Generalized Particle Systems

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Abstract

We discuss a general framework for systems of self-propelled particles conceptualized under the theory of dynamical systems and, by considering agent-based models under the same framework, we highlight a fundamental equivalence between them. We exemplify the general definitions given by applying them to two simple models that display interesting, emergent behavior. Finally, we suggest an use case for the given generalization, arguing that by understanding it as a metamodel, one becomes more apt to explore a specific class of dynamical systems, aiming to find systems that might help improving our understanding of fundamental topics in complexity science.

Introduction

The two primary inspirations for this work were the Primordial Particle Systems (PPS, hereafter) (Schmickl et al., 2016) and *Clusters* (Ventrella, 2020; CodeParade, 2018). Both deal with mostly deterministic particles systems with mainly local interactions, the former being more complicated of a system than the latter. The interest on such systems arises from the fact that both of them exhibit non-trivial, emergent macroscopic behavior, despite their seemingly overall simplicity. These systems fall under the concept of an already known and studied family of dynamical systems, namely, self-propelled particles systems (SPPS), which are central to the discussion we present in this work.

The central idea we wish to pursue is to consolidate a kinetic post-newtonian theory, like slightly suggested in (Helbing, 2001), founded, particularly, on the generalization of particle systems with arbitrary dynamics. By 'dynamics' we wish to imply pretty much everything that can influence or determine the behavior of such particles: external/environmental forces, various kinds of interactions between the particles themselves, richer internal states (for instance, instead of only having masses, we could admit particles to have things like memory Nagai et al. (2015), internal energy storages Schweitzer et al. (1998) or any other kind of arbitrary quantities), non-homogeneous sets of particles – as in *Clusters* –, interactions between the elements and the environment wherein the dynamics unfolds etc.

Generalizations are, usually, intrinsically interesting. If not immediately useful, they tend to, at least, shed some light and promote some insight over relations between things once deemed unrelated. The theoretical exploration we present has for motivation, besides the intrinsic benefits generalizations tend to provide, to promote, in accordance with some previous works (Axelrod, 2006; Hinkelmann et al., 2011), an unification.

SPPS are not generally considered under the convenient agent-based framework, although they are commonly seem as related, oftentimes being self-driven particles called agents. A probable reason for this lack of usage of a notoriously convenient framework is that SPPs are older subjects of study, whereas agent-based modeling gained the spotlight somewhat recently. Another one is that while the study of SPPs usually falls under the lens of physicists, agent-based models (ABMs) tend to be used by a wider variety of researchers, probably reaching its peak usage by complexity scientists.

That notwithstanding, it seems very natural to consider SPPS as systems of agents, which is evidently useful since agent-based modeling provides a higher level description of the dynamics found in SPPSs. Conversely, agent systems can also be seem as SPPS, which might be less interesting precisely due to the fact that instead of a simpler, higher level view of the system, we get a more complicated one. But, as it is often the case, the interplay between these two perspectives, on higher and lower levels of abstraction, might be more revealing than an unilateral focus on either one.

The fact that both SPPS and ABMs display interesting, complex, behavior (like emergent macroscopic properties and behavior, self-organization/self-organized criticality) while still retaining relative simplicity cast them as particularly interesting objects of study in research areas such as complexity science and artificial life.

The suggested unification, thus, is also motivated by the belief that by highlighting, in a more mathematically abstract level, the common nature of these various systems, one is left with at least two useful things: the promotion of a tighter integration between different research areas, which should imply an accentuated sharing of methods and techniques; evidentiate the fundamental aspects, shared by all such systems, aiming to guide the exploration of the infinite variety of existent models, which, hopefully, might further develop our comprehension over profound topics such as (artificial) life, complexity, emergency, self-organization and self-organized criticality, non-linearity, chaos etc.

Of particular interest, one such generalization has the potential to allow us to survey 'model spaces' in order to find out, instead of parameters under which a system manifests interesting behavior, families of models that do so, not unlike what was done in Hovey (2020, 2021), where the model space of life-like cellular automata is mapped. Each set of rules defines, effectively, a model; the cited work, therefore, presents an example of a methodology we here suggest. That a more systematic approach to such explorations is of any interest is strongly suggested by recent works such as Briliantov et al. (2020).

