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Graph-cellular automata: a generalised discrete urban and regional model

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Abstract. A new type of dynamic spatial model is described: graph-cellular automatoa (graph-CA). First, the proximal model of space and geo-algebra are briefly introduced. Then, the graph-CA model is described, with an emphasis on understanding it as a reworking of the proximal model of space and also of geo-algebra. It is shown that graph-CA with particular structural properties defined in terms of the relationships between subsets of cells are a useful generalisation of traditional cellular automaton (CA) which enable meaningful descriptions of model structure to be developed. This enables further development of novel types of model in the same 'family' while retaining links to simpler, better understood examples. It is further argued that the derivation of the graph-CA from both the graph and CA formalisms permits the simultaneous use of well-developed ways of describing model structure and process dynamics, and that this could form the basis of a research programme into the elusive relations between the two. The relationship of graph-CA to other discrete models is briefly discussed, and a classification scheme which indicates the particular geographical interest of such models is suggested.

1 Introduction

Cellular automata (CA) models of urban and regional change have, in recent years, become commonplace (White, 1998). Many have been presented in the pages of this journal, including a number in a special issue (Batty et al, 1997). Briefly, a CA consists of a lattice (often a grid), a set of allowed cell states, and a transition rule specifying changes in cell state which occur at discrete time steps. Each cell's state is determined at each time step according to its own current state and the state of neighbouring cells in the lattice (or cell space). Cell neighbourhoods are uniformly defined across the cell space, typically including a cell's immediate neighbours in the lattice. The (nongeographical) example par excellence is Conway's Game of Life (Poundstone, 1985), which exhibits bewilderingly complex global behaviour based on only two allowed cell states and confoundingly simple transition rules. Such unexpectedly rich global behaviour is one of the attractions of the approach as a basis for building urban and regional models, since global structure in a CA system is often seen to emerge out of purely local interactions between cells (Couclelis, 1985; 1988). This is attractive because it matches our intuitive sense that much human spatial activity is not centrally planned or organised, but arises from the responses of various actors—residents, developers, planners, politicians—to local circumstances. It also holds out some promise of deeper insight into the enduring mystery of the relationship between processes at the microlevel and the macrolevel of geographical and economic activity.

Although the rigid 'classic' CA has been used in some urban and regional models (especially in work by Batty and Longley, 1986; Batty and Xie, 1997), it is generally regarded as rather restrictive, and various 'relaxations' have been introduced. In the urban context, some of these are considered by White (1998, pages 112 – 113). In various applications cells may be nonuniform including, for example, different suitabilities for

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development (Clarke et al, 1997). In some cases cell nonuniformity extends as far as using the CA to generate a dynamic development potential at each cell, which is then used to assign sequentially new development determined *outside* the CA (White and Engelen, 1997). This effectively introduces asynchronous cell update, a significant departure from the formalism. Cells which have a fixed state—a variant of the nonuniform cell approach—have also been introduced, to cope with the problem of model 'edge-effects' (White and Engelen, 1993). Furthermore, neighbourhoods may extend beyond immediately adjacent cells (Clarke et al, 1997; White et al, 1997), with distance-decay effects, and cell transition rules are usually probabilistic. All this variation certainly enhances the realism of CA-based models, and the likelihood of their more widespread adoption in operational settings. However, this is achieved to the detriment of the more general and elusive insights which the simple CA formalism originally promised.

One way out of the impasse is to develop and explore systematically particular, well-defined variations of the CA formalism. This is a major motivation for introducing the graph-CA, which formalises one CA variation in which cell neighbourhoods may be nonuniform across cell space. The potential of such a spatial 'relaxation' of the formalism has previously been raised in the context of proximal spatial models by Couclelis (1997). She discusses the relationship between proximal space, cellular automata as they have been used in urban and regional models, and a formalisation of those models—geo-algebra (Couclelis, 1997; Takeyama, 1996; 1997; Takeyama and Couclelis, 1997). Adopting the same conceptual framework as Couclelis, in this paper I rework the proximal model of space as a particular kind of cellular automaton—a graph-CA or irregular CA. The graph-CA is thus also an alternative formalism to geo-algebra. It is likely that each formalism will be more useful than the other in some (but not all) contexts. In any case, graph-CA, like geo-algebra, are a useful generalisation of CA models, and many existing and possible cellular urban models may be regarded as implementations. It is further argued that the graph-CA, as presented in this paper, provides some useful conceptual tools with which to unpick the knotty problem of the relationship between structure and process, form and function. This has been a recurrent theme of this journal, and perhaps this paper may suggest approaches to some of the questions about relating structure and process posed in a recent editorial (Batty, 1999). The approach may also provide a basis for geocomputational theory and investigation—a recent concern of this journal (Couclelis, 1998)—as has been suggested elsewhere (O'Sullivan, 1999).

In section 2 the proximal model of space, and the geo-algebra formalism are introduced and described, to pave the way in section 3 for the introduction of graph-CA as an alternative formalisation of proximal space. The next three sections then show how understanding graph-CA as graphs, as CA, and as simultaneously graphs *and* CA, respectively, enables a range of new perspectives and approaches. In section 4 the potential for description and investigation of model structures understood as graphs is discussed. A particular graph-CA structure is also described—the multi-graph-CA—which further demonstrates the generality of the graph-CA approach for building a variety of spatial models. In section 5 some ideas from dynamical studies of strict CA which may be usefully applied to this wide range of models are reviewed. This paves the way for a consideration in section 6 of the potential for investigating the relations *between* structure *and* process in graph-CA models. This discussion is contextualised by reference to a framework wherein graph-CA are related to other discrete models, and by reference to research in other fields which demonstrates both that it is possible to relate structure to dynamics using models of this type, *and* that there is a

niche for specifically geographical (perhaps *geo*computational) research in this area. Some brief conclusions are offered in section 7.

2 The proximal model of space and geo-algebra

The proximal model of space and geo-algebra has been presented in a number of papers by Couclelis and Takeyama (Couclelis, 1997; Takeyama, 1997; Takeyama and Couclelis, 1997), and also in Takeyama's (1996) doctoral thesis. These ideas are derived in part from a consideration of the relevance of absolute and relative models of space (Couclelis, 1997) and also as a generalisation of Tomlin's (1990) map algebra. The interested reader should refer to these sources for full details of the concepts and their development; the essentials are presented here to allow the introduction of the graph-based cellular automaton (graph-CA) as a reworking of these ideas, which enables new approaches to the dual problems of implementing dynamic spatial models and developing our understanding of spatial systems.

