Can agent-based systems and their computational implementations be isomorphic?

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1. Introduction: the problem and its context

The purpose of constructing agent-based simulations representative of some interesting or useful reality appears to rest upon the following key propositions:

- 1. We are interested in quantitative measurements of collective phenomena different than those obtained by averages.
- 2. Many examples of collective systems exhibit collective behavior, defined as outcomes where the individual degrees of freedom have been non-trivially (i.e. non-additively) reduced and transformed when moving from the *scale of the agents* to the *scale of the system*. We name this reduction as *emergence*.
- 3. Agents are at least as rich as particle systems, which opens new significant questions regarding the nature of the mathematical devices required to represent them.
- 4. Agent-based systems produce outputs amenable to visualization and fine-grained data analysis.

To that end, we also appear to be interested in establishing a difference between social agent-based systems (SABS), agent-based models (ABM) of those agents, and ultimately implementations of such models (ABMI). For the purpose of grounding the discussion, let us define a social agent-based system loosely as a system composed of active entities for which a significant portion of their internal resources is devoted to information representation and communication. Social agent-based systems are neither formal nor computational; these are the objects of which properties are to be investigated. The goal with them is, to the best of our intellectual capabilities, to gain sufficient information capable of unveiling their laws and the architecture and ultimately derive laws (or at least law-like expressions) that lead to prediction, explanation or retrodiction. Of these, most interesting situations share at least these properties:

1. agents contain some internal form of representation of themselves, others and their environment; this representation may be trivially null, or structurally and functionally rich

- 2. agents are dynamical entities, governed by internal laws that dictate, most generally, the trajectory of their internal representation
- 3. agents are situated in space within an environment possibly with its own governing dynamics
- 4. the environment has finite resources of some sort, whether it is space itself viewed as a resource, its dimensionality or its contents; the finiteness of resources is characterized in terms of extrema emerging from interactions of some sort, most frequently measurements, other times purposeful transformations of local aspects of the environment
- 5. agents experience the passing of time in some form of another as measured by a locally accompanying device known as a *clock*; the clock can be used to uniquely label local events only
- 6. clocks measure the passing of time only *indirectly* by means of some approximate form of effectful, periodic and regular motion
- 7. agents are locally constrained spatially by an immediate vicinity in terms of the effective distance where their actions can have an impact on the environment or other agents
- 8. locality constraints appear to have led, at the moment of investigation, to information representation and communication mechanisms
- 9. agents contain a repertoire of behaviors that, although possibly rich in variety, remains finite
- 10. individual behaviours are often modulated either by environmental inputs, by the agent's internal representation, or by information sent from other agents
- 11. within the instruction repertoire, communication behaviors exist that specify how to send information, when, and most significantly, what to send
- 12. information gathering, representation and communication are often lossy processes: information gains are limited by intrinsic or extrinsic randomness, by limitations of the agent's memory or by how signals are distorted by the environment which is often an active entity itself
- 13. the action of agent appears to be guided by three clearly distinguishable classes of dynamics:
 - a. those that modulate specific behaviors; these may appear to either depend on continuous or discrete variables and have a corresponding response
 - b. those that trigger communication; these appear to depend on the evaluation of conditions that resemble a phase transition insofar a threshold is required to move from the state of non-communication to one of communication
 - c. those that selectively change the frequency of application of either (a) or (b) based on changes of the internal representation; we may call the collection of dynamics as *learning* or meta-dynamics

From this description, it is clear that our ability to capture aspects of the reality of social agents is immediately constrained by our ability (a) to measure and distinguish which patterns of action correspond to relevant macroscale variables, (b) to measure and distinguish individual patterns of action that correspond to microscale variables, (c) to preserve the most representative

variables when faced with increasing selection complexity, (d) to obtain at each level sufficient data in correspondence with the structural and algorithmic complexity of that level (i.e. in proportion to the system's requisite variety), (e) to find suitable formal representations with associated denotational and operational semantics such that the expression and testing of hypothesis is possible, (f) adequate means of re-enacting the formal specification thus far obtained in ways that facilitate visualization and analysis of results, and (g) a mechanism that permits testing of various hypotheses.

Suppose as a thought experiment that the probability of success as a function of outcomes resembling real scenarios can be assigned to each of these steps (in reality, there is no objective way to assess this), and focus on the probability of performing an optimal reduction. To test the experiment, suppose naively that we are only 90% successful at each step; we are soon faced with the fact that by the end of the process our outcomes are indistinguishable from coin tossing. More realistically, the expectation of the representational error upon these numbers in real scientific tests is that:

