Journal of Molecular Graphics and Modelling 50 (2014) 44–49

Contents lists available at ScienceDirect

Journal of Molecular Graphics and Modelling

journal homepage: www.elsevier.com/locate/JMGM

Topical Perspectives

VCMM: A visual tool for continuum molecular modeling

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ARTICLE INFO

Article history:
Accepted 8 March 2014
Available online 28 March 2014

Keywords:
Continuum molecular modeling
Visualization
Visual analysis
Unstructured mesh
Numerical solvers

ABSTRACT

This paper describes the design and function of a visualization tool, VCMM, for visualizing and analyzing data, and interfacing solvers for generic continuum molecular modeling. In particular, an emphasis of the program is to treat the data set based on unstructured mesh as used in finite/boundary element simulations, which largely enhances the capabilities of current visualization tools in this area that only support structured mesh. VCMM is segmented into molecular, meshing and numerical modules. The capabilities of molecular module include molecular visualization and force field assignment. Meshing module contains mesh generation, analysis and visualization tools. Numerical module currently provides a few finite/boundary element solvers of continuum molecular modeling, and contains several common visualization tools for the numerical result such as line and plane interpolations, surface probing, volume rendering and stream rendering. Three modules can exchange data with each other and carry out a complete process of modeling. Interfaces are also designed in order to facilitate usage of other mesh generation tools and numerical solvers. We develop a technique to accelerate data retrieval and have combined many graphical techniques in visualization. VCMM is highly extensible, and users can obtain more powerful functions by introducing relevant plug-ins. VCMM can also be useful in other fields such as computational quantum chemistry, image processing, and material science.

1. Introduction

In biomolecular simulation studies, the explicit solvent methods treat the solvent in full atomic detail, and the implicit solvent methods represent the solvent through its average effect on the solute. Explicit solvent methods are demanding a large number of freedom because they offer a very detailed description of the solvent and ions, whereas implicit solvent methods enjoy the advantage of reduced degrees of freedom. The Poisson–Boltzmann (PB) equation represents a typical implicit solvent model, and provides a simplified continuum description of the discrete particle (e.g., water, ion, and even protein molecule) distributions in solution, as well as the electrostatic interaction of a solvated system at equilibrium state [1–3]. The Poisson–Nernst–Planck (PNP) model provides a continuum description of the non-equilibrium electrodiffusion process of ion transport in solution [4].

Finite difference and finite volume methods dominate the methodologies used in PB solvers in biochemical and biophysical communities. These solvers are based on structured meshes, and the molecular surface is used to define the map of the dielectric function. However, the position of the molecular surface is usually not precisely computed and constructed, and the normal direction of the molecular surface is not calculated, which leads to a neglect of the continuity conditions on the solution. In recent years, there are much research efforts on the boundary element methods (BEM) and finite element methods (FEM) (e.g., see [2,5–13]). With the presence of surface mesh conforming to the molecular boundary, the solutions of these methods automatically satisfy the continuity conditions at the molecular boundary, hence leading to more accurate results. Unlike finite difference methods using structured grid, those methods are based on unstructured mesh, which will lead to many new issues in visualization and data analysis/management.

Visual analysis is an important part of scientific computations. There have been many tools for molecular visualization. Pymol [14] and VMD [15] are among the most popular ones nowadays. GRASP is another program with particular emphasis on the display and manipulation of the surfaces of molecules and their electrostatic properties [16]. However, these software packages lack the capability of unstructured mesh management and visual analysis of numerical results based on unstructured mesh. Furthermore, these packages do not provide functions for BEM and FEM simulations. Therefore, a molecular visualization tool with these functions is an urgent need.

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http://dx.doi.org/10.1016/j.jmgm.2014.03.006
1093-3263/

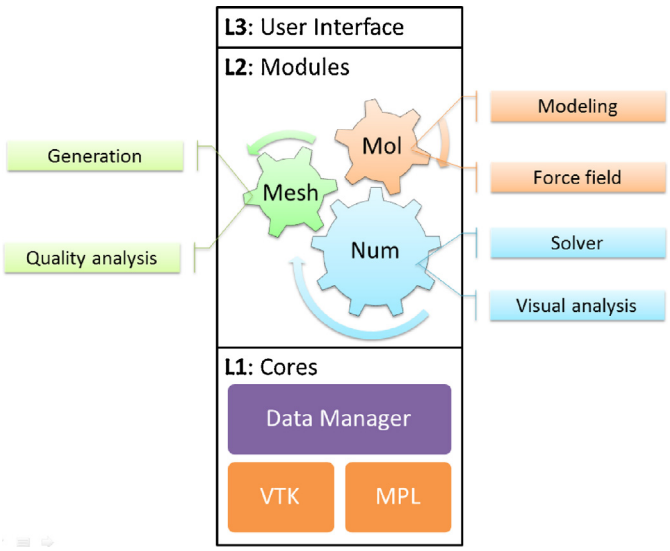

Fig. 1. Schematic design of the VCMM architecture.

