MULTI-AGENT SIMULATORS: FLEXIBLE TOOLS TO REPRODUCE COLLECTIVE BEHAVIORS

I. the use of force-fields

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Abstract: This is the first part of a report on the use of a multi-agent simulator able to show the influence of various types of environmental factors, in the form of force fields, on the collective behavior of a numerous population of agents. The applications include a toy-model of the Big Bang theory, the structural changes induced on a cell population and a longitudinal study of medical students' training. As for qualitative simulations of complex, collective behaviors, the multi-agent approach appears fully justified by its flexible and straightforward implementation. However, a great enhancement of its heuristic power is foreseeable, due to the relatively easy account even of sophisticated environmental effects and cooperative interactions.

1 INTRODUCTION

It is nowadays generally accepted that the emergence of complexity (Holland, 1996; Laughlin, 2005) is the rule and not an exception in most natural phenomena. From the viewpoint of classical, deterministic mathematical models, the unpredictable behavior of complex systems provides severe limitations to their quantitative assessment. However, an alternative and ”systemic” perspective relying upon statistical (Rodgers and Nicewander, 1988) and simulation studies (Accornero and Capozza, 2009) of their dynamic features, opens new avenues in the field. At the macroscopic observation level, complexity can be linked to the collective behaviour of lower-level elements obeying a relatively simple set of rules (Ferber, 1999; DeToni and Bernardi, 2009). Thus, any intuitive and affordable approach to the simulation of a population-dynamics dependent on the interactions among the constitutive elements as well as on the influence of environmental factors, is most welcome.

Figure 1 (left) shows in the evolving landscape of modern informatics the relatively recent appearing of strategies and computational approach more and more appropriate to reproduce complex functions and collective behaviors. Among the several software tools available in this frame the multi-agent-based simulators (MAS) are endowed with a relatively smooth learning curve and a considerable flexibility (Colosimo, 2008; Dzitac and Barbat, 2009). In particular, the Netlogo system (Wilenski, 1999) has the advantage of being: multienvironment, frequently enriched and updated by an active users-community and, last but not least, free-software.

The general philosophy inspiring multi-agent simulators is reminiscent of cellular-automata (Wolfram, 2002), namely collections of ”colored” cells on a grid of specified shape whose color evolves through a number of discrete time steps depending on the color of the neighboring cells. That basic idea is generalized including the possible influence of each cell in the grid on the behaviour of the agents located in that cell. A natural way to account for the influence of environmental factors upon the agents’ dynamic behaviour, is to represent such factors in the form of space-dependent force fields[1], and make the agents responsive to them. Some obvious applications include temperature/pressure gradients, chemical diffusion, electromagnetic/gravitational interactions, etc. discussed at length in the rich library of Netlogo examples.

In this paper three examples of using a multi-agent simulator in quite different contexts will be presented, spanning from a toy-model of cosmological flavor to more serious attempts to reproduce a cellular conformational change and a students performance. The relatively easy adaptation to such contexts of the same basic routine, which describes the influence of the force-fields on the agents dynamics, is obtained by means of a standard technique in the Netlogo environment, that is associating the force-fields to the properties of the spatial grid where the agents move (Figure 1, Right).

