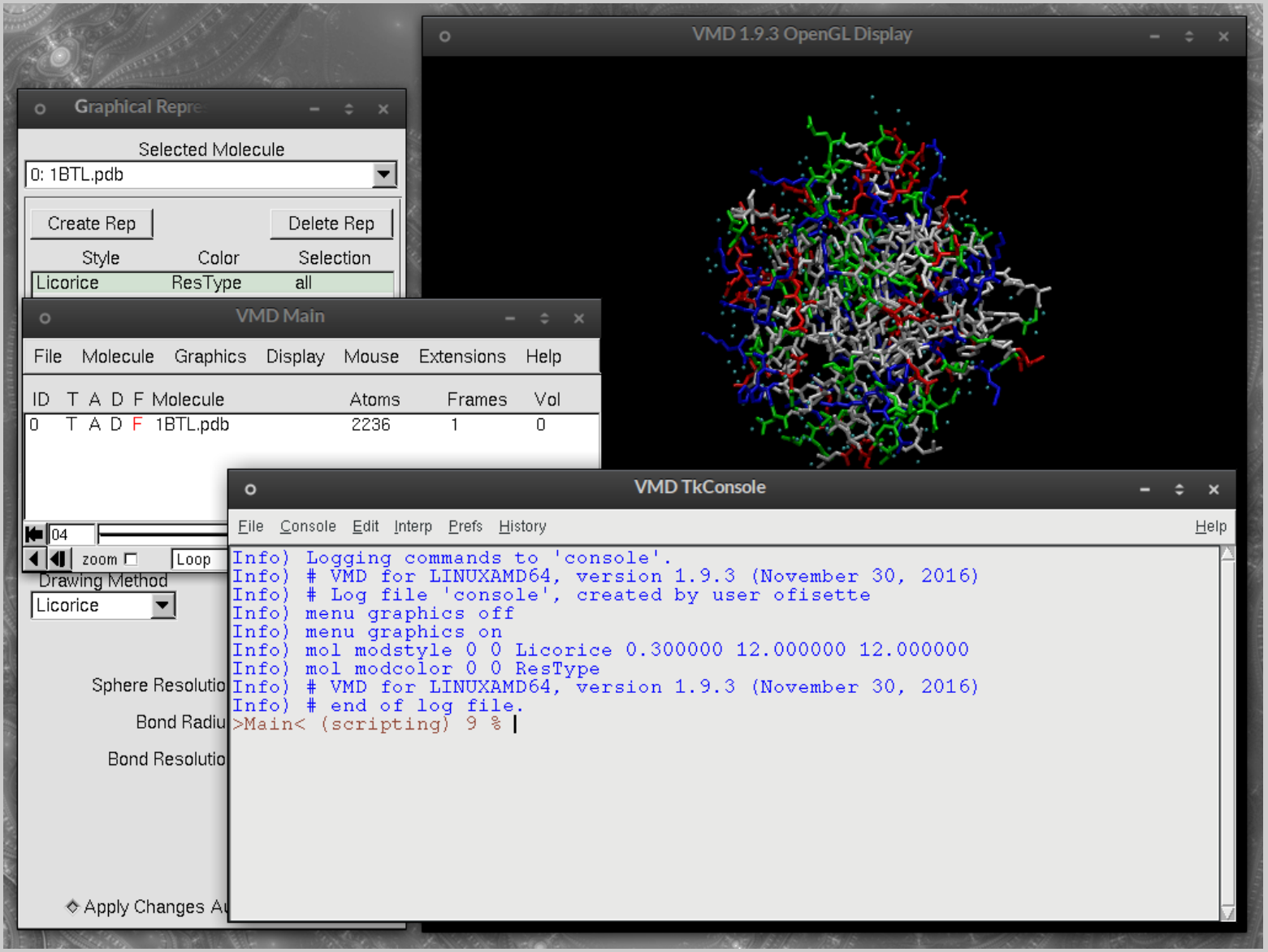
Tk Console


VMD 1.9.3 OpenGL Display
Graphical Repre
Selected Molecule
0: 1BTL.pdb
Create Rep
Delete Rep
Style
Color
Selection
Licorice
ResType
all
Selected Atoms
all
Draw style
Selections
Coloring Method
ResType
Drawing Method
Licorice
Sphere Resolutio
Bond Radiu
Bond Resolutio
Apply Changes Au
Extensions
Help
Frames
Vol
1
0
VMD TkConsole
File
Console
Edit
Interp
Prefs
History
Help
Info) Logging commands to 'console'.
Info) # VMD for LINUXAMD64, version 1.9.3 (November 30, 2016)
Info) # Log file 'console', created by user ofisette
Info) menu graphics off
Info) menu graphics on
Info) mol modstyle 0 0 Licorice 0.300000 12.000000 12.000000
Info) mol modcolor 0 0 ResType
>Main< (scripting) 9 %

