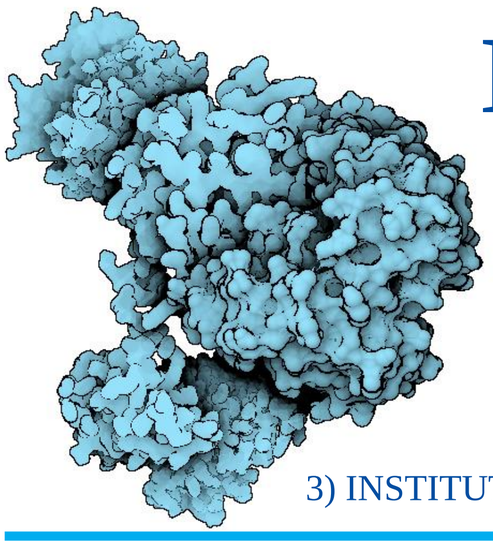
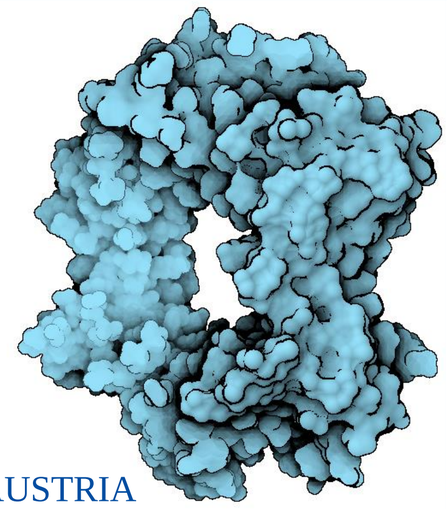


Importance Driven Visualization of Molecular Surfaces



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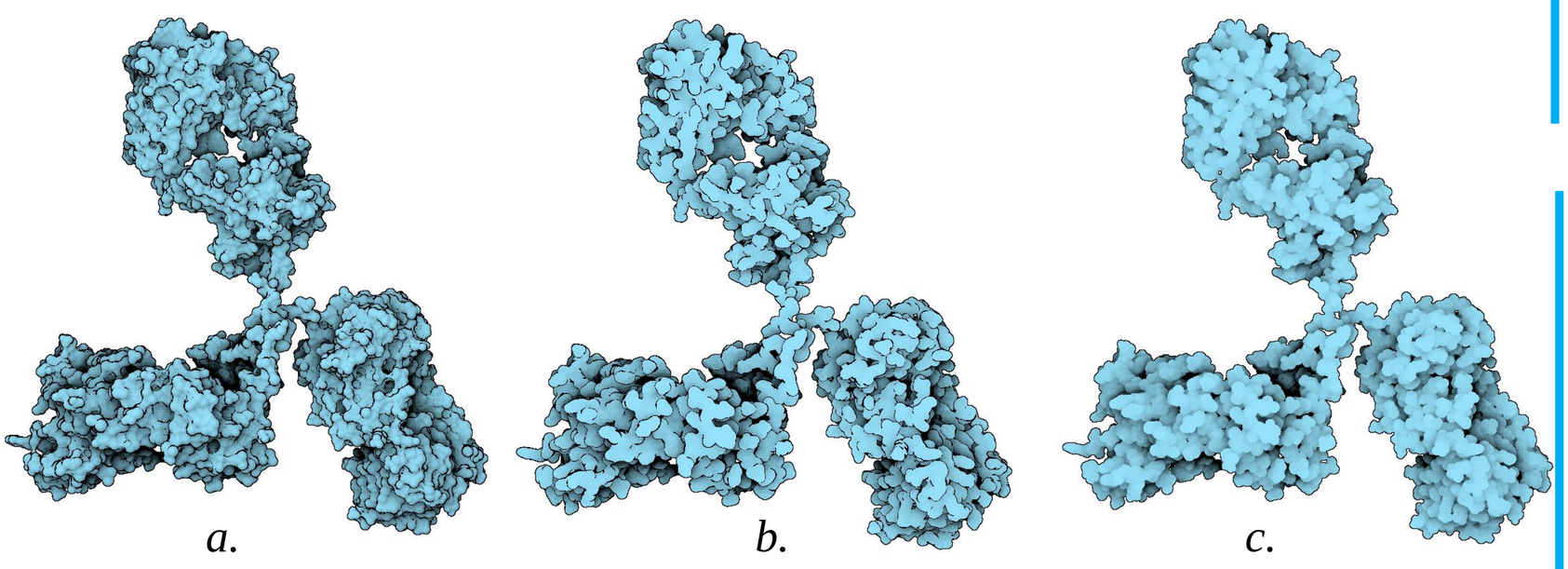
Molecular Visualization

