Adaptive Mesh Generation For Molecular Modeling

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Goals

• Inputs: PDB/PQR files
• Outputs:
  – Molecular surface mesh
  – Tetrahedral meshes
    • Interior mesh
    • Exterior mesh
    • Both

• Good Properties:
  – High quality
  – Smooth
  – Feature-preserving
  – Adaptive
Related Work

- LBIE (Prof. Chandrajit Bajaj, UT-Austin)

Zhang, Bajaj, and Sohn, 2005

Related Work

- Tetgen (Dr. Hang Si, Weierstrass Institute, Germany)

From Tetgen website: http://tetgen.berlios.de/examples.head.html
Related Work

- MSMS (Prof. Michael Sanner, Scripps)

Our Approach: Outline

1. Input
   - PDB Coordinates
   - 3D Volumes
   - Initial Meshes
   - Quality Improvement
   - Mesh Coarsening
   - Terra Generation

2. Output
**Generate Volumes from PDB/PQR**

- Using a Gaussian kernel function

\[ F(\vec{x}) = \sum_{i=1}^{N} e^{-\frac{\|\vec{x} - \vec{x}_i\|^2}{2r_i^2} B_i} \]

- \( x_i \): coordinate (center)
- \( r_i \): radius (user given)
- \( B_i \): blobbiness (-0.5)
- \( N \): number of atoms (thousands to tens of thousands)

- Discretize the function: spacing distance per pixel/grid (0.5 Å/grid)

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**Generate Surfaces from Volumes**

Volume/Surface generated for 1CID molecule
Mesh Quality Improvement

- Angle-based Method

\[ \tilde{X} = \frac{1}{\sum_{i=1}^{M} e^{-\kappa \alpha}} \sum_{i=1}^{M} e^{-\kappa \alpha} X_i \]

- Feature-preserving using local structure tensor

\[ \tilde{X} = X + \sum_{k=1}^{3} \frac{1}{1 + \lambda_k} ((\tilde{X} - X) \cdot e_k) e_k \]

Before quality improvement  
After quality improvement
Mesh Coarsening

• Feature-preserving coarsening

\[ L(X)^\alpha \left( \frac{\lambda_2(X)}{\lambda_1(X)} \right)^\beta < T_0 \]

\[ \sum_{i=1}^{N} \begin{pmatrix} n_{x}^{(i)} & n_{y}^{(i)} & n_{z}^{(i)} \\ n_{x}^{(i)} & n_{y}^{(i)} & n_{z}^{(i)} \\ n_{x}^{(i)} & n_{y}^{(i)} & n_{z}^{(i)} \end{pmatrix} \]

\[
\begin{align*}
L(X): & \text{ maximal edge length connected to } X \\
\lambda_1: & \text{ the largest eigenvalue} \\
\lambda_2: & \text{ the second largest eigenvalue} \\
\alpha, \beta: & \text{ user-defined weights} \\
T_0: & \text{ user-defined parameter}
\end{align*}
\]
Mesh Coarsening

Before coarsening
(34,858 nodes and 69,712 triangles)

After coarsening
(6,449 nodes and 12,894 triangles)

Mesh Smoothing

• Normal-based Smoothing

\[ \tilde{X} = \frac{1}{\sum_{i=1}^{n} w_i} \sum_{i=1}^{n} w_i R(X; e_i, \theta_i) \]

• Anisotropic Feature-preserving Smoothing

\[ \tilde{n}_i = \frac{1}{\sum_{j=1}^{3} e^\kappa(n_i \cdot n_{ij} - 1)} \sum_{j=1}^{3} e^\kappa(n_i \cdot n_{ij} - 1)n_{ij} \]
Mesh Smoothing

Before mesh smoothing

After mesh smoothing

Surface Mesh: Final Results

1CID
Tetrahedron Generation: 1CID

Hierarchical Meshing: 1BVP

T0 = 0.1 (26842 nodes)  T0 = 0.7 (9,480 nodes)
Results: 1BVP

T0 = 0.2 (23102 nodes)

Mesh Generation from Molecules

(mACH: 8,109 atoms)

(42,964 nodes 181,103 tetrahedra) (Yu et al, FEAD 2008)

(22,753 nodes 45,502 triangles) Tetgen
Demo using UCSF Chimera