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Chapter 4: Incremental Territorial Modelling

**Clémentine Cottineau, Paul Chapron, Marion Le Texier and Sébastien Rey
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Cities and territories are complex entities which geography approaches at a mesoscopic scale, between the level of social individuals and that of regional or continental groups. Therefore, cities and territories are considered both as products emerging from local social interactions and as "collective agents" supporting higher level interactions, such as interurban interactions. For instance, while such interactions originally stem from individual choices, they are organized according to the aggregated and emerging properties of cities. This duality (in the representation of territories and the representation of their interactions) matters in the dynamic modelling of cities¹ and geographical territories. .

A central question is therefore how to represent cities and territories in the models. Symbolic representation options (distribution of densities, functions, size and mesh size for example) are at the heart of the geographical discipline, yet there has been little thought given to this question in the history of modelling. The relative lack of discussion about the representation of territories in geographical models is likely due to the appropriation of theories, methods and models from other disciplines whose focus was not the territory. In this chapter, we seek to illustrate the importance of territorial representation by referring to a substrate closer to the discipline: cartographic modelling. Indeed, the choices of representation in maps, familiar to geographers, can constitute a first guide for territorial modelling.

A second challenge is to produce models which adequately represent the urban and territorial dynamics themselves: local evolutions or territorial stylized facts. For example, some models simulate the evolution of land use in specific cities (Chaudhuri and Clarke 2013), while others attempt to reproduce the emergence of segregation in general (Schelling, 1969) or the hierarchical evolution of a generic city system (Sanders *et al.* 1997; Reuillon *et al.* 2015). These two modelling perspectives lead to important differences in the genericity of the resulting model, its explanatory power, its re-applicability and its level of detail. In this sense, a reflection on the situated and partial status of the explanation in the field of geography can help modellers build models and evaluation protocols which are adapted to the simulation objective and the target territory.

The aim of this chapter is to present the main issues with embedding territorial representation and territorial dynamics in simulation models. First we depict current scientific practices, illustrated and illustrate them with select model examples. Second, propose a singular and reproducible modelling strategy, which aims specifically at describing a territorial system and its evolution. This strategy relies on multi-modelling or incremental modelling. This chapter ends with a presentation of the limits and opportunities of this approach, with a discussion of its applicability interest to different case studies.

¹ Dynamic modelling refers here to all models which produce a temporal evolution, such as differential equations or dynamic simulation, as opposed to statistical and static models, for instance.

1. The map and the territory

"Models are, by definition, a simplification of some reality which involves distilling the essence of that reality to some lesser representation." (Batty and Torrens 2001, p.28)

1.1. Modelling as one map: selection and schematization

The geographer's emblem - the map - being a 'simplified and conventional representation of all or part of the earth's surface' (Joly 1976), is already a model of territory and territorial organisation. Cartographic theory and graphic modelling can therefore provide insights into the representation of cities and territories in dynamic models of geographical space.

A map is a model because it is impossible to represent all the detailed elements of a territory on it, unless the map is at the 1:1 scale. In every other case, the cartographer has to generalize the information by reducing the quantity of this information to be represented on the map (selection), and by simplifying the qualitative information with respect to the objective of the map (schematisation).

"Generalisation [...] applies both to the creation of the base map and to the processing of information. Generalisation simultaneously combines selection, schematisation and harmonisation, the respective roles of which vary according to the type of map (topographic map, thematic map), the purpose of the map (dissemination map, scientific map, didactic map) and the scale of publication (format) which conditions the entire process." (Béguin and Pumain 1997, p.32)

In practice, the cartographic selection process consists in choosing which elements to represent and which ones to omit. Taking a road map as an example, the layout of roads, the location of tolls and cities are generally sufficient, whereas geological, agronomic or meteorological elements are not selected as this information is not relevant in the usual context of road map use. In the context of the dynamic modelling of a territory or city, the selection operation corresponds to the identification by the modeller of the essential elements and agents involved in the phenomenon under study. The model can be made more complex during the research, but it always remains schematic compared to reality. It is therefore a matter of prioritising the elements most relevant to the research question, otherwise the model might not be able to provide adequate answers.

To guide the selection operation, the literature distinguishes between two standard approaches. The first one is the well-known principle of parsimony (or Ockham's razor principle): the simplest model which reproduces the target dynamics is always preferred. The opposite approach consists of representing in more realistic details the territorial system studied and its hypothesised mechanisms. Depending on the modelling objectives (and the methodological bias of the modeller), the compromise can favour one approach or the other. The comparison between the SIR model², in its most traditional version, and the MicMac model (Banos *et al.* 2017) illustrates this point. Each of these models aims to simulate the spread of an epidemic within a population. In the first case, this population is divided into compartments (Susceptible, Infected and Recovered agents) linked by a series of differential equations describing the transition rates from one group to another. This mathematical model allows to examine the effect of contamination and to predict the the number of agents belonging to each of the three groups over time. It is an aggregated model (the general population is subdivided into three groups, whose characteristics are studied without explicitly describing the individuals who compose them) and an a-spatial model (the location of individuals and

² SIR is a classical epidemiological model of disease spreading which considers three possible states for social agents: Susceptible, Infected and Recovered.

groups is not modelled). The analytical resolution of the classical SIR model based on differential equations requires a continuous representation of time. In the MicMac model, the rules of the general epidemiological model are still defined according to an aggregated SIR model, but MicMac additionally describes the mobility of some individuals responsible for the spread in a disaggregated way, i.e. by spatialising agents. Mobility is defined on a long-distance range between cities, whereas for each city, an SIR model simulates the number of individuals infected, susceptible to be infected or recovered from infection at a given time. The relative proximity between cities is represented by a graph (whose links are airways and nodes are cities), whose topology and size can be modified. The model is solved numerically by simulation, using discrete time steps, i.e. the state of the population is computed at each step (interval) of time. Other models go even further in the level of details required for simulating the spreading of an epidemic. This is the case, for example, with the MOMA model (Model Of Mosquito *Aedes aegypti*, Maneerat and Daudé 2017), which represents the biological and behavioural characteristics of the vectors of dengue fever, yellow fever, chikungunya and Zika virus: the *Aedes aegypti* mosquitoes. This agent-based model is defined at the micro-geographic level: that of the environment perceived by the mosquito in movement. The behaviour of mosquito agents depends on their own attributes as well as on the attributes of the environment, whereby local geographical patterns (e.g. the presence of ponds) influence mosquito dispersal. It should be noted that despite a relatively high level of detail, this model remains generic since it is transferable from one geographical context to another.

