Exploration methods for simulation models

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Abstract

We recall first in this chapter to what extent simulation models are an absolute necessity in social sciences and humanities, which can only very exceptionally require to experimental sciences methods to construct their knowledge. Models open the perspective to simulate social processes by replacing the complex interplay of individual and collective actions and reactions to the situations they make emerge by simpler mathematical or computational mechanisms, fostering an easier understanding of the relations between causes and consequences of these interactions and to make predictions. The formalisation through mathematical models able to offer analytical solutions being most often not possible in order to provide satisfying representations of social complexity (Jensen, 2018), computational models based on agents are more and more used. For long the limited computational capabilities of computer have forbidden to program models taking into account interactions between large numbers of entities geographically localized (individuals or territories). In principle these models should inform on the possibilities and conditions of the emergence of given configurations defined at a macro-geographical level from interactions occurring at a micro-geographical level, within systems with a too much complex behavior to be understood by a human brain. This however requires to study the dynamical behavior of these models including non-linear feedback effects and verify they produce plausible results at all stages of their simulation. This necessary stage of the exploration of the dynamics of algorithms remained rather rudimentary until the end of the last decade, when algorithms including more sophisticated methods such as evolutionary computation and the use of distributed high performance computing have allowed a significant qualitative leap forward in the validation of models, and even an epistemological turn for social sciences and humanities, as suggest the latest applications realized with the OpenMOLE platform described here.

1 Social sciences and experimentation

Experimentation played a significant role in the construction of natural sciences, since it consists in simulating material, physical, chemical or biological processes, through the use of apparatus imagined by researchers to select, often by isolating them, chains of facts that are simpler than the ones occurring in a complex reality. The confrontation of results of these experiments to observational data, partly or totally foreign to the data used to construct the experimental apparatus, is considered as bringing a proof of truth or of accuracy of the explicative reasoning at the basis of the model construction, more or less robust depending on the quality of the fit between model predictions and observations. We however know that the accuracy of a model predictions is not sufficient to fully validate the correspondance between the explicative mechanism imagined by the builders of the experimental apparatus and processes at work in the studied system, but this remains a crucial stage in the construction of models and theories enriched by observations.

In social sciences and humanities, the elaboration of experimental apparatus is highly problematic since it is confronted to numerous practical and ethical obstacles. Ethical and political critic questions the manipulation of individuals and the usurpation of their freedom. These concerns which are typical of the scientific ontology and deontology (being part of what is nowadays called integrity) have surely not avoided in practice manipulations, in a positive way or not, operated during historical times by actors with a political, cultural or economical power to make decisions which were more or less well informed "scientifically" (see at all historical periods writings by "counsellors of the prince" such as Bodin, Machiavel, Botero, etc. to give a few among the ones having dealt with the planning of territories) and to proceed to "experiments" of governance structures or of technological or cultural innovations which results could be evaluated in some case as beneficial and in others as catastrophic. The evaluation of the efficacy of decisions complicates because of the justifications brought by the actors themselves with their "self-fulfilling prophecies" (Rist, 1970). The often recalled difficulty of the evaluation of public policies is also increased by the uncertainty in the limits between the action and its context, both in space and in time.

Driving change in social systems, whatever the scale of interventions, remains a costly and risky operation, therefore difficultly acceptable by science for deontological concerns. Very few scientists therefore engage in "research-action" projects. A controversy has thus opposed in the sixties in France the advocates of an "applied geography" with a good knowledge of the "field" but sometimes with conservative trends, to the defenders of an "active geography" which would be more implied in the transformation of society. Sometimes, for example to contribute to the definition of policies for balancing metropolitan areas in France (operation by the *Délégation l'Aménagement du Territoire et l'Action Régionale* in 1964), geographers participating in the studies such as Michel Rochefort more particularly, did rely on scientific works, without having the courage to make it explicitly open (in this specific case central place theory by Walter Christaller). Contemporary geographers are less reluctant to exhibit a concern to help decision making in the most informed way possible given the state of their knowledge. They often then make the choice to use simulation models operated in silico by computers. Computer simulation thus became a substitute to experimentation. It is not a coincidence if among researchers in social sciences, geographers have very early found an interest in it: the diversity of multiple data sources (landscapes, populations, built environment, etc.) which they use to account of modifications of terrestrial interfaces by societies, the often large spatial extent of territories they study at the regional, national, or global scales, explain their need to make use of computing to organize this large quantities of information and to understand the dynamics they represent.

2 Geographical data and computational capabilities

The first simulation models in geography were firstly computed "by hand" in the fifties. It is not a coincidence if these models all deal with stylized facts which translate the regularities most frequently observed in the organisation of social space, and which are consequences of the "first law of geography" summarized as such already in 1970 by the American geographer Waldo Tobler: "everything interacts with everything, but two closer things have more chances to make contact than two more distant things". The power of attraction by proximity occurs in all social processes transforming the social space, which are constrained by an "obligation of space". This term was forged by Henri Reymond already in 1971 in a formalisation of issues in geography, who stated as first principle that societies have the tendency to transform the surface of the Earth which is heterogenous, rough and discontinuous, in an organized space exhibiting higher homogeneity and continuity, and making regularities emerge, due to the fact that two objects can not occupy the same place. Stating that individuals and societies have the highest probability to choose occupying the closest locations, both because these are better known and also because they yield economies on costs (physical, financial, and cultural) to travel the distance, may certainly be the strongest theoretical proposal of geography. It can be identified in any spatial configuration implying to distinguish a center and a periphery, which are observed at any level of the geographical space, from the local to the global.

The first simulation models in geography have thus dealt with processes for which the choice of the closest, among the place with which an interaction is expected, is a highly salient anthropological constant, either to observe the effects of an innovation before imitating it, according to the spatial theory of the diffusion of innovations by Hagerstrand (1957), or for the choice of destination places for a migration (Hagerstrand, 1957; Morrill, 1962, 1963). Models already in 1954 rely on the proposal by the American geographer Edward Ullman to construct a geography as the science of spatial interactions. This concerns more particularly trade relations, which have first lead to the empirical test of statistical models, as the so-called "gravity model", before being integrated into urban models which were first static (Lowry, 1964) and then dynamical (Clarke and Wilson, 1983; Wilson, 2014; Allen and Sanglier, 1981; Allen, 2012).

