EASAL: efficient atlasing, search and analysis of assembly landscapes under short-ranged potentials using geometrization, stratification and Cayley convexification.

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We present a versatile, powerful and efficiently computable representation of the topology and geometry of 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 of assembly) amenable to state-of-the art developments in convex analysis, semidefinite programming, combinatorial rigidity, and algebraic topology/geometry of configuration spaces. The mathematically refined perspective helps to formally delineate the graded increase in complexity - of the underlying finite, geometrically constrained configurations - from assembly to folding. EASAL/CayCon 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.

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