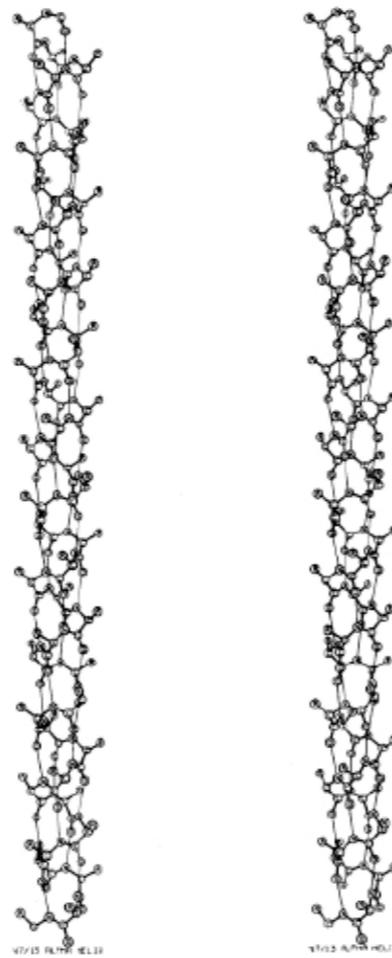
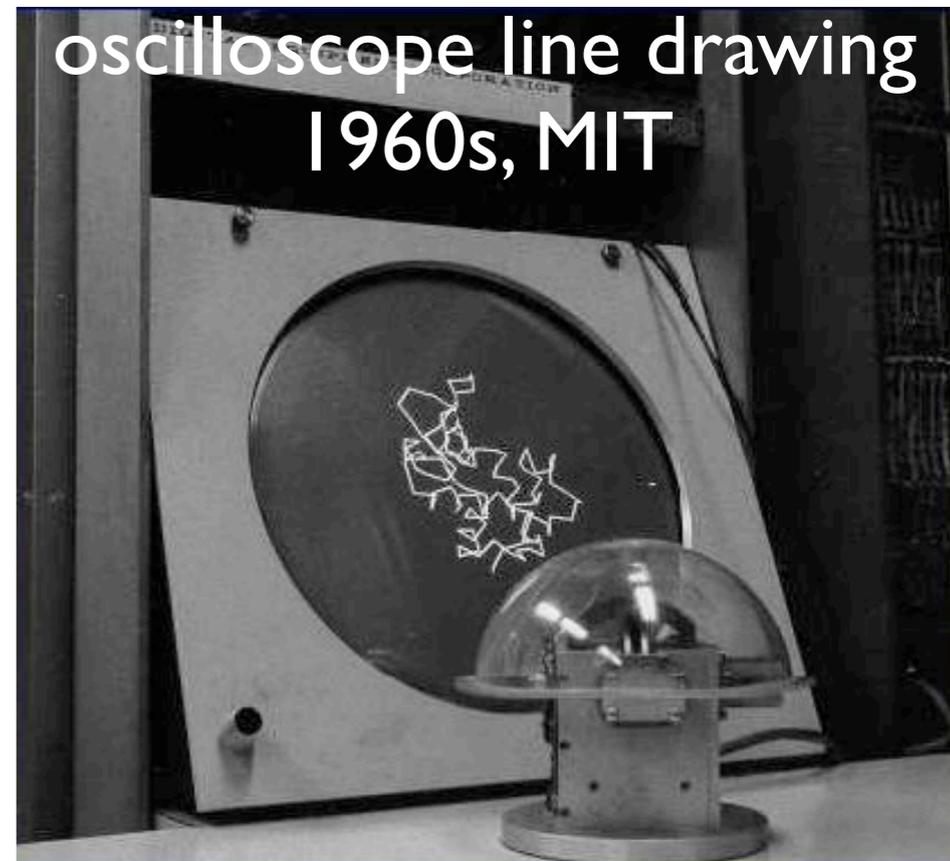


M. Feughelman, R. Langridge,
 W.E. Seeds, A.R. Stokes, H.R.
 Wilson, C.W. Hooper, M.H.F. Wilkins,
 R.K. Barclay, and L.D. Hamilton,
 "Molecular Structure of Deoxyribose
 Nucleic Acid and Nucleoprotein,"
Nature **175** 834-838 (1955).

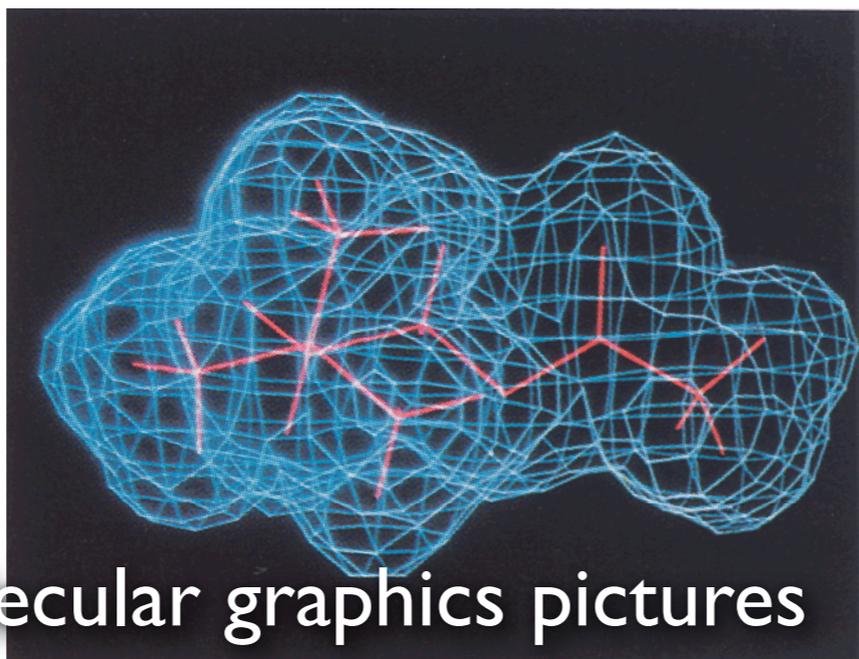
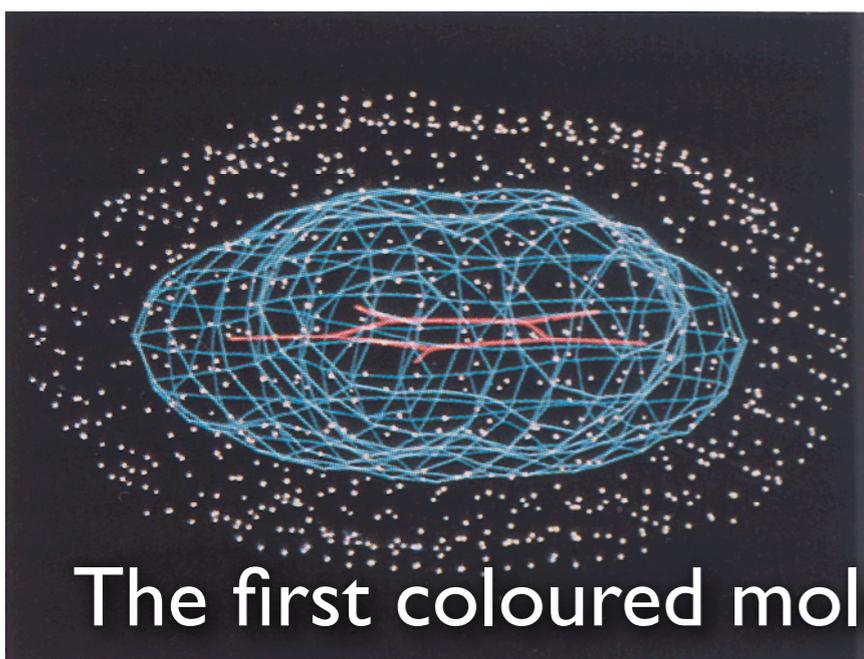
**Molecular Structure
 of DNA - 1955**



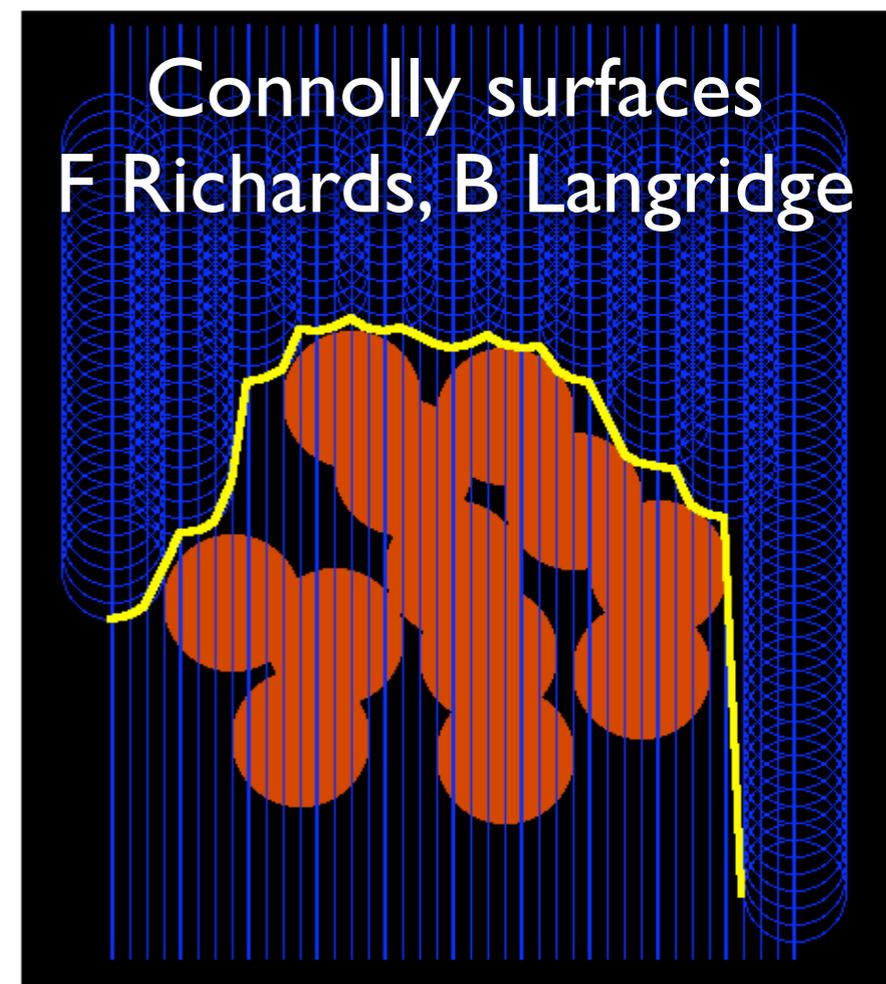
**ORTEP, C Johnson
 1970**



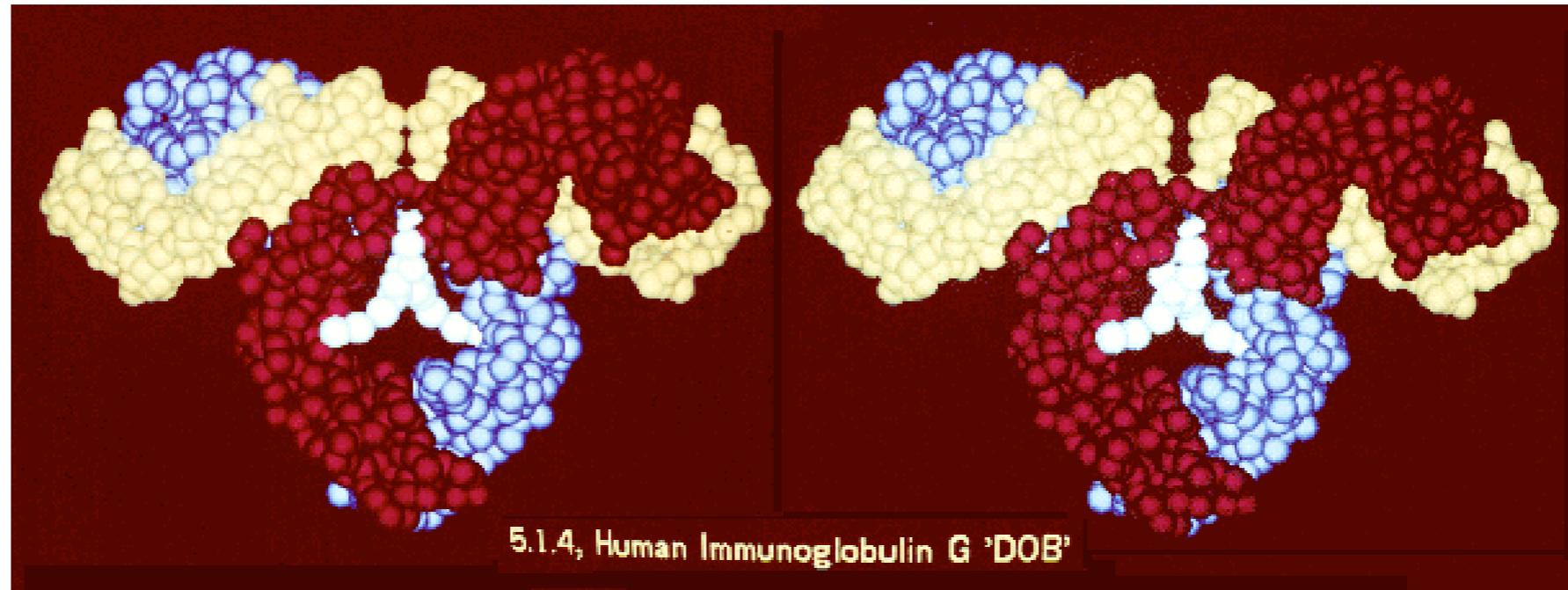
**Connolly surfaces
 F Richards, B Langridge**



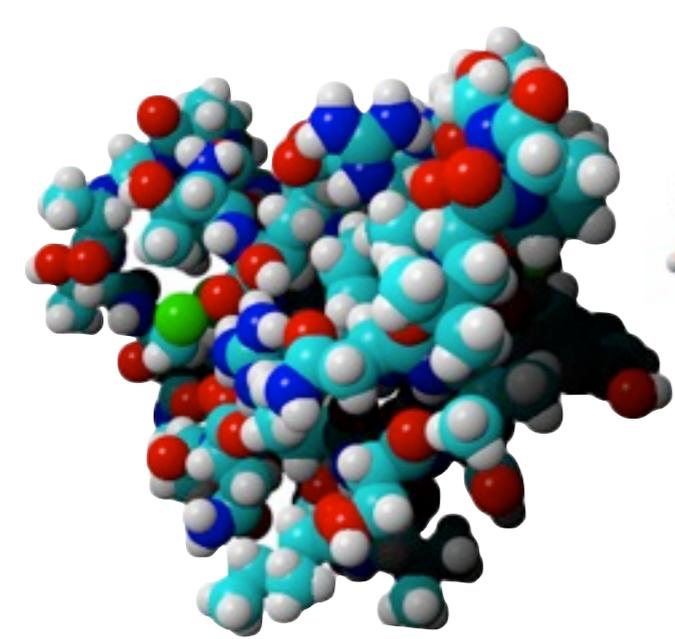
The first coloured molecular graphics pictures