A later generation of models playing in a more complex way with effects of proximity has intensively used cellular automatons. Measures of spatial auto-correlation, which translate in a positive or negative way attraction or concurrency effects linked to proximity are in that context used to test the plausibility of simulated configurations for land-use changes, and in particular urban growth (White and Engelen, 1993; White et al., 2015), or moreover the spread of epidemics in the geographical space (Cliff et al., 2004).

But the development of these models has been very early impeded by the computational capabilities at this time, since the explicit representation of spatial interactions increases as the square of the number of geographical units considered. Therefore, the statistician Christophe Terrier had to segment his Mirabelle program (*Mthode Informatise de Recherche et d'Analyse des Bassins par l'Etude des Liaisons Logement-Emploi*) processing household survey data provided by INSEE in 1975 before being able to simulate the clustering into employment centers of resident populations as a function of work-residence commuting between all 36,000 French communes (Terrier, 1980). Our first simulation model of interactions between cities aimed at reproducing their demographic and economic trajectories influenced by urban functions on a period of 2000 years could only accept a maximum of 400 cities on a personal computer (Bura et al., 1996; Sanders et al., 1997). The increase of computational possibilities has been relatively slow, allowing to consider around one thousand cities in 2007 with the Eurosim model (Sanders et al., 2007) or the Simpop2 models applied by Anne Bretagnolle on Europe and United States (Bretagnolle and Pumain, 2010). Furthermore, the experimentation method with these models stayed at an experimental stage for long, requiring am increased attention in the modification "by hand" of parameter values, which are only very rarely directly observable, and which thus must be estimated through the plausibility of model dynamics. However, equations for urban dynamics models integrate non-linear relations which produce numerous bifurcations, forcing to laborious trial-and-error loops in the estimation procedure (Sanders et al., 2007). This consequent work limits the number of simulations from which the estimation obtained can be judged as satisfying, and more importantly once the model is therein calibrated, there remains a relatively high uncertainty regarding the quality of results obtained.

3 A new generation of simulations

The end of the nineties was to modify completely the working environment of researchers, the diffusion of internet and then mobile phones and finally of massive data produced by diverse numerical sensors having in return rapid and intense effects on the increase of computational power which had allowed these disruptive technological innovations. Simulation models can then integrate considerable quantities of interactions between localized entities chracterized by a large diversity of attributes. Still fifteen years ago, Gleyze (2005) was forced to conclude that network analysis in the case of the Parisian transportation network were "limited by computation". To give a single example of the quantitative leap forward in the increase of computational capabilities and their consequences on the higher confidence given to the models in consequence, we can mention the pioneering work in numerical epidemiology realized by Eubank et al. (2004) to simulate through the EpiSims and TRANSIMS models the daily trajectories on a transportation network of commuting of a million and a half individuals between around 180,000 places in the virtual city of Portland, in order to predict transmission pathways of an epidemics starting from interpersonal meeting probabilities in social networks organized as "small worlds". The epidemics can rapidly propagate to the whole city despite the number of contacts by individual remain low (fifteen in maximum (Eliot and Daudé, 2006)).

Simulation platforms are elaborated such that the largest number of researchers even not specialized in computer science can elaborate agent-based models. NetLogo (Tisue and Wilensky, 2004) is amongst the most famous. It is generic and allows to access multi-agent simulations without a deep knowledge in algorithmics, thanks to its simple programming language and the integrated builder of graphic user interface. Other platforms which are more specialized such as GAMA (Grignard et al., 2013) are immediately elaborated to propose a coupling with geographic information systems. However, the confidence in results obtained from simulation models goes along with an increase in the size and the number of experiments required, i.e. of the amplitude of numerical experiments. Despite the fact that these platforms integrate basic tools for a first step towards such a change in scale, a need for a dedicated "meta-platform" has naturally emerged.

3.1 A virtual laboratory: the OpenMOLE platform

Since 2008, the OpenMOLE software has been conceived to explore the dynamics of multi-agent models (Reuillon et al., 2010, 2013), and rapidly simulation models in general. It inherits from the development of a previous software SimExplorer (Amblard, 2003; Deffuant et al., 2003) which already provided to users an ergonomic interface for the conception of experience plans and gave access to distributed computing. OpenMOLE was generalizing SimpExplorer in the beginning in particular by enabling the parallelisation of large workflows. OpenMOLE (`https://openmole.org/`) is a collaborative modeling tool in constant evolution: "*a permanent effort for genericity has allowed to realize in a few years a pragmatic, generic, and proofed platform for the exploration of models of complex systems under the form of a dedicated language, both graphical and textual, exposing consistent blocks at the appropriated level of abstraction for the design of numerical experiments distributed on simulation models*" (Schmitt, 2014).

Procedures (or workflows) proposed in OpenMOLE are described in a manner independent from the models and are thus reproducible, reusable and exchangeable between modelers. A market place is integrated to the software, similarly to the model library included in NetLogo, and allows users to collect exploration scripts that can act as template or example, in highly diverse thematic fields and for all methods and languages implemented in OpenMOLE (for example for the thematic fields calibration of geographical models, analysis of biological networks, image processing for neurosciences).

It is useful to mention the use by OpenMOLE of a Domain Specific Language (DSL) (Van Deursen and Klint, 2002) to write exploration workflows. This practice consists in the construction of a notation and rules specific to the domain of a given problem. It is in a way a programmation language dedicated in that case to model exploration and associated methods. This language is naturally not created from scratch, but comes as an extension of the underlying language, i.e. the Scala language in the case of OpenMOLE. A reduced number of keywords and primitives fosters an easier use even for a user with no knowledge in programming, and furthermore the DSL remains highly flexible for the advanced user who can use Scala programming. According to Passerat-Palmbach et al. (2017), the DSL of OpenMOLE is one of the key elements of its genericity and accessibility.