In the proximal conception of space, the significant features of a location are not just those local to the location itself, but those which result from its being part of a global spatial structure. The place that a location occupies in space—its *site*—is distinct from its *situation*, which describes its location relative to other locations (Couclelis, 1997). The concept of proximal space attempts to accommodate both site and situation in its central notion of the *neighbourhood*. According to Takeyama (1996, pages 16 – 17):

> "In proximal space, the [spatial] information is geo-referenced as in absolute space, but to each location is attached a representation of the relative space of which it is a part. While the key notion in absolute space is the geo-referenced item, and in relative space, the spatial relation, the key notion in proximal space is the neighbourhood."

Furthermore, a neighbourhood is defined by relations of *nearness* between spatial elements, and nearness in turn depends on both (spatial) adjacency *and* (functional) influence. A location's neighbourhood consists of all those other locations which may influence it, whether through proximity or functional relations. The close affinity between this view and that embodied in the neighbourhood relationships of CA-based models is clear.

The proximal model is capable of encompassing both absolute and relational conceptions of space, which have long competed for dominance in geographical theory. This is not the place to reprise such long-running arguments. It suffices to point out that proximal space seems wholly commensurate with recent developments in geographical theory (see Sack, 1997; and even, perhaps, Harvey, 1996). The proximal approach also draws attention to two aspects of spatial phenomena. First, spatial phenomena are not mere collections of spatially referenced objects, contingently related by their geocoordinates, as in a strictly absolute view of space; the construction of a proximal spatial model requires us to recognise this fact and explicitly construct a set of relations amongst the entities under consideration. The relations we construct are, in turn, dependent on our theories about the phenomena we are modelling. Second, some relations are usually more important than others, depending on the problem domain, and on the particular sorts of phenomena of interest; again, a proximal view requires us explicitly to acknowledge this fact. The necessarily true observation of an extreme relational view, that everything is related to everything else, so that every single location is—in some sense—a mirror of all space, is thus avoided.

According to Takeyama and Couclelis (1997, page 77), "Geo-Algebra aims to provide a rigorous common formalism for map analysis and spatial modelling". The clear implication is that it also provides a formalisation of proximal space,

a connection made explicit by Couclelis (1997). The formalism conceives of a map M as a set of tuples or *geo-units*, each of which consists of a location l_i and a value m_i which attains at that location:

$$M = \{\langle l_i, m(l_i)\rangle\}\,. \tag{1}$$

The terminological confusion is unfortunate (and no coincidence), but the tuples in M may be thought of as generated by a *mapping* $m(l)$: $L \rightarrow V$ from the set of locations $L = \{l_i\}$ to a set of state values $V = \{m(l_i)\}$.

Any arbitrary structure may be defined on the set L, although the initial presentation of the formalism by Takeyama and Couclelis (1997) assumes a regular grid for simplicity. A regular grid is equivalent to continuous two-dimensional space in the limit where $L =$ $\times$, and denotes the set of real numbers. Similarly, the set V may be generalised to a multivariate case where

$$V = \prod_{i=1}^{z} V_i\,, \tag{2}$$

when the formalism also accommodates the multilayer map concept familiar from GIS.

Within this framework, it is easy to define unary map operations which apply at each location l_i, and are effectively global functions on M, defined such in terms of a local function f' on the value of M at each location in L:

$$\mathrm{f}(M) = \{\langle l_i, \mathrm{f}'[m(l_i)]\rangle\}\,. \tag{3}$$

Binary operations such as addition, subtraction, and multiplication can be defined between maps on the same location set L. For example, if V is the set of real numbers , then the addition operation between two maps M and N can be defined such that

$$M + N = \{\langle l_i, m(l_i) + n(l_i)\rangle\}\,, \tag{4}$$

which is the pairwise addition of values in each map by location. This is the core idea in Tomlin's (1990) map algebra, which geo-algebra extends. Maps where V is a simple mathematical set are a special case, and it is more general not to restrict the tuples in M in this way so that $\langle l_i, m(l_i)\rangle$ may be any location–value pair. In this case, elements in L may be geometric entities representing geographical objects 'on the ground', and V may be any set of complex structures representing the current states at those locations. Note that the mapping notation still applies, so that $m(l_i)$ denotes the state in V which attains at location l_i in map M.

This generalisation enables us to include the effects of spatial relations between locations in L—a step vital to geo-algebra's ability to represent the proximal model of space and cellular automata—by admitting the introduction of the *metarelational map*. A metarelational map, R, is a map where a *relational map* is associated with each $l_i \in L$. A relational map, denoted R_i, is the set of all those locations in L which influence location l_i. R_i can be represented by a binary map on L, in which all influencing locations have value 1, and all other locations have value 0. Thus, the metarelational map is given by

$$R = \{\langle l_i, R_i\rangle\}\,,$$

$$R_i = \{\langle l_i, r_i(l_i)\rangle | r_i(l_i) \in \{0, 1\}, \quad \forall l_i \in L\}\,. \tag{5}$$

The metarelational map is thus the means by which "a representation of the relative space of which it is a part" is associated with each location (recall the quote from Takeyama, above).

The metarelational map R may be used in the calculation of nonlocal map functions. First, an intermediate *valued* metarelational map $M \otimes R$ is calculated, in which each location l_i is associated with the set of *values* which attain at its influencing locations:

$$\left.\begin{aligned} M \otimes R &= \{\langle l_i, X_i\rangle\}, \\ X_i &= \{\langle l_i, x(l_i)\rangle | x(l_i) = m(l_i) r_i(l_i)\}. \end{aligned}\right\} \tag{6}$$

Any nonlocal map function may then be defined as a function on $M \otimes R$.

Within this framework, the regular lattice of a CA is represented by a metarelational map R_{CA} in which each location's relational map can be defined with reference to a single, local neighbourhood operator ('orthogonally adjacent grid cells', for example). The CA transition rule is then equivalent to a function on the valued metarelational map $M \otimes R_{\mathrm{CA}}$ which produces a new map M at time $(t+1)$ from the original map M at time t:

$$M_{t+1} = \mathrm{f}(M_t \otimes R_{\mathrm{CA}}). \tag{7}$$

Taken together, the location set L, value set V, the metarelational map R, and the above transition function f constitute a dynamic map which may represent any CA. Details of the representation of CA in geo-algebra are provided by Takeyama (1997) and Takeyama and Couclelis (1997).

The important additional freedom which geo-algebra provides in the construction of a cellular model, is that neighbourhoods need not be defined similarly for all cells. *Any* metarelational map R may be used to represent different structures of spatial and functional relations between locations, and the modeller is not restricted to metarelational maps in which location neighbourhoods are defined uniformly across all $l_i \in L$.