Dynamical systems, self-propelled particles and agent-based models

In this section we shall introduce what we understand by a dynamical system and provide our description of systems of self-propelled particles in a general fashion. After that, we will discuss the formalization of ABMs as dynamical systems, in accordance with (Hinkelmann et al., 2011). The overarching goal is to emphasize the shared abstract structure SPPSs and ABMs have, when considered as dynamical systems.

In a more abstract sense, we consider a an autonomous dynamical system to be the action of a monoid T over a set S, that is, an autonomous dynamical system $\mathcal{D}$ is defined as:

Definition 1 ((Autonomous) Dynamical System)**.** Let $\mathcal{S}$ be a set and T a monoid. An *autonomous dynamical system* $\mathfrak{D}$ is the (left) action of T on $\mathcal{S}$, i.e., the map

$$\begin{aligned}\mathfrak{D} : T \times \mathcal{S} &\to \mathcal{S}\\ (t, x) &\mapsto \mathfrak{D}_t(x).\end{aligned}$$

From the monoid action axioms, it follows that, if we let $T = (\mathcal{T}, *)$, with e as T's identity, and consider $\mathfrak{D}(t, x)$, we have that

$$\begin{aligned}&\mathfrak{D}(e, x) = x;\\ &\mathfrak{D}(t, \mathfrak{D}(s, x)) = \mathfrak{D}(s * t, x)\end{aligned}$$

which yields $\mathfrak{D}_{s*t}(x)$.

Considering, more concretely, the definition above, we could think of the movement of a point in $\mathbb{R}^2$ as

$$\begin{aligned}\mathfrak{D} : T \times (\mathbb{R} \times \mathbb{R}) &\to (\mathbb{R} \times \mathbb{R})\\ (t, \mathbf{x}) &\mapsto \mathfrak{D}_t(\mathbf{x}).\end{aligned}$$

where, generally, if $\mathbf{x} = (x, y)$, we must specify two auxiliary functions $\phi_t, \psi_t : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ such that $\mathfrak{D}_t(\mathbf{x}) = (\phi_t(x, y), \psi_t(x, y))$. One thing we would like to point out is the fact that such simple models are not as simple as they seem, at least not if one is to consider them as a dynamical system. To exemplify that and to start developing our intended generalization, let us consider, now, as an example, the model given at Schmickl et al. (2016), which is highly similar to the canonical Vicsek model Vicsek et al. (1995), but, instead of updating the direction of a particle based on the average direction of its neighboring particles, it does so, in fact, in an arguably more complicated way. A fixed radius r set, the direction $\theta_i(t)$ of the i-th particle, with position $\mathbf{x}_i(t)$, in the PPS is updated accordingly to the following dynamical rule:

$$\theta_i(t + 1) = \alpha + \beta \cdot N_i(t) \cdot \mathrm{sgn}(R_i(t) - L_i(t))$$

where α is a fixed rotation parameter, globally associated to every particle, β is a fixed coefficient that modulates the degree the direction of the particles change. $N_i(t)$ is the size of the neighborhood of $\mathbf{x}_i(t)$ at the instant t, whereas $R_i(t)$ and $L_i(t)$ are the number of neighbors on the right and left hemisphere of the particle in question. These dynamics imply much less smoother changes in direction than Vicsek's model, and the interesting emergent behaviors found there are discussed in Schmickl et al. (2016).

Considering the laws of motion that define the PPS in their fullest form, for a given constant speed v, we have that

$$\begin{aligned}&\theta_i(t + 1) = \alpha + \beta \cdot N_i(t) \cdot \mathrm{sgn}(R_i(t) - L_i(t));\\ &\mathbf{x}_i(t + 1) = \mathbf{x}_i(t) + (\cos\theta_i(t), \sin\theta_i(t)) \cdot v\end{aligned} \tag{1}$$

