Geometric Modeling of Nano Structures with Periodic Surfaces

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Abstract. Commonly used boundary-based solid and surface modeling methods in traditional computer aided design are not capable of constructing configurations with large numbers of particles or complex topology. In this paper, we propose a new geometric modeling scheme, periodic surface, for material design at atomic, molecular, and meso scales. At molecular scale, periodicity of the model allows thousands of particles to be built efficiently. At meso scale, inherent porosity of the model represents morphology of polymer and macromolecule naturally. Model construction and operation methods are developed to build crystal and molecular models based on periodic surfaces.

1 Introduction

To accelerate the development of nanotechnology, computer aided design tools are critical to solve the “lack of design” issue, meaning that no extensive and systematic design of nano systems is available compared to other traditional engineering domains such as mechanical mechanisms and electronic circuits. Computer aided nano design (CAND) is to enable engineering design, traditionally at the component and system levels, to be extended to nano scales. CAND helps to set functional objective, construct model, simulate and optimize design, and guide laboratory effort during physical property implementation.

Existing atomic and molecular simulation methods such as density function theory, molecular mechanics, Monte Carlo, and molecular dynamics and related tools enable scientists to visualize molecular structure and behavior, calculate properties such as electrical conductivity, elasticity, and thermodynamics, as well as to simulate reactions between molecules. This simulation-based approach saves time and resources of conducting real experiments to study material properties and interactions of molecules, which has started being used in drug and material design. Material properties can solely be calculated, and the results become the input of bulk-scale finite element analysis. Nevertheless, lack of efficient compound construct methods for large quantities of atoms and molecule becomes the bottle-neck of CAND. A good initial geometry is required to find optimal molecular configuration in simulation. Providing chemists good geometry conformation that is reasonably close to true minimum energy is highly desirable to save simulation time and lessen the risk of trapping into local minima.

Based on the observation that hyperbolic surfaces exist in nature ubiquitously, we propose a new geometric modeling scheme, periodic surface model to support
multi-scale modeling and simulation. This surface model is based on non-Euclidean geometry that allows for rapid model construction ranging from atoms to polymers. Model construction and operations are introduced to create compounds with thousands of elements or structures with complex topology. It takes a generic approach to explore symmetric tiling and packing of loci surfaces in 2D hyperbolic space and subsequently map into conventional 3D Euclidean space. 3D structures can also be built with foci searching based on surface envelops.

In the rest of the paper, Section 2 gives a background of molecular scale geometric modeling and minimal surface in nano structures. Section 3 introduces periodic surface modeling and associated operations. Section 4 describes the symmetric tiling methods to create mapping from 2D hyperbolic space to 3D Euclidean space, followed by the surface enclosure method of model creation in Section 5.

2 Background

2.1 Molecular Scale Geometric Modeling

At the molecular scale, atoms and particles are represented by geometry (coordinates of positions in Euclidean space) and topology (connection between atoms). Traditionally used visualization methods are space-filled, wireframe, stick, ball and stick, and ribbon models, as illustrated in Fig.1.

![Fig. 1. Different types of visualization models for molecules](image)

To reduce graphic processing time, there has been some research on molecular surface modeling [1]. Lee and Richards [2] first introduced solvent-accessible surface, the locus of a probe rolling over Van der Waals surface, to represent boundary of molecules. Connolly [3] presented an analytical method to calculate the surface. Recently, Bajaj et al. [4, 5] represent solvent accessible surface by NURBS (non-uniform rational B-spines). Carson [6] represent molecular surface with B-spline wavelet. These research efforts concentrate on boundary representation of molecules mainly for visualization, while model construction itself is not considered.

In order to support design and analysis from both material and engineering perspectives, computational models need to accommodate the need of model construction at multiple levels from atomic, to molecular, meso, and bulk scales. Traditional boundary representation of objects is not efficient for geometric modeling at nano scales. Creation of parametric model for multi-scale uses instead of simple “seamless zooming” is important.