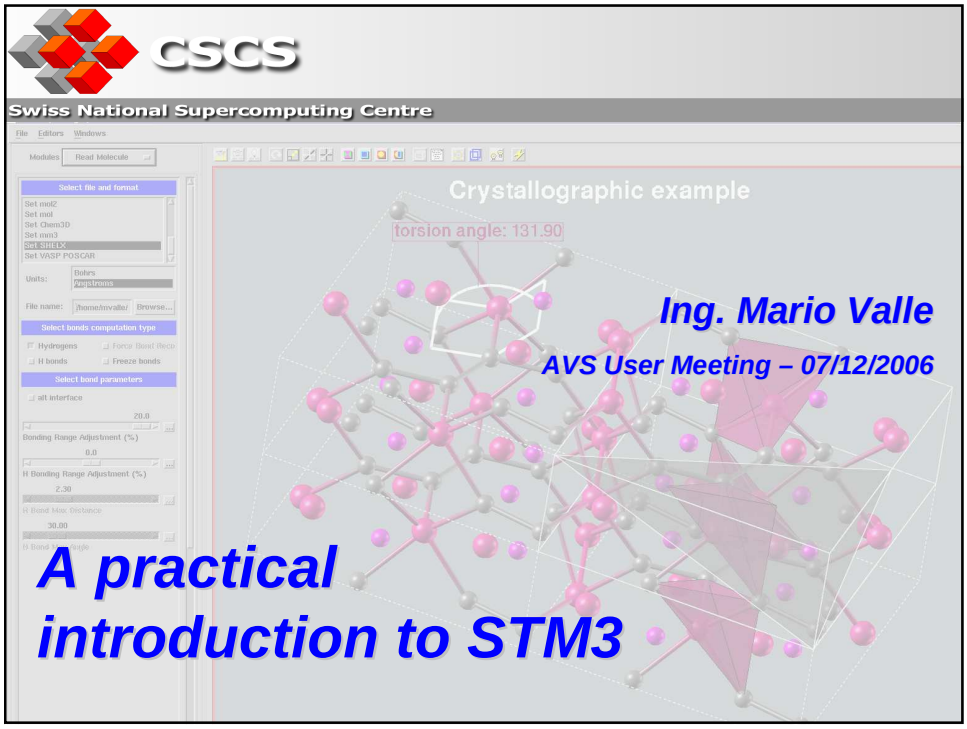
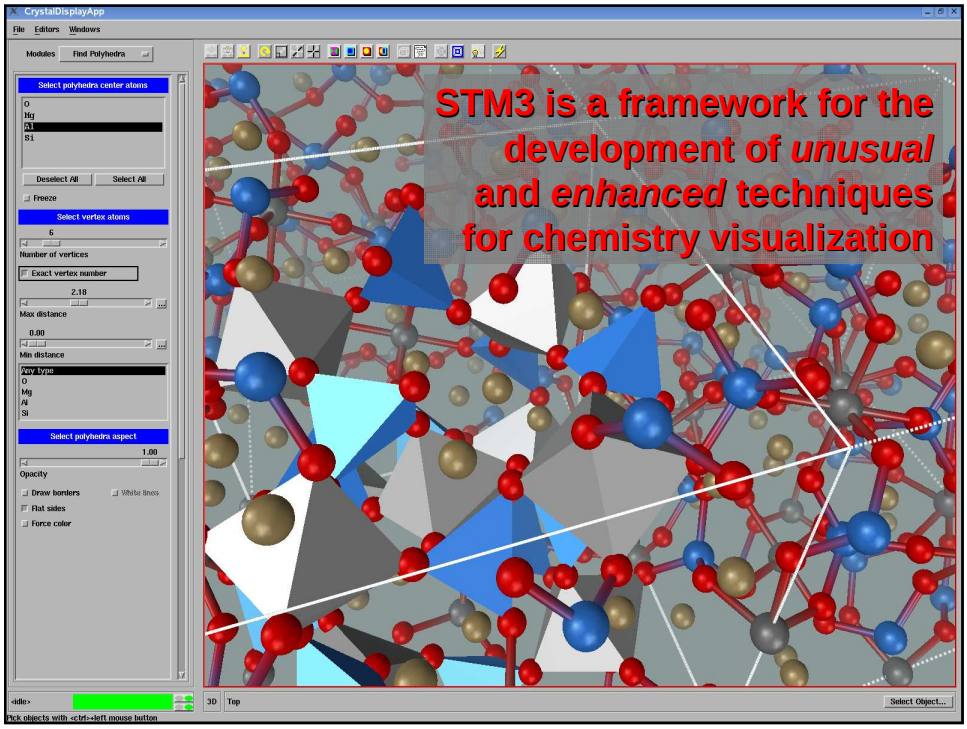
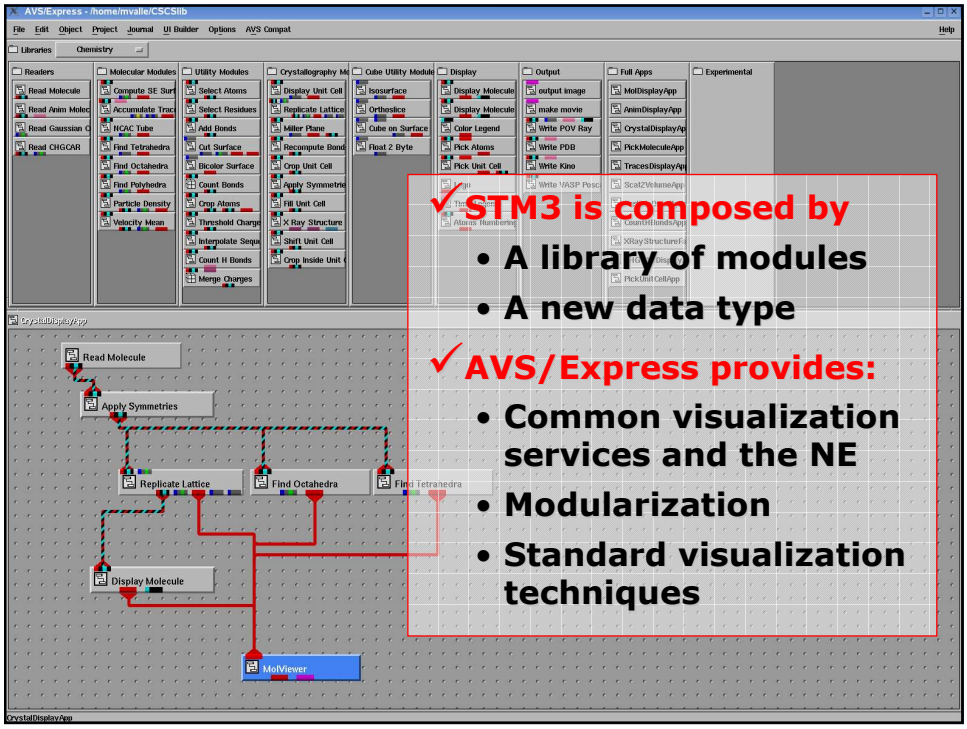

CSCS
Swiss National Supercomputing Centre
Crystallographic example
torsion angle: 131.90
Ing. Mario Valle
AVS User Meeting – 07/12/2006
A practical introduction to STM3


CrystalDisplayApp
File Editors Windows
Modules Find Polyhedra
Select polyhedra center atoms
Deselect All
Select All
Freeze
Select vertex atoms
Number of vertices
Exact vertex number
Max distance
Min distance
Select polyhedra aspect
Opacity
Draw borders
White lines
Flat sides
Force color
STM3 is a framework for the development of unusual and enhanced techniques for chemistry visualization
Select Object...

