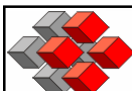


**✓ STM3 is composed by**

- A library of modules
- A new data type

**✓ AVS/Express provides:**

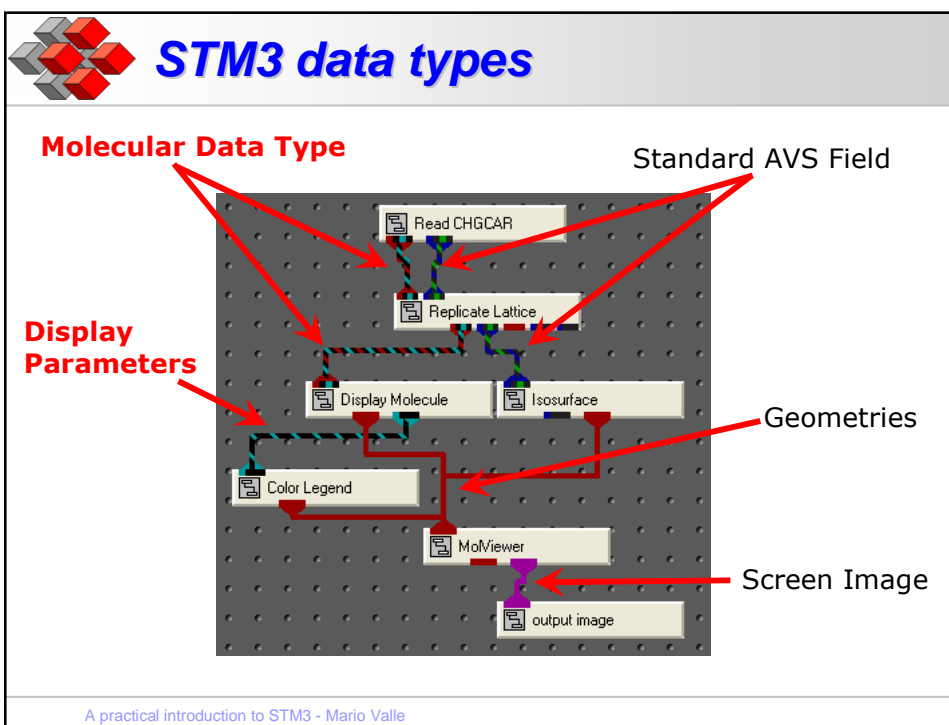
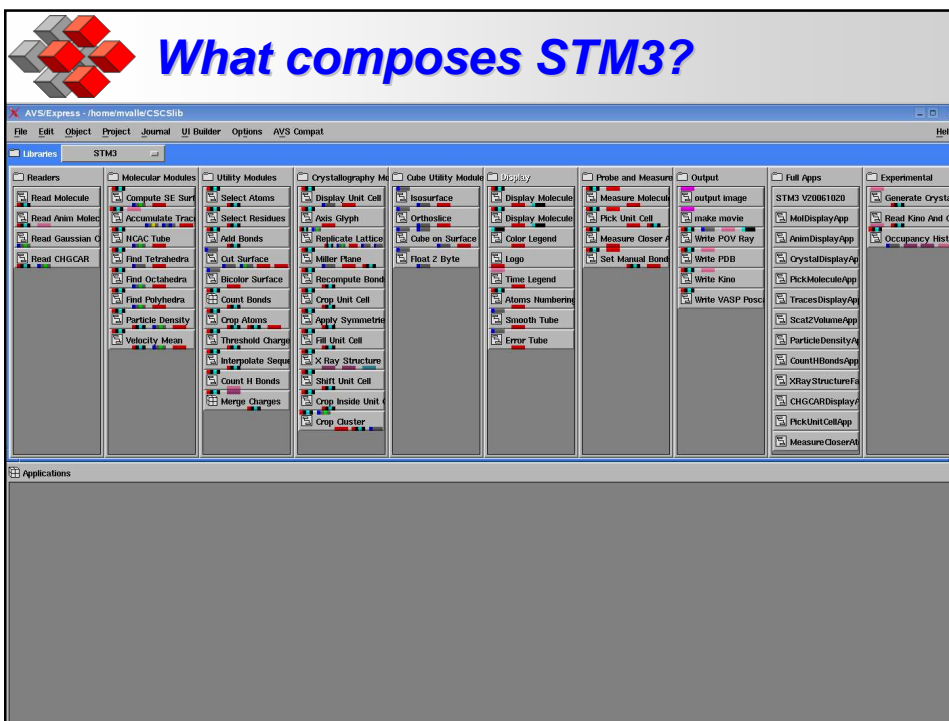
- Common visualization services and the NE
- Modularization
- Standard visualization techniques

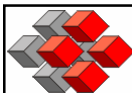


## Workshop Agenda


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

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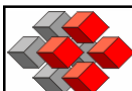




