Solid Rock

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Making Movies: Chimera

- Basic commands
- Spin/rock
- Center
- Increase quality
- Creating animations
- Volume rendering
- Morphing

Making it simple

- Open chimera
  - Load molecule(s)
  - Tools → Utilities → Movie recorder
    - Record
    - Move molecule
    - Stop
    - Make movie

Automatic movement

- Favorites → Command Line
  - **turn y 3 120**
- Tools → Utilities → Movie recorder
  - Record
  - Press enter on command line
  - When done press Stop and Make Movie

Basic commands

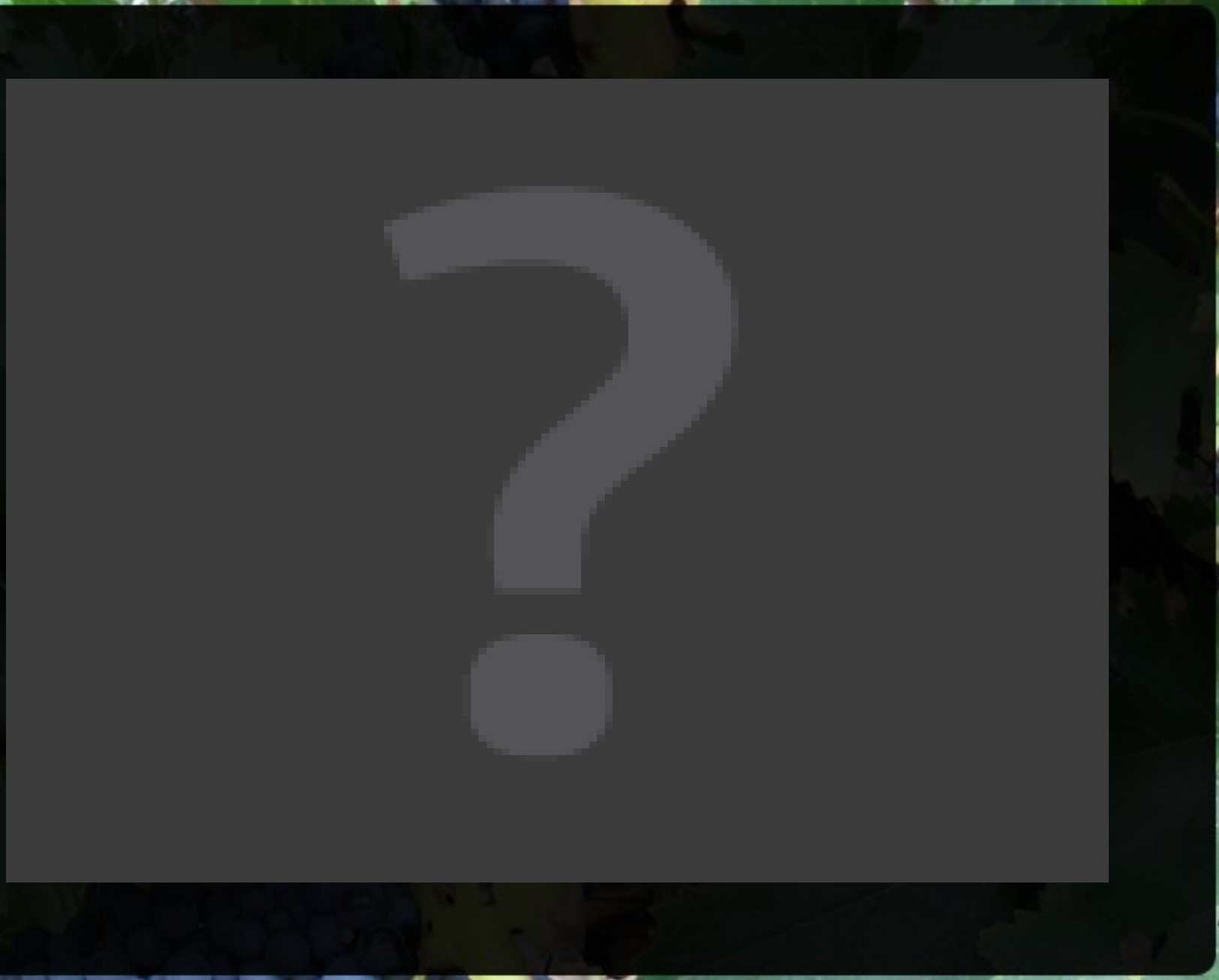
- You can use several commands separated by a ';'
  - movie record
  - movie stop
  - movie encode
- General form: **movie** *action options*
  - **movie record directory** *dir1/dir2/.*
    supersample *3* **size** *w,h* **raytrace** *true*
  - **movie encode mformat** *mp4* **output** *mymv*