3 Graph-cellular automaton models

We now consider an alternative mathematical formalisation of the same proximal model of space. This approach attempts to retain the intuitive simplicity of the cellular automaton formalism, without losing all of the greater generality offered by the geo-algebra framework. The key to understanding the relationship between the two approaches is to realise that *the spatial structure underlying any proximal spatial model is conveniently described and understood as a graph*. Further, we may think of any *dynamic* proximal model as a cellular automaton process running on a graph, or as a graph-CA.

First, we introduce some notation for graphs (for an introduction to the mathematical theory of graphs see Wilson, 1996). A graph G consists of two sets $V(G)$ and $E(G)$. $V(G)$ is a set of *vertices* (or nodes) $\{v_1, v_2, ..., v_n\}$, where n is the size of the graph. $E(G)$ is a set of *edges* (or links) between the vertices, where each edge e is an unordered pair of vertices $\{v_i, v_j\}$, written $v_i v_j$, for brevity. The *neighbourhood* of a vertex $v_i \in V$ is the set of vertices $N(v_i)$ which are joined to v_i by edges in E:

$$N(v_i) = \{v_j | v_j v_i \in E(G)\}. \tag{8}$$

In a simple graph, edges are undirected so that $v_i v_j \equiv v_j v_i$, and *loops*—edges which begin and end at the same vertex—are not admitted. However, in the current context it is preferable to admit both *directed edges* or *arcs* and loops, so that $v_i v_j \not\equiv v_j v_i$, and $v_i v_i$ may be a member of $E(G)$. In the context of such a *directed graph*, it is also useful to distinguish between the *in-neighbourhood* $N_{\mathrm{in}}(v_i)$ of vertices connected by arcs *towards* v_i, and the *out-neighbourhood* $N_{\mathrm{out}}(v_i)$ of vertices connected by arcs *from* v_i, that is

$$N_{\mathrm{in}}(v_i) = \{v_j | v_j v_i \in E(G)\}, \tag{9}$$

$$N_{\mathrm{out}}(v_i) = \{v_j | v_i v_j \in E(G)\}. \tag{10}$$

If the loop $v_i v_i$ exists then v_i is a member of both its own in-neighbourhood and of its out-neighbourhood.

Formally, then, a graph-CA model consists of a directed graph G, and a set of allowed cell (or vertex) states $S = \{s_j\}$. G consists of spatial elements represented by the vertex set $V(G)$ and directed relations between those elements represented by the arc set $E(G)$. In any graph, the neighbourhood of a vertex v_i consists of all the other vertices (or locations) in $V(G)$ to which it is adjacent. In the context of building a dynamic proximal model we may regard the in-neighbourhood of v_i, $N_{\text{in}}(v_i)$ as the set of influencing locations. We use a '(t)' superscript to indicate the particular state attaining at a vertex, or the collective state in a neighbourhood, at time t, as opposed to the set of allowed states S and its elements $\{s_j\}$ (with no superscript). Thus, $s_i^{(t)}$ is the state of location v_i at time t, and the cellular automaton aspect of the model is incorporated according to

$$s_i^{(t+1)} = \mathrm{f}[S_i^{(t)}], \tag{11}$$

where $S_i^{(t)}$ is the set of states of the in-neighbours of v_i at time t, that is,

$$S_i^{(t)} = \{s_j^{(t)} | v_j \in N_{\text{in}}(v_i)\}. \tag{12}$$

Note that $S_i^{(t)}$ will always be some combination of the allowed cell states in S. Also, in most cases, $v_i v_i \in E(G)$, so that $v_i \in N_{\text{in}}(v_i)$, and the state of a location at time $(t+1)$ is partly dependent on its state at time t, as we would expect.

3.1 Graph-CA as a reworking of geo-algebra

The relationship between this description and geo-algebra should be immediately apparent. The set of allowed cell states S, is equivalent to the set of possible location values V in geo-algebra, and can be similarly generalised to the multivariate case. Each vertex $v_i \in V(G)$ in the graph-CA, has a set of influencing vertices $N_{\text{in}}(v_i)$ in the same way as the local relational map R_i of geo-algebra represents those locations which influence location l_i. The metarelational map of geo-algebra is equivalent to the complete set of graph arcs $E(G)$ which defines all the in-neighbourhoods of influencing locations.

We can also see this if we consider the *adjacency matrix* $\mathbf{A}$ of a graph G. $\mathbf{A}(G)$ is defined such that

$$\mathbf{A}(G) = [a_{ij}], \qquad \text{where } a_{ij} = \begin{cases} 1, & \Longleftrightarrow v_i v_j \in E(G), \\ 0, & \text{otherwise.} \end{cases} \tag{13}$$

The adjacency matrix of a directed graph may be asymmetric with $a_{ij} \neq a_{ji}$. Now, if we write each location's relational map R_i as a vector $\boldsymbol{R}_i$.

$$\boldsymbol{R}_i = \begin{bmatrix} r_{1i} \\ \vdots \\ r_{ji} \\ \vdots \\ r_{ni} \end{bmatrix}, \tag{14}$$

where $r_{ji} = 1$ if location l_j influences l_i, and 0 otherwise—as in equation (5)—then the equivalence between the metarelational map R and the graph G can be seen from the

fact that $\mathbf{A}(G)$ may be written

$$\mathbf{A}(G) = \begin{bmatrix} a_{11} & \dots & a_{n1} \\ \vdots & \ddots & \vdots \\ a_{1n} & \dots & a_{nn} \end{bmatrix} \equiv \begin{bmatrix} \boldsymbol{R}_1^T \\ \vdots \\ \boldsymbol{R}_n^T \end{bmatrix}. \tag{15}$$

These equivalences between the graph-CA and geo-algebra formalisms are summarised in table 1. The equivalence of the two approaches is no coincidence: their close correspondence arises from a common origin in a desire to represent dynamic, proximal spatial models.

In considering the usefulness of the graph-CA formalism it now makes sense to examine it from three perspectives: first, graph-CA are graphs; second, they are a variety of CA; and third they are *both* graphs *and* CA. Each of these aspects is considered in turn in the sections which follow.

Table 1. The direct equivalence relationships between the graph-CA and geo-algebra formalisms.

Graph-CA		Geo-algebra	
element	notation	element	notation
Vertex set	$V(G)$	Locations	L
Allowed states	S	Values	V
In-neighbourhoods	$N_{\text{in}}(v_i)$	Local relational maps	R_i
Graph arcs	$E(G)$	Metarelational map	R

4 Graph-CA as graphs: understanding model structure

The graph-CA formalism has an advantage over geo-algebra in its ability both to suggest structural forms for cellular models which could be built, and to allow model structures to be described, compared, explored, and represented in various ways. The graph-theoretic framework enables us to specify model structures concisely. This is demonstrated below where some further graph-theoretic ideas are introduced in section 4.1 and are used as the basis for a discussion of potential model structures in section 4.2. Further generic tools provided by graph theory which assist in model description are discussed in section 4.3.