We can also remark that one of the main assets of OpenMOLE is the transparent access to High Performance Computing environments (HPC). The increase in computational capabilities already described can in practice be implemented physically under different forms for the modeler: local server, local computation cluster, computation grid (network of multiple clusters, such as the European computing grid EGI), cloud computing services. Their use requires in most cases advanced computer science knowledge which are generally inaccessible to the standard modeler in geography. OpenMOLE integrates a library allowing to access most of these computing facilities, and their integration in the DSL is totally transparent for the user. The user script can then be tested on the local machine and then scaled on the HPC environments by modifying a single keyword in it.

The presentation of how to use the DSL and to elaborate scripts is out of the scope of this chapter, and we refer the reader to the online documentation of OpenMOLE for examples of scripts and model explorations. We simply recall the fundamental components of an exploration script: (i) the definition of prototypes, which correspond to parameters and outputs of the model, and which will take different values during the experiment; (ii) the definition of tasks, including model execution but that can also be for exemple pre- or post-processing tasks - the tasks covering a high variety of languages (scala, java, NetLogo, R, Scilab, native code such as python or C++); (iii) the description of methods to be applied (exploration by sampling, calibration, diversity search, etc.) which will act on the values of prototypes and will launch the considered evaluation task (mostly the model); (iv) a specification of the data gathered as an output of script execution (simulation data being often massive, a selection through this stage is crucial); and (v) the definition of the computation environment on which the method will be launched.

The platform aims at considerably extending practices of generative social science proposed by Epstein and Axtell (1996), which considers each multi-agent model as an artificial society, yielding macroscopic behaviors from assumptions made on microscopic behaviors. Numerical experiments that can be considered follow a change in scale, and the questions asked to the model evolve in a qualitative way. According to Schmitt (2014), who used the OpenMOLE platform to develop with Rey-Coyrehourcq (2015) the SimpopLocal model aimed at simulating the emergence of a system of cities, the virtual laboratory represented by this platform "*is not anymore only the simulation model and the hypothesis it simulated (i.e. the artificial society). It also contains the methods, tools and modeling procedures adapted to the conception and the exploration of the model and which practice creates as much knowledge and theoretical feedbacks than the conception of the model itself. This virtual laboratory is thus furthermore resembling a real research laboratory with an experimental desk (the model to conceive and explore), the assumptions of a researcher (the geographical processes translated into model mechanisms), methods (the iterative modeling method and aided by intensive computation), tools (the procedure for automatic exploration and any other experience plan integrated in OpenMOLE), all this gathered in a single room, the modeling platform SimProcess [an alternative name for the framework in which OpenMOLE in inserted] (Rey-Coyrehourcq, 2015)*".

In comparison to general protocols as the one introduced by Grimm et al. (2005) to describe all the stage of the modeling process, principles applied in OpenMOLE mostly innovate regarding the potentialities without precedent to explore the dynamical behavior of simulation models. Two main innovations rely in the systematic application of optimization meta-heuristics, mainly genetic algorithms, to rapidly test the largest possible number of combinations for model parameter values, and in the simultaneous distribution of simulations on multiple machines of a computation grid, what allows to considerably reduce the length of experiments without which it would become quickly prohibitive.

The choice of genetic algorithms as an optimization heuristic is justified by their efficiency in the context of multi-objective optimization problems. Moreover, the island distribution scheme (populations evolving independantly during a given duration) is particularly suited to a distribution on grid, each node making a subpopulation evolve, which is regularly fetched, merged into the global population, and from which a new subpopulation is generated and sent on the node. This type of algorithms furthermore extends relatively well to stochastic models, even if this aspect still implies a certain number of open problems (Rakshit et al., 2017). Following Rey-Coyrehourcq (2015), these methods are situated within the larger context of Evolutionary Computation, and the scala library MGO developed simultaneously to the platform and which allows to implement evolutionary algorithms in it, has been conceived to be easily extended to other heuristics in Evolutionary Computation, opening totally the possibilities for the inclusion of new methods in OpenMOLE.

Reuillon et al. (2013) describe the fundamental principles of the platform, whereas Pumain and Reuillon (2017) give a contextualisation of the different uses in the frame of simulation models for systems of cities. According to R. Reuillon cited by Raimbault (2017a), the philosophy of OpenMOLE is articulated around three axis: the model as a "black box" to be explored (i.e. methods which are independent from the model), the use of advanced exploration methods, and the transparent access to intensive computation environments. These different components are in a strong interdependence, and allow a paradigm shift in the use of simulation models: use of multi-modeling, i.e. variable structure of the model such as it was presented in chapter 4 (Cottineau et al., 2015), change in the nature of questions asked to the model (for example full determination of the feasible space (Chérel et al., 2015)), all this allowed by the use of intensive computation (Schmitt et al., 2015). The different methods available in that context will be illustrated below in concrete examples. The online documentation gives a broad overview of the available methods in the most recent version of the software and of their articulation within a standard context.

We consider a simulation model as an algorithm producing outputs from data and parameters as inputs. In that frame, we recall that in an ideal case, all the following stages should be necessary for a robust use of simulation models.

1. Identification of principal mechanisms and of crucial associated parameters, also with their variation range suggested by their thematic signification if they have some; identification of indicators to evaluate the performance or the behavior of the model.

2. Evaluation of stochastic variations: large number of repetitions for a reasonable number of parameters, assessment of the number of necessary repetitions to reach a certain level of statistical convergence.

3. Direct exploration for a first sensitivity analysis, if possible statistical evaluation of relations between parameters and output indicators.

4. Calibration, targeted algorithmic exploration through the use of specific algorithms (Calibration Profile (Reuillon et al., 2015), Pattern Space Exploration (Chérel et al., 2015)).

5. Feedbacks on the model, extension and new multi-modeling bricks, feedbacks on stylized facts and theory.

6. Extended sensitivity analysis, corresponding to experimental methods currently in construction and integration into the platform, such as for example the sensitivity to meta-parameters and to initial spatial conditions proposed by Raimbault et al. (2018).