The cartographic simplification operation consists in schematising the layout or symbolic representation of certain elements as one changes scale or adds more information to the map. On a map of Norway, for instance, at a large scale, the coastline will be complex and fjord outlines may appear. At the European scale, however, Norway is usually generalised and its boundaries are sketched with about a hundred more or less straight segments. In the same vein, territorial modelling schematises and simplifies the dynamics and representation of these objects. For example, 'as the crow flies' distance is often used in neighbourhood perception and transport cost assessment operations, even though it is recognised that large-scale human travel rarely conforms to Euclidean distances. Similarly, 'as the crow flies' distances are often calculated between centroids of geographical units rather than between barycentres of the population in spatial interaction models (Wilson 1971), which is considered a minor difference which simplifies modelling and computation. The main difficulty for the modeller is to know when this schematisation can be considered neutral with regard to the functioning of the model and its objectives and when it does not, even though it simplifies the calculations and the time management of the simulation. This problem, called the "representativeness of hypotheses according to objectives" is difficult to assess in general terms (Varenne 2013; Rey-Coyrehourcq 2015), especially since there is a tendency towards pluriformisation in current modelling practice, i.e. the hybridisation of formalisms (differential equations and agent based models, for example) within the same model.

Dynamic territorial models developed in geography therefore often differ from visual and procedural modelling methods which aim, among other things, at reconstructing urban landscapes from laser imaging and scanning (Musialski *et al.* 2013) or generating urban spaces of realistic shape and appearance using generative grammar (Parish and Müller 2001). These approaches, mainly oriented towards applications in cinema or video games, could nevertheless constitute an important development in geography and planning. The UrbanSim model (Waddell 2002) is perhaps most illustrative of this trend. In its most recent version, UrbanSim offers a 3D visualization platform which has the stated objective of facilitating the understanding of territorial dynamics by policy makers and the public. More recently, C. Slager and B. de Vries (2013) proposed a tool for the automated generation of spatial configurations "*with a high level of detail and realism*" for the evaluation of urban development projects, while SimPLU3D (Brasebin 2014) is aimed at simulating realistic residential built forms through the formalisation of local urban planning regulations. The latter models of territorial dynamics are based on intangible information (projections, planning,

regulations), which require ad-hoc modelling, and cannot be carried out by simply selecting or mapping available data. More generally, for a territorial model to work, its spatial components must be modelled, formalised and then used *as inputs to of* the model before the model dynamic processes can be simulated.

1.2. The representation of territory as an input of the model

Geographical models feature elements to represent territories which are more or less numerous and more or less schematic. Historically, models in urban geography modelling took inspiration from other disciplines. This has affected the way cities and territories are represented in models ever since. In particular, urban models have inherited from many ramifications of the "systemic project" (Pouvreau 2013; Rey-Coyrehourcq 2015; Varenne 2017). Physics and chemistry from the 1970s had a particularly strong influence on French urban geography for instance:

"with, on the one hand, Allen's work within the theoretical framework of Prigogine's dissipative structures, and on the other hand, that of Weidlich and Haag (1983) within the framework of the synergetics developed by Haken (1983), and finally that of Wilson (2000) who offered a theoretical basis based on the concept of entropy to the classical models of spatial interactions" (Sanders 2013, p.834)

Because of this disciplinary legacy, *"although the "cybernetic" phase of the systemic project [has] made it possible shift the focus from the entities to their interactions, and to clearly differentiate between the simple measurement of evolutions (a kinetics) and dynamics themselves (including an interpretation of the factors controlling this evolution)"* (Pumain 2013, p.13), early models of urban geography³ have tended to over-represent stock characteristics of territories (e.g. population, the numbers of jobs) in a fictional and abstract space. These early models also tended to under-represent the strictly territorial characteristics, reducing cities to interconnected points and the space between them to a uniform Euclidean field. The points were generally connected by flows which depended on the geometric distance between the points, and it was often not even necessary to represent space at all in the model, the coordinates of city-points being sufficient to calculate the distances and therefore the flows. This legacy has fostered the development of geographical models in which geographical space is isotropic and uniform, unlike its empirical equivalent. As a matter of fact, most of the scientific corpus of human geography aims to highlight the heterogenous distribution of human activities and the 'roughness' of the space which supports them.

The reintroduction of explicit geographical structures into dynamic models is therefore an important issue for territorial modelling, both because it is part of the geographer-modeller's job description and because, as a framework and support for agent interactions, such geographical structures and variations at the initialisation of the model have an influence on the simulated outputs. For example, A. Banos (2012) reveals the effect of the shape and structure of the urban network on the extent of spatial segregation obtained in the Schelling model, at constant parameter values. J. Raimbault *et al.* (2019) reach similar conclusions when varying the initial distribution of residential density on which the Schelling model is simulated. The challenge of this geographical structure integration also extends to the way the phenomena at work on these structures is observed: I. Thomas *et al.* (2017) show, for example, how the choice of boundaries and scale of the system represented in LUTI models can affect the results obtained, while M. Le Texier and G. Caruso (2017) reveal the impact of aggregation levels on the dynamics of Euro coins diffusion.

In addition to the model sensitivity to initial spatial conditions, i.e. to the representation of the territory supporting the modelled interactions as a fully-fledged input to the simulation process, the degree of

³ In Lowry's or Forrester's models, for example.

abstraction of the empirical fact to be represented also changes the requirements of territorial models. A. Banos and L. Sanders (2013) identify two main dimensions which differentiate dynamic models: a dimension of abstraction and, orthogonally to it in a 2D plan, a dimension of parsimony. The parsimony dimension, generally reduced to the opposition between KISS⁴ and KIDS⁵ models introduced by B. Edmonds and S. Moss (2004), contrasts parsimonious models (such as Schelling's⁶) to more complicated and complete models (such as MATSIM⁷). One end of the spectrum aims at understanding and schematically explaining fundamental processes; while the other end tends to favour realistic representations of systems and the prediction of future or alternative outcomes given the variations of certain conditions (scenario approach). The orthogonal dimension of Banos and Sanders – cf. Chapter 2 of this book as well – contrasts general and abstract models (for example: models of segregation) to particular models (for example: models of the distribution of social groups in the Paris area in the 2000s). As a matter of fact, the abstraction of processes does not necessarily imply the abstraction of territory, as shown by the application of the Schelling model to the city of Yaffo, whose digitized building footprints were characterised by a realistic distribution of population by religion (Benenson *et al.* 2009). By contrast, complete models can be applied to stylized spaces. An example of this practice is the application of the new geographical economy to linear cities or two-region world models (Fujita *et al.* 1999).

Finally, the representation of cities and territories as inputs of a model can be hybrid. Instead of representing all the elements of a given geographical level in the same way, the modeller can choose to vary the representation level according to the distance to the agent or object whose action is simulated. For example, in a model of trade between countries, the use of a 'rest of the world' category along with single country partners may correspond to this hybrid strategy. For computational reasons, A. Hagen-Zanker and Y. Jin (2012) have offered a similar strategy: their spatial interaction model implements adaptive zoning. The areas far away from the considered area are aggregated into groups which are larger the further away they are, in order to produce flows of comparable size to that of the flows between nearby areas. Such an adaptive zoning is probably more appropriate to represent human geographical perception than the uniform mesh sizes generally used in territorial models. It thus constitutes an interesting avenue for research from a conceptual as well as a computational point of view.

