TOWARDS THE GLOBAL: COMPLEXITY, TOPOLOGY AND CHAOS IN MODELLING, SIMULATION AND COMPUTATION

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ABSTRACT

Topological effects produce chaos in multiagent simulation and distributed computation. We explain this result by developing three themes concerning complex systems in the natural and social sciences: (i) Pragmatically, a system is complex when it is represented efficiently by different models at different scales. (ii) Nontrivial topology, identifiable as we scale towards the global, induces complexity in this sense. (iii) Complex systems with nontrivial topology are typically chaotic.

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1. Introduction

Although the concerns of modelling and simulation can be quite different [1], both support a pragmatic definition of complexity: A system is complex if it is represented efficiently by different models at different scales. This idea is commonplace, reflected in the way we organize our understanding of the world around us into physics, chemistry, biology, psychology, economics and political science at (roughly) increasing size scales. The goal of this paper is to explain a recently demonstrated difficulty with multiagent simulations of complex systems at the social science end of this spectrum [2] by placing it in the context of (possibly more familiar) models and simulations of complex systems at the natural science end.

We begin by showing that this definition of complexity is more than subjective. In Section 2 we consider the hierarchical algorithm of Barnes and Hut for simulation of gravitationally interacting particles [3]. Their multiscale algorithm is more efficient, in a very precise sense, than naïve direct simulation. Large scale states are described by total mass and average position of particles, so the model is similar at different scales. We describe this situation as simplicity. For more complicated systems, as we increase in scale towards the global, we may identify states with nontrivial topology. The presence of such states can lead to a different and more efficient model at the larger scale; topology induces complexity.

The purest example of this phenomenon might be topological geons in quantum gravity [4]: prime components of the spacelike 3-manifold comprise localized nontrivial topology and can be modelled as particles. The intellectual heritage of this model includes Lord Kelvin's theory of atoms as knotted vortex lines [5]. That theory was mistaken, of course, but it was motivated by Helmholtz's mathematical analysis of hydrodynamical vortices [6]. Vortices alone are topologically nontrivial states, in terms of which the equations for fluid mechanics can be recast and which are utilized in very practical vortex simulations of fluid flow [7]. We explain this in Section 3, remarking on the efficiencies gained by use of a hierarchical algorithm. While demonstrations of improved simulation efficiency are not available for all the systems we consider, these two examples reenforce the belief, based on the conceptual adequacy of different models at different scales, that the systems are indeed complex.

Multiagent systems are discrete, in contrast to PDE models for fluid mechanics. To develop our theme of topology induced complexity for application in the former, we must explain how it can occur in non-continuum systems. In Section 4 we consider the homogeneous sector of a multispecies reaction-diffusion model in chemistry/population biology. This model, analyzed by Ruijgrok and Ruijgrok [8], illustrates our first two themes: (discrete) topology induces complexity in the sense of a different efficient model at the global scale.

The same nontrivial discrete topology—a cycle—is ubiquitous in formal models of economics and political science: In Sections 5 and 6 we describe two fundamental results—

Sonnenschein, Debreu, and Mantel's excess demand theorems [9] and Arrow's voting theorem [10]—which guarantee the existence of cycles in market and voting models, respectively. We also expand our third theme: systems with topologically induced complexity are typically chaotic. In particular, we explain the precise mathematical sense in which aggregation by voting makes multiagent simulations chaotic [2].

But the aggregation processes which scale multiagent simulations towards the global are usually market mechanisms or voting rules; thus such systems are typically complex, and, according to the results described in Section 6, chaotic. In the final section we discuss the consequences of this phenomenon and mechanisms which might be implemented to control it.

2. Hierarchical efficiency

Simulation of interesting natural or social systems compels careful attention to the efficiency of the algorithms used. Algorithms which are exponential in the size of the system are essentially useless, and even for polynomial algorithms, decreasing the leading exponent reduces runtime by orders of magnitude. The simulations of concern here typically consist of a large number N of fundamental objects interacting according to rules which model the dynamics of the system under investigation. Algorithmic efficiency is thus determined by runtime as a function of N.

