Suggested citation:
Hewitt, R., & Díaz-Pacheco, J. (2017). Stable models for metastable systems? Lessons from sensitivity analysis of a Cellular Automata urban land use model. *Computers, Environment and Urban Systems*, 62, 113-124.

Stable models for metastable systems? Lessons from sensitivity analysis of a Cellular Automata urban land use model.

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Abstract

This research suggests that the degree of variability in a Cellular Automata (CA) urban land use model application may be linked to the application's suitability for modelling complex urban systems. Although highly stable models may be perceived as desirable, because they produce reliable, realistic-looking land use simulations, there is a risk that they may not be able to simulate true urban complexity. To test this hypothesis, variability was analysed through a sensitivity analysis in which a calibrated CA land use model application was modified repeatedly to produce a range of model variants with different characteristics. Since model scale is a key attribute known from literature to strongly influence model results, sensitivity analysis was conducted with reference to the scale-related elements (cell resolution, neighbourhood effect) in the model. Variation was found to be slight even between applications having widely differing cell resolutions and neighbourhood distance decay effects. It is contended that this is not an application-specific question, but a feature of these types of models more generally, where simple rules, strong constraints and a low degree of stochastic variation tend to produce highly stable simulation outcomes. To address the question of whether such stable model applications are really suitability for simulating urban complexity, the applications are discussed with relevance to three key indicators of complexity; 1) spontaneous emergence, 2) bifurcation; 3) critical transitions. Finally, we ask whether the requirement of metastability necessary for calibration of such models violates the assumption of freedom from systemic constraints that would allow true complexity to be simulated. Some suggestions are made as to how these issues might be resolved in future, allowing a new generation of models to emerge.

Highlights

- Cellular automata (CA) land use models are analysed from a systems perspective.
- Highly stable models may be perceived as desirable but there is a risk that they may not be able to simulate true urban complexity.
- To test this hypothesis, a sensitivity analysis is carried out for a CA model application by changing cell resolutions and neighbourhood effects.
- Though the sensitivity analysis suggested that the application was quite stable, key characteristics of complex systems could be identified.
- These kinds of models are not presently able to simulate critical transitions of the kind found in some Agent-based models.
- The ability of these models to simulate true complexity depends on the individual case and is sometimes overstated.
- While highly stable model applications may be suitable for some specific cases,, model constraints should be relaxed for exploratory purposes.

Introduction

Cellular Automata (CA) models of land use change are popular and useful tools for simulating complexity in urban systems (e.g. White and Engelen 1993, Clark et al 1997, Besussi et al 1998, Batty and Torrens 2001). Early model applications were able to simulate complex patterns of urban growth, self-organization and change (White and Engelen 1993, Clark et al 1997). However, it has since become common practice to apply constraints to the CA model to improve realism and application to real world problems. Though this has arguably made the models much more useful, no detailed research is available about the degree to which constraints may limit the CA's ability to simulate complexity. A highly constrained CA model may jettison this capability completely and predictably return only a few basic patterns. A sensitivity analysis, therefore, is useful in a CA model, not so much to ensure that model behaviour is stable, but rather to ensure that it is not so stable as to prevent any possibility of that some of the more interesting features of complex systems (emergence, bifurcation, critical transitions) might appear.

In this paper this question is addressed by developing, calibrating, validating, and undertaking detailed sensitivity analysis on a land use model for the region of Madrid, using the well-known and widely used Cellular Automata (CA) modelling framework developed by White and co-workers (e.g. White and Engelen 1993, White et al 1997, White and Engelen 2000 etc), in its most widely known software implementation, Metronamica.

Research Background

Modelling complexity in Urban systems

The theory of cities as complex systems has been attributed to Peter Allen (e.g. Allen and Sanglier 1981; cited by Portugali 2013) but is rooted in earlier developments in systems theory (e.g. Churchman 1968) and far-from-equilibrium thermodynamics (Prigogine 1980). In a landmark paper, White and Engelen (1993) showed that a computer model based on Cellular Automata (CA) could be used to generate realistic simulations of urban systems in which key features of complex systems identified in the earlier literature, e.g. spontaneous emergence of patterns, bifurcation, and irreversible state transitions (e.g. Prigogine 1980, Allen and Sanglier 1981) were clearly present. White and Engelen's model provided a template for simulation of complex patterns of urban change, and has since seen many applications around the world (e.g. Barredo et al 2004; Lajoie and Hagen-Zanker 2007; Wickramasuriya et al 2009). Since its initial development the model has been adapted to include, in particular, a constraint on the number of cells that transform at each time step (Demand); the influence of infrastructure networks (Accessibility); biophysical factors such as terrain slope or aspect (Suitability); and planning restrictions (Zoning). Despite these additions, the CA transition rules set (Neighbourhood dynamics) and the stochastic perturbation term (v), remain at the core of the model. However, at present, it remains unclear to what extent these additional constraints can be applied before the CA is effectively overpowered and produces only predictable outcomes. In this paper, we address this question with respect to three specific characteristics of complexity identified in earlier models:

1. Bifurcation. As Prigogine (1996) has noted, bifurcation is a key property of far-from-equilibrium systems. In such a system, fluctuations, produced for example, by dissipative processes, can lead the system to "choose" between alternate states or pathways. If bifurcation occurs repeatedly as part of a process chain, the system takes on a branching structure giving rise to a very large number of possible end states which are unpredictable *ex ante*. Bifurcations in the model described here are the result of a random process introduced through the stochastic factor (*v*) which affects the land use allocation decisions. Thus a land area that was not especially attractive for a particular land use may suddenly become so. Cells are allocated in the next time step to this new pole of attraction, causing a cluster. The neighbourhood effect caused by the new cluster causes this cluster to grow. Since the demand is exogenously defined true spatial bifurcations can occur, because land allocated to this new cluster cannot now be allocated anywhere else. The system has been transformed in a way that could not have been predicted.. This behaviour is described by White and Engelen (1997, p. 244) in their model of the island of SimLucia. A forest area on the northeast of the island was converted to agriculture in around 20% of the simulations, a result of a random allocation in an area where potential for this transition to occur was already high.

2. Emergence. For the purposes of this article, we define emergence simply as "the capability of the model to produce isolated spatial structures beyond the influence of the cell neighbourhood". This is a characteristic of all classic urban CA models (e.g. Clarke and Gaydos 1998, White 1998) and is also an observable property of cities

themselves. We argue that a model that does not show emergent behaviour may not be suitable for simulating urban complexity.

3. Critical transitions. In theory, a self-organising system with highly innovative emergent properties and very strong bifurcations could produce transitions at the level of the system itself, causing flips from one state to another. With respect to CA models, the special bifurcation case described above in the SimLucia model (White and Engelen 1997) might arguably also be a case of a critical transition, since, although the forest to agriculture conversion only occurred around 20% of the time, when it did, it seemed to be because the stochastic variability had caused a critical threshold to be crossed. However, it could be argued that to differentiate critical transitions from bifurcations, a state change would need to be observed at the level of the system. In the case described it's not clear that the forest-to-agriculture conversion described actually caused a significant system transformation. Clearly, though, where emergence and bifurcations can be convincingly demonstrated, the possibility that this behaviour may eventually culminate in a critical transition should not be ruled out.

Aims

The aim of this work is therefore to explore how variability in the scale of the model, reflected through the cell resolution and the neighbourhood effect, influences a land use model's capacity to simulate land use change, and how this may determine the usefulness of the model for simulation of complex urban systems. As a starting point for our analysis, we make three basic assertions:

1) The basis of the CA model is spatial interaction in the cell neighbourhood (neighbourhood dynamics), and this is the principal determinant of the model's dynamic behaviour.

2) Neighbourhood dynamics, do, on their own, produce spatial patterns readily identifiable as “complex”, as demonstrated by the previously mentioned work of White and colleagues. These patterns are generated by the allocation of land use to cells according to a cell's potential for that land use, The complex spatial patterning is affected by the stochastic factor but unrelated to the externally generated demand.

3) The introduction of other spatial constraints like Accessibility, Suitability and Zoning, as is typically done when calibrating a standard Metronamica application,

may reduce the model's capability to simulate complexity and decrease the usefulness of model applications.

Methods

The area selected for the analysis is the Madrid region (Figure 1), a Spanish Autonomous Community and province with around 6 million inhabitants. This region was chosen because of the extraordinarily dynamic land use change that the region has undergone during recent decades (until the beginning of the current economic crisis around 2008), and because a highly detailed land use database documenting this change has recently become available (Diaz-Pacheco and Garcia Palomares 2014).

