Finding the optimal nets for self-folding Kirigami

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The synthesis of three-dimensional polyhedral shells at the micron and nano scales is key for encapsulation and drug delivery. Inspired by the Japanese art of Kirigami, where hollowed structures are obtained from cutting and folding a sheet of paper, lithographic methods have been developed to form shells from two-dimensional templates of interconnected panels. The potential is enormous, for a wide range of shapes and sizes can be obtained. Ideally, the unfolded templates (nets) should spontaneously self-fold into the target structure to reduce production costs and achieve large-scale parallel production.

The optimal nets are the ones that maximize the number of vertex connections, i.e., vertices that have only two of its faces cut away from each other in the net. Previous methods for finding such nets are based on random search and thus do not guarantee the optimal solution. Here, we propose a deterministic procedure. We map the connectivity of the shell into a shell graph, where the nodes and links of the graph represent the vertices and edges of the shell, respectively. Identifying the nets that maximize the number of vertex connections corresponds to finding the set of maximum leaf spanning trees of the shell graph. This method allows not only to design the self-assembly of much larger shell structures but also to apply additional design criteria, as a complete catalog of the maximum leaf spanning trees is obtained.

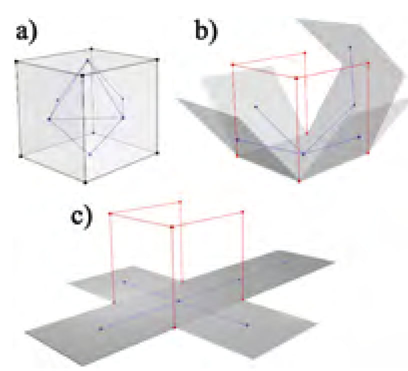

FIGURE 1
Net of a cubic shell. (a) The cubic shell is mapped into a shell graph (black), where nodes and links of the shell graph are the vertices and edges of the polyhedron, respectively. In the face graph (blue), the nodes are the shell faces and the links connect pairs of adjacent faces. To unfold the shell into a two-dimensional template (net), one needs to remove a set of shell edges (e.g., red links in (b) and (c)).

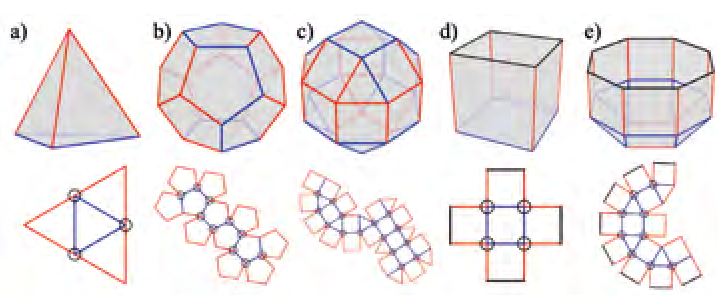

FIGURE 2
Five examples of shells and of one of their nets corresponding to a cut that is a maximum leaf spanning tree: a) tetrahedron, with four faces and nine edges, it has four maximum leaf spanning trees, but only one non-isomorphic; b) dodecahedron, with twelve faces and thirty edges, it has 1980 maximum leaf spanning trees, but only 21 non-isomorphic; c) small rhombicuboctahedron, with 26 faces and 48 edges, it has 1536 maximum leaf spanning trees, but only 32 non-isomorphic; d) open cubic shell, with five faces and twelve edges, it has only one maximum leaf spanning tree e) small rhombicuboctahedron with the top nine faces removed and 17 faces, 36 edges and 20 nodes remaining, it has 720 maximum leaf spanning trees, but only 90 non-isomorphic. The black circles in the nets indicate the vertex connections.