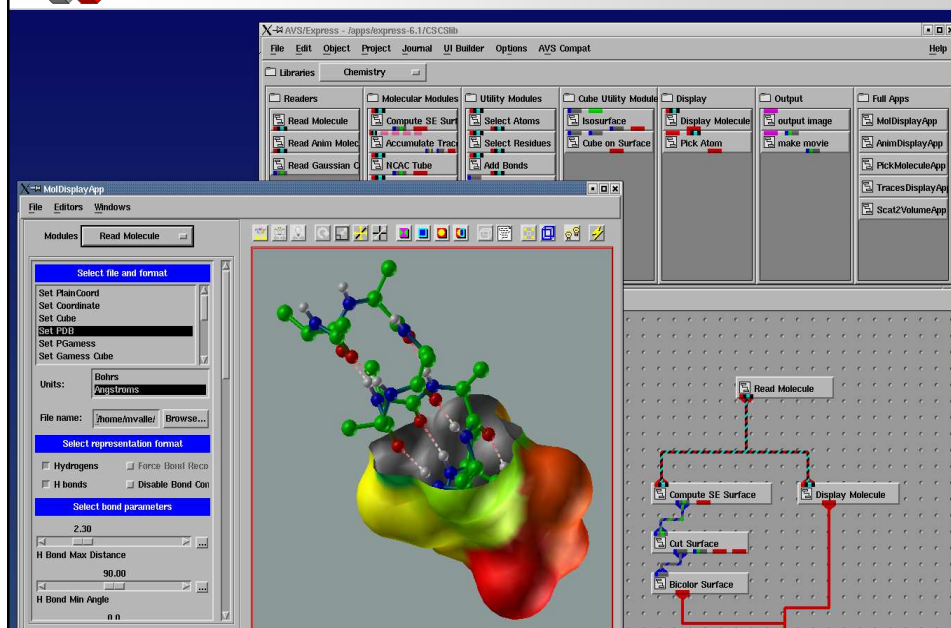
## Start STM3 (and 2" tutorial)

- 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.

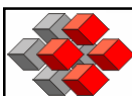
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## AVS/Express behind the scenes

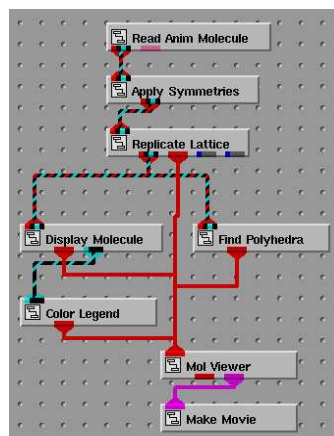


The screenshot displays the AVS/Express software interface. The main window shows a 3D molecular model of a protein-ligand complex. The interface includes a menu bar (File, Edit, Object, Project, Journal, UI Builder, Options, AVS Comput, Help) and a toolbar. On the left, there are several panels: 'Libraries' (Chemistry), 'Readers' (Read Molecule, Read Anim Molec, Read Gaussian C), 'Molecular Modules' (Compute SE Surf, Accumulate Trac, NCAC Tube, Add Bonds), 'Utility Modules' (Select Atoms, Select Residues), 'Cube Utility Module' (Isosurface, Cube on Surface), 'Display' (Display Molecule, Pick Atom), 'Output' (output image, make movie), and 'Full Apps' (MolDisplayApp, AnimDisplayApp, PickMoleculeApp, TracesDisplayApp, Scal2VolumeApp). The 'MolDisplayApp' window is open, showing a 'Modules' dropdown menu set to 'Read Molecule'. The 'Select file and format' section includes options for 'Set PlainCoord', 'Set Coordinate', 'Set Cube', 'Set PDB', 'Set PGness', and 'Set Gaussess Cube'. The 'Units' section shows 'Bohrs' and 'Angstroms'. The 'File name' field contains 'home/mvalle'. The 'Select representation format' section has checkboxes for 'Hydrogens', 'Force Bond Recs', 'H bonds', and 'Disable Bond Con'. The 'Select bond parameters' section shows '2.30' for 'H Bond Max Distance', '90.00' for 'H Bond Min Angle', and 'n n' for 'H Bond Min Angle'.

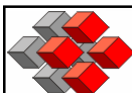


## AVS/Express applications

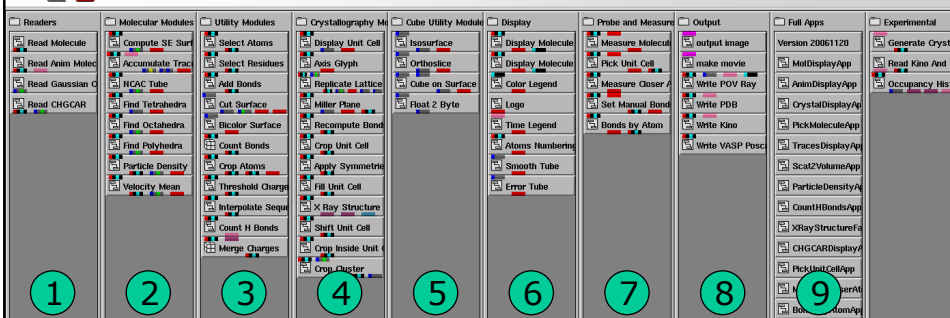
- Each module starts when receives all the needed data
- An application can use STM3 and standard AVS/Express modules together
- Connection ports (popup gives info and help)
- Colors related to data type
- The user interface automatically docks in the right place



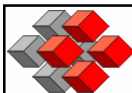
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## STM3 modules



- Readers for various, static and dynamic, chemical file formats
- Modules that compute various derived structures
- Manipulation of molecules, like atom selection
- Unit cells, periodic lattices and symmetries support
- Volumetric data visualization and manipulation
- Final rendering of molecular data and legends
- Probe, interaction and measurements
- Output to image files, movies and other formats
- 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>

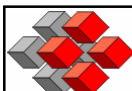
- **A (marketing) brochure on AVS/Express**

[http://www.avs.com/software/soft\\_t/avsxps.html](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>

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## 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**

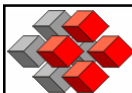
- It is more a LEGO construction box
- More power and flexibility comes at the expense of no point-and-click interface

- **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

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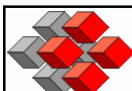




