LBIE Tutorial

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Contents

LBIE

This is the user documentation for LBIE v2.0. This is to help both new users familiarize themselves with the software, and to provide a comprehensive list of functions to everyone. There is a separate programmer documentation available for those interested in extending the functionality of LBIE, which is an open source software. LBIE was developed at the Center for Computational Visualization under Dr. Chandrajit Bajaj, at the University of Texas at Austin.

Chapter 1

Introduction

The development of finite element simulations in medicine, molecular biology and engineering has increased the need for quality finite element meshes. Although there has been tremendous progress in the area of surface reconstruction and 3D geometric modelling, it still remains a challenging process to generate 3D meshes directly from imaging data, such as Computed Tomography (CT), Magnetic Resonance Imaging (MRI) and Signed Distance Function (SDF). For accurate and efficient finite element calculations, it is important to have adaptive and quality geometric models with minimal number of elements. The studied object may have complicated topology.

LBIE-Mesher (Level Set Boundary Interior and Exterior Mesher for molecule) [1-4] is an interactive program for 3D mesh extraction and rendering from volume data. In the program, error tolerances and isovalues can be changed interactively. LBIE-Mesher can extract adaptive and quality 2D (triangular or quadrilateral) meshes over isosurfaces and 3D (tetrahedral or hexahedral) meshes with isosurfaces as boundary surfaces directly from volumetric imaging data. LBIE-Mesher can generate 3D meshes for the volume interior to an isosurface, the volume exterior to an isosurface, or an interval volume between two isosurfaces.

1.1 Installation

Please install LBIE and perform the functions described in the rest of the tutorial to learn more about the software. LBIE is open source and should be available for download from CCV's software download page. It has been tested under windows, linux and MAC. You will need the following

- A windows or linux operating system.
- QT and a C++ compiler.

Once you have downloaded the source, you can compile it using either the QT's Makefiles (the .pro files) or the project workspace files (for windows).

There are some subtle problems which could come up when compiling and linking LBIE. Here are some solutions.

- Download and install QT. There is a free version for Linux.
- Make sure that the variables QTDIR and QTLIB are defined.

1.2 The main user interface

In Figure 1.1, we show an exterior tetrahedral mesh generated for a molecule. The different regions in the user interface are

- The rendering area is the top part of the user interface, and it runs using OpenGL.
- Properties area is the bottom part of the user interface. You can choose different mesh types, normal calculation methods, isovalues and error tolerances.