Were one dare to consider the above equations under the rigorous definition of a dynamical system, what they would get is

$$\begin{aligned}\mathfrak{D}[\alpha, \beta, r, v] : T \times (\mathbb{R} \times \mathbb{R})^n &\to (\mathbb{R} \times \mathbb{R})^n\\ (t, \mathbf{X}) &\mapsto \mathfrak{D}_t(\mathbf{X}).\end{aligned}$$

with $\mathbf{X}$ being a $N \times 2$ matrix consisting of all of the system's particles and by $[\alpha, \beta, r, v]$ we denote the model parameters. The above, nonetheless, implies the necessity of some further specification, since it is not the case that $\mathfrak{D}_t$ is the same for every row $\mathbf{x}_i$ in $\mathbf{X}$. Indeed, since each particle has its own neighborhood, which depends on the positions of every other particle, the equations in (1) hide a mathematical complexity that seems to be, from time to time, overlooked. What we would actually have for the 'state update' function in this case looks more like

$$\begin{aligned}\mathbf{x}_i(t + 1) = F[\alpha, \beta, r, v, t](&\mathbf{x}_i(t), \mathbf{x}_0(t), \ldots, \mathbf{x}_{i-1}(t),\\ &\mathbf{x}_{i+1}(t), \ldots, \mathbf{x}_n(t))\end{aligned} \tag{2}$$

Analytically, we could functionally define $N_i(t)$ with aid of an auxiliary function

$$\delta_r(d) : \mathbb{R} \to \{0, 1\}$$

$$\delta_r(d) = \begin{cases} 1, & \text{if } x \le r \\ 0, & \text{otherwise} \end{cases}$$

So as to obtain $N[r,i](t) = \sum_{j\neq i}\delta_r(||\mathbf{x}_i(t) - \mathbf{x}_j(t)||)$. With this, denoting, for convenience, $\mathbf{x}_0(t),\ldots,\mathbf{x}_{i-1}(t),\mathbf{x}_{i+1}(t),\ldots,\mathbf{x}_n(t)$ as $(\mathbf{x}_j)_{j\neq i}$, we have, considering together equations (1) and (2):

$$\begin{aligned}
&F[\alpha,\beta,r,v,t](\mathbf{x}_i(t),(\mathbf{x}_j)_{j\neq i}) = \\
&\mathbf{x}_i(t) + (\cos(\alpha+\beta\cdot N[r,i](t)\cdot \mathrm{sgn}(R_i(t) \\
&- L_i(t))), \sin(\alpha+\beta\cdot N[r,i](t)\cdot \mathrm{sgn}(R_i(t) \\
&- L_i(t)))) \cdot v \\
&= \mathbf{x}_i(t+1)
\end{aligned} \tag{3}$$

On the other hand, agent-based models are usually described in more qualitative terms, what, despite helping handling the above problem, tend leave simulations as the main method of studying such systems, which in turn leads to a hindered usage of mathematical analysis tools. A thorough discussion over this topic is given at Hinkelmann et al. (2011), wherein ABMs are effectively written as dynamical systems, not unlike what was done here. Essentially, they are seem as dynamical systems with local update functions: given a collection of variables $\{x_i\}_{i\in I}$, $\#I = n$ taking values in some field $\mathbb{F}$, we associate to each x_i an update state function $f_i : \mathbb{F}^n \to \mathbb{F}$ that takes inputs in the vicinity of x_i. This conducts to the dynamical system given by $f = (f_1,\ldots,f_n) : \mathbb{F}^n \to \mathbb{F}^n$. This idea is further developed until it yields an actual definition of an agent-based model.

Our emphasis, here, nonetheless, is to proceed with our discussion concerning the generalization of SPPSs, with results that, we believe, very closely relate to ABMs. Consonant with such purpose, we shall now consider the case where we have a variety of types of particles, as in *Clusters* or, more precisely, as discussed in CodeParade (2018)

In this model, that seems not to have a formal publication, there are three types of particles, with somewhat simple interactions between them.