1.3. The representation of territory as an output of the model

Although territorial modelling generally targets fidelity to the represented city or territory, the simulation of territorial dynamics can be based on objects and concepts which do not exist or cannot be assessed in reality, but which serve as "stepping stones" to explain observed processes. In other words, the model can be used to explore the possible dynamics leading to configurations empirically observed, using the register of explanation by way of analogy (Workman 1964). The objects and dynamics selected by the modeller to feature in a model must be integrated into the reflection as an attempt to reconstruct a complex reality whose entire functioning cannot be observed. This bias being acknowledged, it is more important to focus on the coherence of this selection and its possible effects on the model outcomes rather than on the realism of an element in itself. In other words, it should not be forgotten that we are operating on an electronic substrate (the simulator) where the meaning and dynamics of the selected elements have very little to do with their complexity of their functioning in reality (Bulle 2005). Such assessments must be tested (by sensitivity analysis) to be confirmed.

⁴ Keep it Simple, Stupid!

⁵ Keep it Descriptive, Stupid!

⁶ The Schelling model is a classic and very parsimonious multi-agent model of urban segregation. It has two mechanisms: 1/ the agent assesses her satisfaction with the composition of her neighbourhood, and 2/ she moves to a new location if her minimum satisfaction rate is not reached where she currently resides.

⁷ In MATSIM, the city is represented with dwellings of different sizes and rents, commercial premises with variable lease levels, transport networks described by their geographical location, bus schedules, individuals with different time budgets and many other attributes.

However, whatever the realism of the dynamics modelled from the input territory, and whatever its status (empirical territory at a past date, abstract space, originally undifferentiated territory), the output territory produced by the model is assessed with regards to its ability to satisfy some requirements defined ex-ante (or by iteration) by the modeller. These requirements can be of two kinds.

On the one hand, the objective of the model may be to reproduce a trajectory which has been observed empirically. In this case, it is necessary to define the selection of elements to be simulated and what a 'good simulation' is in terms of deviation from this empirical situation. In the case of MATSIM transport models for instance, the configuration to generate is the distribution of daily mobility flows, by means of the organisation of their activity schedules and locations. The share of poorly estimated flows and maximum delays is used to distinguish between "good" and "bad" simulations. In the case of the Anasazi model, the configuration to generate is the extinction of the settlement (Dean et al. 2000). The generation of the observed trajectory is necessary although not sufficient to validate the model (Hermann 1967 ; Amblard *et al.* 2006 ; Rey-Coyrehourcq 2015).

On the other hand, the objective of the model may be, rather than to simulate an empirical trajectory, to generate one or more "stylised fact(s)". Since N. Khaldor (1961), the typical regularities of a domain have been referred to as stylised facts. Without being scientific laws, these stylized facts can be compared to the generalisations or empirical laws of the classical scientific approach (Harvey 1969). An example of a stylised fact in the geography of cities is the hierarchical distribution of their size, and more precisely according to a power function of exponent $\alpha \sim -1$ of their rank, the rank being the position of cities in the list of populations by decreasing order (Zipf 1949). The interpretation (Sanders 2012) and the expected value of the parameters of this power function vary according to disciplines, territories, time periods and ways of estimating it (Rosen and Resnick 1980) but the general aspect of the distribution and the regularity of the hierarchy persist. This is why some models take the generation of this stylised fact as an indication of a successful simulation (Cottineau 2017). In this case, even if the modelled cities have some economic, social and technical attributes which can be used to reflect the simulated configuration, the characteristic selected to qualify the model output is reduced to the distribution of their size (Sanders *et al.* 1997). It is in this sense that the territory represented as an output of the model can diverge from the territory represented as an input of the model, and from the territory used by the model and transformed by the modelled dynamics. The territory represented as an output is thus only a subset of this intermediate territory modified by the model (Figure 1).

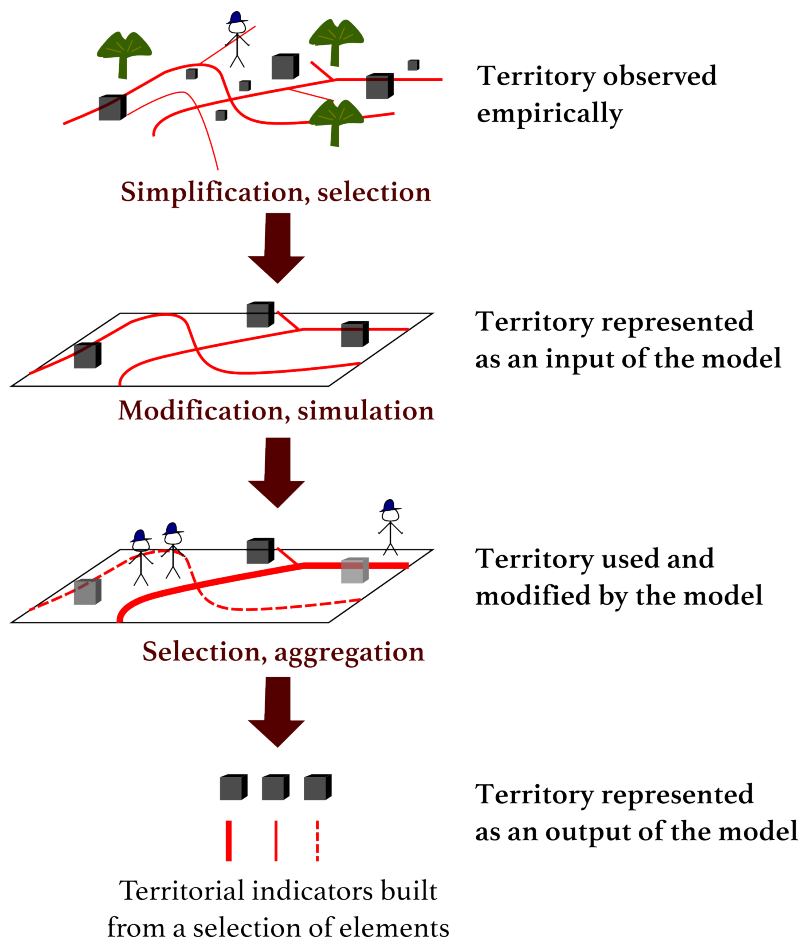


Figure 1: Different representations of the territory during the modelling process

The question of identifying stylised facts and their importance in the construction and evaluation of models is not limited to geography. Ecologists, for example, are among the pioneers in developing methods and tools to expose the process of model building and evaluation. On the descriptive level, the ODD formalism⁸ (Grimm *et al.* 2010) is now widely used to support models in interdisciplinary publications. Even more to the point of model validation, ecologists rely on the POM methodology⁹ (Grimm *et al.* 2005) and the notion of patterns (or stylised facts) to qualify 'good' models according to their ability to exhibit several stylised facts simultaneously. This method suggests using observed patterns as filters to compare and evaluate different model structures. In this sense, V. Grimm and U. Berger (2016a) speak of a modelling logic aimed at structural realism¹⁰ which is different from a search for reality. Models which generate the greatest number of patterns simultaneously are considered better in this framework. The POM approach is intended for models which simulate stylised facts, and whose expectations are numerous and detailed. This specification of expectations through *patterns* protocols allows to both reintegrate and assess hypotheses in an incremental and non-linear model-building process. The *path dependency* inherent to model-building is thus questioned (Augusiak *et al.* 2014; Grimm and Berger 2016b), but the methodology allows to filter more efficiently the "good" models. Indeed, if there several relevant processes can generate generate a single given stylized fact,, exhibiting simultaneously several distinct stylised facts is a criterion which greatly reduces the number of model candidates. The number of simple relevant processes

⁸ Overview, Design concepts, and Details.