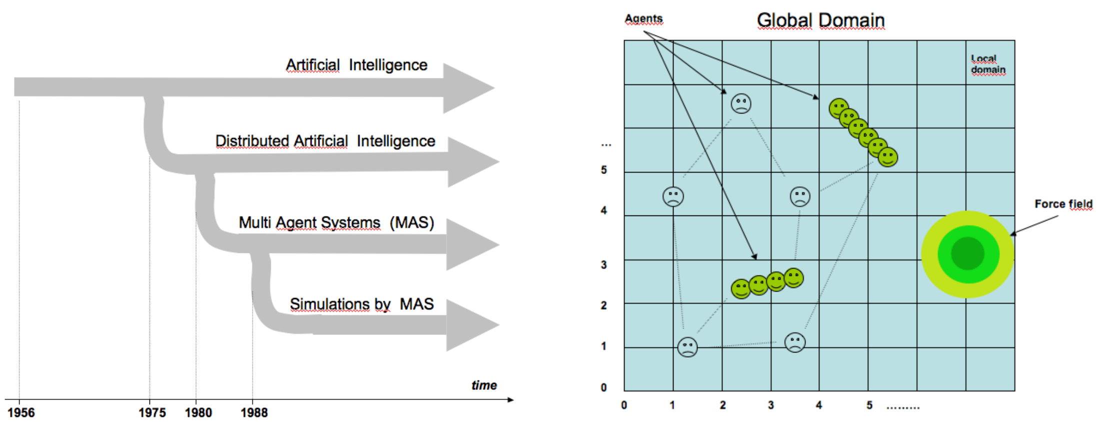

Figure 1: *Left:* Development of multi-agent simulators (MAS) from other similar disciplines (Modified from De Toni and Bernardi, 2009) *Right:* The space (global domain) in which agents move is a grid of variable size where each single location (local domain) can be endowed with specific features, like attractive/repulsive ability caused by force-fields of defined intensity and shape.

[1] of course, time-dependence can be introduced too, with a little more effort

2 METHODS

The simulators used in this work were implemented in the Netlogo programming environment (Wilenski, 1999). A nice feature of this interpreter is that it allows, at expense of a minimum programming effort and computational delay, to arrange the algorithms so that the values of many working parameters can be changed on the fly, during a running simulation. This is extremely useful in the cumbersome optimization of the parameter values if a data fitting is in order, which in most cases cannot be done by autonomous, iterative procedures. The unifying element for the three examples which will be discussed below, is the presence of force-fields affecting the dynamic behavior of the agents. In the present version of our simulators the fields are time-invariant and the spatial dependence of their intensity is of the form:

$$FF_d = FF_o e^{-d} \tag{1}$$

where *FFd* is the force-field strength at distance *d* from the source *FFo*.

The numerical resolution of such space dependence is directly proportional to the granularity of the agents' world, namely the grid where they move (Figure 1, Right). We typically used a 400 * 400 square grid, and agent populations of up to several thousands elements. Such values represent a reasonable compromise between computational burden and statistical reliability of the simulation results. Under these conditions, a single run of the simulator in the case of students performance took approximately 4 minutes on an Apple MacIntosh personal computer (2.53 GHz).

In order to show the effects of force-fields on a bunch of random moving agents, we present in figure 2 an easy to grasp example: a crude representation of at least part of the message conveyed by the Big-Bang theory of the origin of the universe (Weinberg, 1986). The most impressive feature of such theory is not difficult to realize by means of a MA simulator, provided that: i) the agents are initially concentrated in the same location (Figure 2, panel A), and ii) the explosion which is supposed to give birth to the universe is visualized as a random, isotropic and progressive distribution of agents in all the available space (panel B, and C). In this frame, some spectacular events like stars birth or black holes may be reproduced, as shown in Panels E and D, respectively. In both cases