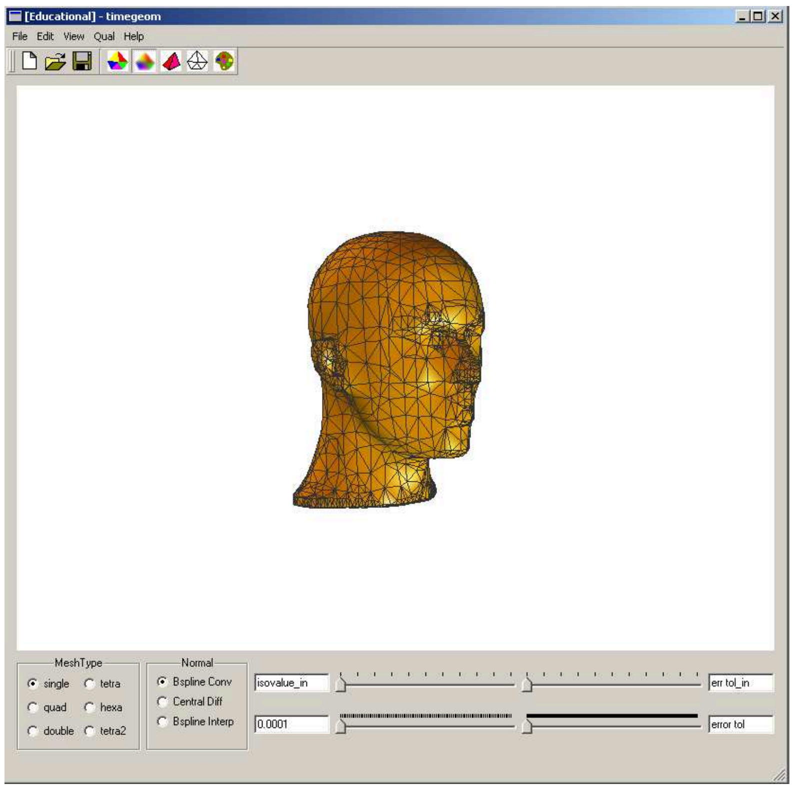


Figure 1.1: The main user interface of LBIE. In this figure, the top part shows the rendering area where data is rendered, and the bottom part is the Properties widget where the properties of the selected data set are shown.

Chapter 2

Functionalities

LBIE allows users to compute functions including surfaces/volumes and surface/volume functions like isosurfaces, normal, area, and volume. For molecules, LBIE first optimizes the radius for each atom, and constructs volumetric data using the Gaussian summation. After that, various types of meshes can be extracted from the volume data, and the quality is improved. The distribution of some functions such as electrostatic potential can be shown over extracted molecular surfaces.

2.1 Functions

LBIE is both a visualization and computational toolkit for volumetric data. Some of the main features include

- Open source software for rendering volumetric data sets. It has been tested on CT, MRI and SDF data sets.
- Written in C++, with a QT front end. The same code should work on multiple platforms, including Windows and Linux.
- Reads in rawiv formats.
- Produces adaptive and quality boundary element meshes and interior/exterior finite element meshes.
- Produces high quality images using High-end graphics cards functionalities.
- Wireframe and smooth shaded isosurfaces.
- Computes metrics including surface areas and volumes.

2.2 Mesh type

The user can choose different mesh types to generate in the main user interface. There are six options:

- single - Generates triangular meshes for one isosurface.
- tetra - Generate tetrahedral meshes for the volume interior to one isosurface.
- quad - Generates quadrilateral meshes for one isosurface.
- hexa - Generate hexahedral meshes for the volume interior to one isosurface.
- double - Generates triangular meshes for two isosurfaces.
- tetra2 - Generate tetrahedral meshes for the interval volume between two isosurfaces.

2.2.1 Triangular/tetrahedral mesh generation

A top-down octree subdivision coupled with the dual contouring method is used to rapidly extract adaptive 3D finite element meshes with correct topology from volumetric imaging data [2]. The edge contraction and smoothing methods are used to improve the mesh quality. The main contribution is extending the dual contouring method to crack-free interval volume 3D meshing with feature sensitive adaptation. Compared to other tetrahedral extraction methods from imaging data, our method generates adaptive and quality 3D meshes without introducing any hanging nodes.

2.2.2 Quadrilateral/hexahedral mesh generation

LBIE uses an algorithm described in [1] to extract adaptive and quality quadrilateral/ hexahedral meshes directly from volumetric data. First, a bottom-up surface topology preserving octree-based algorithm is applied to select a starting octree level. Then the dual contouring method is used to extract a preliminary uniform quad/hex mesh, which is decomposed into finer quads/hexes adaptively without introducing any hanging nodes. The positions of all boundary vertices are recalculated to approximate the boundary surface more accurately. Mesh adaptivity can be controlled by a feature sensitive error function, the regions that users are interested in, or finite element calculation results. Finally, a relaxation based technique is deployed to improve mesh quality.

2.3 Normal calculation

Three normal calculation methods are provided in LBIE: Bspline convolution, central difference and Bspline interpolation.

2.4 Isovalue and error tolerance

Isovalues and error tolerances can be controlled interactively in the main user interface by dragging the bar and by typing a value in the small window. The isovalue is controlled by the left bar, and the right bar controls error tolerances. The top row controls the inner surface, and the bottom row controls the outer surface.

2.5 Cutting plane

A bar on the bottom is used to adjust the position of the cutting plane.

2.6 Interior/Exterior mesh

The button "Exterior" on the tool bar is used to switch the visualization way - interior or exterior. If you click "Exterior" button and open a new file. The visualization way becomes "Exterior" as shown in the figure 1.1.