Tk Console

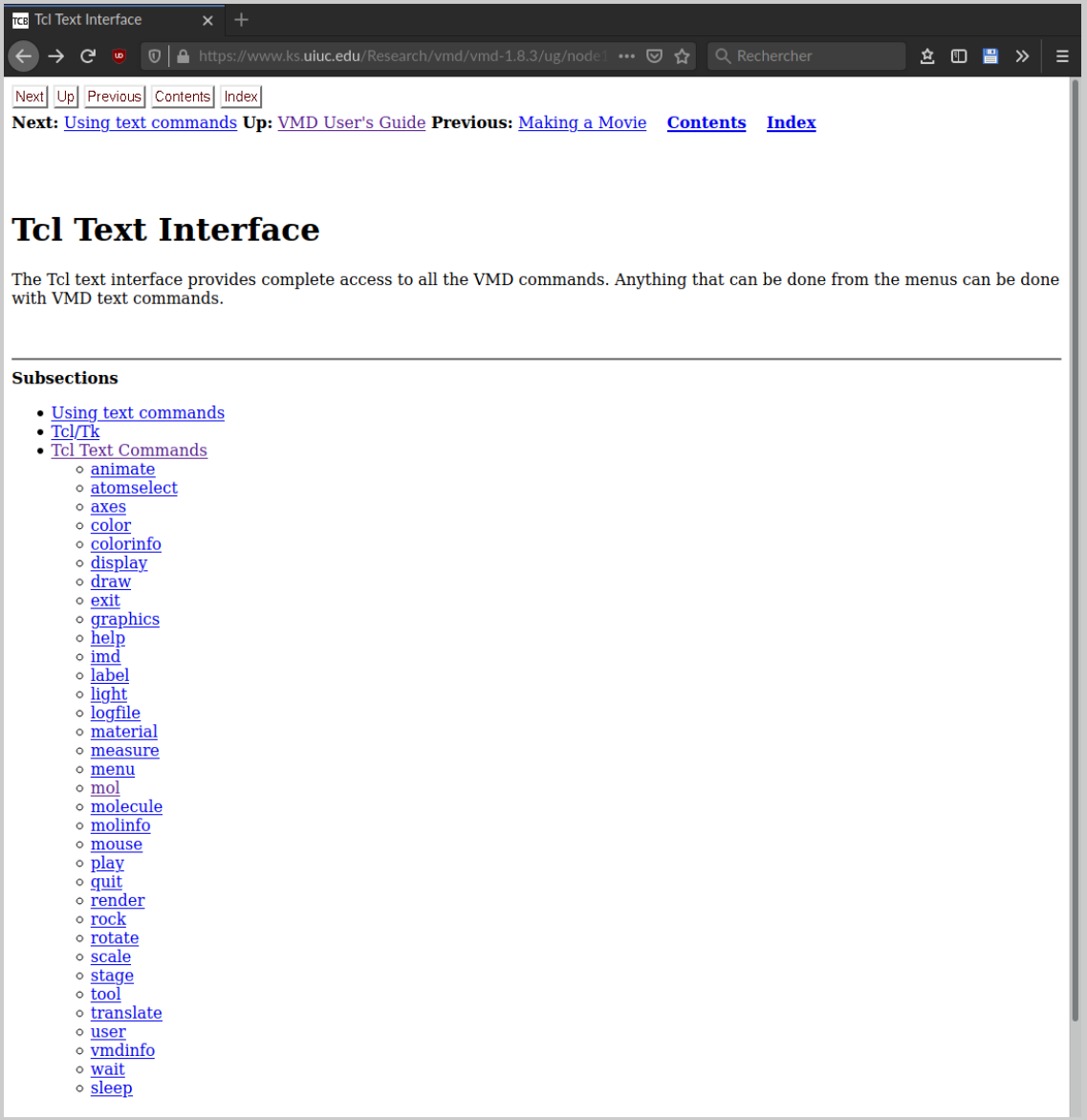

VMD 1.9.3 OpenGL Display
Graphical Repre
Selected Molecule
0: 1BTL.pdb
Create Rep
Delete Rep
Style
Color
Selection
Licorice
ResType
all
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
New Molecule...
Load Data Into Molecule...
Save Coordinates...
Load Visualization State...
Save Visualization State...
Log Tcl Commands to Console
Log Tcl Commands to File...
Turn Off Logging
Render...
Quit
Atoms
Frames
Vol
2236
1
0
speed
Sphere Resolutio
Bond Radiu
Bond Resolutio
Apply Changes Au
VMD TkConsole
Help
sole'.
) # VMD for LINUXAMD64, Version 1.9.3 (November 30, 2016)
) # Log file 'console', created by user ofisette
) menu graphics off
Info) menu graphics on
Info) mol modstyle 0 0 Licorice 0.300000 12.000000 12.000000
Info) mol modcolor 0 0 ResType
>Main< (scripting) 9 %

Tk Console


VMD 1.9.3 OpenGL Display
Graphical Repre
Selected Molecule
0: 1BTL.pdb
Create Rep
Delete Rep
Style
Color
Selection
Licorice
ResType
all
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Frames
Vol
0 T A D F 1BTL.pdb
2236
1
0
04
zoom
Loop
Drawing Method
Licorice
Sphere Resolutio
Bond Radiu
Bond Resolutio
Apply Changes Au
VMD TkConsole
File
Console
Edit
Interp
Prefs
History
Help
Info) Logging commands to 'console'.
Info) # VMD for LINUXAMD64, version 1.9.3 (November 30, 2016)
Info) # Log file 'console', created by user ofisette
Info) menu graphics off
Info) menu graphics on
Info) mol modstyle 0 0 Licorice 0.300000 12.000000 12.000000
Info) mol modcolor 0 0 ResType
Info) # VMD for LINUXAMD64, version 1.9.3 (November 30, 2016)
Info) # end of log file.
>Main< (scripting) 9 %

VMD User's Guide: Tcl Text Interface

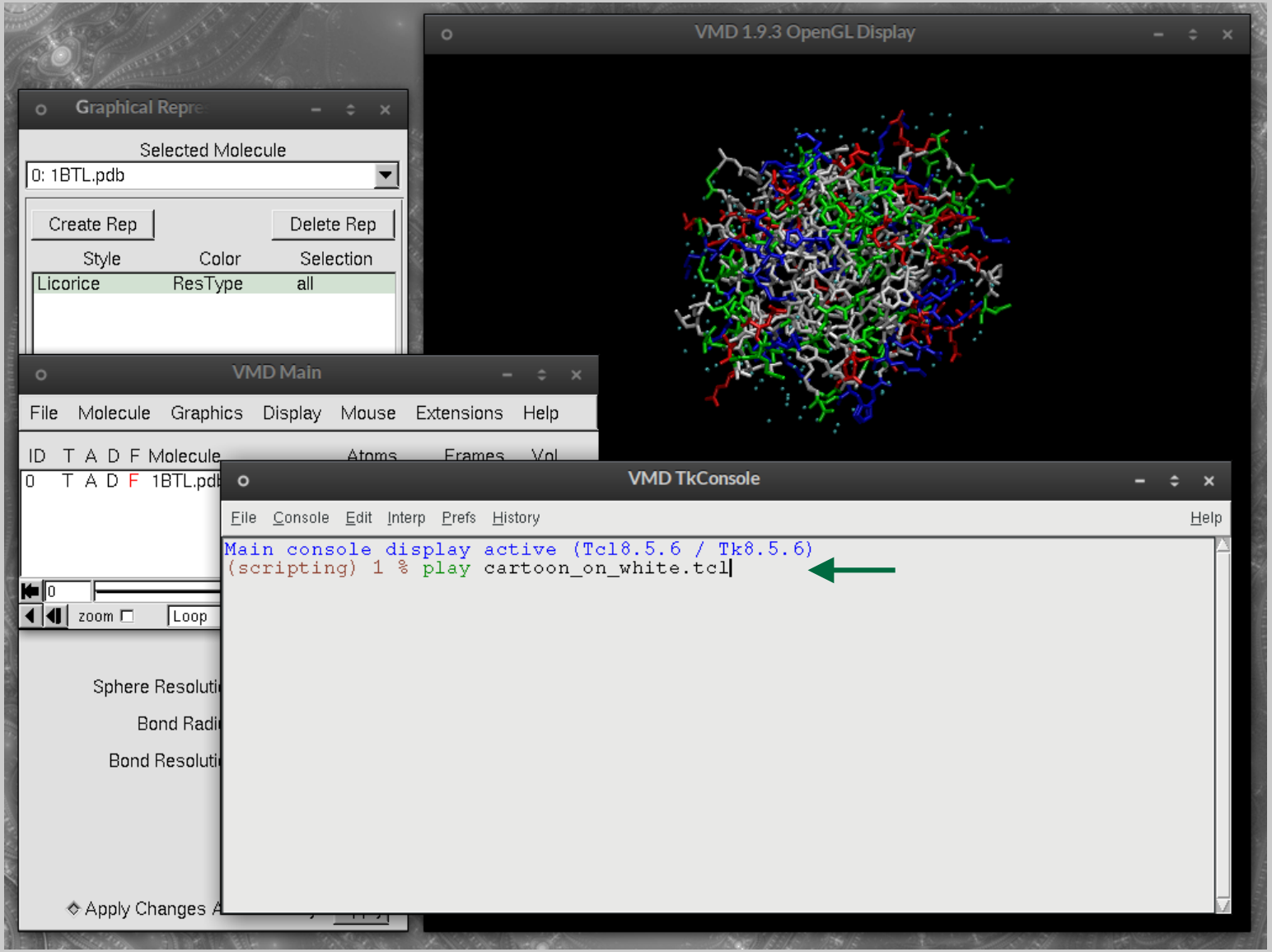
https://www.ks.uiuc.edu/Research/vmd/current/ug/node117.html



