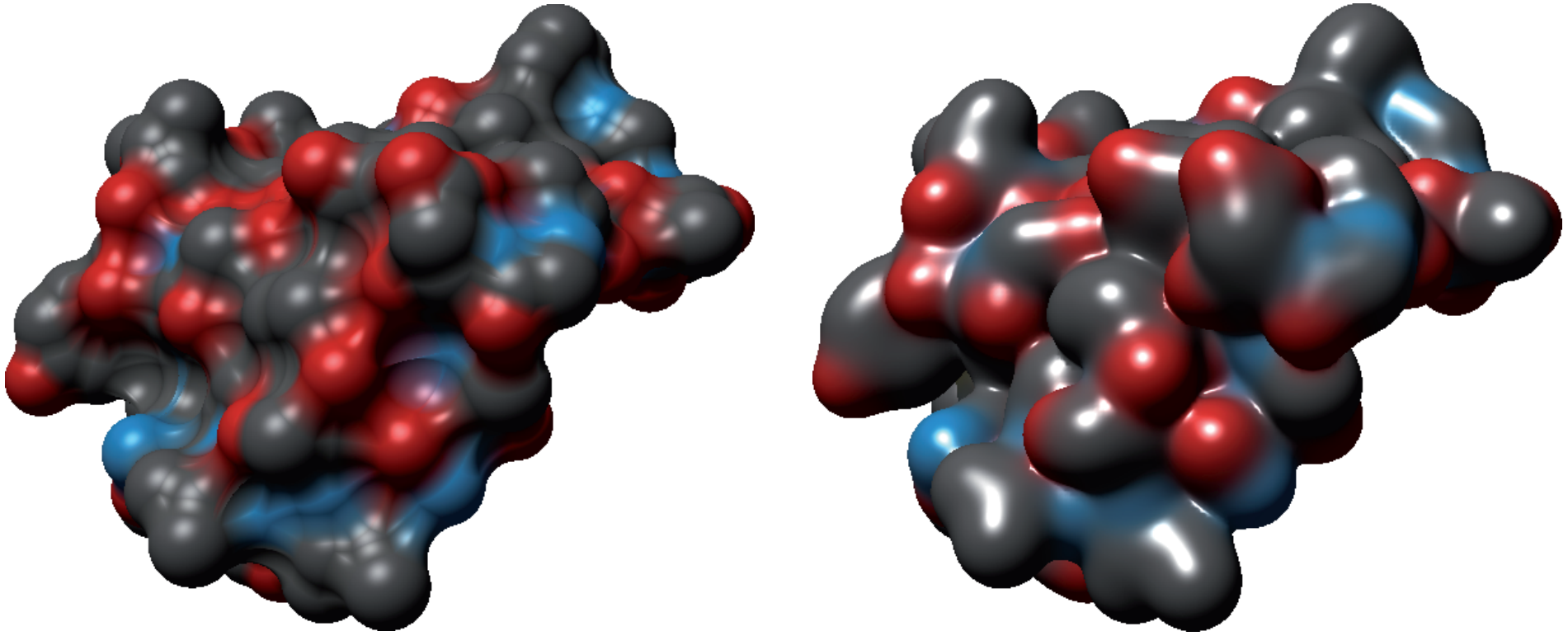
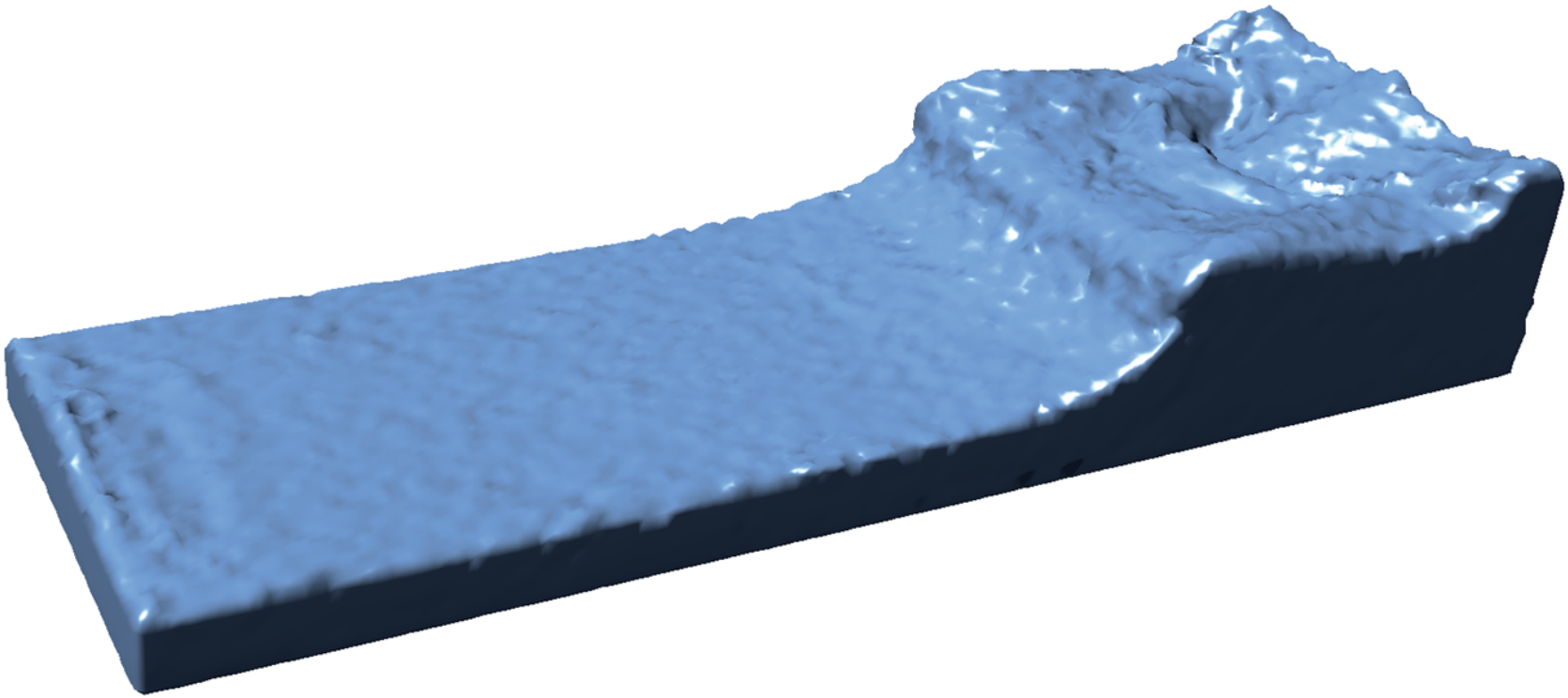
M. Krone, J. E. Stone, T. Ertl, K. Schulten: „Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories“.



