Molecular Surface Computation

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Introduction

Among the geometric representations commonly used in molecular visualization, surface mesh representations are particularly useful since they can be created from many types of input data. Several useful surface representations types can be generated by isosurface extraction algorithms applied to volumetric density map data acquired via X-ray crystallography, cryo-electron microscopy, or by synthesis from atomic coordinate data. As progress continues to be made in reconstruction and modeling of large biomolecular complexes (4096^3 voxel density maps, 10^7 atom molecular models), visualization and analysis tools must utilize parallel processing and GPU accelerated computation in order continue to operate effectively.

Description

Although many algorithms exist for the purpose of calculating molecular surfaces, the natural strengths of the GPU hardware and broad applicability of surface algorithms based on isosurface extraction techniques make them an excellent starting point for GPU acceleration with CUDA. There are a number of well known algorithms for isosurface extraction which could be selected for this project. The Marching Cubes and Marching Tetrahedra algorithms can be adapted for use on a GPU. These algorithms find and compute density isovalues along the edges of rectangular or tetrahedral cells, and reconstruct the triangulated surface(s) passing through each cell. Since each grid cell can be considered independently of others, there is a great degree of data parallelism available for a GPU accelerated CUDA implementation. Although the grid cells can be calculated independently, elimination of redundant memory accesses will necessitate a carefully planned parallel decomposition.

Objective

The proposed project will require implementing two variants of a GPU accelerated isosurface extraction algorithm. The first version will operate on pre-computed volumetric density maps. The second version will be a minor variation of the same algorithm, computing densities on-the-fly from a set of atom coordinates, using Blinn's "Blob" electron density approximation. Test density maps will be provided, ranging from 64^3 up to 1024^3 voxels or more. Equivalent complexity atomic coordinate datasets will be provided for use with the on-the-fly variant of the isosurface extraction algorithm. The extracted surface mesh will be returned to host memory. The key goals of the GPU accelerated implementation are to achieve high performance, efficient use of

GPU hardware resources, and to report on limitations of the hardware for the selected isosurface extraction algorithm.

Background

No specialized knowledge is necessary to work on the application, since the algorithms are well known and extensive reference materials and source code are available. Having some background in computer graphics will be helpful when reading published literature.

Resources

Algorithm references, papers, and sample code will be made available online: http://www.ks.uiuc.edu/Research/vmd/projects/ece498/

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