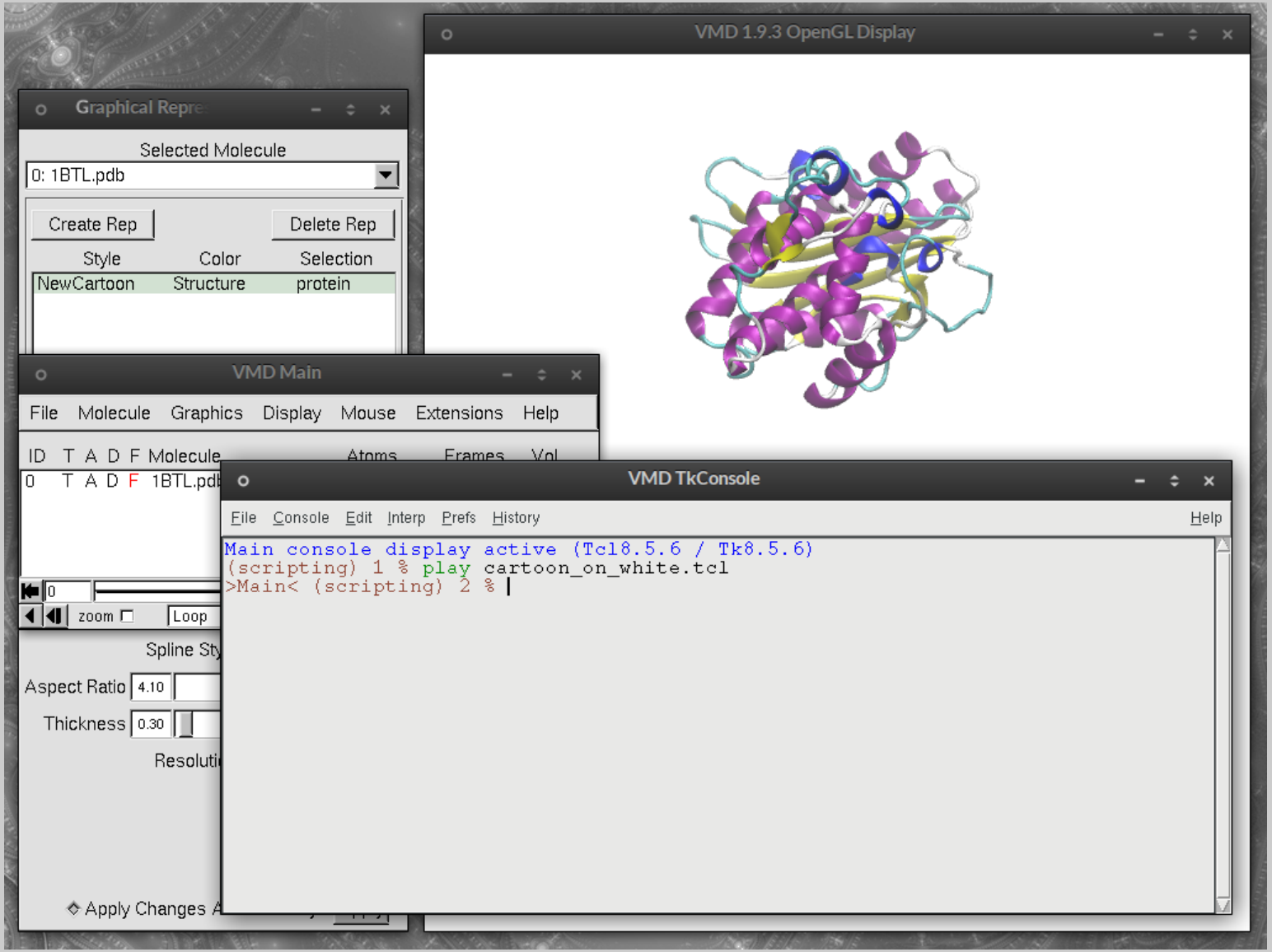
Tcl scripts

```
 1 # Global parameters
 2 display projection orthographic
 3 color Display Background white
 4 axes location Off
 5
 6 # Delete default representation
 7 mol delrep 0 top
 8
 9 # Show protein as cartoon, color by secondary structure
10 # (thickness, resolution, aspect ratio, spline type)
11 mol representation NewCartoon 0.3 10.0 4.1 0
12 mol color Structure
13 mol selection {protein}
14 mol addrep top
~
~
~
~
~
~
~
~
~
~
~
~
"cartoon_on_white.tcl" 14L, 365C écrit(s)                    14,14         Tout
```

Tcl scripts


VMD 1.9.3 OpenGL Display
Graphical Repre
Selected Molecule
0: 1BTL.pdb
Create Rep
Delete Rep
Style
Color
Selection
Licorice
ResType
all
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Frames
Vol
0 T A D F 1BTL.pdb
zoom
Loop
Sphere Resoluti
Bond Radi
Bond Resoluti
Apply Changes
VMD TkConsole
File
Console
Edit
Interp
Prefs
History
Help
Main console display active (Tcl8.5.6 / Tk8.5.6)
(scripting) 1 % play cartoon_on_white.tcl

Tcl scripts


VMD 1.9.3 OpenGL Display
Graphical Repre
Selected Molecule
0: 1BTL.pdb
Create Rep
Delete Rep
Style
Color
Selection
NewCartoon
Structure
protein
VMD Main
File
Molecule
Graphics
Display
Mouse
Extensions
Help
ID T A D F Molecule
Atoms
Frames
Vol
0 T A D F 1BTL.pdb
zoom
Loop
Spline Sty
Aspect Ratio
4.10
Thickness
0.30
Resoluti
Apply Changes A
VMD TkConsole
File
Console
Edit
Interp
Prefs
History
Help
Main console display active (Tcl8.5.6 / Tk8.5.6)
(scripting) 1 % play cartoon_on_white.tcl
>Main< (scripting) 2 %

vmdrc Initialisation file

- You can create a Tcl script that will be “played” when VMD starts.
  - UNIX: *$HOME/.vmdrc*
  - Windows: *$HOME/vmd.rc*
- This enables customisation
  - Display options
  - Keyboard shortcuts
  - Colour definitions

vmdrc Initialisation file

```
# Global parameters
display projection orthographic
color Display Background white
axes location Off

# Keyboard shortcuts
user add key a "axes location off"
user add key A "axes location lowerleft"

# Universal palette
# blue (blue)
color change rgb  0 0.00 0.47 0.72
# red (orange red)
color change rgb  1 0.96 0.25 0.00
# 2 gray
# orange (dark yellow)
color change rgb  3 0.99 0.63 0.00
# yellow (bright yellow)
color change rgb  4 0.94 0.89 0.26
# 5 tan (dark blue)
color change rgb  5 0.00 0.30 0.45
# 6 silver
# green (green)
color change rgb  7 0.00 0.62 0.45
# 8 white
# pink (pink)
color change rgb  9 0.89 0.49 0.68
# cyan (sky blue)
color change rgb 10 0.25 0.75 1.00

# Show main window
menu main on
                                                          13,18         Tout
```