Before introducing yet more formal description in the next section, it is useful to pause and consider figure 1 (see over). This illustrates a graph-CA model of the gentrification process in a small urban fragment (see O'Sullivan, 2000, for details). Some of the flexibility which the 'spatial relaxation' of cellular automata provides is especially clear. *Any* set of spatial elements, not just cells in a grid, may be built into a model of this type (compare the examples in Takeyma, 1997). The main proviso is that the elements can be meaningfully related to one another by relations of influence (in this case predominantly relations of spatial nearness), provided plausible transition rules can be devised. Furthermore, the choice of which relations count—which graph edges to include—becomes an integral part of the modelling process, intimately related to the development of model transition rules. The modeller must bring to bear theories about the process under investigation as its effects operate across space. In fact, we may regard the proximal model of space as represented in graph-CA, as one possible formal expression of Gould's portrayal of the geographer's view of space:

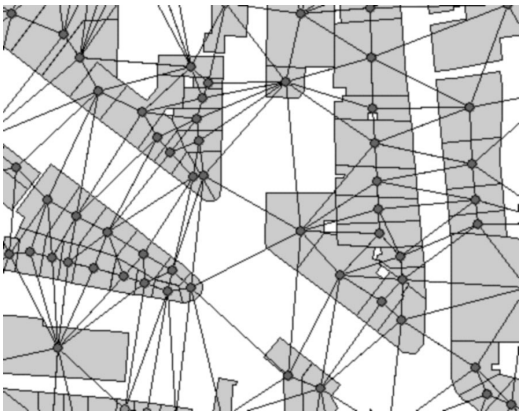

Figure 1. A portion of a graph-CA model. 'Cells' in this model are individual buildings and the graph structure shown represents cell neighbourhoods which are used to determine the evolution of particular cell states.

> "... we start with the idea that this strange no-thing [space] is structured by other things, which we relate in various ways to each other, and which we measure as various distances to each other as the fancy takes us according to our purpose of utility, curiosity, or ambition" (1997, page 128).

4.1 Multigraph-CA

A further sense of the riches unlocked by the graph-CA formalism is best provided after a little more dry formalism has been introduced in the shape of the *multigraph-CA*. It should be emphasised that a multigraph-CA is *not* an extension of the graph-CA formalism. Rather, it is a description of a structure to which a particular graph-CA may conform. The multigraph-CA allows us to envisage various model structures which might be built or observed, which seem likely to have very different dynamic properties. Following the formal description of multigraph-CA below, some of these potential model structures are described and discussed in section 4.2.

A multigraph-CA is a graph-CA G which may be partitioned into a set of z subgraphs $\{G_1, ..., G_\mu, ..., G_z\}$. Each subgraph G_μ is made up of a set of vertices

$$V_\mu(G_\mu) = \{v_{\mu 1}, ..., v_{\mu n_\mu}\}, \tag{16}$$

where $n_\mu = |G_\mu|$, and a set of arcs

$$E_\mu(G_\mu) = \{v_{\mu i} v_{\mu j} | v_{\mu i}, v_{\mu j} \in V_\mu\}, \tag{17}$$

Usually, the partition of G will be nonoverlapping, so that no vertex is a member of more than one set, thus

$$V_\mu \cap V_\nu = \emptyset, \qquad \forall \mu, \nu, \tag{18}$$

although this need not always be the case. Each 'subgraph-CA' G_μ has a distinct cell (vertex) state set S_μ and may thus have CA-like transition rules defined on it, as for a simple graph-CA [refer back to equations (9) to (12)].

As described so far, there is no interaction between the subgraph-CA in G. This is introduced by defining further arc sets *between* the vertex sets in G where

$$E_{\mu\nu} = \{v_{\mu i} v_{\nu i} | v_{\mu i} \in V_\mu \wedge v_{\nu i} \in V_\nu\}. \tag{19}$$

By using this notation, the set of arcs in graph G_μ is written $E_{\mu\mu}$. Equation (19) implies that $E_{\mu\nu} \subseteq V_\mu \times V_\nu$. The whole graph-CA $G(V, E)$ has vertex set

$$V = \bigcup_{\mu=1}^{z} V_\mu , \tag{20}$$

and arc set

$$E = \bigcup_{\nu=1}^{z} \bigcup_{\mu=1}^{z} E_{\mu\nu} . \tag{21}$$

In the overall graph-CA the influencing neighbourhood on which the CA rules are defined may be made up of cells (vertices) both *within* the same subgraph-CA, and from *other* subgraph-CA so that

$$N_{\text{in}}(v_{\mu i}) = \bigcup_{\phi=1}^{z} \{v_{\phi j} | v_{\phi j} v_{\mu i} \in E_{\phi\mu}\} . \tag{22}$$

Note that since $N_{\text{in}}(v_{\mu i})$ may contain vertices from a number of subgraphs G_ϕ in G, each with states defined on a different state set S_ϕ the definition of transition rules may become fairly complex—if only because there are likely to be more cell states defined by the collection of sets $\{S_\phi\}$ than by a single state set S.

4.2 Interpretations of the multigraph-CA

As described, a multigraph-CA is no different from a simple graph-CA except that not all possible states are allowed at all cells, a situation which could attain in any graph-CA where not all state transitions were possible. However, if we place further limitations on the interrelations and properties of the various subsets of vertices and edges defined above, we may interpret the resulting graph-CA in a range of ways, both spatial and aspatial, and use these interpretations as a basis for the construction of interesting urban and regional models. Some of the possibilities are discussed below.

4.2.1 *Hierarchical graph-CA*

If the subgraphs in G can be ordered so that

$$E_{\mu\nu} = \emptyset \iff |\mu - \nu| > 1 , \tag{23}$$

then we may regard the multigraph-CA as *hierarchical* or layered. In a hierarchical graph-CA the subgraphs in G may be regarded as organised in a sequence of layers, with no arcs joining vertices in nonadjacent layers. A representative three-layer model of this type is illustrated in figure 2(a) (see over). The most obvious spatial interpretation of such a model in an urban context is that the lowest layer G_1 is some subdivision of an urban system into small units (as in figure 1), and successive layers $G_2, \ldots, G_z$ represent successive higher level aggregations of elements in the layer below. In this particular interpretation $|V_\mu| \leqslant |V_{\mu-1}|$, although this need not be true in general.

