

**CSCS**  
Swiss National Supercomputing Centre

# Beyond Ball-and-Stick

## What scientific visualization can do for chemistry users

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## Do you like this?

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## No! We pretend a lot of graphic

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## ChemViz current usage

Movies for conference talks

Nice images for publications

FRANCESCO GARAVIOLLO – ETH ZÜRICH

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## So why this tutorial?

Analysis of the current visualization usage in chemistry show it is limited to present results and common representations.

Today we will try to:

1. Go beyond visualization intended only as a method to produce nice images
2. Go beyond thinking that chemical visualization is exclusively ball-and-stick

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## How?

- Starting from visualization fundamentals and then applying to chemistry problems.
- Hearing your experiences, complains and requirements to shape the CSCS chemistry visualization offer

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## Tutorial agenda

- 13.30 – 14.20 **Part 1: Using vision to think**  
(how visualization can help your research)
- 14.20 – 14.50 **Workshop: New horizons with Horizon** (1<sup>st</sup> part)  
(collect current status of affairs) **Your input needed!**
- 14.50 – 16.00 **Part 2: Practical chemistry visualization**  
(some ideas on data and tools)
- 15.30 – 15.40 **Coffee Break**  
(how a good chat can help your research)
- 16.00 – 16.30 **Workshop: New horizons with Horizon** (2<sup>nd</sup> part)  
(what are your needs?) **Your input needed!**

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## What hopefully you will take home

1. New ideas that maybe give rise to new research directions and new work methodologies for you
2. Requests for new and interesting services from the CSCS Visualization Group

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## Resources

- <http://www.cscs.ch/~mvalle/ChemViz/#Tutorial2005>
  - Slides
  - Software pointers
  - Results from workshop
    - Be patient, not everything is already available.
    - Contributions and ideas are welcome
- General material on visualization  
<http://www.cscs.ch/~mvalle/visualization/>
- And you can contact me at: [mvalle@cscs.ch](mailto:mvalle@cscs.ch)

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**Let start!**