- Molecular data are obtained through molecular dynamics on the initial set of atoms.
- One way to analyze the molecular data is through molecular surface visualization.
- We exploit three popular surface models: *a.* Solvent Excluded Surface (SES), *b.* Gaussian Kernel Model, *c.* van der Waals Surface*)*.



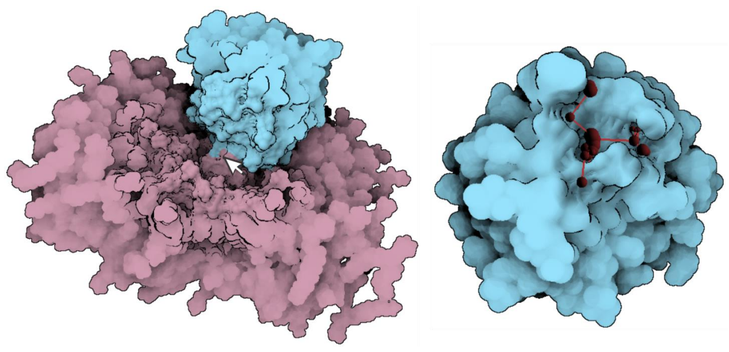
a. *b.* *c.*

Approach

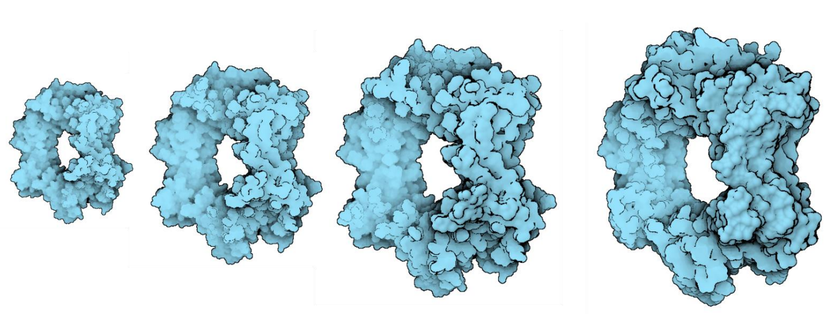
- Combinations of different molecular surface representations and shading styles in level of detail (LOD) manner [1].
- LOD is determined by the importance function defined by the camera distance.
  - **Model**: Closest to the viewer we aim at providing a maximum of relevant information related to the structure and binding sites. Farther away from the viewer, we are smoothly changing the visual representation to an approximation of SES through Gaussian kernels. Farthest away from the viewer, we employ the least detailed representation via simple spheres.
  - **Shading**: For shape detail, we employ local diffuse shading model. For relative depth, we employ ambient occlusion. Ordinal depth cues are communicated with contour rendering and the figure-ground ambiguity is resolved with silhouette rendering. We have a specific distribution of visual cues for each level of detail.

Results

- Through our LOD concept we are able to boost the rendering performance of molecular models by 5-10x.



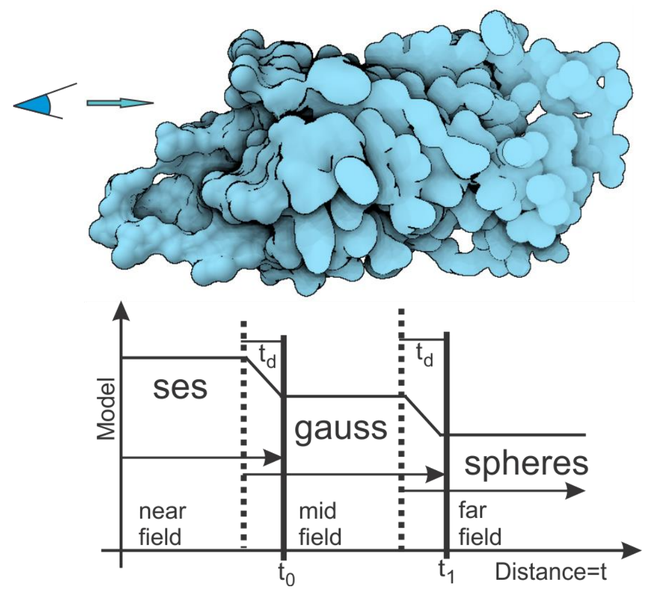
Two different versions of the LOD function. Individual fields are determined through mouse based interaction (left), and via a distance from the cavity centerline (right).