In some cases, some stages to not necessary take place, for example the evaluation of stochasticity in the case of a deterministic model. Similarly, each step take more or less importance depending on the nature of the question asked: calibration will not be relevant in the case of fully synthetic models, whereas a systematic exploration of a large number of parameters will not be necessary in the case of a model aimed at being calibrated on data.

In order to better illustrate this general presentation of the platform and associated methods, we propose in the following of this section to precisely develop the example of the SimpopLocal model, which genesis has been tightly linked to the one of the platform, and which has been candidate for the development and the application of diverse methods.

3.2 The SimpopLocal experiment: simulation of an emergence in geography

The SimpopLocal model has been conceived to represent emergence of systems of cities such as it has been observed in five or six regions of the world around 3000 years after the emergence of agriculture practices in sedentary societies (Marcus and Sabloff, 2008). The purpose is to explain the emergence not only of "the" city but indeed of "systems of cities" since we know that cities already at this time were never isolated but already organized as networks in the territory of each of these antic "civilisations". The most recent publications by archeologists insist in a certain continuity of processes which led to the settlement of hunter-gatherer populations, gathered in hamlets and villages and then to the apparition of cities in some of these regions. The development of agriculture has been concomitant to a considerable increase of population densities and of the size of human groups in these countries (the density switch from 0.1 person per square kilometre to to, i.e. a factor of 100 between the two orders of magnitude), ans also a complexification of the political organization and of the social division of labor. This very slow process of accumulation of ressources and of concentration of populations is done through chains including numerous feedbacks with many fluctuations in growth, due to the frequent adversary events that are natural catastrophes and the predations of neighbor groups. Because of the slow rate of transformations and their frequent interruptions, archeologists now sometimes contest the name of "neolithic revolution" which was proposed in 1942 by Gordon Childe (Demoule et al., 2018, p. 159).

However, geographers still identify the apparition of cities as an emergence, or a "bifurcation" for two main reasons: first it did not systematically occur in all regions where agriculture was practiced, therefore two evolution regimes for settlements systems are possible and historically viable (agricultural only regions and with villages may have functioned for centuries and still exist nowadays in a residual way in some forests and on pacific islands for example), therefore the territorial regime including cities indeed constitutes a specific "attractor" in the dynamic of ancient settlements systems; secondly the evolutive trajectory which led to the birth of cities translates an important qualitative change (an emergence) with a significant increase of the diversity of social functions associated to habitats and also a considerable broadening in the scale of the life of relations: commercial exchanges which are done there at a more or less high distance allow thus the cities to be less dependent of a "site" of local resources as are agricultural villages, and to develop the assets of a geographical "situation" exploiting the wealth of a network of sites more and more distant (Reymond, 1971).

The SimpopLocal model aims at reproducing this remarkable aspect of the dynamic of settlement systems, which invariably produces an amplification of the hierarchical differentiation between habitats defined in the literature as a major stylized fact: already in any system at any place and at any time of history or prehistory, the size distribution of inhabited places (measured by population or spatial extent, or even the diversity of functional artefacts) is statistically highly dissymmetrical, including numerous very small agglomerations and only few very large agglomerations following a relatively regular distribution of the type of a Zipf law or log-normal law (Fletcher, 1986; Liu, 1996). This hierarchical schema is a structural property (magnitude of the size of entities) at the macroscopic level which is relatively persistent in time whatever the local fluctuations intervening at the level of entities. The SimpopLocal model is conceived to test the hypothesis introduced in the evolutive theory of urban systems (Pumain, 1997), which explains this structural characteristic by an urban growth process in average proportional to the size attained, and its amplification through the creation of multiple technological and social innovations inducing the growth and the diversification of wealth which diffuse among the places put in relation by any sort of exchanges.

The SimpopLocal model is first inspired by the statistical model which constitutes a first excellent approximation of the evolution of populations in a system of cities, by simulating urban growth as a simple stochastic process which makes the size of each city vary in a way proportional to its size and leads to a lognormal distribution of urban populations (Gibrat, 1931). The high quality of this elementary statistical model relies in the fact that it uses as "explanation" of growth the already acquired size, which expresses both the accumulated wealth and the attraction and resilience capabilities of the inhabited place (in some sense this corresponds to a model following the concept of "endogenous growth" proposed by economists). But SimpopLocal is conceived, as the preceding models of the "family" of multi-agent Simpop models (Bura et al., 1996; Sanders et al., 2007), to palliate to the incapacity of the Gibrat model to predict the trend of a growth larger than expected observed everywhere for largest cities located in central places of networks (Moriconi-Ebrard, 1993) and the exaggeration of the inequality between city sizes (Pumain, 1997; Bretagnolle and Pumain, 2010). These deviations to the Gibrat model are linked to long-range correlations (Rozenfeld et al., 2008) induced by spatial interactions. The influence of these amplifies the hierarchical differentiation between sizes of cities participating to exchanges in an urban system (Favaro and Pumain, 2011). The Simpop models include this effect by introducing, in an exogenous way to the model and at different times in the simulation, new urban functions which select some cities or are integrated by these in a continuous adaptation process to these innovations. In comparison to other Simpop models, SimpopLocal introduces two novel elements: it uses an abstract representation of successive innovation waves and gathers all in a single object "innovation". A second originality consists in making the innovation creation process endogenous by linking it to the size of the inhabited place, which is assumed to amplify in a non-linear way the emergence of new technical, social or cultural forms (with a creation probability varying as the square of populations being present or in relation). This more parsimonious of the model construction allow to significantly redue the number of parameters and authorizes thus more systematic exploration and evaluation.

3.3 Implementation of SimpopLocal, from NetLogo to OpenMOLE

SimpopLocal has been initially developed under the NetLogo language, and then redeveloped with the Scala programming language. The simulation with NetLogo has the advantage of the ergonomy of the interface which allows to numerically and graphically follow the modifications impacted on macroscopic variables describing the state of the system, but rapidly showed its limits in terms of possible experiments. The manual method of trial-and-error to set parameter values was difficultly capable of avoiding "cascades" of urban growth leading to city size increments too much larger for the historical period that it tried to simulate. The reprogramming in Scale and the integration into the OpenMOLE platform were to allow a more refined and complete exploration of model behaviors.