⁹ Pattern Oriented Modelling.

¹⁰ The aim is to try, through a set of good practices, to capture as best as possible the actual functioning of a system and to establish testable predictions, which also implies being able to measure the difference between this capture and reality. The term also refers to the previous discussion about internal coherence (Bulle, 2005).

which can generate such a configuration is probably finite, and decreases with the number of independent stylised facts considered.

All in all, we see that the formalism, structure and explanatory dimension of a model depend on the modelled issue and the purpose of the research. However, the status of geography as a historical science brings additional aspects to the discussion of the general and the particular, which we now discuss in Section 2. A model is not so much "*what is being sought as such, but what facilitates the search for information about a real or fictional system, as part of a process of representation, knowledge, conceptualisation, design or transformation.*" (Varenne 2008). This is an idea that has been around for a long time among modelling geographers (Sanders 2000), for whom the content of a model is what counts when it comes to explanation.

2. Generality and specificity: explaining by ways of geographical models.

Although there is a variety of reasons to model social systems, including learning, communicating and formalising hypotheses, etc. (Varenne 2013), the main reason is to explain the modelled phenomenon (Epstein 2008).

"Literally, to explain ('expliquer') is to get out ('ex') of your folds ('plis') and to formulate hypotheses is to propose "a way of unfolding" ('déplier'). But to propose a way of unfolding is to situate oneself within a constructed world, the geographical world, and to use a language as unambiguously as possible so that the unfolding process is coherent. " (Raffestin 1976, p.85-6)

C. Raffestin considers the quantitative revolution in geography as a way of specifying the chosen way of unfolding, and thus making the geographical explanation falsifiable and predictive. Moreover, with the incorporation of the principles of cybernetics, the theory of self-organization and complexity, the relationship to the diversity of territories as well as its origin changed (Pumain 2003). Explaining by ways of territorial modelling thus embeds the notions of historical contingency and non-ergodicity (section 2.1) and makes the distinction between general, specific and singular trajectories (section 2.2).

2.1. Historical contingency and non-ergodicity.

Any scientific explanation should produce falsifiable statements and predictions. In social sciences, the generic and predictive nature of theories and explanations is sometimes challenged on the grounds that general laws cannot apply to human behaviour nor to its collective expression in space and time. In geography, because of the multivariate nature of the disciplinary objects, explanation must account not only for the phenomena under study (urbanisation, the demographic transition, etc.), but also for their variation of expression over time and space. Explanation is therefore often multifaceted, combining systemic, ecological, functional and causal analysis (Harvey 1969).

"Even if they result in distinct geographical configurations, spatial frames are organised by temporal processes which reproduce or maintain the stability of this structure in its various components. The explanation of the durability of a combination lies not so much in the strength of the associations which bind its components together, but in the subtlety of the evolving principles by which the structure, incrementally and continuously, and in all its components, adapts to change and sometimes also helps to bring it about. Therefore, very quickly, this theoretical quest implied knowing how to move from the observation of regularities to the

analysis of processes, from the identification of "combinations" or structures, to the study of the change likely to produce and transform them." (Pumain 2003, p.7-8)

Assumptions about the irreversibility of time and the unpredictability of the future underlie the non-ergodic property of territorial models (Pumain 2010b). This property implies that "*all possible states for all cities [and all territories] are [not] accessible to each of them*" (Pumain 2010b, p.60), due to the evolving processes of diffusion and specialisation which guide territories along "paths" of evolution rather than towards a predictable end state. For example, observing cities of different sizes at a given time is not equivalent observing a typical city during its historical growth path.

By adopting the paradigm of synergetics and complexity, i.e. a modelling universe where "*the same equations are capable of generating a very broad diversity of forms and evolutions*" (Pumain 2005, p.15), the contingency of observed patterns corresponds no longer to the historical contingency which produces the complete trajectory of a territory through a succession of singular events, but rather to a contingency which directs the system towards one or another of its possible trajectories, at the whim of bifurcations, and that a complex model allows to explore.

"The theory of self-organisation makes us understand how identical general processes are likely to produce different effects and structures, depending on the initial conditions and values of the parameters which control interactions and their evolution." (Pumain 2003, p.16-17)

The complexity paradigm therefore invites us to rethink the distinction between general, specific and singular trajectories (Durand-Dastès 1991), as well as the situated or partial nature of models which apply only to a single case study or predict only one type of outcome. The diversity of the results produced by a territorial model when varying its initial conditions and parameter values slightly allows to reinforce the extent of its applicability when the results correspond to known empirical situations, and to provide information on possible futures not yet realised, as well as to identify situations of falsification of the theory.

"It is of course important to ensure that a model is able to reproduce the patterns it is designed to explain. And it is equally important, following Popper's argument, to look for simulations that may have the power to falsify the model, those which display an association of input values and output patterns which contradicts data." (Chérel *et al.* 2015, p.1)

Without rejecting Popper-Hempel's Hypothetico-Deductive (HD) and Nomologico Deductive (ND) models as a whole, as Passeron (2006) did for sociology, geographers prefer to rely on a multiplicity of knowledge building regimes to enhance the toolset and methods of so-called "qualitative" and "quantitative" work (Pumain 2005; Sanders 2000 ; Varenne 2014; Rey-Coyrehourcq 2015). In other words, deductive reasoning would by no means be the only way to produce scientific reasoning. For example, J-M Besse (2000) proposes to value abductive logic¹¹ allowing a "progression of meaning", a "progression in elucidation" which leaves room to interpret the cognitive aspects in the course of reasoning when it comes to keeping or rejecting an hypothesis:

¹¹ For S. Catellin (2004): "*The starting point of abduction is a fact perceived as surprising, which is therefore against expectations, against habit, or against what was previously taken for granted. Abduction consists in selecting a hypothesis A likely to explain fact C, so that if A is true, C is explained as a normal fact. In other words, abduction is a normalization procedure of a surprising fact. It is an effort of reasoning that is undertaken when there is a rupture in our system of expectations, an "imaginative" reasoning that uses our knowledge. Abduction is part of a process logic and not a calculation logic, it refers to a context and a culture, to a social habitus.*" Other definitions of abduction and their relationship to modelling are discussed by S. Rey-Coyrehourcq (2015).

