Modelling of quasi-coherent displacement in chain-like bodies' movement

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Introduction

Chain-like bodies' movement is a phenomenon which is common in nature. One of the most interesting processes linked to the chain-motion is the translocation through a pore in membrane. It can be observed e.g. in rapid DNA and RNA sequencing techniques, controlled drug delivery process or gene therapy.

Many different algorithms for the simulation of the chain-like structures movement can be found in literature. However, it seems to be reasonable to create an efficient algorithm which can reflect the chain behaviour as well as possible. Therefore, the sequential algorithm for the modeling of the chain-like bodies' motion (SA-CLS) was proposed in literature.

Here, the following extensions of SA-CLS algorithm are presented:

- ❖ Compression Propagation Mechanism
- ❖ Movement-Direction Preference Mechanism

Compression propagation mechanism

In the previous version of SA-CLS the tension propagation mechanism has been incorporated. The tension stress apears in structure when the distance between consecutive segments during the move is bigger then the tension parameter (T_p). Analogous, the compression stress appears when the distance between consecutive segments during the move is smaller than compression parameter (C_p). The move is continued as long as the distance between consecutive segments is lower that C_p or/and greater then T_p, so till the tension or/and compression of the CLS exists. The illustration of the compression propagation mechanism and tension propagation mechanism influence on the chain motion are Figs 1 and 2.

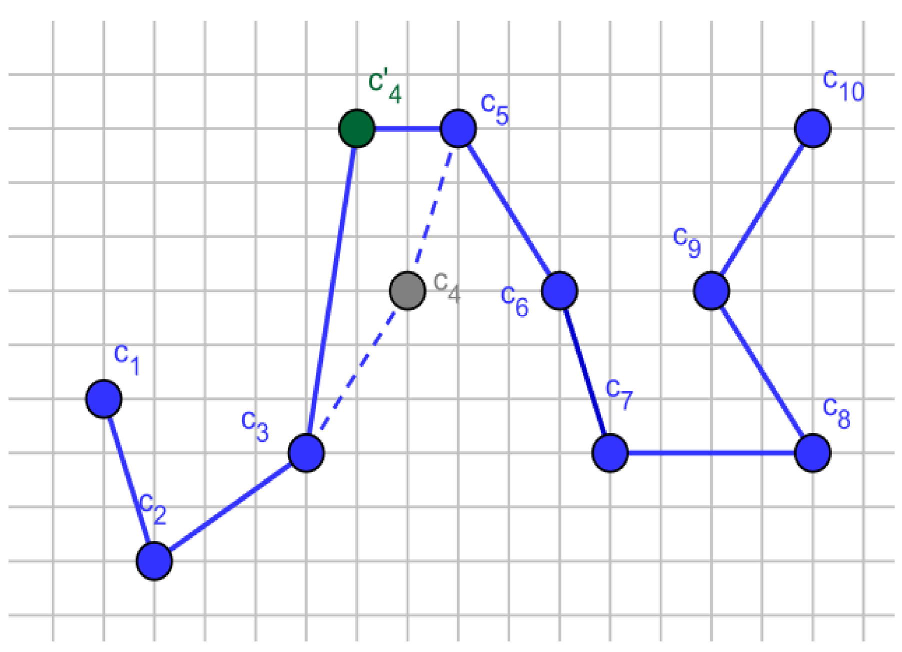

Fig. 1. The first step of the chain. c_4 – segment chosen to move as the first segment; c'_4 – a new position of segment c_4 .

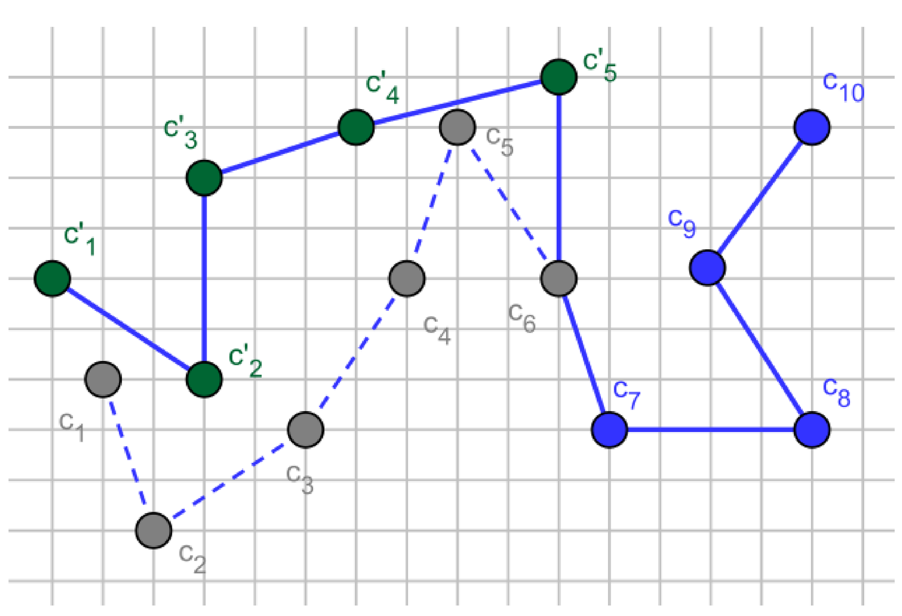

Fig. 2. New positions of segments caused by a tension or compression stress assuming that parameter C_p equals 2 and parameter T_p equals 4.