We can further refine our interpretations of such a model with reference to the relations between the various subgraphs. In the general hierarchical case, described by equation (23), influential relations between adjacent layers are mutual, so that over time, various feedback effects are likely. If only within-layer and upward arcs exist, that is $E_{\mu\nu} = \emptyset \iff \mu > \nu$, we may think of the hierarchical graph-CA as a *bottom-up* network of relations of influence, wherein the state of an element in any layer is influenced only by other elements in its own layer or the layer below; if $E_{\mu\nu} = \emptyset \iff \mu < \nu$ then the network of relations is *top-down* and element states are only affected by other elements in the same layer or the layer above.

Such hierarchical models seem likely to be of use in exploring a broad range of geographical systems. The relationships between globalisation and changes at

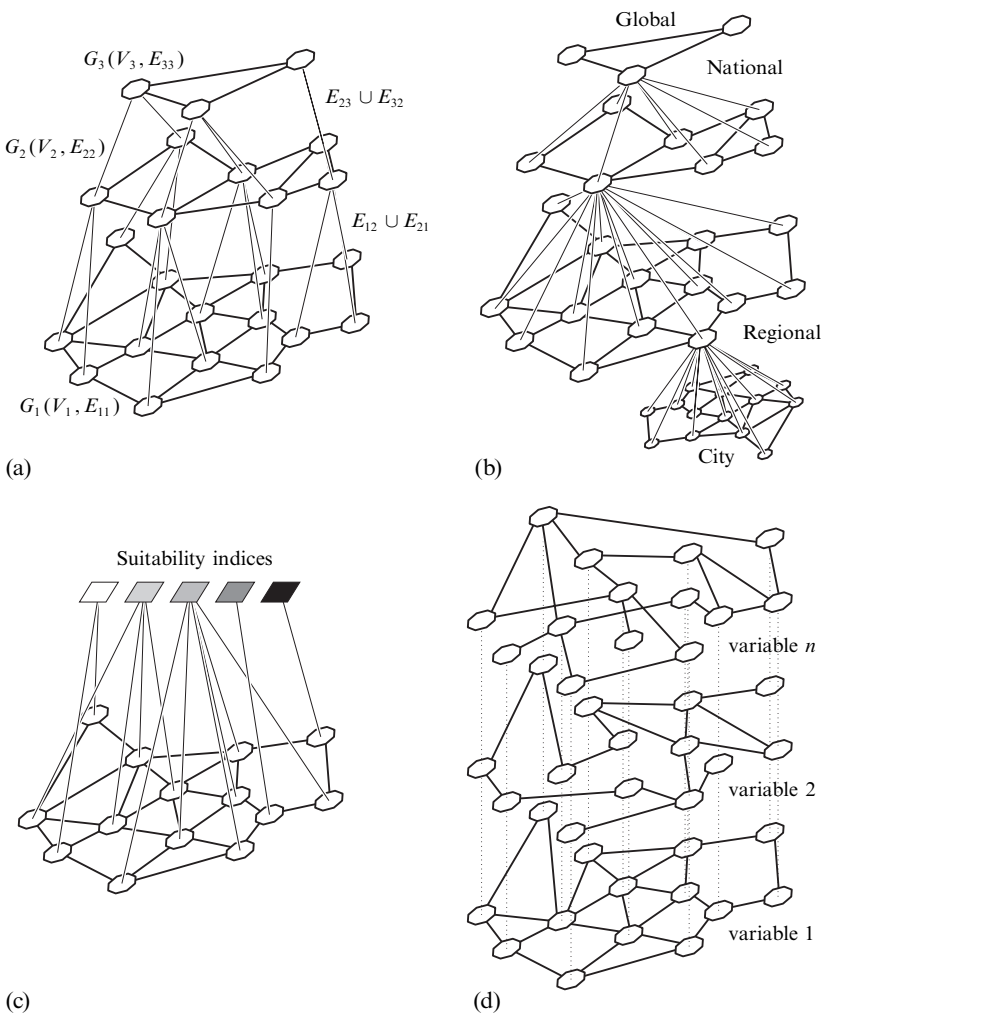

Figure 2. Generalising CA using the graph-CA concept. Note that arcs are shown as undirected edges for clarity. (a) A three-layer hierarchical graph-CA, (b) a hierarchical graph-CA in which only one element in each level is modelled in detail at the next level down, (c) a nonhomogeneous graph-CA where suitability indices are represented as a subgraph, and (d) a multivariate graph-CA (dotted lines indicate that vertices in each layer are identical; arcs between layers are not shown, for clarity).

national, regional, and local scales are frequently commented upon, and a hierarchical graph-CA seems well-suited for exploring the dynamics of spatial systems with this type of organisation. There would be no requirement in such a model for lower layers to be complete, so that, for example, a neighbourhood could be modelled in detail (again, see figure 1), set in its urban, regional, national, and global contexts, without other cities being modelled to the same level of detail. This possibility is schematically illustrated in figure 2(b). Note that this approach could, with care, allow the development of a modular model framework.

The hierarchical graph-CA is thus a very general model structure. The generality of the graph-CA formalism may be further demonstrated by reinterpreting two common, operational modifications of CA as multigraph-CA also.

4.2.2 *Nonhomogeneous (zoned) graph-CA*

As mentioned previously, a frequent deviation from the strict constraints of classic CA models in urban modelling is to have nonhomogeneous cells. A frequent instance of this is the assignment of a 'suitability' index to each cell based on the process under investigation. For example, in their urban growth model of the San Francisco Bay area, Clarke et al (1997) introduce land slope as a generalised measure of the suitability of individual cells for urban development. This interacts with the current demand for land so that the maximum land slope of cells which may host urban growth varies. This may be interpreted as a multigraph-CA—see figure 2(c)—if we divided the vertex set into two subsets, so that one represents a conventional (grid-based) CA, and the other consists of vertices each representing a finite, discrete suitability index. Each vertex in the conventional CA subgraph then has one in-neighbour in the suitability index subgraph, which affects its state transitions as the model runs. In principle, a number of discrete-valued cell properties could be associated with a standard cellular model in this way. Note that, as shown in the figure, there might be no arcs internal to the subgraph representing suitability values, which are therefore fixed. If this were not the case, the suitability layer might itself be a cellular model of some nonspatial process.

