



Good morning! I'm Mario Valle,  
I'm working at Swiss National  
Supercomputing Centre, and I'm not  
a chemists, but...



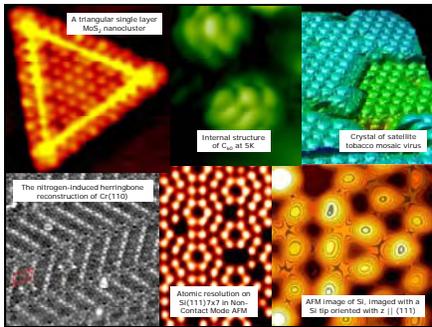
... I interact with various chemists  
and help various chemist groups.  
And I know that all of them are  
visual people.  
They love to scribble everywhere, to  
draw diagrams, to teach using  
images and models



They love to invent representations,  
to reason, to teach, to explain



Why?  
Why this love for visual  
representations?



Why? If today they can see the  
atoms.  
Like painting instead of  
photography: seems no low fidelity  
representation is needed anymore.



So why?  
Because it is not simple to see your  
object of study  
Because you use more  
computational chemistry, more  
numbers and less laboratory  
Because there are plenty of tools  
that help make data visible  
But over all considerations...

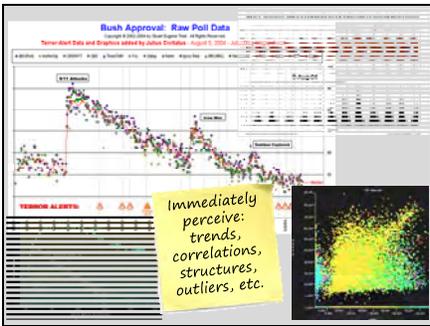




A supercomputer trained by million of years of difficult survival, when was “interesting” to spot barely visible predators.



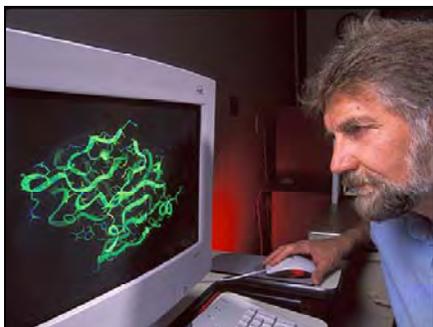
Today we do not spot predators, but we still immediately, without rational effort, see structures and regularities around us



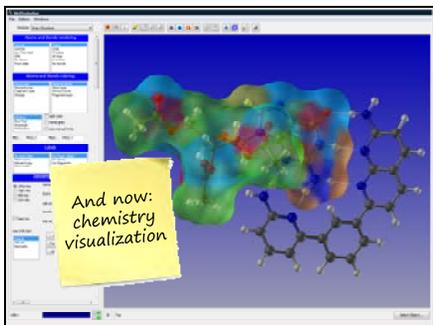
Regularities and structures hidden in our data...



...after the art of visualization  
adapts numbers...



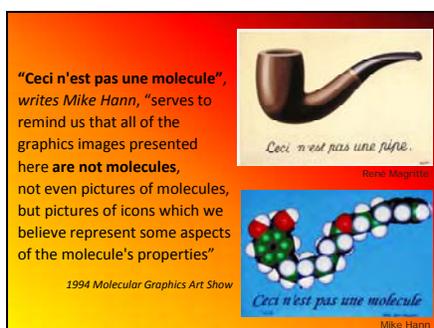
...to our perception



So, chemistry visualization.  
When we open a visualization tool  
to look at a molecule or see a  
beautiful image during a  
conference...



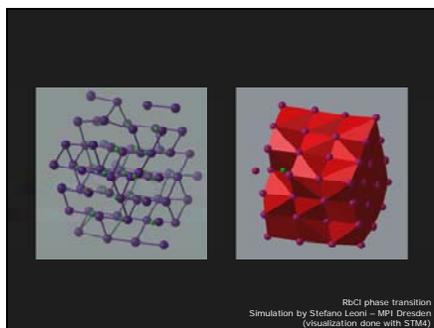
...do we think about what lies behind the image or behind a ball and stick representation?  
Do we think what else our tool should provide to make our research more effective?