## Before starting: STM3 evolution

- 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

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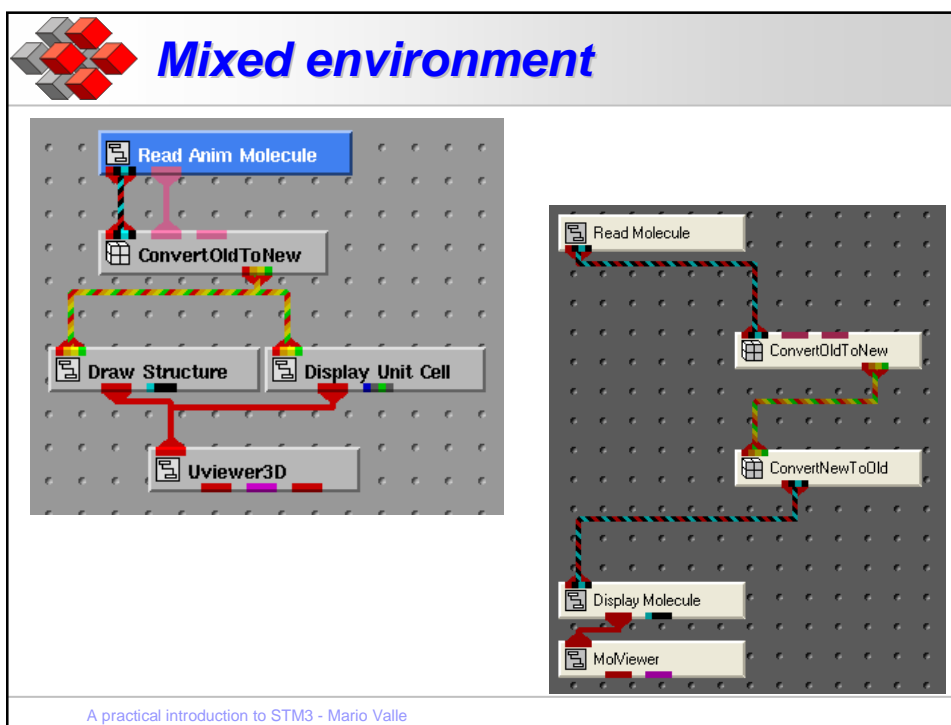
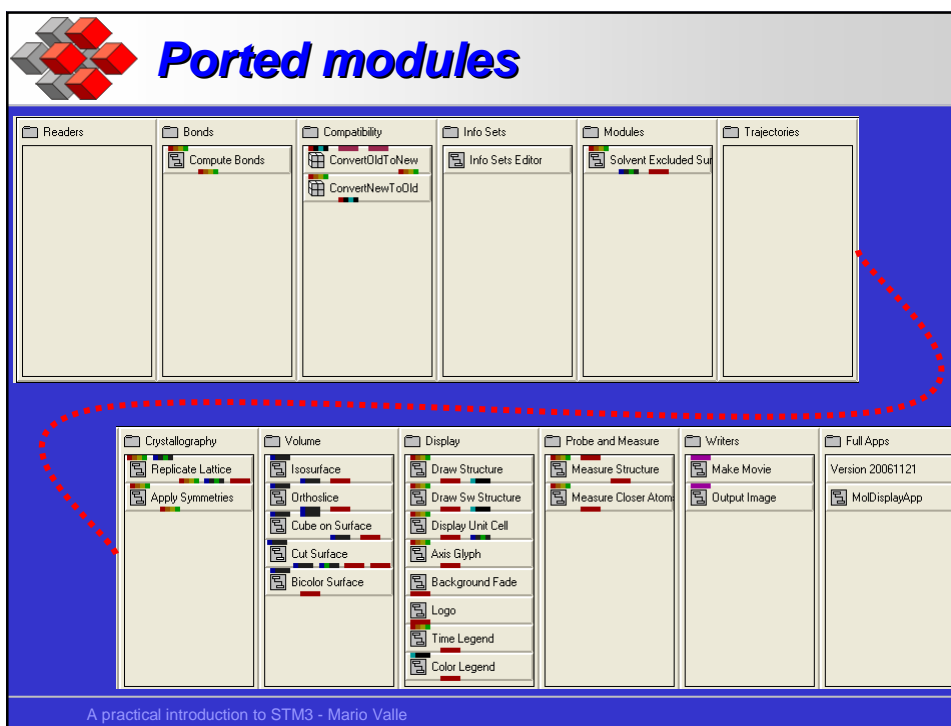
## Ported STM3 modules