Early stereo pictures



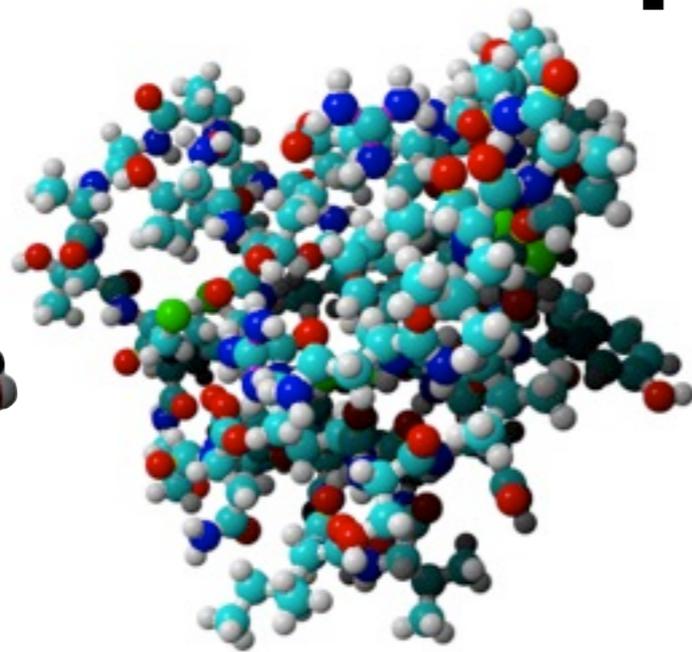
Standard representations



CPK spheres

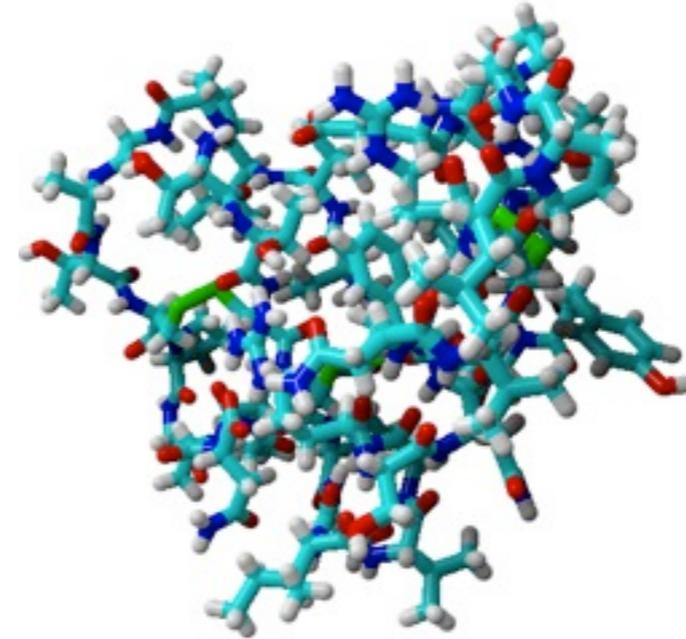
31k / 10k

vertices / faces



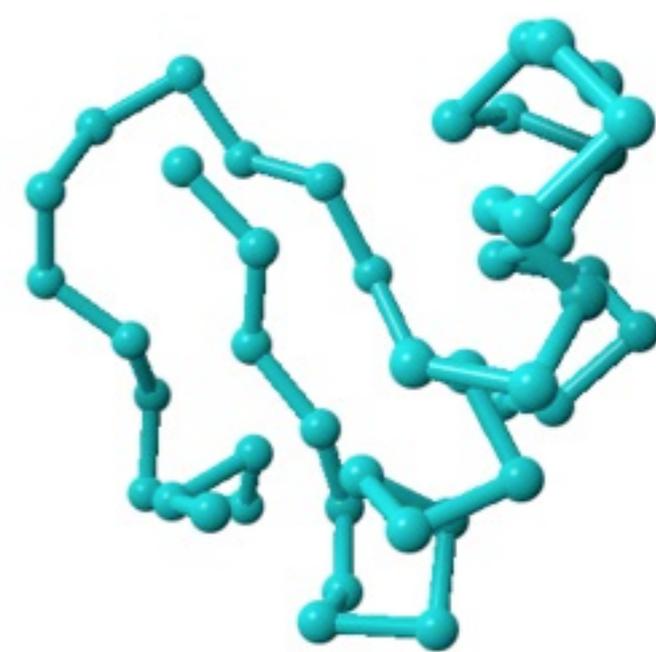
ball & stick

112k / 37k



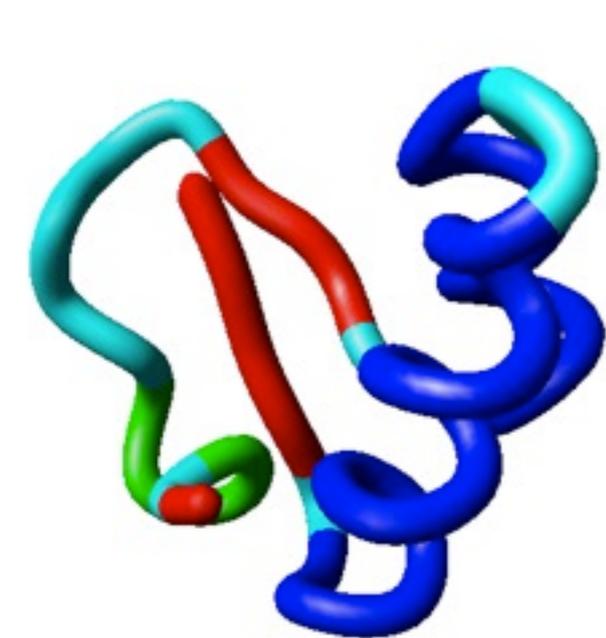
licorice

112k / 37k



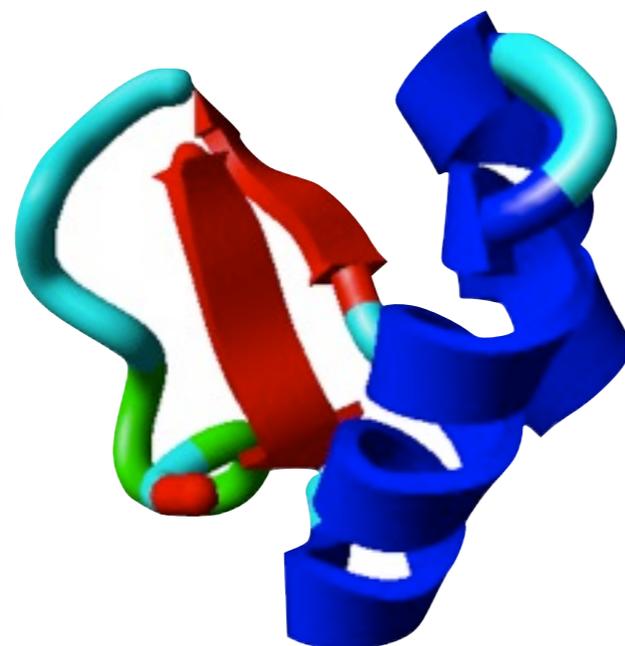
trace

11k / 4k



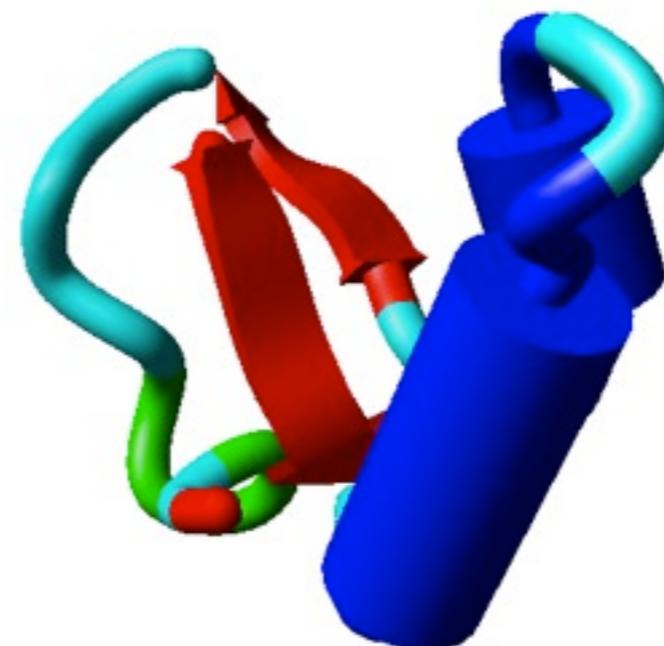
tube

33k / 11k



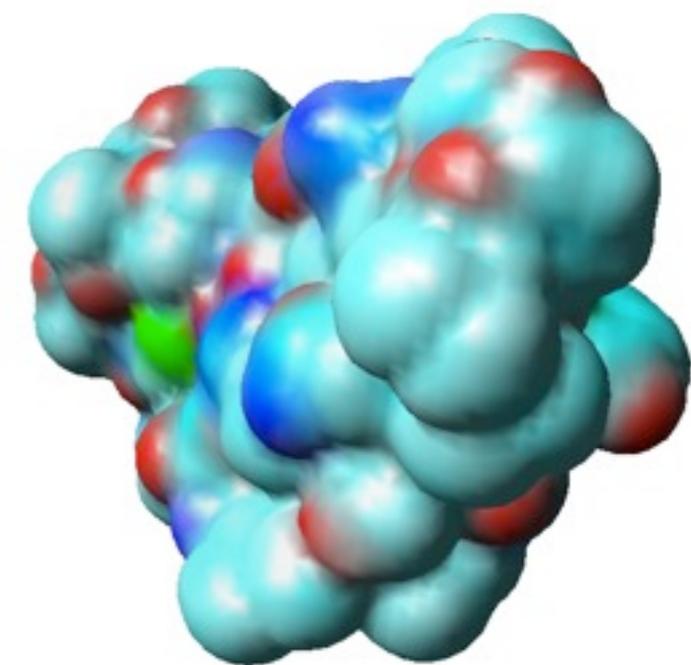
ribbon

68k / 23k



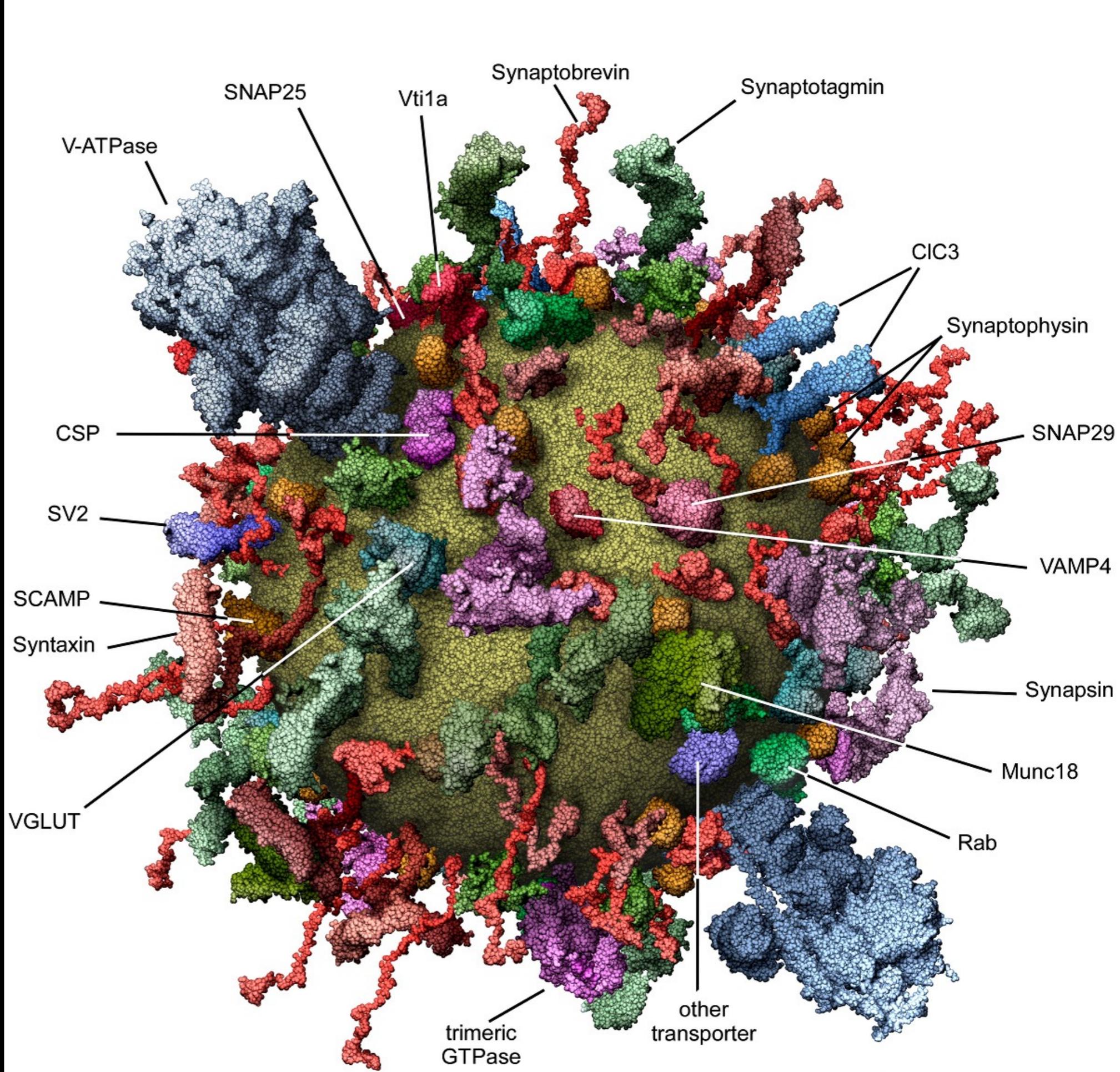
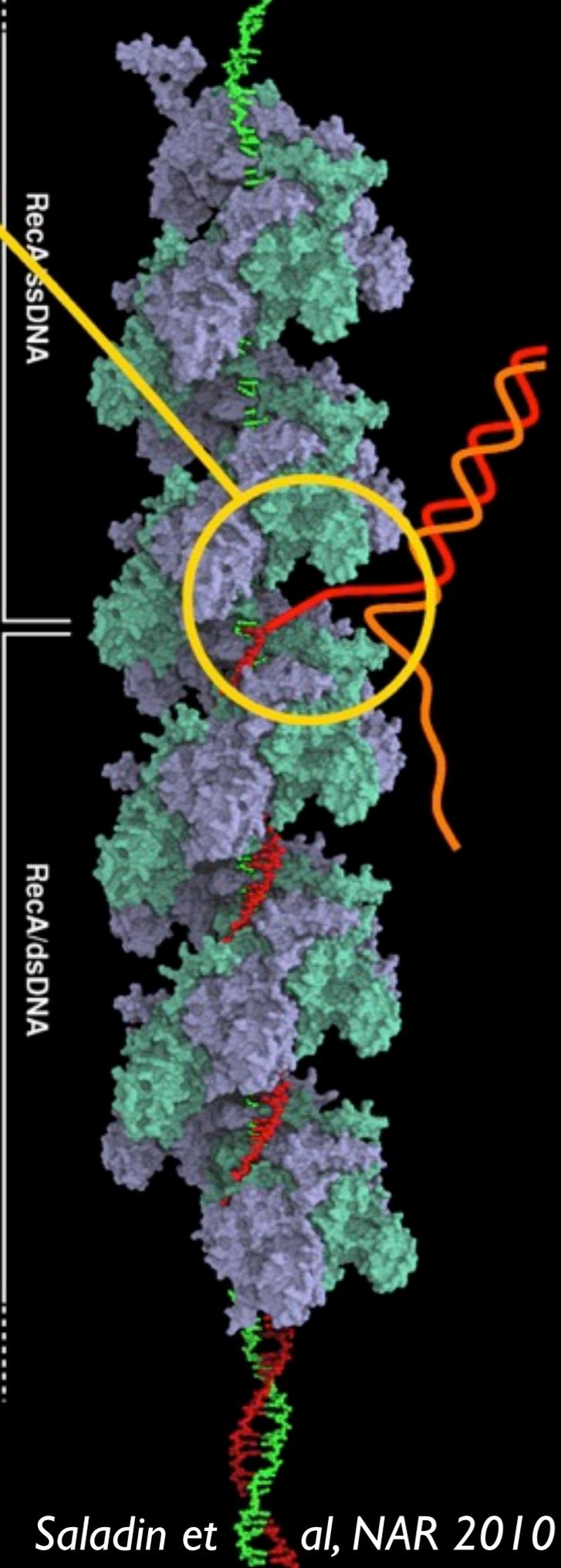
cartoon

