1117-92-343 **Meera Sitharam*** (sitharam@cise.ufl.edu), University of Florida, CSE bldg, P.O. box 11-6120, Gainesville, FL 32611-6120. *Geometrization, Stratification and Convexification for Atlasing Molecular Assembly Configuration Spaces.*

Abstract: We present a versatile, powerful and efficiently computable representation of the topology and geometry of molecular assembly configuration spaces under short-ranged potentials, using the standard concept of Geometrization, a classical concept of Stratification and a new concept of Convexification using Cayley or distance parameters (abbr: CayCon technique). The representation makes search and the computation of path, volumes and other measures (needed for free energy, configurational entropy, and kinetics pathways of assembly) amenable to state-of-the art developments in convex analysis, semidefinite programming, combinatorial rigidity, and algebraic topology/geometry of configuration spaces. EASAL (Efficient Analysis and Search of Assembly Landscapes) is a method that has been successfully used in predicting crucial interactions driving assembly of 3 types of viruses, and in computing path, area and volume integrals useful for kinetics of assembly of hard-sphere clusters. Detailed studies comparing its performance and resource usage with standard MC-based sampling clearly demonstrate its efficacy. We anticipate that hybrids of EASAL/CayCon with currently standard MC/MD based methods will soon become de rigeur for predictions related to assembly. (Received January 17, 2016)