"As such, much of science's task would not primarily consist of seeking deductive causes and sequences, but in organising points of view and frames representing the situations it aims to account for. In other words, before seeking to explain and demonstrate successions of causes and effects, science is concerned with illuminating situations by abductively making meaningful connections. Science does not only seek to demonstrate, but also to enlighten." (Besse 2000)

This logic is explained and operationalised for the modelling practices of geographers (for example, see Banos 2013).

2.2.General/specific/singular

The opposition between general and particular features or trajectories is at the root of scientific theory building, since theories aim to account for particular cases by linking them to a general "law" through the explanation process. However, in the field of social sciences, but also of "historical" sciences to which even geology could belong (Harvey 1969), the distinction made by A. Bouvier (2011) between the individual and the singular (or unique) is essential. Indeed, while the general case derives from the standard application of the model in the abstract case, it can only be compared to the particular cases of empirical reality. These particular cases may exhibit characteristics deriving from the general model, i.e. shared characteristics based on the presence of common attributes (for example, capital cities share a common particular attribute and tend to be larger than the average city in a given country). The singular case "*escapes generalisation*" (Sanders 2013, p.12) and requires the use of historical explanation to understand its evolution (for example, Vienna is bigger than other Austrian cities but we need some knowledge about the Austro-Hungarian Empire to understand why). This distinction between general, particular and singular is interesting to approach the modelling of cities and territories, because it allows us to compare the results of a model with *particular* geographical configurations, observable and measurable on empirical data, but also to highlight the singularities of some trajectories at the end of an iterative process of model complexification. While the empirical analysis of particular cases aims to increase in generality by common categories identification or classification, the complexification approach reflects the opposite path: a "descent from generality". At the end of this path, the residual trajectories which the model cannot predict are deemed singular.

Hence, the model as well as the methodology of its construction can facilitate the explanation of a geographical phenomenon in general (for example, the differentiation of city sizes in a country), in particular (the evolution of city sizes in a socialist country, in a developing country etc.) and in 'singular' (the contemporary Chinese evolution). In section 3, we present an incremental and modular approach to model-building, based on the MARIUS modelling experience. We detail the steps and issues involved in this construction.

3. Incremental territorial modelling

"Traditional models get the present right and are then used to predict the future. In contrast, [...] Simulation enables [complex systems models] to generate different outcomes, which under some circumstances might appear to be different futures but really define a space of different model outcomes. The way this space is generated is not simply through systematic variations in parameter values, which is the time honored methods of model calibration in the case of traditional models, but through varying the model structures within some limits, that is usually varying the rules that encode different processes into the model, thus simulating different experiments within a kind of virtual laboratory." (Batty et Torrens 2001, p.32)

In the spirit of this programmatic quotation, the method we present aims to separate the explanation of the geographical pattern under study into more or less independent mechanisms, which are more or less general or specific to the geographical object being modelled, in order to combine them into a single, modular model. This model is evaluated both in terms of the empirical geographical configuration it has to simulate and in terms of how well it matches with more general stylized facts about the object under study. The methodological question raised by this incremental approach is the following: how can we build 'realistic' models with regard to empirical data and stylized facts, which integrate successively (and simultaneously) a richer information on their processes and on the diversity of their geographical expression?

We propose a six-step approach. First, we consider the identification of the scale of analysis, of the configuration to simulate and of the stylized (section 3.1). Subsequently, we address the question of collecting and categorizing the various existing explanations (section 3.2), then prioritizing them with respect to the generality of their explanatory power (sections 3.3 and 3.4). Finally, we describe how models are implemented in a modular manner (section 3.5), combined, simulated and compared with the empirical data and stylized facts prepared for their evaluation (section 3.6).

3.1. Identifying the object, scale, configuration and stylized facts

The first step in incremental territorial modelling consists in defining the research question, identifying the objects, the geographical scale and the target evolution to be depicted by the model. There are a multitude of territorial models because there are an infinite number of geographical questions. For example, there are pedestrian flow models, oriented towards emergency evacuation analysis (Zheng *et al.* 2009) which are different from the pedestrian models aimed towards the optimisation of dense areas such as stations (Hoy *et al.* 2016). Other pedestrian models focus on the emergence of urban riots, with particular applications in London in the United Kingdom (Davies *et al.* 2013) or Kibera in Kenya (Pires and Crooks 2017). The resulting models are sometimes similar, often incompatible and always contingent on the research team producing them. We therefore suggest, in addition to the documentation of ODD models (Grimm *et al.* 2010) allowing their communication, diffusion and potential reuse by others, that modellers make an extensive 'modelography' (Schmitt and Pumain 2013) of existing theoretical and applied models before they start building *yet another model* (O'Sullivan *et al.* 2016). The re-use of models cannot generally be direct, as each model answers a specific research question. The rather uncommon practice of *model docking* is interesting in this respect (Wilensky 2007), because it consists in realigning models developed with different objectives by showing that they can produce, and therefore partly explain, similar *patterns*. The practice of reuse with modifications, which is certainly demanding because of the reproducibility efforts it involves (Grimm *et al.* 2010 and 2014; Rey-Coyrehourcq *et al.* 2017), should be much more frequent than it is now, because it fosters the accumulation of knowledge (Pumain 2005 and 2009; Rey-Coyrehourcq 2015).

Once the object of the model has been identified, it is necessary to decide whether the model is expected to simulate a singular empirical configuration, a particularity of this configuration, or the general underlying process expressed through the geographical configuration. A two-fold ambition may be to build a model which is capable of reproducing both the particular configuration which motivated its development as well as the empirical variations of the phenomenon, thus demonstrating its general explanatory power. In this case, the objectives for evaluating the model have to identify both requirements and to characterise their level of generality/particularity, for example by distinguishing between general objectives ('obtaining a distribution of city sizes according to a power law'), particular objectives ('obtaining a concave distribution for socialist countries) and singular objectives ('reproducing the distribution of the former USSR at a particular date'). This definition/explanation of *patterns* is essential in the search of the mechanisms to be modelled as well as for conducting a rigorous and reproducible evaluation, especially for a POM type of evaluation.

3.2. Gathering the different theoretical explanations

In concrete terms, the search for explanations of the targeted phenomenon and their modelling can start from the object studied and the existing models and theories reported in the literature (may it be about urban riots, the risk of marine flooding or social segregation,), but also from the geographical scale of this object or from the type of evolution at stake. In the case of the approach which starts from scales, the review of existing models at a given scale (for example the city, the agricultural plot or the globe) allows to explore processes and themes which are not considered directly but which may have an effect on the pattern to be simulated and play a role in the explanation. In the case of the approach by types of evolution, a comparison between models from different disciplines can be fruitful. For example, the process of size hierarchisation of interacting elements is generated by stochastic dynamics in mathematics, preferential attachment dynamics in network physics or by increasing returns in economics. These different approaches can serve as competing and complementary model candidates to explain the demographic differentiation between cities, companies or archaeological settlements (Pumain 2006; Sanders 2012).

