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Some theoretical issues on computer simulations¹

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Abstract

The subject of this paper is the development of mathematical foundations for a theory of simulation. Sequentially updated cellular automata (sCA) over arbitrary graphs are employed as a paradigmatic framework. In the development of the theory, we focus on the properties of causal dependencies among local mappings in a simulation. The main object of study is the mapping between a graph representing the dependencies among entities of a simulation and a graph representing the equivalence classes of systems obtained by all possible updates.

1 Introduction

Computer simulations are “composition engines”, that compose the actions of “entities” or “actors” with respect to a certain support-structure and are typically used for prediction and analysis. Consequently, a key question for a “theory of simulation” is to analyze *how* this composition is actually works, meaning: how does it depend on the actors/agents and on the actual dependency structure among them? Sequential dependencies, for example, are an issue in non-cooperative game theory [16]. Accordingly the primary focus of a theory of simulation is on the properties that result from composition of causal local interactions among individual entities. In order to assure generality, given a collection of local mappings and an update schedule, by hypothesis we assume entities to exist inherently—whether or not the mappings are specifically associated with software agent/actors, sites in a lattice, or otherwise. Accordingly, we make no essential reference in the theory to any particular method of local

representation in a simulation. For mathematical convenience and without loss of generality relative to simulation viewed as ordered composition of local maps, in this paper we utilize sequential updates of cellular automata (sCA) [21] over graphs as a paradigmatic framework for locality and sequentiality. We actually define a sCA over a graph (c.f. [23] for a similar approach that considers CA over Cayley graphs), X , by associating to each vertex i , a state $x_i \in \{0, 1\}$ and a local map f_i defined on the states of the i -neighbors and x_i , and which returns the state y_i . Application of local maps f_{i_k} in a particular order then induces a sequential CA (sCA) over a graph. This setting allows us to express the locality by adjacency in X and sequentiality by the different orders in which the vertices can be updated. For example, update sequences can be introduced for standard (i.e., a CA updated in parallel according to a nearest neighbor rule and closed boundary conditions) CA [18, 7, 1]. This yields an sCA over Circ_n (the circle graph on n vertices). In fact, every CA (over Circ_n) can be derived from a sCA over $2n$ vertices.

The line of thought of the paper as it relates to simulation is as follows. First basic terminology and the ansatz are introduced. Then the dependency graph and its local mappings are introduced. The dependency graph induces another graph (an update graph) wherein vertices are permutations of mapping update orders, and components imply functionally equivalent update orders. Relationships between these two graphs are proven where the dependency graph is viewed as a random graph (a probability space) that induces a random update graph. Hamiltonian paths in one graph imply isolated points in the other, and a single threshold function exists for the occurrence of both a Hamiltonian path and connectivity in the dependency graph [15, 5, 4, 3, 12]. This corresponds to the occurrence of isolated points in the update graph.

The interpretation relevant to simulation is that if the local mappings have more than very sparse dependencies in an update time interval, then, with probability one, unique update sequences, nearly a notion of a specific script, will be necessary to produce a given dynamical system. The number of components in the update graph is studied which obviously corresponds to the number of dynamical systems that a collection of co-dependent mappings can generate. The existence and the length of a path in the random update graph $U(G_{n,p})$ between two update orderings, e.g., update schedules, is analyzed. In fact, this equivalence can be tested in polynomial time. Further, the average size of a $U(G_{n,p})$ -component is computed. The relevance to simulation is that given two update orders, one can determine if they are in the same component; that is, if they produce the same dynamical system. We emphasize that this determination is made based on analysis of the structure of the causal dependencies among local mappings and not by measurements in the state space of those mappings or their composition. Last, the update is viewed from a categorical point of view rather than as a random variable. These results address the essential foundational issues of computer simulation, generation of system dynamics by composition of local maps and congruence of simulations, in a very general way and points to strategies for development of the theory. Full proofs of all results can be found in [9].

