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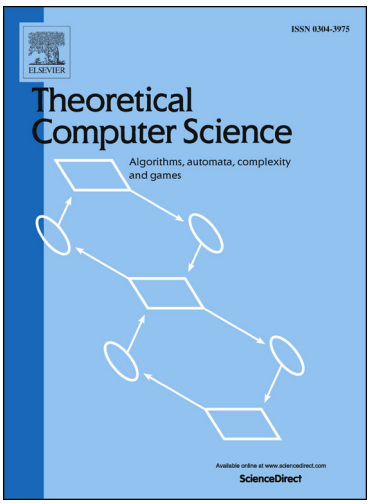

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Computational modeling of the kinetic Tile Assembly Model using a rule-based approach

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Abstract

The (abstract) Tile Assembly Model (aTAM), is a mathematical paradigm for the study and algorithmic design of DNA self-assembly systems. It employs the use of so-called DNA-tiles, which are abstractions of experimentally achievable DNA nanostructure complexes with similar inter-matching behaviours. To this day, there are about half-dozen different experimental implementations of DNA tiles and their sub-sequent algorithmic assembly into larger complexes, see e.g. Reif et al. 2012. In order to provide further insight into the assembly process, the aTAM model has been extended to a kinetic counterpart (kTAM). Although there is a wide abundance of different variants of the abstract model, e.g., stage, step, hierarchical, temperature-k, signal-passing, etc. (see e.g. Patitz 2012), numerical simulations of the kinetic counterpart have been performed only for a few types of these systems. This might be due to the fact that the numerical models and simulations of kTAM were almost exclusively implemented using classical stochastic simulation algorithms frameworks, which are not designed for capturing models with theoretically un-bounded number of species. In this paper we introduce an agent- and rule-based modeling approach for kTAM, and its implementation on NFsim, one of the available platforms for such type of modelling. We show not only how the modelling of kTAM can be implemented, but we also explore the advantages of this modelling framework for kinetic simulations of kTAM and the easy way such models can be updated and modified. We present numerical comparisons both with classical numerical simulations of kTAM, as well as comparison in between four different kinetic variant of the TAM model, all implemented in NFsim as stand-alone rule-based models.

1. Introduction

Recent advances in DNA-based nano-technology have opened the way towards the systematic engineering of inexpensive, nucleic-acid based nano-scale