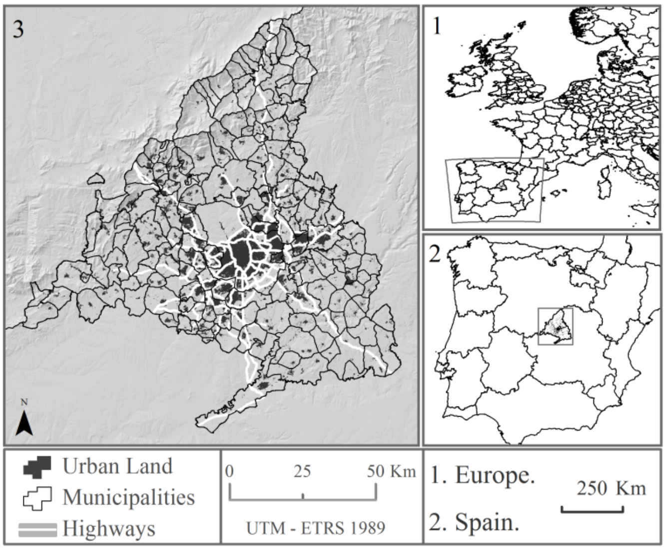


Figure 1. Location of Madrid region

Source: Díaz-Pacheco and Gutiérrez, (2013)

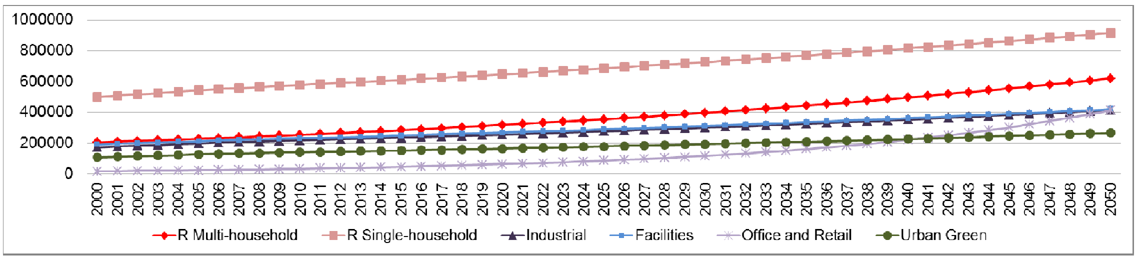
To carry out the sensitivity analysis, a Cellular Automata (CA) urban land use model was built and calibrated for the case study area. The land use dataset used in the model was Madrid Land Use (Diaz-Pacheco and Garcia Palomares 2014), a large detail scale cartographic database of land use and land cover information for the Madrid Region, covering the time periods 2000, 2006 and 2009. The Madrid Land Use dataset comprises 12 land use classes of which 7 are urban.

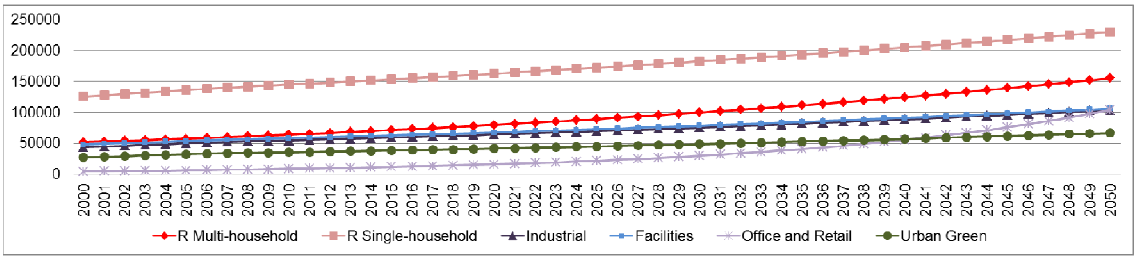
The modelling framework adopted was that found in Metronamica, a popular land use modelling software, which implements the CA modelling approach of White and collaborators (White and Engelen 1993, White et al 1997, White et al 2000 etc). In this model, the distribution of land use in a given area is represented as a raster map in which each cell has a value which represents a land use. The value of the cells can change according to a set of transition rules computed by a simple equation in which the geographic effect of a cell over its neighbours (attraction or repulsion between land use cells) represents the main driving force of change in the system. A random parameter to incorporate a degree of stochasticity into the model is also introduced. Accessibility (e.g. distance to road networks) and suitability (e.g. degree of terrain slope) parameters are introduced to align the model with the characteristics of the study region. Finally a zoning parameter can be also added to allow the influence of policies or planning scenarios to be introduced into the simulation. New cells are allocated at each step of the model on the basis of the transition potential computation (Eqn 1) until cell demand (determined exogenously) is exhausted or all available cell space is used up.

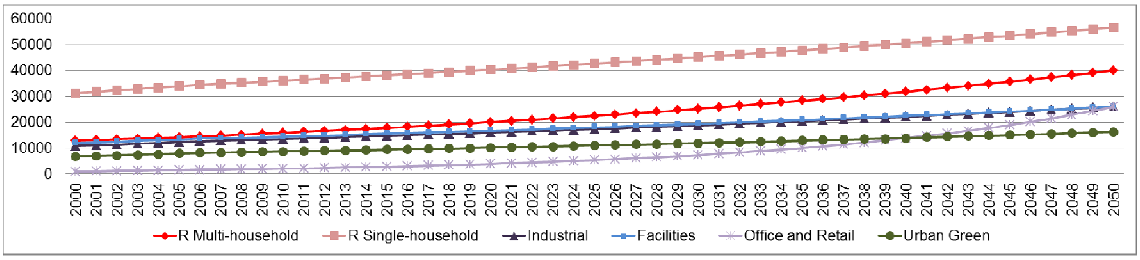
Land use demand Δ is calculated for each yearly timestep by Δt_2-Δt_1/t_2-t_1, where Δt_1 is the number of cells for each land use in the land use map of the simulation start date, Δt_2 is the number of cells for each land use in the land use map of the simulation end date, t_1 is the simulation end year and t_1 is the simulation start year. For simulations of future dates where Δ is unknown, it is determined in various ways; e.g. by extrapolating the historic linear growth tendency, through growth scenarios, or as in this case, by using population projections to estimate the required urban area at the future date (Fig. 2)

The demand is essential to the model's functioning, since without land to allocate, nothing can change. However, the demand is not, on its own, responsible for the model's dynamic behaviour – this is controlled by the interaction of land uses at varying distances modelled through the neighbourhood rules. While complex spatial interactions are more *evident* in the case of larger land demand, but this demand does not affect where they will be located..

Figure 2: Demand in cells for 2000-2050, computed by compound annual growth. Top: 25mx25m resolution, Center: 50mx50m resolution, Bottom: 100mx100m resolution.







The transition potential is specified as:

$P_j = N_j A_j S_j v_j Z_j$ [Eqn 1]

Where:

P_j : Is the transition potential

A_j: The accessibility from cell *j* to any element of the transport network

N_j: Is the neighbourhood calculated by a function of a weighted sum to express the influence of the state of a cell *j* over a specific group of cells into a specific range of distance. The *neighbourhood rules* are user-defined forces of attraction and repulsion that decay over distance (Figure 8). The influence score for the neighbourhood effect (N) is a relative, not an absolute measure and is unbounded ($-\infty \leq N \leq \infty$).

S_j: Is the suitability of the cell *j* for changing to a specific state

Z_j: Is the zoning status (land policies, planning, restrictions…) for the cell *j*

and:

v_j: Is a random parameter which introduces stochastic perturbations on cell *j* defined by the expression:

$1 + (-\ln(1 - R))^{\alpha}$ [Eqn. 2]

where R is a number from the Uniform distribution in the range 0-1, and α is the scale of the stochastic effect, where 0 = no effect.