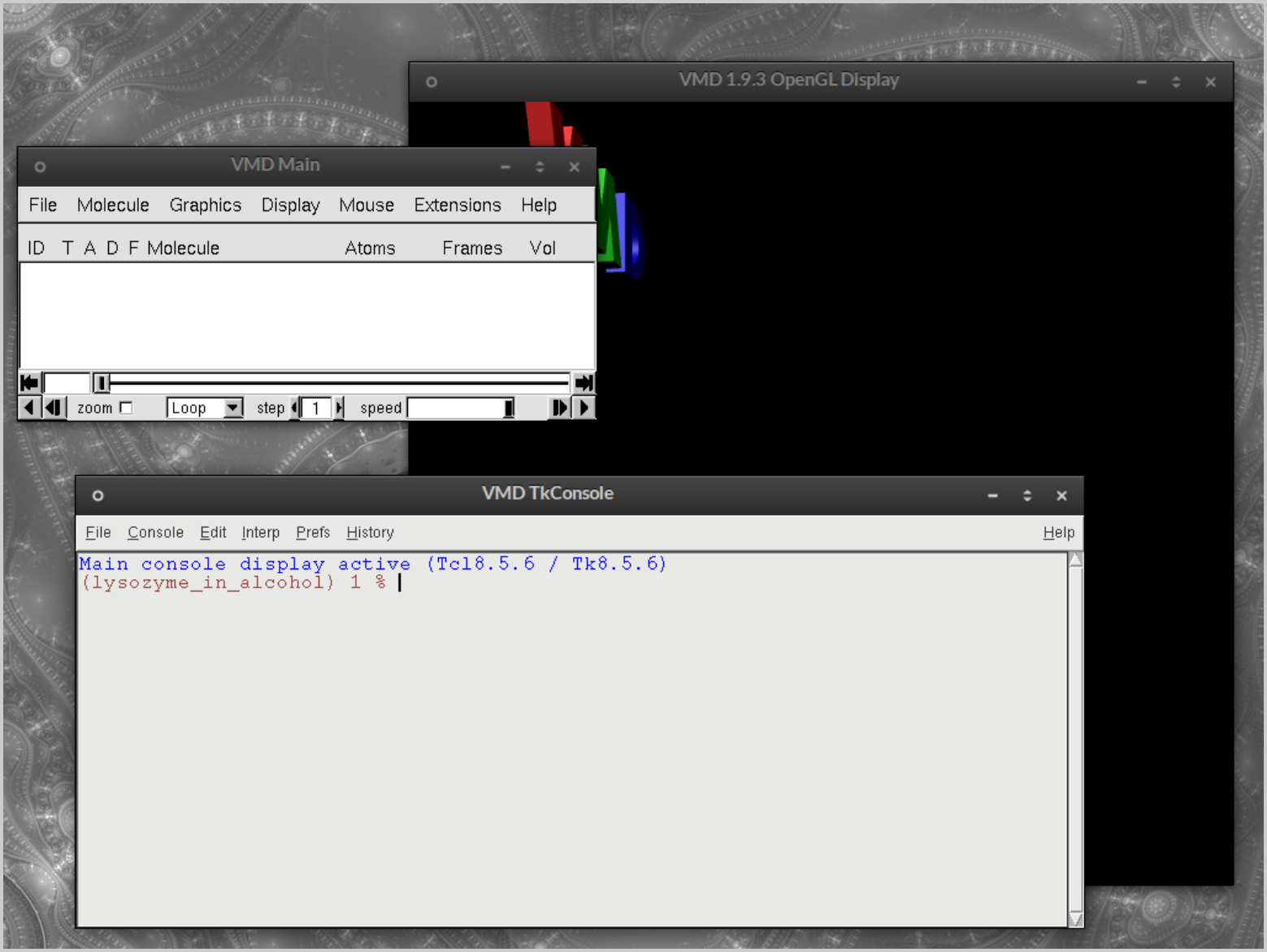
Contents

- Basics
  - Loading structures
  - Representations
  - Atom selections
  - 3D navigation
- Drawing methods
- Materials and colouring
- Image rendering
- Trajectories
  - Troubleshooting
  - Post-processing
- Movies
  - Using the “Movie Maker”
- Scripting
  - Tk Console
  - Tcl scripts
  - *vmdrc*
- **Combining trajectories, movies, and scripting**

Combining trajectories, movies, and scripting

- Objective
  - Animate a trajectory of lysozyme unfolding in ethanol solvent
  - Rotate the viewpoint while the trajectory advances
  - Recalculate secondary structure at each trajectory frame
  - Produce an MP4 movie with the H.265 codec
- Strategy
  - Animate in Movie Maker with a user-defined procedure (Tcl script)
  - Render TGA frames from the Movie Maker
  - Encode the movie outside VMD with *ffmpeg* (Bash script)

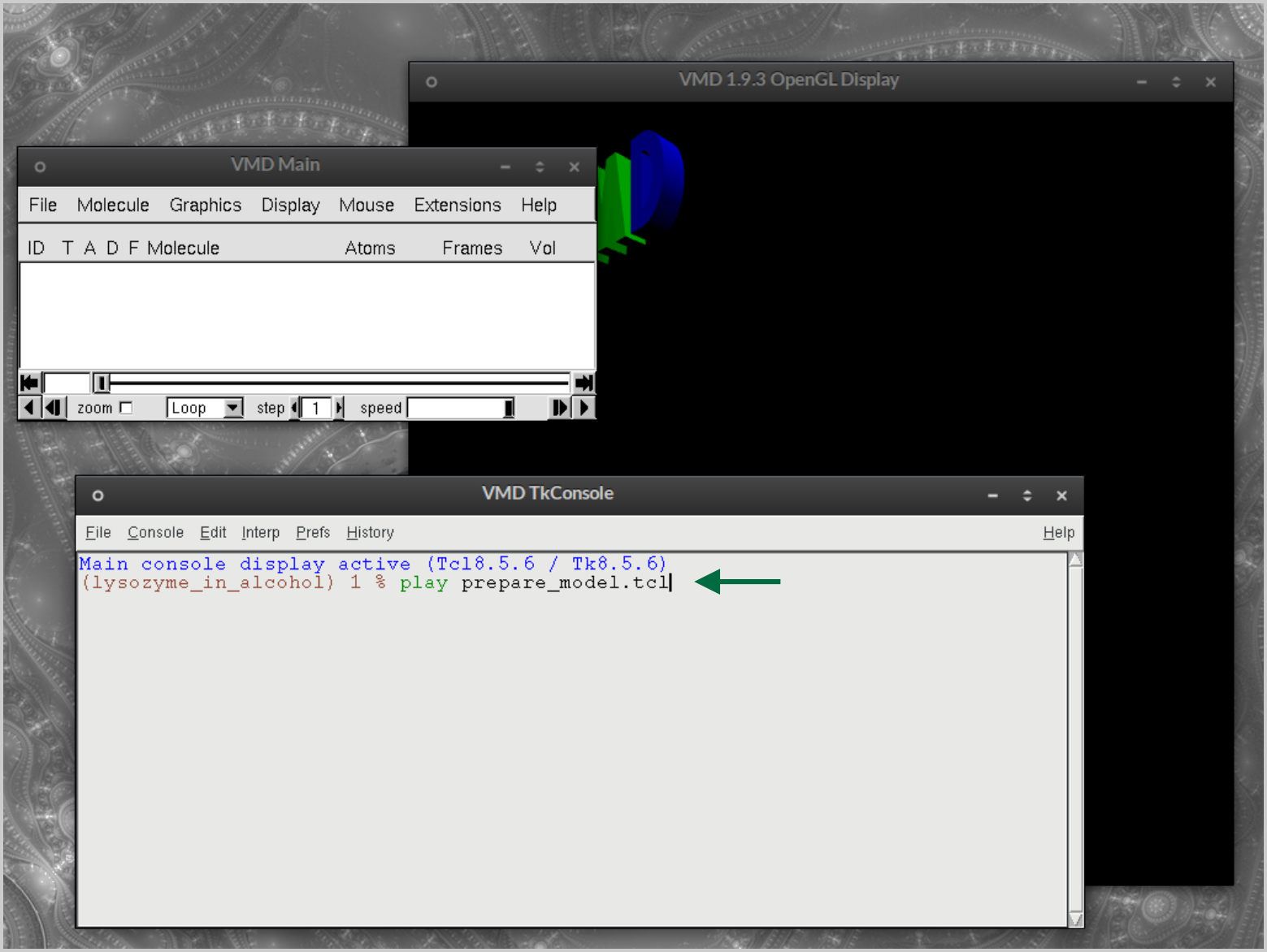
Combining trajectories, movies, and scripting