Automatic recording

- The problem lies in hand switching
- Let us use the command line:
  - movie record ; turn y 3 120 ; **wait**; movie stop
  - movie encode output mymovie

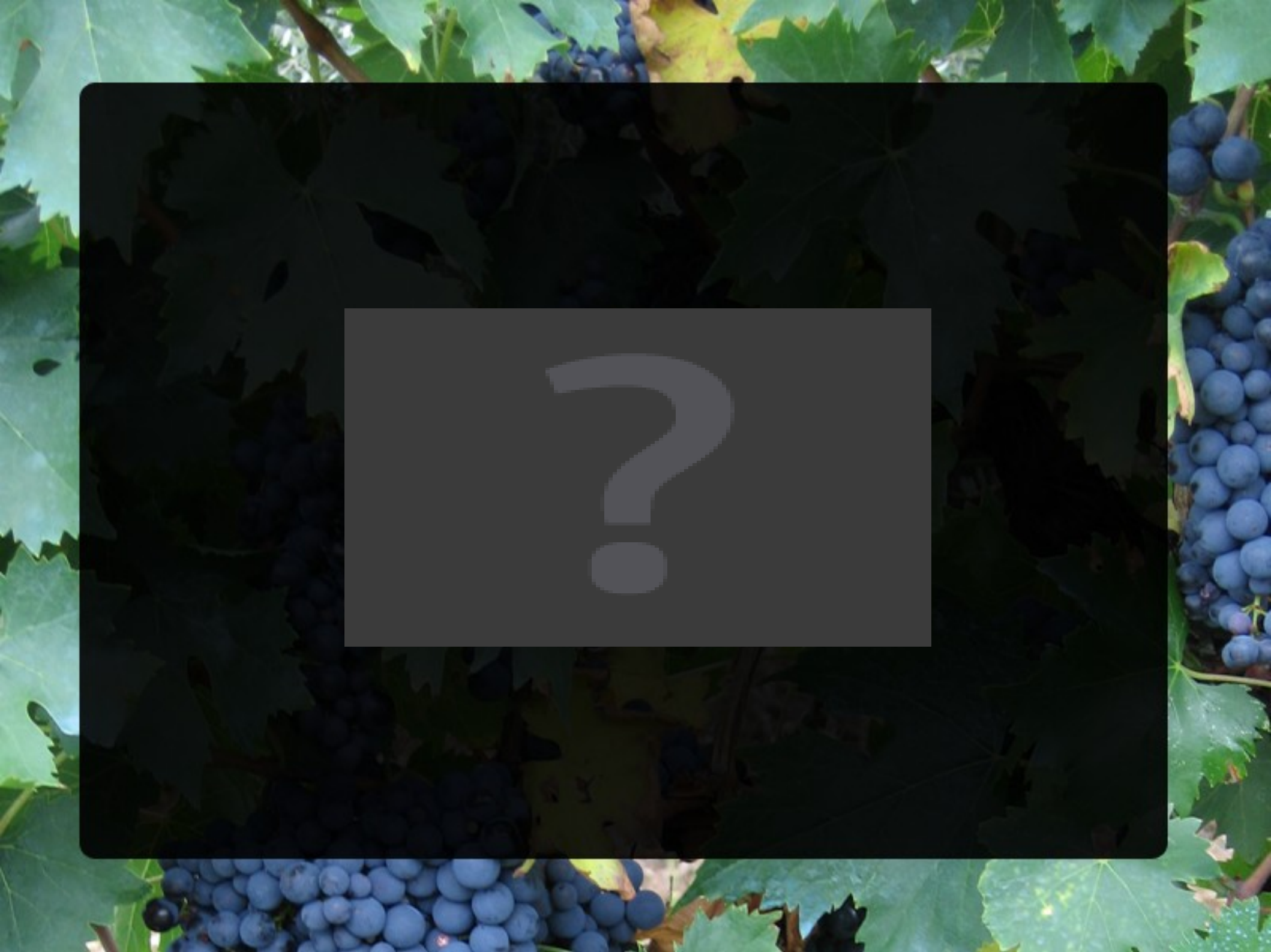
Controlling movement

- You can use any visualization command between **movie** commands
- Remember to **wait** for a long command to finish before issuing the next
- Try rocking instead of spinning
  - movie record; rock y 3 68; wait; rock x 3 68; wait; movie stop; movie encode output mymovie.mov



Control animation

- You can use any visualization command
  - On the menu
  - On the command line
- Better if you define layout first
  - Change window size
  - Presets → Interactive 1
  - Select → residue
  - Actions → set pivot...



Control animation (2)

- windowsize 640 480
- preset apply interactive 1
- cofr :GLN
- movie record ; rock y 3 68 ; wait ; rock x 3 68; wait ; movie stop ; movie encode output mymovie.mov
- You can put everything in a script file **.cmd** and load it with **File → open**

Improving quality

- Record with supersampling (e.g. 3): draw at a bigger size and resize down
  - movie record supersample 3
- Record at desired size
  - movie record size 640,480
- Increase output bit rate for a given window size, 640x480: 200 (low), 1000 (medium), 6000 (high)
  - movie encode bitrate 10000
- Use appropriate encoding (e.g. mov, mp4)
- Add fill frames

Raytracing

- Very slow, may hang GUI for > ~200 frames
- Produces a POVray file for each frame and renders it using POVray

```
windowsize 640 480
~ribbon
show :GLN
repr sphere
color byelement
reset
set bg_color black
movie record supersample 3 raytrace true
 wait 10 ;rock y 3 68; wait; rock x 3 68; wait; wait 10