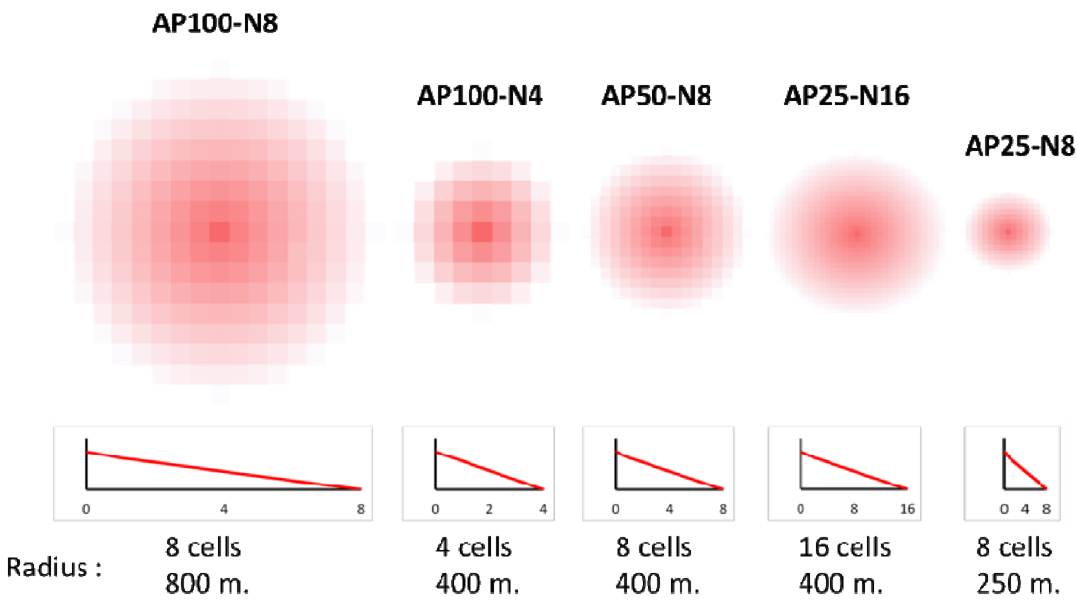
The model employs a *tabula rasa* approach whereby *all cells in the model* are allocated at *each* timestep. Thus the only way to ensure persistence of the same function land use in the model at multiple timesteps is to make this land use strongly attractive to itself (Fig 7), such that it will be almost always be allocated in its old location before new locations are considered.

The application presented here does not incorporate zoning parameters in order to give as much freedom to the system as possible. Thus transitions are determined according to Eqn 1 by neighbourhood rules, accessibility and suitability only, with occasional stochastic perturbations introduced by the random factor. Table 1 shows the 5 simulations generated.

To calibrate the model, transition rules were established through a trial and error approach, informed by previous analysis of land change processes in the region (Diaz-Pacheco and Garcia Palomares 2014), and applied to the starting land use map (2000) to generate simulations of the land use map for 2006. The transition rules were modified until acceptable goodness of fit, according to standard statistical measures - Kappa Simulation (K_{sim}), Fuzzy Kappa Simulation (K_{simF}), Fractal Dimension (FD), and Clumpiness (C) - as well as visual inspection, was achieved. Statistical testing was carried out in the Map Comparison Kit Software (Visser and De Nijs 2006). The first of these, $K_{sim,}$ is useful for determining the number of cells that have been correctly simulated, taking into account only those parts of the map in which change has actually occurred (Van Vliet et al 2011), the second, K_{simF}, is a modified version of K_{sim} which applies fuzzy set theory to include similarity of location (Van Vliet et al 2013b) while the remaining two measures are used for determining the degree of spatial similarity between elements in the simulated map and the real map (White, 2006). The validity of the transition rules obtained in this way for the period 2000-2006 were tested by running model simulations for a second time period 2006-2009 and testing against the map for 2009. This process is known as validation (Van Vliet et al 2013a). Once acceptable calibration and validation values had been obtained for the base model application, which had a 50x50 cell resolution and an 8 cell neighbourhood (AP50-N8, see Table 1), four variants of the model were created (AP25-N8, AP100-N8, AP25-N16 and AP100-N4; see Table 1). In the new model applications, the model's key parameters, the scale of the cell grid represented and the scale of the neighbourhood effect, were modified. The new applications were then tested using the procedure, and the statistical indices, described above. In this way, the effect of significant parameter variations could be measured. Finally, future land use simulations were run to the year 2050 for each application.

Table 1: Scale changes in neighbourhood for each application

Application id:	AP100-N8	AP100-N4	AP50-N8	AP25-N16	AP25-N8
Resolution	**100x100**	**100x100**	**50x50**	**25x25**	**25x25**
Feature of changes	Doubled resolution Equal radius in cells Unequal radius in meters	Doubled resolution Unequal radius in cells Equal radius in meters	Original	Halved resolution Unequal radius in cells Equal radius in meters	Halved resolution Equal radius in cells Unequal radius in meters
Cell radius	8	4	8	16	8
Meter radius	800	400	400	400	250
Number of cells	197	49	197	788	197
Area in m^2	1,970,000	490,000	492,500	492,500	123,125



To test the effect of changing the scale of the neighbourhood rules (N), the neighbourhood influence over distance was held constant in one set of applications by modifying neighbourhood cell size according to the resolution, and changed in another set of applications by holding neighbourhood cell size constant as global cell resolution was varied (Table 1).

The strength of the random perturbation introduced by the parameter *v* can be modified by the user, by changing the value of the scale factor, exponent α (see Eqn 2). Low scale factors tend to produce highly deterministic simulations while high scale factors tend to produce a high number of random transitions. To test the extent to which spatial allocation behaviour was determined by the random effect, simulations to 2050 were carried out for a range of values of α (Fig. 5).

Accessibility is empirically calibrated for each simulated land use through a distance decay function. In the case of the Madrid application, the distance to different elements of the transport network, like the highways, roads, train stations and metro stations was introduced. The accessibility values are introduced in a similar way for each application, but in this case the values between the nearest and the furthest distance considered to the network (roads, rail, highway, metro stations...) is automatically computed by the software through a distance decay function. To ensure that the Accessibility was the same for all applications distances were doubled or halved in order to adapt the function at each application, e.g. if in the 50x50m application was considered a value for the road influence at 200m to the residential land cells, in the 100x100m application this value was doubled to 400m. to respect the proportionality demanded by the size of the cell. Network weight values (to reflect the different relative importance of networks to different land uses) were kept equal for all applications. The only Suitability factor included is the slope of the terrain, since this was found to be the only physical suitability factor of importance to urban land change in this region. Suitability was held constant in all model applications. The long term effects on the base model application (50x50m resolution) of including parameters Accessibility and Suitability in the model were tested for the year 2050 (Fig. 6).

Results of calibration and validation of the initial 50x50m application

Calibration was considered to be complete once values of 0.144 had been obtained for K_{sim}. The values considerably outperform a null or neutral model (RAMD25, 50, and 100) generated by the Random Constraint Match procedure implemented in the Map Comparison Kit (Hagen-Zanker and Lajoie 2008). The model was considered acceptably validated at 0.113 (Table 2). These values are comparable with published values considered acceptable in other applications of the model (e.g. Van Vliet et al 2013a, Hewitt et al 2014).

Table 2: Values of the indices used for calibration and validation of the 50m base application.

Index	AP50-00-06	AP50-06-09	RAMD50
Kappa simulation	0.144	0.113	-
R. Multi-household Clumpiness Difference	-0.0226	-0.0023	-0.0811
R. Single-household Clumpiness Difference	-0.0018	0.0071	-0.0754
Industrial Clumpiness Diference	0.0235	0.0029	-0.1196
Facilities Clumpines Difference	-0.0183	-0.0093	-0.0856
Office and Reatil Clumpiness Difference	0.0112	0.0081	-0.2593
Urban Green Clumpiness Difference	-0.0361	-0.0081	-0.1115
Fractal Dimension Difference	0.0070	0.0013	-0.0268
	CALIBRATION Data06-Sim06	VALIDATION Data09-Sim09	BENCHMARK

Both clumpiness and mass fractal dimension are often employed in landscape ecology to analyse landscape structure. In this research, these metrics allow the spatial similarity of the simulated map and reference map to be assessed. Clumpiness is a measure of the degree of dispersion/aggregation of the patches in an image according to their type (McGarigal, 1994). Mass fractal dimension measures the degree of “linearity” of elements in the map in which plane filling objects like circles or squares will have a value of 2.0 and a line will have a value of 1.0 (Gardner et al, 1987). As goodness of fit improves, both clumpiness and mass fractal dimension approach the values in the comparison map.

For both clumpiness and mass fractal dimension, the calibrated and validated application achieved similar values and both outperform a random land use map used as benchmark (Table 2). The same is true for the clumpiness index, tested for each one of the simulated land uses. Once the simulation produced by the 50m application was considered suitable to reproduce the land use patterns of change, its scale characteristics were modified according to the procedure previously described in order to evaluate their effects on the model (Table 1).