Consider the problem of simulating the (Newtonian) gravitational dynamics of N particles. Each particle exerts a force on every other particle and is subject to the sum of the forces exerted on it by all the other particles. The most straightforward algorithm would compute the N(N-1)/2 pairwise forces, sum the forces on each particle, and then evolve each particle accordingly, at each timestep. This algorithm involves no approximations beyond the finite precision computer representation of real numbers; it provides an accurate $O(N^2)$ description of the dynamics.

Barnes and Hut showed, however, that by aggregating the particles into a hierarchy of clusters of increasing sizes, the average run time can be reduced to $O(N \log N)$ with bounded error [3]. Their algorithm works by dividing up the volume of space containing the particles into a tree of cubical cells: Starting with a cube large enough to contain all the particles, at each timestep consider the particles in some (arbitrary) sequence. While the particle lies in the same cube as any previous particle, subdivide that cube into eight cubes of half the linear size. Now assign to each non-empty cube a 'cluster-particle' with the total mass of the particles in that cell, and locate the cluster-particle at the center of mass of those particles. On average, constructing the tree of cells and cluster-particles requires $O(N \log N)$ steps.

The force on a given particle is now computed recursively by working down the tree: If a cluster-particle lies in a cube of size l, is distance d from the particle, and $l/d < \theta$ (a constant), compute the force it would exert; if not move down to the next smaller cluster-particles in the tree and repeat. This algorithm approximates the force on a particle, with

bounded error (depending on θ), in an average of $O(\log N)$ steps. The average runtime per timestep is thus $O(N \log N)$ for the whole algorithm.

In this description 'average' refers to possible particle configurations with respect to a uniform probability distribution on the cube. When the particles are literally clustered, as in the simulation Barnes and Hut present of two interacting clusters, additional efficiencies obtain. Even in this case, however, the larger scale representation is essentially similar to the smaller scale one; the system is simple.

3. Topology induces complexity

Fluid flow provides our first example of a system with different representations at different scales. Disregarding the fact that real fluids are composed of molecules, which are composed of atoms, ..., and should, by virtue of that multiscale description alone, be complex systems, let us take the system to be defined by the Navier-Stokes equations:

$$\partial_t v + v \cdot \nabla v = -\nabla p + \nu \nabla^2 v$$
$$\nabla \cdot v = 0.$$

together with appropriate boundary conditions. Here v is the velocity field of the (incompressible) fluid, p is the pressure, and ν is the viscosity. Immense effort has, of course, gone into simulating the Navier-Stokes equations [11], whose solutions range from laminar to turbulent flow.

The configuration variable in this system, the velocity field, can be topologically non-trivial: there may be, for example, vortices, i.e., closed loops in the flow. Their presence is measured by the vorticity $\omega := \nabla \wedge v$ [6], in terms of which the first equation above can be rewritten as

$$\partial_t \omega = \nabla \wedge (v \wedge \omega) + \nu \nabla^2 \omega,$$

eliminating the pressure. The inverse of the Poisson equation defining vorticity is the Biot-Savart law; it gives v as a function of ω and allows the system to be reformulated entirely in terms of the vorticity. This is a different, although entirely equivalent, model for fluid flow.

When the flow is restricted to two dimensions the vorticity has only a single (orthogonal) component so the configuration variable for the model is a (pseudo-)scalar field. As such it can be approximated by a superposition of delta functions, or more physically, by a collection of point vortices with circulations c_i :

$$\omega(r,t) pprox \sum_{i=1}^{N} c_i \delta(r - r_i(t)).$$

Even before the advent of digital computers Rosenhead simulated fluid flow using this approximation [12]: For inviscid flow, the velocity of each vortex is the value of the velocity

field at its present location; this is given in terms of the vorticity field by the Biot-Savart law. Notice that a straightforward algorithm for this computation would be $O(N^2)$. Just as in the simulation of gravitating particles considered in Section 2, the vortex positions can then be integrated forward in time.

There are several problems with this procedure: While it is correct for inviscid flow, the singularities in the vorticity field make the errors in time integration difficult to control when the point vortices pass too close to one another. (We anticipate the results of Section 6 by remarking that such systems with only a few vortices have been shown to be chaotic [13].) This problem can be resolved to some extent by implementing a 'cloud-in-cell' technique [14] which also improves the runtime for solving the Poisson equation to $O(N) + O(M \log M)$, where M is the size of an approximating spatial mesh. Alternatively, and at the same time modifying the model so as to be able to simulate viscous flow, the point vortices can be replaced with 'vortex blobs' in which the vorticity has a fixed but nonsingular distribution [15]. Hald has shown that the error can be controlled in simulations of inviscid flow with such models [16].