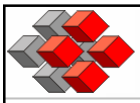


✓ **STM3 is composed by**

- **A library of modules**
- **A new data type**

✓ **AVS/Express provides:**

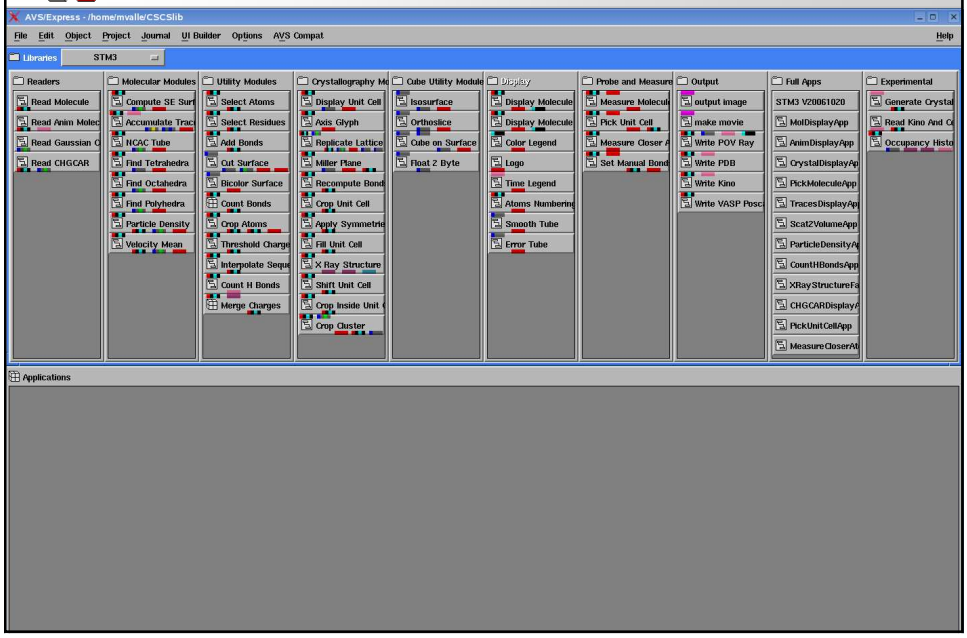
- **Common visualization services and the NE**
- **Modularization**
- **Standard visualization techniques**



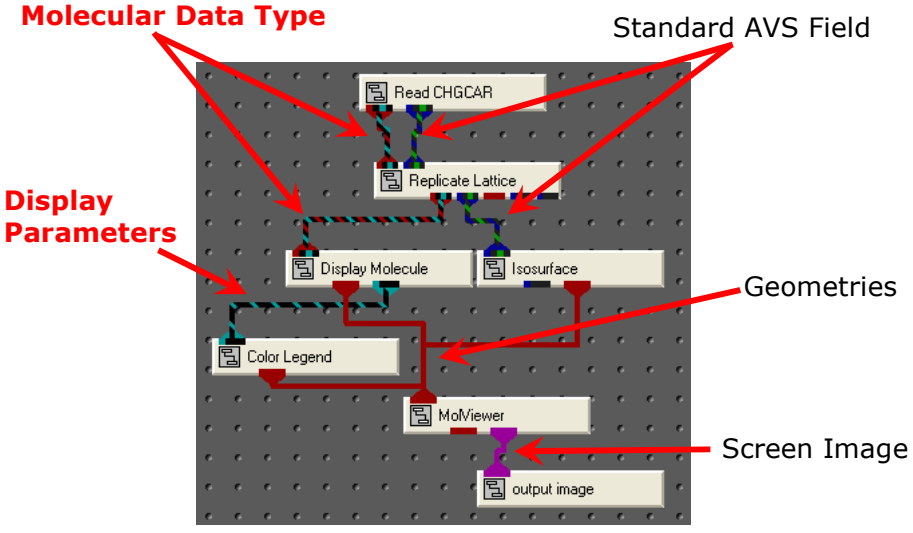
Workshop Agenda

1. Start AVS/Express and open STM3 library
2. Basic functions (single and multiple static structures)
3. Dynamic structures
4. Volumetric data
5. Crystallography support
6. Output production (movies and images)
7. Other modules
8. Extensibility

What composes STM3?



STM3 data types



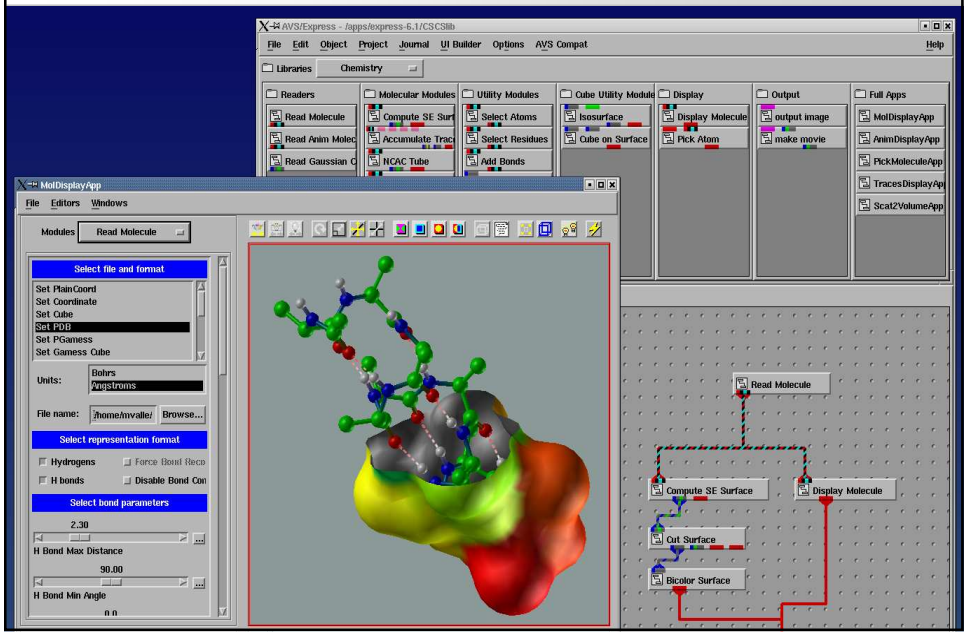
Start STM3 (and 2" tutorial)

- Launch AVS/Express (with STM3 included):

```
$ source /usr/local/userenv/express.csh
$ express                (Linux)
C:\> cd CSCSlib
C:\CSCSlib> go.bat (Windows)
```

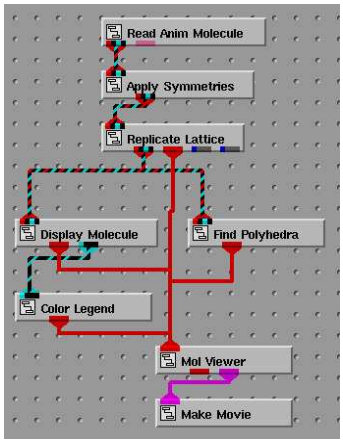
- Special cases: **`./go-viz`** **`./go -nohw`**
- Go To Libraries ➠ STM3
- Then go to the rightmost column (Full Apps)
- Drag the MolDisplayApp block in the area below marked Applications
- In the window that pops up select the file format (e.g. PDB) and read a file.
- Mouse rotate. Middle Mouse Button+Shift: Zoom. +Ctrl: Pan. Reset with the button.
- With the Modules drop down menu select Display Molecule and change the molecule appearance.

