Complexity and modularity in a simple model of self-assembling polycubes

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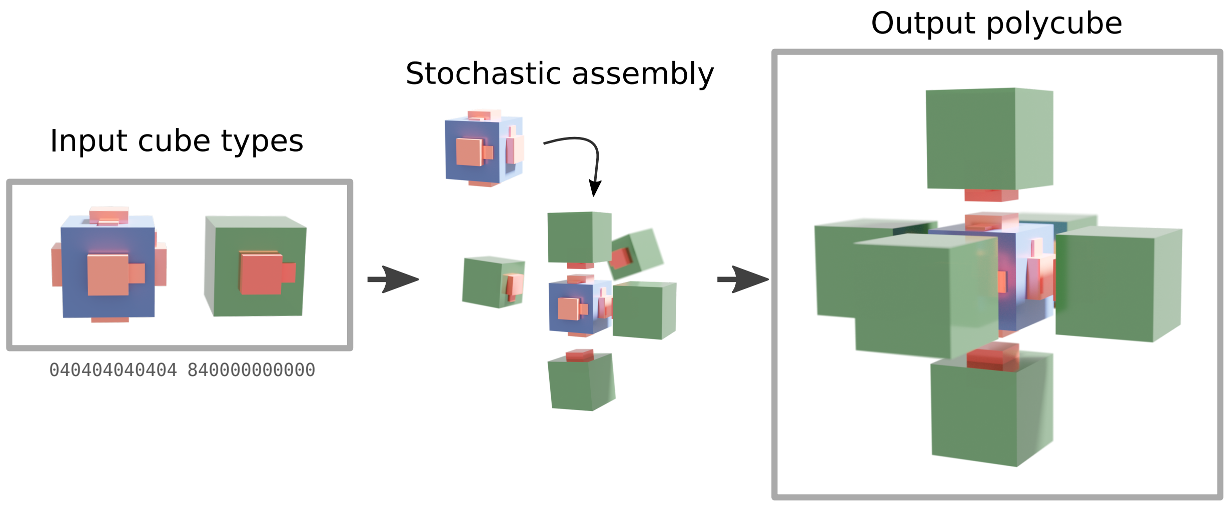
It seems intuitively clear that some shapes will be easier to self-assemble than others. Recent theoretical results based on algorithmic information theory (AIT) [1,2] have quantified this intuition by predicting that the number of inputs that lead to a particular output shape scales exponentially with the Kolmogorov complexity of the simplest input needed to make such a shape. Here we study this very general prediction using a simple model of 3D polycube structures whose assembly is controlled through face-face interaction rules.

The model, which is a 3D generalisation of the 2D polyomino model [3,4], stochastically assembles instances of specified input cubes on a lattice, as illustrated in the figure to the right. Each face of the cubes can have an oriented patch, binding to another patch of corresponding colour and orientation. Starting with an instance of the first cube in the available set, additional cubes are stocastically attached wherever a bond can be made.