4.2.3 *Multivariate cell states*

Takeyama and Couclelis (1997, pages 88–89) show how a dynamic, multivariate CA-based model can be conceptualised and constructed in geo-algebra. The ability to cope with multivariate states is important in urban models given the rich diversity of elements which will constitute any subdivision of a city. This depends on extending the multivariate value at each location (see equation 2 above) to a z-layer metarelational map, so that it becomes a family of metarelational maps,

$$R = \left\{\{R_{11} \ldots R_{1z}\}\ldots\{R_{i1} \ldots R_{iz}\}\ldots\{R_{z1} \ldots R_{zz}\}\right\} . \tag{24}$$

This is closely related to the subdivision of the arc set of a multigraph-CA into subsets $E_{\mu\nu}$ as described by equation (19) above. We can see that if we drop the restriction on overlapping subgraphs [that is, ignore equation (18)] then it is perfectly possible for a multigraph-CA G to have vertex subsets $\{V_1, \ldots, V_z\}$ such that $V_\mu \equiv V(G)$ for all $\mu \in \{1, 2, \ldots, z\}$. Since each vertex subset V_μ has a distinct state set S_μ, different arc sets may be defined internal to and between each 'layer' as before, and the graph-CA formalism can then represent multivariate cell states in the same way as geo-algebra. Figure 2(d) is a schematic representation of this approach.

Finally, one further extension of the graph-CA concept is possible, regardless of whether it is a multigraph-CA or not.

4.2.4 *Mutation of graph-CA models*

Since graph-CA models are potentially variable in their cell states, their rule sets, *and* their spatial (graph) structure, it is a relatively simple matter to condition changes in the graph structure on the existence of various local neighbourhood states. Such changes would be dependent on the types of relationships represented by arcs in the underlying graph. In a relatively clear cut case, where arcs represent transport links between settlements, new arcs might be introduced when two settlements had reached a certain size, to reflect their mutual influence. Of course, there are complications. The appearance of new arcs between otherwise unrelated vertices implies the introduction of CA rules which do not operate on the current neighbourhood alone, a significant step down the slippery slope towards model complication and confusion. However, in the context of operational models which aim at some sort of realism, the potential for mutation of the underlying model structure may be of significant interest. It is noteworthy that we may interpret some of Allen's (1997) models as graph-CAs capable of

mutation in this sense. Semboloni (2000) has conducted some experiments with a mutable, irregular CA approach to urban growth modelling which indicates the potential of the approach. An attractive feature of this type of model is that it makes the spatial structure of a model over time dependent on spatial processes, so that the two become mutually constitutive. This is an exciting possibility given the dominance of such dialectical conceptualisations in geographical theory [see, for example Soja (1989) who discusses the 'sociospatial' dialectic, together with later formulations of the same basic idea].

Combining some of the above suggestions—especially spatial hierarchy and structural change of the model—would certainly result in substantially more complex models, but is nevertheless an intriguing, further possibility.

4.3 Describing graph-CA model structure using graph theoretic measures

Whether a graph-CA model can be regarded as a multigraph-CA or not (this will depend greatly on the intentions of the model builder), the fact that *any* graph-CA model is running on a graph is in itself significant, because it immediately provides access to ways of describing, measuring, and exploring the model structure in graph theoretic terms. This is a by-product of the generality of the graph abstraction (for a sense of the widespread use of graphs, see Beineke and Wilson, 1997; Haggett and Chorley, 1969; Jungnickel, 1999; Krafta, 1994; 1996; Krüger, 1979a; 1979b; Wassermann and Faust, 1994).

The diagrams in figure 3 are intended to distinguish three distinct kinds of structural measure, which can be identified. Figure 3(a) shows a 'typical' graph. One of the most obvious questions to ask about a graph is, "which are the most important vertices?" One answer to this question is to define various measures of *centrality*, as schematically illustrated in figure 3(b) where paler greys indicate more central vertices according to some criteria. Another approach to the structural description of graphs is to identify particularly tightly interrelated subsets of the graph vertices—generically termed *cohesive subgroups* and illustrated in figure 3(c). A third aspect of graph structure relates to the identification of *structurally equivalent* vertices. Such vertices occupy similar positions in the graph's structure (end vertices with only one neighbour

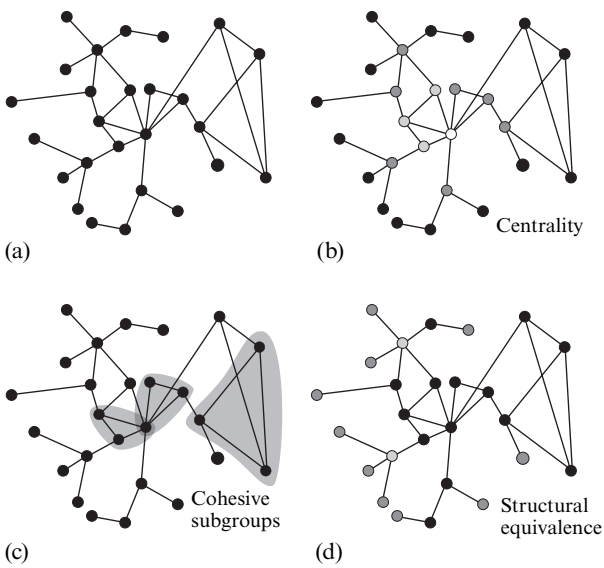

Figure 3. Various kinds of graph structural measure illustrated.

are an obvious example). This is schematically illustrated in figure 3(d). Various methods and measures for defining these three broad descriptors of graph structure in particular cases have been developed (see Wassermann and Faust, 1994). Additionally, recent developments in visualisation techniques, particularly in the automated drawing of graphs so that their structure becomes more visually apparent, also deserve attention in this connection (see Tollis et al, 1999) since they may enable structural features to be identified which are not immediately describable in terms of any of these measures.

The important point is not that any particular measure of graph structure be used, since different measures are likely to reveal similar patterns in any individual case (Donninger, 1986), but that the generality of the graph representation of a relational system, together with its widespread adoption in various disciplines, means that a range of approaches are readily available to the modeller. We return to this point in section 6.

5 Graph-CA as a variety of cellular automata: understanding model dynamics

CA are a well-understood class of discrete dynamic model, and graph-CA are a variation on that theme. This aspect of urban CA-based models has generally not been emphasised by researchers in the field, who have tended to emphasise the interactive and visual appeal of building CA-like models.

