1096-VL-1406 **Wufeng Tian*** (wtian@crimson.ua.edu), Tuscaloosa, AL 35487, and **Shan Zhao** (szhao@bama.ua.edu), Tuscaloosa, AL 35487. *A fast ADI algorithm for geometric flow equations in bio-molecular surface generation.*

A new alternating direction implicit (ADI) method is introduced to solve potential driven geometric flow partial differential equations (PDEs) for bio-molecular surface generation. For such PDEs, an extra factor is usually added to stabilize the explicit time integration. Based on a scaled PDE model, there are two existing ADI schemes involved with cross derivative terms that have to be evaluated explicitly. It affects the stability and accuracy of these ADI schemes. To overcome these difficulties, we propose a new ADI algorithm based on the un-scaled form so that cross derivatives are not involved. The proposed ADI algorithm is validated through benchmark examples with analytical solutions, reference solutions, or literature results. Moreover, quantitative indicators of a bio-molecular surface, including surface area,surface-enclosed volume and solvation free energy, are analyzed for various proteins. The proposed ADI method is found to be unconditionally stable and more accurate than the existing ADI schemes in all tests. This enables the use of a large time increment in the steady state simulation so that the proposed ADI algorithm is very efficient for bio-molecular surface generation. (Received September 16, 2013)