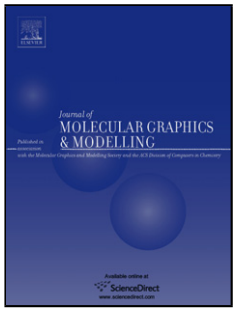

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High quality rendering of protein dynamics in space filling mode

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Abstract

Producing high quality depictions of molecular structures has been an area of academic interest for years, with visualisation tools such as UCSF Chimera, Yasara and PyMol providing a huge number of different rendering modes and lighting effects. However, no visualisation program supports per-pixel lighting effects with shadows whilst rendering a molecular trajectory in space filling mode.

In this paper, a new approach to rendering high quality visualisations of molecular trajectories is presented. To enhance depth, ambient occlusion is included within the render. Shadows are also included to help the user perceive relative motions of parts of the protein as they move based on their trajectories. Our approach requires a regular grid to be constructed every time the molecular structure deforms allowing per-pixel lighting effects and ambient occlusion to be rendered every frame, at interactive refresh rates. Two different regular grids are investigated, a fixed grid and a memory efficient compact grid.

The algorithms used allow trajectories of proteins comprising of up to 300,000 atoms in size to be rendered at ninety frames per second on a desktop computer using the GPU for general purpose computations. Regular grid construction was found to only take up a small proportion of the total time to render a frame. It was found that despite being slower to construct, the memory efficient compact grid outperformed the theoretically faster fixed grid when the protein being rendered is large, owing to its more efficient memory access patterns. The techniques described could be implemented in other molecular rendering software.

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