These simulations demonstrate that two dimensional hydrodynamics is therefore a complex system according to our operational definition: Not only are there efficient algorithms at different size scales, as presaged by our discussion of gravitating particles, but the system is modelled differently at each scale—by a velocity field, by a collection of vortices, and by a distribution of vorticity on a mesh. Topology will play this role—inducing new models at more global scales—for the rest of the discussion.

4. Finite topology

Vortices in fluids contain cycles—closed continuous flow lines. But continuity of this sort is not necessary for nontrivial topology. Moving away from physics to a model for a system in chemistry or population biology, consider three species (types of particles) with interactions*

$$A + B \rightarrow 2A$$
, $B + C \rightarrow 2B$, $C + A \rightarrow 2C$.

We notice immediately that there is a kind of cyclicity inherent in this set of reactions. Ruijgrok and Ruijgrok have analyzed a system of such particles which are simultaneously interacting according to

$$A + 2B \rightarrow 3B$$
, $B + 2C \rightarrow 3C$, $C + 2A \rightarrow 3A$,

with relative rate α [8].

Since each of the reactions conserves particle number we can normalize to population densities A + B + C = 1. Since A, B and C are all positive, the configurations of the system can be represented by points in the interior of an equilateral triangle with side

^{*} Delightfully, Sinervo and Lively have observed populations of lizards competing according to very similar rules [17].

 $2/\sqrt{3}$: for any point inside this triangle the sum of the altitudes A, B and C to the three sides is 1. The evolution of the system is a flow on the triangle, described by the system of three ODEs obtained from

$$\dot{A} = A(B - C) + \alpha A(AC - B^2)$$

by cyclic permutations of (ABC).

Notice that the center of the triangle A = B = C = 1/3 is an equilibrium point. When $\alpha = 0$, the product P := ABC is left invariant by the flow: all the solutions are periodic orbits along the closed curves P = const. In general,

$$\frac{1}{P(t)}\frac{\mathrm{d}P(t)}{\mathrm{d}t} = -\frac{9}{4}\alpha r^2(t),$$

where r(t) is the distance from the center of the triangle. Thus for $\alpha < 0$, the center (1/3, 1/3, 1/3) is a stable equilibrium, while for $\alpha > 0$ it is unstable; the $\alpha = 0$ model is not structurally stable.

Although we have not introduced the formalism for finite topological spaces, this analysis motivates identification of the cyclicity of the two sets of reactions as topological nontriviality; certainly this cyclicity can induce cycles in the evolution of the system. Moreover, in the sense that the system can be represented globally as a cycling 'ecology', or one at a stable or unstable equilibrium, rather than only in terms of individual, interacting particles, it is complex.

5. Economics and politics

Thinking of the preceding system as a model in population biology leads us towards social science models of multiple interacting agents. By now we should expect cycles to occur in these systems—and they do, in very similar ways. We begin by considering an example, due to Scarf [18], which indicates difficulties with the general equilibrium model in economics [19].

In this model there are multiple agents with initial endowments $w_i \in \mathbb{R}^k_{\geq 0}$, where the components of w_i represent amounts of k goods. The prices of these goods are represented by another vector $p \in \mathbb{R}^k_{\geq 0}$, so the initial wealth of agent i is $p \cdot w_i$. By exchanging goods according to prices p, agent i can afford any commodity bundle $x \in \mathbb{R}^k_{\geq 0}$, provided $p \cdot x \leq p \cdot w_i$.