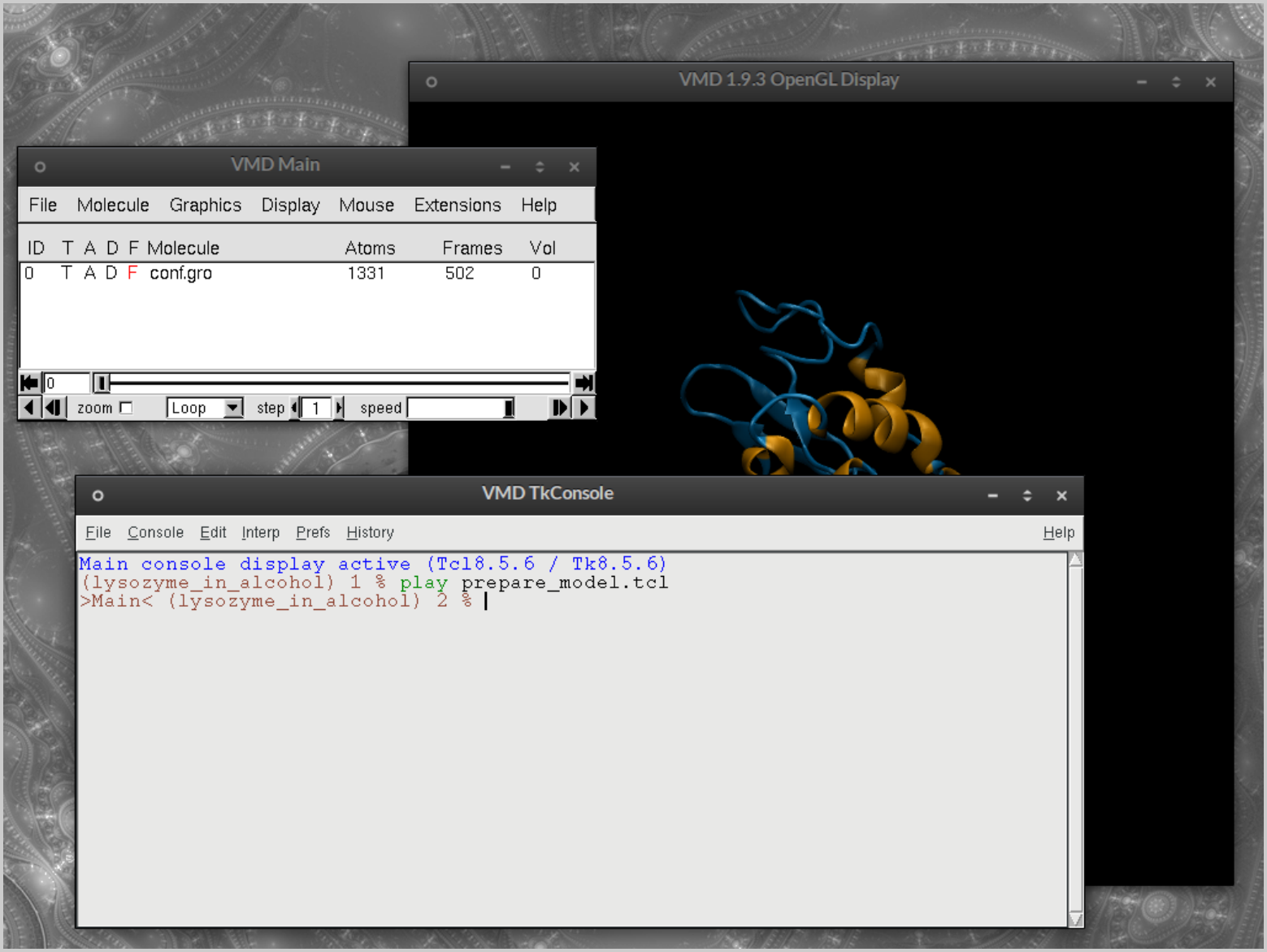
Combining trajectories, movies, and scripting

```
# Load topology and trajectory
mol new conf.gro
mol addfile traj.xtc waitfor all

# Universal palette
color change rgb  0 0.00 0.47 0.72
color change rgb  1 0.96 0.25 0.00
color change rgb  3 0.99 0.63 0.00
color change rgb  4 0.94 0.89 0.26
color change rgb  5 0.00 0.30 0.45
color change rgb  7 0.00 0.62 0.45
color change rgb  9 0.89 0.49 0.68
color change rgb 10 0.25 0.75 1.00

# Global parameters
display projection orthographic
color display background white
axes location off

# Delete default representation
mol delrep 0 top

# Show protein as cartoon, color by secondary structure
mol representation NewCartoon 0.3 10.0 4.1 0
mol color Structure
mol selection {protein}
mol addrep top

# Trajectory smoothing
mol smoothrep 0 0 5

# Secondary structure colours
color Structure "Alpha Helix" orange
color Structure 3_10_Helix orange
color Structure Pi_Helix orange
color Structure Extended_Beta blue
color Structure Bridge_Beta blue
color Structure Turn blue
color Structure Coil blue

# Go to the first frame (topology)
animate goto 0

# (Re)calculate secondary structure
vmd_calculate_structure top
                                                    45,27         Tout
```

Combining trajectories, movies, and scripting



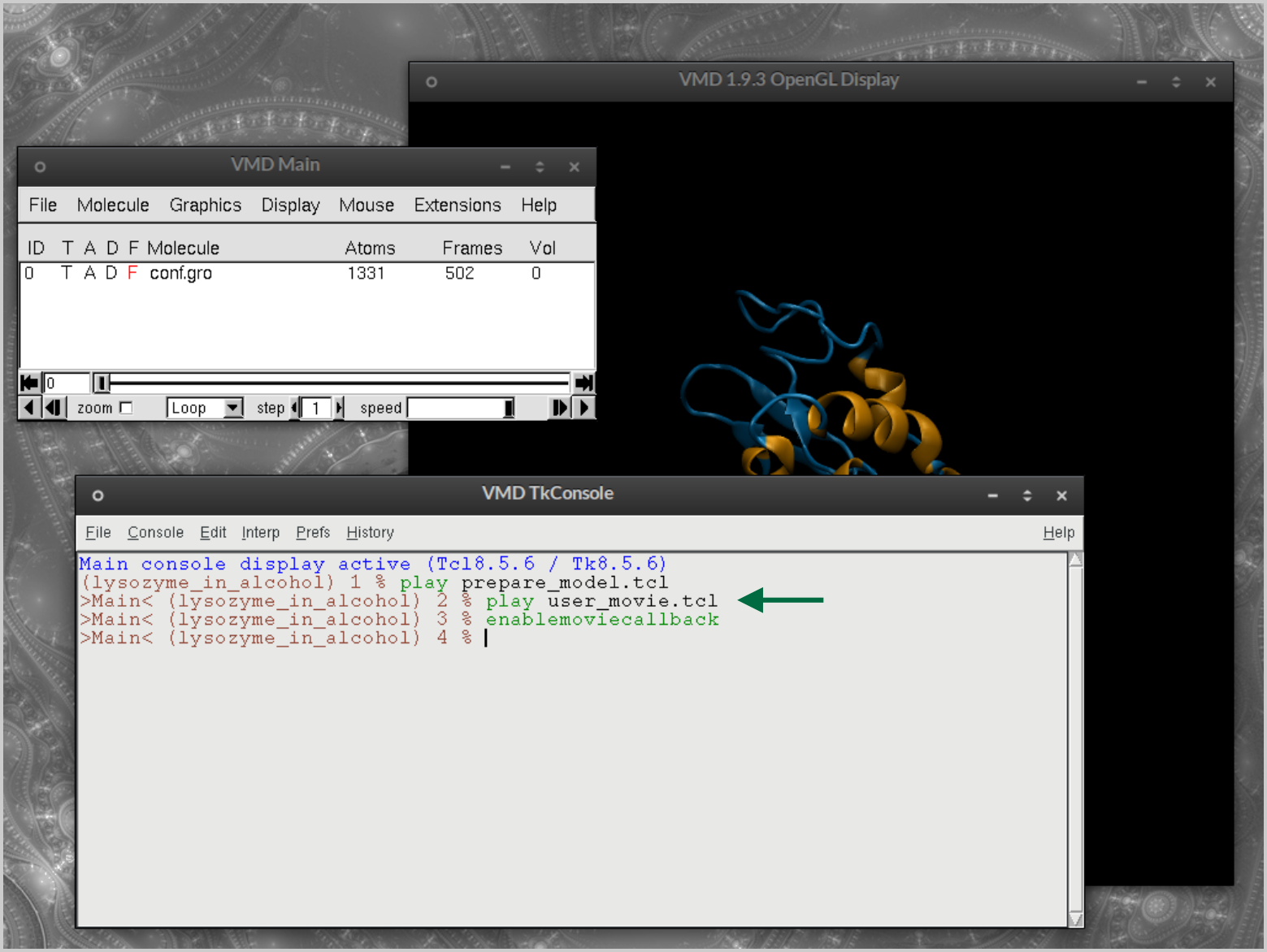
Combining trajectories, movies, and scripting