AVS/Express behind the scenes

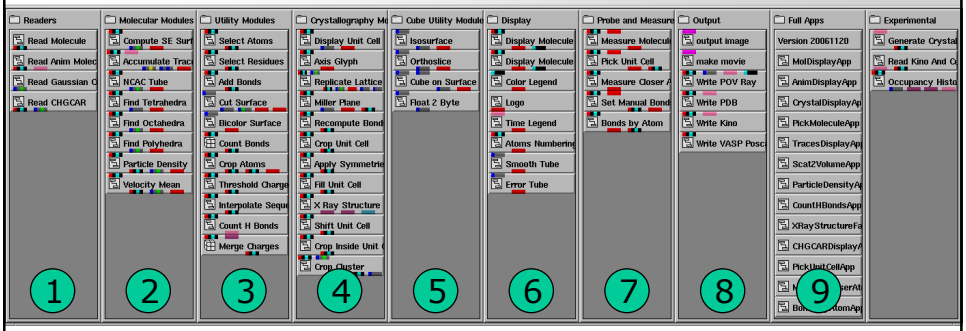


AVS/Express applications

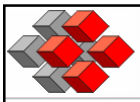
- Each module starts when receives all the needed data
- An application can use STM3 and standard AVS/Express modules together
- Connection ports (popup gives info and help)
- Colors related to data type
- The user interface automatically docks in the right place



STM3 modules



1. Readers for various, static and dynamic, chemical file formats
2. Modules that computes various derived structures
3. Manipulation of molecules, like atom selection
4. Unit cells, periodic lattices and symmetries support
5. Volumetric data visualization and manipulation
6. Final rendering of molecular data and legends
7. Probe, interaction and measurements
8. Output to image files, movies and other formats
9. Ready to run applications (plus display of STM3 version)



STM3 resources

- **STM3 overview and image gallery page**

  http://www.cscs.ch/projects/AVSChemistry.php

- **The list of current STM3 modules**

  http://www.cscs.ch/~mvalle/ChemViz/doc/STM3/

- **The STM3 paper**

  M. Valle, **STM3: a chemistry visualization platform,**
  Zeitschrift für Kristallographie, vol. 220, no. 5-6, pp. 585-588, 2005

- **The Blog and Wiki resources**

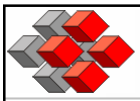
  http://chemviz.blogspot.com/
  https://twiki.cscs.ch/bin/view/TWiki/ChemViz

- **A (marketing) brochure on AVS/Express**

  http://www.avs.com/software/soft_t/avsxps.html

- **A user level AVS/Express course**

  http://www.cscs.ch/~mvalle/AVS/XP-intro-en.html



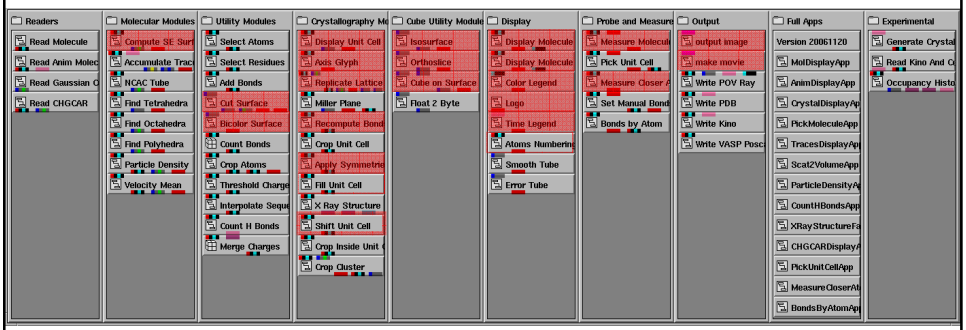
Before starting: what STM3 is not

- A complete chemistry visualization tool
  - It grows depending on user requests. If something is not requested, it is not be added.
  - Remember, STM3 goal is not to replace existing tools
- A simple, end user tool
  - It is more a LEGO construction box
  - More power and flexibility comes at the expense of no point-and-click interface
- A tool for a specific chemistry field (biochemistry, MD, crystallography, etc.)
  - Again functionalities depend on the requests
  - But it is precisely its goal to be cross-field

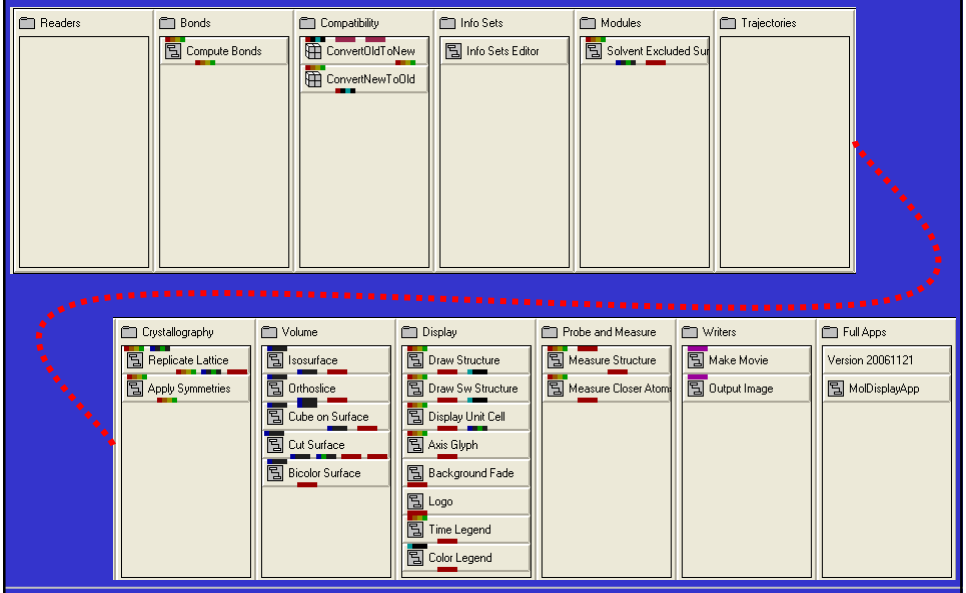
Before starting: STM3 evolution

- I'm working on the STM3 evolution, tentatively called (guess what?) STM4
- Something already exist. I will show examples during the tutorial
- But is still too early to switch over (for example there is no updated documentation)
- Anyway the same concepts and almost the same modules will be available
- And more: with a pair of conversion modules, current and future modules could be mixed