The agents also have preferences among the different goods, modelled by utility functions $u_i: \mathbb{R}^k_{\geq 0} \to \mathbb{R}$; $u_i(y) \geq u_i(x)$ means that agent i prefers commodity bundle y to bundle x. We assume that for each agent i, $\{y \in \mathbb{R}^k_{\geq 0} \mid u_i(y) \geq u_i(x)\}$ is a strictly convex set and that $\nabla u_i \in \mathbb{R}^k_{>0}$. At given prices p, agent i maximizes utility with a commodity bundle $x_i(p)$ satisfying $\lambda p = \nabla u_i(x_i(p))$, for some $\lambda > 0$; this bundle is the agent's

demand. Notice that any rescaling of p can be absorbed into λ ; we follow tradition and rescale so that $p \cdot p = k$, although we could equally well rescale p so that $p \cdot (1, \ldots, 1) = 1$; in either case we refer to the price simplex of possible price vectors. The excess demand of agent i at prices p is $x_i(p) - w_i$; the aggregate excess demand $v(p) := \sum_i (x_i(p) - w_i)$ is a continuous vector field on the price simplex.

The aggregate excess demand defines a flow on the price simplex according to $\dot{p} = v(p)$. That there is always an equilibrium point v(p) = 0 for such a flow is a consequence of Brouwer's fixed point theorem [20]; this is the topological content [21] of the Arrow-Debreu approach to the existence of competitive equilibria [22]. Scarf demonstrated, however, that such equilibria can be globally unstable [18]: Consider the utility function in a k = 3 good economy defined by $u_1(x) = \min(x_1, x_2)$. Suppose this is the utility function for agent 1 and that there are two more agents with utility functions obtained from u_1 by cyclic permutations of (x_1, x_2, x_3) . Let the initial endowments of the three agents be (1, 0, 0) and its cyclic permutations, respectively. Then the first component of the aggregate excess demand is

$$v_1(p) = \frac{-p_2}{p_1 + p_2} + \frac{p_3}{p_3 + p_1};$$

the other two components are obtained by cyclic permutation of (p_1, p_2, p_3) .

The center point $p_1 = p_2 = p_3 = 1$ is an equilibrium point and, just as in the $\alpha = 0$ case of the example discussed in the preceding section, the product $p_1p_2p_3$ is left invariant by the flow. Thus the system has no stable equilibrium. While the utility functions used in this example are convex, but not strictly convex, and the initial endowments are at an extreme, Scarf showed that there is a family of such models (just as there was in Section 4) which have strictly convex utility functions and inital endowments nonzero in each good, but which are also globally unstable [18].

In this economic model the discrete cycle of utility functions leads to continuous cyclic orbits just as the discrete cycle of reaction equations did in Ruijgrok and Ruijgrok's model. But suppose there are only a finite number of states for the system. This is the situation in political science models where each agent's utility function is replaced with a preference order among a finite set of alternatives: a relation, denoted \geq , which is complete (for all pairs of alternatives $a \geq b$ or $b \geq a$) and transitive (if $a \geq b$ and $b \geq c$ then $a \geq c$) [10]. When $a \geq b$ and $b \geq a$, the agent with this preference order is indifferent between a and b; when only $a \geq b$, say, the agent strictly prefers a and we write a > b.

The analogue of the aggregate excess demand is a map f from preference profiles (lists of the agents' preference orders) p to directed graphs f_p . A directed edge $a \leftarrow b$ in f_p indicates that for profile p the map f chooses alternative a over alternative b. We call f a voting rule if for all profiles p, f_p is complete (for all pairs of alternatives $a \leftarrow b$ or $b \leftarrow a$) and Pareto (if $a \geq b$ in each preference order in p then $a \leftarrow b$ in f_p).

More than 200 years ago Condorcet recognized that there are potential problems with voting rules, namely that aggregation might produce cycles rather than a definitive

outcome [23]. For example, suppose that there are three alternatives $\{a, b, c\}$ and three agents rank them in the orders a > b > c, b > c > a, and c > a > b. Given a choice between b and a, a 2:1 majority prefers a; if they are offered the opportunity to switch from a to c, again a majority will vote to do so; finally a majority also prefers b to c, completing a cycle. This cycle exists in the directed graph f_p corresponding to the majority voting rule; it is the discrete analogue of the continuous cyclic orbits we have seen in the two preceding systems.