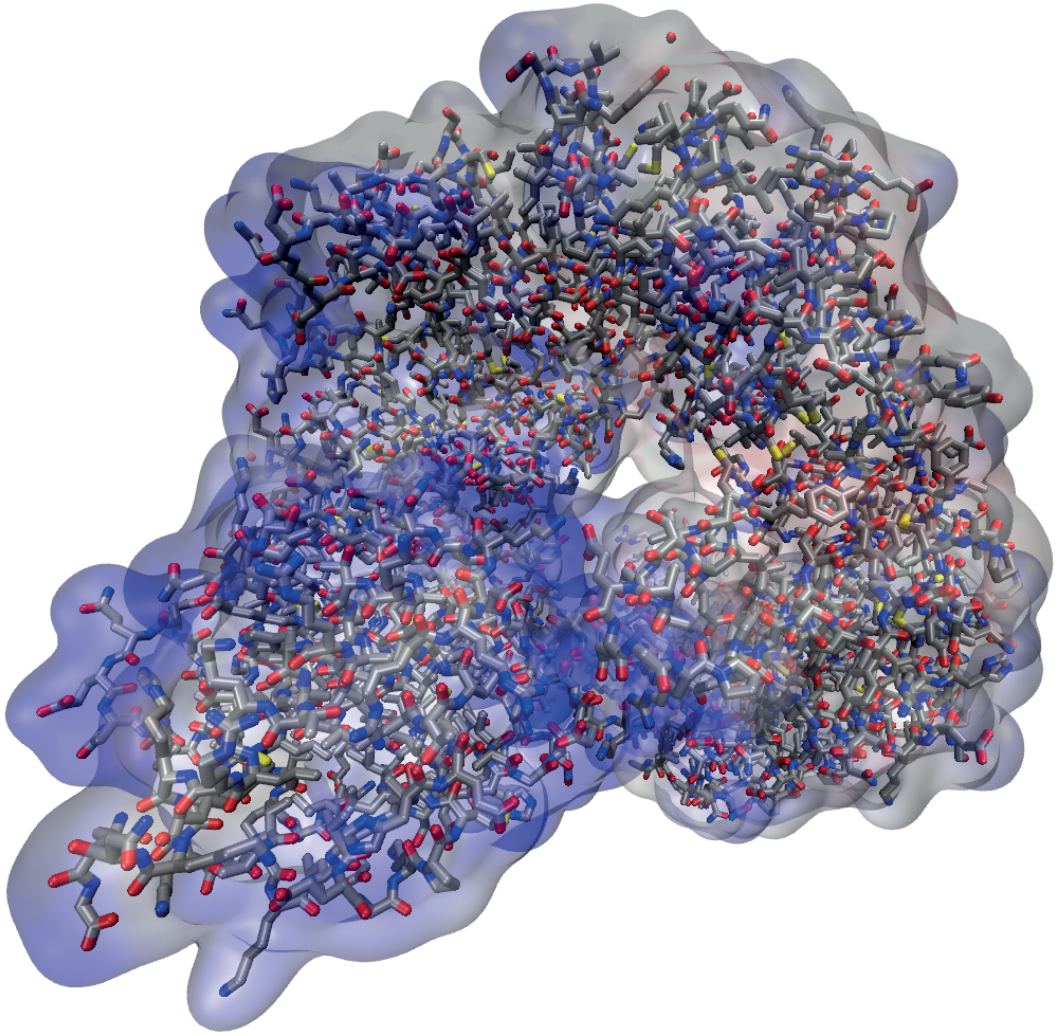
Comparison between Solvent Excluded Surface (left) and our method (right).
PDB-ID: 1CRN (http://www.pdb.org)