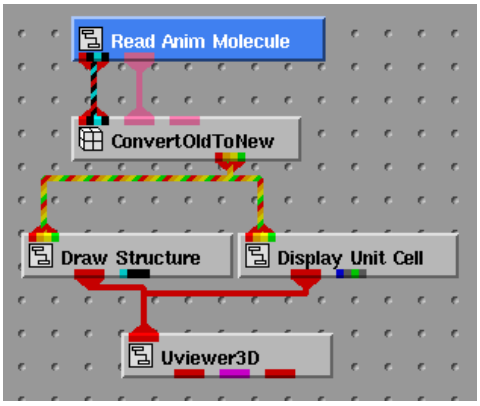
Ported STM3 modules

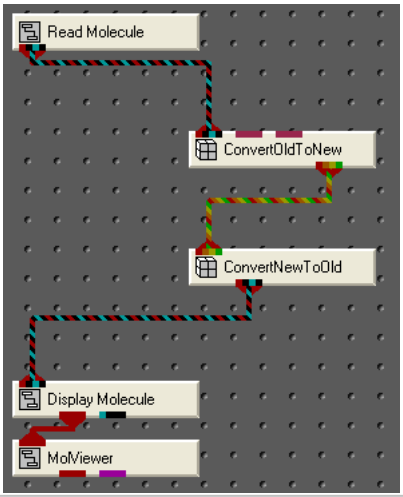


Ported modules



Mixed environment





Look at a static structure

Goal

- Look at a static structure experimenting with various rendering modes

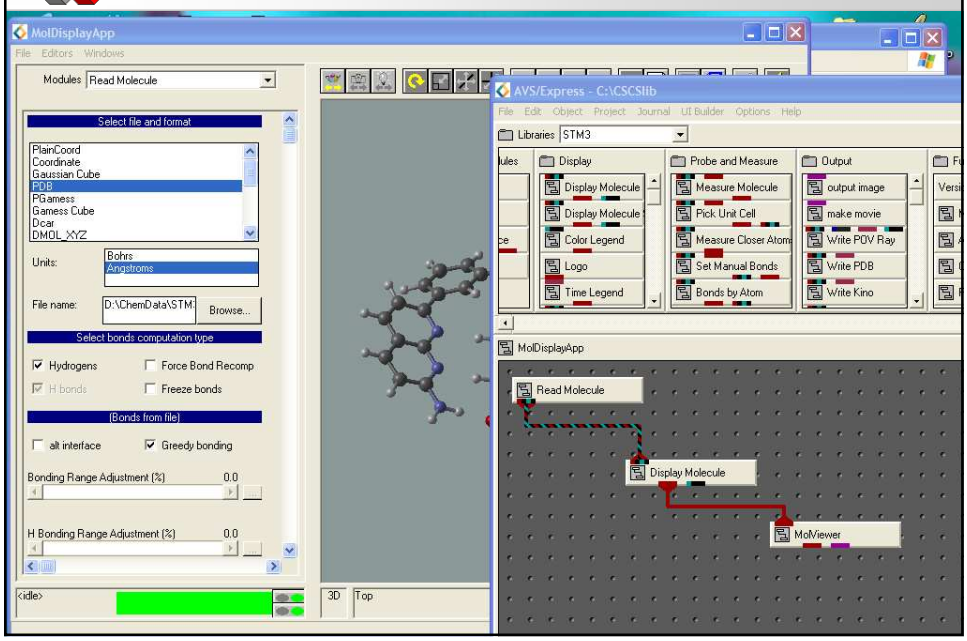
How

1. Instantiate MolDisplayApp
2. Look at its structure (double click on the application)
3. Load G-host.pdb
4. Play with reader options
5. Play with rendering options

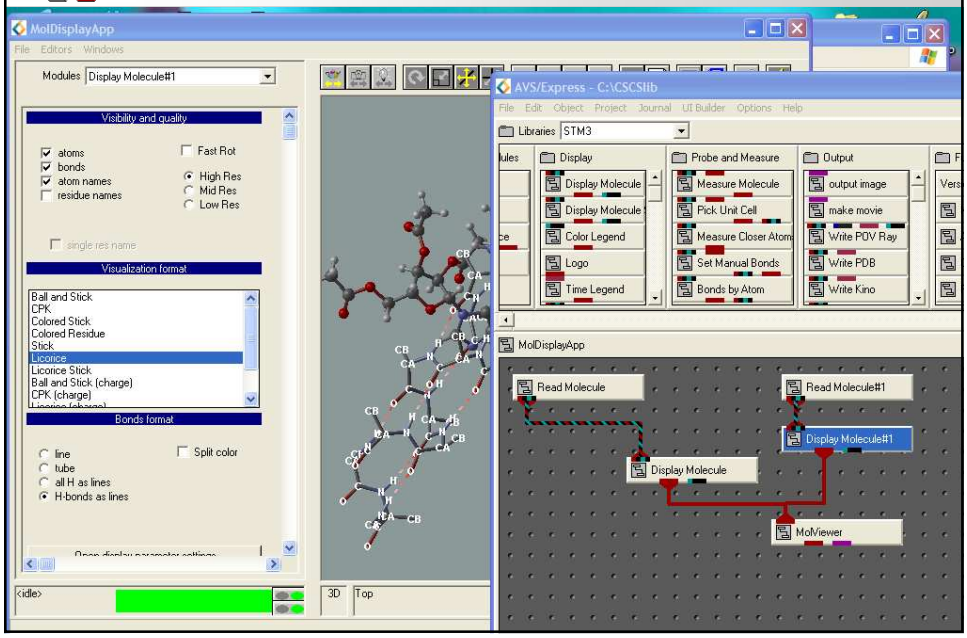
Bonus

1. Add a second molecule
2. Try the STM4 MolDisplayApp

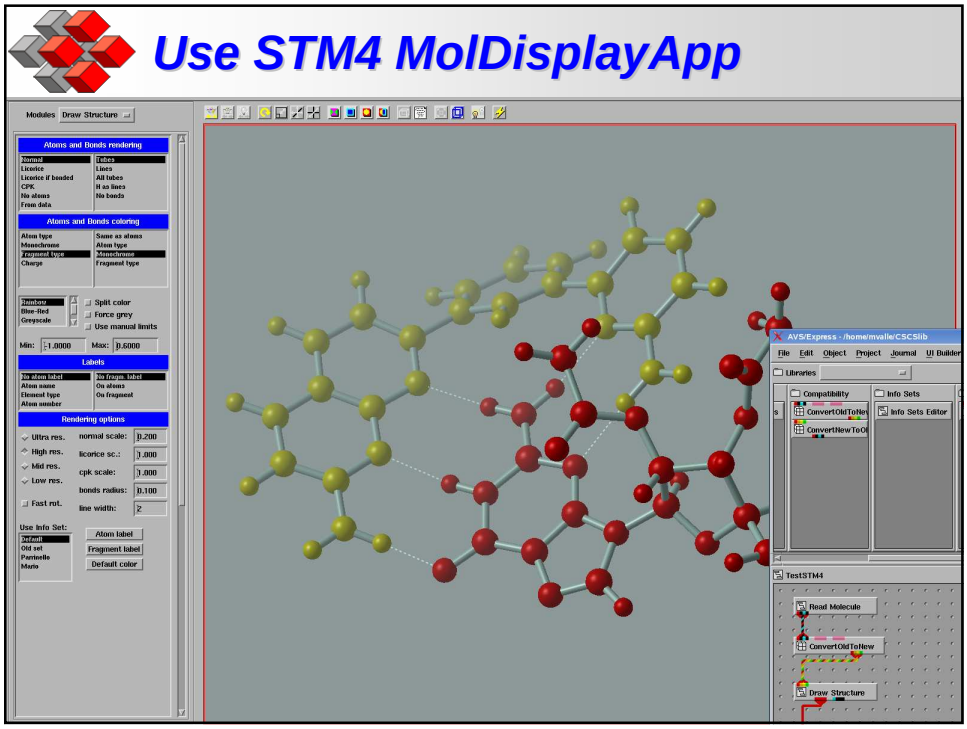
Look at a static structure



Two static structures



Use STM4 MolDisplayApp



Crystallography support

Goal

- Look at a static structure experimenting with various crystallographic support modules

