

W0037

Approximating Short-Range Lee-Richards Molecular Surfaces by Blurring. Peter N. Zhivkov, Herbert J. Bernstein, Dowling College, Oakdale, NY 11769, USA.

In 1971, Lee and Richards defined a molecular surface as the surface resulting from rolling a probe sphere on the van der Waals surface of a molecule. Much of the molecular surface is identical to the van der Waals surface, namely where the probe contacts only one atom, but a large amount of additional computation is needed when the probe contacts two or more atoms at the same time. Geometrically the van der Waals surface consists of intersecting spherical segments. When the probe rolls between pairs of atoms, toroidal segments need to be generated. When the probe touches three or more atoms at the same time, spherical triangular segments need to be generated. Accurate calculation and rendering of these additional surface segments is computationally demanding and limits the size of structures for which molecular surfaces can be rendered in real time. We propose an alternate approach to rendering of the short range toroidal segments by blurring pixels in the z-buffer of a van der Waals surface rendering. Computational efficiency is gained by avoiding any rendering of toroidal segments buried within the surface and by replacing a full calculation of the visible short-range toroidal segments with a localized averaging of pixels from van der Waals surfaces of adjacent atoms. The blurring is limited to the intersecting regions, so the overall surface edges remain sharp. This produces a very different image from molecular surfaces simulated by blurring an entire image to a coarser resolution. The technique lends itself well to combination with analytic calculation of toroidal segments between atoms that are too far apart for blurring to be workable and analytic calculation of spherical caps that are large enough to be seen. In addition, this blurring technique helps in comprehending the van der Waals surface by suppressing the visual distractions of the intersections between atoms when one does not wish to expend the computational resources to render the entire molecular surface.

Work supported in part by NSF grants EF-0312612 and DBI-035281.