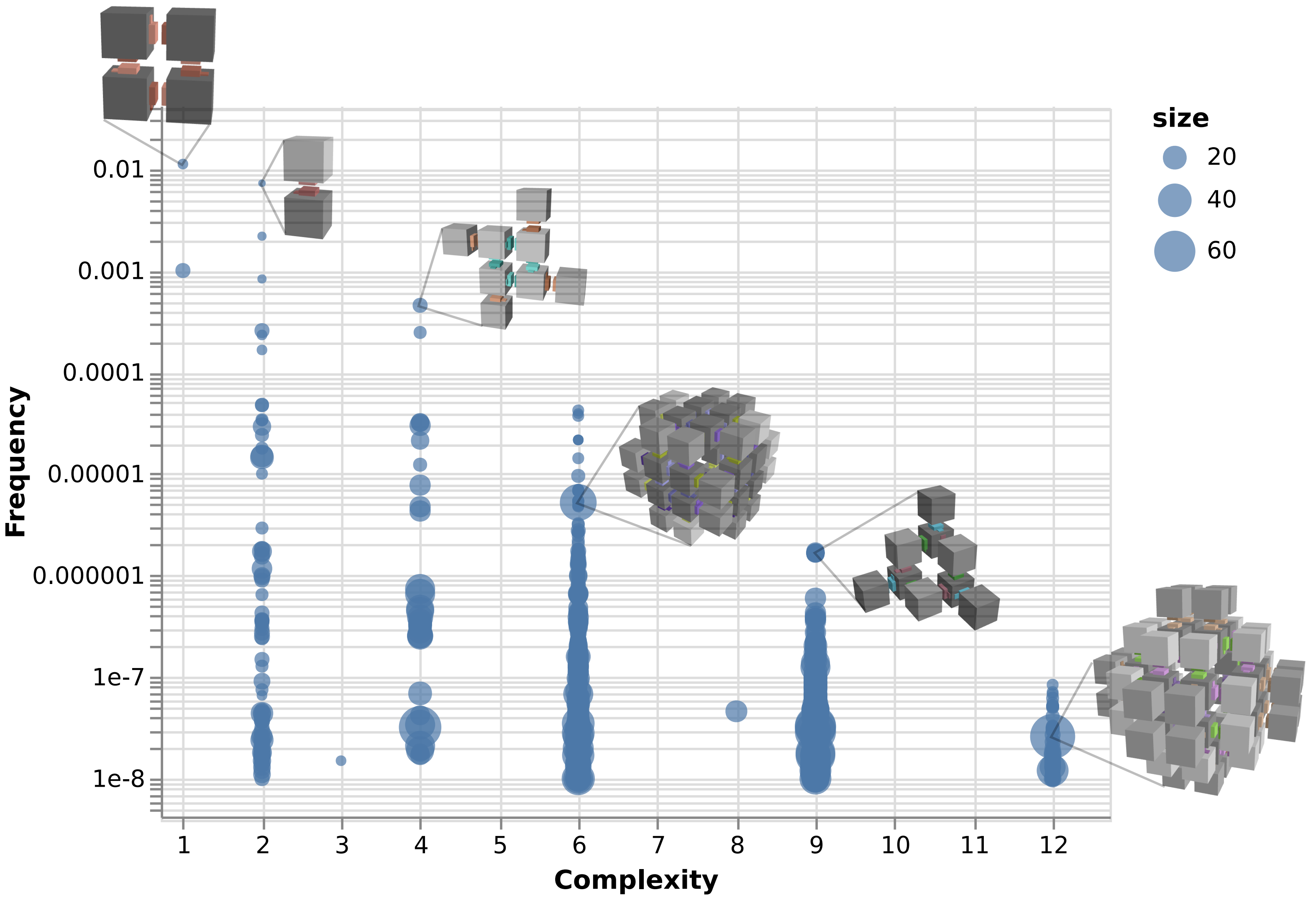


The patch orientation is in any of four possible rotations:  , while the patch colour can be any integer number n and will bind to -n.

With enough patch colours and cube types, any polycube shape could be assembled, allthough some will need a much larger input than others. At most, you would use a unique cube type for each position and a unique colour for each connection, but with symmetry and modularity you can simplify the input significantly. Following previous studies, we search for the simplest input that assembles a given structure, comparing that with the frequency at which the structure is found by random sampling.

A billion random inputs were uniformly sampled from the space of all possible rules with at most eight cube types and eight colours. The inputs that assembled deterministically and with a bounded size were then grouped by their output polycube shape. The complexity of each such polycube was then denoted as the number of cube types times the number of colours needed in he simplest input found to assemble that output.

By plotting this notion of complexity (a proxy for Kolmogrov complexity) against the frequency at which each polycube shape was found in the random sampling, a power-law distribution emerges in agreement with the predictions in [1, 2], as can be seen in the figure to the right.



Since low-complexity polycubes occupy a much larger portion of the available input space than complex ones, it can be argued, as in [5], that they should be more robust, since a change in the input is more likely to not affect the output. Thus, these findings could help guide the design of large-scale self-assembled nanostructures, both in the sense that simple structures tend to be easier to assemble, but also by making assemblies more robust.

References

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