M. Krone, J. E. Stone, T. Ertl, K. Schulten: „Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories“.



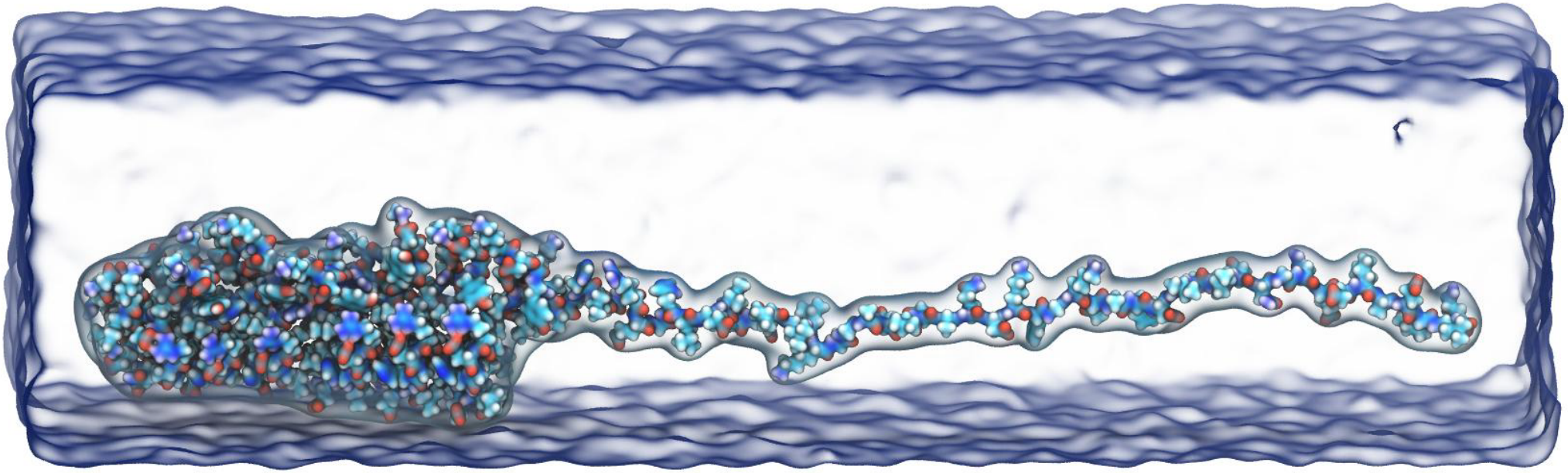
Computational Fluid Dynamics data set from a Smoothed Particle Hydodynamics (SPH) Simulation (200,000 particles)