RESULTS

The influence of the stochastic factor

The results of the sensitivity test for the stochastic factor are shown below. Low randomness has been compared with medium randomness (Fig. 3; right) and with high randomness (Fig. 3; far right). All tests were performed for Neighbourhood and random factor only, so as to provide the maximum freedom possible to the model. Fractal dimension statistics for these tests are given in Table 3.

These results allow some interesting conclusions to be drawn:

1. Randomness is not responsible for the presence of complex behaviour in the model, cell resolution seems to be much more important. This is because at higher cell resolutions more cells are allocated, and thus there are more opportunities for emergence and bifurcations. Note how emergent structures can be clearly identified in the highly deterministic simulation for 25m cell resolution (Fig. 3, top left. , sim 2050 α 0.1, see the bottom right corner of the madrid region), while the same structures are not present in the α 0.1 simulations for larger cell sizes.

2. High randomness can prevent the formation of new complex structures by producing excessive scattering. Thus, although emergence is present and bifurcations are evident, model behaviour is so dynamic that emergent cells do not grow into recognisable clusters. This suggests that, contrary to what might logically be expected, adding more randomness may make the spatial pattern *more* stable (but more and more noisy) until a critical threshold is exceeded and underlying patterns are completely out-competed by very high random values everywhere. This behaviour is most pronounced for values of α >0.9, and is therefore not easily observable in Fig. 3.

3. Clumping and dispersion seem to be more strongly related to cell size than to randomness. Note how the bottom row of simulations are significantly more clumped than the top row of simulations, which show a tendency towards dispersion (Table 3).

The cluster rank-size plot (Figure 4) supports these results, showing that with increasing α, more small clusters are generated. By this indicator, simulations deviate further and further from the data as α is increased. The Fractal dimension comparison results (Table 3) also support this conclusion.

Table 3: Fractal dimension comparison results for simulations under different values of α. Here, the fractal dimension index for all the active land uses in the map for simulations of the year 2050 under different values of α has been compared with the map of the same land uses in 2000. Note how the global difference increases with increasing α.

Cell Size	Data Map 2000	Sim2050 α= 0,1	Diff. Data	Sim2050 α = 0,5	Diff. Data	Sim2050 α =0,9	Diff. Data	Random Map	Diff. Data
25X25	1.41018	1.39543	0.01475	1.41508	0.0049	1.43608	0.0259	1.43953	0.02935
50X50	1.47777	1.46284	0.01493	1.47799	0.00022	1.4903	0.01253	1.50459	0.02682
100X100	1.52587	1.51499	0	1.52748	0.00161	1.53686	0.01099	1.54465	0.01878

Higher Absolute Difference   Lower Absolute Difference

Sim= simulation   Diff. Data= Global Difference in Fractal Dimension with Data Map

Figure 3: Simulations to 2050 (25x25; 50x50; and 100x100) changing values of α to 0.1; 0.5; and 0.9 (left) and comparing location results between simulations α=0.1; α=0.5 and simulations α=0.1; α=0.9 (right)

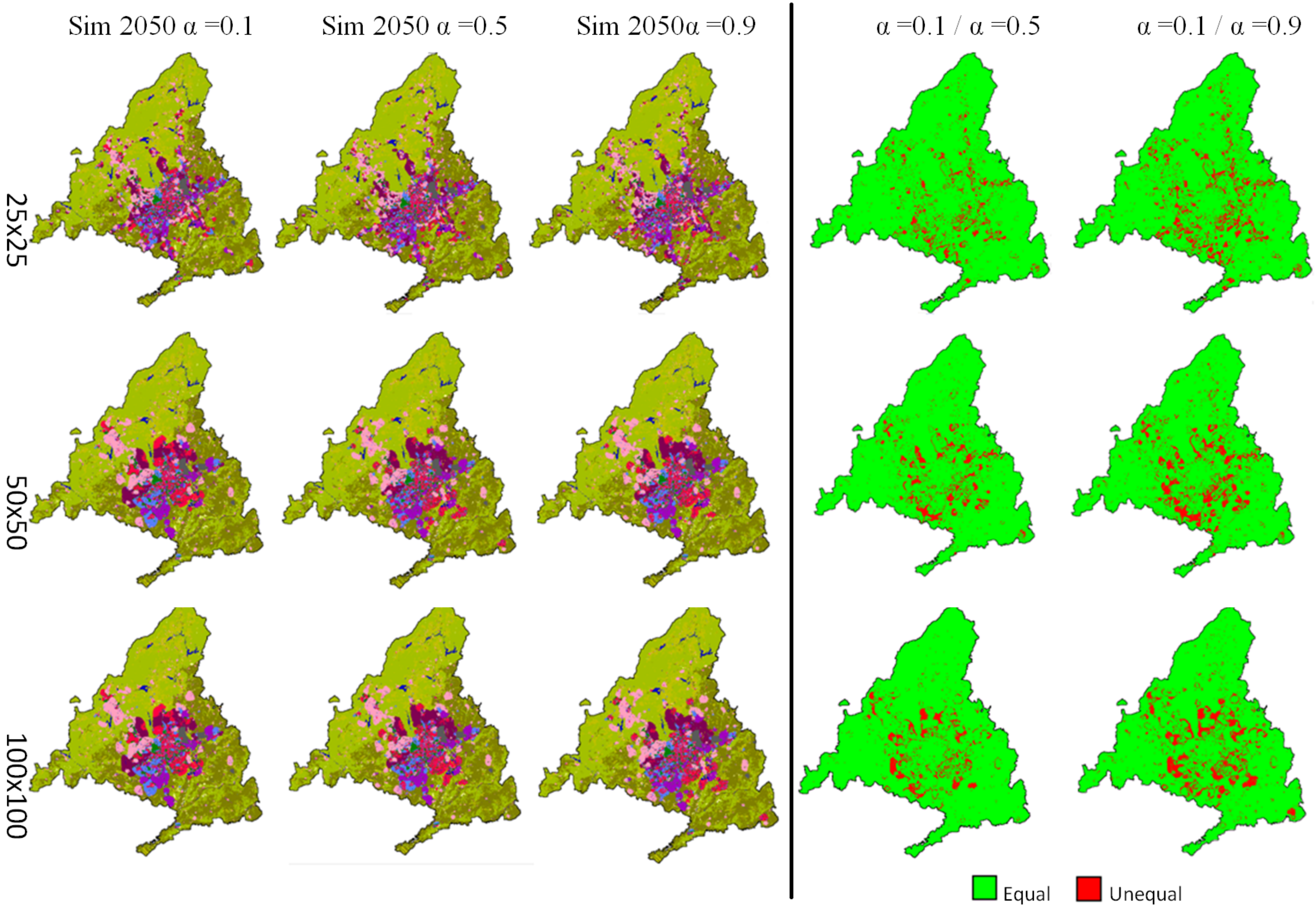
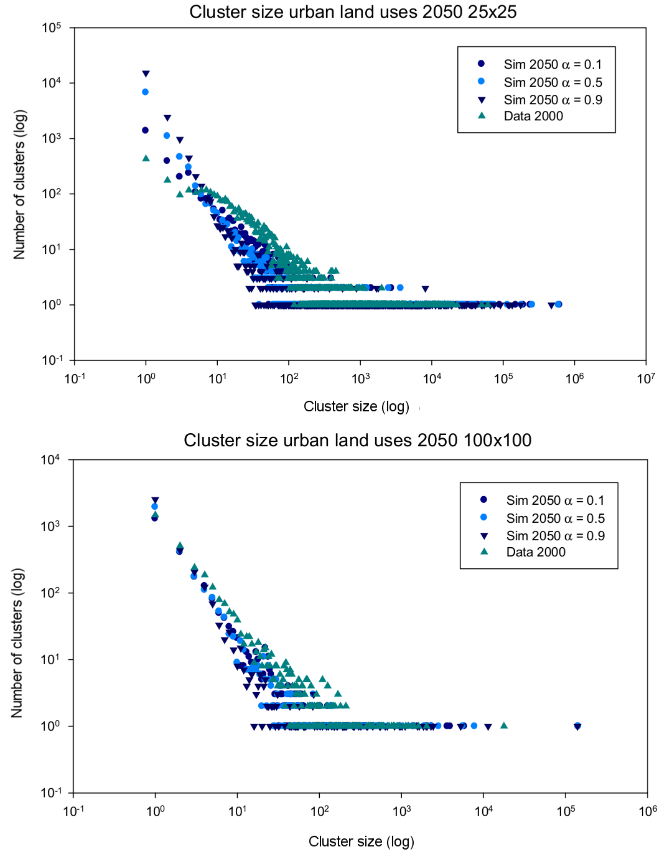


Figure 4; cluster size-frequency plot for different values of α and two different cell resolutions.