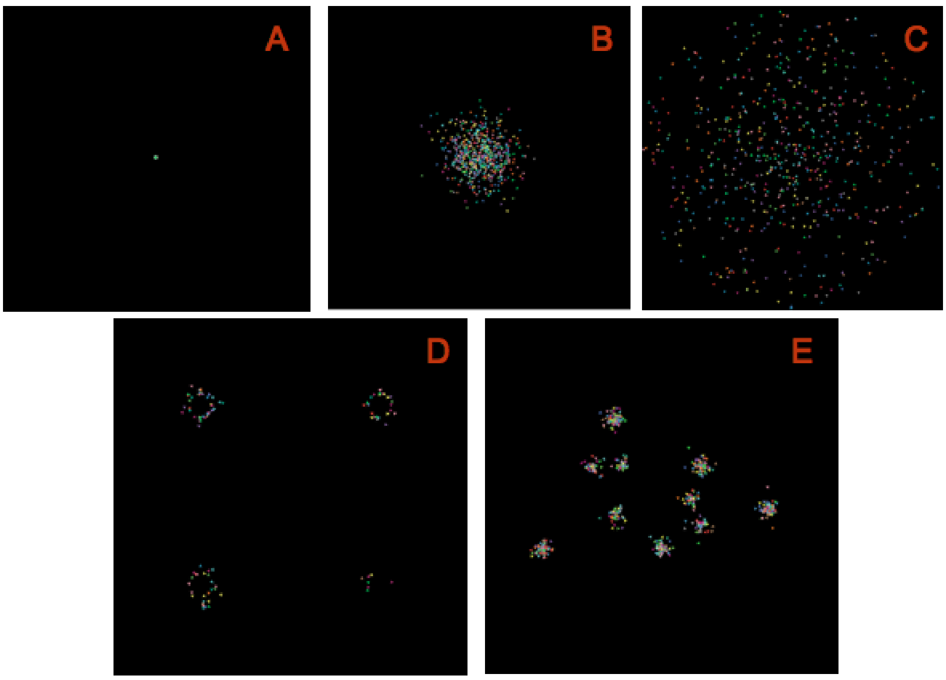

Figure 2: Random spreading of the agents from a single initial location (panel A) leads to an isotropic, progressive distribution of matter in all the available space (panels B, C) . The moving agents can be attracted by the 'black holes' simmetrically located in the four quadrants, which make their luminescence disappear (panel D), or condense in a number of randomly chosen locations, thus producing 'stars' (panel E).

the visual effect is a consequence of the action exerted by attractive fields on moving agents, which disappear when in the attraction range of ”black holes”.

It is worth remembering that, for the sake of simplicity, the spatial dependence of the attractive force-field has been defined in terms of an exponential decay (see eq. 1) and not as an inverse function of the square distance. Even the intensity dependence of the fields on the mass of the aggregating agents has not been taken into account. Although of serious prejudice for the physical reliability of the Big Bang toy-model, the issue is not relevant for the two applications discussed in what follows.

3 RESULTS

3.1 Structural changes in cells.

Since the pioneering work of M. Perutz on hemoglobin (Perutz, 1970), the structural rearrangements caused by a number of physico-chemical factors in biological macromolecules are the basis of any mechanistic model of their functional regulation (Wyman and Gill, 1990). According to a crude but quite useful approximation, the rate of switching from one conformation (C_1) to another (C_2), namely $C_1 \longrightarrow C_2$, can be associated to that of a simple first order process ruled by a kinetic constant k_1, namely $v_1 = k_1 * [C_1]$, where the square brackets indicate molar concentration. If the switch is reversible, the same reasoning applies to the reverse process, $C_1 \longleftarrow C_2$, leading to an equilibrium condition when $v_1 = k_1 * [C_1] = v_2 = k_2 * [C_2]$. Thus, under equilibrium conditions the relative proportion of C_1 to C_2 is given by k_2 / k_1.