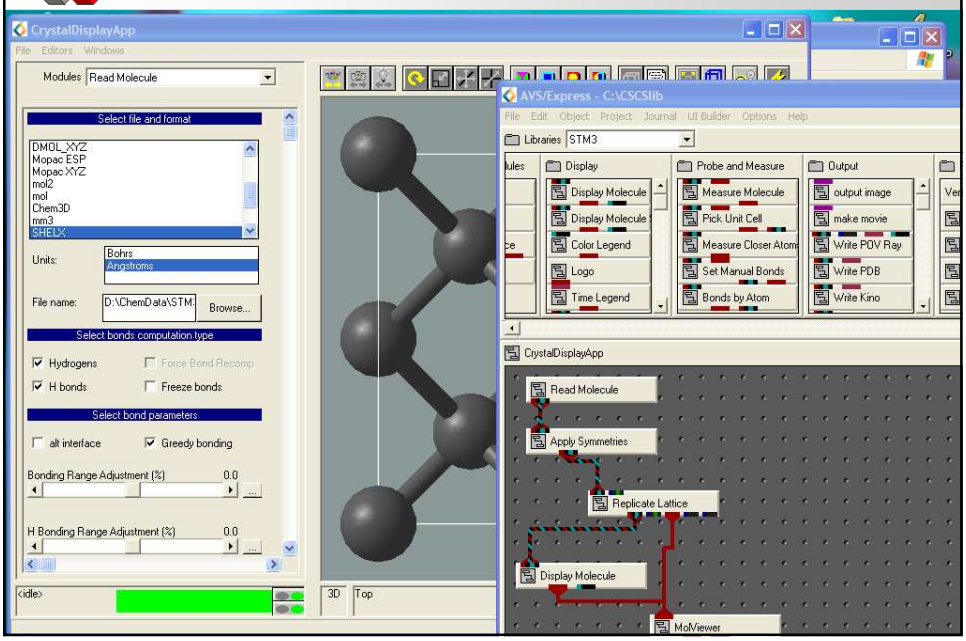
How

1. Instantiate CrystalDisplayApp
2. Look at its structure
3. Load diamond.res using SHELX format
4. Disable symmetries
5. Play with cell replication options

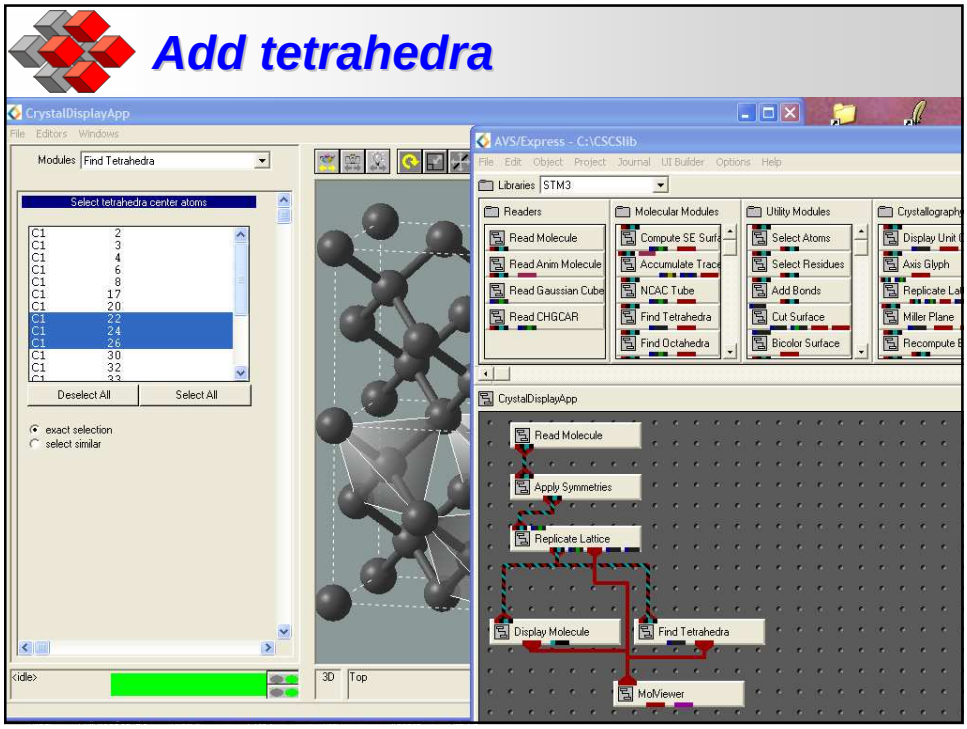
Bonus

1. Add tetrahedra
2. Build the same network in STM4 starting from MolDisplayApp
3. What are the differences between STM3 and STM4 versions?

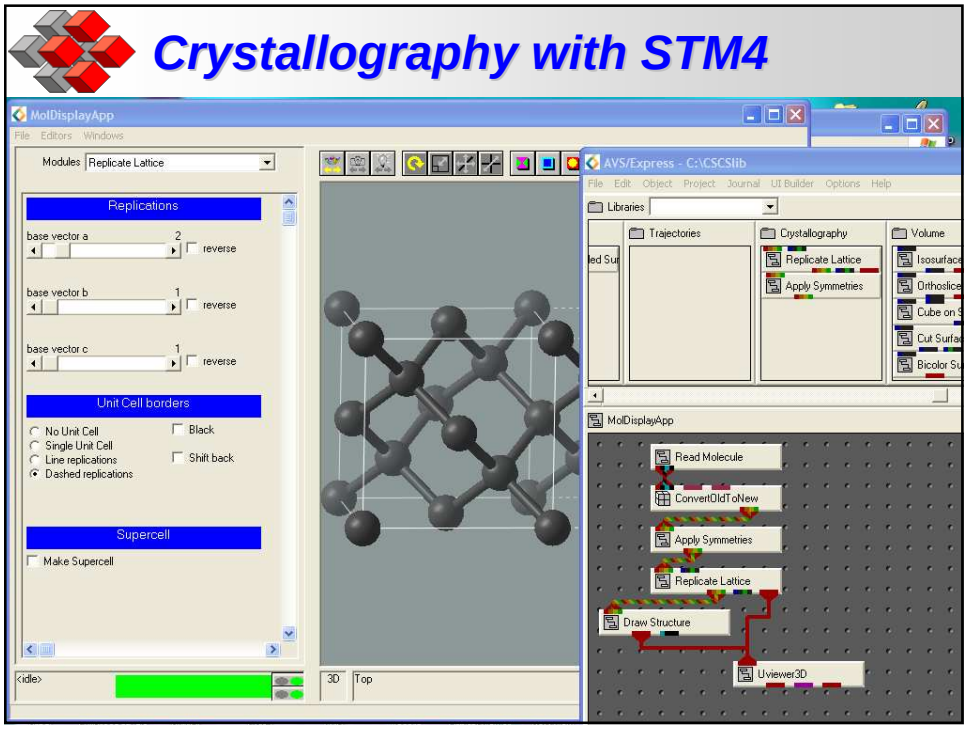
Crystallography support



Add tetrahedra



Crystallography with STM4



Volumetric data

Goal

- Look at a static structure and its associated volumetric data experimenting with various volume visualization techniques