23k / 8k



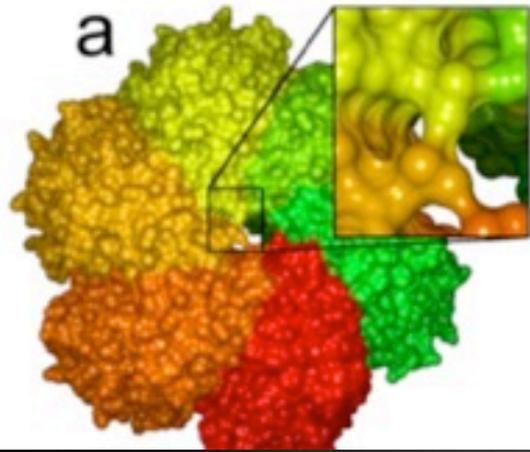
surface

50k / 17k

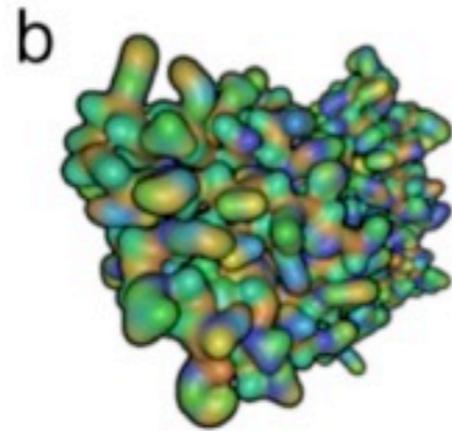


New developments on GPUs

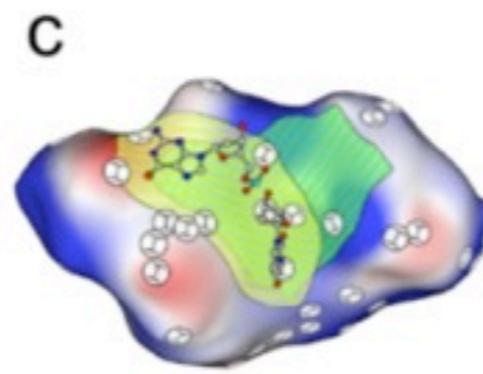
SURFACES



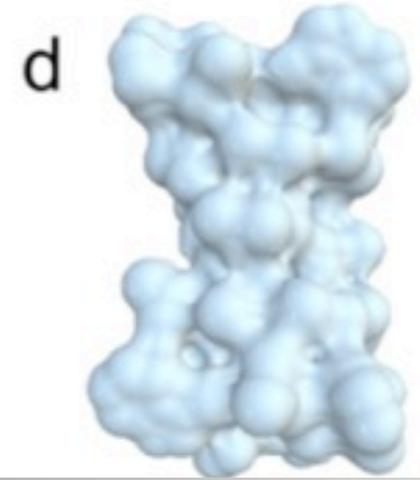
Connolly / ray-casting



metaballs / ray-casting

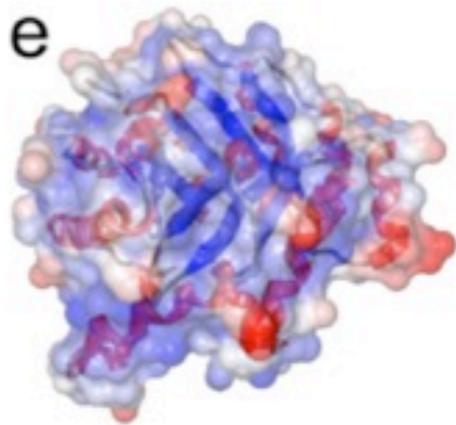


abstracted

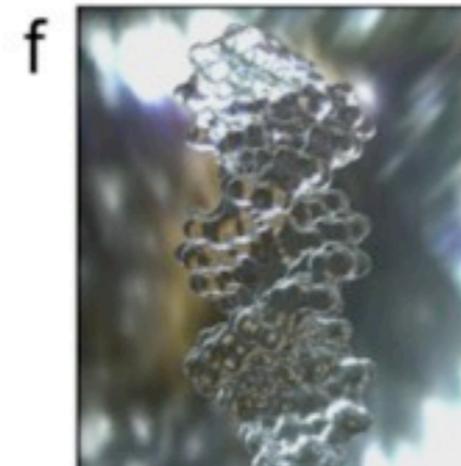


skin / ray-casting

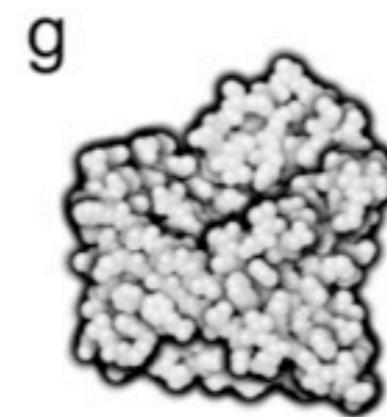
LIGHTING



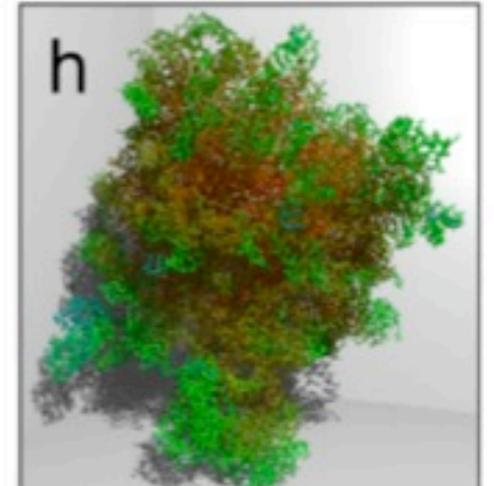
transparency



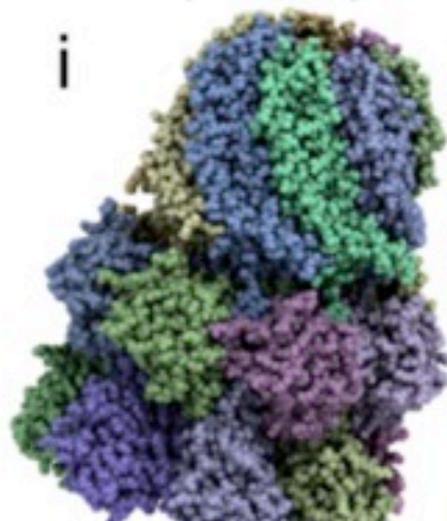
high dynamic range



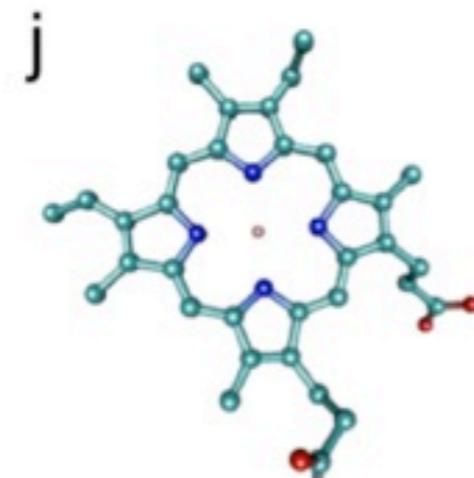
halo effect



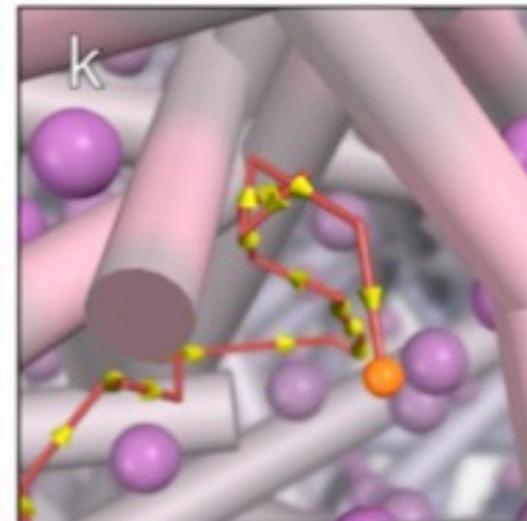
global shadowing



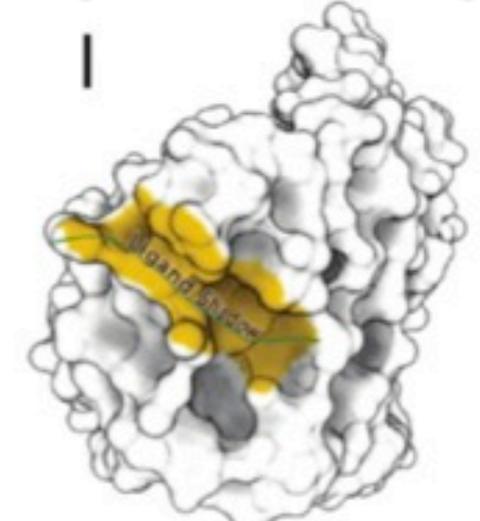
ambient occlusion



*ray-casted CPK
& HyperBalls*



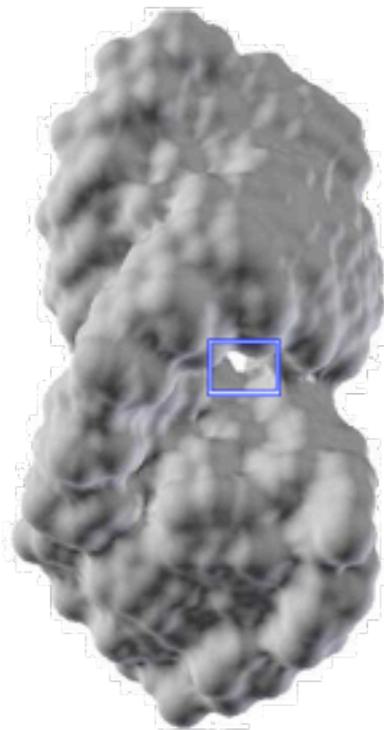
dof / desaturation



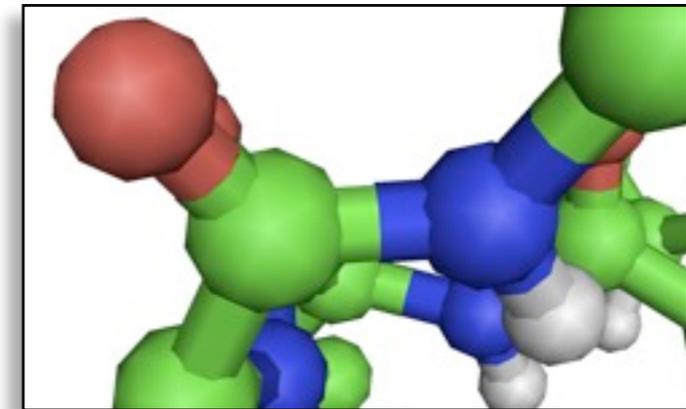
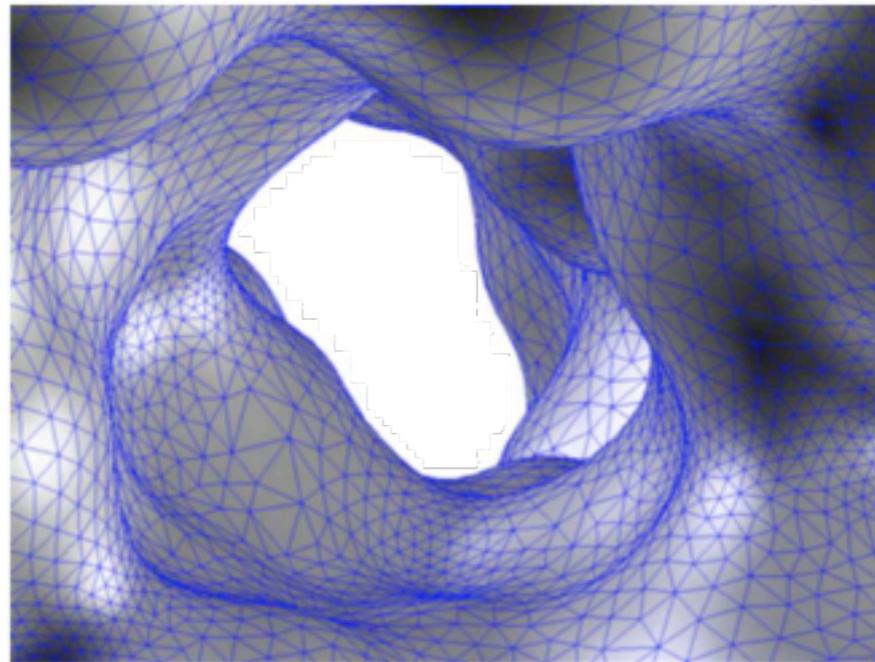
3D annotation

Mesh-based molecular representations

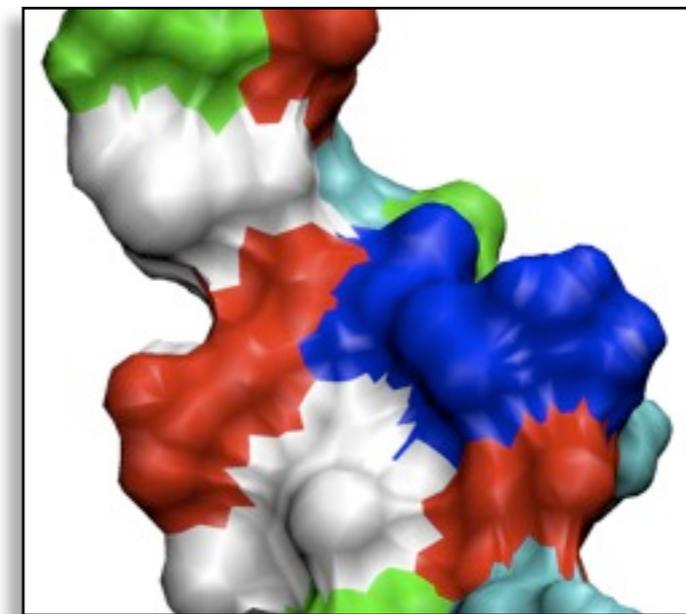
- **Surface triangulation: a discrete model**
 - slow and not very precise



Molecular Skin Surface ¹



Ball & Stick (PyMol²)



Molecular Surface (VMD³)

1. H-L Cheng, X Shi, Quality mesh generation for molecular skin surfaces using restricted union of balls, IEEE Visualization, 2005, 399-405.