- a. Detecting errors and biases during data gathering and variable selection is the most onerous task, but statistics can at least bound the fidelity of each measurement
- b. Even if microscale variables are poorly measured, the degeneracy present in the respective bridge equations from the microscale to the macroscale can lead -except in cases of extraordinarily poor luck- to commensurate, and ideally equivalent results.
- c. Selection complexity can be tamed at the expense of restricting the size of the environment volume, the richness of agent repertoires, the timescales or the sources of randomness when these are proven to be systematic and ineffectual. Proving so, however, often entails significant efforts.
- d. We often consult with success the enriched arsenals of mathematics for small systems; however, for reasons that have become increasingly apparent since 1970, the common language of differential equations appears to be increasingly unsuitable to deal with the complexity of systems beyond active matter, least human systems.
- e. The rise of cyberinfrastructure and powerful personal computing systems have democratized experimentation through agent-based models. However, computational science in general (not only computational social science) remains poorly developed in conceptual terms. We lack a robust, unified theory of simulation capable of interrogating particular simulation instances for answers about their ability to uncover social laws and principles. We also lack a proper theory of computational reproducibility that operates from the ground up instead of asking reproducibility from artifacts that were not constructed to satisfy it.
- f. Hypothesis testing is a well-founded discipline that, under suitable conditions, provides the necessary answers. Yet, the dilemma resides in the word *suitable*. Normality, independence, homocedasiticy, and linearity are often but illusions that render parametric statistics moot. The dependence of the significance of p-values in relation to F-measures on the specific structure of problem instances is but one of many examples of the latter. More recently, non-parametric statistics have arisen as a response.

All of these factors, when all elements align, can render computational outcomes that are testable, and moreover, representative of a social reality. We are further concerned in those cases with the question of whether these successes are scalable conceptually, operationally and computationally. We are also concerned about the possibility of identifying the sources of failure for those systems where, even for small scales, success could not be achieved.

Up to this point, we have not questioned the most fundamental of our premises: that the research program set before us of finding social primitives and using them to derive realistic facts is valid. Historically, several counter-arguments have been stated which fall under three large categories. First, that the richness of the repertoire of anything more complex than a social insect can either pose serious mathematical or computational intractability. Second, that the reality of the social transcends formal representations. Third and last, that limited information and randomness during measurement processes prevent us from gaining the necessary insights required to even construct the models. Our argument in favor of such research program contests these others by taking an ab initio stance. We start by stating that independently of how we partition natural, social or artificial systems, the laws of Nature are never suspended at any scale. Moreover, their action is concurrent and relative for all involved locations, and the ability to identify something in particular depends on Liebniz's principle of identity of indiscernibles: two objects are equal only when all their properties are equal. If two agents share the same state, position and dynamics at a specific time, they must be the same. As a consequence, and knowing that for every interaction between entities we are justified to postulate mediating fields, particles or messages, we seem also justified to adopt a relational view of space where no frame of reference is privileged².

As stressed by Lee Smolin³, even large cosmic structures are connected to the smallest aspects of reality at all times, yet their architecture -in terms of spatial and temporal organization-appears seamless. Equally effortlessly for Nature, all scales are present during any given action, but our selection for the reference frame of observation can reveal specific constraints and aggregations. What we call critical phenomena and self-organization at one scale can become a single element of self-organization in another one; this is how topological defects are characterized⁴. At this point, it is worth noting that self-organization and emergence seems to depend on the balance between the requisite variety of the repertoire per entity and the number of entities required to satisfy a thermodynamic limit. Since social systems appear to emerge only at the scale of complex living systems with some capability of representation of the self and of others, and since the laws of Nature are never suspended, it is only logical to assume that the "new" (partially observed) laws of social systems are only new in the sense that we are just

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¹ Leibniz, G.W., 2012. Philosophical Papers and Letters: a selection (Vol. 2). Springer Science & Business Media.

² Northrop, F.S., 1946. Leibniz's theory of space. Journal of the History of Ideas, pp.422-446.

³ Smolin, L., 1995. Cosmology as a problem in critical phenomena. In Complex systems and binary networks (pp. 184-223). Springer, Berlin, Heidelberg.

⁴ McCoy, J.H., Brunner, W., Pesch, W. and Bodenschatz, E., 2008. Self-organization of topological defects due to applied constraints. Physical review letters, 101(25), p.254102.

starting to observe them, but not new in the sense of being ontologically independent from the hierarchy of laws we use to understand the rest of the universe. Moreover, similarly to how quantum mechanical laws constrain classical ones⁵ although less straightforwardly, we should naturally expect laws below the social to restrict the set of possible worlds, necessary to prevent the effective infinities that tend to appear when the only method of analysis is enumeration. Concretely, we conjecture that social primitives exist as the result of self-organized systems with structural and functional complexity sufficient for actionable local information representation and transmission mechanisms to manifest; moreover, we conjecture that these social primitives are discoverable and that the novelty associated with their discovery must be interpreted in the context of an inferred hierarchy of phenomenologies and laws, whatever the inference mechanism may be. We finally conjecture that a minimally representative set of social primitives exists such that observed collective behavior of social agent-based systems can be reasonably captured by compositionally applying these primitives.

