

STM3: a chemistry visualization platform

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Received July 5, 2004; accepted July 30, 2004

*Chemical visualization / Integration platform /
STM3 Computer code / Computational crystallography*

Abstract. To support CSCS research users we built STM3, a software platform on which advanced chemistry visualization techniques can be integrated. Its main goal is not to replace existing tools, but to provide functionalities not covered by them. STM3's unusual characteristic among chemistry visualization tools is its ability to combine chemistry and general visualization techniques in the same view. STM3 is built on top of a proven visualization environment (AVS/Express) that lets CSCS's visualization staff concentrate its efforts on developing new technologies rather than investing time on graphical and user interface implementation issues.

Introduction

CSCS is the Swiss National Supercomputing Centre that provides, develops and promotes technical and scientific services for the Swiss research community on the fields of high-performance and high-throughput computing.

Researchers in the Molecular Dynamics and Crystallography areas master very well standard visualization tools and produce by themselves their images and animations. To go beyond any routine processing of their data, they are invited by the CSCS staff to propose new visualization scenarios, which we develop under their supervision.

To support those users and to collect and reuse the new functionalities already created for them, we decided to build a framework in which more *esoteric* or *unusual* features can be quickly prototyped and implemented without replicating all the functionalities of standard chemistry visualization packages such as VMD [1], RasMol [2], gOpenMol [3], etc. The STM3 web page [4] provides some examples of those unusual functionalities.

Another important decision taken has been to avoid developing everything from scratch, but instead to integrate chemistry specific modules inside AVS/Express [5], a commercial visualization environment. AVS/Express is a very powerful programming environment that combines state-of-the-art data visualization algorithms with advanced

graphics and animation tools. The added modules follow the same architecture and rely on the same data model as the native visualization components. The development effort is thus minimal.

This strategy brings us three important benefits: 1) we can concentrate on the solution of chemistry problems delegating the rendering and visualization support to the specialized base tool (AVS/Express); 2) we base our development efforts on the *rapid prototyping* features of AVS/Express to enable efficient and close collaboration with our users; 3) the user choices are not restricted to functionalities specific to crystallography or molecular dynamics; they can also use standard visualization techniques from other fields like Computational Fluid Dynamics [6, 7] (see Fig. 3).

This platform has been called STM3 to recall its origins. In 2001 the *See The Molecule* project (a.k.a. STM) [8] was made available to the AVS community at the International AVS Center [9] by Ken Flurchick et al. of the North Carolina Supercomputing Center. STM3 reuses the project idea and some of its readers' code, but its overall structure has been completely reengineered. And, by the way, STM acronym has nothing to do with Scanning Tunneling Microscopy.

Visualization

Architecture

STM3 is built inside AVS/Express and so shares its application architecture. An application is built in AVS/Express selecting modules from a set of libraries and dragging them to a working area (Fig. 1). Each module implements a specific visualization technique or data transform algorithm. The modules are connected together to form a network. Data of a specific type are shared on each connection. Each module starts executing as soon as its input data is valid. This paradigm lets the user concentrate on problem solving issues instead of technical program structure problems. AVS/Express provides also everything related to graphical rendering (lights, surface properties, stereo and immersive visualization support) and user interaction (position manipulation and object picking). Another service provided is the creation of movies and images.

STM3 integrates in this architecture its set of modules and adds a data type that describes atomic structures to

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connect them (i.e. a new connection type). Atomic structures are rendered in various selectable forms: ball&stick, licorice, colors related to atom type or charge, H-bonds, etc. Other structures of interest to crystallography, like tetrahedra and octahedra, are rendered as graphical objects with selectable color and transparency.

Standard visualization modules can be used together with STM3 ones. They operate on Gaussian [12] cube data or on non chemical data, like fluid dynamic solvers output. An example of this kind of integration is the already cited [6]. There are no predefined limits on the number of structures that can be visualized together.

Data formats

STM3 provides readers for various common chemistry file formats. Static formats accepted are PDB [11], Gaussian Cube, SHEL-X [13], VASP [14] and less common ones like GAMESS, MOL and CHEM-3D. For dynamic trajectories, STM3 can read various forms of multi frame PDB, DCD [15], DL_POLY [16], VASP and some in house formats.

Other formats can be easily integrated if the need arise and if the format is sufficiently documented. In addition,

we have the freedom to ‘tune’ some readers to the idiosyncrasies of local format usage.

Services offered

Roughly speaking, the STM3 modules can be subdivided in various areas (the complete list is on [4]): picking of atoms with measurement of distances, angles and torsion angles (an example is visible in Fig. 1). Structure selection and cropping (atoms and residues). Crystallography support (symmetries, unit cells and replications, structure visualization, planes). Organic chemistry (molecular surfaces and skeletons). Molecular dynamics (trajectory interpolation, traces). Special functions (volumetric density, bonds count).