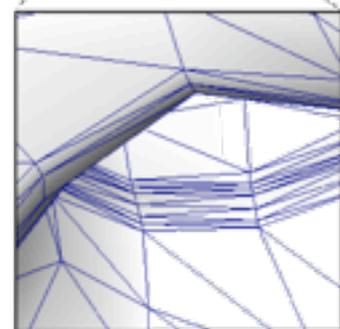
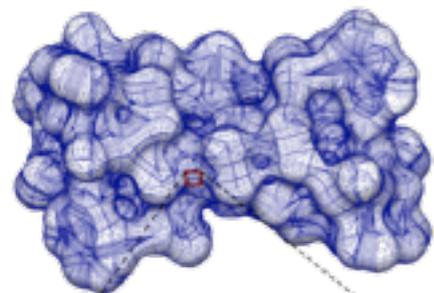
2. PyMOL, Molecular Graphics System, Version 1.2, Schrödinger, LLC

3. W Humphrey, A Dalke, K Schulten, VMD: Visual Molecular Dynamics, J. Mol. Graph. 14(1996) 33-38.

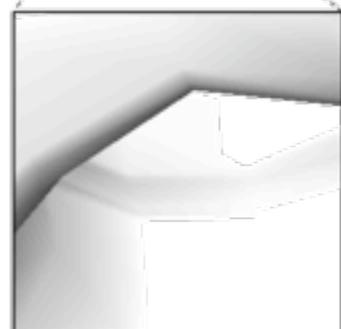
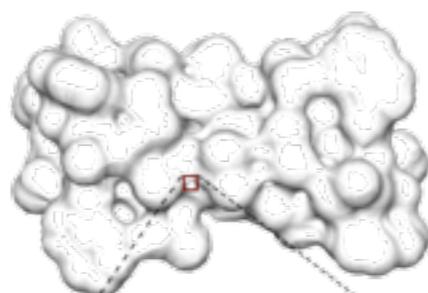
Ray-casted molecular representations

- GPU ray casting: a «*vectorial*» model
 - Pixel-precise (rather fast).

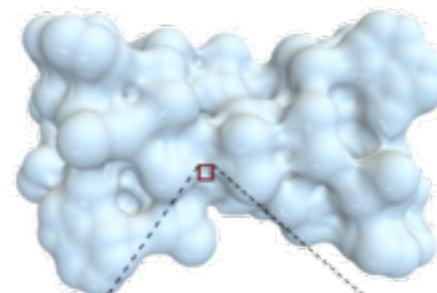
Gramicidin A (*side*)



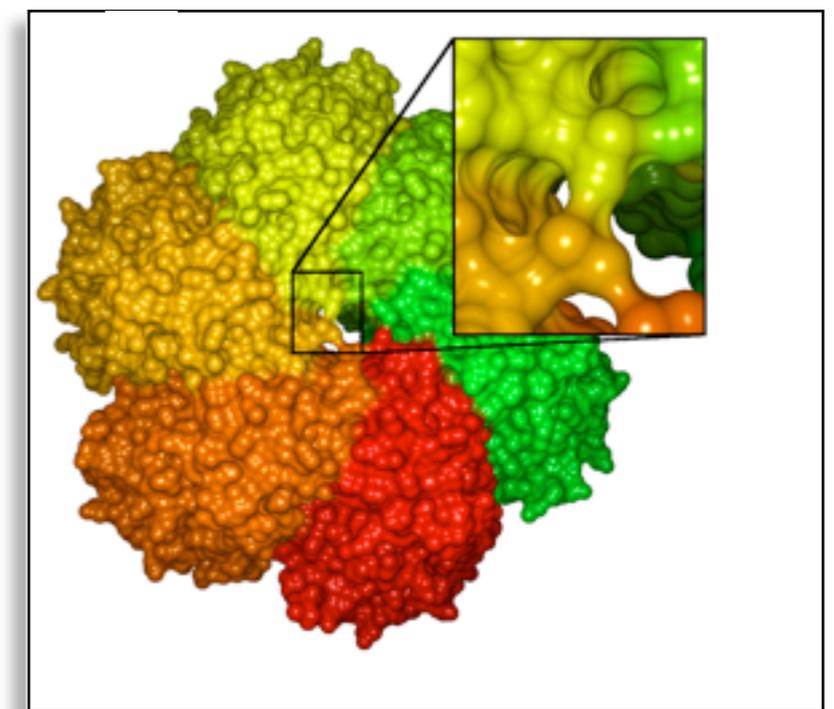
Triangulated
(with Wire Frame)



Triangulated



Ray Casted



• **Molecular Surface²**

• **Molecular Skin Surface¹**

1. M. Chavent, B. Levy, and B. Maigret, *J Mol Graph Model* **27** (2), 209 (2008). 2. M. Krone, K. Bidmon, and T. Ertl, *IEEE Trans Vis Comput Graph* **15** (6), 1391 (2009).

Extending ray casting to classical molecular representations: Ball & Stick, VdW...

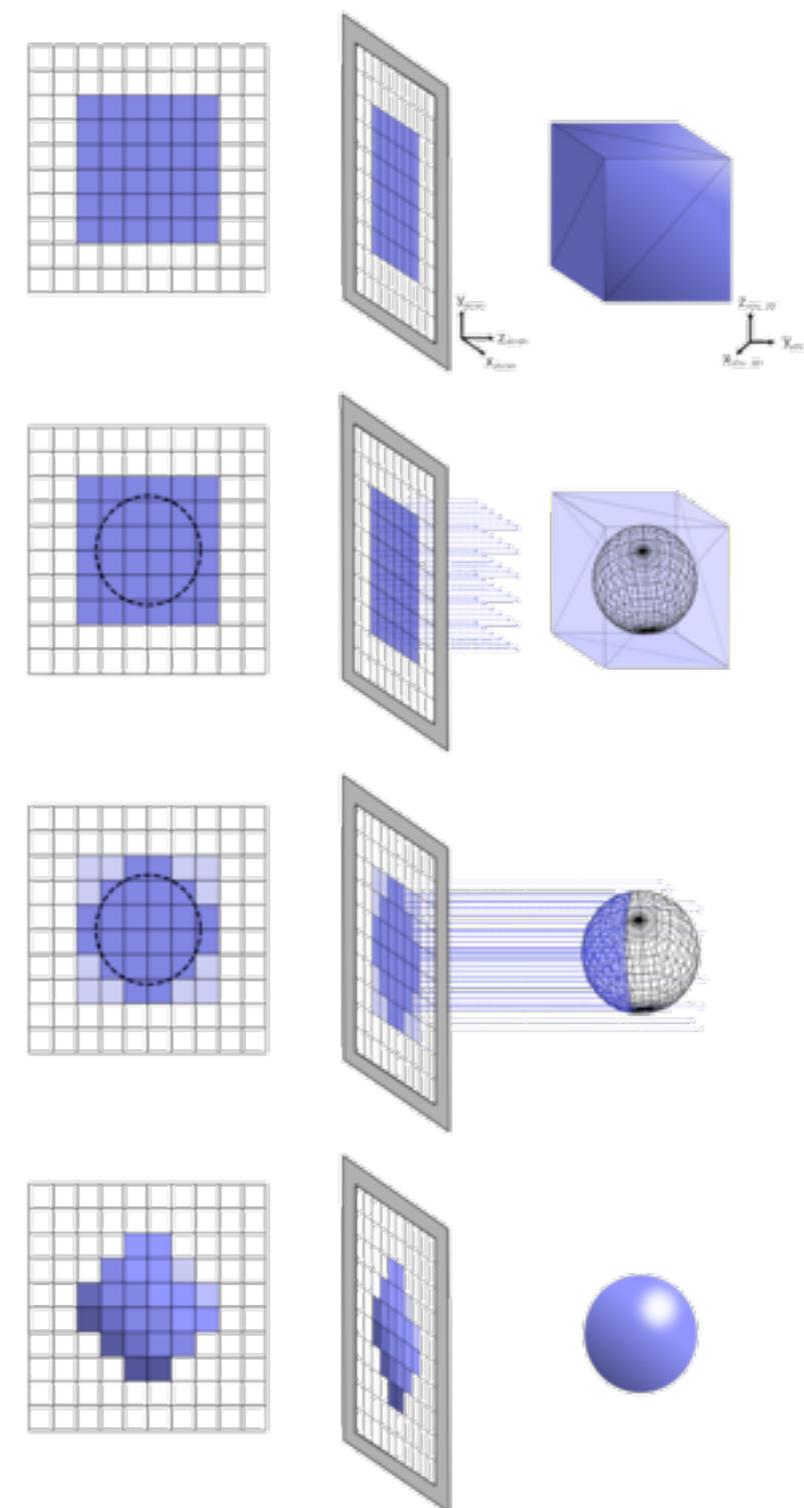
- GPU ray casting: the principle

- Represent an OpenGL cube.

- Cast rays from the screen.

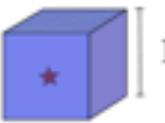
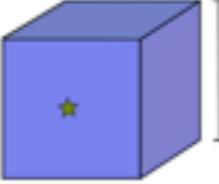
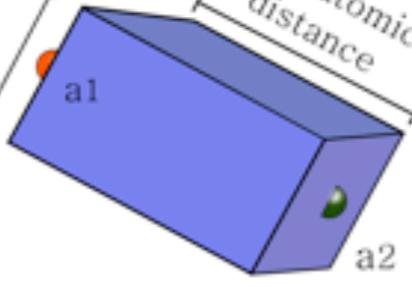
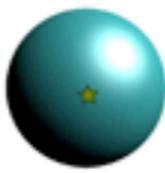
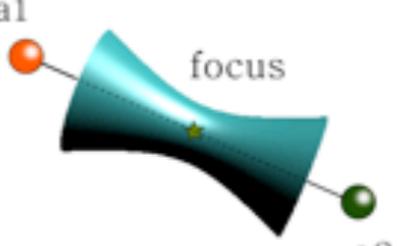
- Consider intersecting rays/surfaces.

- Remove pixels where no intersection with the sphere is observed + lighting.

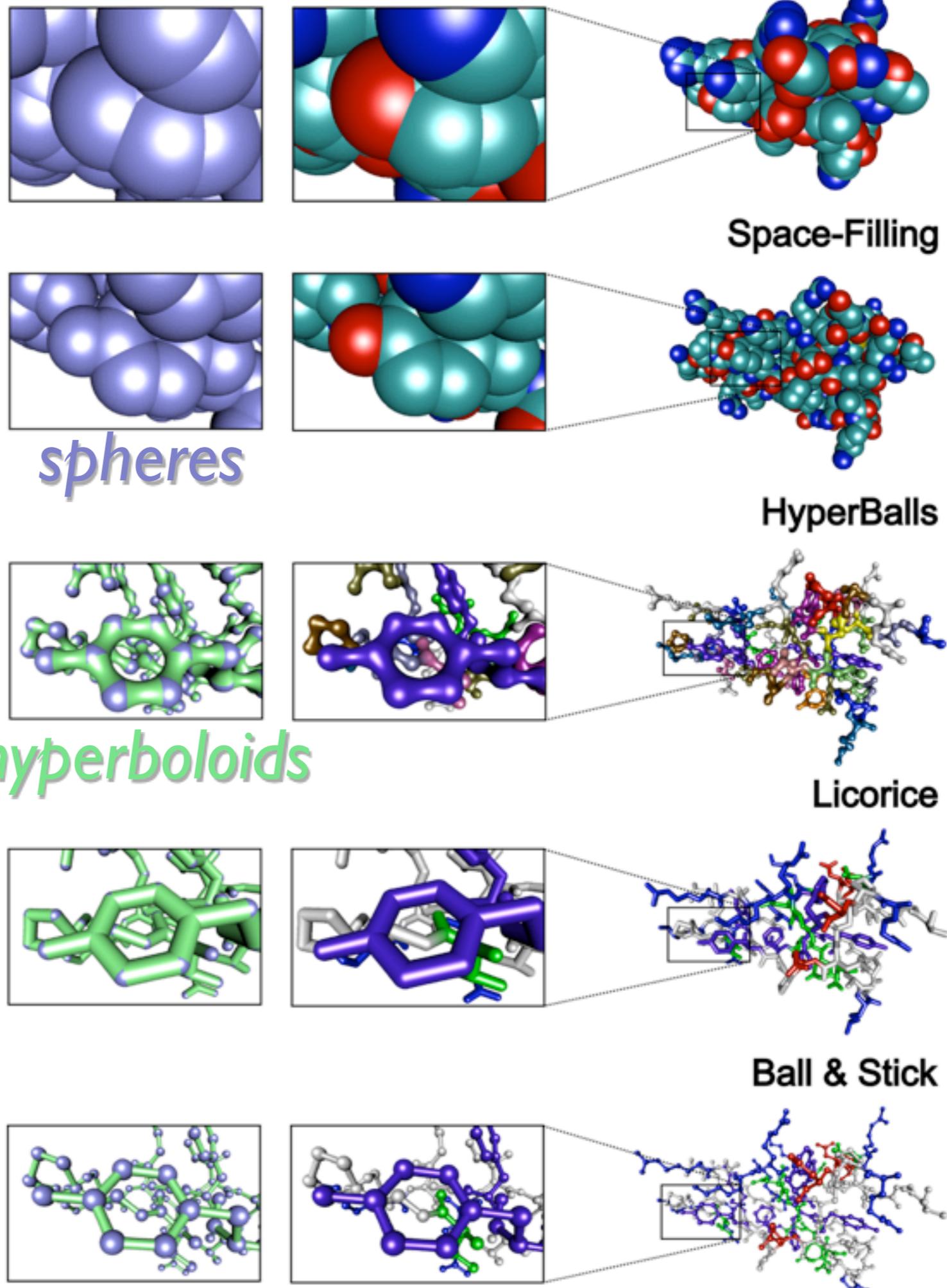
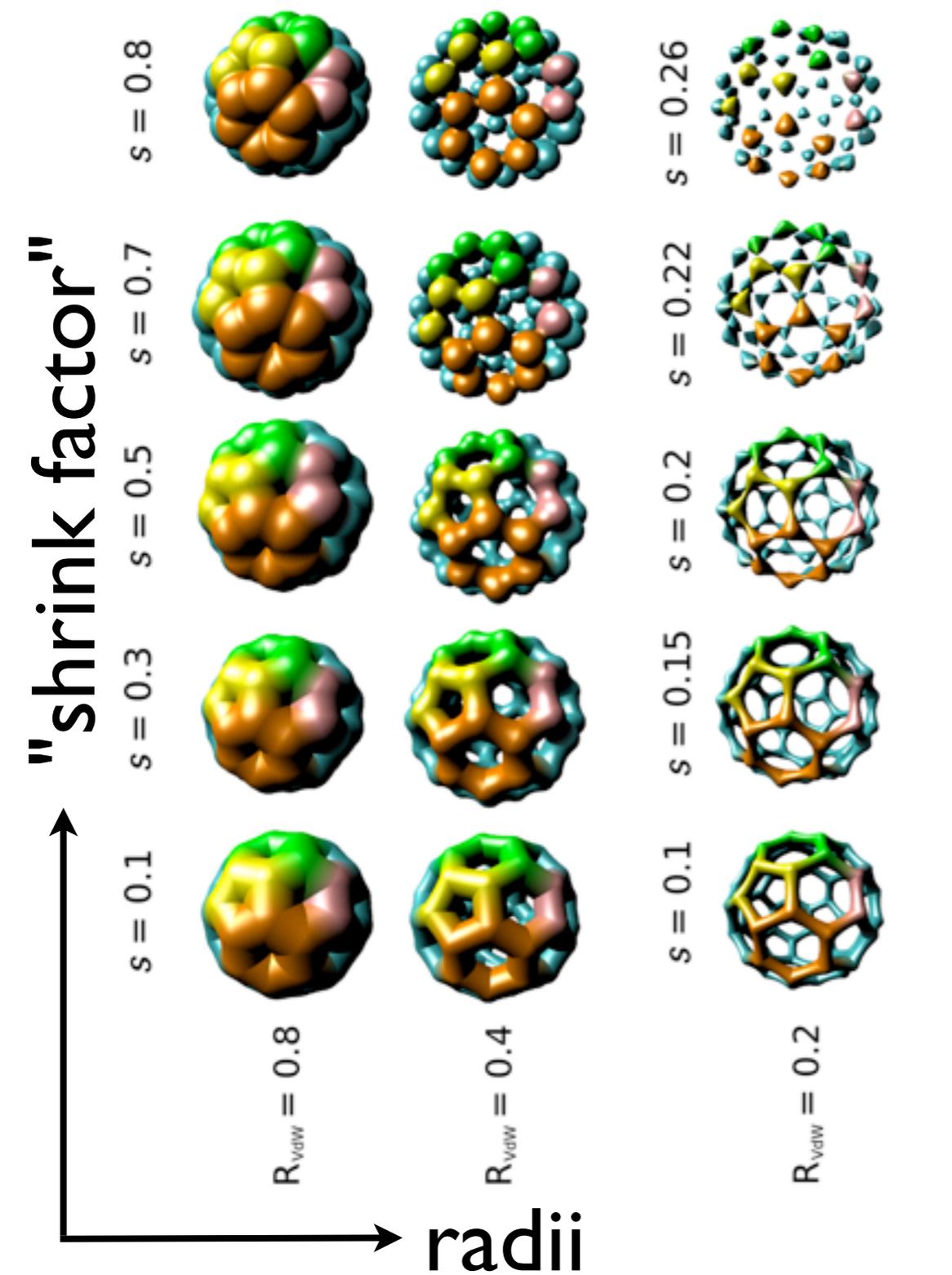


Extending ray casting to classical molecular representations: Ball & Stick, VdW...