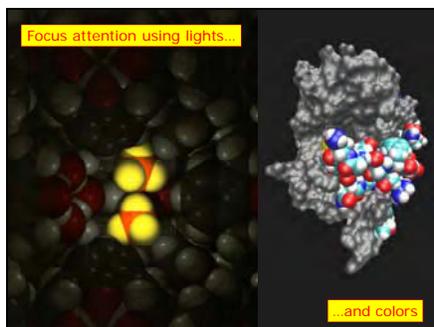
First we should remember that we are working with metaphors, graphical metaphors, not with something real.  
And metaphors give you a freedom not available in other visualization fields



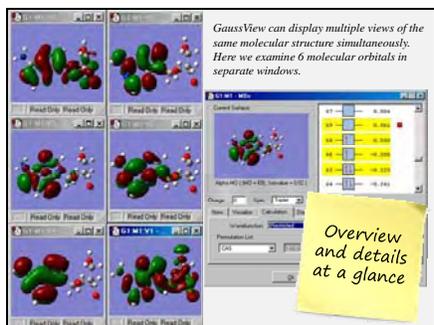
Freedom to remove unneeded details, distractions, irrelevant things to highlighting the important parts



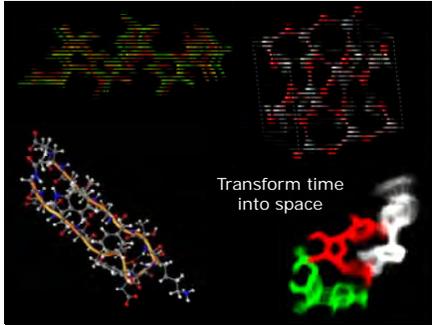
Graphical metaphors reveal non obvious things, like a crystal transition from cubic to octahedral. The two movie show exactly the same data, but how different the understanding!



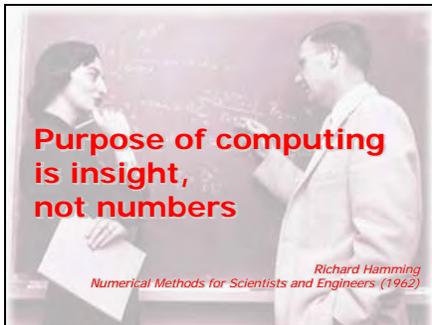
Colors and lights help focus attention



Tools support holistic view of your data. You can see all of them at a glance enabling comparison



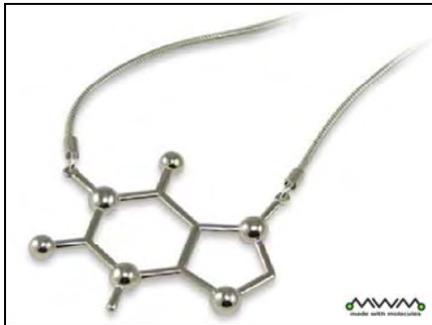
The same with time.  
Visualization let us transform time into space to look at the whole phenomena



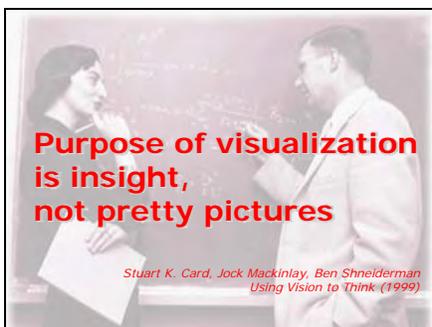
The goal is to understand. Don't forget this!  
Richard Hamming more than 40 years ago reminded us that the purpose of computing is to create insight, to make discoveries.



And visualization should facilitate the scientist's discovery work.  
Instead there are a lot of scientists that restrict its scope to only producing nice images for conferences or publications...



...or to produce jewelry. Nice, but...



...we tend to forget visualization as a discovery tool. Yes, communication is a valid role for visualization, but it is not the only one or the principal one. Paraphrasing Hamming, the visualization community try to remember us the role of visualization.



So, visualization helps insight, tools support visualization and chemists are avid consumers of graphical representations. So what should I expect from a visualization tool?