2.7 Function visualization

The distribution of some functions can be shown over isosurfaces. For example, LBIE reads the electrostatic potential data, then show its distribution over over molecular surfaces.

2.8 Quality improvement

In LBIE, geometric flows are used to smooth the surface and improve mesh quality with feature preserved [4]. For surface meshes, the surface diffusion flow is selected to remove noise by relocating vertices in the normal direction, and the aspect ratio is improved with feature preserved by adjusting vertex positions in the tangent direction. For volume meshes, besides the surface vertex movement in the normal and tangent directions, interior vertices are relocated to improve the aspect ratio. Our method has the properties of noise removal, feature preservation and quality improvement of surface/volume meshes, and it is especially suitable for biomolecular meshes because the surface diffusion flow preserves sphere accurately if the initial surface is close to a sphere.

Chapter 3

Data formats

LBIE reads volumetric data. The main interface on selecting File - Open from the main menu is as shown in Figure 1.1. Filename is the full path and name of the data set to be opened.

3.1 Loading volumetric data

Volumetric data (rawiv, rawv, dx, mrc) format can be loaded directly to LBIE. The size of the volumetric data should be $(2^n + 1)^3$ cube because we are using octree data structure.

About CCV's rawiv, rawv file formats, please read about CCV's data formats here: rawiv,rawv file format description

3.2 Loading function data

The distribution of function can be loaded from different volumetric formats (rawiv).

3.3 Various meshes output

When you click "Save" button, the generated mesh will be saved in a file. The output mesh is in raw,rawnc format.

About CCV's raw, rawnc file formats, please read about CCV's data formats here: raw,rawnc file format description

3.4 Generating pictures

The generated meshes are rendered in the rendering area, the user can make snapshots of the meshes.

Chapter 4

Examples

4.1 Loading volumetric data

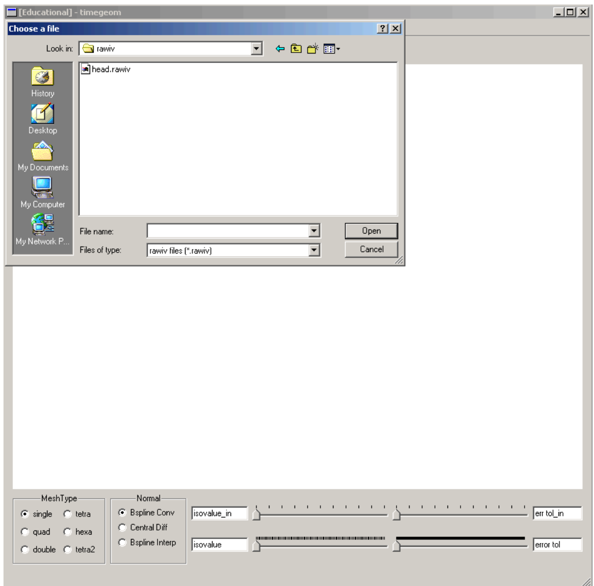
You can click the open file button and the file openning dialog will pop up. Then open a volumetric rawiv file. LBIE will automatically make a mesh as shown in the figures 4.1(a) and 4.1(b).

4.2 Different meshes

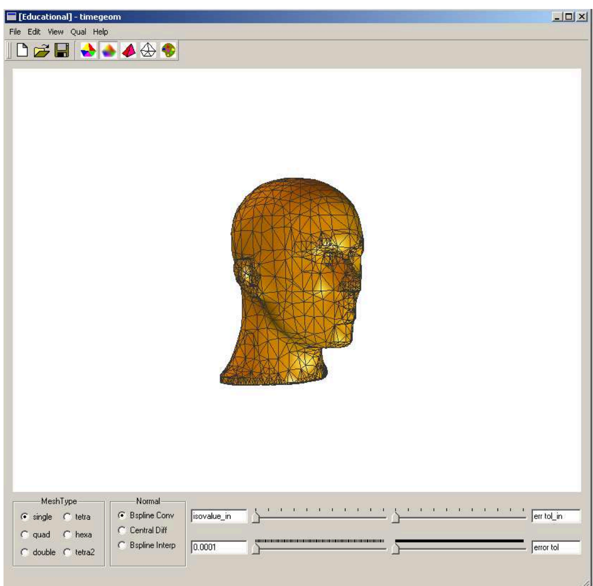
Different mesh types are shown in the figures 4.1(b),4.2,4.3,4.4,4.5 and 4.6.