6. Complexity and chaos

These social science models, therefore, have features in common with the natural science models we considered in Sections 2, 3 and 4. At the more global scale defined by the aggregation mechanisms, the set of agents may be replaced by a cyclic (sub)market and a cyclic decision process, respectively. Of course, if the utility functions of the economic agents are such that the aggregate excess demand is representable as the excess demand for a single agent then the market has a unique stable equilibrium. Similarly, given a voting rule, the preferences of the agents may cohere to the extent that there is a definitive outcome; even more simply, the voting rule might be dictatorial, i.e., dependent only on the preferences of a single, specified agent. In all of these cases the model at the global scale is similar to the individual agent model; the topology is trivial and the systems are simple.

We emphasize, however, that complexity is inherent in social aggregation: The theorems of Sonnenschein, Mantel, and Debreu show that for two or more goods and at least as many agents, the aggregate excess demand can be any continuous vector field on the price simplex [9]. In particular, the flow need not have a stable equilibrium: As we have seen already in two dimensions, even though the Poincaré-Bendixson theorem precludes more complicated behaviour [24], the limit set may include cycles. If there is any time dependence from external effects, and in higher dimensional markets, the Kupka-Smale theorem [25] implies that chaotic dynamics is structurally stable; systems with a unique or stable equilibrium point are far from generic.

For completely discrete voting models, Arrow's theorem imples that for more than two agents, under a reasonable condition* on voting rules, any which are not dictatorial must contain cycles [10]. We recently showed that in the latter situation, not only is the system complex, but it is also chaotic in the mathematical sense [2]: The topological entropy [26], defined to be

$$\lim_{n\to\infty} \frac{1}{n} \log(\text{number of } n\text{-periodic orbits in } f_p)$$

is positive exactly when there is a cycle in f_p ; beyond identifying the existence of chaos, it quantifies 'how chaotic' the system is. Averaged over the space of voter preferences, the topological entropy measures the complexity of a voting rule, and averaged over voting

^{*} This is the independence of irrelevant alternatives, namely that the relation between a and b in f_p depend only on the relations of a and b in the preference orders in p.

rules, it measures the (lack of) coherence among voter preferences [2].

7. Consequences

Aggregation rules define the way models of social systems scale towards the global. The larger scale model may be similar to the smaller scale one, as is the case for a dictatorial voting rule, for example. In equivalently simple physical models, rescaling simply renormalizes the state variables and their interactions, but introduces no new ones. Complexity emerges when nontrivial topology exists at the more global scale. This is a cycle in each of our examples, and it induces qualitatively different models in both natural and social systems.

The attendant chaos has profound consequences for simulations of these systems: Fine grained prediction is impossible—only certain statistical properties of the evolution are robust. This fact is appreciated heuristically in some of the economics and sociology literature [27], but seems to receive less emphasis in discussions of specific multiagent simulation platforms [28]. It will, nevertheless, determine to which problems such programs can be applied successfully.

Systems of multiple software agents, interacting to effect some (un)intentional distributed computation, are subject to exactly the same analysis. Whether their interactions are decision theoretic [29] or market oriented [30], designers and users must be aware of the possibilities for complexity and chaos. Even when the artificial agents are physical—autonomous robots [31]—attempts at designing coordinated action [32] should be informed by these same considerations.

Particularly in the context of deploying interacting software or hardware agents for some specific task, but also in the context of modelling or simulating multiagent social systems, success may depend on controlling the degree of chaos in the resulting complex system. As we noted at the end of the last section, the topological entropy, for example, measures how chaotic a system is and allows us to identify the sources of complexity, but this alone is insufficient for control. There are several possibilities: We have primarily considered immutable agents; there are also models with adaptive agents [33] which one might hope to have better generic behaviour. The population biology example of Section 4, however, models a particular kind of adaptation, so chaos is probably no less generic in complex adaptive systems. Agents with 'higher' rationality have also been modelled [34]; these are agents which make internal models for the behaviour of the other agents with which they interact. This approach, while possibly more realistic for modelling human agents, seems to flirt with self-reference and undecidability [35], and must, at best, constrain the depth of the internal models to achieve acceptable computational efficiency [36]. Most generally, it seems that models for complex social systems should include some form of 'back reaction' from the more global aggregation scale to the local individual agent scale. Such a back reaction might affect the agents' preferences or the way they interact, but must be carefully implemented to model interesting complex systems which balance precariously between simplicity and extreme chaos.

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