M. Krone, J. E. Stone, T. Ertl, K. Schulten: „Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories“.



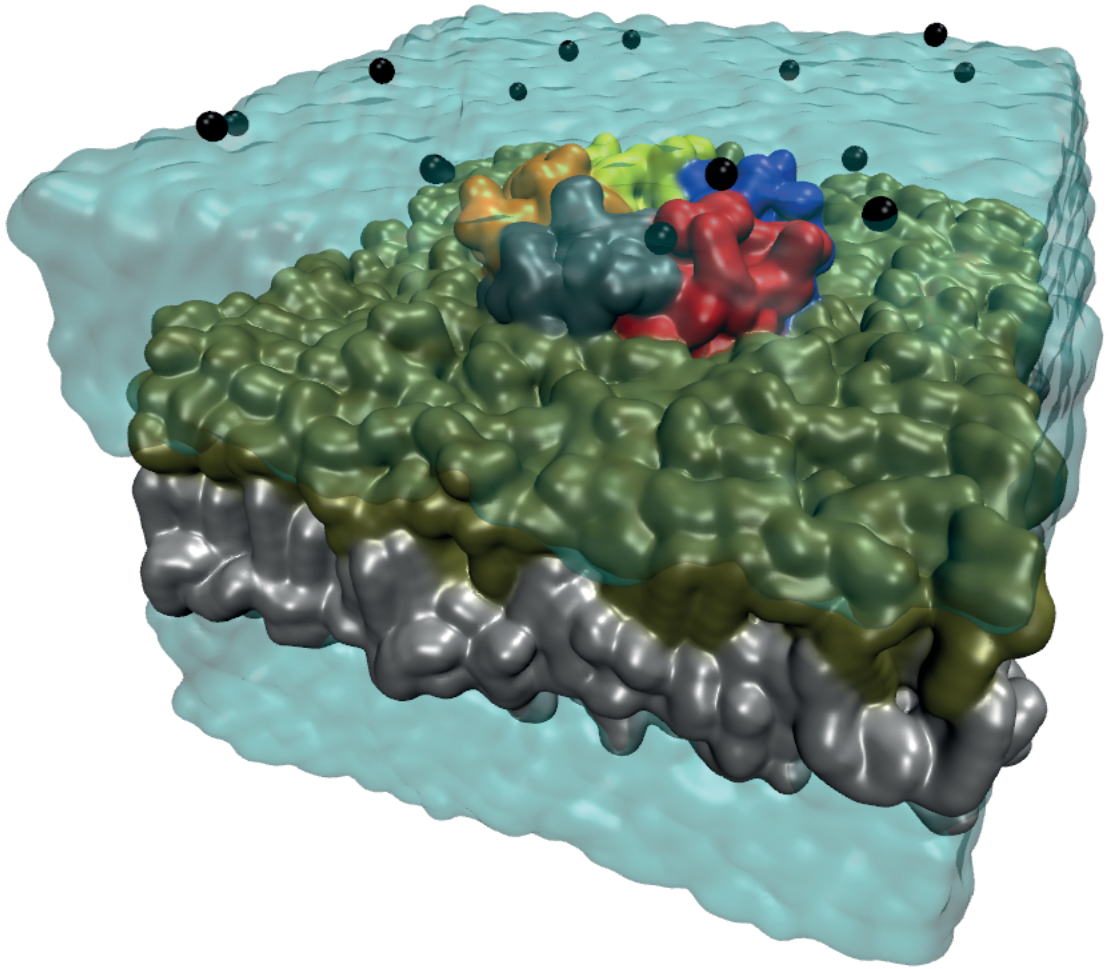
Molecular Surface of a protein (PDB-ID: 1QGK, ~7,000 atoms) used for the comparison with Dias et al. [DG11]. The density map resolution was set to 0.5 Angstrom (as in [DG11]). In this screenshot, the surface is blended with a stick representation of the protein.