To simplify common visualization tasks a set of pre-built applications is provided.

Output formats

STM3 is mainly used as an exploratory tool in which the user interacts with the on screen visualization. Nevertheless, at the end of a study high quality images and animations are often needed.

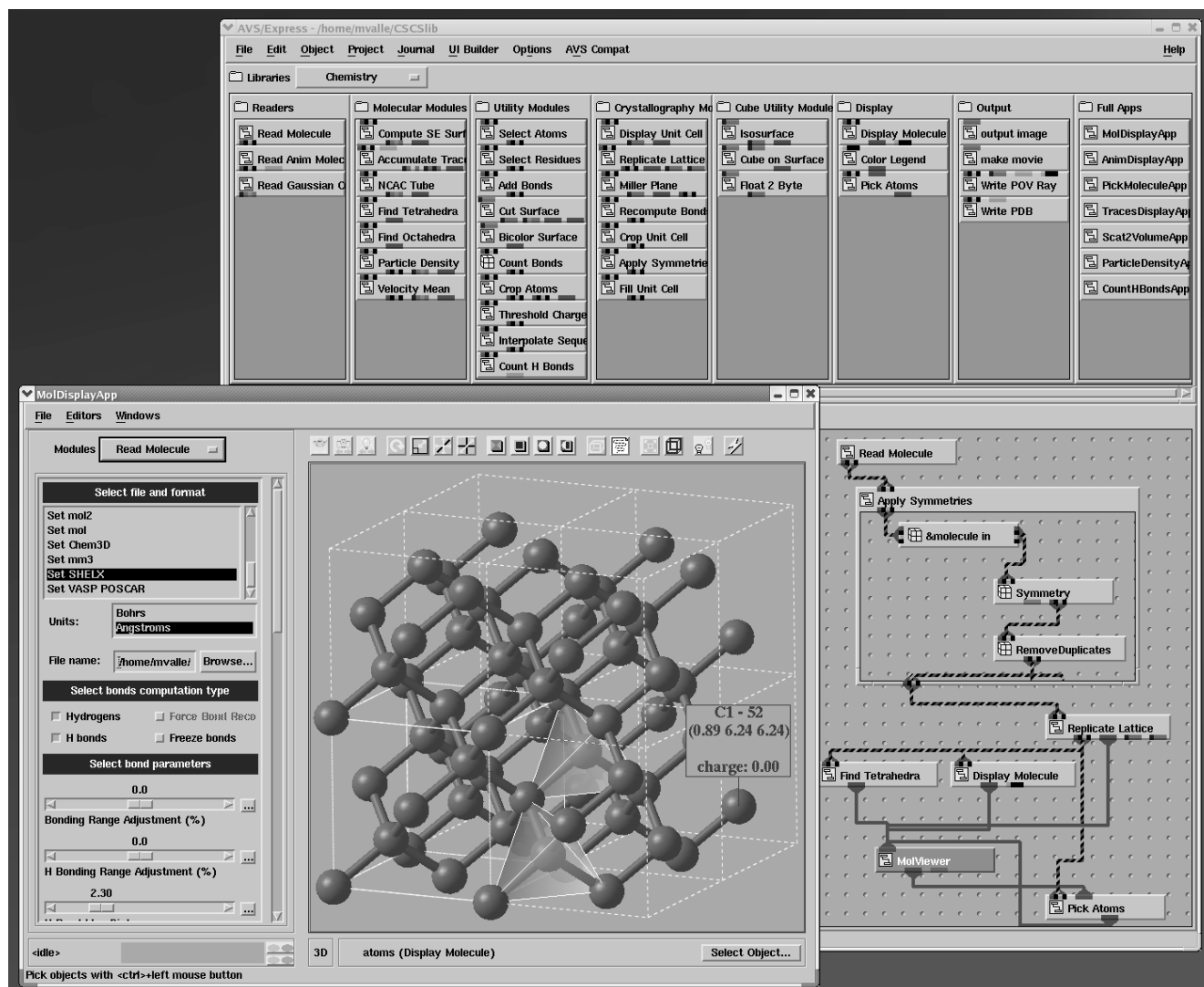


Fig. 1. STM3 toolkit inside AVS/Express. Visible are the library of modules (top), the programming area (right) and the viewer with modules user interface (left).

STM3 can save the visualization as high quality images, or can output a scene for raytraced PovRAY [10] offline rendering. Animations can be saved as MPEG or AVI movies.