4.3 Mesh quality improvement

You can use different techniques to improve the quality of the mesh. The figures 4.3 are an example.



(a) select a rawiv file



(b) after loading

Figure 4.1: Loading a rawiv file

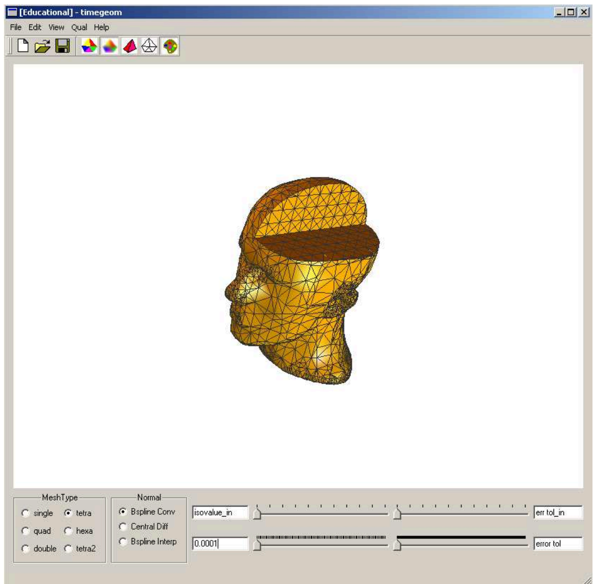


Figure 4.2: Tetrahedral mesh

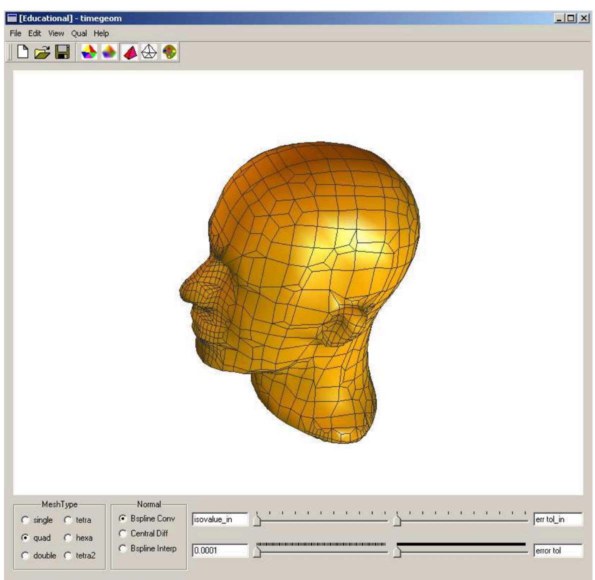


Figure 4.3: Quadrilateral mesh