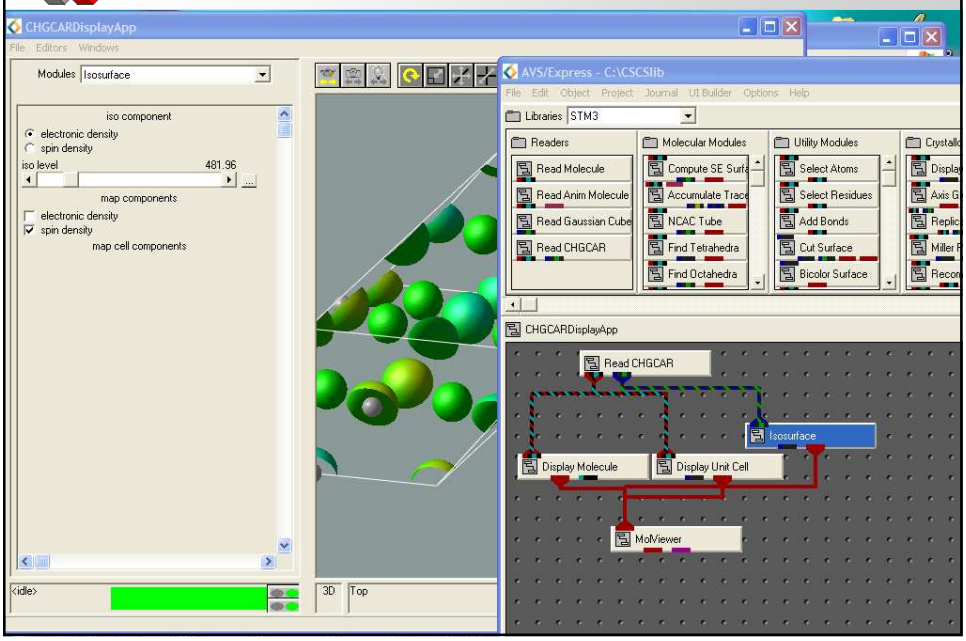
How

1. Instantiate CHGCARDisplayApp
2. Look at its structure
3. Load CHG-magnetic (setting before the “magnetic” toggle)
4. Add a Display Unit Cell module
5. Play with Isosurface parameters

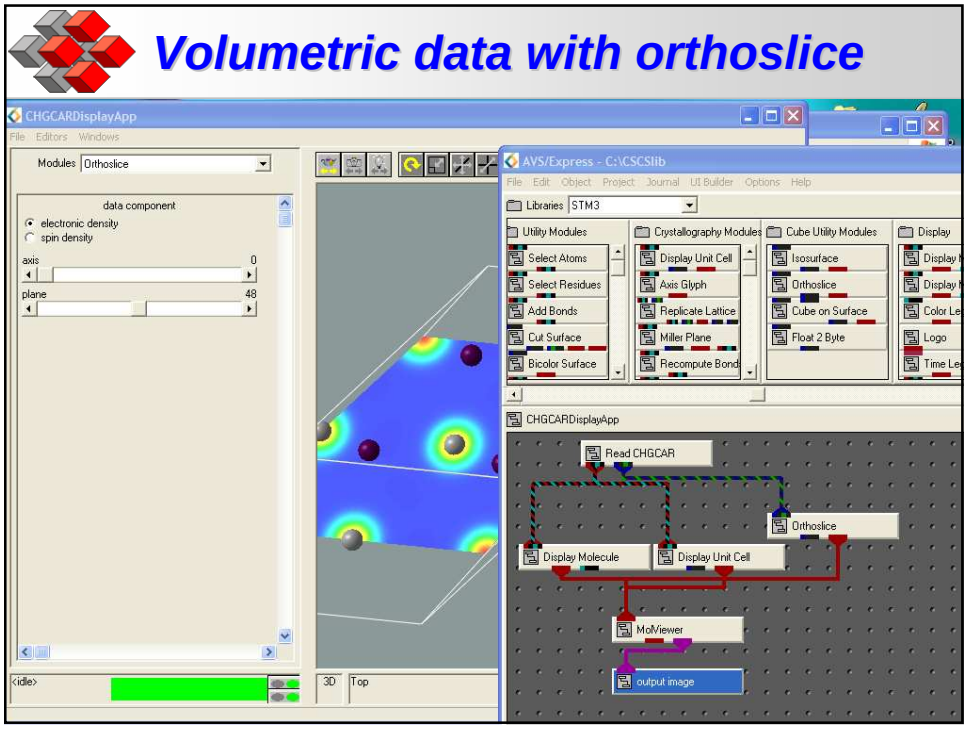
Bonus

1. Add Orthoslice
2. Save a screenshot of the resulting visualization
3. Use volume render (under Main → Mappers) + Float 2 Byte

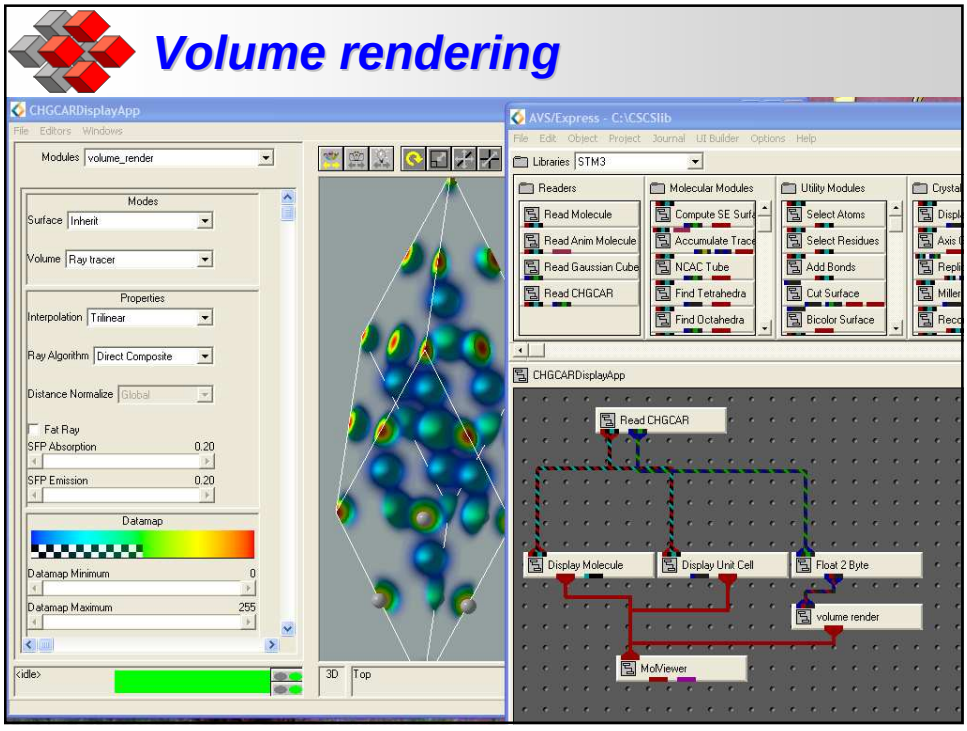
Volumetric data



Volumetric data with orthoslice



Volume rendering



Dynamic structures

Goal

- Look at a dynamic structure experimenting with movie creation and animation techniques