Methodologically, we must deal with the problem of computer implementations of models, their representativeness of the model and transitively of the phenomenon, and their epistemological robustness. We suspect that the representativeness of the implementation with respect to the model depends on the ability to understand how the action described by a particular ABM maps onto a given type system and its inferential mechanism. The mapping, more properly, acts as additional laws of discrete nature that induce information loss of various kinds⁶. One of the most obvious examples is the effect of using various *float* types of variable word length on the accuracy of stiff systems; while recent efforts to overcome the difficulties of the IEEE-754 standard for floating point arithmetics have been amply discussed and implemented, they have not yet reached the world of agent-based modeling and simulation. We therefore assume that most of the work in the area is constrained by current FPU designs and their programming languages counterparts. An immediate consequence of this is that information loss may artificially introduce effects that end up manifesting at large as deviations from realism. Many of the techniques found in numerical methods as well as new ones such as uncertainty quantification⁷ may help prevent such mishaps.

Epistemological robustness is more elusive, but we suspect progress can still be made. For instance, except when ABM models are provably equivalent to some form of diffusion or propagation by showing the existence of (a) a correct mapping between the ABM and a Lagrangian (particulate) model and (b) a subsequent mapping between such Lagrangian and an Eulerian (field-based) model, sequential time updates should be discouraged. If a model can be reduced to an Eulerian form, then the computation reduces to a system of partial differential equations applied over an arbitrary refined grid. The latter is equivalent to saying that, for some small time scale, the correlation of sequences of events in the same location

⁵ Bohr, N. and Rosenfeld, L., 1976. Collected Works: The Correspondence Principle (1918-1923) (Vol. 3). North Holland.

⁶ Backhouse, R., Chisholm, P., Malcolm, G. and Saaman, E., 1989. Do-it-yourself type theory. Formal Aspects of Computing, 1(1), pp.19-84.

⁷ Smith, R.C., 2013. Uncertainty quantification: theory, implementation, and applications (Vol. 12). Siam.

 $< x(t), x(t+\delta t), x(t+2\delta t), ...>$ and adjacent events in space $< x_1(t), x_2(t), x_3(t), ...>$ equals zero. As long as the discretization of the grid preserves this property, sequencing should not be expected to significantly impact the outcome. Phenomenologically, this is also equivalent to a memory-less system: memory entails correlation, and selective information loss. Incidentally, many of the principles and ideas found in irreversible thermodynamics⁸ should be directly applicable to the study of ABMs. Hence, we expect that ABMs where agent trajectories are influenced by the effects of some form of memory should be susceptible to changes in the sequence of events at each time step. If a sufficiently similar (reaction-)diffusion model⁹ can be found for a given ABMs, the sensibility of orderings may manifest as a difference in the variance of the spatial distribution of suitable observables.

Considering all aspects up to this point, a sound research program on social primitives as a new foundation for computational social science appears to necessarily concern itself with at least some of the following theoretical issues:

- How do we formally characterize the notion of representativeness between SABS and ABMIs?
- How do we measure and represent sufficient relevant aspects of the reality of a SABS to construct an ABM? How do we rigorously evaluate measurements from macroscale and microscale observables?
- How do we define social primitives intuitively and formally? How do we identify them from experimental data? How do we obtain a minimally useful set of social primitives?
- Are social primitives compositional? Is compositionality affected by scale, understood as the combination of number of agents and degrees of freedom, and topology?
- Can ABMs be classified depending on the social primitives and overall conceptual and operational architecture?
- Given a model containing a minimally useful set of social primitives, how can we determine its sensitivity to non-functional implementation aspects such as event discreteness vs. continuity, global vs. local time or procedural event ordering?
- Given an ABMI, what conditions of its construction guarantee its reproducibility? Is model correctness a requirement for reproducibility?

Our main hypothesis may finally be stated as follows: is it possible to prove the equivalence between SABS based on the notion of social primitives and ABMIs such that an isomorphism can be identified and used to find equivalence classes for ABMs? Moreover, by using an approximate (weak) version of the univalent axiom¹⁰ at the core of homotopy type theory stating that equality is commensurable with equivalence, and topos theory as the compositional theory

⁸ Dewar, R.C., Lineweaver, C.H., Niven, R.K. and Regenauer-Lieb, K., 2013. Beyond the Second Law. Entropy Production and Non-Equilibrium Systems.

⁹ For an example, see: Rida, S.Z., El-Sayed, A.M.A. and Arafa, A.A.M., 2010. Effect of bacterial memory dependent growth by using fractional derivatives reaction-diffusion chemotactic model. Journal of Statistical Physics, 140(4), pp.797-811.

¹⁰ Voevodsky, V., 2010. The equivalence axiom and univalent models of type theory. Talk at CMU, pp.172-187.

of space- and time-dependent action, it is possible to precisely state how ABMs map onto programming language semantics, and furthermore how examination of certain spaces of collective action may be rendered unnecessary thanks to better understanding of the abstract structure of the interplay between hierarchies of laws and constraints.