2 Terminology

Let X be a finite undirected graph with vertex set $\mathbf{v}X$ and edge set $\mathbf{e}X$. Two adjacent vertices P, Q are called *extremities* of an edge y and a subgraph $Y < X$ is called *induced*, if $P, P' \in \mathbf{v}Y$ are adjacent in Y if and only if P, P' are adjacent in X . A *path* in X is a multi-set $(Q_1, y_1, Q_2, \dots, y_n, Q_{n+1})$, where $Q_i \in \mathbf{v}X$, $y_i \in \mathbf{e}X$, Q_i and Q_{i+1} are extremities of y_i . The *length* of a path is the number of edges in the multi-set $(Q_1, y_1, Q_2, \dots, y_n, Q_{n+1})$; the *distance* $d_X(P, Q)$ between X -vertices P, Q is the minimal length of a X -path connecting P, Q or ∞ if there is no such path. Suppose $|\{Q_1, \dots, Q_n\}| = n$; the path $(Q_1, y_1, Q_2, \dots, Q_n, y_n, Q_1)$ corresponds up to isomorphism to a graph, which we refer to as Circ_n , the circle graph on n vertices. A graph X is called *connected* if any two vertices occur in an X -path. X -subgraphs induced by maximal connected subsets of vertices are called *components*. Let Y be a subgraph of X ; the set of $X \setminus Y$ -vertices that are adjacent to some vertices of Y , is called the *Y -vertex-boundary*, $d_X Y$. We denote

the *ball* of radius k in X by

$$\mathcal{B}_k(i, X) = \{j \mid d_X(i, j) \leq k\}. \quad (2.1)$$

A *random graph* [14, 15, 5, 2] is a finite probability space consisting of subgraphs of a base graph X . E.g. take $X = K_n$, the complete graph over n vertices, and consider subgraphs $Y < X$ with the underlying probability $\mu_{n,p}(Y) = p^{|\mathbf{e}Y|}[1 - p]^{\binom{n}{2} - |\mathbf{e}Y|}$. We denote the random graph $(\{Y < K_n\}, \mu_{n,p})$ by $G_{n,p}$. Its elements are obtained by selecting each K_n -edge with independent probability p . Let $p_n, q_n : \mathbb{N} \rightarrow [0, 1]$ be probabilities. A *threshold function* of a property $(\#)$ of a random graph is a probability p_n such that: for n tending to ∞ , the probability of the set of subgraphs having $(\#)$ fulfills a 1-0-law: for $\lim_{n \rightarrow \infty} (q_n/p_n) = 0$: $\lim_{n \rightarrow \infty} \mu_{q_n}\{H \models (\#)\} = 0$ and for $\lim_{n \rightarrow \infty} (p_n/q_n) = 0$: $\lim_{n \rightarrow \infty} \mu_{q_n}\{H \models (\#)\} = 1$. A n -cube Ω_2^n is a graph whose vertices are n -tuples (x_1, \dots, x_n) , $x_i \in \{0, 1\}$ and two vertices are adjacent if they differ in exactly one coordinate. We will abbreviate *almost surely* by a.s. and write for functions $f : \mathbb{N} \rightarrow \mathbb{R}$, $g : \mathbb{N} \rightarrow \mathbb{R}$: $f = O(g)$ iff $\lim_{n \rightarrow \infty} \frac{f(n)}{g(n)}$ exists and $\lim_{n \rightarrow \infty} \frac{f(n)}{g(n)} = c > 0$, in particular $f \sim g$ for $\lim_{n \rightarrow \infty} \frac{f(n)}{g(n)} = 1$ and $f = o(g)$ iff $\lim_{n \rightarrow \infty} \frac{f(n)}{g(n)}$ exists and $\lim_{n \rightarrow \infty} \frac{f(n)}{g(n)} = 0$. Further we make use of the following result on sums of independent random variables, $Z_n = \sum_{i=1}^n z_i$, where each z_i has values in $\{0, 1\}$ [8, 2]. Then, $\forall c > 0 \exists c_1 > 0$:

$$\mu_n\{ |Z_n - \mathbb{E}[Z_n]| > c\mathbb{E}[Z_n] \} \leq e^{-c_1\mathbb{E}[Z_n]}. \quad (2.2)$$