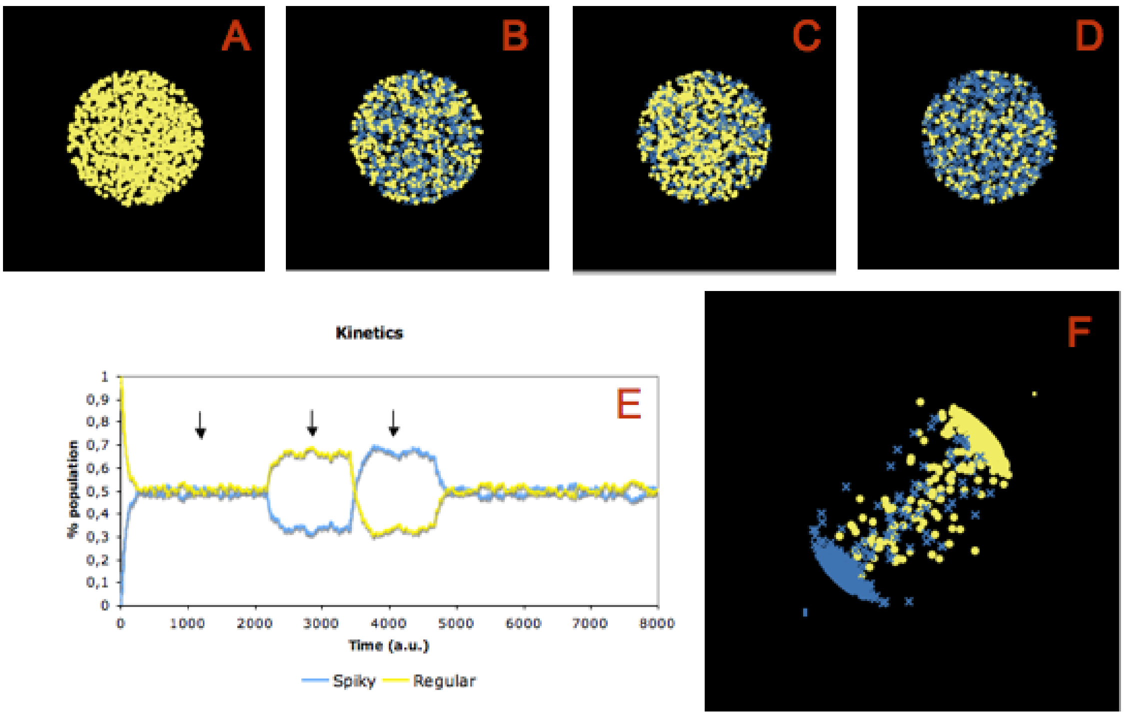

Figure 3: *Dynamics of conformational changes.* A 100% ’regular, yellow’ population of agents (pretty similar to a cell population in a Petri dish, panel A) at t_0 undergoes a reversible transition to a ’spiky, blue’ state . The yellow/blue ratio at equilibrium, as defined by the rates of the direct and inverse change, is about 1, 2 and 0.5 in panels B, C and D, respectively (see also the text). Panel (E) shows the time course of an overall process including the transitions A⟶B⟶C⟶D⟶A, and the arrows indicate, from left to right, the equilibrium state in B, C and D. Panel E shows the clustering of ”regular” and ”spiky” agents induced by specific force-fields. The field sources are indicated by small dots of the corresponding color, located outside the agents moving area.