The model represents the evolution of settlement units dispersed in a zone large enough to count a few thousand of inhabitants but limited enough in surface to ensure the possible connection between the inhabited places with the transportation means available at this time (this could be for example ancient Mesopotamy or antic meso-America). The simulation space is composed of around hundred inhabited places. Each place is considered as a fixed agent and is described by three attributes: the location of its permanent habitat (x, y), the size of its population P and the resources available in its local environment. The quantity of available resources R is quantified in population units and can be understood as the carrying capacity of the local environment to sustain a population, which varies as a function of competencies to exploit resources that the local population acquired, thanks to the innovations it created or received from other inhabited places. However, the exploitation of resources is done locally and the share or the exchange of goods or of people are not explicitly included in the model. Each novel innovation created or acquired by an inhabited place develops its competencies in exploitation. The entity innovation corresponds here as a significant abstract invention socially accepted, which can be a technical innovation, a discovery, a social organisation, new habits or practices, ... Each acquisition of an innovation by an inhabited place brings the possibility to overpass its carrying capacities, and therein yields a demographic growth.

The model was conceived to be the most parcimonious possible by minimizing the number of attributes of agents (which are inhabited places) and the parameters controlling their evolution. The average orders of magnitude given by the work of archeologists were directly used to fix at around 4000 years the duration of the transition period between an agricultural settlement system and an urban settlement system, to estimate an annual average variation rate of population at around 0.02% per year, and to consider that the size of the largest inhabited place in the system would change from around hundred to around 10,000 inhabitants. On the contrary, the values of the five other parameters could not be estimated from the literature and had to be deduced from simulation experiments. These parameters are the probability to create an innovation through an interaction between two persons in the same place, of the diffusion probability of an innovation through an interaction between two persons from two different places, of the intensity of the dissuasive effect of distance on these interactions between places, of the impact of an innovation on population growth (which is a consequence of an increase of available resources) and of the maximal possible dimension of an inhabited place (measured in terms of population or available resources) which intervenes in the logistic growth equation retained as a generic model of an evolution still very strongly constrained by local resources. Equations summarizing the model and tables defining precisely parameters and their action are detailed in Schmitt (2014) and Pumain and Reuillon (2017).

We define an initial value of population and resources of inhabited places, and the interaction network between them is created. Then at each stage of the simulation, mechanisms for population growth and innovation diffusion are applied. The impact of innovations on the efficacy of resource extraction is computed. This loop is iterated until the stopping criteria is reached: in this case after 4000 steps or when an arbitrary maximal number of innovations is reached. We observe the evolution of the settlement system state defined at the macro-geographic level through the distribution of the size of inhabited places, summarized by the slope of the rank-size distribution. The model uses some parameters which are probabilities and is stochastic, therefore a same set of parameter values can yield quite different results. An automatized method to make the value of parameters vary and interpret the results obtained has been progressively elaborated through a collaboration between computer scientists and geographers.

3.4 Calibration and validation

The automation of the exploration of dynamics produced by simulation models with the OpenMOLE platform uses genetic algorithms which realize in a systematic way the variations of parameter values which were before done "by hand" by the researcher. The distribution of computation tasks on a grid infrastructure (a network of computers) furthermore allows to operate this very high number of combinatorial operations while significantly reducing the computing time, through the parallel processing of information. But putting this new form of model experiments into practice also assumes an intervention of the thematic researcher, which has to select the precise objectives that the model has to satisfy, whereas a supplementary refinement of the exploration method can lead to an increase in trust given to the scientific assumptions of the model.

Calibration as optimization through genetic algorithms

Calibration is a procedure aiming at minimizing the discrepancy (called fitness) between the behavior simulated by the model and the behavior observed empirically, by making the unknown model parameter values vary in an incremental way. Stonedahl (2011) has recalled the difficulties of this exploration which rapidly becomes fastidious when it is done by hand, because of the multiple bifurcations occurring in models in which most of mechanisms linking variables are non-linear. An exhaustive exploration of the parameter space can not be conceived since it would require a too large computation time, which follows an exponential growth in the number of these parameters.

As these procedures also produce large quantities of results, they furthermore impose to use dedicated methods to process and visualize informations produced by simulations. A whole suite of softwares must thus be elaborated to enable the researcher to discover the main schemes for dynamics associated to the variations of model parameters.

This is where suited algorithms can be used, by understanding the calibration issue as an optimization problem. Genetic algorithms have been used to calibrate multi-agent systems in several domains as therapeutic evaluation (Castiglione et al., 2007), ecology (Duboz et al., 2010), economics (Espinosa, 2012; Stonedahl and Wilensky, 2010), or hydrology (Solomatine et al., 1999). Despite of the the frequent use of multi-agent systems in social sciences, this method has not been applied very often (Heppenstall et al., 2007; Stonedahl and Wilensky, 2010). This type of numerical experiment indeed requires that quantitative objective are defined in order to evaluate if simulation results are compatible to results expected from expert knowledge, and the enormous computation load must also be managed while optimizing a fitness function candidate to very large stochastic fluctuations (Di Pietro et al., 2004).

In the case of SimpopLocal, which has five unknown parameter values (even their order of magnitude can not be estimated from empirical data), three "objective functions" had to be defined. These characterize a simulation result at the macro-geographical level and correspond to stylized facts which order of magnitude were established from archeological and historical knowledge: the final distribution of city sizes must be log-normal (not far to a Zipf's law), the maximal size of the largest city must be around 10,000 inhabitants, for a simulation duration corresponding to 4000 years.