Although the tools of analysis for cellular automata are less well developed than for graphs, they are still considerable. Since the most significant observable fact about CA is their unpredictable and varied dynamic behaviour, theoretical work on CA has concentrated on developing ways of understanding this behaviour. Wolfram's (1983) paper is a key contribution. He conducts a phenomenological survey of the behaviour of the simplest class of CA imaginable: linear CA with just two allowed cell states, where each cell has its immediately adjacent cells as neighbours. His surprising finding is just how varied the behaviour of even such simple examples can be. Based on this and the investigation of further, only slightly more complex cases (five cell neighbourhoods, with three or four allowed cell states), Wolfram suggests that four qualitative classes of behaviour can be identified: class-1 CA evolve in a short period of time to a unique homogeneous state; class-2 CA may attain final states which exhibit periodicity over time; class-3 CA evolve to aperiodic *chaotic* behaviour which, although it is totally deterministic, is unpredictable, except with complete knowledge of the initial state; and class-4 cellular automata exhibit *complex* behaviour. Such behaviour has hierarchical structure. Class-4 behaviour is characteristic of systems capable of computation, which may be 'programmed', and are therefore capable of arbitrarily complicated behaviour. In fact, much of the theoretical and practical interest of CA rests on the existence of class-3 and class-4 cases, whose behaviour may be analogous to that of unpredictable physical, chemical, biological, and social systems.

Significantly, Wolfram also proposes a method for quantitatively characterising the behaviour of these (and potentially any) CA, based on the observation that the time evolution of some measure of system disorder will be different for the four classes. In particular, class-3 systems will produce long-term, apparently random system change at a high level of disorder, whereas class-4 systems exhibit long-term variations where periods of disorder are interspersed with periods of order. Disordered and ordered regimes are likely to interact unpredictably over time.

Wolfram (1984) suggests that an entropy measure may be used as the basis of a method for classifying CA into behavioural classes, and defines a 'spatial set entropy' as

$$S(X) \;=\; -\frac{1}{X}\sum_{j=1}^{s^X} p_j \log_s p_j \,, \tag{25}$$

where p_j denotes the frequency of occurrence of each of the s^X possible neighbourhood states in sequences of cells of length X, with s allowed cell states. This measure is in the range 0 to 1, where 0 indicates a very ordered arrangement of cell states and 1 indicates a completely disorganised arrangement of states. Note that the measure is applied over some sequence length of cells, X. A particular configuration of cell states may seem random at $X = 1$, but exhibit order at some other value of X. The suggestion of a measurement method is critical to any attempt to extend Wolfram's work beyond simple one-dimensional CA whose temporal evolution is very easily explored in contrast with two and higher-dimensional cases (this issue is explored more thoroughly in O'Sullivan, 2001).

Note that statistical measures of the entropy type have appeared in the geography literature (Batty, 1974) but have been used relatively little in practice (Morrill, 1995, provides a rare example). Wolfram's usage is distinct from these, partly because summation is carried out over cell *neighbourhood* states, not individual cells, but also, more importantly, because he is concerned with the *time evolution* of the measure, and not with its value at any particular moment. Note also that it helps if we do not focus too closely on the precise 'meaning' of entropy in this context [the entropy concept has a long history of use and misuse across a variety of disciplines as Couclelis (1984) makes clear]. Wolfram's use of the concept is primarily for the ability of its functional form to measure the (dis)order in a frequency distribution, but also has close affinities with Shannon's entropy from communication theory.

As in section 4, the important point is not the particular measures used in any particular case, but the observation that CA dynamic behaviour is describable with reference to well-understood ideas about dynamic complexity. Of course, it may also be that animations and other visualisations of the behaviour of a model provide insights and ideas not clear from a measure of the kind discussed here. The key issue is that by virtue of their being close cousins of simple CA, graph-CA models are *also* amenable to investigation in the way which Wolfram describes.

6 Graph-CA as *both* graphs *and* CA: theoretical structure-process research using graph-CA

We now turn to a novel opportunity for further research which is enabled by the graph-CA formalisation of certain types of discrete model. We have already seen that the advantage of the graph-CA approach is not in the formalisation per se, but in the ways of thinking about aspects of the resulting models which are provided by its joint derivation from graphs and cellular automata. A graph-CA may be characterised in terms both of its structure represented by a graph, and also of its dynamic behaviour by adapting ideas from research into CA. Work on the behaviour of CA gives us a way of thinking about the dynamics of spatial processes. Graph-CA, by also admitting the use of measures of graph structure, thereby enable investigation of the influence of spatial structure on spatial process dynamics. The graph-CA therefore enable explicit exploration of relationships between the structure of spaces in which processes unfold and the sorts of dynamic behaviour which occur. This may shed light on long-standing concerns about the relationships between spatial structures and spatial dynamics, and represent a specifically *geographical* avenue for research into the dynamics of complex systems. This potential has been clearly signposted in previous sections, and we can now expand on the possibility.

As a preliminary step, it is useful to consider the place of graph-CA models relative to similar and related models. In figure 4 three types of discrete model—cellular automata, graph-cellular automata, and Boolean networks—are schematically related to one another. This helps to place these models in a research context, and suggests the

particular relevance of graph-CA models to *geographical* and *geo*computational research. Cellular automata themselves are the most closely related models to graph-CA. Another kind of discrete model—the Boolean network—is also related. A Boolean network consists of a directed graph of vertices, each of which may be in either the 'on' or 'off' state. Note that in a classic Boolean network, only two vertex states are allowed (hence the term 'Boolean'), however the idea can clearly be extended to multivalent logics. The state of each vertex at time $(t + 1)$ is determined by the states of its in-neighbours in the graph at time t. This is very much like a graph-CA. However, in a Boolean network, the rules relating each vertex's state to its in-neighbourhood state need not be the same throughout the network.

Figure 4 indicates two axes of variation among these models. First, it is possible for the spatial structure of the discrete model elements (the cell space, lattice, or graph structure) to be homogeneous or invariant from location to location, or to vary across the system. Conventional CA are stationary in this sense, whereas graph-CA models are not. Boolean networks are also nonstationary in this sense. Second, the rules representing processes in a model may be stationary or nonstationary. Both CA and graph-CA models are stationary, whereas Boolean networks are nonstationary. Note, however, that as a graph-CA model's cell space structure departs further from stationarity, it is unlikely that its process rules can be regarded as absolutely stationary. This is because there is an unavoidable interaction between the size of cell neighbourhoods and the impact of process rules, because it is difficult (if not impossible) to express rules so that they can be considered invariant across a range of neighbourhood sizes, from only a few cells, to (perhaps) tens or even hundreds of cells.

The framework of figure 4 identifies the particularly geographical interest of graph-CA models, because it draws attention to the fact that the main axis of variation between CA and graph-CA models is spatial. This implies that investigating the changes which occur in the transition from a CA to a graph-CA model may shed light on the specifically spatial effects in such discrete models. We can further see that exploration of the effect of spatial structure on spatial dynamics is possible at two distinct levels—the global and the local.