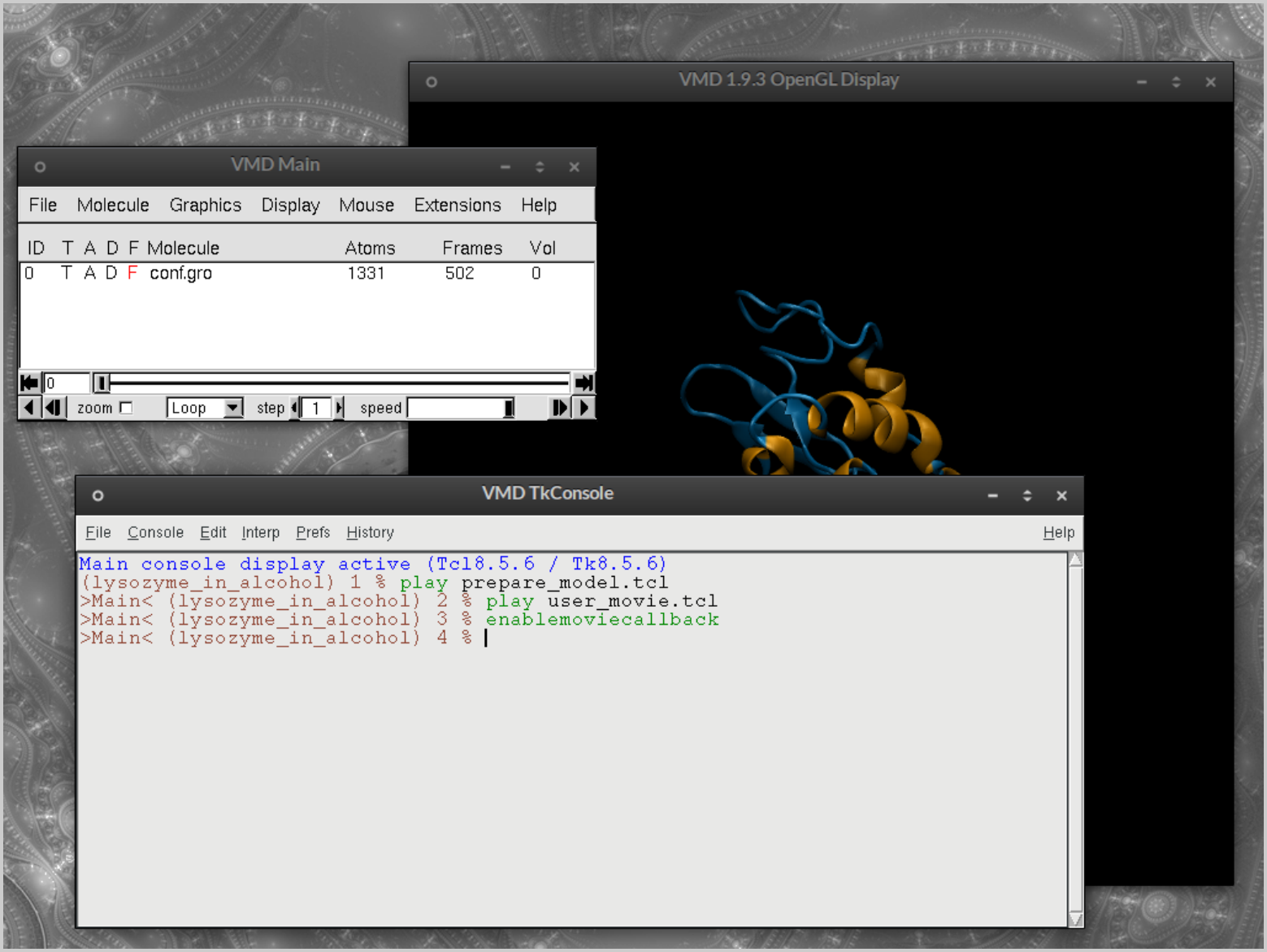
Combining trajectories, movies, and scripting

```
 1 ## User-defined movie frame update callback procedure, invoked every time
 2 ## a movie frame is rendered.
 3 proc moviecallback { args } {
 4   puts "User-defined movie frame update callback frame: $::MovieMaker::userframe
 5  / $::MovieMaker::numframes"
 6
 7   animate next
 8   vmd_calculate_structure top
 9   rotate y by 0.2
10 }
11
12 ## Easy-to-use proc to enable the user-defined movie frame callback
13 proc enablemoviecallback { }  {
14   trace add variable ::MovieMaker::userframe write moviecallback
15 }
16
17 ## Easy-to-use proc to disable the user-defined movie frame callback
18 proc disablemoviecallback { } {
19   trace remove variable ::MovieMaker::userframe write moviecallback
20 }
21
~
~
~
~
~
"user_movie.tcl" 21L, 651C                                    21,0-1        Tout
```

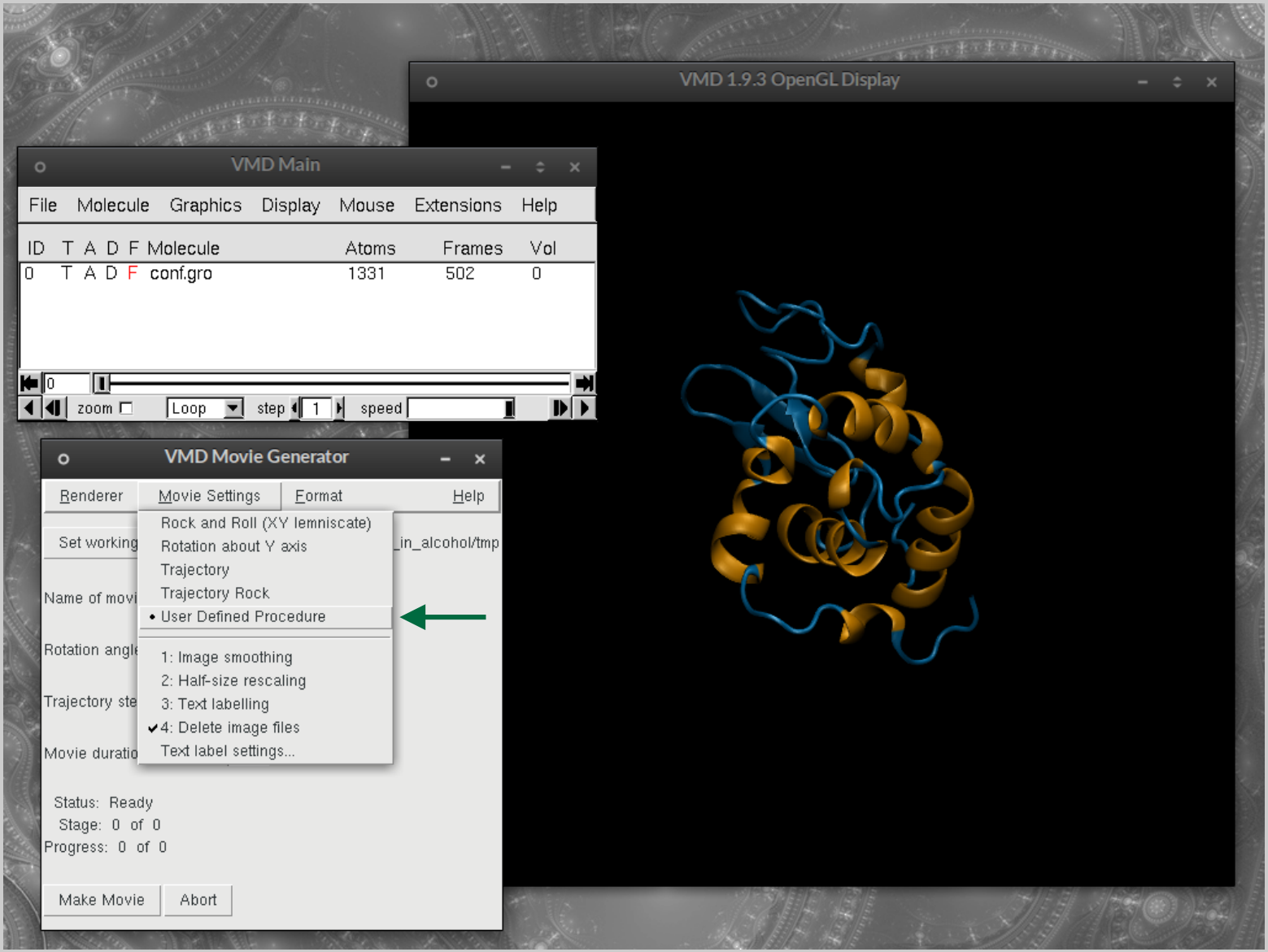
Combining trajectories, movies, and scripting



