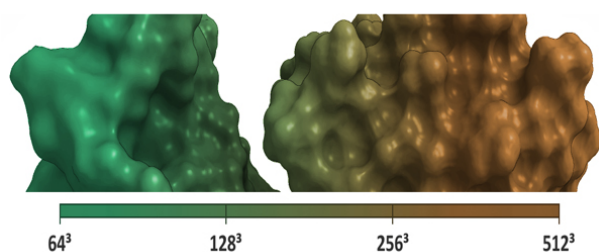


# Interactive GPU-based Generation of Solvent Excluded Surfaces

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The Solvent Excluded Surface (SES) is a popular molecular representation that gives the boundary of the molecular volume with respect to a specific solvent. SESs depict which areas of a molecule are accessible by a specific solvent, which is represented as a spherical probe. Despite the popularity of SESs, their generation is still a compute-intensive process, which is often performed in a preprocessing stage prior to the actual rendering (except for small models). For dynamic data or varying probe radii, however, such a preprocessing is not feasible as it prevents interactive visual analysis. Thus, we present a novel

approach for the on-the-fly generation of SESs, a highly parallelizable, grid-based algorithm where the SES is rendered using ray-marching. By exploiting modern GPUs, we are able to rapidly generate SESs directly within the mapping stage of the visualization pipeline. Our algorithm can be applied to large time-varying molecules and is scalable, as it can progressively refine the SES if GPU capabilities are insufficient. In this paper, we show how our algorithm is realized and how smooth transitions are achieved during progressive refinement. We further show visual results obtained from real world data and discuss the performance obtained, which improves upon previous techniques in both the size of the molecules that can be handled and the resulting frame rate.