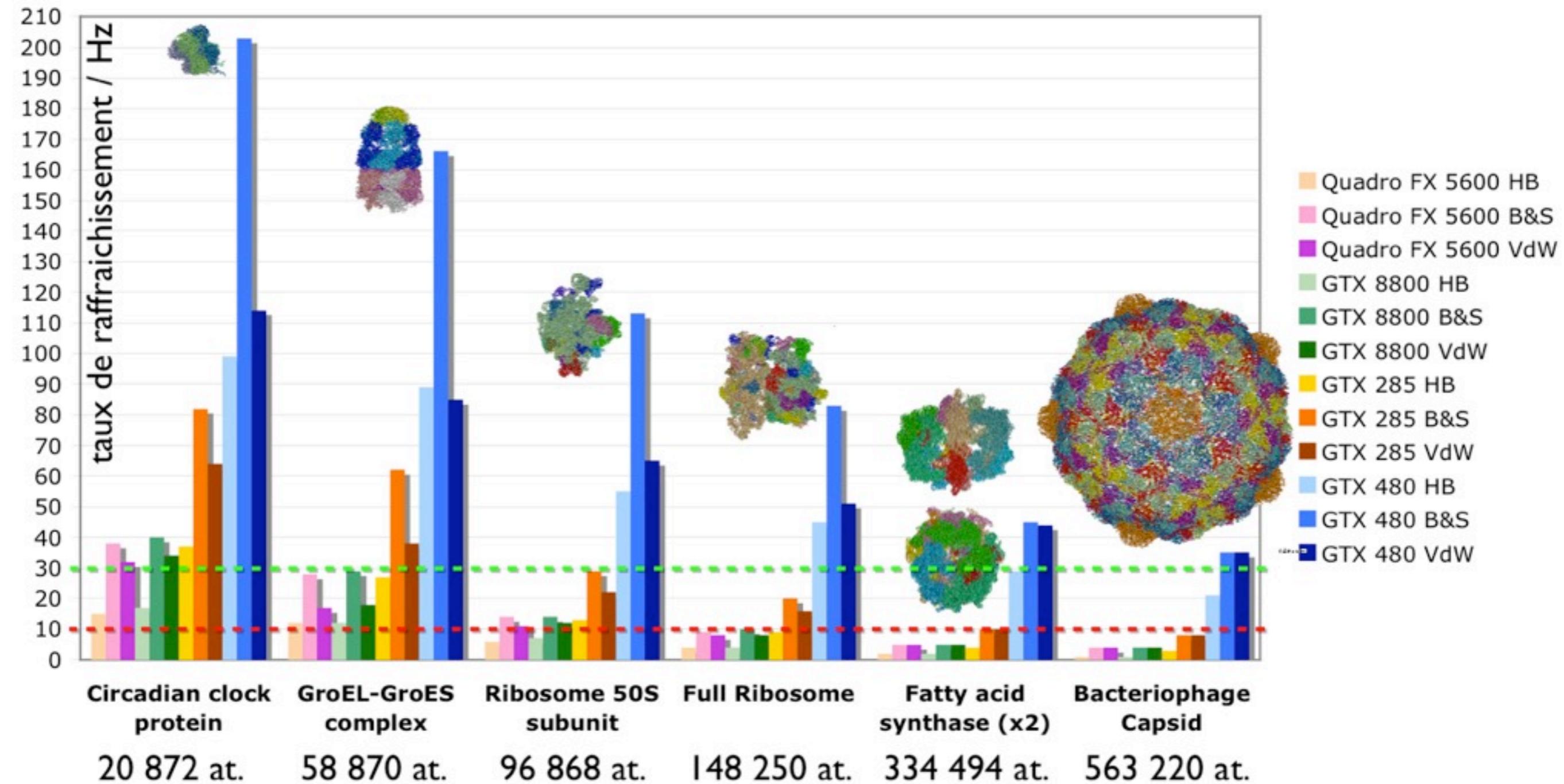
- Draw the different primitives (2): graphical pipeline

	<i>Sphere Representation</i>	<i>Bond Representation</i>	<i>Sphere Rendering</i>	<i>Bond Rendering</i>	
Graphical pipeline	CPU	<p>For each atom :</p> <ul style="list-style-type: none"> - Fill Texture1 with atom Id. - Fill Texture2 with position. - Fill Texture3 with radius. - Fill Texture4 with color. <p>- Create a cube of 1 \AA^3 at (0;0;0).</p>	<p>For each link :</p> <ul style="list-style-type: none"> - Fill Texture1 with atom Id. - Fill Texture2 with position. - Fill Texture3 with radius. - Fill Texture4 with color. <p>- Create a cube of 1 \AA^3 at (0;0;0).</p>	 <p>Origin (0,0,0)</p>	 <p>Origin (0,0,0)</p>
	Vertex Shader	<p>For each Vertex :</p> <ul style="list-style-type: none"> - Translate Vertex from (0;0;0) environment to atom position environment using textures 1 & 2. - Calculate Ray origin and direction. 	<p>For each Vertex :</p> <ul style="list-style-type: none"> - Translate Vertex from (0;0;0) environment to atom position environment using textures 1 & 2. - Scale the cube to transform it in a paralepiped. - Calculate Ray origin and direction. 	 <p>atom center</p>	
	Fragment Shader	<p>For each Fragment :</p> <ul style="list-style-type: none"> - Calculate Ray intersection using sphere equation, radii stored in Texture 3 with Id stored in Texture1. - Discard unnecessary pixels. - Depth Calculation. - Coloring using Texture4. - Normal calculation & Lighting. 	<p>For each Fragment :</p> <ul style="list-style-type: none"> - Calculate Ray intersection using hyperboloid/cylinder equation, radii stored in Texture 3 with Id stored in Texture1. - Discard unnecessary pixels. - Clip link. - Depth Calculation. - Coloring using Texture4. - Normal Calculation & Lighting. 	 <p>atom center</p> <p>spheres</p>	 <p>HyperBalls</p> <p>hyperboloids</p>

