Flexibility of Subdivided Polyhedral Complexes

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A *subdivided polyhedron* is the graph obtained by adding vertices on some of the edges of the 1-skeleton of a polyhedron. We also consider subdivided polyhedral complexes, which are collections of polyhedra connected into a topological complex along faces (as in a **beehive**).

We use these graphs to define abstract *molecules*, by placing *atoms* at the vertices and *bonds* along the edges. One of the simplest examples is the subdivided *cube* with many inter-connected cycles and few degrees of freedom, introduced and used in Thorpe and Lei [6] as a benchmark for testing the ROCK-software approach to sampling molecular conformations of proteins.

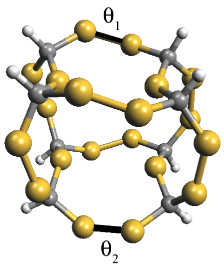


Figure 1: The 2dof cube molecule.

Generating coherent molecular motions for structures with many inter-connected cycles is a challenging computational problem, for which several heuristics have been proposed. In [4], we use a collection of such abstract molecules with few degrees of freedom to test our approach and compare it with ROCK[2].

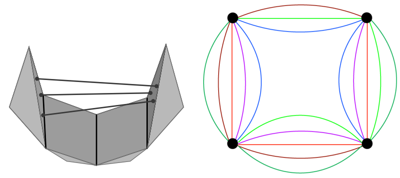
In this paper, we describe an algorithm for systematically generating and analyzing the flexibility of subdivided polyhedral complexes. We have used it to create a comprehensive database of *abstract molecules* serving as benchmarks in the comparison of loop-closure heuristics for random motion generation: our models are annotated with information regarding their dependent, rigid or flexible substructures.

Body-and-hinge structures. Molecular structures maintain the bond lengths, and it is tempting to interpret them as *bar-and-joint frameworks* (where the rigid bars are allowed to rotate around their connecting *joints*).

Mechanically, the correct model is that of *body-and-hinge structures*. These are collections of rigid bodies connected by hinges, which allow rotations about hinge axes. With this model in mind, an atom is viewed as a rigid body, and the bonds attached to it rigidly as *hinges*.

A *body-and-bar structure* is built from rigid bodies connected by rigid bars placed generically; by using the observation that a hinge can be represented by 5 bars [5], every body-and-hinge structure can be interpreted as a body-and-bar structure. A body-and-bar structure induces a graph, with a vertex associated to each body and an edge to each bar.

A rigid structure is *minimally rigid* if the removal of any bar results in a flexible structure. Otherwise, the structure



(a) (b)

Figure 2: (a) Generic minimally rigid body-hinge-and-bar structure. (b) Corresponding graph decomposes into 6 edge-disjoint spanning trees.

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may contain *overconstraints*, i.e., bars whose removal does not affect the flexibility or rigidity of the structure; the *dependency degree* of a structure is the number of overconstraints in a structure. A flexible structure contains *rigid components*, or maximal rigid substructures.

Tay's Theorem [5]. A structure is (generically) rigid in 3D if and only if the associated graph is a the edge-disjoint union of 6 spanning trees.

Graphs that are decomposable into k edge-disjoint spanning trees belong to the family of *sparse* graphs, those graphs on n vertices with $kn - l$ total edges and $kn' - l$ edges induced on any subset of n' vertices. In [3], we generalize the 2D pebble game algorithm of Jacobs and Hendrickson [1] to sparse graphs.The algorithm starts with an empty copy of the graph and inserts independent edges one at a time; *rejected* edges correspond to overconstraints.

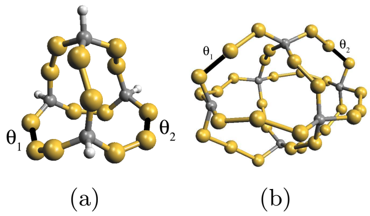

Figure 3: The 2dof tetrahedron and octahedron molecules, with an annotated pair of rotatable bonds.

Subdivision. For any edge, a *subdivision* is performed by introducing a new vertex along it; the original edge is removed and two new edges are added, attaching the new vertex to the endpoints of the original edge.

Lemma 1 Each subdivision of an overconstraint reduces the dependency degree by one.

Corollary 2 Given a minimally rigid structure, each subsequent subdivision produces one degree of freedom.

Algorithm. Begin with a randomly generated planar graph, interpreted as a body-and-hinge structure. Run the $(6, 6)$-pebble game on the graph associated with the structure, attempting to insert groups of 5 edges (originally one hinge) at a time. If some, but not all, of the 5 edges for a hinge are rejected, mark the hinge as containing overconstraints. At the end of the game, if edges were rejected, *subdivide* a marked hinge (an edge in the original graph) and play the pebble game again.

Iterate until there are no overconstraints and the structure is minimally rigid.

Continue subdivision to introduce degrees of freedom.

Figure 3 shows two of the models generated by the algorithm; both the subdivided tetrahedron and octahedron have two degrees of freedom.

References

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