The influence of scale and cell size

The comparison results between the data for 2006 and simulations for the same year are shown in Table 4.

Table 4: Map comparison results for applications. Abbreviations: AP50-25-100: applications and resolutions; RAMD50-100-25: random simulations and resolutions.

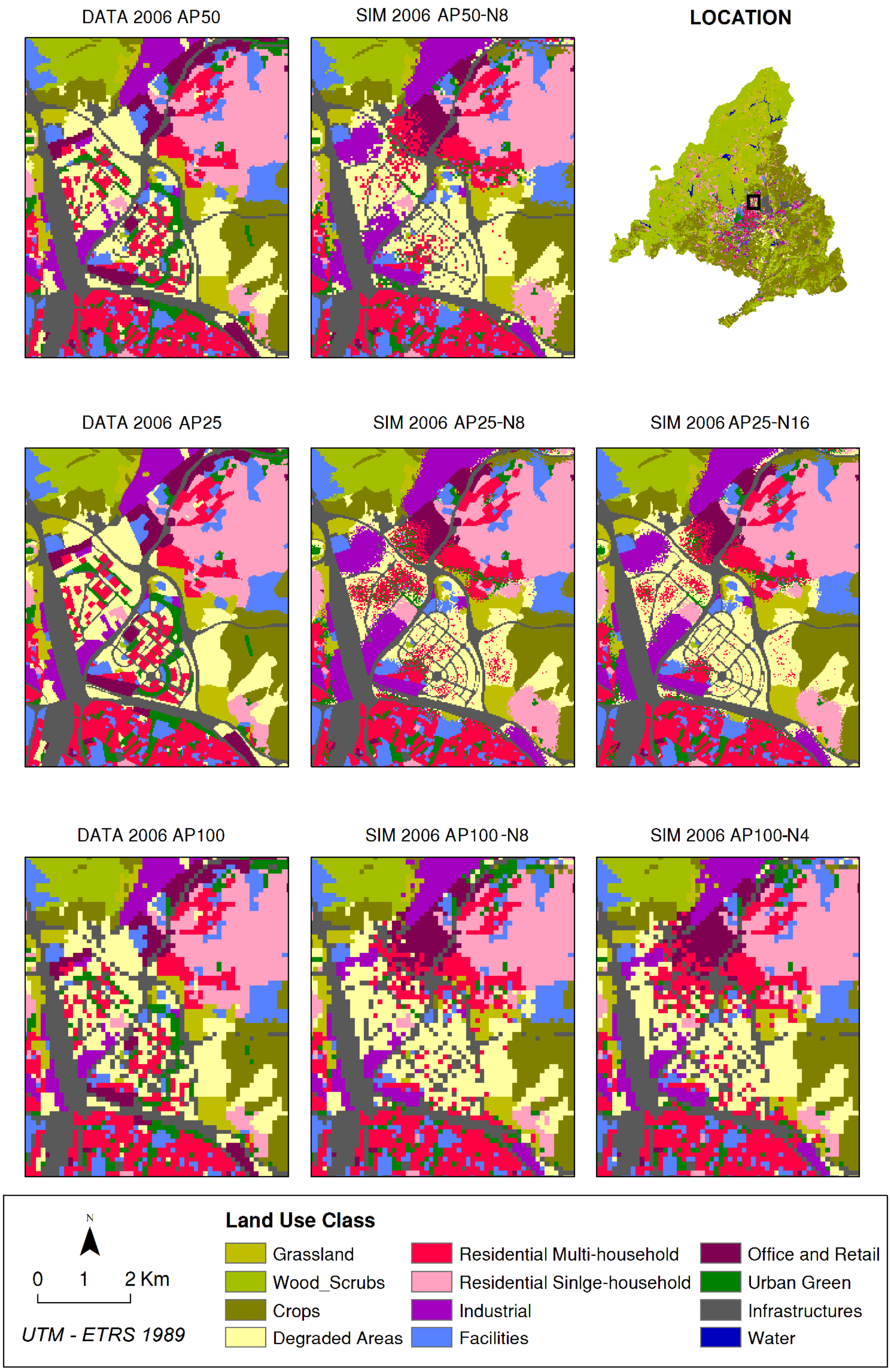
	Applications					Benchmarks		
Index	**AP50-N8**	**AP25-N8**	**AP100-N8**	**AP25-N16**	**AP100-N4**	**RAMD50**	**RAMD100**	**RAMD25**
Kappa simulation	0.144	0.149	0.116	0.146	0.158	-	-	-
R. Multi-household Clumpiness Difference	0.0226	0.0430	0.0050	0.0400	0.0007	0.0811	0.0602	0.1017
R. Single-household Clumpiness Difference	0.0018	0.0079	0.0111	0.0192	0.0250	0.0754	0.0643	0.0867
Industrial Clumpiness Diference	0.0235	0.0020	0.0409	0.0111	0.0409	0.1196	0.0991	0.1352
Facilities Clumpines Difference	0.0183	0.0290	0.0065	0.0567	0.0044	0.0856	0.0609	0.1054
Office and Retail Clumpiness Difference	0.0112	0.0156	0.0731	0.0284	0.0835	0.2593	0.1981	0.3007
Urban Green Clumpiness Difference	0.0361	0.0642	0.0108	0.0849	0.0099	0.1115	0.0752	0.1550
Fractal Dimension Difference	0.0070	0.0108	0.0053	0.0157	0.0003	0.0268	0.0182	0.0299

According to the map comparison indices used, the simulation results from all of the different applications (apps) for 2006 could be considered acceptable. Both the 25m app with the 8 cell neighbourhood radius and the 100 m. app with the 4 cell neighbourhood radius actually improve on the original 50 m 8 cell neighbourhood radius app (Table 4). For clumpiness, the difference between the clumpiness of the data and clumpiness of the simulations is comparable across all the applications, and better than the random simulation used as a benchmark. The same is true of the fractal dimension index. In some cases the scale-modified apps achieve slightly better values than the initial app of 50m (e.g. in AP100-N4, clumpiness for multi-household and facilities classes). However, better performance of some categories tends to be compensated by poorer performance for others. Taken overall, the differences between the scale-modified apps and the original app are not great enough to be able to claim that any of the modified applications are significantly better or worse than the original 50m app.

A visual comparison between the land use data maps for 2006 and the simulations produced by the different applications (Fig. 5) supports the impression given by the statistical comparisons (Table 4). This figure shows simulated (centre and right hand column) and real (left hand column) land use for an enlargement of a highly urbanized (mainly residential) area in 2006. The middle column of Fig. 5 shows the apps with different resolutions (25m, 50m and 100 m) and the same neighbourhood radius in cells (N8), such that the distance decay of the neighbourhood effect is halved (SIM 2006 AP25-N8) and doubled (SIM 2006, AP25-N8) respect to the initial calibration (SIM 2006, AP50-N8) as a result of the change in cell size. The right hand column then shows the effect on the calibration of maintaining the distance decay of the neighbourhood effect the same as in the initial calibration (SIM 2006, AP50-N8), by increasing or decreasing the number of cells in the neighbourhood.
It is interesting to note that no simulation seems to be much better or worse than any other. Some classes, e.g. Residential Multi-household are not simulated very successfully in any application. This is probably because all locations in this residential area were equally favourable, being close to existing urban areas, on suitable land and close to transport networks.

The relationship between cell-size and the size of the land parcels is also clearly shown. While it is not really possibly to identify the “correct” resolution statistically, the 50m resolution simulation seems to provide more realistic-looking results than the 25m and 100m resolution simulations because the cell size is a closer match to the size of the actual land parcels. This demonstrates the limitations of the statistical comparison methods and emphasises the importance of visual inspection when choosing the right resolution for a given application.

Fig. 5: Comparison of data 2006 (all with 8 cell neighbourhood radius) and simulations for 2006 from the different apps. Abbreviations: SIM: simulation; AP25-50-100: application and resolution; N4-8: neighbourhood and radius.



Discussion

Why is there so little variation between simulations?