To support future development of structure editing, a writer of PDB format files is provided.

Implementation

STM3 code is written in portable C++ and is freely available in source and precompiled form. The underlying AVS/Express framework guarantees its portability to various platforms: Linux, Windows, standard Unix and Mac, but to date STM3 specific code has been tested only on Linux, Windows and SGI IRIX.

STM3 uses the Library for Approximate Nearest Neighbor Searching (ANN) [17] for bonds computation and SgInfo [18] for symmetries. STM3 integrates also external tools for specific functions: the first one has been MSMS [19] to compute molecular surfaces.

Some use cases

STM3 is present behind the scene in various papers and scientific works. Here are just some examples that highlight the tool philosophy; other examples can be found on the STM3 web page [4].

The work of Churakov and Wunder [20] visualize the spatial distribution of the positions occupied by H in a topaz crystal using volume rendering techniques (Fig. 2). The module developed specifically for this work has been generalized and now is available to all STM3 users. Werder [6] uses an iterative method to model flow around a carbon nanotube that switches between a continuous fluid dynamic solution and an atomistic one. Visualization relies

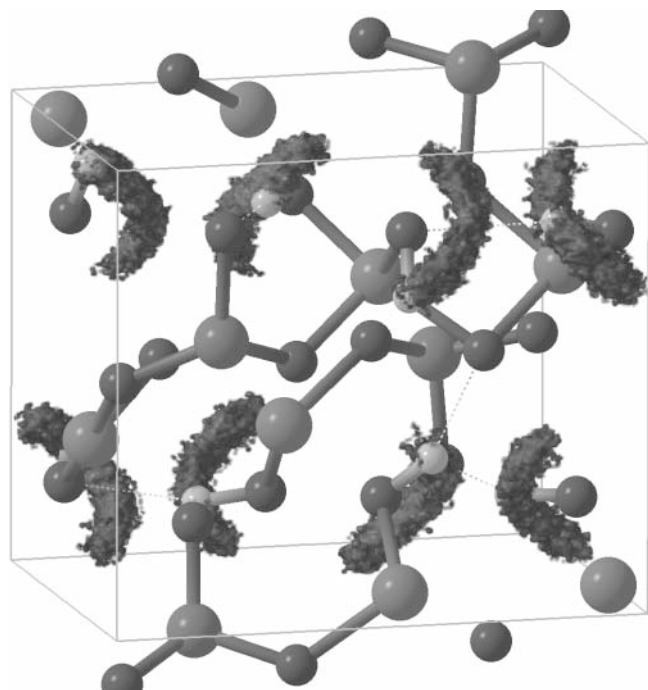


Fig. 2. Atom position traces visualization.

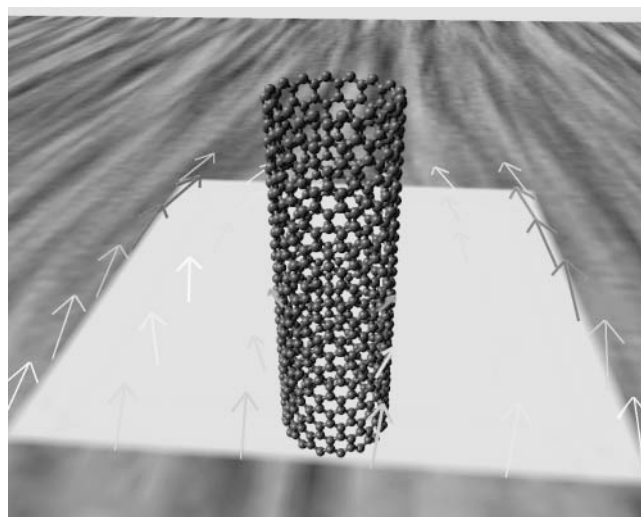


Fig. 3. An example of integration between STM3 molecule rendering and continuous vector field visualization (from [7]). The hole is the domain of the atomistic solution.

on the STM3 ability to integrate chemistry and general visualization techniques (Fig. 3).

Conclusions and future work

STM3 is constantly evolving based on user requests. STM3 main strength relies in offering integration support of unusual functionality instead of providing a rigid, pre-compiled set of functions. AVS/Express' support for rapid prototyping means that STM3's future evolution can be easily tailored based on user involvement.

On the other hand, this approach generates a steeper learning curve. We try to counteract this with user training and including a broader set of pre-built applications.

Planned developments are in the area of structure modeling and on simpler user interaction with the tool.

The code is freely available from the author. The only prerequisite is the installation and licensing of AVS/Express.

Acknowledgments. A special thanks to Jean Favre for first introducing the original STM at CSCS and for defining its development strategy.

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