Let S_n be the symmetric group over n letters. We write $(1, 2, \dots, n-1, n)$ as id and set

$$\forall \pi \in S_n : \text{Inv}(\pi) = |\{(i, k) \mid i < k \wedge \pi(i) > \pi(k)\}| \quad (2.3)$$

that is $\text{Inv}(\pi)$ is the number of *inversions* of the permutation π . For a pair (i, k) with $\pi(i) > \pi(k)$ we say (i, k) is an *inversion-pair* (i.p.) of π [13].

3 Sequential cellular automata over graphs

A *cellular automaton* (CA) [21, 18] of size n (with closed boundary conditions, i.e. cell i depends on $i - k \bmod n, \dots, i + k \bmod n$) is a dynamical system

$$g : \mathbb{F}_2^n \rightarrow \mathbb{F}_2^n, \quad g[(x_1, \dots, x_n)] = (y_1, \dots, y_n) \quad (3.1)$$

where \mathbb{F}_2^n is a n -dimensional vector space over \mathbb{F}_2 . The map g is induced by *parallel application* of a *local rule* f , that is, a mapping

$$f : \mathbb{F}_2^{2k+1} \rightarrow \mathbb{F}_2, \quad f(x_{i-k \equiv n}, \dots, x_{i+k \equiv n}) = y_i. \quad (3.2)$$

Here, local means that the coordinate y_i depends only on $x_{i-k \equiv n}, \dots, x_{i+k \equiv n}$ for small k . In particular, the locality of a nearest neighbor CA corresponds to the adjacency relation of the *circle graph* Circ_n with vertex set $\{1, \dots, n\}$ and $k = 1$. Next we define sequential CAs over regular graphs. In certain analogy with a classic CA with nearest neighbor rule, where $X \cong \text{Circ}_n$, a sequential CA (sCA) is a quadruple $(X, \mathbb{F}_2, (f_i)_X, \pi)$, where

- X is a regular graph with $\mathbf{v}X = \{1, \dots, n\}$ and vertex degree m
 - \mathbb{F}_2 is the set of *states* of an X -vertex
 - f_i, X is a *local map*: $f_i, X : \mathbb{F}_2^{m+1} \rightarrow \mathbb{F}_2$
- $$f_i, X(x_{i_1}, \dots, x_{i_{m+1}}) = y_i \quad i_1 < i_2, \dots, i_m < i_{m+1}$$
- $i_k \in \mathcal{B}_1(i, X)$ where i_1, \dots, i_{m+1} are X -vertices and $\mathcal{B}_1(i, X)$ is defined by (2.1)
- π is a permutation, or ordering $\mathfrak{O}(\pi)$ according to which the local maps f_i, X are applied.

The mapping $(x_{i_1}, \dots, x_{i_{m+1}}) \mapsto y_i$ is referred to as the *update* of x_i . The local maps f_i, X induce maps $F_i, X : \mathbb{F}_2^n \rightarrow \mathbb{F}_2^n$ in a natural way:

$$F_i, X((x_j)_j) = (x_1, \dots, x_{i-1}, y_i, x_{i+1}, \dots, x_n). \quad (3.3)$$

where $y_i = f_i(x_{i_1}, \dots, x_{i_{m+1}})$. The induced maps $F_i, X : \mathbb{F}_2^n \rightarrow \mathbb{F}_2^n$, $F_j, X : \mathbb{F}_2^n \rightarrow \mathbb{F}_2^n$ allow the formation of products $F_i, X \circ F_j, X$. Now, choosing an ordering \mathfrak{O} of the X -vertices a complete update of $\mathbf{v}X$ corresponds to a product

$$\prod_{i=1}^n F_{\pi(i), X} : \mathbb{F}_2^n \longrightarrow \mathbb{F}_2^n, \quad \pi \in S_n. \quad (3.4)$$