The experiments with the random factor (Fig. 3, Fig. 4) show that, even over long time periods, the cell size is ultimately more important in terms of map structure and pattern than the level of randomness in the model. This supports the widely held view (e.g. Ménard & Marceau 2005; Jantz and Goetz 2005) that cell resolution is very important to the spatial behaviour of CA models. However, when this was specifically tested by significantly varying both the the scale of the underlying grid and scale of the neighbourhood effect for a range of otherwise identical simulations, no major differences were found in model goodness of fit to data. Four possible explanations can be advanced for this:

1) The cell neighbourhood is not the key change driver.
2) The relative scaling up or down of the map objects through the changing resolutions affects both the simulation map and the comparison map equally.
3) The neighbourhood influence declines very steeply and that all important interactions take place at near distances.
4) The calibration phase is too short for major differences to emerge.

These are considered as follows:

1) The cell neighbourhood is not the key change driver

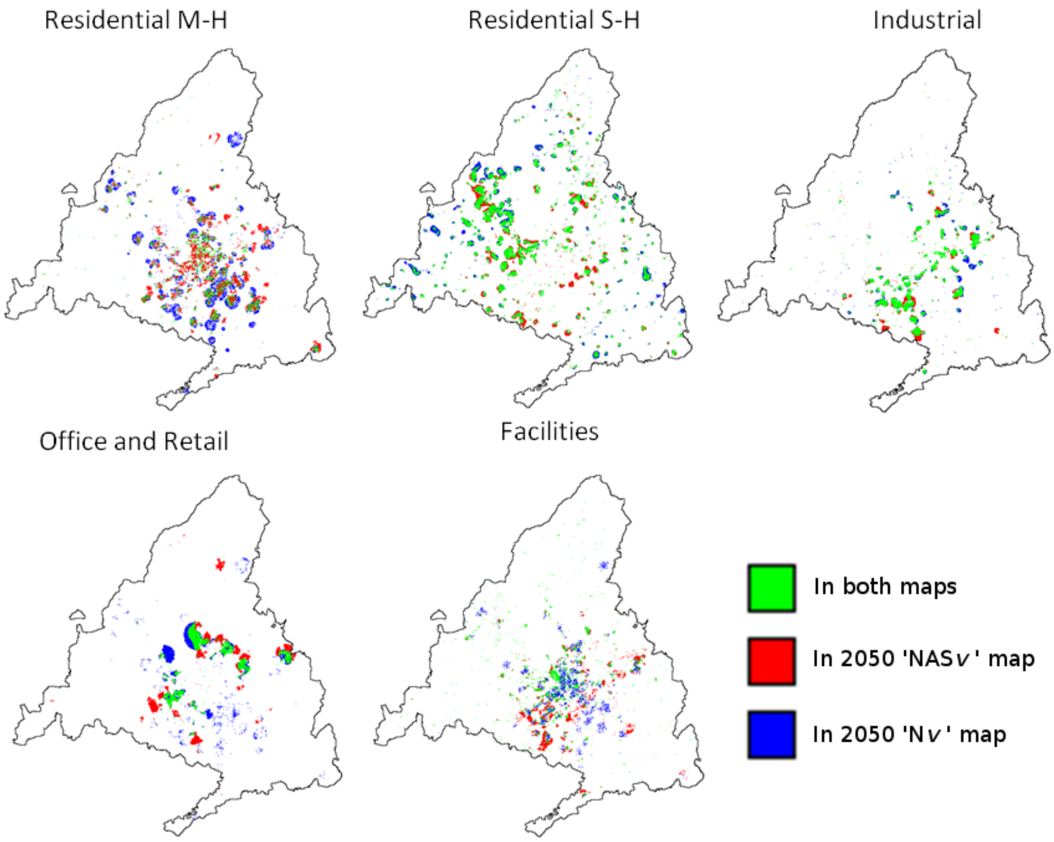
The major driver of dynamic change in models of this type is typically the spatial interaction in the cell neighbourhood. However, since major changes were made to the spatial interaction rules in the different applications, it is possible that the low degree of variation between them could be explained by the spatial interaction effects being “cancelled out” or overruled by other model blocks like suitability or zoning. However, this cannot be the correct explanation here, since zoning is absent in all applications, and suitability is limited to a slope map, in which virtually all regions in the Madrid metropolitan area are highly suitable. In any case, all the applications outperform the benchmarks in which land change is randomly allocated in the immediate vicinity of patches of the same land use (Table 4). Adding accessibility, either alone or with suitability to a null model does not greatly improve goodness-of-fit (see Table 5). These factors make it clear that the cell neighbourhood *is* a highly important driver.

Table 5: Running the model adding factors where N is Neighbourhood, A is Accessibility, S is Suitability and v is random, and testing the results with the kappa simulation (K_{sim}) and fuzzy kappa simulation (K_{simF}.) indices.

Factors	$\mathbf{K_{sim}}$	$\mathbf{K_{simF}}$
Neighbourhood **Random*	0.124	0.139
Neighbourhood * Accessibility * *Random*	0.141	0.155
Neighbourhood * Accessibility *Suitability * Random	0.144	0.158

This conclusion is further supported when we compare the simulations for 2050 with each other (Fig. 6). A model application in which Accessibility and Suitability parameters are included (2050 'NAS*v*' map, red in Fig. 6) does vary significantly from a Neighbourhood * random only model (2050 'N*v*' map, blue in Fig.6), but not for all classes. Residential Single Household and Industrial land uses have already found a relatively stable allocation pattern under Neighbourhood * random only. Neighbourhood is therefore the most important determinant of location for these land classes, and while Accessibility and Suitability parameters play a greater role in spatial allocation for the other classes shown, the high coincidence in some areas (in green in Fig. 6) further testifies to the importance of Neighbourhood in determining model dynamics.

Figure 6: Map comparison by land use categories. Simulations 2050. NAS*v* against N*v*. M-H = Multi-Household, S-H = Single Household.



2) The relative scaling up or down of the map objects through the changing resolutions affects both the simulation map and the comparison map equally.

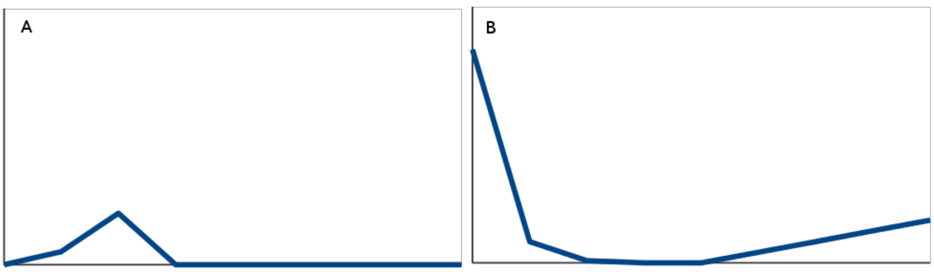
The second explanation seems plausible for comparison between applications within the same rules set (e.g. equal cell radius with unequal distance radius, or unequal cell radius with equal distance radius) but does not offer a good explanation for the similarity in goodness-of-fit across the rules sets. Since the comparison maps are the same for both rules sets at each resolution, for this explanation to hold true, it would be necessary to observe more substantial differences between the two rules sets.

3) The neighbourhood influence declines very steeply and that all important interactions take place at near distances.

The third explanation has more merit and seems to offer a plausible reason for the similarity in goodness-of-fit scores between simulations with quite extreme differences in scale, e.g. AP100-N8 and AP25-N8 (100x100m apps with 800m neighbourhood distance radii and 25x25 apps with 200m neighbourhood distance radii respectively). For this set of applications, if neighbourhood rules were actively determining the land use pattern at all distances, a linear decrease in accuracy of the simulation for the individual land use classes would be expected, since thematic classification accuracy is known to decrease linearly as raster cell size size increases (Carver and Brunsdon 1994). However, since the K_{sim} statistic does not measure agreement across the entire map, only of change areas, it may be that simple neighbourhood rules at close distances, maintained across all model applications are sufficient to reproduce the most important patterns of change, and for this reason, these patterns are extremely stable throughout all the applications.

Although the pattern statistics are slightly dissimilar between calibrations they seem adequate in each case, and always outperform the benchmarks (Table 4). For clumpiness in particular this is likely to be due to the fact that it is the *type* of rule (Fig. 7) not the influence values or the length of the tail that determine the degree of aggregation of the resulting pattern:

Figure 7: Two rules for a land use's attraction to itself. A; tends to produce scattered (disaggregated) patterns; B: tends to produce large, clumped patches. The x axis represents distance, typically not more than 8 cells, while the y axis is the neighbourhood influence value assigned by the user, which is unbounded, but typically might be between 0 and 10000 for attraction effects, with negative values for repulsion effects. As a consequence, since the shape of the neighbourhood rules has been maintained, the degree of aggregation remains comparable across simulations.



