Motivation: Voronoi Diagrams of Spheres

- Not extensively investigated
- Lack of robust algorithms
- Especially for non-general position and disconnected Voronoi edges
- Many current applications simplify the problem
  - Assume that all atoms are 3D points
- Example application: Proteins
  - Voronoi diagrams are often used to analyze structural properties of molecules

Background

- Bisectors of spheres
  - The locus of points that are equidistant from two spheres
  - Either a plane or a hyperbolic surface
  - Assumption: no completely contained spheres
  - (allow partially intersecting)
- Voronoi diagrams of spheres in 3D
  - The surface of a Voronoi cell is the lower envelope of its corresponding bisectors
  - In general position, numbers of spheres contributing to:
    - Voronoi vertex: 4; Voronoi face: 3; Voronoi edge: 2; Voronoi cell: 1
    - In non-general positions, there are more contributing spheres

Sampling Rays and Calculating Bisectors

- Sampling rays from spheres
  - Parameterizing bounding cube for each sphere (uniformly subdivided domains in u and v)
  - Each face of the bounding cube maps to 1/6 of the sphere
  - Shoot rays from the sphere center through each u-v point
  - Ray function:
    \[ r(t) = r(x(t), y(t), z(t)) = 0 + t \cdot n \]
- Calculating the bisector functions
  - The bisector surfaces between two spheres:
    \[ \frac{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2 - R_1^2}{(x-x_1)^2 + (y-y_1)^2 + (z-z_1)^2 - R_1^2} = 1 \]
  - Transforming to implicit hyperbolic surface equation:
    \[ A_1 x^2 + B_1 y^2 + C_1 z^2 + D_{1xy} + D_{1xz} + D_{1yz} + E_x + E_y + E_z + F + G = 0 \]

Calculating Sample Points on Voronoi Faces

- Combining ray functions and bisector functions
  - For the “base” sphere in each Voronoi cell, test all bisectors corresponding to each ray shot from the base sphere
  - Each ray either shoots to infinity or intersects the lower envelope at a Voronoi face sample point
  - Solve the functions:
    \[ u \cdot t^2 + b \cdot t + c \geq 0 \]
    \[ A_2 x^2 + B_2 y^2 + C_2 z^2 + D_{2xy} + D_{2xz} + D_{2yz} + E_x + E_y + E_z + F + G = 0 \]
- Visualization of color-coded face sample points per base sphere
  - The color of each sample point is decided by its corresponding sphere
  - Base sphere as black
  - We also get color code on u-v domain (bounding cube)

Determining Presence of Voronoi Vertices

- U-V grid cells
  - Each group of four neighboring face sample points on the bounding cube
  - “Marching” through the grid cells, check if the four corners have three or more different colors
  - Three or more colors \( \rightarrow \) the corresponding Voronoi faces may intersect in a Voronoi vertex

Calculating Voronoi Vertices’ Position

- Newton-Raphson method in 3 variables
  - Calculate xyz coordinates of Voronoi vertex in each 3-color grid cell
  - Equivalent to solving three bisector equations simultaneously
  - Use the average of xyz coordinates of the four corners of the grid cell as start point for iteration
  - Def: 3x3 Jacobian

Results

- Handling non-general position and large inputs
  - A Voronoi cell containing a high-order degree Voronoi vertex
  - Voronoi diagrams of Protein Data Bank ID “1bh8” consisting of 2161 atoms
  - Timing results (seconds) for face samples and Voronoi vertices

Contributions and Future Work

- A novel approach to compute Voronoi diagrams of spheres
  - Sample based + lower envelope + GPU parallel computing
- Accurately calculate Voronoi vertices’ geometry
  - Use the samples to initialize numerical iteration
  - Guarantee the accuracy within user-defined tolerance
- This algorithm is robust for
  - Thousands of input spheres representing actual protein molecules
  - Spheres not in general position, handling Voronoi vertices with degree greater than four
- Future work:
  - On u-v domain (bounding cube), trace Voronoi edges by particular color patterns
  - Apply approach to more complex primitives