Figure 3 shows how a population of agents all in the same (yellow) state at time = t_0 (panel A), undergoes a reversible shift to another (blue) state, reaching different equilibria ruled by different $k_1 : k_2$ ratios. Such ratios are 1 : 1; 0.7 : 0.3 and 0.3 : 0.7 in panels B. C and D, respectively, where k_1 rules the yellow—►blue rate. In panel D the global time course of the considered process is reported and the arrows indicate the three equilibrium states. Such a simulation exercise can be obviously approached through the corresponding set of differential equations, available in this case. However, the appealing feature of the MA simulator remains the straightforward , intuitive connection with the statistical nature underlying any first-order kinetic process: for example, when k_1 = 0.7 the switch from C_1 to C_2 of each member of the agents population is provided by the following couple of lines:

```
  ask agents
 [ if color=yellow and random 100  <  70 [ set color=blue]  ]
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where random < 100 is a random integer between 0 and 99.

Connecting structural and functional properties has always been one of the most unifying and useful ways to describe and predict the behavior of living systems, independent of size and specific features. This entitles the use of the above modeling approach at different dimensional levels and, in particular, in the case of cellular populations where phenotypical (structural) changes may reflect events of huge physiological and pathological relevance. More specifically, having in mind the changes in cellular and tissue architecture associated to neoplastic transformations (Bizzarri et al., 2011), the two types of agents in the shown simulations have been characterized by both different color (yellow/blue) and shape (regular/'spiky'). Due to the crucial influence on the cells behavior attributed to a manifold of exogenous (environmental) factors, it also appears of special interest the easy reproduction of that influence by means of external force-fields, as exemplified in figure 3 (panel F). The aggregation induced by different force-fields on a specific cell type is just one of the many relevant effects which could be made more and more realistic as far as their type and specificity is concerned.

As a matter of fact, some relatively slight improvements in the simulator would produce relevant predictions, amenable to experimental tests. Such improvements, under work now, mainly deal with a precise modeling the influence of gravitational-fields, cell density and various chemical factors on the conformational switch.

3.2 Students' performance.

Improving the learning performance is the obvious goal of the teaching staff in any educational institution and often implies the choice among different options in planning a systematic tutorship program. In large-scale institutions (like medical schools) the challenge is to take into consideration a vast number of environmental conditions of potential effect on the performance, in conjunction with the vastly different expectations, motivations and cultural backgrounds of a numerous and heterogeneous population of students.

This frame discourages the use of classical mathematical-modeling in favour of an approach more appropriate to problems typical of social dynamics (Hegsellman and Flache, 1998). Thus, we set up an MA simulator in which the goal of agents is to get across a "training-area" and reach the target of graduating in a predefined time, corresponding to the expected training length (6 years for medical students). If they don't reach the goal, they are considered as 'dropouts'. The agents' individual features are the following:

- a (randomly distributed) energy they need to move. This representes the individual MOTIVATION.
- a moving speed, representing the moving 'EFFICIENCY'.
- the ability to feel the attractive force-fields, located outside the training area. This represents a DEEPER MOTIVATION (Professional Tuning), somehow related to a specific medical field. This feature is related with cultural maturation and only appears in biennium II and III.

Each of the above mentioned features can be affected by some external factor, thus allowing to check the efficacy of any specific tutorship in terms of increased learning performance.

Figure 4 depicts the training-area in the form of a green circle surrounded by light blue and yellow circular crowns of identical surface, which represent the first, second and third biennium, respectively, of the total length of the medical course (6 years). Outside the training-area are located the attractive fields (marked by A, B, C, D) which provide the student a preferential direction in their moving.

Figure 5 summarizes the results of: first, fitting some actual data concerning a cohort of students (freshmen in 2001) in the first medical faculty of Sapienza (Rome University) with a properly tuned set of parameters in

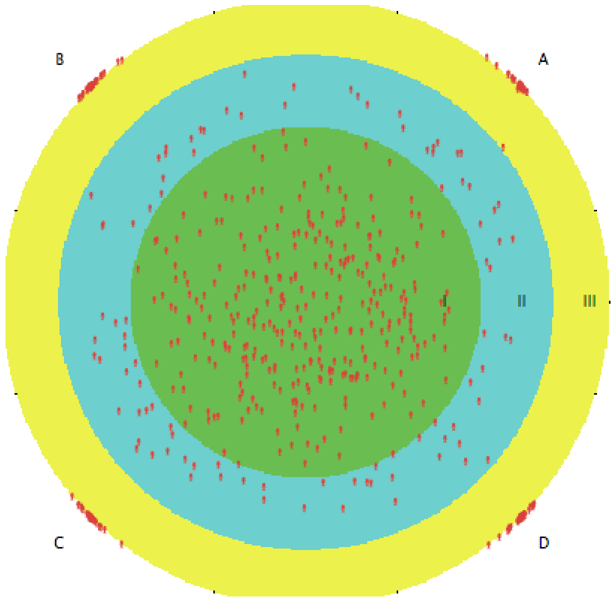

Figure 4: *A students' performance simulator.* The three circular regions of different color and identical surface represent the three fractions (biennium I, II and III) in which the six years training of italian medical students is traditionally divided. Starting from the innermost (green) area as freshmen the students task is to reach the white area out of the yellow region, that is to graduate, within the 6^{th} year of training. Several options are available, in the form of different tutorship strategies, to help sluggish students in getting such goal. In the absence of any tutorship, the fraction of students able to graduate within the predefined dead line is relatively low (about one third, in the student cohort starting in 2001 - see figure 5). In the simulation such clever students aggregate outside the yellow region in the close vicinity of the attractive fields (A, B C D) which represent a combined effect of motivation, efficiency and professional tuning (see the text).