movie stop
movie encode mformat mp4 bitrate 10000 output 08-raytrace.mp4
```

Animation

- Start by marking all needed positions:
  - savepos start
  - center :GLN; savepos centered
  - ~select 0; move x 30; move y 40; turn x 90; select 0; savepos unbound
- Chimera moves among positions with **reset**. If more than one frame is requested, linear interpolation will be used.

Prepare world

- Select initial position
- Select conformation/display
- Add labels:
  - 2dlabel create title “XX” xpos 0.3 ypos 0.9 color white
- Select background color
  - set bg_color gray
- etc...

You can do anything...

- While recording:
  - Add/remove surfaces
  - Fade in/out objects
  - Identify Hydrogen bonds
  - Color by any criteria
  - Change display modes (CPK, surface..)
  - Anything!

Getting it done

- Work on a script
  - Prepare positions
  - Set up initial scene
  - Comment out (#) movie record
  - Keep on adding commands until OK
  - Add movie stop; movie encode
  - Uncomment movie record
- Load script

Volume rendering

- You can also animate volumetric data
  - e.g. from EMSD:1321
    - open #0 emdbID:1321
    - volume #0 level 127
    - volume #0 color yellow
    - movie record
    - rock x 3 68; rock y 3 68
    - roll 1,1,0 3 68
    - movie stop; movie encode

Morphing

- You can morph among different structures too:
  - morph start #0.1
  - morph interpolate #0.2
  - …
  - morph interpolate #0.10
  - morph movie
  - movie record
  - coordset #1 1, ; wait; movie stop; ...

Morphing example

- Fetch by ID: PDB:1az6
- Tools → Structure comparison → Morph conformations
- Add → Add all variants, then add again variant #1
- Action on create → Hide conformations
- Create
- Play


That's all, folks!
QUESTIONS?