Sketch

• There has been a long time interest in systems of particles with more complicated dynamics than those that we arise from physics alone.
• These systems often display, even with rules as simple as those that describe systems of physical particles moving under newton's laws, much richer behavior.
• In fact, they are in many ways essentially the same thing as agent-based models, which gained the spotlight in recent years and offer indeed a great framework for modeling complex systems.
• Being able to understand ABM as dynamical systems is great. Dynamical systems are older and have lots of tools.
• On the other hand, frameworks such as holonic systems might help simplifying physical models, since they deal of manners of providing descriptions of ensembles of agents and such, in a similar way to that used in physics, for instance, when aggregating particles in quasi-particles.
(quasi-particles as generalized particles; the possibility of aggregating some subsets of particles in a system as another particle – just like in holonic systems)

• It is common, in complexity science, to emphasize the surprisingly intricate behaviors that arise from somewhat simple rules, generally describing local interactions. The fact that these emergent phenomena are surprising is kinda undeniable. But we would like to point out another fact: that these simple rules are, very often, not as simple as they seem. That is not to diminish the mysterious beauty such phenomena have, but only to suggest a different look on them, one that, we believe, could improve our understanding of how such systems work and through which mechanisms do they develop such surprising behaviors. It might be the case that admitting that they are not *that* simple could lead us from a staggering astonishment to an enlightened contemplation.

• Complex systems are pretty damn complicated in mostly all of their aspects, from bottom up and conversely. But that is not all that there is to it. Flock models, for instance, suggest much the contrary. Birds are complicated systems, whereas flocks are quite simple. The point is quite different there: the emergent behavior is non-trivial, the uncoordinated coordination is fascinating, but it happens by means of much complex systems, like birds, acting like simpler agents, following simple rules.

Some particles, agents and dynamical systems

• Argue that SDPS are kinda in the intersection between DSs and ABMs.

Dynamical systems

Autonomous, Nonautonomous, Discrete, Continuous

Agent-based models as dynamical systems and conversely

• Relate DS with ABMs, show differences and similarities.

Flock model as dynamical system and as an agent model

• Exemplify with flock model.

The generalized model

Pretty examples

• Show implementations of the generalized model.

Conclusions

References

Axelrod, R. (2006). Agent-based Modeling as a Bridge Between Disciplines. In *Handbook of Computational Economics*, volume 2, pages 1565–1584.

Brilliantov, N. V., Abutuqayqah, H., Tyukin, I. Y., and Matveev, S. A. (2020). Swirlonic state of active matter. *Scientific Reports*, 10(1):1–13.

CodeParade (2018). Particle Life - A Game of Life Made of Particles. Retrieved March 9, 2021, from https://www.youtube.com/watch?v=Z_zmZ23grXE.

Helbing, D. (2001). *The Wonderful World of Active Many-Particle Systems*, pages 357–369. Springer Berlin Heidelberg, Berlin, Heidelberg.

Hinkelmann, F., Murrugarra, D., Jarrah, A. S., and Laubenbacher, R. (2011). A Mathematical Framework for Agent Based Models of Complex Biological Networks. *Bulletin of Mathematical Biology*, 73(7):1583–1602.

Hovey, K. (2020). Digital Astronomy with Cellular Automata. Retrieved January 7, 2021, from https://kylehovey.github.io/blog/automata-nebula.

Hovey, K. (2021). CA Nebula. Retrieved January 7, 2021, from http://kylehovey.github.io/automata-nebula-explorer/index.html.

Nagai, K. H., Sumino, Y., Montagne, R., Aranson, I. S., and Chaté, H. (2015). Collective motion of self-propelled particles with memory. *Physical Review Letters*, 114(16):1–6.

Schmickl, T., Stefanec, M., and Crailsheim, K. (2016). How a life-like system emerges from a simplistic particle motion law. *Scientific Reports*, 6(October):1–15.

Schweitzer, F., Ebeling, W., and Tilch, B. (1998). Complex motion of brownian particles with energy depots. *Physical Review Letters*, 80(23):5044–5047.

Ventrella, J. (2020). Clusters. Retrieved December 23, 2020, from http://www.ventrella.com/Clusters/.

Vicsek, T., Czirók, A., Ben-Jacob, E., Cohen, I., and Shochet, O. (1995). Novel Type of Phase Transition in a System of Self-Driven Particles. *Physical Review Letters*, 75(6):1226–1229.