Names: Neil Gupta, Gargi Kher

Dalphaball Paper: https://link.springer.com/content/pdf/10.1007/s00454-004-1099-1.pdf

Abstract: For computational biological modeling, it is important to implicitly represent solvent molecules so that we can get more accurate data about a molecule's interaction with the solution it's in. Hydrophobicity is the measure of a molecule's repulsion to water, and can be represented as the sum of weighted atomic surface areas. The derivative of these areas give important information regarding forces influencing the movement of the molecule in solution. This paper derives formulas for Solvent Exposed Surface Area so that we can better model molecules in solution.

Introduction/Motivation for Paper:
-background on motivation
-have been earlier attempts at this problem (faster at solving, less accurate)
-One of the early methods for calculating protein hydrophobicity was introduced by Richmond in 1984. Still makes use of spheres, but doesn't use Alpha Shapes, uses Gauss-Bonnet theorem. Still makes use of gradients to decrease calculation times. This method has been improved on since then. (Richmond 1984). One of the biggest ways this method has been improved is by using Alpha Shapes - which will be discussed later in the paper.
-Another way (used in Rosetta) is the Shrake-Rupley algorithm (1993), which draws a mesh of points a small distance from the molecule (usually 1.4 Angstroms). It then counts the number of points that are on the surface, and multiplies by the approx surface area that each point represents. Later work has optimized the position of these dots to more accurately calculate the surface area. (Legrand, Merz)
-Briefly mention importance of Implicit solvation models (representing solvent as continuous rather than individual molecules)

Model:
-explain that molecules are represented as balls and each ball has a center (vertex) with a radius and is bounded by a sphere (this is how the paper simplifies representing molecules).
-explain effective potential eq'n
-explain a bit more about Alpha Shape theory/ Delaunay triangulation: Generally, molecules are modeled as balls in space. We'll take center of balls to be vertex of triangles. (Edelsbrunner 1995)
-linear map and power diagram
-explain derivation of solvation energy formula

Assumptions for Derivations:
-We are assuming that water is continuous rather than modeling it as individual molecules. Each atom is represented as a sphere.
-No influence of polarity
-Spherical electron clouds

Derivation:
-Two types of area theorems:
1. Direction Preserving motion
2. Distance Preserving motion
   (For both): Explain how each motion is defined. Explain what F means, and what we are assuming about the spheres. We could insert an image of or draw our own image. Explain what the variables mean, and talk about how they derived distances and used Archimedes' principle to get the areas.
-Area derivative theorem
   ● Explain how this is a sum of direction preserving and distance preserving motion equations.
-Weighted area derivative theorem
   ● Explain how this is different from Area derivative theorem. We might not have to go as in-depth as above because they're similar.
-also explain discontinuity cases/ maybe elaborate on just a few

Terms:
   -State **z** is 3n dimensional, represents the position of n balls.
   -Power Diagram is the set of power cells, each of which contains points who are closest To a given atom
   -Power cell represents the set of points in the sphere surrounding the atom or   "ball" that minimize the power distance, or distance between a particular point and a sphere. The power distance is given by $||x-z_i||-rad^2$

Discussion:
-Run Dalphaball on ~200 pdbs (proteins from the Protein Data Bank database)
-Results from our run (Runtime and accuracy)
-Explain how authors found this implementation compared to existing algorithms (How fast, accurate)
-See how Dalphaball was implemented in the Rosetta software for protein design and modeling (a modern software)
-Anything else that might be interesting to find in the future/any improvements

Conclusion:
-Elaborate on results from our pdb runs, talk about how solutions to a problem like this will always be a balance between accuracy and speed.

Resources:
https://link.springer.com/content/pdf/10.1007/BF02574053.pdf (Edelsbrunner 1995) - Mostly using this to help explain Alpha Shapes geometrically, won't use the proofs.
https://www.sciencedirect.com/science/article/pii/0022283684902316(Richmond 1984) one of the first analytical methods for computing surface areas.

https://onlinelibrary.wiley.com/doi/abs/10.1002/jcc.540140309 (Le Grand, Merz 1993)
Shrake-Rupley algorithm (Used in Rosetta)