The 'cartography' of competing and complementary explanations is not new or necessarily related to territorial modelling: the pioneers of dynamic modelling in the 1960s (Levins 1996; Hermann 1967) already considered a diversity of mechanisms and the advantage of dynamic modelling to decide between them. R. Levins (1966) for example listed and linked prey-predator models of the Lotka-Volterra type with theories postulating the effect of competition between species and food chain models to map a 'cluster of models' able to exhibit the emergence of ecological communities. In general, the verification of theories by comparing alternative explanations is a common epistemological practice which, although different from the Popperian and Kuhnian approaches, applies to geography as well as to other sciences (Harvey 1969). For example, in urban geography, C. Cottineau et al. (2015a) identify five mechanisms which can explain the differentiation of city sizes over time: the effect of spatial interactions and the hierarchical diffusion of innovations; self-reinforcing effects of city size differences; site effects and the presence of natural resource deposits; the effects of situations (on transport networks in particular); and territorial effects, i.e. linked to a political organisation of solidarity on a defined space, such as a region or state.

Once the mechanisms are listed, we claim it is important to hierarchise their supposed importance in order to organize the implementation of the model, and especially to make testable assumptions about the explanatory power of the different mechanisms. One way of doing this may be to prioritise the mechanisms according to a subjective (although not arbitrary) assessment of their general or system-specific nature, as well as to separate interaction mechanisms between geographical agents from interaction mechanisms between agents and their geographical environment.

3.3. Hierarchising the interaction processes between agents

Hierarchising interaction mechanisms between agents is an important step in most modelling approaches, but is rarely mentioned in the published results of the model. A notable counter-example though is the presentation of the Sugarscape model in J. Epstein and R. Axtell's (1996) book. Starting from a simple model, the authors describe in successive chapters the increasing complexity of behaviours available to the simulated agents, from static agents harvesting a local resource to mobile, gendered agents capable of building up food stocks and transmitting them, trading, reproducing and polluting. In the example of the MARIUS model simulating the differentiated evolution of city populations in the former Soviet Union (Cottineau *et al.* 2015b), the interaction mechanisms between city-agents are hierarchised from the most general one (i.e. exchanging value according to a gravity model), to the one most particular to the study space (i.e. socialist economic planning and the

exclusive specialisation of cities in the production of goods for the entire country). In between, we find the mechanisms of territorial perequation, the memory of exchanges or the diversification of urban functions (cf. axis 1 on Figure 2). This hierarchisation has enabled us to choose which mechanisms to implement and evaluate first.

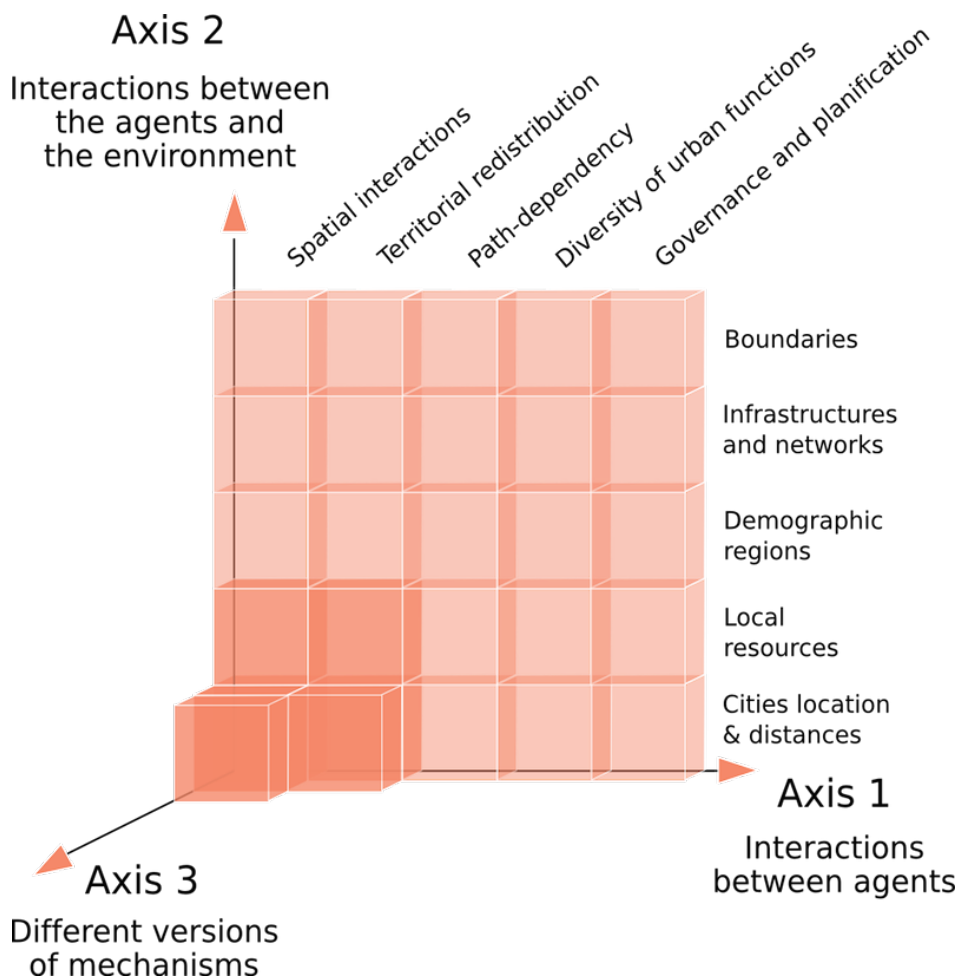


Figure 2. Hierarchy of mechanisms potentially explaining the urbanisation dynamics of the former Soviet Union over the past fifty years. Source: Cottineau et al, 2015, JASSS

3.4. Hierarchising the interaction processes between agents and their environment

The hierarchisation of interaction processes between agents and their environment is a particularly important aspect for territorial modelling. Indeed, this dimension of differentiation relate to both the level of detail with which the model's environment is represented (from a simple uniform grid to an empirical cadastre representing individual plots) and also to the richness of the agents' geographical behaviour. The detailed description of an urban environment makes it possible to model more realistic navigation behaviours (as in the policing model of Camden (Wise and Chen 2016) or contagion (Perez and Dragicevic 2009) whereas the addition of localised data on the agricultural potential of cultivated plots makes it possible to accurately reproduce the agricultural production dynamics of Amerindian societies (Dean *et al.* 2000).

In the example of the MARIUS model, the interaction mechanisms between city agents and the Soviet environment are hierarchised from the most general one (the effect of distance on interactions), to the most specific to the study area (the modification of borders over time). In between lay intermediate

mechanisms such as the local presence of raw materials, the macro-regional differentiation of demographic regimes and the impact of transport infrastructure on the calculation of time-distances (cf. axis 2 on figure 2). This hierarchy was produced on the basis of a prior statistical analysis of the evolution of these cities, observed over a long period of time.