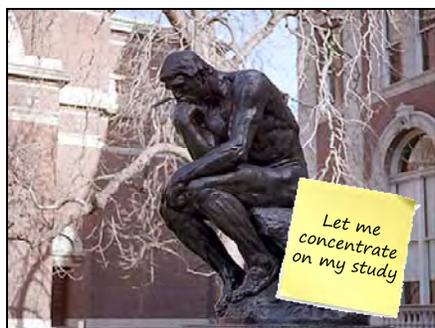
The tool, pardon, the discovery environment that I envision should let me play with the data, looking at them from various sides



The tools should adapt at my own discovery style and needs and not force me to adapt to the tool idiosyncrasies



A tool that helps manage may data, my reference sources and, why not, helps me to prepare my publications.



In conclusion, an environment that supports my research and help me concentrate on the science aspect of my study.



So in chemistry visualization I expect to find tools that support all this, tools that are at the forefront of visualization research. But also a quick survey show...

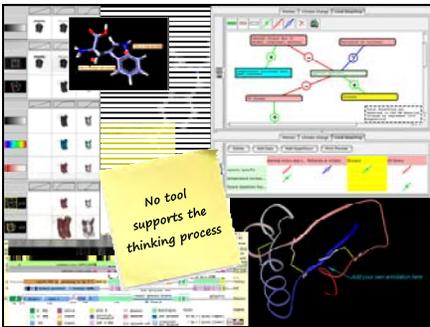


... that they lag behind!





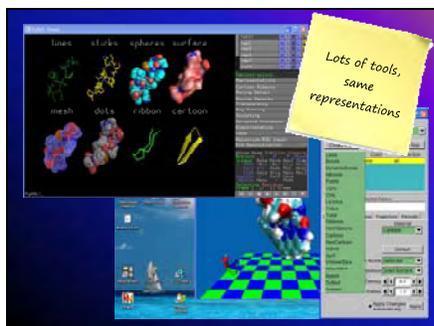
...and post-it based integration with the thinking process. Not to speak of paper databases and finger-pointing collaboration.



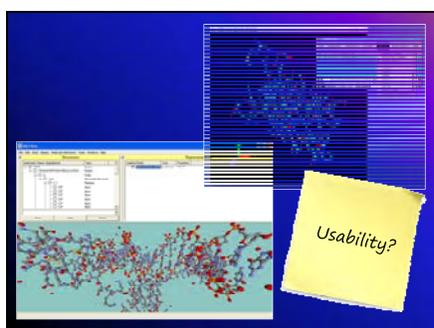
In this area tools are severely lacking. Even a simple thing like putting annotations is available only in some commercial tool. Never seen instead support to creativity or reasoning.



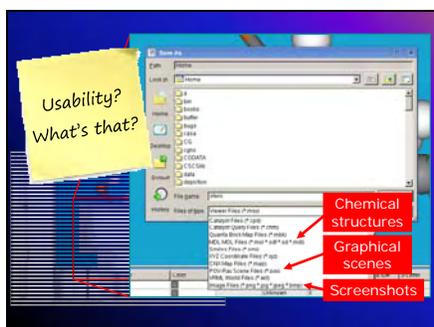
And then, conformity like a sheep's herd....



...tools provide almost exactly the same representations and the same functionalities



And interaction support? A tool should be almost invisible in my opinion.  
 But also very good tools like VMD needs two hand to navigate around a molecule  
 And tools for which the visual part seems not the most precious thing to show.  
 Not to speak of the 'Star Trek' graphical rendering.

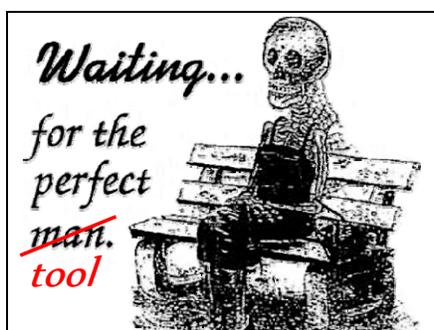


Interfaces that seems an heap of functionalities. Everything together. So why don't use a single menu labeled "Do" and put everything under it?



Last, but not least, the difficulties to understand data that various tools have.

Chemists are very creative in inventing data formats... without thinking of the consequences...