Suppose now we have a subgraph $Y < X$ such that $\mathbf{v}Y = \mathbf{v}X$. Although Y is not regular we can define maps $f_{i, Y}, F_{i, Y}$ analogous to f_i, X, F_i, X if

- $f_{i, Y} : \mathbb{F}_2^{m+1} \rightarrow \mathbb{F}_2$, $f_{i, Y}(x_{i_1}, \dots, x_{i_{m+1}}) = y_i$, $i_1 < i_2, \dots, i_m < i_{m+1}$, $i_k \in \mathcal{B}_1(i, X)$, and
- $f_{i, Y}$ does *not* depend on $X \setminus Y$ -neighbors.

Note that in the extreme case $\mathbf{e}Y = \emptyset$, the maps $f_{i, Y}$ only depend on the vertex i itself. In complete analogy to (3.3) we then induce the maps $F_{i, Y}$ and the time evolution of Y -vertices is obtained by iterating $\prod_{i=1}^n F_{\pi(i), Y} : \mathbb{F}_2^n \longrightarrow \mathbb{F}_2^n$, $\pi \in S_n$. Each factor $F_{\pi(i), Y}$ is a mapping that updates the state of vertex $\pi(i)$ as a function on all $\pi(i)$ neighbors in Y and that leaves all other Y -vertex states invariant.

Let us next assume that $Y < X$ and $\mathcal{F} = \{F_{1, Y}, \dots, F_{n, Y}\}$ are fixed. Then it is natural to ask which permutations leave a given product $\prod_{i=1}^n F_{\pi(i), Y}$ invariant.

Given two permutations $\pi, \pi' \in S_n$, it is important to note that the equality

$$\prod_{i=1}^n F_{\pi(i), Y} = \prod_{i=1}^n F_{\pi'(i), Y} \quad (3.5)$$

is due to either (a) symmetries of the maps F_i or (b) the structure of X . In this paper we will not address (a), instead we will elaborate (b) in some more detail. First, $\forall \{\pi(i), \pi(j)\} \in \mathbf{e}[Y] \exists F_{\pi(j), Y}, F_{\pi(i), Y}$

$$F_{\pi(j), Y} \circ F_{\pi(i), Y} \neq F_{\pi(i), Y} \circ F_{\pi(j), Y} \quad (3.6)$$

and second $\forall F_{\pi(j), Y}, F_{\pi(i), Y} : \{\pi(i), \pi(j)\} \notin \mathbf{e}[Y]$

$$F_{\pi(j), Y} \circ F_{\pi(i), Y} = F_{\pi(i), Y} \circ F_{\pi(j), Y}. \quad (3.7)$$

Taking an abstraction of this situation we may then replace a product $\prod_{i=1}^n F_{\pi(i), Y}$ by the corresponding permutation π . Moreover, we can introduce a neighborhood relation by saying that two permutations $\pi = (i_1, \dots, i_n)$ and $\pi' = (i'_1, \dots, i'_n)$ are adjacent iff there exist two consecutive indices i_k, i_{k+1} such that $i_k = i'_{k+1}$, $i_{k+1} = i'_k$ and $i_j = i'_j$, otherwise. This approach leads to the definition of the *update graph* $U(Y)$ whose components imply certain *equivalence classes* of sCA over Y . We will formally define update graphs in the next section.

4 Update graphs

In this section (see [9] for proofs) we establish a mapping U , that assigns to an arbitrary graph Y with $\mathbf{v}Y = \{1, \dots, n\}$ an *update graph*, $U(Y)$, whose vertices are permutations, (i_1, \dots, i_n) , $i_k \in \mathbf{N}_n$. It is straightforward to show that every transposition of consecutive vertices i_k, i_{k+1} with $\{i_k, i_{k+1}\} \notin \mathbf{e}Y$ leaves the product of arbitrary local maps $\prod_{i=1}^n F_{i, Y}$ invariant.