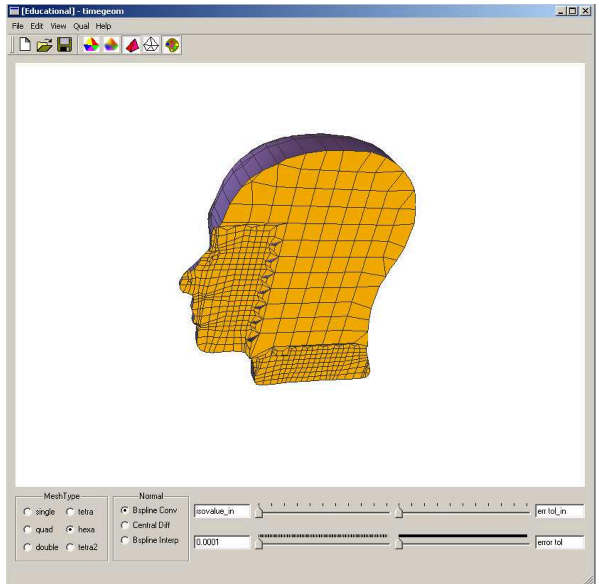


Figure 4.4: Hexahedral mesh

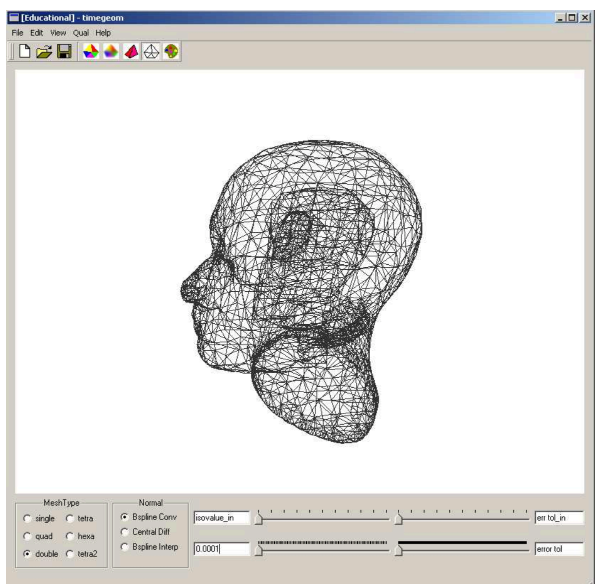


Figure 4.5: Double layer triangular mesh

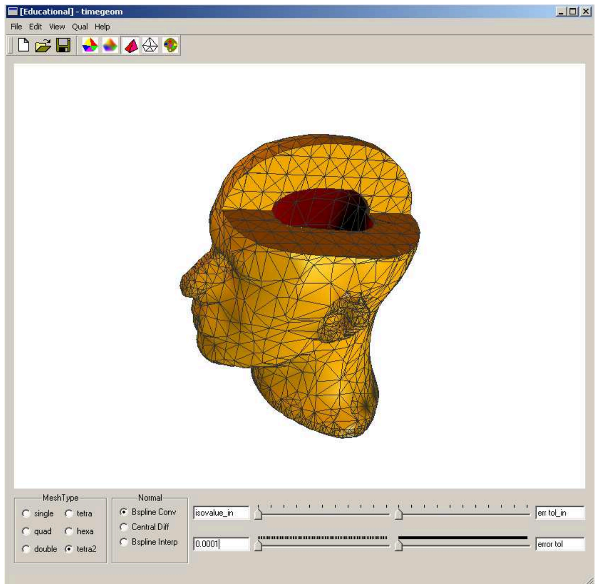


Figure 4.6: Double layer tetrahedral mesh

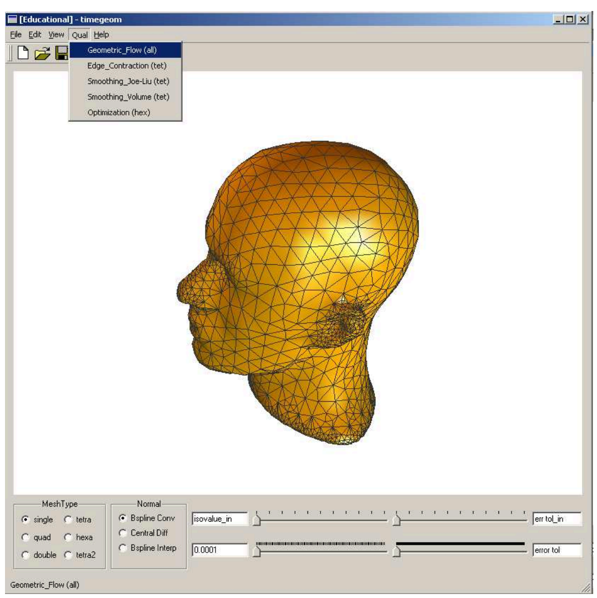


Figure 4.7: Quality improvement

Acknowledgements

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