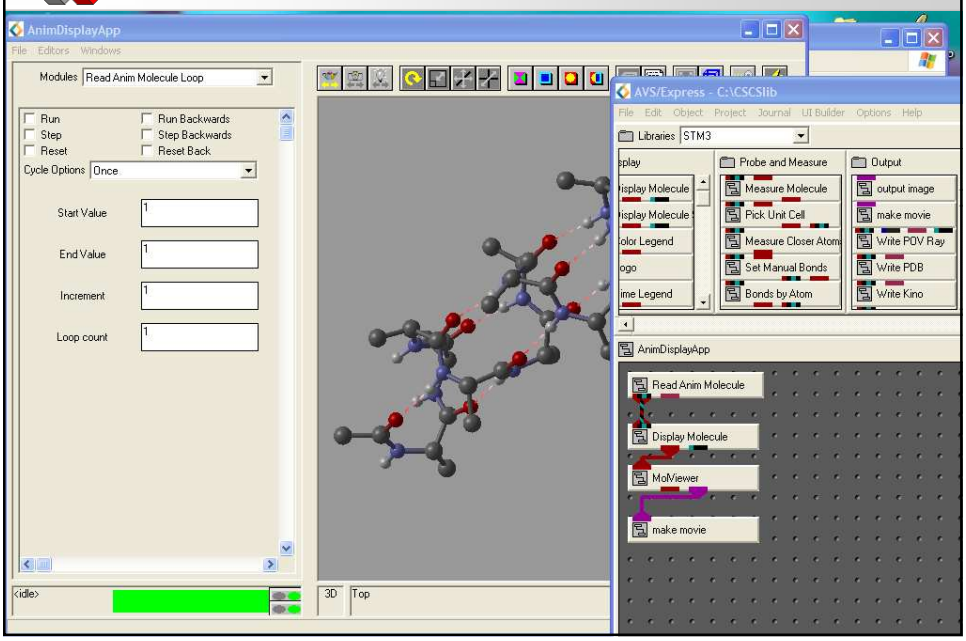
How

1. Instantiate AnimDisplayApp
2. Look at its structure
3. Load alanine.pdb and alanine.dcd (as DCD)
4. Animate it
5. Save a movie of the animation