Readers	Molecular Modules	Utility Modules	Crystallography Modules	Cube Utility Module	Display	Probe and Measure	Output	Full Apps	Experimental
<input checked="" type="checkbox"/> Read Molecule	<input checked="" type="checkbox"/> Compute SE Sur	<input checked="" type="checkbox"/> Select Atoms	<input checked="" type="checkbox"/> Display Unit Cell	<input checked="" type="checkbox"/> Isosurface	<input checked="" type="checkbox"/> Display Molecule	<input checked="" type="checkbox"/> Measure Molecule	<input checked="" type="checkbox"/> output image	<input checked="" type="checkbox"/> Version 20061120	<input checked="" type="checkbox"/> Generate Crystal
<input checked="" type="checkbox"/> Read Anim Molec	<input checked="" type="checkbox"/> Accumulate Trac	<input checked="" type="checkbox"/> Select Residues	<input checked="" type="checkbox"/> Axis Glyph	<input checked="" type="checkbox"/> Orthoslice	<input checked="" type="checkbox"/> Display Molecule	<input checked="" type="checkbox"/> Pick Unit Cell	<input checked="" type="checkbox"/> make movie	<input checked="" type="checkbox"/> MailDisplayApp	<input checked="" type="checkbox"/> Read Kino And C
<input checked="" type="checkbox"/> Read Gaussian C	<input checked="" type="checkbox"/> NCAC Tube	<input checked="" type="checkbox"/> Add Bonds	<input checked="" type="checkbox"/> Replicate Lattice	<input checked="" type="checkbox"/> Cube on Surface	<input checked="" type="checkbox"/> Color Legend	<input checked="" type="checkbox"/> Measure Closer	<input checked="" type="checkbox"/> Write POV Ray	<input checked="" type="checkbox"/> AnimDisplayApp	<input checked="" type="checkbox"/> Occupancy Histo
<input checked="" type="checkbox"/> Read CHGCAR	<input checked="" type="checkbox"/> Find Tetrahedra	<input checked="" type="checkbox"/> Cut Surface	<input checked="" type="checkbox"/> Miller Plane	<input checked="" type="checkbox"/> Float 2 Byte	<input checked="" type="checkbox"/> Logo	<input checked="" type="checkbox"/> Set Manual Bond	<input checked="" type="checkbox"/> Write PDB	<input checked="" type="checkbox"/> CrystalDisplayAp	
	<input checked="" type="checkbox"/> Find Octahedra	<input checked="" type="checkbox"/> Bicolor Surface	<input checked="" type="checkbox"/> Recalculate Bonds		<input checked="" type="checkbox"/> Title Legend	<input checked="" type="checkbox"/> Bonds by Atom	<input checked="" type="checkbox"/> Write Kino	<input checked="" type="checkbox"/> PickMoleculeApp	
	<input checked="" type="checkbox"/> Find Polyhedra	<input checked="" type="checkbox"/> Count Bonds	<input checked="" type="checkbox"/> Crop Unit Cell		<input checked="" type="checkbox"/> Atoms Humberbox		<input checked="" type="checkbox"/> Write VASP Posc	<input checked="" type="checkbox"/> TracesDisplayApp	
	<input checked="" type="checkbox"/> Particle Density	<input checked="" type="checkbox"/> Crop Atoms	<input checked="" type="checkbox"/> Apply Symmetry		<input checked="" type="checkbox"/> Smooth Tube			<input checked="" type="checkbox"/> Scat2VolumeApp	
	<input checked="" type="checkbox"/> Velocity Mean	<input checked="" type="checkbox"/> Threshold Charge	<input checked="" type="checkbox"/> Fill Unit Cell		<input checked="" type="checkbox"/> Error Tube			<input checked="" type="checkbox"/> ParticleDensityAp	
		<input checked="" type="checkbox"/> Interpolate Sequ	<input checked="" type="checkbox"/> X Ray Structure					<input checked="" type="checkbox"/> CountHBondsApp	
		<input checked="" type="checkbox"/> Count H Bonds	<input checked="" type="checkbox"/> Shift Unit Cell					<input checked="" type="checkbox"/> XRayStructuresFa	
		<input checked="" type="checkbox"/> Merge Charges	<input checked="" type="checkbox"/> Crop Inside Unit					<input checked="" type="checkbox"/> CHGCARDisplayAp	
			<input checked="" type="checkbox"/> Crop Cluster					<input checked="" type="checkbox"/> PickUnitCellApp	
								<input checked="" type="checkbox"/> MeasureCloserAt	
								<input checked="" type="checkbox"/> BondsByAtomApp	

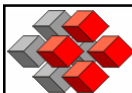
- ☒ Ported
- ☐ Not ported
- ☐ Working on

Updated 2006-12-01

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## Look at a static structure

