Meeting: 1003, Atlanta, Georgia, AMS CP 1, AMS Contributed Paper Session

1003-65-1478 **Mark S. Korlie*** (korliem@mail.montclair.edu), Department of Mathematical Sciences, Montclair State University, Montclair, NJ 07043. *A 3-D Molecular Mechanics Simulation of Cracks and Fractures in a Solid under Stress.* Preliminary report.

Lennard-Jones potential type formulas are used to derive dynamical equations for the molecules in a rectangular solid. The resulting systems of nonlinear ordinary differential equations are then used to simulate the evolution and propagation of cracks and fractures in the solid. For application, we use a 3-D solid ice, where the ice molecules are stressed. Computer examples compare dynamical responses when the solid has a slot or does not have a slot. The mechanisms for both cracks and fractures development are presented and discussed. (Received October 05, 2004)