Approximate Simulations of Cortical Microtubules using Dynamical Graph Grammars

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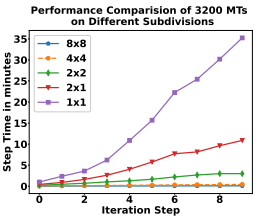
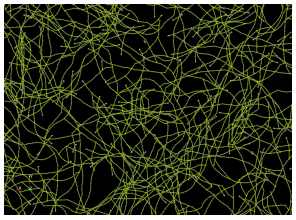
***Abstract*— Dynamical graph grammars (DGGs) are capable of modelling and simulating the dynamics of the cortical microtubule array (CMA) in plant cells by using an exact simulation algorithm derived from the master equation; however, the exact method is slow for large systems. We present an approximate simulation algorithm that is compatible with the DGG formalism, implement a simulator, and run an experiment using a DGG for the CMA. The approximate algorithm is faster than the exact and our experiment leads to the formation of a network in the long-time behavior.**

***Index Terms*— Plant Cells, Cortical Microtubule Dynamics, Graph Algorithms, Computational Modeling, Master Equation**



(a) Performance Comparision



(b) Long-time Behavior

Fig. 1: (a) Performance results (qualitative behavior observed over runs), and (b) Long-time behavior of DGG CMA.

I. Background

Dynamical Graph Grammars (DGGs) [1] allow for an expressive and powerful way to declare a set of local rules to model a complex, dynamic system with graphs. DGGs can be mapped into a master equation, a phenomenological set of first order linear differential equations governing the time evolution of joint probability distributions of state variables of a dynamic system. DGGs can be simulated exactly using an exact algorithm [2] that includes the Gillespie algorithm [3]. Similar to Gillespie, the exact algorithm becomes slow for large systems. Using operator algebra [2], an approximate algorithm for spatially embedded graphs can be derived.

In plant cells, the cortical microtubule array (CMA) plays an important role in cell division and shape [4]. Since microtubules (MTs) are polymer chains, they have a natural representation as a graph. Cortical microtubules (CMTs) in the CMA undergo dynamics such as treadmilling, zippering, induced catastrophe and crossover [5] - all of which can be represented as DGG rules.

II. Results

In this work, we have developed and implemented an approximate algorithm for accelerating the simulation of spatially embedded DGGs, and analyzed performance of an experimental DGG for the CMA. Our simulator is also capable of running the exact algorithm. In figure 1a we show a stack up of performance using the exact (1x1 case) and approximate (remaining cases) for the CMA DGG. The approximate algorithm allows for speedup by breaking the system into well-separated reaction sub-systems and firing some rules out of order at the cost of accuracy. In figure 1b, we demonstrate the long-time behavior of the CMA DGG. We started with 3200 fully disconnected MTs and let the simulation run until a long-time steady state was reached.

III. Conclusion

DGGs can be used to simulated biological systems using a simulation algorithm derived from a master equation. We have introduced an approximate algorithm to improve performance over the exact at the cost of accuracy. We were able to demonstrate the speedup and simulate dynamics by implementing a CMA DGG, which forms a network.

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