3.5. Implementing mechanisms and their formal alternatives

Figure 2 presents a third axis of organisation of mechanisms, for a given level of representation of the agents, their interactions and the environment: the dimension of formal alternatives for a given theoretical explanation. A pioneering example of exploring mathematical variants of the gravity model comes from S. Openshaw (1983 and 1988). During the 1980s, he has implemented an "automatic geographical machine" which automatically generated combinations of gravity models (using logarithmic, exponential or power functions assigned to the population, for example) to be estimated using empirical data on inter-zone flows. Since then, model docking movements have headed to a similar direction, although less systematically, by aligning models from different disciplines and issues, but producing equivalent results (Axtell *et al.* 1996). More recently, J. C. Thiele and V. Grimm (2015) suggested ecologists should explore existing models more systematically, break them down and explore their modifications in order to capitalise on previous efforts, but also to improve the robustness of models re-implemented and tested by several research teams.

We could add a fourth dimension, often ignored: the technical implementation of mechanisms, since the decomposition of mechanisms into computer algorithms naturally gives way to interpretative variations. When modelling the behaviour of interacting social entities (actors or collective agents) in a territory, an additional dimension along which mechanisms can differ is the cognitive capacities of the agents. The hierarchy can be organised with respect to the amount of information they have (complete or limited) or to the complexity of their individual reasoning or behaviour: from the purely reactive agent to an agent who, on the basis of perceptions that she confronts with her beliefs, plans her actions according to their expected effects. Finally, for models based on "highly" social agents, we can consider an additional dimension according to the complexity of social organisations, from the colony of undifferentiated agents to organisations structured by roles, groups and rules which are themselves hierarchical (Bouquet *et al.* 2015).

We assume that the evaluation of alternative formalisms of mechanisms can be done in parallel with the evaluation of models of different structures (with more or less mechanisms describing interactions between agents and with the environment). To do this, it is necessary to set up the most robust possible strategy for combining, simulating and evaluating models.

3.6. Combining, simulating, comparing

The perk of subdividing the explanation into different mechanisms lies in the fact that we can implement basic "building blocks", each of which representing a candidate mechanism (and its formalism), and combine them into a modular model. The modularity of the model must therefore be transcribed using a programming language which allows the automated combination of bricks and conveys the information about the parameters required by each combination to execute the model.

In this respect, during our experiment with the MARIUS model, we used the computer notions of "trait" and "dependency injection" (also known as Cake Pattern¹²) of the Scala programming language to generate all possible combinations of building blocks (64 combinations in this case), to which a

¹² This is a way to extend the functionalities of the methods of an object class (here: the mechanisms) according to the context in which they are called (here: the particular combination of bricks forming a model). See also (Rey-Coyrehourcq 2015) for an example of the use of these technologies.

structure identifier is assigned (Cottineau *et al.* 2015a). This identifier is used as a meta-parameter when assessing the performance of simulation results against empirical data. This assessment is done by measuring the distance between the simulated city populations and the (post-)Soviet cities population data, and relating this performance to the model structure, i.e. its content in terms of combined mechanisms, which this identifier condenses. This experiment allowed to analyse which are the most probably needed mechanisms to simulate the evolution of the city populations in the former Soviet Union, according to their presence in the most efficient models at different levels of complexity (estimated, for example, by the number of blocks of mechanisms present in the model combination). In particular, it was shown that the mechanism reflecting the process of rural migration to urban centres (or urban transition) was the most important to account for the differentiation of Soviet city sizes between 1959 and 1989, whereas the mechanism of natural resources extraction appeared to be the most important after 1991, confirming in this case the previous insights regarding the post-Soviet urbanization.

We believe that this experimentation can be generalised to other territorial models and that it presents interesting opportunities in terms of robustness analysis (each combination of mechanisms being confronted with the others) and offormalised knowledge accumulation (using the qualification of the explanatory power of each mechanisms). However, multi-modelling (i.e. the combination of different mechanisms and their competing evaluation) presents significant challenges. Section 4 offers a discussion of some of these challenges.

4. Challenges and limits of multi-modelling

“The data requirements, problems associated with parameter estimation, and possible magnifications of parameter errors [make spatially explicit] models an onerous process.” (Wiegand *et al.* 2004)

Among the main challenges of multi-modelling are the human and computational costs, due in particular to the high number of possible combinations which grows more than proportionately with the number of building blocks the choice, number and order of these building blocks and the absence of standardised methods for comparing models of different structures.

4.1. The combinatorial curse

"Combinatorial explosion" is one of the challenges that modellers have faced for a long time. The high number of possible model combinations implies lengthy calculations to evaluate the model (calibration, sensitivity analysis, robustness) but also to analyse and interpret these results. Indeed, the more descriptive and complete the modelling is, the more numerous the alternatives of formalisation are, and the higher the number of building blocks to combine. The number of combinations increases geometrically. In the MARIUS case, with one base mechanism and five additional mechanisms, the multi-model resulted in $2^6 = 64$ possible combinations¹³. Its calibration required more than 400,000 hours of calculation¹⁴.

If we were to implement C. Cottineau's project (2018, p. 20) on urban inequalities based on the twelve mechanisms identified in the literature as candidates for explaining the dynamics of economic inequalities in cities, we would arrive at $2^{12} = 4096$ possible model structures. The tools for analysis and interactive visualisation of the results developed for MARIUS (Pumain and Reuillon 2017) would

¹³ The number 2 refers to the possible states of the mechanisms, i.e. active or passive in the model, while the number 6 refers to the number of distinct mechanisms.

¹⁴ Distributed on a computing grid using the OpenMole platform (Reuillon *et al.* 2013).

not be sufficient to manage such a level of complexity. The method is therefore envisaged as a prototype and a methodological approach rather than as a universal modelling standard.

4.2.Human and technical costs

Since the pioneers of the 1980s, enormous progress has been made on the issue of computing infrastructure, both in terms of hardware and software. Despite this, the difficulty of accessing computational structures for social sciences studies (Banos 2013; Rey-Coyrehourcq 2015) and the constancy of the computational cost associated with model exploration are constraints that still need to be addressed. The design and implementation of a software chain that supports (a) the automatic generation of a tree of possible combinations from a multitude of heterogeneous building blocks, (b) the evaluation of this tree on distributed computing platforms with adapted methodologies, and (c) an automatic re-composition of the bricks of the tree formulated in (a) on the basis of relevant evaluation criteria, remains to date the result of an *ad hoc* modelling process. To become affordable, this complex engineering will have to be integrated in the form of new construction primitives within modelling platforms (NetLogo, Gama, etc.). This also allows us to discuss the human cost of such an undertaking. Indeed, a project like MARIUS required about two years of work by three young researchers (doctoral and post-doctoral) funded on the ERC GeoDiverCity project. This experience of interdisciplinarity is described in (Chapron *et al.* 2014; Pumain and Reuillon 2014; Rey-Coyrehourcq 2015; Pumain 2018).

