Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Frustration in Condensed Matter and Protein Folding S LORELLI, A CABOT, N SUNDARPRASAD, C BOEKEMA, San Jose State University — Using computer modeling [1-3] we study frustration in condensed matter and protein folding. Frustration is due to random and/or competing interactions. One definition of frustration is the sum of squares of the differences between actual and expected distances between characters. [3] If this sum is non-zero, then the system is said to have frustration. A simulation tracks the movement of characters to lower their frustration. Our research is conducted on frustration as a function of temperature using a logarithmic scale. At absolute zero, the relaxation for frustration is a power function for randomly assigned patterns or an exponential function for regular patterns like Thomson figures. These findings have implications for protein folding; we attempt to apply our frustration modeling to protein folding and dynamics. [4,5] We use coding in Python to simulate different ways a protein can fold. An algorithm is being developed to find the lowest frustration (and thus energy) states possible. [6,7] Research supported by SJSU & AFC. [1] AK Dewdney, *Scientific American* (1987) 112. [2] C Boekema *et al, Hpf Interact 26* (1990) 345. [3] I M Suarez *et al,* Conf Proc 2nd Woodward Conference, Springer Verlag NY 1990; Am Phys Soc Bull 35 (1990) 548. [4] J Claycomb & JQP Tran, *Introductory Biophysics* (2010). [5] LN Mazzoni & L Casetti, *Phys Rev Lett* (2006) [6] JL Van Hemmen, *Phys Rev Lett* 49 (1982) 4109. [7] M Mezard *et al*, Spin Glass Theory and Beyond. *World Scientific* (1987).

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Date submitted: 11 Nov 2016 Electronic form version 1.4