In Fig. 1 it can be seen that the distance between initial position of c_5 and the final position of segment c_4 (c'_4) is smaller then C_p = 2. Therefore, the compression stress apeared and segment c_5 moved to its new position c'_5 which is illustrated in Fig. 2. Moves of remaining segments are caused by appearing a tension stress.

Movement-Direction Preference Mechanism

Implementation of the movement-direction preference mechanism causes that the direction of the moving-segment-step depends on the position of the segment which has been moved previously. The moving segment is pulled (or pushed) in the direction of the previously moved segment (its new position). To implement this mechanism additional parameter has been introduced that determines the impact of the previous step on the next one. Important value which also has an influence on the whole mechanism functioning is the angle between vectors $\overrightarrow{w_1} = \overrightarrow{c_i c_{i+1}}$ (or $\overrightarrow{w_1} = \overrightarrow{c_i c_{i-1}}$) and $\overrightarrow{w_2} = \overrightarrow{c_i c_i'}$, where c_{i+1} (c_{i-1}) is the previous segment which made a step, c_i is the segment which currently makes a step and c_i' is its new position. The examplary angles are presented in Fig. 3 and Fig. 4.

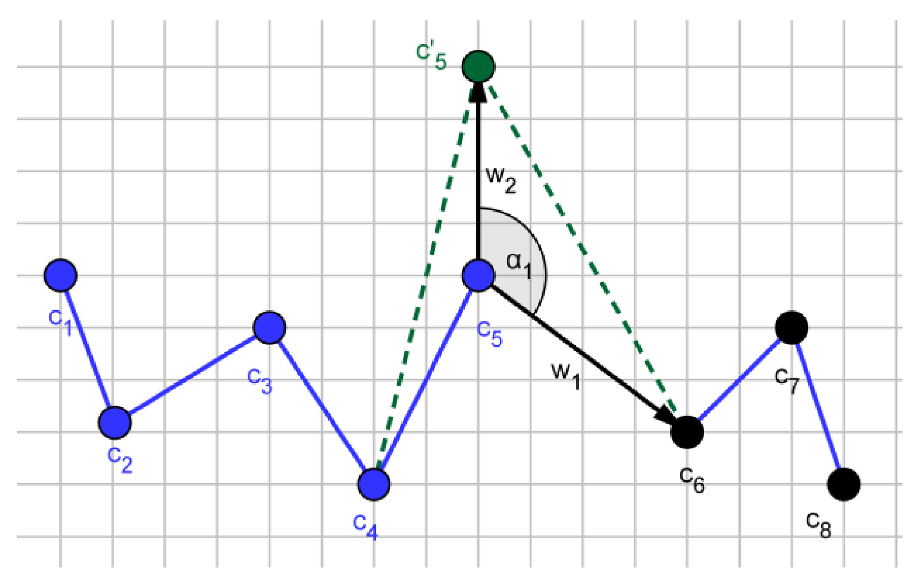

Fig. 3. Exemplary angle which is considered when the step direction is chosen – the case of obtuse angle.

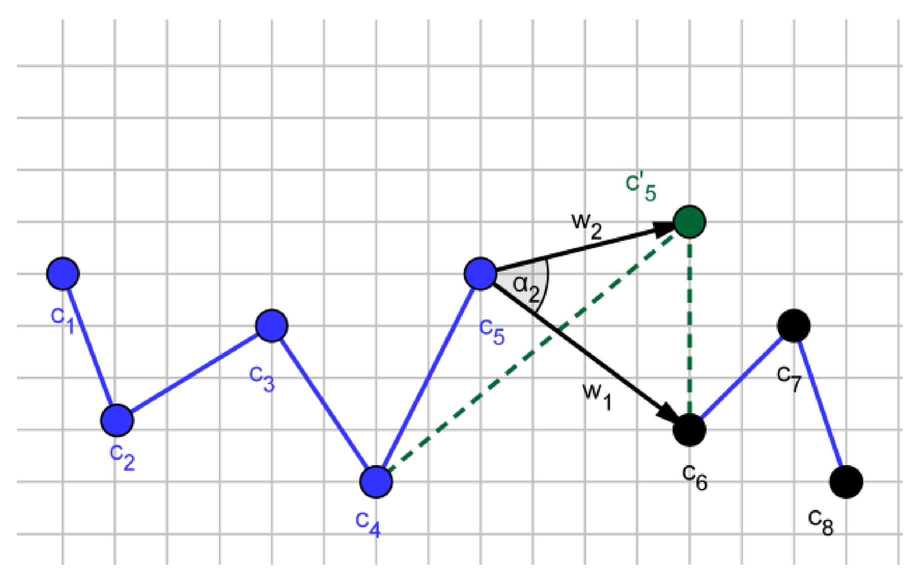

Fig. 4. Exemplary angle which is considered when the step direction is chosen – the case of acute angle.

Fig. 3 and Fig. 4 show two different possibility of new c_5 position. It should be noticed that the greater the value of cos(α), the higher probability of the step in vector w_2 direction. Therefore, the new position of c_4 presented in Fig. 4 is more probable than position presented in Fig.3, because $\cos(\alpha_1) < \cos(\alpha_2)$.

Final remarks

The results of studies confirm that presented mechanisms significantly affect the simulation process. They provide a possibility of more accurate settings of the structure and environment parameters. Moreover, obtained results show that introduced parameters have observable impact on the translocation time.

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