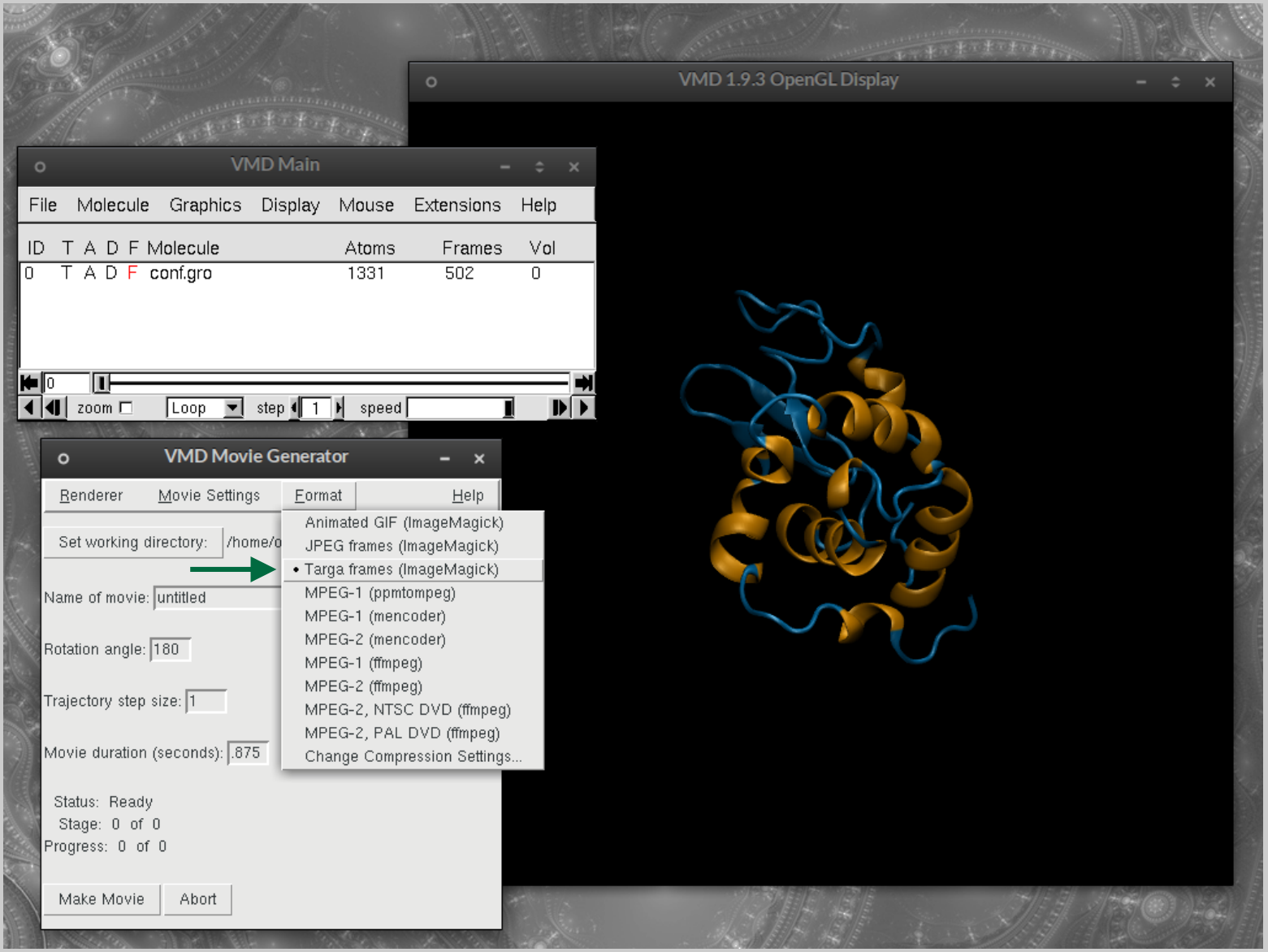
Combining trajectories, movies, and scripting



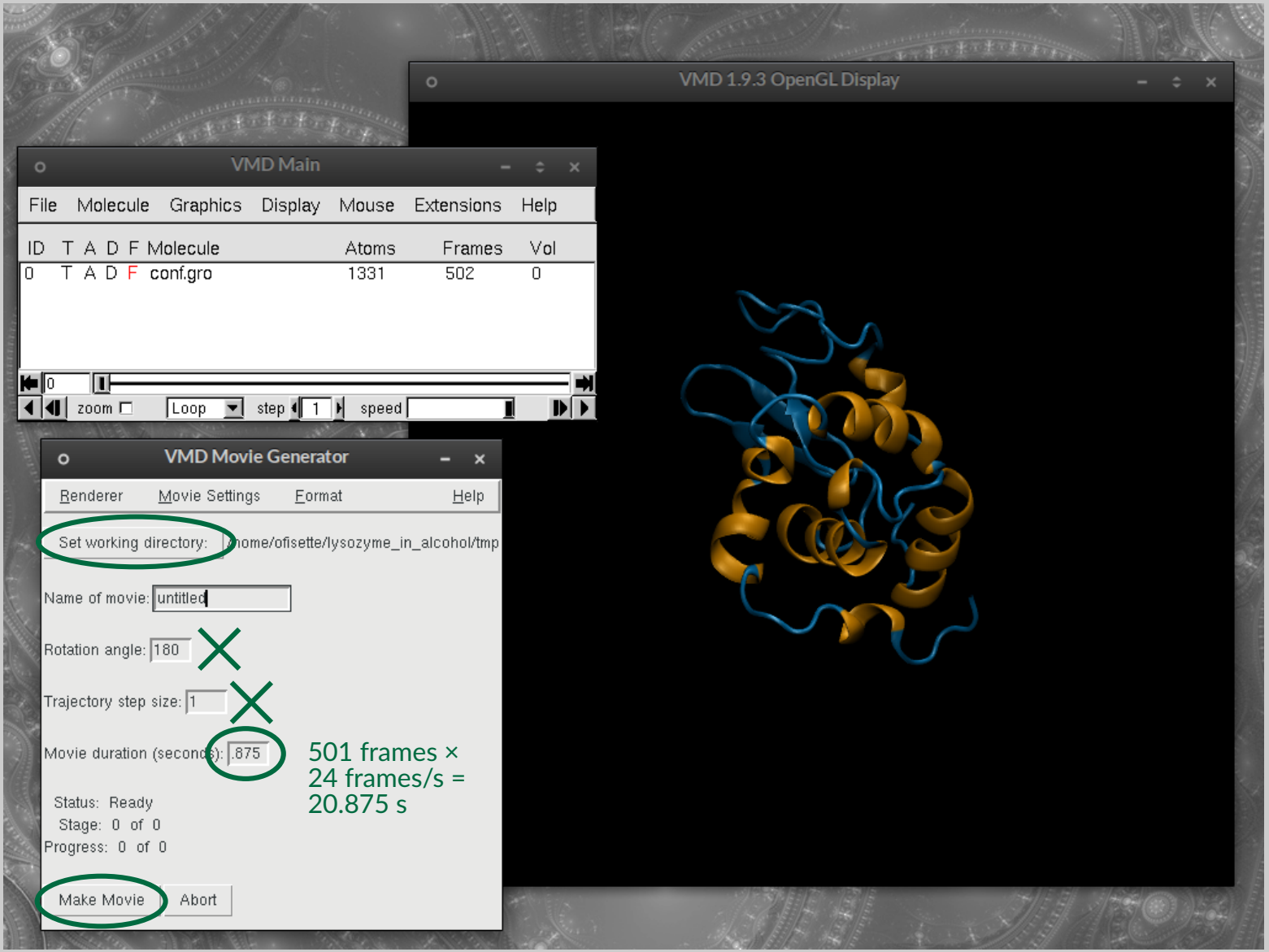
Combining trajectories, movies, and scripting