This requirement of defining objective functions could be considered as a strong constraint on the epistemological validity of the model, it seems indeed to contradict the assumption of an open evolution for systems of cities. Indeed, this intermediate computation step corresponds to a condensate of knowledges, a minimal requirement on the representativity and the plausibility of model behavior in comparison to all dynamics of systems of cities that could be considered (at the historical period of the emergence of cities). The result in terms of evaluation of simulations should allow to advance in the knowledge of inter-urban interaction processes susceptible to produce this general dynamic at the macroscopic scale of the system, such a theoretical reconstitution corresponding then to what some physicists describe as an "inverse problem".

A rather broad numerical domain is established a priori for each of the five parameters. Each parameter set combining a value for each parameter is evaluated depending on the simulation outcome it produces. This evaluation measures the proximity between simulation outputs and objective functions defined for the model and provides thus a measure of the ability of a given of parameters values set to reproduce the stylized facts of which the simulation must be the closest. The parameter values receiving the best evaluations are then used as a basis to produce new parameter sets which are then tested.

Exploration of the parameter space under objective constraints

The SimpopLocal model being stochastic, simulation results vary from one simulation to the other for the same parameter values. In consequence, the evaluation of parameter values according to the three objectives must take into account this variability. We verified that around hundred simulations for each parameter set was enough to capture this variability without increasing too much computation time.

To each objective function corresponds a measure of the evaluation to the quality of the simulated result. The ability of the model to produce a log-normal distribution is measured by the distance between the simulated distribution and a theoretical log-normal distribution with the same average and standard deviation following a Kolmogorov-Smirnov test. The maximal population objective quantifies the ability of the model to produce more or less large cities, the result of a simulation being tested by computing the distance between the size of the largest city and the expected value of 10,000 inhabitants: $|(\text{population of the largest agglomeration} - 10,000)/10,000|$. The objective of the duration of the simulation duration quantifies the ability of the model to generate an expected configuration in an historically plausible time window. The distance between the number of iterations of the simulation and the expected value of 4000 steps for the simulation is computed: $|(simulationduration - 4000)/4000|$. These three computations of errors are normalized in order to enable the comparison the degree of satisfaction of a simulation regarding each of the three objectives. But the aggregation of the three computations which would produce a single global quality measure is not possible , a multi-objective algorithm is necessary to determine which simulations are the most satisfying to approach the expected final configuration. This type of algorithm computes compromise solutions such that no solution dominates all the others for all objectives. These solutions are called Pareto compromises and are together part of what is called a Pareto front.

The use of global exploration methods such as the one of genetic algorithms to calibrate a multi-agent model (and in particular a stochastic multi-agent model) implies a very high computation cost (Sharma and Singh, 2006). Such a computation charge is too voluminous to be executed on local computers, and supercomputers have a high cost and are not easily available for most of research laboratories. Computer grids provide a solution to these issues of intensive computation. However, distributing computation at such a large scale requires to orchestrate the execution of ten of thousands of model instances on computers distributed in the entire world. The cumulated probability of local failures and the issue of sharing to workload in an optimal way on the grid make its use very difficult for a non-specialized researcher as described above. It is in particular to overcome these difficulties that the OpenMOLE platform has been conceived (Reuillon et al., 2010, 2013). This exemple of the calibration of the SimpopLocal model shows well to what extent OpenMOLE helps modelers to overcome the technical and methodological gap which separates them from high performance computing.

The infrastructure of the European Computation Grid allowed to use a computing power such that half a billion simulations of the model have been executed for the calibration of SimpopLocal, without which it would have required around 20 years of computation with a single computer.

The Calibration Profile, a significant leap forward for social sciences

The result of the calibration process ensures only that the model is able to reproduce stylized characteristics of the emergence of a system of cities, with a relatively precise evaluation of parameter values which altogether contribute to produce this evolution. But it does not tell anything on the frequency to which parameter sets produce plausible behaviors, and to what extent each parameter contributes to modify the model behavior. It would be interesting for example to know at which point some parameter values avoid the system to reach a plausible behavior, and to not be restricted to know only a single "optimal" parameter values set.

A new method has been elaborated to represent the sensitivity of the model to the variations of a single parameter, independently of the variations of all other parameters (Reuillon et al., 2015). Using an objective function computing a single numerical value describing the quality of the calibration for the model, the profile algorithm computes the calibration error the lowest possible when the value of a given parameter remains fixed and all others are free. The algorithm computes this minimal error for the full variation domain of the parameter studied. For each value of a parameter, the algorithm aims at identifying parameter values for other parameters which produce the best fit of the model to the expected data (the smallest error possible). A plot gives then the variations of this optimal fit value as a function of the variations of the parameter studied. The calibration profile shows then different possible forms for this curve. When it exhibits a clear inflexion in the lowest values for the calibration error, for a relatively small domain of variation for the parameter studied, it is possible to conclude that the order of magnitude of the parameter was truly identified which satisfies to the expectations in terms of model behavior. If one of these curves remains flat, it indicates that the parameter has no effect on the local behavior of the model and thus can be removed from it. Therefore, in the case of SimpopLocal, a parameter thought as the duration of life of an innovation was finally excluded since variations remained without effect on the quality of fit of the model, all things being equal regarding the variations of the other parameters (Schmitt, 2014). This provides thus the possibility to evaluate to what extent the mechanisms invented to construct the model are not only sufficient, but also necessary to produce the expected behavior. Naturally within the limits of the theoretical framework and of the selection of stylized facts which were kept, it is the first time that researchers in social science can reach such an essential scientific conclusion, thanks to a validation method finally efficient for multi-agent simulation models. This is an enormous progress from the epistemological point of view for social sciences - surely still within the theoretical framework given by the objects, attributes and mechanisms selected by researchers as representatives of the system observed.

A complementary form of model validation could then be imagined if historians and archeologists would try to recalibrate it from their observations. Indeed, the estimated parameter set contains values which indeed provide the expected dynamic for a settlement system but which are not absolutely fixed, they are relative one to the other on the one hand and to the synthetic data introduced on the other hand. If these are modified to be compatible with an historically observed settlement system, the ability of the model to simulate its development would then be confirmed, not only by reconstructing the trajectories of the evolution of population of the considered inhabited places, but also by keeping the relative orders of magnitude of parameters which yield this dynamic.