### Goal

- Look at a static structure experimenting with various rendering modes

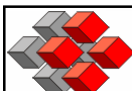
### How

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

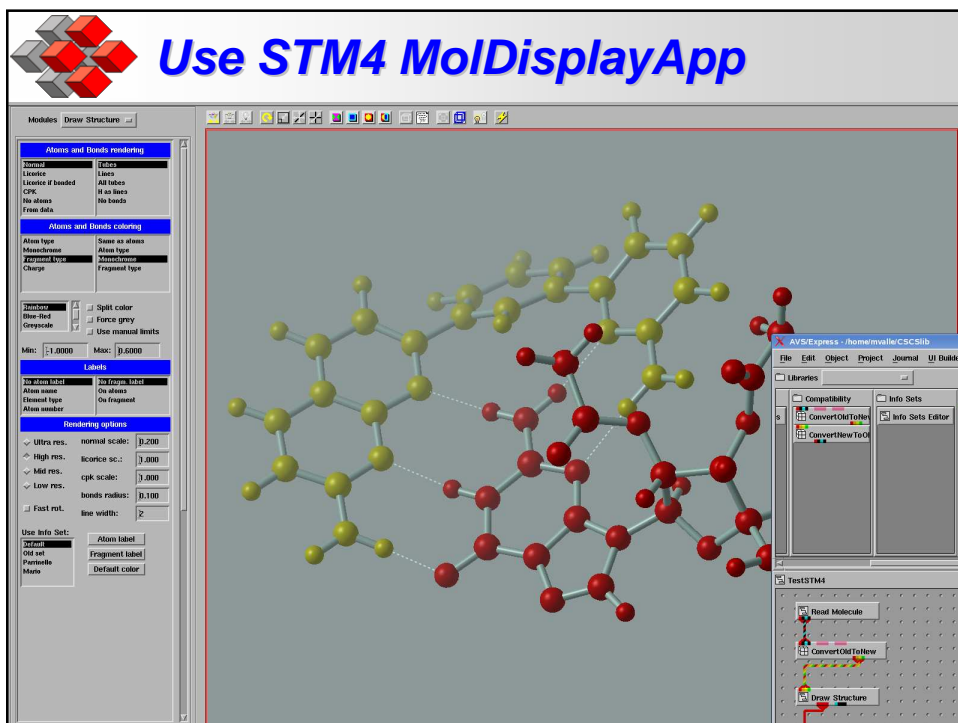
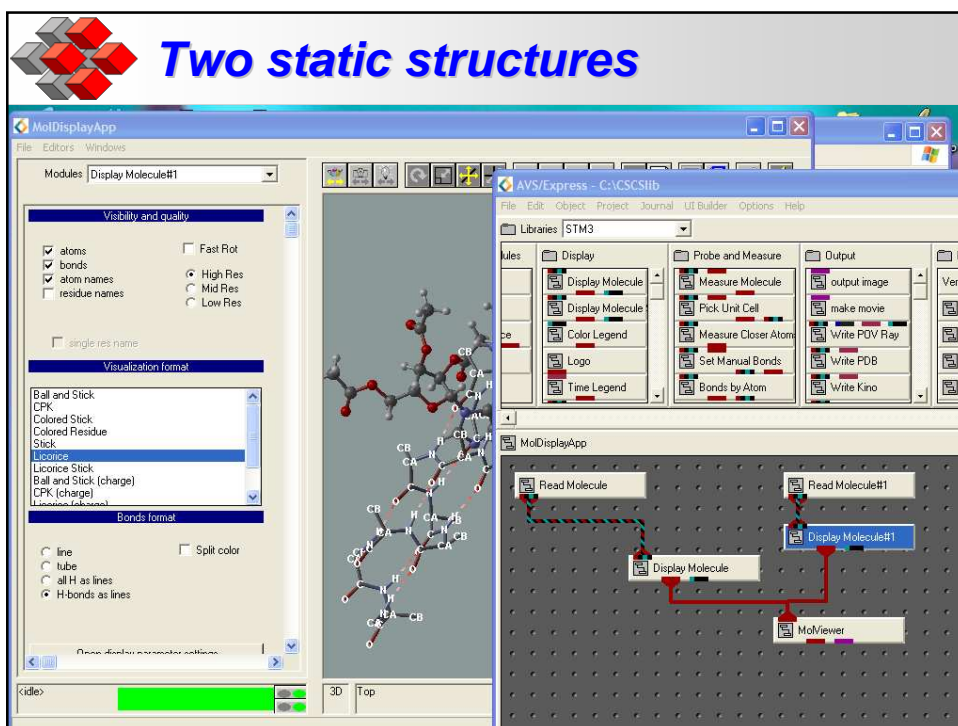
### Bonus

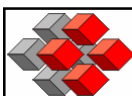
1. Add a second molecule
2. Try the STM4 MolDisplayApp

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## Look at a static structure





## Crystallography support

### Goal

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

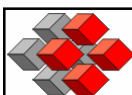
### How

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

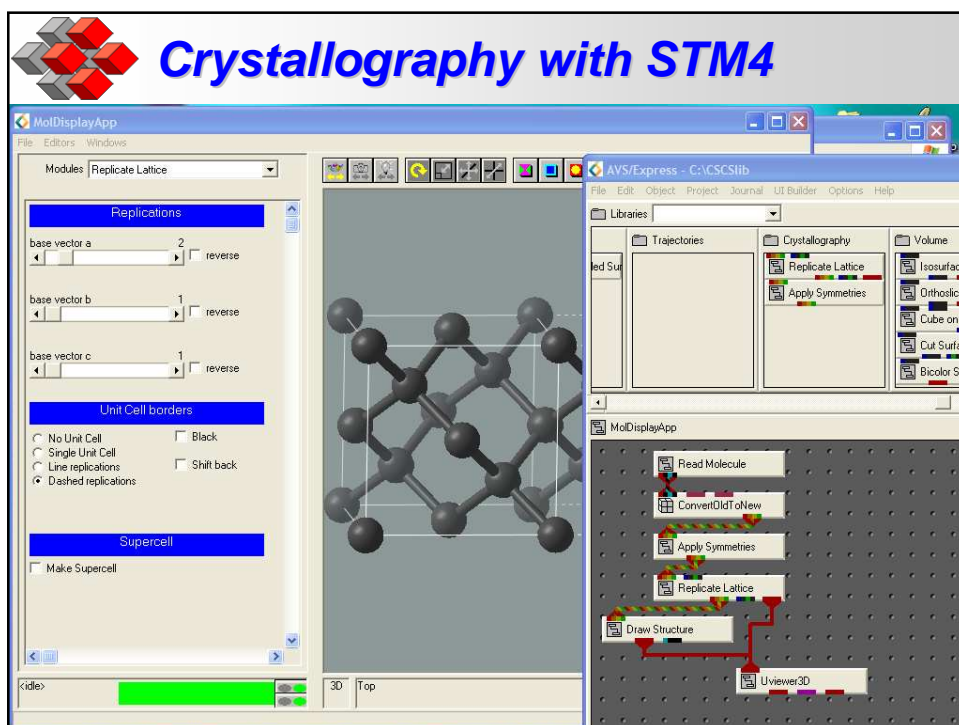
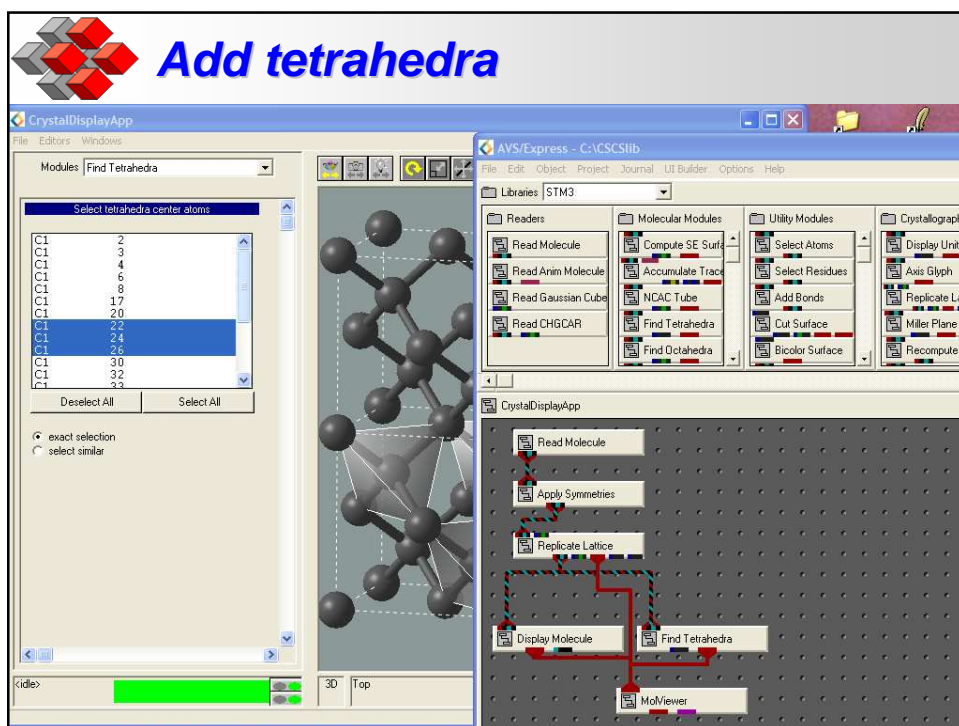
1. Add tetrahedra
2. Build the same network in STM4 starting from MolDisplayApp
3. What are the differences between STM3 and STM4 versions?

