Path Finding In Sphere Based Assembly Configuration Spaces Using EASAL

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The EASAL software implements a suite of algorithms for understanding in $\mathbf{R}^3$ the structure and geometric properties of two point sets that are pairwise constrained by distance intervals. The algorithms generate, describe and explore the configuration spaces of these constraint systems using classical results for stratification of configuration spaces, new results for efficient sampling by convex parameterization and intuitive visualization. We study a special case of this problem when the rigid point sets are sets of non-colliding spheres.

EASAL stratifies the assembly configuration space into various regions called active constraint regions. This stratification produces an atlas that can be used to find assembly paths between configurations. The path topology of the assembly configuration space is crucial for understanding assembly kinetics. In this talk we will discuss the algorithms used in finding such paths in the configuration space of assembling molecules.