Knots!

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Method of mapping the knots is suggested. Prospective biological implementations are discussed.

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Method

Mathematical description of knot in this approach presents a list of symbols (*i.e.* metric), each of which corresponds to a certain opening in a hollow scaffolding used to construct the knot. As a proof of concept, rigid 5 x 5 x 5 bamboo-straw-made cubic scaffolding was used to develop the knot building approach (Fig. 1). Sequence of symbols in metric exactly follows the sequence of openings a body of knot (*i.e.* strand, rope, …) should go through in the scaffolding in order to construct the knot. Openings of the scaffolding should have been conventionally labeled. As an example, a following labeling system may be used for cubic scaffolding. Each opening of the scaffolding cube is labeled as x^{i}_{j} where x is one of the letters: a, b, c, d, f, or g, depending on which facet of the cube an opening belongs to. Upper index i denotes the row and the lower index j the column.

For example, label g_3^1 stands for the opening in the first row and third column of G- facet. Facets are labeled A, B, C, D, F, G in such a way as openings a_1^1 then b_1^1 then c_1^1 then d_1^1 then f_1^1 then g_1^1 follow each other clockwise, being viewed from one of the vertices along its space diagonal (Fig. 2).

The method is best explained with mapping a simple overhand knot [1]. As one can see (Fig. 3), to build the knot a working end of the rope should consequently go through the openings:

(in c_5^4) → (out f_2^5) → (in g_1^1) → (out c_5^1) → (in b_1^2) → (out g_4^1).

Thus, the metric of simple overhand knot is: $5\, c_5^4\, f_2^5\, g_1^1\, c_5^1\, b_1^2\, g_4^1$, where number in front indicates size of the cubic scaffolding.

Concluding Remarks

(i) Clearly, the approach described here is not limited to the *cubic* scaffolding. Any particular geometry of scaffolding should help the best in solving a mapping task it serves.

(ii) Easily *reassembled* scaffoldings would be more usable among knot enthusiasts to convey a knot building scheme: assemble scaffolding → construct the knot of interest → disassemble the scaffolding without breaking the knot.

(iii) It is just a question of size of scaffolding to choose in order to perform a correct mapping of however sophisticated knot is.

(iv) To make sure metrics are unique and unambiguous with one-to-one metric-to-knot correspondences, a unified mapping system should be developed similar to one, recommended by IUPAC to name organic molecules. Nevertheless, a couple of rules were already found empirically:

1) cross sections of rope and opening should not mutually differ too much;

2) sections of the rope between the openings inside the scaffolding should be straight and do not touch each other.

(v) Current approach will certainly allow one to establish one-to-one relations between the sequences of building units in biological polymers (*e.g.* proteins) and their folding patterns. Indeed, the endeavor would involve two conceptual steps:

1) mapping the folding patterns of all known biological polymers;

2) big data analysis with the help from AI to reveal statistical correlations between sequences of building units in biological polymers and sequences of symbols in polymers' metrics. Once realized, the program above would allow one to tailor and manufacture medical cure for pretty much any genetic disease from hemophilia to aging, following general scheme:

constructing desired folding pattern → mapping the pattern → decoding the metrics into the actual sequence of building units → synthesizing the pharmaceutical remedy required.