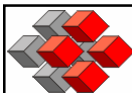
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## Crystallography support

The screenshot displays the CrystalDisplayApp interface. On the left, a 'Modules | Read Molecule' panel is active, showing a list of file formats (DMOLXYZ, Mopac ESP, MopacXYZ, mol2, mol, Chem3D, mm3, SHELX) with SHELX selected. Below this, there are fields for 'Units' (Bohrs, Angstroms), 'File name' (D:\ChemData\STM), and 'Select bonds computation type' (Hydrogens, H bonds, Free Bond Recomp, Freeze bonds). Further down, 'Select bond parameters' includes 'all interface' and 'Greedy bonding' options, along with 'Bonding Range Adjustment (%)' and 'H Bonding Range Adjustment (%)' sliders. The central 3D view shows a ball-and-stick model of a molecular structure. On the right, the 'AVS/Express - C:\CSCStib' window is open, showing a 'Libraries | STM3' panel with various tools like 'Display Molecule', 'Measure Molecule', 'Pick Unit Cell', 'Measure Closer Atoms', 'Set Manual Bonds', 'Bonds by Atom', 'output image', 'make movie', 'Write POV Ray', 'Write PDB', and 'Write Kino'. At the bottom right, a 'CrystalDisplayApp' window shows a workflow diagram with steps: 'Read Molecule', 'Apply Symmetries', 'Replicate Lattice', 'Display Molecule', and 'MolViewer'.