Proposition 1 Let Y be a subgraph of a regular graph X with $\mathbf{v}Y = \{1, \dots, n\}$ and $\pi = (i_1, \dots, i_n)$, $\pi' = (i'_1, \dots, i'_n)$ two permutations of its vertex set. Suppose there exists a sequence of transpositions (s_k, s_l, \dots, s_h) , where $s_j = (j, j+1)$ and $m+1 = |(s_k, s_l, \dots, s_h)|$, such that

$$\begin{aligned} s_k \pi &= (i_1, \dots, i_{k+1}, i_k, \dots, i_n) = \pi^1 \\ s_l \pi^1 &= (i_1^1, \dots, i_{l+1}^1, i_l^1, \dots, i_n^1) = \pi^2 \\ &\dots \\ s_h \pi^m &= (i_1^m, \dots, i_{h+1}^m, i_h^m, \dots, i_n^m) = \pi', \end{aligned}$$

with $\{i_k, i_{k+1}\}, \{i_l^1, i_{l+1}^1\}, \dots, \{i_h^m, i_{h+1}^m\} \notin \mathbf{e}Y$. Then we have

$$\prod_{r=1}^n F_{\pi(r), Y} = \prod_{r=1}^n F_{\pi'(r), Y}.$$

Accordingly, our construction is an adequate framework in which to study the equivalence class problem for sCAs. We next give the formal definition of update graphs $U(Y)$ for arbitrary graphs Y :

Definition 1 Let Y be a graph with $\mathbf{v}Y = \{1, \dots, n\}$. The update graph $U(Y)$ over Y has vertex set S_n and two vertices $(i_1, \dots, i_n), (h_1, \dots, h_n)$ are adjacent iff $\exists j \in \mathbb{N}_{n-1} : (i_j, i_{j+1}) = (h_{j+1}, h_j), i_m = h_m$, else $\wedge \{i_j, i_{j+1}\} \notin \mathbf{e}Y$.

For a graph Y we refer to the graph having $\mathbf{v}Y$ as vertex set and an empty edge set as Y_\emptyset . Obviously, $U(Y_\emptyset)$ is a $n-1$ regular graph with diameter $\binom{n}{2}$ and we have $U(Y) < U(Y_\emptyset)$. Further, let $Y < X$ be a subgraph of a regular graph X , and let $C_n^{(1)}, C_n^{(2)}$ be two $U(Y)$ -components, then there exists a Y -edge $\{i, k\}$ such that $C_n^{(1)}$ -vertices can be written as $\pi_1 = (\dots, i, \dots, k, \dots)$ and $C_n^{(2)}$ -vertices $\pi_2 = (\dots, k, \dots, i, \dots)$ respectively. According to (3.6) there exist local maps $F_{Y,i}, F_{Y,k}$ such that $F_{i,Y} \circ F_{k,Y} \neq F_{k,Y} \circ F_{i,Y}$. If, for example, all maps $F_{r,Y}$ are bijective we conclude from this

$$\prod_{r=1}^n F_{\pi_1(r), Y} \neq \prod_{r=1}^n F_{\pi_2(r), Y}.$$

That is, for any two $U(Y)$ -components, $C_n^{(1)}, C_n^{(2)}$, there exist local maps such that induced sCA over Y w.r.t. $C_n^{(1)}, C_n^{(2)}$ -vertices are different.

Lemma 1 Let Y be a graph and $U(Y)$ be the update graph, defined as above. Then, $U : \{Y < X\} \rightarrow \{U(X) < U(X_\emptyset)\}$ is injective.

The assignment $Y \mapsto U(Y)$ allows us to study the relation between actual dependencies of a family of local maps and the corresponding induced dynamics, without exhaustively enumerating rule space.

A natural and general framework for this question is to assume that $X = K_n$, the complete graph over n vertices, and to consider the random graph $G_{n,p}$. U can be viewed as a random variable over $G_{n,p}$, which induces a random graph $U(G_{n,p})$ as follows

$$U : G_{n,p} \rightarrow (\{U(Y)\}, \mu_U), \quad Y \mapsto U(Y), \quad (4.1)$$

where $\mu_U(U(Y)) = \mu_{n,p}(Y)$. According to lemma 1 μ_U is well defined.

