1046-92-1080 **Chandrajit Bajaj*** (bajaj@cs.utexas.edu), Department of Computer Sciences, 1 University Station C0200, Austin, TX 78712, and **Guoliang Xu** (xuguo@lsec.cc.ac.cn) and **Qin Zhang** (zqyork@ices.utexas.edu). *Molecular Solvation Models and Minimal Surfaces.*

Molecular surfaces of proteins and other biomolecules are often modeled as smooth analytic interfaces separating the molecule from solvent (an implicit solvation model). These analytic solvation models are often of high genus with a myriad of interconnected tunnels and pockets with openings (mouths). All these interfaces are biochemically significant as pockets are often active sites for ligand binding or enzymatic reactions and tunnels are often solvent ion conductance zones. In this talk, we present a general characterization of these solvation interfaces and approximately model them as piecewise minimal surfaces, namely, the solution of non-linear elliptic or biharmonic partial differential Euler-Lagrange equations obtained from the minimization of high-order energy functionals. This is joint work with members of my research group, in particular Guoliang Xu and Qin Zhang. (Received September 15, 2008)