## Volumetric data

### Goal

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

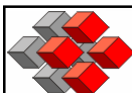
### How

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

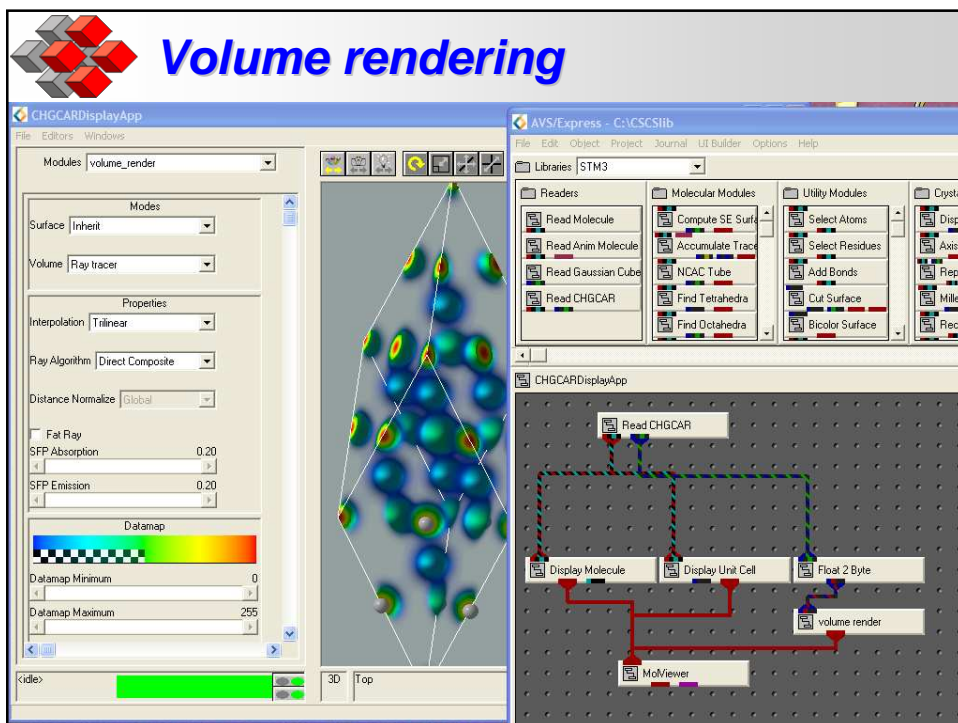
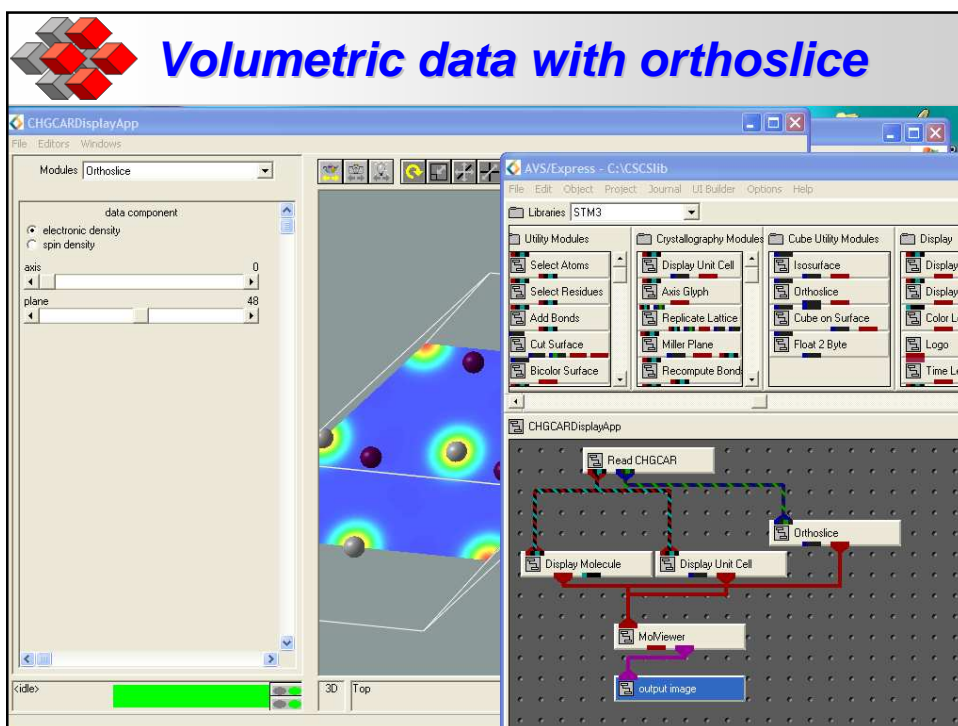
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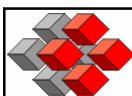


## Volumetric data

The screenshot displays two software windows. The left window, titled 'CHGCARDisplayApp', features a 'Modules' dropdown set to 'Isosurface'. It includes controls for 'iso component' (radio buttons for 'electronic density' and 'spin density'), an 'iso level' slider set to 481.96, and checkboxes for 'map components' (electronic density, spin density) and 'map cell components'. The central 3D view shows a molecular structure with green isosurfaces. The right window, 'AVS/Express - C:\CSCSlib', shows a 'Libraries' dropdown set to 'STM3' and a 'Modules' panel with categories like Readers, Molecular Modules, Utility Modules, and Crystals. The 'CHGCARDisplayApp' window is also visible in the background, showing a workflow diagram with modules like 'Read CHGCAR', 'Display Molecule', 'Display Unit Cell', and 'MoViewer'.







## Dynamic structures

### Goal

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

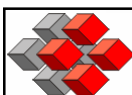
### How

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-C $\alpha$ -C tube (backbone) and change its color
2. Compute the Solvent Excluded Surface (does not work on Mac)

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## Dynamic structures

AnimDisplayApp

File Editors Windows

Modules | Read Anim Molecule Loop

☐ Run ☐ Run Backwards  
☐ Step ☐ Step Backwards  
☐ Reset ☐ Reset Back

Cycle Options: Once

Start Value: 1  
End Value: 1  
Increment: 1  
Loop count: 1

AVS/Express - C:\CSCSlib

File Edit Object Project Journal UI Builder Options Help

Libraries: STM3

Display Molecule  
Color Legend  
Logo  
Time Legend

Probe and Measure  
Measure Molecule  
Pick Unit Cell  
Measure Closer Atom  
Set Manual Bonds  
Bonds by Atom