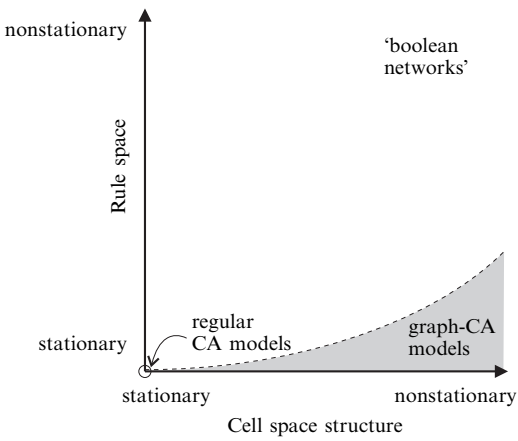

Figure 4. Graph-CA in relation to other discrete cellular models. Graph-CA have nonstationary spatial structure, but stationary transition rules. However spatial structure and rules are not wholly independent so that very irregular structures prevent definition of truly stationary transition rules.

6.1 Global relations

As discussed in section 4, it is possible to consider the structure of the graph which underlies a graph-CA model both in terms of the interrelations which may exist between defined subsets of the vertices—the multigraph-CA approach—and also by using theoretic measures of various aspects of graph structure. Either of these approaches, together with more exploratory approaches based on visualisations of various redrawings of the graph could be adopted in trying to understand whether there are systematic relationships between model structures and model dynamics. For example, by using vertex centrality measures, we could quantify the extent to which a model is centralised on particular cells. The relationship between such measures of overall graph structure and the dynamic behaviour of various graph-CA running on it may be of interest. In the simplest case we might hope to find a relationship between some centralisation measure and the Wolfram class of the graph-CA. Perhaps more realistically, as was implied in the discussion of hierarchical graph-CA, we could examine the differences between bottom-up and top-down hierarchical models. Examples of similar research are Kauffman's (1984) random Boolean networks and, more recently, investigations of the behaviour of 'small world' networks by Watts and Strogatz (1998). Both Watts and Strogatz's and Kauffman's work focus on particular system architectures which differ greatly from likely geographical—or proximal—graph-CA models. Nevertheless, these cases establish the possibility of making general, yet useful, statements about the relationship between a system's overall global structure understood as a graph, and its dynamic behaviour.

In more recent work examining the behaviour of CA running on small world networks, Watts (1999, page 187) comments that "... it is natural to ask whether or not high-performance CAs can be developed *by varying the coupling topology of the automata instead of their rules*" [original emphasis]. The relationship between Watts's concerns and interesting research questions for graph-CA models—can relationships be found between the structure of the graph in a graph-CA and dynamic behaviour of the model?—is clear. Obviously, Watts's interest is expressed in terms appropriate to an engineering problem, whereas the geographical research proposed here is concerned with developing an understanding of already existing real-world spatial systems. Research is ongoing on graph-CA models which adopt this global approach, examines the issues raised in more detail, and presents some initial results suggesting that the relationship between model structure and dynamics can, indeed, be fruitfully explored in this way (O'Sullivan, 2001).

6.2 Local relations

Another aspect of the structure–process investigation of a graph-CA model is to examine whether there is a relationship between *local measures of individual elements* in the graph and their *individual* dynamic behaviour. Questions such as "which vertices (cells) are most influential in determining model outcomes?", and "are the most central vertices (cells) more or less stable in their states than peripheral vertices?", or "do structurally equivalent vertices in the model behave in similar ways?" then become a rich source of ideas and hypotheses in seeking to examine the model and its behaviour. The various kinds of graph structure measures discussed in section 4.3 could all be brought to bear in this approach. We might find that members of different cohesive subgroups in the graph behave differently, that vertices which belong to different structural equivalence classes behave differently, or that there is a relationship between vertex centrality and behaviour. Any of these localised relationships might also produce significant insights into the way in which the model behaves globally, and therefore into the way in which those aspects of the world being modelled behave. These sorts of

relationships are akin to the usual concerns of the spatial modeller or analyst to find relationships between locational variables and behaviour, albeit with more of an emphasis on the system dynamics. The current approach is a potentially useful new way of thinking about these issues.

7 Conclusions

The graph-CA model clarifies aspects of geo-algebra, which are somewhat obscured by a focus on formalising the distinction between site and situation, without providing conceptual tools with which this local–global relationship can be properly grasped. Realising that the relationship is precisely represented by the implied underlying graph and making use of that fact is key to the present contribution. The graph-CA approach thereby makes two aspects of the geo-algebra a little clearer. First, underlying spatially generalised CA is a global relational structure, which may be described, measured, and visualised quite independently from the behaviour of the CA. Such description and visualisation enables us conveniently to construct, envisage, and represent further more complex model structures than hitherto. Examples of the possibilities have been provided in section 4.2. Second, *any* set of spatial elements—points, lines, areas, or mixtures of all three—can be built into a proximal model, provided meaningful neighbourhood relations can be constructed among them. Further, such spatial elements need not be space-filling or nonoverlapping, and may in fact consist of interrelated sets of elements at different scales or derived from different perspectives. This aspect has also been emphasised in the discussion of multigraph-CA structures in section 4.

There is also potential value in interpreting at least some of the great variety of 'urban CA' as graph-CA. Realising that there are closer affinities between some of these numerous variations on the CA theme than is immediately apparent—that, in fact, many of them are examples of the same class of model, possibly with describable differences in their relational structures—might also enable us to regain some of the promised insights of simpler strict CA (see also O'Sullivan and Torrens, 2001; Torrens and O'Sullivan, 2001). In this context, the various types of graph-CA model described in section 4 add further to claims for the generality and wide applicability of cellular or discrete models. It also suggests that it may be time to reconsider the continued usefulness of the term 'cellular automaton'—perhaps discrete relational automaton would be a more accurate, less restrictive label.

Whatever we call them, such models can also be usefully examined in relation to well-established ideas about dynamic systems. Then the graph-CA may enable theoretical—as opposed to practical 'model construction'—progress to be made. Here, the usefulness of the graph-CA formalism lies in the link it provides to well-understood and developed tools and concepts for examining *both* the structure *and* the dynamics of the resulting models. It thus opens up the possibility of using the investigative framework suggested in sections 5 and 6, to address long-standing questions about links between the spatial structure of urban and regional systems, and the dynamics of the changes (and continuities) which occur in those systems. Reference to related research in biology and physics has been made which indicates the potential of the approach, and research based on the concepts outlined here is ongoing (O'Sullivan, 2001). Together, these practical and theoretical aspects suggest that the particular relaxation of CA invoked—the allowance of nonregular spatial structure—may have far-reaching and interesting implications for geographical modelling.

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