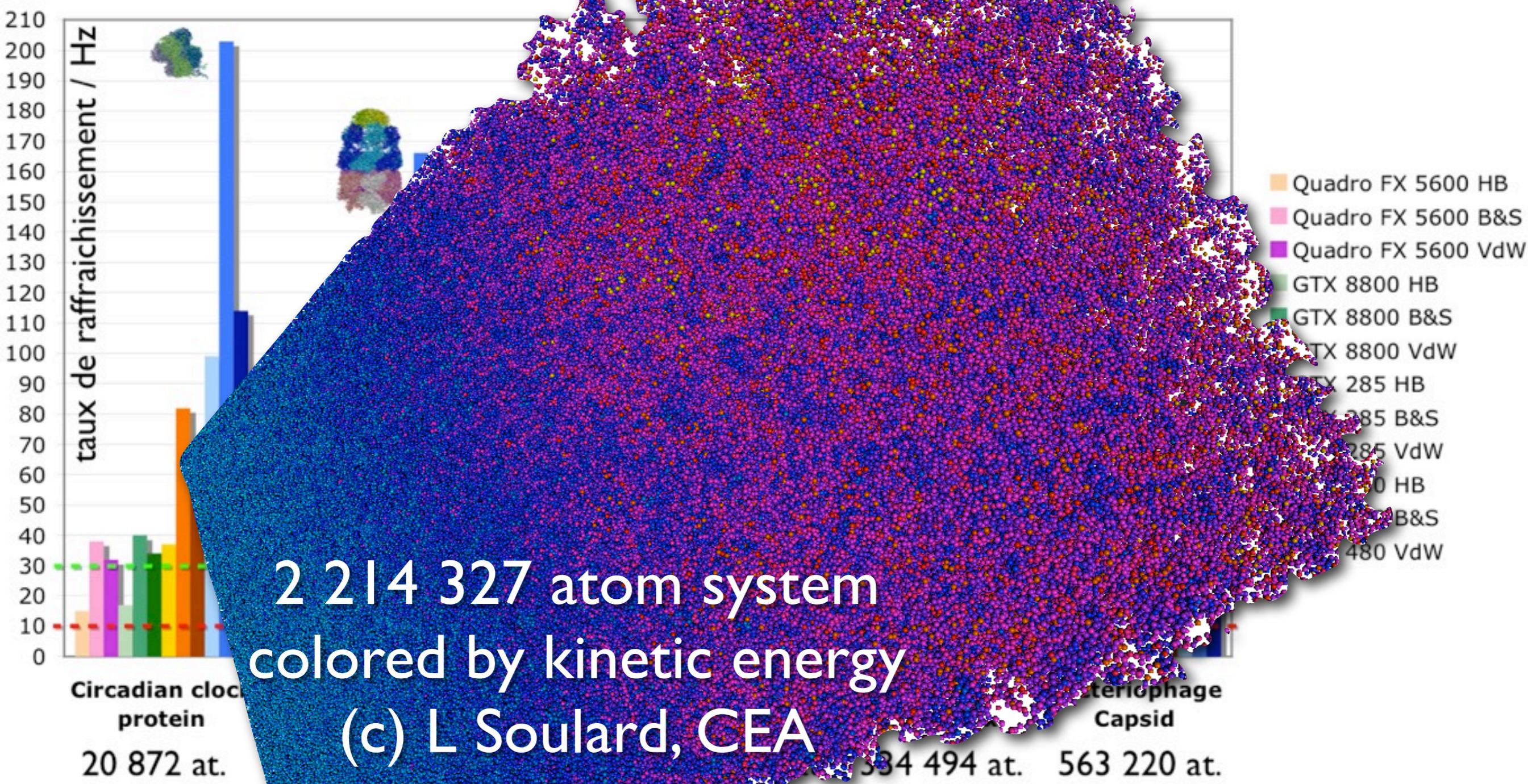
A unified representation



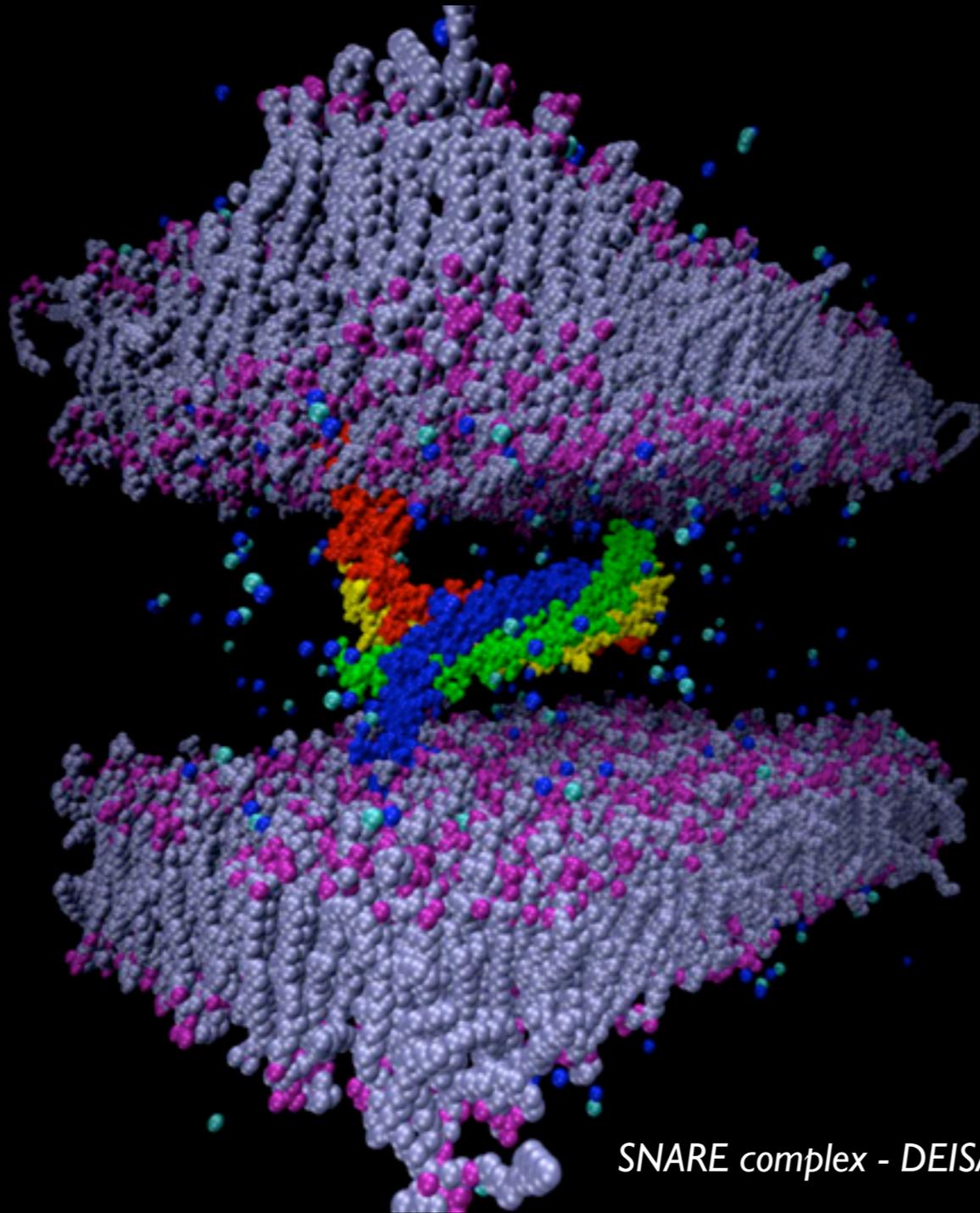
Performance



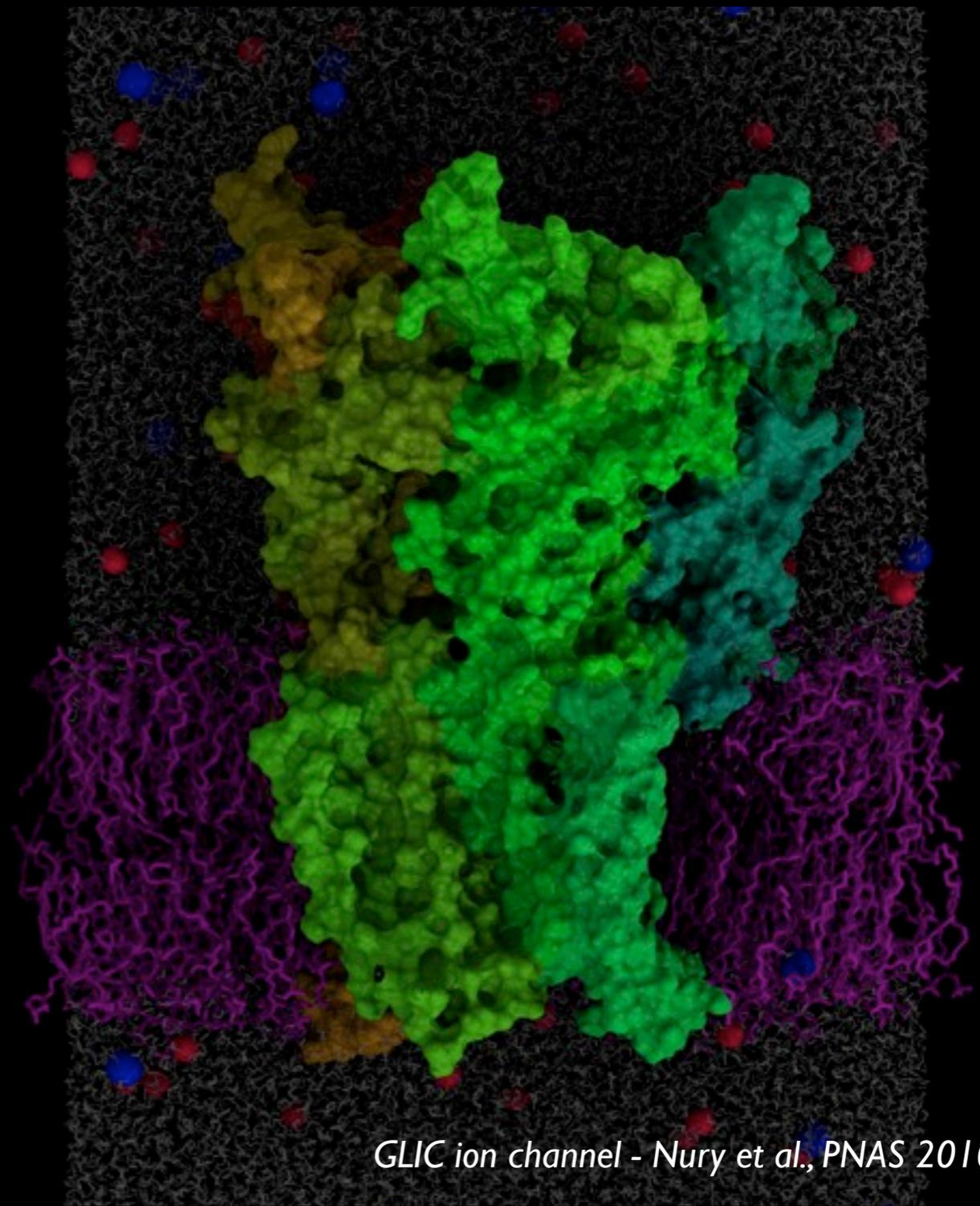
Performance



Large Dynamic datasets



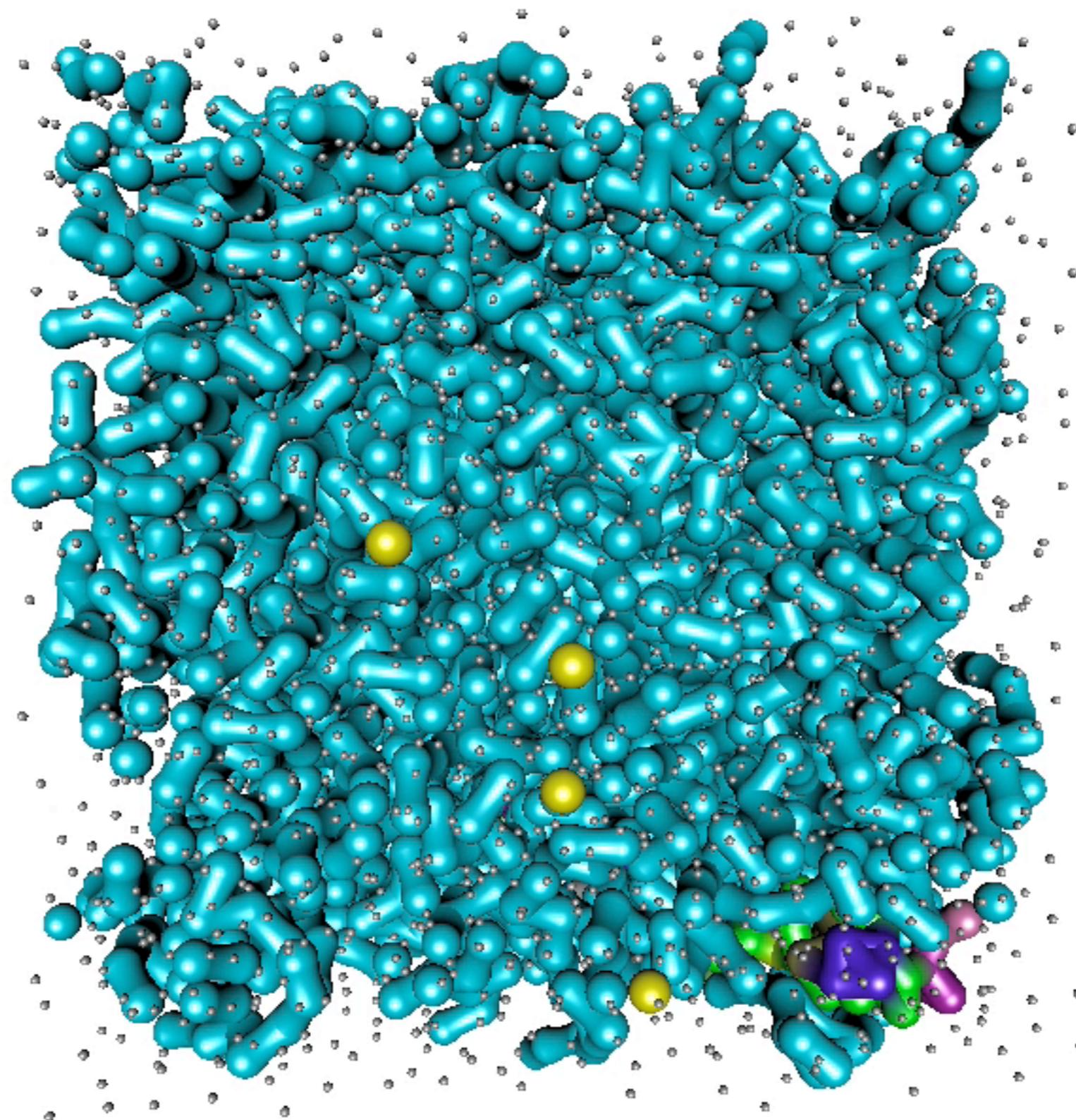
SNARE complex - DEISA DECI



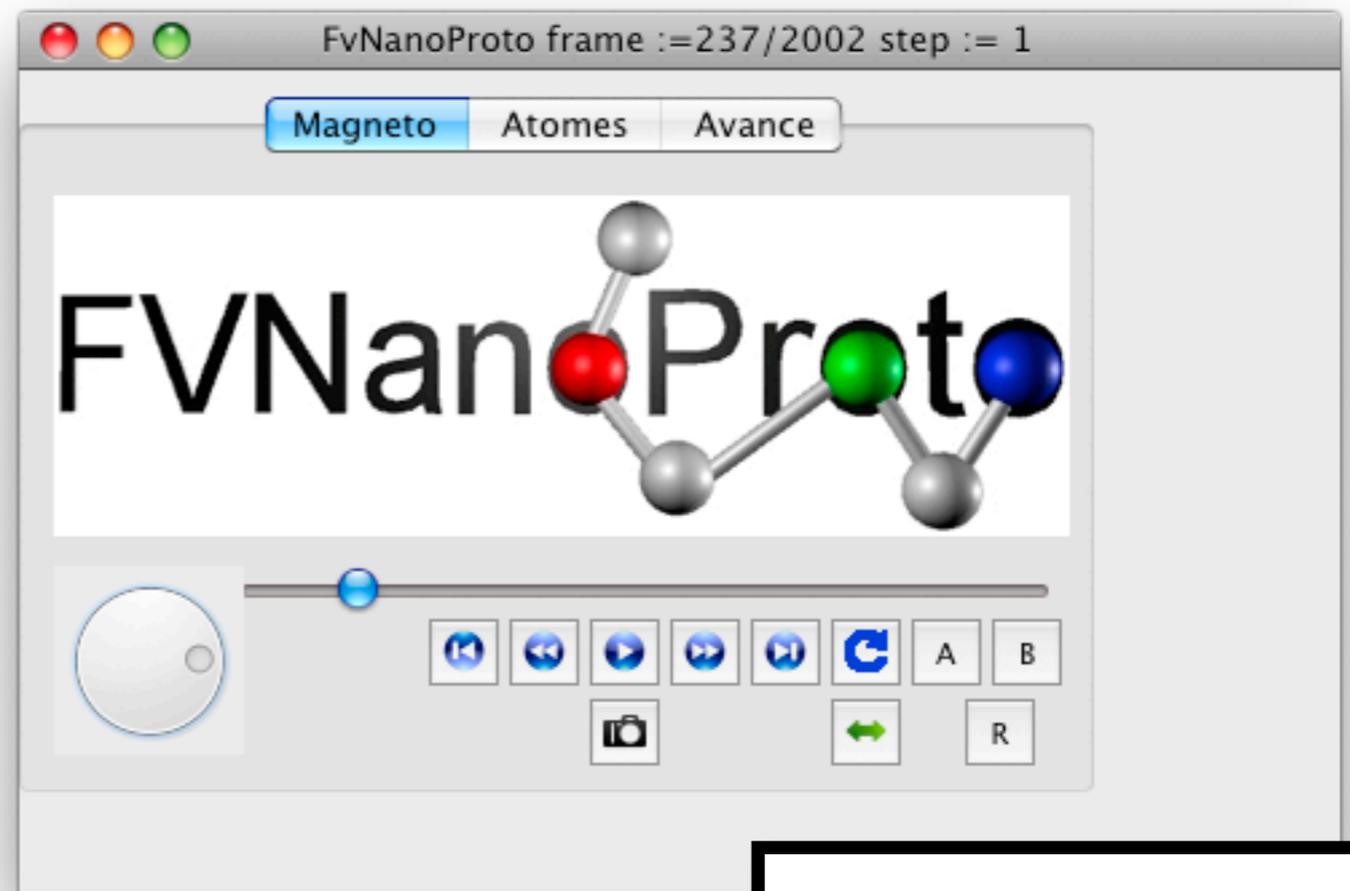
GLIC ion channel - Nury et al., PNAS 2010

- 339 792 atoms
- 75 Gb of data (compressed)
- > 40 000 frames

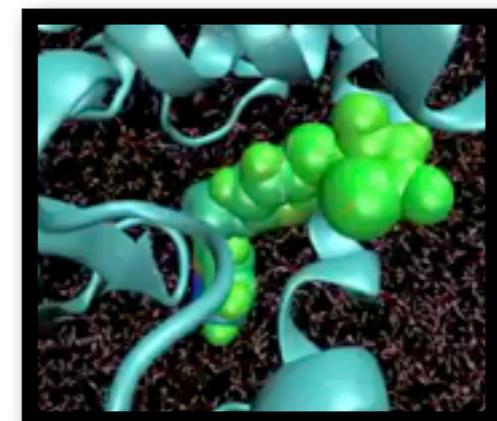
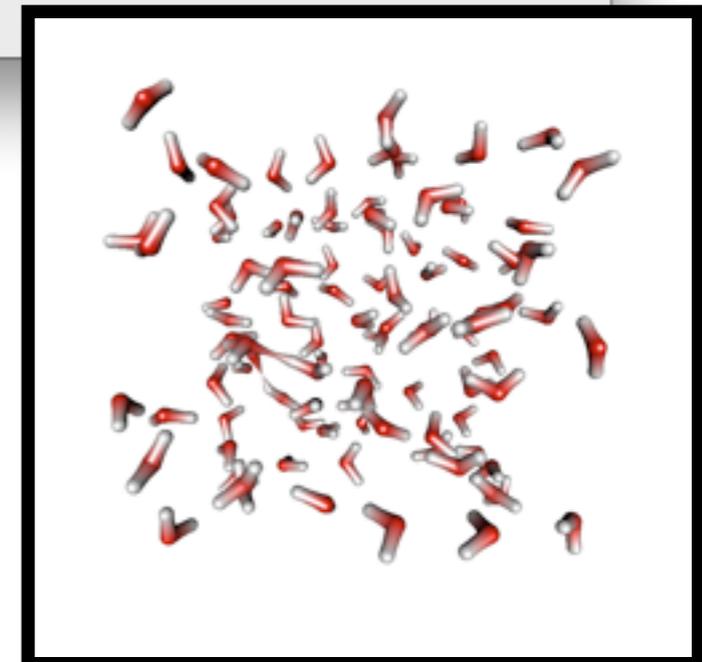
- 198 567 atoms
- 169 Gb of data (compressed)
- > 20 000 frames



Trajectory Viewer



- navigate within trajectory data
- control synchronization and speed
- provide continuous data stream
- add visual analytics options
 - dynamic change of color/representation