Combining trajectories, movies, and scripting



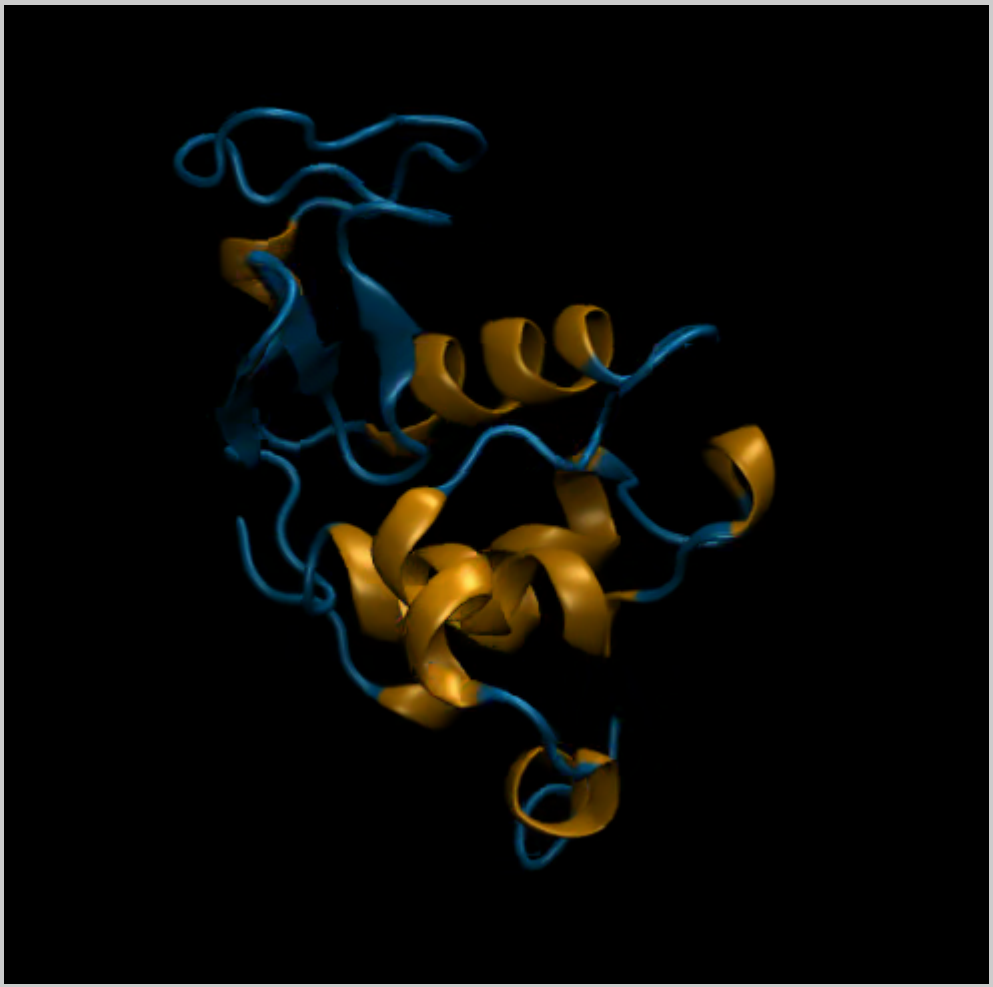
Combining trajectories, movies, and scripting

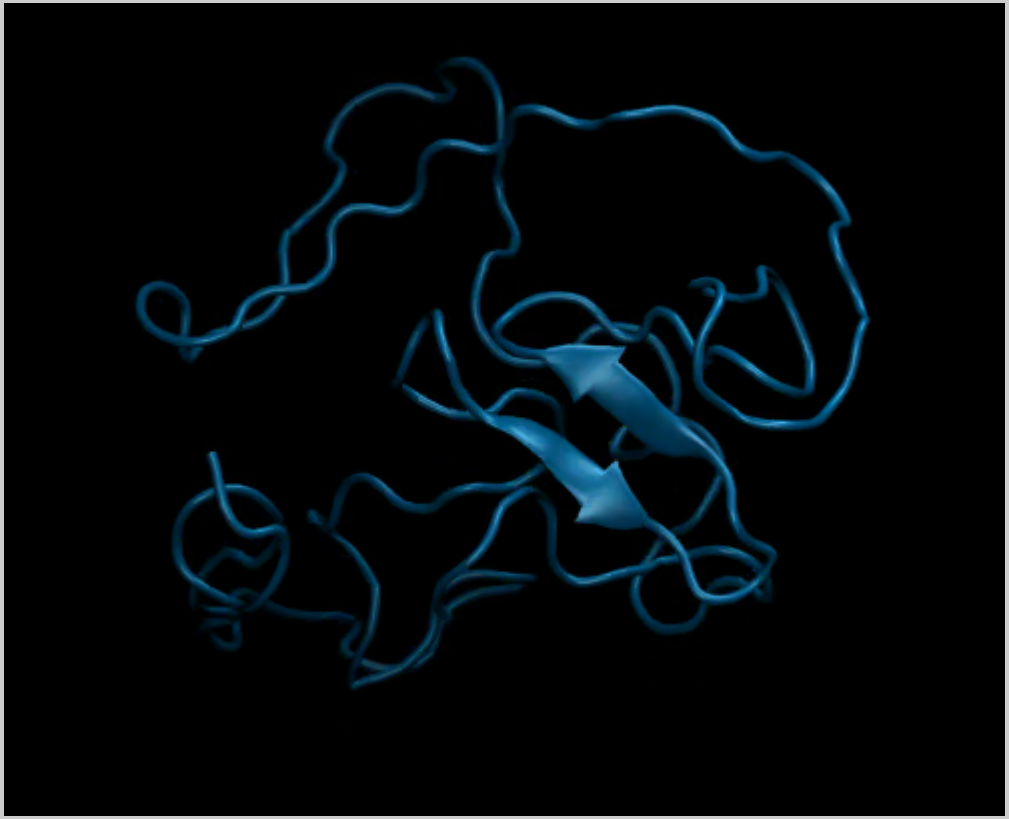


Combining trajectories, movies, and scripting

```
#!/usr/bin/env bash
set -e; shopt -s expand_aliases

ffmpeg -framerate 24 \
       -i "tmp/final.untitled.%05d.tga" \
       -vf vflip \
       -c:v libx265 "lysozyme_ethanol.mp4"
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
~
"encode_movie.sh" 7L, 180C                                    7,42          Tout
```

Combining trajectories, movies, and scripting





Resources

- VMD website
  - *https://www.ks.uiuc.edu/Research/vmd/*
- Using VMD (tutorial)
  - *https://www.ks.uiuc.edu/Training/Tutorials/vmd/tutorial-html/*
- VMD User's Guide
  - *https://www.ks.uiuc.edu/Research/vmd/vmd-1.8.3/ug/*
- Compute Canada Documentation (CC Doc): VMD
  - *https://docs.computecanada.ca/wiki/VMD*
- WestGrid webinar: Molecular visualization with VMD
  - *https://www.westgrid.ca/events/molecular_visualization_vmd*

Questions

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