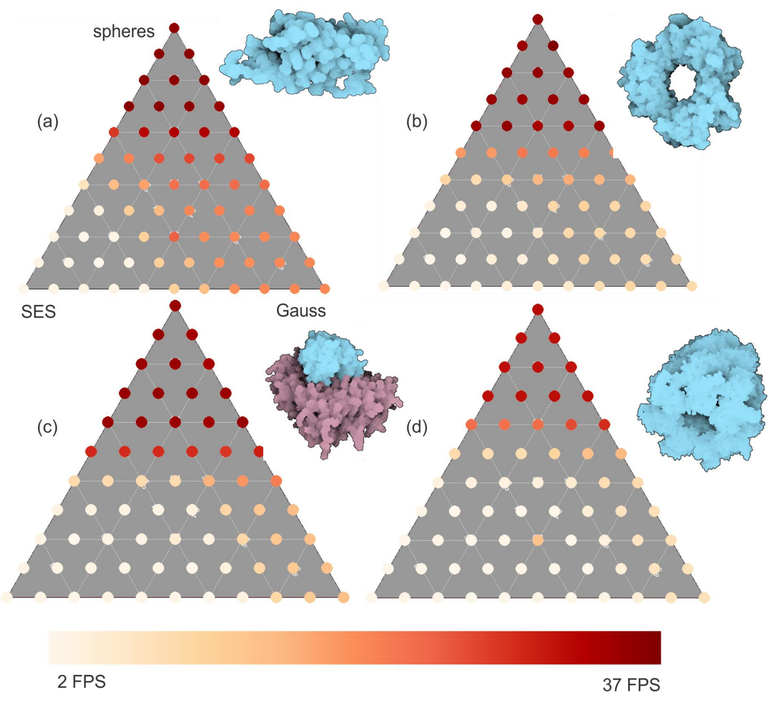
An example of zooming in towards the molecule (proliferatic cell nuclear antigen). When fields are fixed, we obtain more and more details at every zoom level.

Motivation

- Boost rendering performance.
- Introduce *focus and context* technique on molecular surfaces – depict details only when necessary.
- Study illustrative visualization on molecule surfaces.
- Motivated by the workflow proposed by David Goodsell [2].



The organization of the three surface and shading levels according to importance function defined by the increasing distance from the camera. In the overlapping zones, the representations are merged using linear interpolation.



Ternary plots showing performance analysis evaluated on four distinct MD datasets. The analysis is based on the lengths of individual fields The achieved FPS are directly proportional to the lengths of each areas.

Acknowledgments

We give thanks to Nathalie Reuter for providing the molecular dynamics simulation datasets, David Goodsell and Helwig Hauser for giving us the necessary feedback for the overall visualization. This work has been carried out within the PhysioIllustration research project (NFR, #218023). This paper has been also supported by the Vienna Science and Technology Fund (WWTF) through project VRG11-010, and also by grants from the Excellence Center at Linköping and Lund in Information Technology (ELLIIT) and the Swedish e-Science Research Centre (SeRC), as well as VR grant 2011-4113.

References

[1] J. Parulek, T. Ropinski, I. Viola. Seamless Abstraction of Molecular Surfaces, Spring Conference on Computer Graphics (SCCG 2013) , 2013, pp. 120-127

[2] Goodsell, D.S. (2003) Illustrating Molecules. In The Guild Handbook of Scientific Illustration, Second Edition (E.R.S. Hodges, ed.) Chapter 15, pp. 267-270..

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