Implementations

- FlowVR Render

*A Shader-Based Parallel Rendering Framework
Cg-based vertex & fragment shaders*



- VTK-based visualization prototype

Replace CSCS shaders by HyperBalls



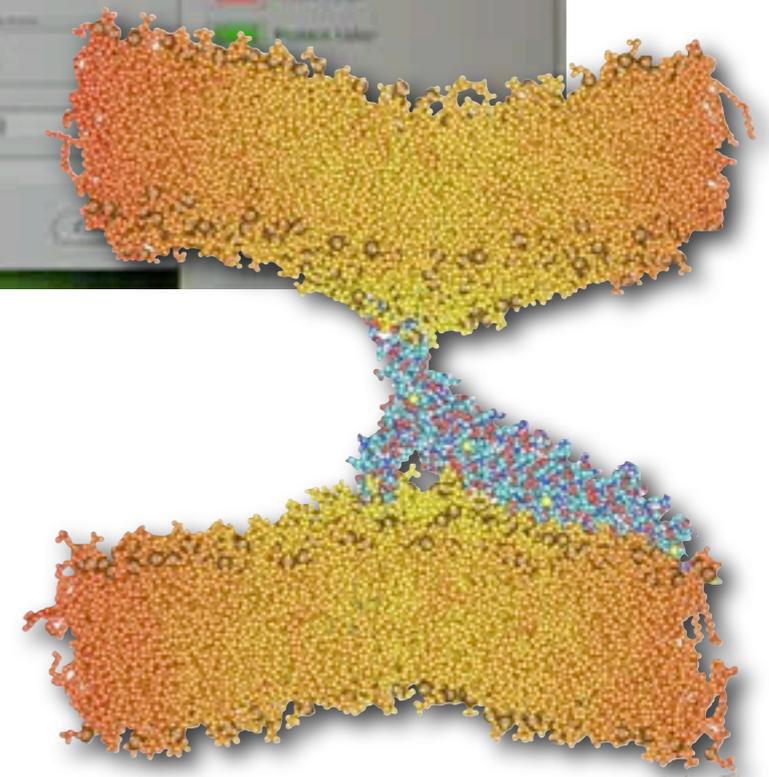
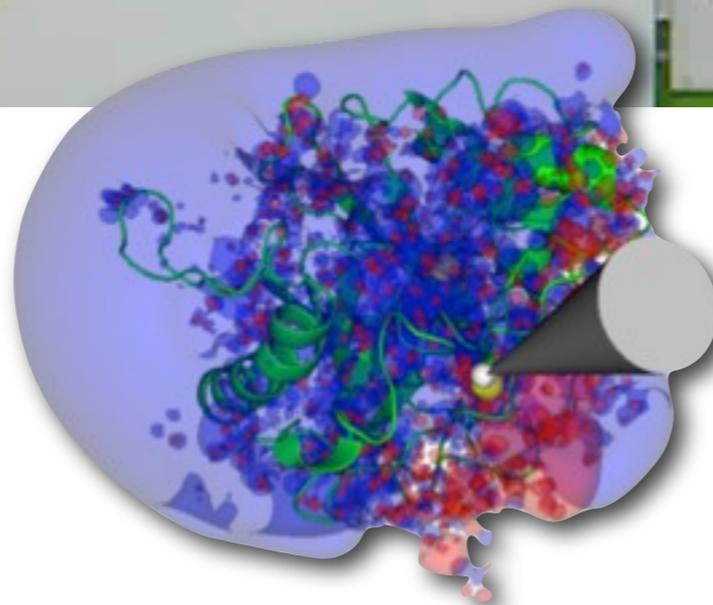
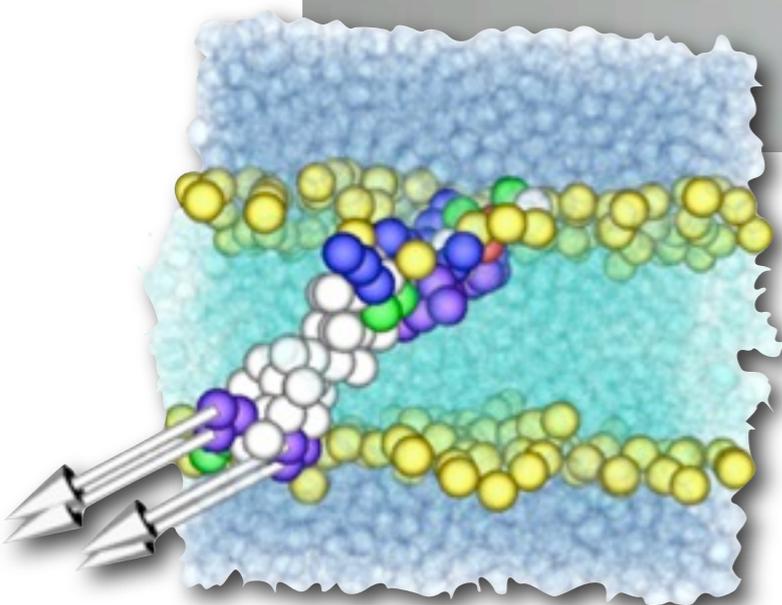
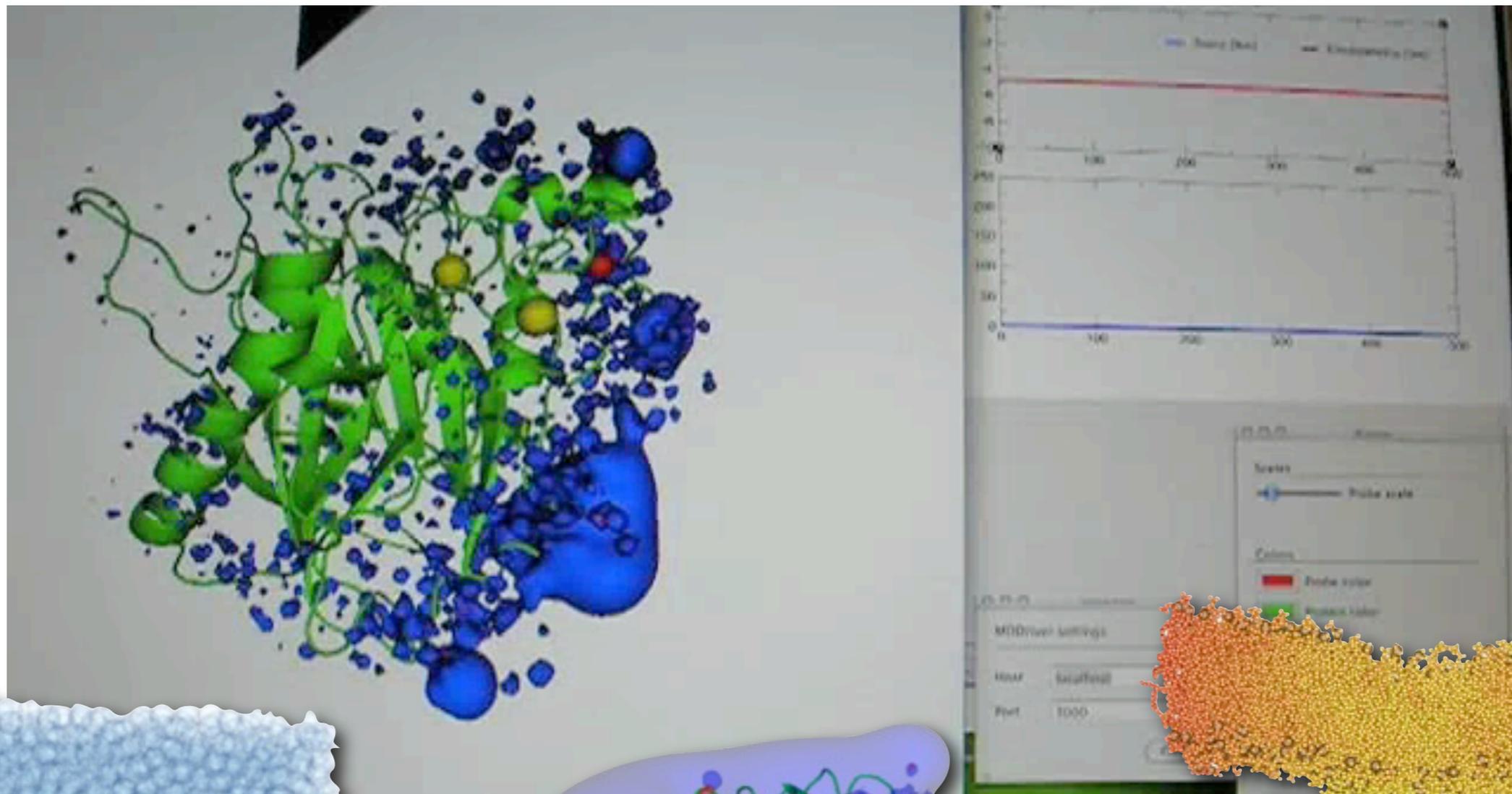
- Graphite

B Lévy's research platform for computer graphics

- Unity3D / SiO2 for mobile devices

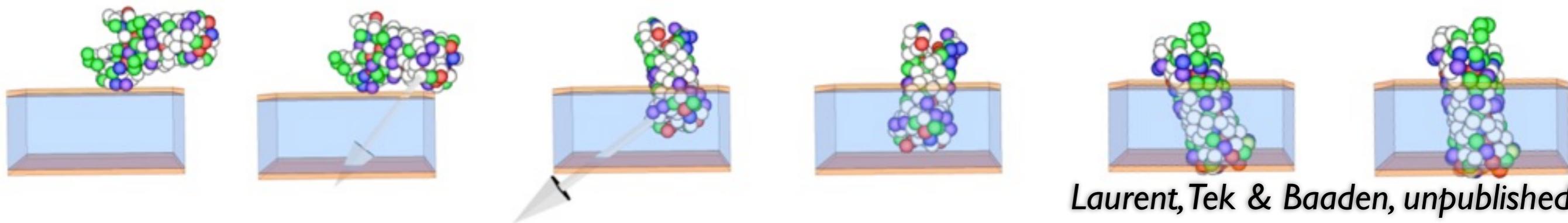
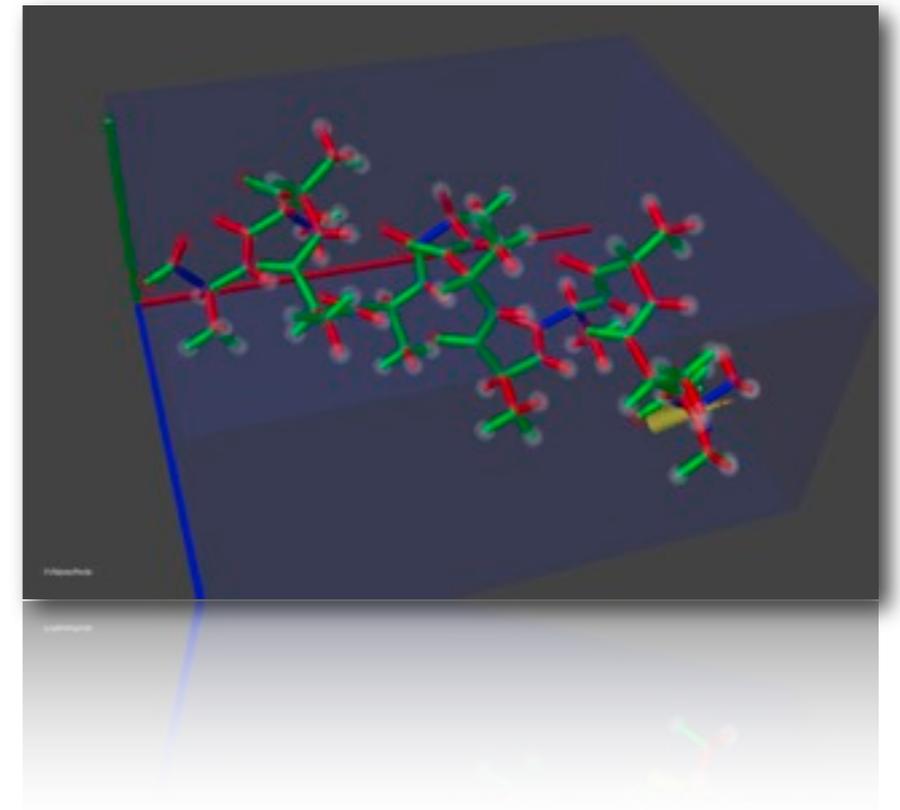
Explore iPhone and iPad capacities

VTK-based visualizer & live energy grapher

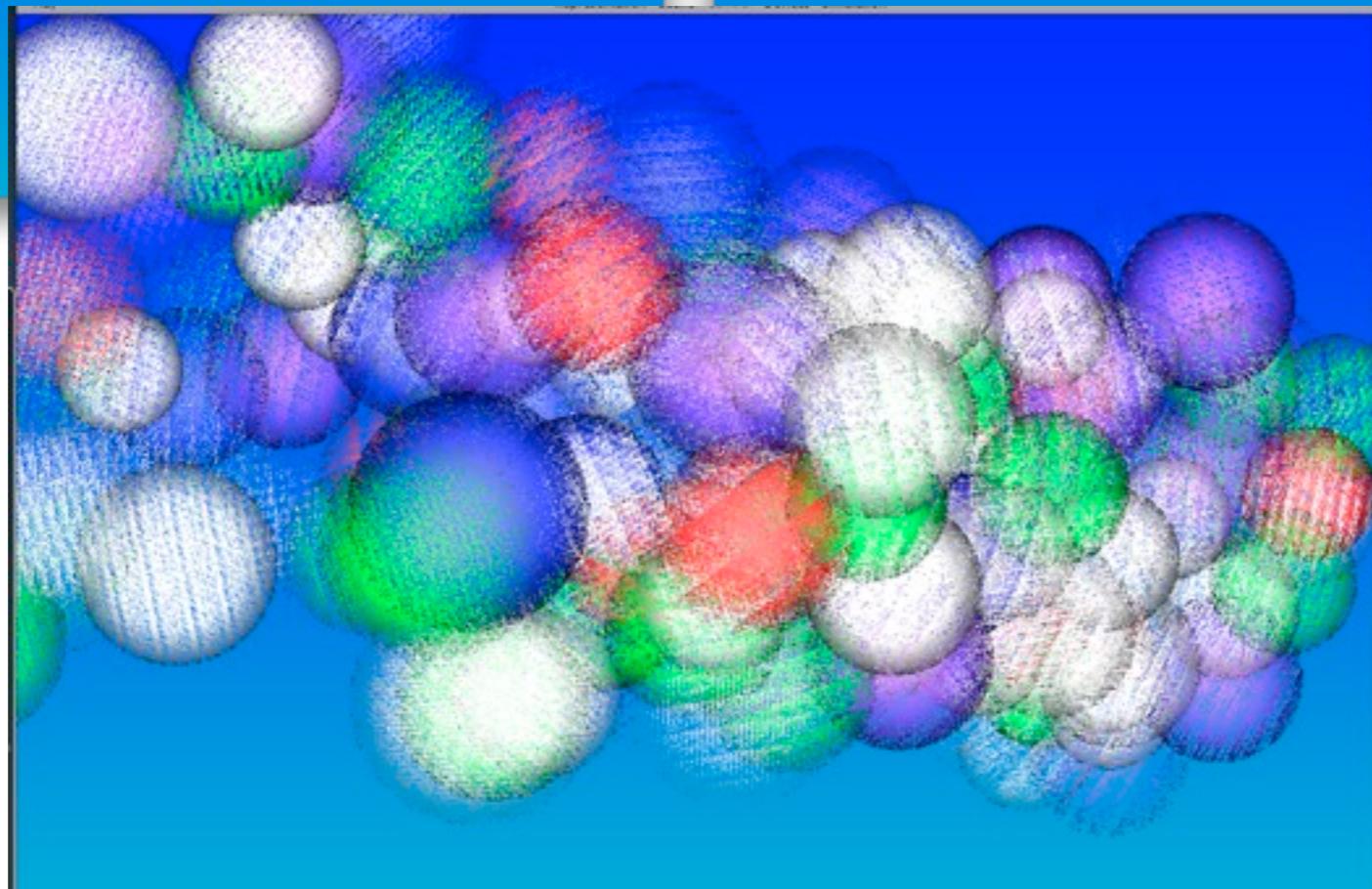
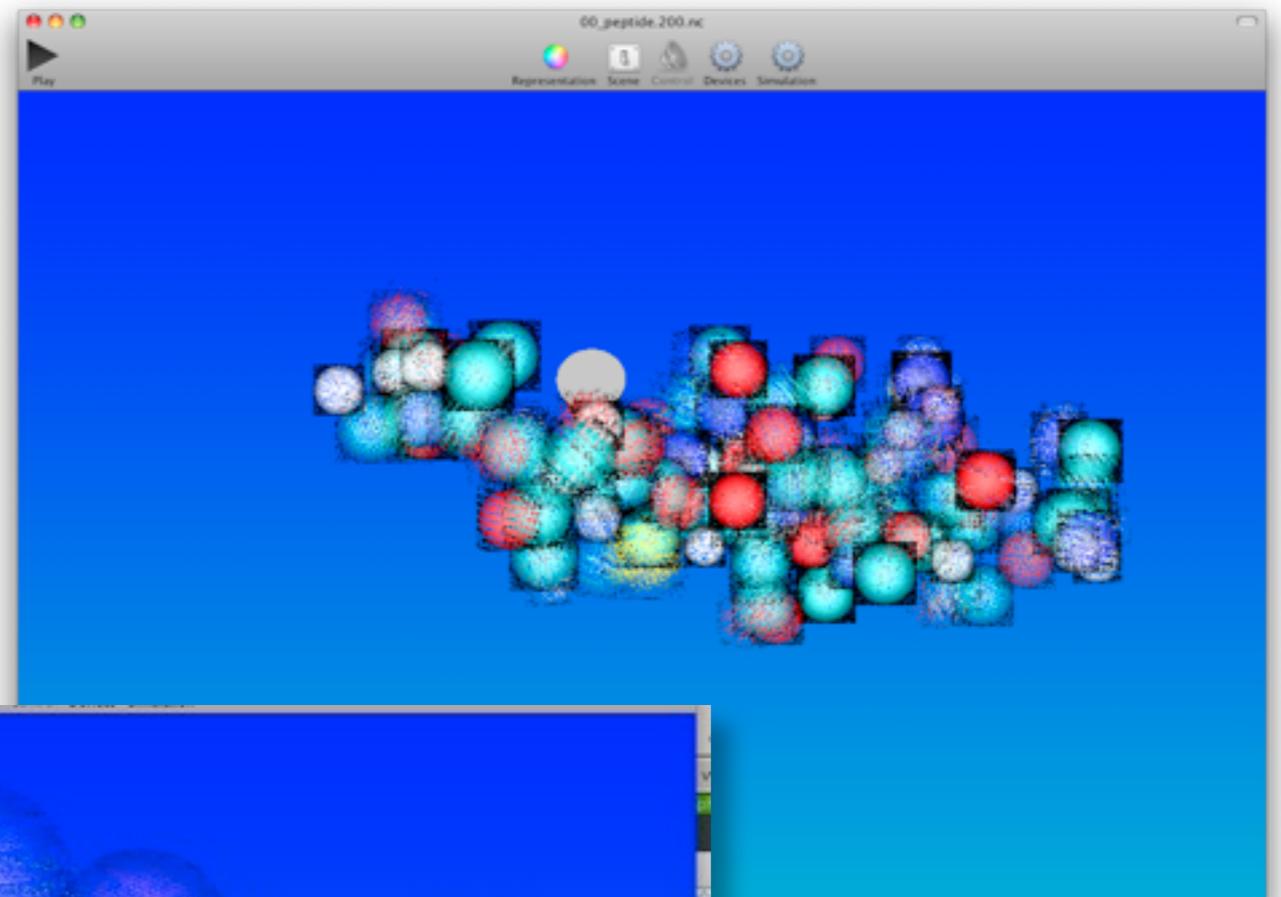
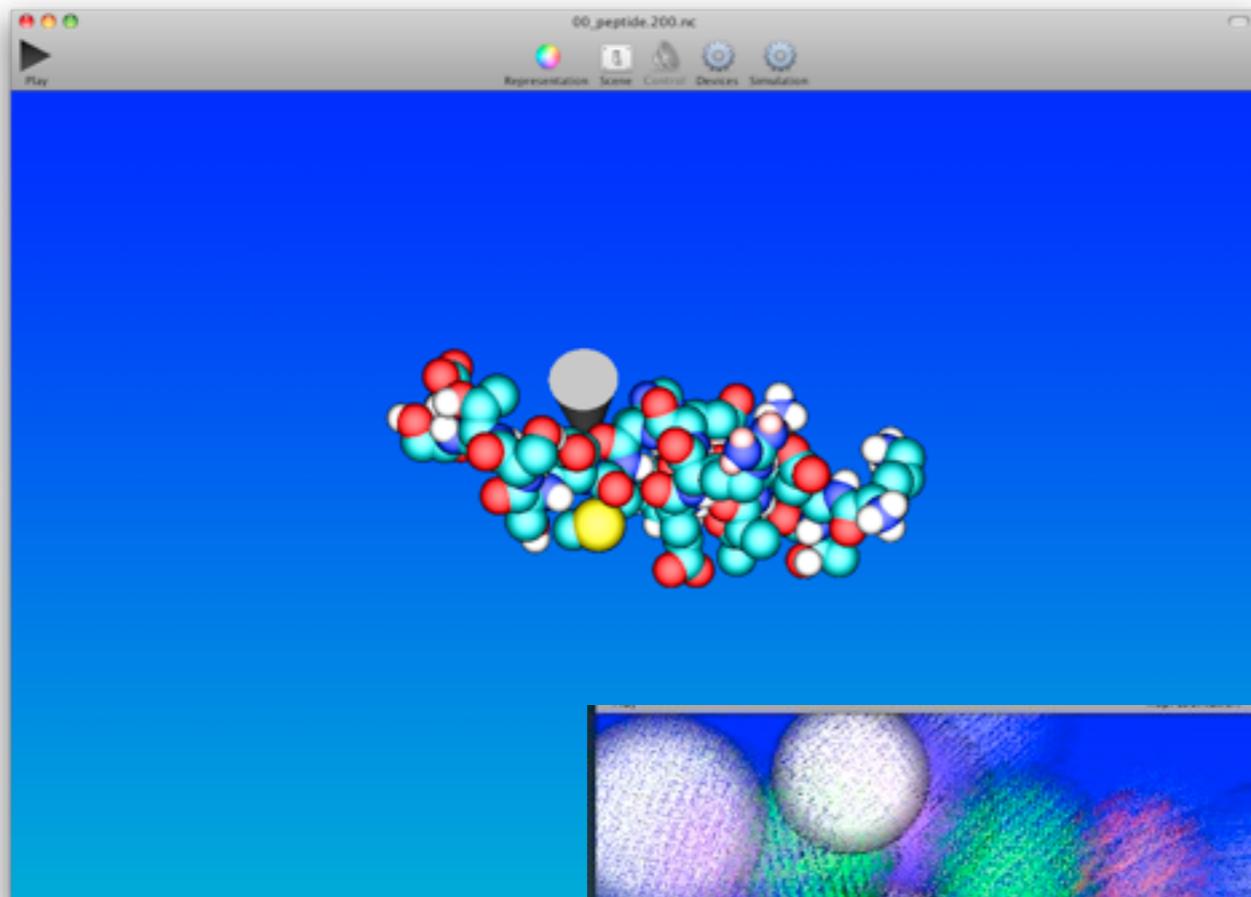