This paper will report a general visual tool, VCMM, for continuum molecular modeling with focal applications of BEM and FEM. We developed a mesh dividing technique based on molecular structure to manage the large molecular mesh, which enables VCMM to have a high efficiency of handling molecular mesh. A variety of visual analysis tools are designed for the numerical results of BEM and FEM solvers. To facilitate the simulation processes, VCMM has integrated into a tool chain. The tool chain includes the following parts:

1 Molecular visualization and force field tools.
2 Surface and volume mesh generation tools.
3 Mesh visualization and analysis tools.
4 BEM and FEM solvers.
5 Numerical results visualization and analysis tools.

The organization of this article is as follows. The design and overview of VCMM are introduced first, followed by a description of the features of each module. We then also give a demonstrating example including a whole process of molecular electrostatic modeling. Finally, we discuss the future outlook, list the availability, and end up with acknowledgments.

2. Design and overview

The frame of VCMM is written in Python and the cores are written in C++. VCMM is designed as a layered architecture as showned in Fig. 1. The first layer contains a data manager and two visual packages: visualization toolkit (VTK) [17] and Matplotlib (MPL) [18]. The data manager is designed to handle various types of data (e.g., PDB [19], PQR, OFF, MESH, and VTK.) and is used in each module and visualization. The second layer is a logical layer, which can control the simulation process. This layer consists of three modules: molecular module, meshing module and numerical module. More details of the three modules will be described later. The third layer is the graphical user interface including user-computer interactions. Currently, VCMM runs on Microsoft Windows and Linux systems.

The main interface window of VCMM is shown in Fig. 2. There are several regions at the user interface including the Menu Bar on the top, the Left Panel on the left side, the Status Bar at the bottom and the Render Area in the middle. These regions are described as below.

- *The Menu Bar*: The menu bar provides access to functions such as opening files, managing data, starting modules and invoking plug-ins.
- *Left Panel*: The left panel is a data manager. A data list and several buttons can be handled by users to manage memory.
- *Render Area*: The Render Area is where the 2D/3D representation of the scene is rendered. Mouse and keyboard interactions are provided in this area.
- *Status Bar*: There are some tips on the Status Bar including error messages, help messages and other information.

3. Modules

3.1. Molecular module

Molecular visualization is a main part of the molecular module. VCMM reads in a molecule coordinate file from the data manager and interactively displays the molecule on the screen in a variety of color schemes and molecule representations. VCMM supports most of the common representations for molecular structures: ball-and-stick, spheres, wire bonds, van der Walls surface and so on. When a user selects the sphere style (Fig. 3(b)), VCMM will adaptively control the resolution of each atom if the molecule has a large number of atoms. In this style, VCMM can display more than one million atoms on a typical PC in 2013.

Continuum modeling requires accurate and complete structural data as well as force field parameters such as atomic charges and radii, which information can be saved in a so called PQR file. In some cases, the molecular structure from PDB does not contain hydrogen atoms, and may even miss a fraction of the heavy atom coordinates. PDB2PQR [20] can provide the force field parameters and add the hydrogen atom and some heavy atoms missed in PDB. VCMM integrates the PDB2PQR package and enriches the database to handle some unusual amino acid types and ion species.

3.2. Meshing module

Meshing module includes mesh visualization, mesh generation and mesh quality analysis. Molecular surface meshing and volume meshing are useful in boundary/finite element modeling of biomolecules. The commonly used meshes are surface triangular mesh and volume tetrahedral mesh.

VCMM is able to render a given mesh in different styles as shown in Fig. 4. A mesh can be displayed as a surface or wire-frame by pressing the shortcut key like in Fig. 4(a) and (b). A surface mesh can be displayed directly, but the interior regions of a 3D volume mesh are difficult to render. In order to overcome this difficulty, VCMM provides some mesh filters to get a part of the mesh as shown in Fig. 4(c) and (d). Plane cutting is the most useful operation and it maintains the integrity of each volume cell. Users are also able to get a part of the mesh by selecting region marks as in Fig. 4(c).

If users have no molecular surface mesh file for input, VCMM can be used to generate it with the integrated mesh generation tools. VCMM contains a tool developed by our group, TMSmesh [21,22], for surface meshing on a molecular Gaussian surface. A Gaussian surface is defined as a level set of the summation of the Gaussian kernel functions. TMSmesh has a linear time complexity with respect to the number of atoms and is capable to handle arbitrarily large molecules (like a virus with more than 1 million atoms) of protein in PDB. In addition, MSMS [23] is another surface mesh generation tool as a plug-in in VCMM. MSMS is widely used for molecular surface triangulation for not huge molecules because of its high efficiency and relatively good quality. Once a surface mesh is obtained, a user can generate a volume mesh conforming to the molecular surface. The volume mesh can be generated