

**RANDOM TRANSITION OF KNOTS: A FIRST STEP
TOWARDS MODELLING UNKNOTTING BY TYPE II
TOPOISOMERASES**

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TOPOII is an enzyme that helps unknot DNA very efficiently with a process called strand-passage. In order to see whether it unknots DNA more efficiently than it can do by performing random strand-passages, we designed a computer algorithm to simulate random strand-passages.

There are two main steps in this simulation, namely, simulating DNA molecules and simulating random strand-passages. For the first step, we model DNA molecules as mathematical knots in the simple cubic lattice Z^3 and we use the BFACF algorithm, which is a type of Monte Carlo methods, to explore all possible configurations. For the second step, instead of performing strand-passages in a three dimensional space, we make use of Dowker codes which are one dimensional characterization of different types of knots.

We identify knot types after random strand-passages by means of Homfly polynomials, which are topological invariants of different types of knots. Finally, this identification enables us to obtain the distribution of knots after any given number of strand-passages.

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