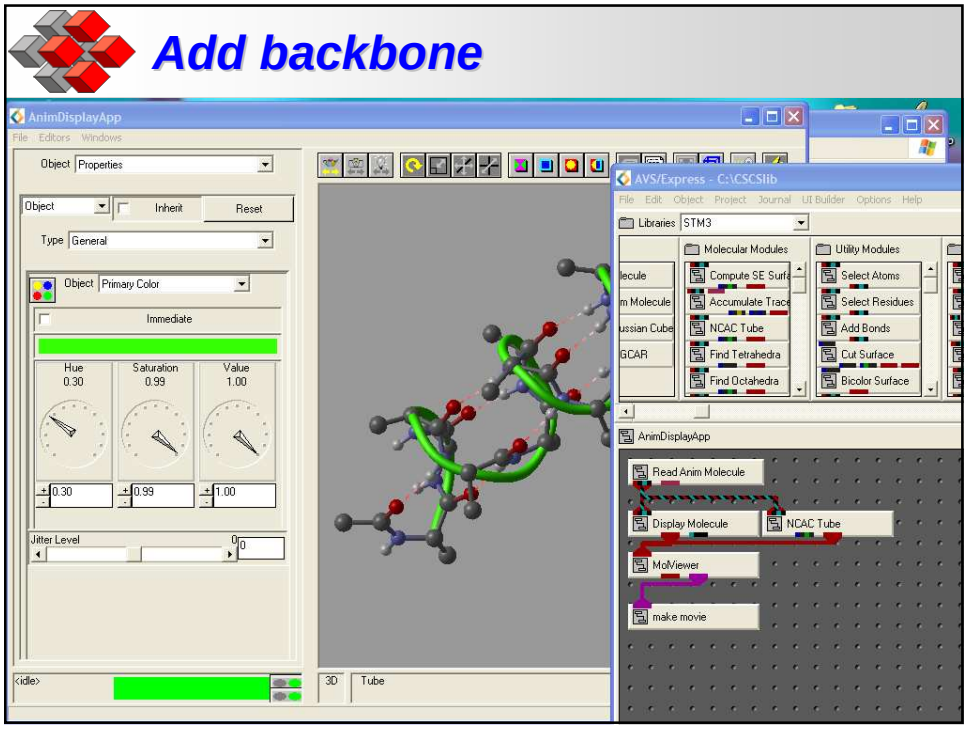
Bonus

1. Add N-Cα-C tube (backbone) and change its color
2. Compute the Solvent Excluded Surface (does not works on Mac)

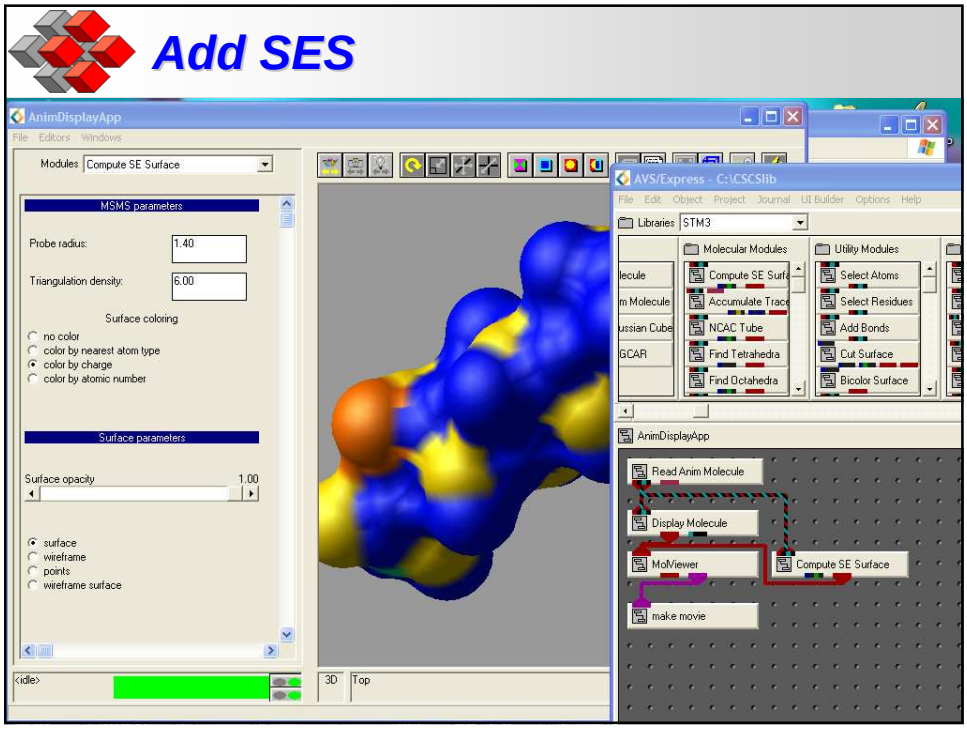
Dynamic structures



Add backbone



Add SES



Context element for output

Goal

- Add context elements to the graphical scene to enhance output production

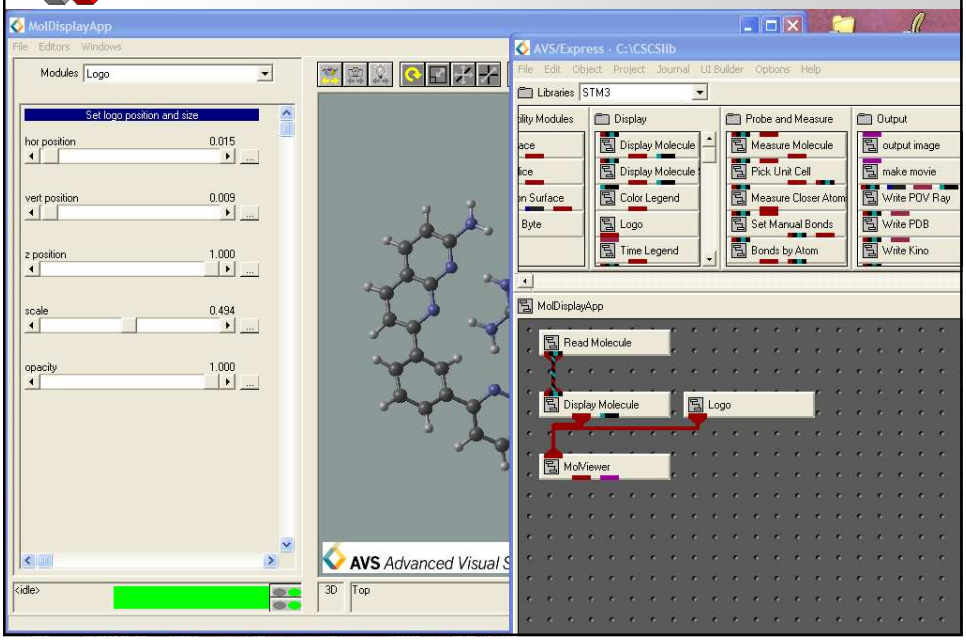
How

1. Instantiate MolDisplayApp
2. Load G-host.pdb
3. Add Logo
4. Add Color legend
5. Output image

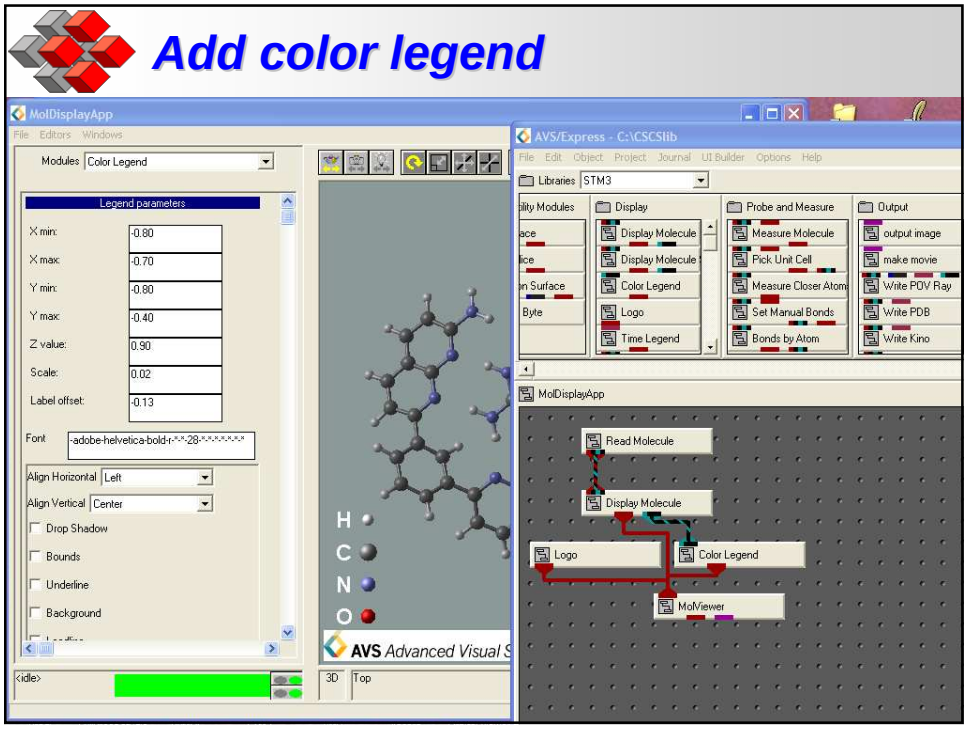
Bonus

1. Add BackgroundFade (under Main → Geometries)
2. Add TextTitle (idem)

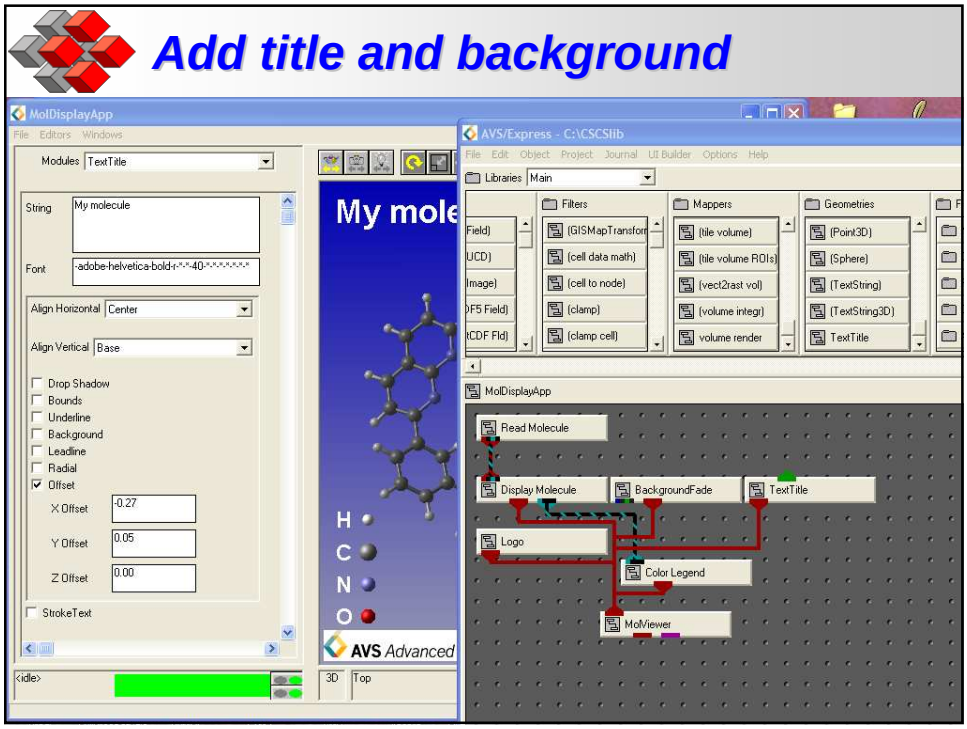
Add Logo

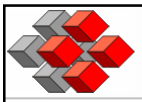


Add color legend



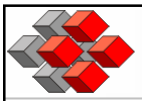
Add title and background





What is missing

- **Charges (file ice-melting.pdb)**
  - Color by charge
  - Threshold
- **Surfaces (file alanin.pdb)**
  - Cut
  - Bicolor surface
  - Surface values mapping
- **Selection (file 1A00.pdb)**
  - Select atoms and residues
  - Crop atoms
- **Interaction (file G-host.pdb)**
  - Pick atoms
- **Special techniques**
  - Traces (file T600unit.xyz)
  - Particle density (file ice-melting.pdb)
  - Velocity density
  - Scat to volume (file Condensation.pdb)
  - X-Ray factors (file 1485.res)



To summarize

- With STM3 you can concentrate on the chemistry, not on the visualization tool
- STM3 needs your creative ideas to grow
- Try it with your data