Proposition 2 The following assertions hold

$$\begin{aligned} \text{for } p = 0 & \quad \mu_{n,0}\{U(G_{n,0}) \text{ is connected}\} = 1. \\ \text{for } p = 1 & \quad \mu_{n,1}\{\mathbf{e}U(G_{n,1}) = \emptyset\} = 1. \end{aligned}$$

These observations lead to the question: what is the evolution of $U(Y)$ as p increases from 0 to 1? For this purpose it is useful to recall an important theorem on Hamiltonian paths in $G_{n,p}$, which was a long standing open problem of Erdős and Rényi [14, 15], solved by Bollobás [4, 3] and independently by Komlós and Szemerédi [12].

Theorem 1 Suppose $p = \frac{\ln(n) + \ln(\ln(n)) + c}{n}$ with $c \in \mathbb{R}_+$, then

$$\lim_{n \rightarrow \infty} \mu_{n,p}\{G_{n,p} \text{ is Hamiltonian}\} = e^{-e^{-c}}. \quad (4.2)$$

As we will see later, $\frac{\ln(n)}{n}$ is the threshold function for the emergence of a Hamiltonian path and connectivity of $G_{n,p}$ [10, 14, 15]. Theorem 1 in particular implies that $p = \frac{c \ln(n)}{n}$ is a threshold function for the existence of isolated vertices in $U(G_{n,p})$.

Corollary 1 Let $p = \frac{\ln(n) + \ln(\ln(n)) + c}{n}$ with $c \in \mathbb{R}_+$, then

$$\lim_{n \rightarrow \infty} \mu_{n,p}\{U(G_{n,p}) \text{ has an isolated vertex}\} = e^{-e^{-c}}. \quad (4.3)$$

Now we turn to the component-structure of $U(G_{n,p})$ as p tends to 1. Again, we can report a duality between the random graphs $G_{n,p}$ and $U(G_{n,p})$. In this context it is worth recalling the main epochs in the evolution of $G_{n,p}$ [10, 14, 15, 5].

Theorem 2 Suppose $p = \frac{c}{n}$ with $c \in \mathbb{R}_+$, then for

$$\begin{aligned} c < 1, \quad & \lim_{n \rightarrow \infty} \mu_{n,p} \{ \text{all components} \leq O(\ln(n)) \} = 1, \\ c = 1, \quad & \lim_{n \rightarrow \infty} \mu_{n,p} \{ \exists \text{ a component} \geq O(n^{\frac{2}{3}}) \} = 1, \\ c > 1, \quad & \lim_{n \rightarrow \infty} \mu_{n,p} \{ \exists \text{ a component} \geq O(n) \} = 1. \end{aligned}$$

For $p = \frac{c \ln(n)}{n}$ with $c \in \mathbb{R}_+$

$$\lim_{n \rightarrow \infty} \mu_{n,p} \{ G_{n,p} \text{ is connected} \} = e^{-e^{-c}}. \quad (4.4)$$

We can now state first properties of U :

Theorem 3 For the random graph $G_{n,p}$ let $U(G_{n,p})$ be the induced random graph. Then $\forall 0 < a < 1$:

$$U(G_{n,p}) \text{ has a component of size} \geq \frac{n!}{2^{[1+a]p \binom{n}{2}}} \text{ a.s.} \quad (4.5)$$

In particular, for $p = o(\frac{\ln(n)}{n})$ and $0 < \epsilon < 1$ we have

$$U(G_{n,p}) \text{ has a giant component} \geq [n!]^{1-\epsilon} \text{ a.s.} \quad (4.6)$$

Proposition 3 Let the random graphs $G_{n,p}$ and $U(G_{n,p})$ be given. Then we have

$$\mu_{n,p} \{ \pi, \text{id} \in U(G_{n,p}) \text{ are connected} \} = (1-p)^{\text{Inv}(\pi)}. \quad (4.7)$$