4 Examples for applications of OpenMOLE: network-territories interaction models

We propose in this section to illustrate the application of the exploration methods included in OpenMOLE and intensive computation to an other thematic question, the issue of interactions between networks and territories. This question has fed numerous scientific debates fir which most of problems remain relatively open. For example, the issue of "structuring effects of transportation infrastructures" (Bonnafous and Plassard, 1974), described by

Offner (1993) as a "scientific myth" invoked to justify the cost of an infrastructure through its spillovers on regional development, and which are not always observed on middle terms, can according to A. Bretagnolle in (Offner et al., 2014) be observed for broader territories and on long times, while taking into account local fluctuations in dynamics of systems of cities. The empirical difficulty to extract general stylized facts together with the conceptual difficulty of geographical entities in relations of circular causality, are avoided through the approach of modeling co-evolution between transportation networks and territories proposed by Raimbault (2018c). The results obtained are closely linked to the use of OpenMOLE and its exploration and calibration algorithms, of which we will give a few illustrations.

The application of multi-objective calibration appears to be essential for the application of models for systems of cities to real situations. For example, Raimbault (2018a) introduce a model for the evolution of a system of cities on long times which is close to the model by (Favaro and Pumain, 2011) but focuses on the effect of the physical transportation network. Growth rates of cities are determined by the superposition of several effects: (i) endogenous growth captured with a fixed growth rate corresponding to the Gibrat model; (ii) interactions between cities through a gravity model; (iii) feedback of flows circulating in the network on traversed cities. This model is calibrated in a non-stationary way in time (i.e. on temporal moving windows in order to take into account the change in nature of urban dynamics such as observed by Bretagnolle and Franc (2018) with for example the mutations of transportation networks) on the French system of cities between 1830 and 2000. To calibrate the model, simulated populations are compared to observed populations. At this stage the use of a multi-objective calibration algorithm (the NSGA2 algorithm implemented in OpenMOLE) is crucial. Indeed, the fit can be for example computed as a mean square error in time and for all cities. However, given the disparities in city sizes due to urban hierarchy, it rapidly occurs that a mono-objective calibration on this error will focus on adjusting the size of largest cities, at the expense of most cities in the system. The addition of a second objective taken for example as a mean square error on logarithms of populations, allowing to take these into account. An important result of (Raimbault, 2018a) is then the emergence of Pareto fronts for these two objectives for all time windows considered. This shows that this type of model must be applied by making a compromise between the adjustment of population for medium-sized cities and populations for largest cities. This result is obtained thanks to the multi-objective optimization with a genetic algorithm in OpenMOLE.

An other application example for methods included in the platform which illustrate its crucial role is given by the search for co-evolution regimes. Following Raimbault (2017b), the study of lagged correlation patterns in time allows to identify typical interaction regimes between variables describing the network and variables describing the territory. More precisely, Raimbault (2018c) defines co-evolution as the existence of circular causal relationships at the level of a population of entities in a given spatial extent. In the case of networks and territories, network properties must be locally caused by the properties of territories and reciprocally. Mono-directional causalities of networks to territories correspond then to "structuring effects" mentioned above. This definition allows to capture the "congruence" Offner (1993) between these objects, in some sense their reciprocal adaptation in a dynamical way. It also yields the construction of an operational method proposed by Raimbault (2017b) which statistically investigates causality links between corresponding variables. In practice, the weak Granger causality notion is used, providing a flexibility regarding the data required and the temporal and spatial frame of estimation. This causality is in our case quantified by lagged correlations between variations of network variables (such as centralities or accessibilities) and variations of territory variables (such as population, employments, real estate transactions, etc.), and the existence of significant extrema at non zero lags gives a sense of causality. A typology of these lagged correlation profiles provides what we call "causality regimes", among which co-evolution regimes in which two variables for territory and network are in reciprocal causality.

The question is then is a given case study to identify the regimes in presence from observed data or from data simulated by a model, and particularly the regimes corresponding to a co-evolution. The demonstration of the existence of such regimes as output of a "co-evolution model" is a priori not expected, since processes included at the microscopic scale for which the influences are indeed reciprocal do not imply a reciprocal causality at the macroscopic scale of indicators, as the models considered are complex and exhibit emergence. This method is applied to a macroscopic model of co-evolution by Raimbault (2018b), which extends the model of (Raimbault, 2018a) by adding rules for the evolution of network capacities. A direct sampling which consists in a random sampling of a fixed number of parameter points (for example through Latin Hypercube Sampling maximizing the discrepancy of points), is a first experiment allowed by OpenMOLE to have an overview of the capacity of the model to produce co-evolution. This experiment provides a certain number of regimes which can potentially be produced by the model, namely 33 regimes among 729 possible regimes for the variable considered, i.e. 4,5% (in this case we consider as territory variable the populations, and as network variables the closeness centrality and the accessibility, what corresponds to six directed couples of variables, and thus $3^6 = 729$ possible configurations since each couple can exhibit a positive, negative or inexistent lagged correlation). We find among these 19 co-evolution regimes, which existence could not be intuitively predicted. The existence and the variety of these regimes is an important result, showing that it is possible to model a co-evolution, in the precise statistical sense given above.

The application of the Pattern Space Exploration algorithm (Chérel et al., 2015) with objective the diversity of produced regimes allows then to considerably extend this conclusion, since it produces 260 regimes (35,7%). This is a typical example where the strong non-linearity of outputs considered can lead to partial or even biased conclusions and where the use of a specific method is crucial. The results are then made more robust and extended thanks to the application of a specific method integrated to the OpenMOLE platform.

This method furthermore allows to compare between them models with a certain confidence in the exhaustivity of solutions obtained. Raimbault (2018d) applies the same approach to the SimpopNet model introduced by Schmitt (2014) which is also a co-evolution model at the macroscopic scale exhibiting a large number of common points with the previous model in particular in the variables considered and thus in the output indicators that can be computed. A smaller number of regimes of interaction and of co-evolution is then obtained, confirming on the one hand that it is not straightforward for a model conceived for co-evolution to effectively produce co-evolution regimes, and on the other hand suggesting that stronger constraints in the evolution rules for the network induce a bigger difficulty to produce a diversity of regimes.