VTK / BioSpagetthi

- **First VTK implementation (2006)**
using vtkSpheres
- **VR devices using vtkVRPN**
Aguilera, Carrard & Guilbaud
- **Performance issues**
Reduce number of actors & ...
- **GLSL shaders by Latapie & Biddiscombe**
CSCS implementation (FastSphere point sprites)
- **some bugs** (ExactSphere).. and no HyperBalls, yet

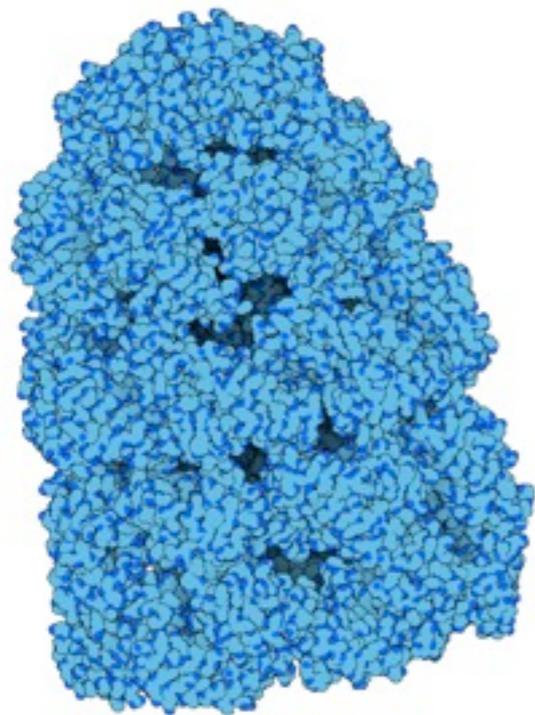


ExactSphere shader bug

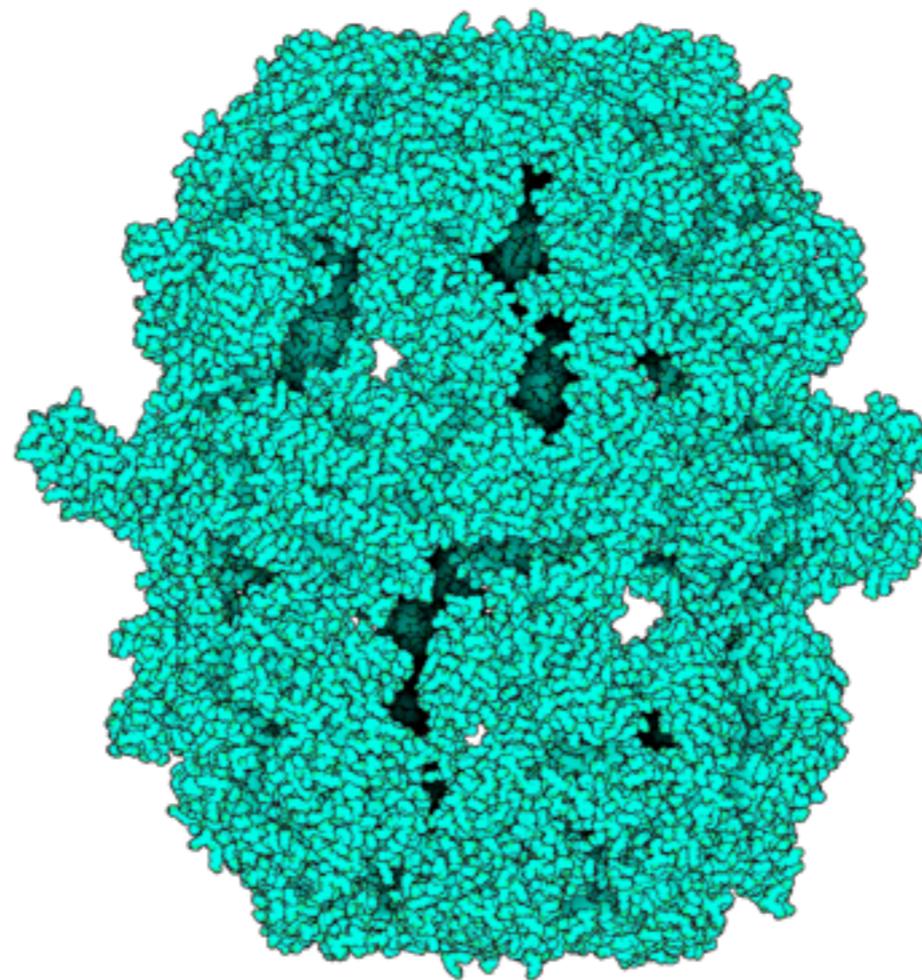


HyperBalls on GPU: outlook on lighting effects

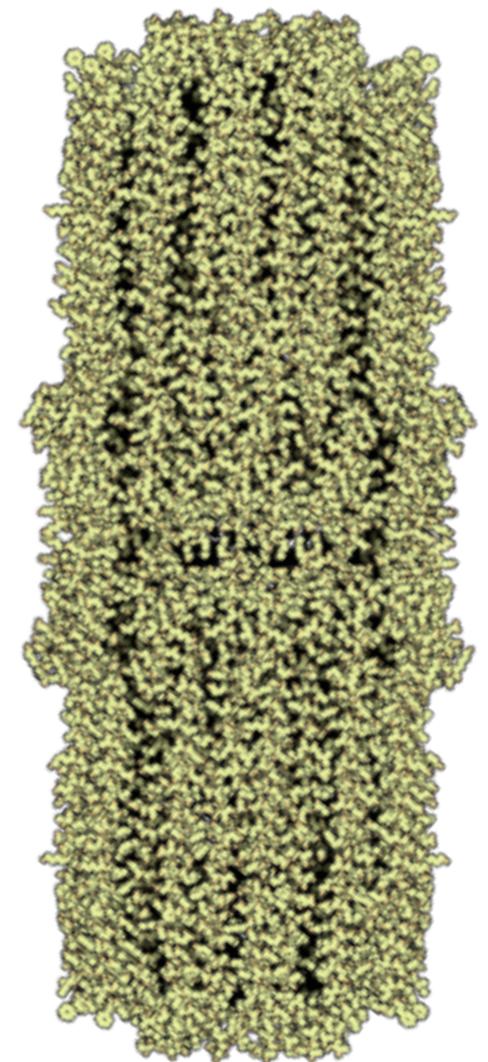
- *Cel shading + Ambient Occlusion :*



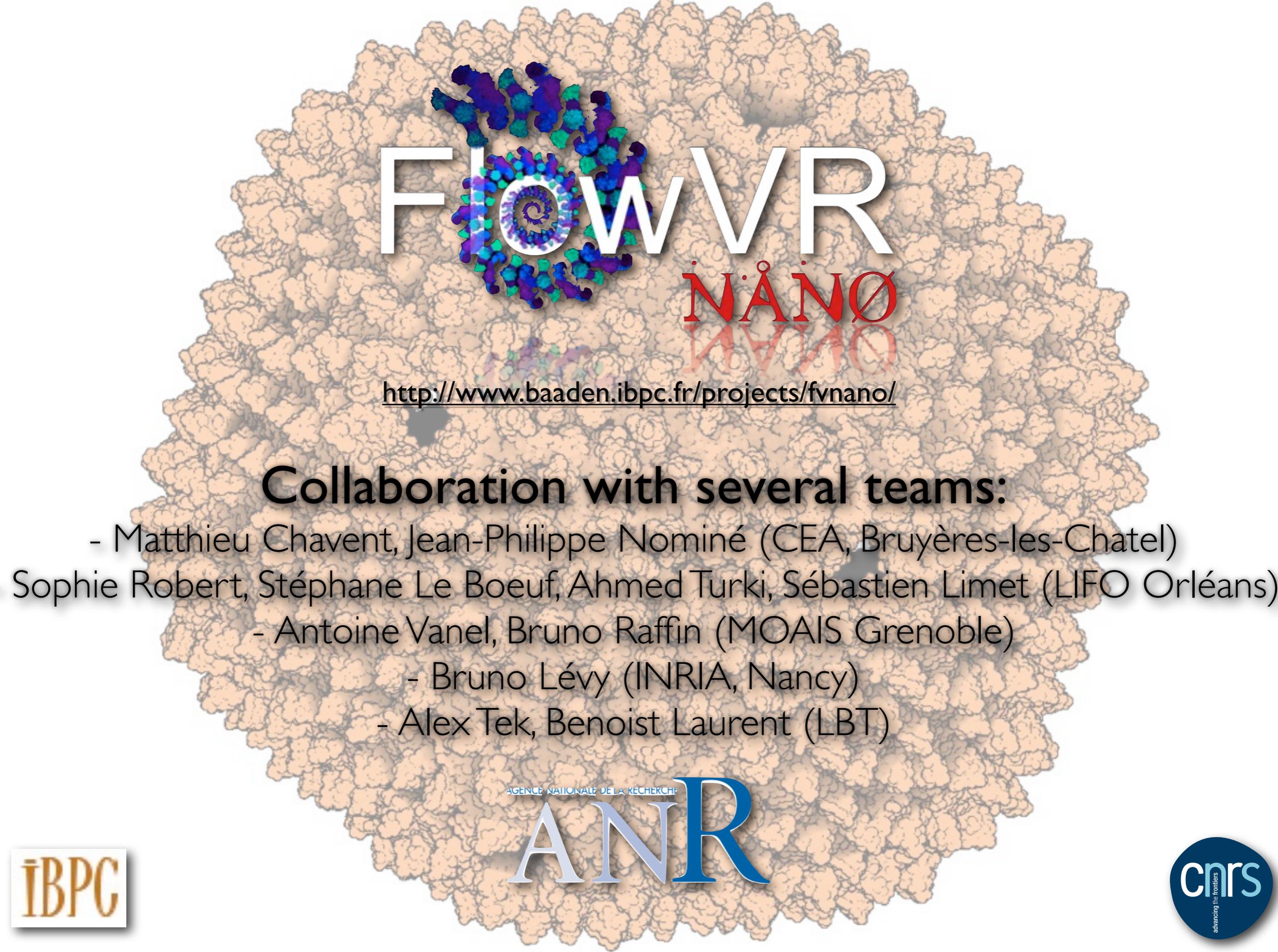
GroEl-GroES (58870 atoms)



Fatty Acid Synthase (166485 atoms)



Cytolisin (53832 atoms)



FlowVR

NANO

<http://www.baaden.ibpc.fr/projects/fvnano/>

Collaboration with several teams:

- Matthieu Chavent, Jean-Philippe Nominé (CEA, Bruyères-les-Chatel)
Sophie Robert, Stéphane Le Boeuf, Ahmed Turki, Sébastien Limet (LIFO Orléans)
- Antoine Vanel, Bruno Raffin (MOAIS Grenoble)
- Bruno Lévy (INRIA, Nancy)
- Alex Tek, Benoist Laurent (LBT)

AGENCE NATIONALE DE LA RECHERCHE

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advancing the frontiers