Reference

1. Geoffrey Budworth, *EverydayKnots*, Metro Books, 2008

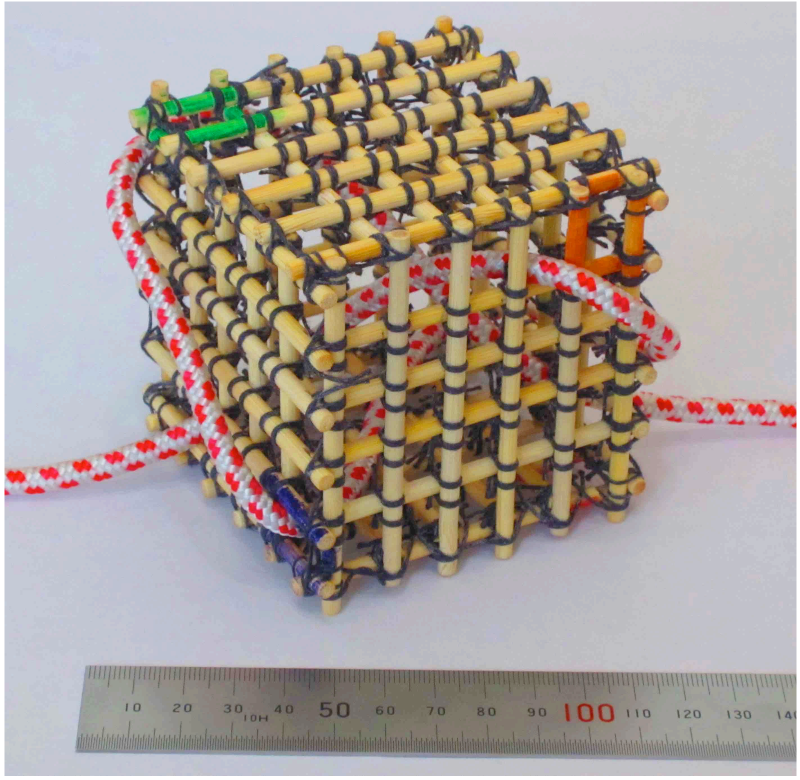

Fig.1 Photo of 5 x 5 x 5 bamboo-straw-made cubic scaffolding

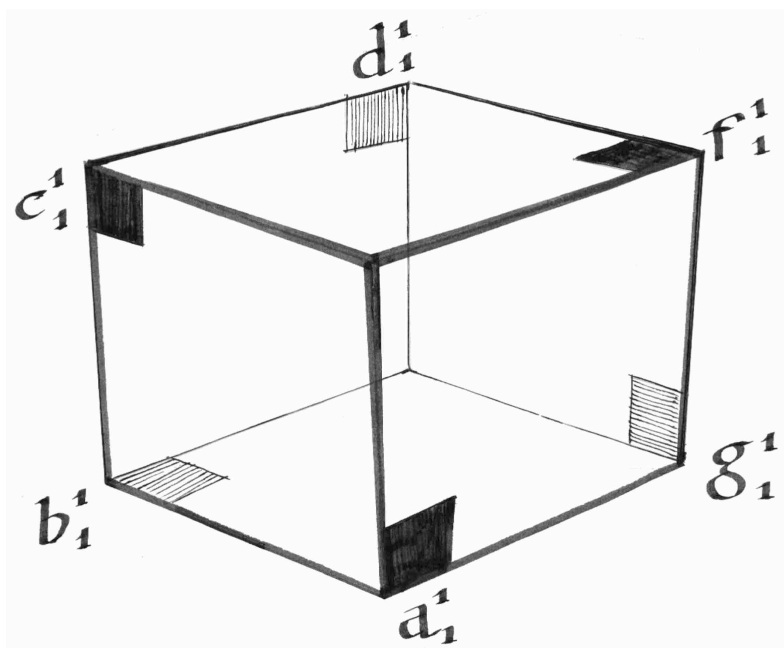

Fig. 2 Labeling openings of the cubic scaffolding

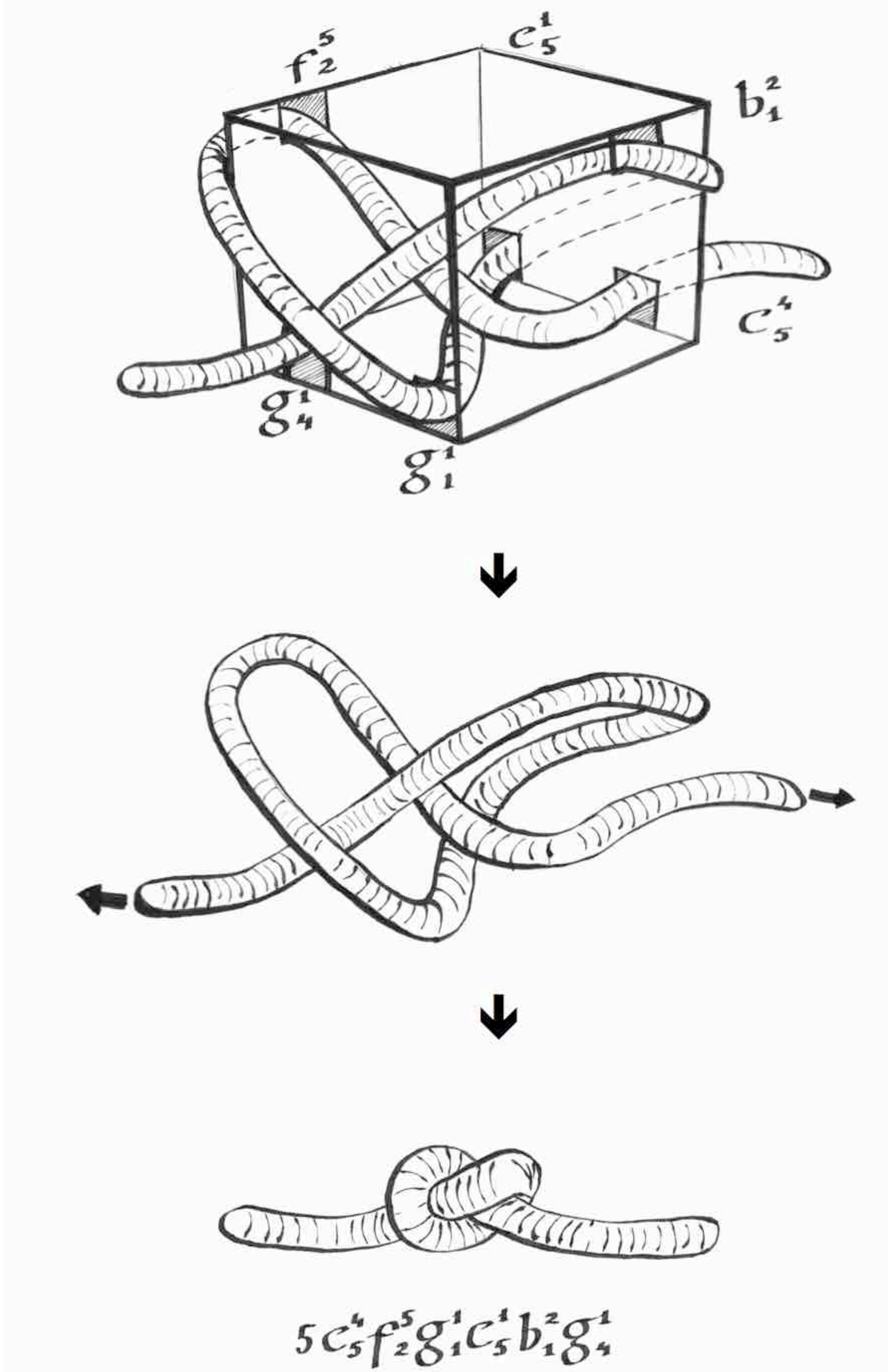

Fig. 3 Mapping a simple overhand knot