5 Perspectives

The elaboration of the OpenMOLE platform has created a research axis, even a research domain, with a specific positioning which one of the remarkable aspects is a high level of interdisciplinarity between social sciences and more technical disciplines such as computer science. According to Banos (2017) this leads to the production of a broader and deeper knowledge (in a way similar to the virtuous spiral between disciplinarity and interdisciplinarity described by Banos (2013)). But also through the philosophy of unique platform (described above, through the strong interaction between the three axis of model embedding, access to innovative model exploration methods, and transparent access to intensive computation environments), the perspectives opened are numerous, as much on the technical side than on the theoretical, methodological or thematic side. We give below a few examples, accounting of a current state of possible futures for OpenMOLE.

5.1 Methods

The extension of available methods is a privileged axis of research linked to the development of OpenMOLE. For example, the exhaustive resolution of inverse problems (Aster et al., 2018) is currently not included. Solving an inverse problem consists in determining all the antecedents of a given objective in the output space of the model. Calibration algorithms solve similar problems but do not ensure the exhaustivity of the solutions produced, what can become a considerable issue in the case of equifinality (Rey-Coyrehourcq, 2015), i.e. of parameter configurations or initial conditions leading through different trajectories to an identical result. An heuristic for inverse problems inspired by the PSE mechanisms is currently being elaborated for an integration into OpenMOLE.

The use of Bayesian inference methods is also a direction developed. Indeed, in the case of strongly stochastic models, and in which the joint distributions have a non standard form, an estimation of the probability distribution of parameters can be provided by this type of method. In the case of simulation models, the method of Approximate Bayesian Computation (Csilléry et al., 2010) allows for a given observed dataset to get the probability distribution of parameters having the most likely produced it. This is therefore an extended calibration with a probabilistic knowledge produced allowing to take into account uncertainty. A specification of this method proposed by Lenormand et al. (2013) with the purpose to reduce the number of simulations in the case of models with a significant computation time, is also being adapted to parallel computation and integrated into the platform.

We can finally mention diverse methodological directions which are also being investigated: (i) the question of high dimensionality is rapidly an issue in the use of the PSE algorithm, since the number of output configurations is potentially victim of the dimensionality curse, i.e. that the time or the size of execution are an exponential function of the number of dimensions (a grid exploration is the simplest example to get a grasp on this phenomenon) - new methods combining dimensionality reduction and diversity search would allow to solve this problem and take into account a much higher richness of outputs; (ii) the question of the sensitivity to initial spatial conditions which was already mentioned (Raimbault et al., 2018) is particularly relevant for geographical models, and a scala library including synthetic generators for population configurations at different scales is currently being implemented, including for example the generators for districts studied by Raimbault and Perret (2019); (iii) the implementation of information criteria for the performance of models, already described in chapter 4, is also being studied, such as the POMIC criteria proposed by Piou et al. (2009).

5.2 Tools

All along its development, OpenMOLE has always been innovative in terms of tools used and developed. The choice of the Scala language to replace Java already in the first versions is an innovative technological choice which is particularly relevant through the functional programming but also object programming possibilities while still keeping the underlying Java infrastructure allowing a high portability without complications depending on the operating system or on the hardware, what is crucial for the distribution of computations of computations on heterogenous nodes of the computation grid. For example, properties such as trait mixing make scala particularly suited to multi-modeling (Odersky and Zenger, 2005). The possibilities offered by object programming are conserved in Scala and can be combined to the abstraction of functional programming, making it a language more powerful in this sense of flexibility than other functional languages such as Haskell (Oliveira and Gibbons, 2010). Furthermore, properties such as implicit conversions or case classes make Scala highly ergonomic for the design of DSL (Sloane, 2008), which as we already described is an essential feature of OpenMOLE.

The issue of program embedding, and by extension of model embedding, remain an active research field in particular in relation with reproducibility. The docker software which uses containers allows to wrap an execution environment in an identical manner whatever the operating system and the hardware. Hung et al. (2016) propose to couple docker with a graphical user interface for scientific reproducibility. Similar softwares such as Singularity are specifically dedicated to the reproducibility of HPC experiments (Kurtzer et al., 2017). The core of the embedding strategy taken by OpenMOLE does not rely on such a software, for example because of performance reasons, but some tasks relying on the execution of binaries or of programs with a complicated environment are embedded in OpenMOLE through a task using docker (for example for the R language task which requires the installation of a full R environment). An improvement of the integration of docker into OpenMOLE is an active research direction which is crucial for the future extension of the genericity of embeddable programs. OpenMOLE is therefore at the edge in technical research regarding scientific reproducibility. In a similar way, the question of scalability of experiments is at the core of the philosophy of the platform, and research are done for example to automatize the deployment of multiple OpenMOLE instances on a cluster and facilitate the use within communities of thematic researchers.

Conclusion

The exploration of simulation models has been progressively established in geography through the intermediary of initiatives such as the development of the OpenMOLE platform. It has been achieved in a highly interdisciplinary and reciprocal framework (win-win relations between computer scientists and geographers), but also through a novel integration of knowledge domains (Raimbault, 2017a), i.e. of empirical, theoretical and modeling knowledges, but also tools and methods which are within each of these domains in strong interaction. The OpenMOLE enterprise and its branch linked to geography in the context of the Geodivercity ERC project witnesses of a novel way to produce geographical knowledge, in a robust evidence-based manner, and suggesting the possibility of scientific proofs in social sciences. Such an emancipation remains to be propagated and the approach to be valorized to realize its potential of future direction of Quantitative and Theoretical Geography, in complementarity with new emerging disciplines of City Science and Urban Analytics described by Batty (2019), but the proof-of-concept is largely validated and provides significant evidence to social sciences to resist the colonizer hegemony of hard sciences such as physics pretending to a monopoly on evidence-based approaches to social systems (Dupuy and Benguigui, 2015).

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