M. Krone, J. E. Stone, T. Ertl, K. Schulten: „Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories“.



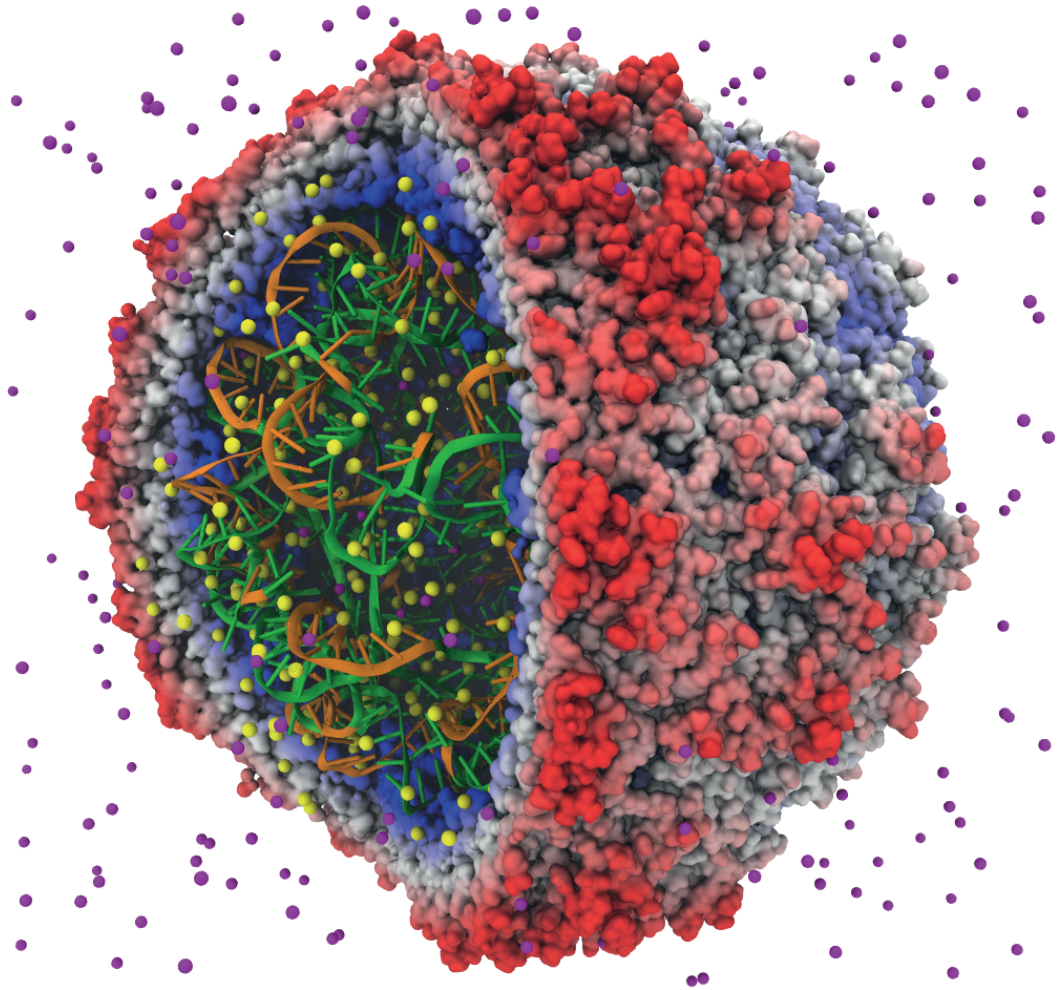
Ankyrin (4,200 atoms) simulated in water (204,600 atoms in total).
While the protein is rendered in atomic detail, the semi-transparent, blue water box is rendered in reduced detail to show the context.

M. Krone, J. E. Stone, T. Ertl, K. Schulten: „Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories“.



Small membrane patch with a transmembrane protein and ions in water (100,000 atoms). Please note that the black ions are not ray casted spheres but also rendered with our method using a density grid resolution of 0.5 Angstrom.

M. Krone, J. E. Stone, T. Ertl, K. Schulten: „Fast Visualization of Gaussian Density Surfaces for Molecular Dynamics and Particle System Trajectories“.



Raytraced surface of the STMV virus capsid data set (147,976 atoms, test data set 1) combined with the interior RNA rendered as ribbons and ions rendered as spheres. The image was rendered using the batch mode Tachyon raytracer which is included in the molecular modeling program VMD (http://www.ks.uiuc.edu/Research/vmd/). The triangulated molecular surface was computed in VMD using our algorithm and can be used for interactive rendering of dynamic data as well as offline ray tracing.