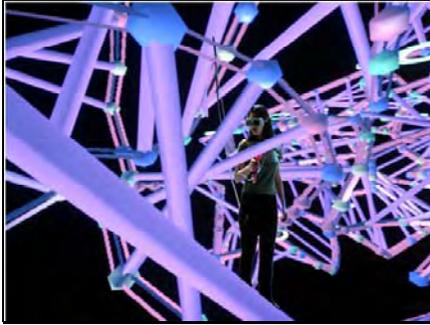
So what we can do?

Should we wait for the perfect tool?

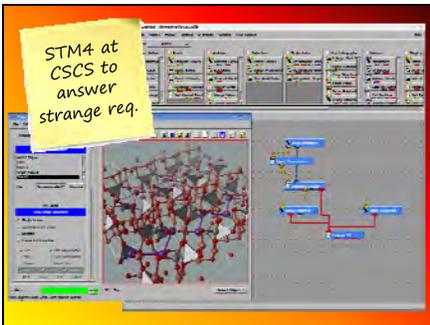
We can wait or we can help!



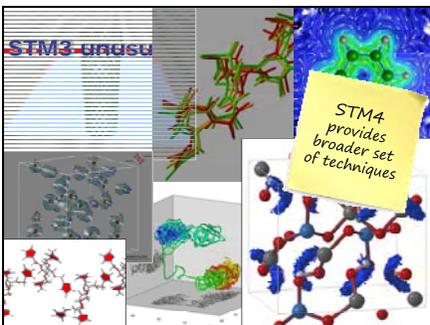
First, debunk myths!



You don't need CAVE, special hardware to improve the tool situation.  
First thing, you should teach and use visualization as a reasoning tool  
Teaching graphics grammar  
Using visualization to analyze your data  
Noting what is missing



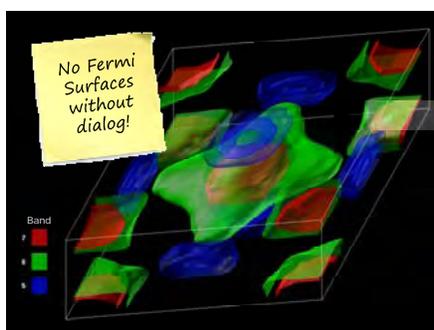
At CSCS I have developed an environment to implement ideas and requests from my users, not another visualization tool.



An environment that offers new data representations and unusual analysis tools.



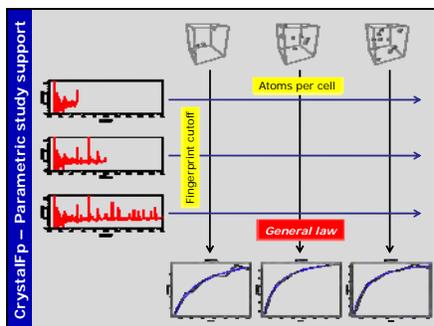
How STM4 grows?  
Speaking with chemists, putting together those two worlds that often do not speak.



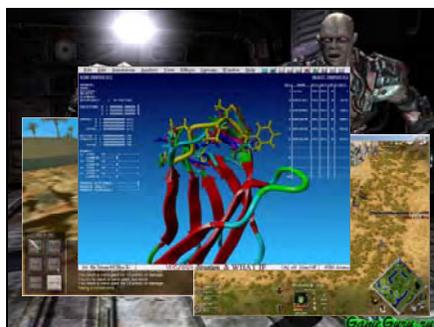
Exchanging knowledge, setting up collaborations, giving to viz people things to work on.  
For example Fermi surfaces in STM4 were added after a professor explained me what are they and why he needed them.



But tools could become better helper if we encourage research in unusual fields, games, new media, games, creativity.  
If we encourage contaminations between disciplines. If we think about our future users.



For example the research I'm involved right now mixes crystallography and high dimensional data analysis and requires parametric study visualization support.



Teachers, use your students videogames passion! Videogames let the gamer concentrate on the action without distractions, help them not to feel lost in their virtual worlds. So, why do not transfer this ideas to our visualization tools? Think about this.



In the meantime, use the existing tools! they are not perfect, but they help! Use them and collaborate to help us produce better visualization support for your research. The result maybe will not be perfect, but sure will be on the way to become more useful. Thank you!