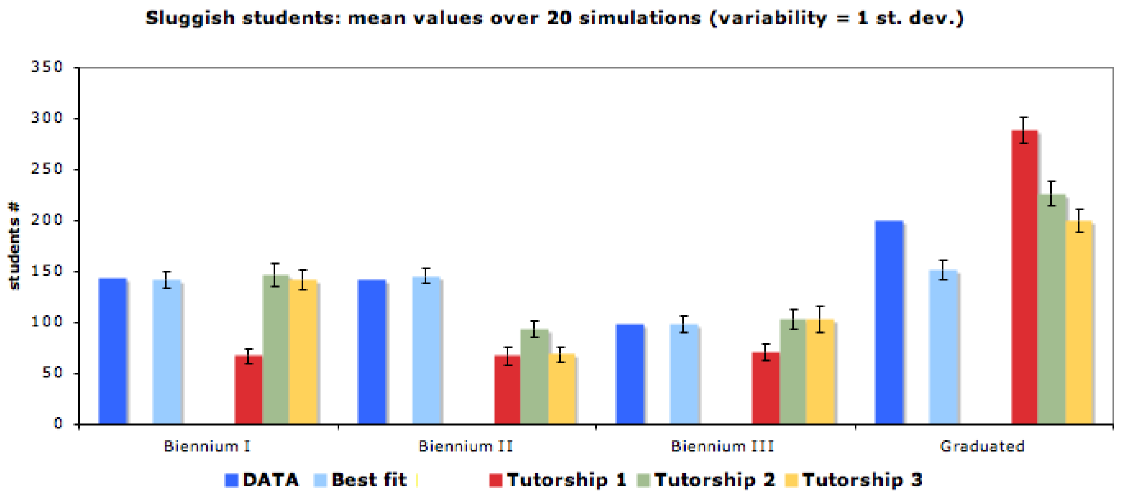

Figure 5: *Tutorship effects on students's performance.* For each temporal fraction of the whole training period (biennium I, II, III) and for the (timely) graduated students the dark and light blue bars represent, respectively, the actual data of the students cohort starting in 2001 (source: INFOSTUD data base of "Sapienza", University of Rome), and of fitting such data by appropriate tuning of the simulator working parameters. A potentially important use of the tuned simulator, namely as a predictor of the effects of different tutorship strategies, is illustrated by the three other bars in each temporal fraction (see the text for further information and data discussion). In all simulated conditions the mean values of 20 trials and the corresponding standard deviation are reported.

our MA simulator [2]; second, simulating of the possible influence on the learning performance, of three different tutorship strategies, specifically acting upon Motivation, Efficiency and Deeper Motivation (Professional Tuning)

[2] the parameters to be tuned are: the time step in the simulator; the values assigned to the initial distribution of motivation among students , and the values of the moving speed in the green, gray and yellow region of the training area

of students, as indicated by the fraction which is graduated in the proper time and of the sluggish individuals left behind in the various regions. Increasing the fraction of motivated students (Totorship 1) looks the most efficient tutorship strategy, since the clear effects appear both in decreasing the number of dropouts in the 3 biennia and in increasing the number of timely graduated individuals. The effects of Tutorships 2 and 3 (affecting efficiency and Deep Motivation) are less clear, although significant, and not equally distributed in biennium I, II and III. In this respect, it is interesting to note that both of them improve the performance particularly in biennium II and in the last part of the course, as shown by the increased number of graduates.

4 CONCLUSION

Obvious as it is, the main utility of multi-agent simulations can be appreciated at the level of two types of problems. The first one concerns a qualitative account of the collective behavior of agents' populations emerging from the underlying features of each agent and of its location on the grid. Another, more ambitious, problem points to the quantitative refinement of the model parameters describing the collective behavior, in the aim to fit at best the observed dynamics in experimental data. Multi-agent simulators undoubtedly provide a more intuitive and rewarding approach to the first type of problems, as compared to the traditional approach based on approximated solutions of differential equations. As far as the second type of problems is concerned, the difference between the two approaches is greatly reduced, and difficult to evaluate in many cases.

The first application discussed in this paper, concerning the cellular context, only aims to a qualitative representation of the considered phenomena. However, it provides a fast, realistic and visual response of the system dynamics to various combinations of factors, potentially useful in the development of new mechanisms and ideas.

As for the second application, concerning the students' performance, the ambition of the simulator exceeds a bit the purely descriptive dimension. In this case, in fact, since the model looks able to reproduce the trend shown by some real data, some prediction of the performance improvement consequent to well defined changes in some specific factors could be proposed and easily tested.

It is very important reminding that in this paper actually only one of the two features typical of the MA simulators, namely the easy account of the influence of environmental factors on the agents behavior, has been exploited by means of force fields. The other feature, namely the reciprocal influence the agents could exert on each other behavior, has not been considered, as yet, although its relevance to increase the euristic power of the simulators in complex and realistic situations, cannot be overestimated. The easiest and most general way to account for that influence is to make the agents' behavior in a given area dependent on the population density in that area. In the context of the Big Bang toy model this would mean accounting for mass dependent attractive interactions. However, in the context of the two applications, both attractive and repulsive interactions among different types of agents could be considered.

As a matter of fact, electromagnetic interactions of various type should greatly affect the dynamics of conformational changes in cells populations, as well as inter-individual interactions of various type influence students populations behavior. Even qualitative modeling of such highly nonlinear effects is a difficult - but extremely exciting - challenge [3].

5 ACKNOWLEDGEMENTS

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[3]The MA simulators used in this paper can be obtained as free-software in the form of applets, upon motivated request to the author.

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