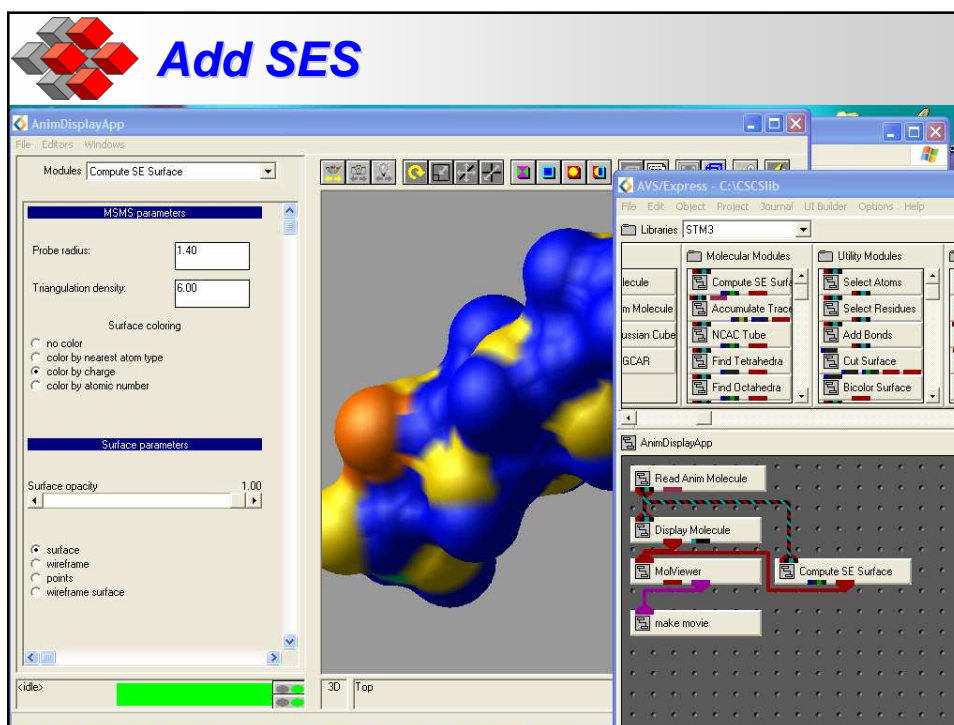
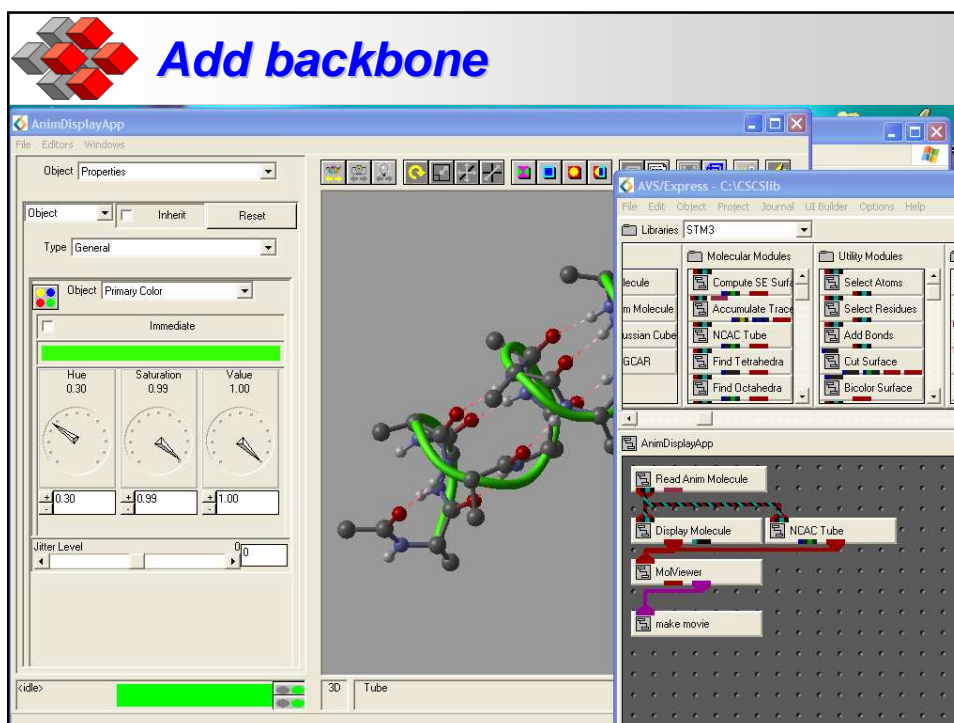
Output  
output image  
make movie  
Write POV Ray  
Write PDB  
Write Kino

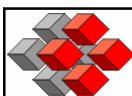
AnimDisplayApp

Read Anim Molecule  
Display Molecule  
MolViewer  
make movie

<idle> 3D Top







## Context element for output

### Goal

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

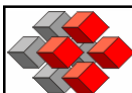
### How

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)

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## Add Logo

The screenshot displays the AVS/Express software interface. On the left, the 'MolDisplayApp' window is open, showing a 3D molecular model of a crystal structure. The 'Modules' list on the left includes 'Logo'. The 'Set logo position and size' panel on the right shows parameters: hor position (0.015), vert position (0.009), z position (1.000), scale (0.494), and opacity (1.000). The 'AVS/Express' main window is on the right, showing a 'Libraries' list with 'STM3'. The 'Display' module is selected, and the 'Logo' module is visible in the 'Display' list. The 'Output' module is also visible, with 'output image' selected. The 'MolDisplayApp' window is in the foreground, showing the 3D molecular model and the 'Logo' module in the 'Display' list.

## Add color legend

The screenshot shows the AVS/Express interface with the 'MolDisplayApp' project open. The 'Color Legend' module is added to the 'Display' group. The 'Legend parameters' panel is visible, showing settings for X, Y, Z, and Scale. The 'Color Legend' module is connected to the 'Display Molecule' module.

**Legend parameters:**

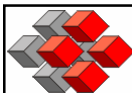
- X min: -0.80
- X max: -0.70
- Y min: -0.80
- Y max: -0.40
- Z value: 0.90
- Scale: 0.02
- Label offset: -0.13
- Font: adobe-helvetica-bold-12-28-xxxxxx
- Align Horizontal: Left
- Align Vertical: Center
- Drop Shadow: ☐
- Bounds: ☐
- Underline: ☐
- Background: ☐

## Add title and background

The screenshot shows the AVS/Express interface with the 'MolDisplayApp' project open. The 'BackgroundFade' and 'TextTitle' modules are added to the 'Display' group. The 'TextTitle' module is connected to the 'Display Molecule' module.

**TextTitle parameters:**

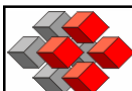
- String: My molecule
- Font: adobe-helvetica-bold-12-40-xxxxxx
- Align Horizontal: Center
- Align Vertical: Base
- Drop Shadow: ☐
- Bounds: ☐
- Underline: ☐
- Background: ☐
- Leadline: ☐
- Radial: ☐
- Offset: ☒
  - X Offset: -0.27
  - Y Offset: 0.05
  - Z Offset: 0.00
- StrokeText: ☐



## 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)

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## 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

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