4) The calibration phase is too short for major differences to emerge.

Results from testing the stochastic factor (Fig. 3, Fig. 4) suggest that changing cell size results in significant differences in the pattern of land use allocation over long time periods. Since no data exist for the year 2050, data and simulations cannot be compared in the same way as for the calibration and validation years (2006 and 2009). For this reason, it's not possible to say whether major goodness of fit differences would have emerged for different scales of application in the case of a long calibration period. Testing this for a study area where land use maps for long historical time periods are available would be a useful next step.

Wider implications for simulation of urban complexity

The land use model discussed has been successfully calibrated and validated (*sensu* van Vliet 2013a) according to all available guidelines and parallels in literature. Even the poorest fitting application outperforms the null model and goodness of fit is comparable with that considered acceptable in other models. The most visually acceptable application seems therefore to be the most appropriate to use for generation of future scenarios. But the very low degree of variation between applications, despite the quite radical changes in scale, particularly in the cell neighbourhood, lead us to question whether the model may be too stable to simulate truly complex behaviour, as characterised by, for example; 1) spontaneous emergence of new land patches; 2) bifurcations, where simulations take different pathways at a particular timestep leading to two (or more) entirely different outcomes; 3) critical transitions or shocks – defined here as sudden state transformations leading to completely new patterns (see, for example, Polhill et al 2016). In the following paragraphs, we ask, with reference to the applications analysed in this paper, to what extent these kinds of models can simulate this kind of behaviour, and what this implies about their suitability for simulating complex urban systems.

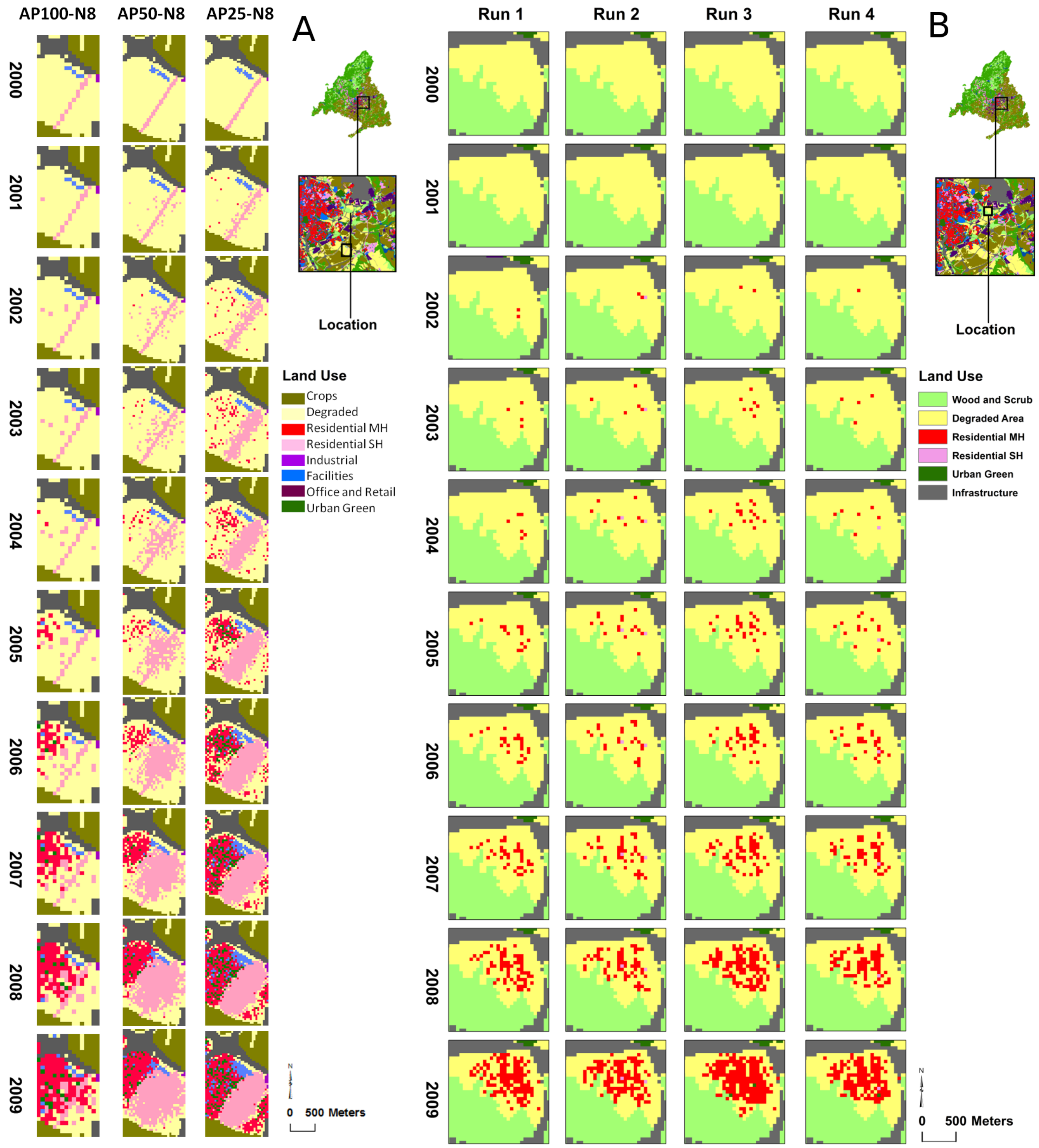
Spontaneous emergence

The action of the stochastic parameter v means that land will sometimes be allocated in cells that are generally otherwise not favoured, being far from existing cells of the same type or having low accessibility. However, it is important to consider that very restrictive suitability or zoning regimes will prevent this occurring, so it is not sufficient just to cite the presence of the stochastic factor as proof that the model is non-deterministic. If demand for land use A is 10 cells, and zoning or suitability restrictions effectively leave only 10 cells free for its allocation, the outcome will be predictable even if there is a high degree of stochasticity in the model. Further, in urban simulation models of this type, it is common for single cells to appear and disappear in subsequent timesteps. However, cells would need to be able to appear and then grow into plausible land use patterns to qualify as truly emergent. In the applications discussed here, the liberal nature of the suitability rules and the absence of zoning mean that no such strong restrictions are present. Indeed, as Fig. 8a clearly shows, spontaneous emergence is present in all applications.

Bifurcation

White et al (2015: 19) provide a useful synthesis of bifurcation in complex systems using the analogy of paddling a canoe upstream. In the metaphor of these authors, bifurcation is the point at which the decision must be taken to paddle the canoe left or right at a branch or fork in the river, with each choice leading to a different outcome. In simulations that show true bifurcation, new urban land use clusters (sometimes arising through spontaneous emergence) would grow and develop in one area in one simulation (taking the left fork of the river) and in a different area in another (taking the right fork of the river). It is clear that a useful model would be expected to generate numerous bifurcations as many land areas may be equally suitable for new land use allocation, just as a real city has many possible futures, not a single predetermined pathway (White et al 2015: 11). In this model application, for example, the poor fit to data of the Residential Multi-household land use class may in fact be due to the presence of multiple suitable locations, resulting in effectively random location decisions. As Fig. 8b shows, in this case, the Residential Multi-household land use class allocation can “flip” between any of these suitable locations at random, which is the equivalent, in the analogy of White et al (2015), of selecting multiple divergent forks of the river. In the normal case, the range of possible future states may be extremely large (a power law distribution x^n, where x the number of available locations and n is the number of cells to be allocated). However, the vast majority of these states are extremely similar to one another, so, from a single rule set, the system does not *per se* function as generator of multiple diverse options. And as the sensitivity analysis indicates, even quite major modifications to key model elements may not increase this diversity. In Fig. 8b, for example, the similarity of the different bifurcation paths end state for the year 2009 is probably due to the strong constraints exercised by slope and accessibility.

Figure 8a (left): Spontaneously emerging clusters over 9 timesteps in different model resolutions. Figure 8b (right): Various model runs showing different configurations of Residential Multi-Household land use simulated by timesteps.