4.3.Subjectivity in the choice of building blocks

Another weakness of multi-modelling is that it is based on a partially subjective choice of implemented increments (or building blocks). Indeed, although the hierarchy of processes follows scientific arguments, it is unlikely that the result will be unanimously accepted, which in itself is a weakness as much as a strength. Moreover, given the combinatorial explosion issue, it seems unwise to aim at exploring the exhaustive set of the possible mechanisms into a multi-model. Our recommendation to the novice multi-modeller would therefore be to favour parsimony in the selection of building blocks after having justified as far as possible the hierarchy of processes described in section 3, by referring to empirical regularities as well as strong theoretical arguments. It is also possible to hope that the reuse and re-evaluation of different blocks of mechanisms will make it possible to characterize their robustness and interest in modelling the geographical object in question, facilitating the choice of robust and efficient increments in the applications tested for subsequent models (Thiele and Grimm 2015).

4.4.Comparing models of different structures

An additional problem of multi-modelling is to take into account the content of the building blocks in their comparative evaluation. Indeed, given the impossibility of defining the likelihood value of each model, traditional statistical analysis tools for model selection, such as Akaike or Bayes information criteria, no longer work in the case of complex territorial simulation.

If we were to reason more simply, by trying to arbitrate between distance from simulation objectives and parsimony, let us imagine the comparison of three models. Model A contains only one mechanism, for example the random growth of economic firms. This mechanism has two parameters: the average growth of firms and the standard deviation of their distribution. Model B contains only one mechanism, namely the growth of firms based on their interactions with other firms. This mechanism is based on three parameters: the range of interactions, the multiplier effect of size and the average growth of firms. Model C contains the combined mechanisms of models A and B, and therefore has four parameters in total. It is easy to consider model C as more complex than models A and B. However, are A and B equivalent (since they have the same number of mechanisms) or not

(since B has more parameters and, probably, more lines of code¹⁵)? The MARIUS experiment (Cottineau *et al.* 2015a) considered them as equivalent, which is probably too simplistic. However, it is not clear how it would always be possible to order the degree of parsimony of different model structures when their number and complexity grow.

The approach of C. Piou *et al.* (2009) is quite different: these authors use the POM method and define an information criterion called POMIC. This indicator is based on the estimation of a deviation measure between the entropy of the model outputs and that of the field data. This solution, applied to different mathematical forms, reflects differences in terms of number of parameters, but no differences in content. It is therefore still difficult to compare the influence of a mechanism involving the consideration of data external to the model with a more parsimonious mechanism on this aspect.

Although we wanted to highlight the limits of the multi-modelling approach in territorial applications, we still believe that this approach is the most consistent with the scientific approach of social sciences in general and geography in particular. Moreover, the advantage of such a method is that it encourages the accumulation of formalised and evaluated knowledge, making it possible to reproduce stylised facts in diverse configurations, reflecting the diversity of territories. This opportunity will necessarily require the sharing of models and their evaluation protocol, and a theorising enterprise: a kind of overarching theory of complex models themselves.

4.5. Sharing and accumulation of knowledge

This overarching theory of multi-agent models is the subject of a research group led by U. Berger, V. Grimm, I. Lorscheid, and M. Meyer¹⁶. The first path envisaged by this group is the documentation, evaluation and sharing of "sub-models" within catalogues of mechanisms implemented in common computer languages. Like the package operation of the R software or the model libraries of the NetLogo software, one can imagine libraries of mechanisms (building blocks) relating to objects and scales of territorial modelling, from which modellers could choose the most interesting combinations for their research question. The challenge is then to standardize the conditions of experimentation: input and output data formats, methods and tools and documentation of model source codes¹⁷, but also the acceptance of these standards in a community that has until now been characterized by a diversity of practices, languages and investigation issues.

Conclusion

This chapter has pointed out the importance of adequately representing cities and territories, but also the dynamic interactions between simulated agents and simulated territories, in complex simulation models. This territorial approach presents specific issues. Therefore, we have detailed the different states a territory can undertake during the modelling process. First, it is abstracted from reality as the modeller assesses which characteristics are the most relevant with respect to the research question - as in cartography. Second, the territorial setting is described using a formalised procedure, i.e. it is transposed into an algebraic system whose structure, scale and level of details are at the heart of the modelling process. We have stressed that initial conditions of this first territorial representation have a huge technical and theoretical impact on the simulation process. As such, the territory is indeed both an *input* and an *output* of the simulation. It is first altered by the mechanisms of the model during simulation, then abstracted again at the end of the simulation when the

¹⁵ A tricky measurement, which only works if language, programming experience and the programmer remain constant during the development of the model.

¹⁶ <http://abm-theory.org/>

¹⁷ Not to mention their openness and free accessibility, execution and modification, as proposed in the GeOpenMod section of Cybergeog magazine <https://journals.openedition.org/cybergeog/26452>

modeller selects which territorial components will be used to qualify the simulation outputs and to measure the correspondance with empirical data and/or stylized facts.

The chapter dealt further with the question of the nature of explanation in territorial simulation. Models of this type intend to explain a geographical phenomenon by combining parametric mechanisms, translated into mathematical structures or computer programs. This formalisation ensures a precise analysis of their independent and combined effects. Such a monitoring allows modellers to assess the variety of potential territorial dynamics as well as to characterise a particular historical trajectory by comparing it to a set of alternative results arising from the same mechanisms. This approach leads to distinguish, in the study of a territory and its models, between the general, the specific and the singular conditions.

Finally, we proposed a modelling strategy which goes beyond the classical definition of a model as a fixed set of mechanisms deriving directly from a research question. Instead, this strategy considers a model as a singular combination of mechanisms selected among a broad collection of potential ones. a classification is made according to their degree of generality (i.e. from the most general to the most specific) and complexity (i.e. from the simplest to the most complex). This allows to better understand the effects of a variation in the model structure on its dynamics and outputs, and therefore to better inform the wealth of information it provides. Other ordering criteria can be used depending of the research question. In this chapter, we have for instance chosen to arrange the incremental mechanisms according to two dimensions: the interactions between entities (cities here) and the spatial resolution of the environment in which interactions take place. However, this method implies significant costs, which we have detailed in the last part of the chapter.

The analysis of existing modelling approaches and of the incremental modelling strategy sought to provide the reader-modeller-geographer with a guide to represent territorial complexity in a progressive and well-reasoned manner, in order to develop a reproducible territorial model and evaluation protocol. The incremental multi-modelling approach tackles the issue of model adequacy with regards to the geographical object under study and it clarifies the elements of the scientific debate in case of alternative explanations as it requires a fine specification of the simulation objectives, of the conditions under which the model operates and of it implementation details. It lays down the foundations for testing and confronting empirical and theoretical hypotheses from simulation models. We believe that this incremental and multi-modelling strategy is very promising and in line with the more general concerns of the agent-based modelling community. However, this method implies high implementation costs as the autmated combination of modular building blocks and their systematic calibration rely on an important technical and computer arsenal, which we have partly discussed in the last part of the chapter and will be further detailed in the following chapter.