Note that the random variable $\text{Inv} : S_n \rightarrow \mathbb{Z}$ is in the limit Gaussian distributed with $\mathbb{E}[\text{Inv}] = \frac{n(n-1)}{4}$ and $\mathbb{V}[\text{Inv}] \sim \frac{n^3}{36}$ [13]. In view of Proposition 3 this observation could allow us to derive results on $U(G_{n,p})$ -components for $p = \frac{c \ln(n)}{n}$ and beyond. A first result in this context analyzes the random variable $C_{\text{id}} : U(G_{n,p}) \rightarrow \mathbb{Z}$:

$$C_{\text{id}}(U(Y)) = |\{\pi \mid \pi, \text{id} \text{ are connected}\}|. \quad (4.8)$$

Proposition 4 Let the random graphs $G_{n,p}$ and $U(G_{n,p})$ be given. Then we have

$$\mathbb{E}(C_{\text{id}}) = p^{-n} \prod_{i=1}^n [1 - (1-p)^i]. \quad (4.9)$$

In particular we have for $p = 1$, $\mathbb{E}(C_{\text{id}}) = 1$ and for $p = 0$, $\mathbb{E}(C_{\text{id}}) = n!$.

We finally give a categorical interpretation of U :

Proposition 5 Let Y be a graph and Y^c be the graph with $\mathbf{v}Y^c = \{1, \dots, n\}$ and $\mathbf{e}Y^c = \mathbf{e}K_n \setminus \mathbf{e}Y$. Let ϕ be a surjective graph morphism, then we have the commutative diagram

$$\begin{array}{ccc} Y_1^c & \longrightarrow & U(Y_1) \\ \downarrow \phi & & \downarrow U(\phi) \\ Y_2^c & \longrightarrow & U(Y_2) \end{array}$$

and for surjective graph morphisms ϕ, ψ holds

$$U(\phi \circ \psi) = U(\phi) \circ U(\psi) \quad (4.10)$$

$$U(\text{id}_{Y^c}) = \text{id}_{U(Y)}. \quad (4.11)$$

5 Discussion

An abstraction of computer simulations viewed as compositions of local mappings that produce global system dynamics has been developed. This perspective allows analysis without detailed formal reference to particular local mappings beyond the fact that they can depend on each other. We employ sequential cellular automata (sCA) over random graphs as a paradigmatic framework for elements of a theory of simulation and show that dynamical systems generated by simulations can be classified by equivalence classes on update sequences. Simulation is only beginning to be seen as an area to be developed formally in computer science, but due to the widespread use of computer simulation, the need for development of theoretical foundations is recognized. The main aspects of a theory of simulation we are concerned with here are locality and sequentiality. Our analysis has focused on the relation between the basic dependency graph Y , whose vertices are updated by local maps (local here being defined by the adjacency in Y), and its update graph $U(Y)$ whose components imply certain equivalence classes of sCA over Y . What distinguishes the approach we take here from what we see occurring in the literature might be summarized by our specific intent to exclude any detail from consideration of the local rules aside from dependencies, the use of random graphs to broadly characterize properties of simulation, the focus on generation of dynamics as primary, and the derivation of mimicry from the basic generative considerations. Mathematically, a rather different, but related view can be found in Z. Róka [23], which reveals interesting insights concerning simulations between CA on different Cayley graphs. The conceptual similarity between Róka's approach and ours consists of a recognition of the im-

portance that structural properties of the representation are influential to the generated dynamics and that equivalent systems can be generated over different structures under certain conditions. However, our setting is not restricted to Cayley graphs over finite groups and their morphisms.

We have discussed in detail how our approach relates to [11, 6, 19, 22]. Moreover, it may be of interest that the mathematical properties observed in this analysis of simulation are related to random graph models of sequence to structure mappings in biomolecules [17], and topics in theory of parallel computing [20]. In particular our theory has interesting implications for gene-regulatory networks, modeled by random Boolean networks. Our results show to what extend a specific order matters, according to which certain genes are activated.

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