Critical transitions or shocks

An interesting example of a critical transition in a land use model can be found in the work of Polhill et al (2016), for the FEARLUS model. In this model, agents (farm businesses) drive agricultural land use change by searching for the most profitable land use, with profitability being influenced by exogenous and endogenous variability such as climate and characteristics of the individual land parcel. Once a profitable land use is found by one agent, other agents adopt the same land use by imitation, which eventually leads to homogenization of land uses and ultimately, a single land use across the whole model. A decline in profitability of the only land use (which, under a heterogeneous land use regime would cause agents to transition to another land use), results in bankruptcy of all agents in the model in a single timestep. In our model, this kind of transition would be almost impossible to simulate. There are two principal reasons for this:

1) The model simulates spatial pattern and location of land use, not quantity. Thus the number of cells to be allocated for each land use at each time step (the *demand*) is determined exogenously in advance and introduced to the model before running the simulations. For the calibration and validation phases of model application development, the demand for each land use is simply the total number of cells for that land use in the second map. For simulation of future scenarios, the demand must be established for the future date by either extrapolating the linear historic tendency or by estimating the demand in some other way, e.g. by consultation with stakeholders, through scenarios, or according to targets established by policy makers. Thus, even where one land use would occupy all of the map space at the expense of others, it is not permitted to do so by the exogenous demand. This is a difficult problem to resolve in the model as currently configured, since while the demand can be set to whatever figure the researcher chooses, this demand is *always* allocated as long as there is space in the map. One way of addressing this would be to determine demand dynamically in a separate model block through the interaction of various factors (e.g. economy, climate or policy), which could include the amount of land use already allocated, thus introducing a feedback loop. In this way, genuinely unpredictable results could be obtained from the interaction of various components, simulating much more realistically the complex behaviour of a true urban system.

2) The process of calibrating and validating the model with reference the historic tendency determines, to a great extent, the path which the model must follow for future dates. This aspect is discussed in detail by Brown et al (2005). These authors note that attaining a close fit to real land use patterns risks overfitting the model and reducing its capability to produce surprises. There is a true paradox here, since a model not fitted to an historical tendency is an uncalibrated model. One possible remedy for this is would be to focus more strongly on generating realistic growth patterns and spatial structures, and less on attaining goodness of fit scores through cell-by-cell comparison methods like K_{sim}. This problem can also be addressed to some extent by using different calibrations of the model for simulating different future scenarios. And even a highly overfitted model should be still able to produce a reasonable variety of complex patterns, since the random factor will generate some bifurcations and, if enough land is allocated, there will be some emergence (Fig. 3, Fig. 8). To escape from this "calibration paradox", it would be necessary to adapt it to allow the spatial interaction rules themselves to evolve over time in response to some kind of exogenous or endogenous but stochastic stimulus. In this way true critical transitions might be generated in cell space at the level of the system – for example, if neighbourhood attraction effects were converted to repulsion effects previously clumped land uses could spontaneously scatter across the territory.

Equilibrium, metastability and innovation

Following the discussion given in the preceding paragraphs with regard to the suitability of these types of models for simulating true complexity, it is possible to ask a more general question – does the preoccupation with generating very accurate simulations of land use patterns, and especially the use of heavy constraints through the suitability and zoning blocks, prevent us from simulating complex behaviour? And, following this question, a second question – does this matter?

To answer these questions, it is instructive to return to systems theory, which, after all, lies at the heart of urban simulation modelling. Winder (2007) observes that a system may be *metastable; i.e.* apparently at equilibrium but susceptible to transformation to a lower energy state under certain conditions, or *innovative*, also apparently at equilibrium but susceptible to transformations not governed by any rule defined from within the system itself. For Winder, both types of systems are complex, but while metastable systems are time-invariant and *computably* complex, innovative systems are *uncomputably* complex because the taxonomies are not preserved across system states. This is relevant to the present work because land use models function under the assumption, explicit or otherwise, that the system represented by the running model is metastable, neither predictably stable nor unpredictably innovative. This is clearly a useful assumption, since a stable model is completely deterministic, while a truly innovative model may disappear, generate butterflies or polar bears instead of land use, or get up and walk around the room. Leaving aside the philosophical consideration that human systems, urban systems included, are probably innovative in nature, the major concern of this paper is that most land use model applications are stable, not metastable. While the land use modelling system described here is capable of metastability, as clearly demonstrated by its ability to generate, among other things, bifurcations and spontaneous emergence, applications that prioritise exact replication of historic land use patterns according to crisp (non-fuzzy) cell-by-cell comparison measures and that strongly restrict certain parts of the model (e.g. through suitability and zoning) are not really, and should not be claimed to be, complex simulation models.

To answer the second question, whether this matters or not depends entirely on the objective of the research in question. A very stable, highly deterministic model may still be useful for planning purposes, since it is often desirable to know which locations are the most highly favoured for new urban development in the near future, given the plausible assumption of a continuation of historic tendencies. On the other hand, if the aim of the research is to explore *what if?* scenarios more broadly, it may be useful to relax the model application's constraints to allow for real complex behaviour.

Suggested modifications to the model to improve ability to simulate complexity

Further to the previous discussion, some modifications to the model can be advanced that may improve its ability to simulate truly complex interaction processes.

Land use demand

Introduce a demand sub-model and feedback loops, perhaps also incorporating a stochastic variable. By establishing land use demand through an exogenous process, as in the FEARLUS model, and then allowing this demand to change, according to economic factors or some other characteristics perhaps together with some random perturbation, it should be possible to replicate the effect of system shocks, even if, in principle, this eventuality is not specifically defined in the calibration process.

Calibration and validation approaches

In calibration and validation, concentrate on pattern and dynamic behaviour instead, and try to avoid cell-by-cell comparison measures like K_{sim}. If cell-by-cell comparison cannot be avoided, use fuzzy instead of crisp measures. It is also recommended to keep suitability and zoning very simple, or leave them out entirely.

Partial validation of each model block in turn

Hewitt et al (2014) apply a stepwise calibration procedure in which each of the key model blocks (Neighbourhood, Accessibility, Suitability, Zoning) is evaluated incrementally in turn. This approach can be used to check that spontaneous emergence is truly occurring by evaluating in detail the number and location of emergent clusters as each model block is applied. This is key to ensuring that excessively restrictive rules in any of the blocks are not shutting out stochastic variability.

Finally, in view of the approach taken in this research, we recommend carrying out a model sensitivity analysis in order to understand the range of variability of which a given model application is capable.

Future work

We suggest the following possible directions for future work:

1. Make specific modifications to the model discussed here to allow for the simulation of critical transitions.
2. Apply spatial metrics to identify the dynamic emergence of complex spatial patterns in real cities, and to try to link these to real historical events or processes.
3. Find ways to communicate uncertainty about results of these models to stakeholder groups (e.g. land planners), rather than imposing more constraints to make model applications “look right”.

CONCLUSIONS

A series of rigorous tests applied to a CA land use model of urban change have demonstrated that, contrary to expectations, major modifications to the scale of the model, either by changing the cell resolution or by changing both cell resolution and neighbourhood transition rules have relatively little effect on the accuracy of the simulation results. This indicates that the transition rules are quite insensitive to neighbourhood distance effects, probably because the most important neighbourhood effects are all occurring at close distances. It is suggested that excessive stability may sometimes limit the ability of these models to simulate complex behaviour. However, despite the apparent insensitivity of the model application investigated, features compatible with simulating complex urban systems were found to be present. Nonetheless, while these kinds of CA land use model are in principle capable of simulating complex behaviour, it does not necessarily follow that any application that applies this modelling framework must automatically be able to do so. In general, it is likely that these models, as habitually applied, are rather more deterministic and quite a lot less applicable to simulation of complex systems than is sometimes admitted. This may not present any problems in some land planning contexts, but is likely to limit the usefulness of these models for freely exploring *what if* tendencies. Some suggestions have been made both around general application good practice and as to how the model could be adapted to improve its ability to simulate true urban complexity. Finally, it is contended that sensitivity analysis should be approached from the perspective of “optimal sensitivity”, since a highly insensitive model may not be capable of producing any surprises, and, as a result, may not, in fact, be useful.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge funding received under remit of the EU FP7 project COMPLEX (project no. 308601). We are also very grateful to editor Itzhak Benenson and to three anonymous reviewers for their constructive and detailed comments and suggestions, as well as to Roger White of Memorial University, Newfoundland, who generously gave up his time and expertise to read and comment at length on the manuscript. All of these contributions have greatly improved this article.

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