Chapter

Multi-Agent Systems, Simulation and Nanotechnology

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Abstract

Multi-agent systems (MAS) are used in investigations with different purposes, mainly in computational simulations. These systems are composed of autonomous software entities, named agents, that act and interact in a shared environment, changing the state of the environment. Simulation environments for nanostructures can be considered essentially reactive, that is, suitable for reactive agent architectures. A significant feature in agent-oriented theory is autonomy, which also exists in small-scale structures such as atoms and molecules, despite the strong interaction. Regarding the organisation of a reactive or cognitive multi-agent system, there are events, constraints and interactions that occur in a nanoscale environment. So, MAS paradigm has methodologies and tools that could guarantee simulations of Brownian motion, at the nanoscale, generating and monitoring collision systems. Experiments for the nanocapsule production and characterisation should be supported by computational simulations, mainly to reduce experiment time, equipment wear and material waste. Therefore, this paper presents how MAS can increase the investigations in nanoscience through simulations of moving bodies.

Keywords: event-driven simulation, nanoparticles, reactive systems, distributed artificial intelligence

1. Introduction

Artificial intelligence is widespread in many areas of knowledge. It increases the quality of processing solutions of different problems. One of the areas in which artificial intelligence can also collaborate is in nanoscience [1], through multi-agent systems.

Nanoscience is the study of phenomena and manipulations of materials at atomic and molecular scales, where properties differ significantly from those at a larger scale. Nanotechnology is concerned with the design, characterisation, production and application of nanoscale structures [2]. Production and characterisation of polymer nanoparticles (PNPs), colloidal dispersion, are processes that require time and technical skills to produce accurate results. Computational simulations in nanoscience have aided in these processes, providing support and agility to achieve better results [3].

In order to help and reduce this gap, a simulation environment for nanocapsules —colloidal dispersion—was designed and built: multi-agent system for polymeric

nanoparticles (MASPN) [3, 4]. This tool can be considered innovative and unprecedented, as it combines event-driven simulation resources and the multi-agent system paradigm. This environment allows the researcher to enter input parameters, visualise particle interactions and monitor whether the dispersion is stabilising or not. The manipulation parameters are amount of particles, maximum and minimum particle sizes, mean particle distribution, zeta potential, pH, polymer, drug and drug content.

There are different types of polymeric nanoparticles (PNP), in which nanocapsules and nanospheres differ according to composition and structural organisation. Nanocapsules are defined by vesicular structures consisting of a thin polymeric shell and a normally oily central cavity where the active substance may be dissolved [5, 6]. Due to this, it is considered a reservoir system, which has a submicron diameter of less than 1 mcm, typically between 200 and 400 nm. The active component may be dissolved in the oily central cavity or may adsorb to the polymer wall [7–9]. Nanocapsules are composed of the drug, polymer, oil, surfactant and water and are produced by different methods with size distributions smaller than 1 μm. The nanometric size generates greater surface area, thus correlating their biological responses [10]. For this reason, the nanoparticles are suitable for applications in composite materials, transport and delivery of drugs and storage of chemical energy, for example, [7, 11]. PNPs attract researchers' attention because their bioavailability, biodegradability and photostability characteristics of drugs, to modulate interaction with cells and tissues, reduce drug adverse effects, increase encapsulation efficiency, increase solubility and reduce therapeutic doses and biological fluids during storage [7–10].

The nanocapsules can be produced with natural or synthetic polymers and can be used to encapsulate bioactive drugs and compounds. In addition, the polymers protect the lipophilic nucleus and control the release of lipophilic drugs. Therefore, the proper choice of the polymer is important to achieve specific purposes and modulate the release and degradation characteristics of the particles [7, 10].

Thus, computational modelling and simulation are resources that can produce accuracy in results, decrease production time and characterisation and preserve the life of laboratory equipment. Modelling and simulations through the multi-agent approach has been used in numerous investigations in biology, chemistry, physics, etc. [12].

We organise the text into sections. Sections 2 and 3 deal with computation applied to nanotechnology, and MAS paradigm focused on computational simulations. Section 4 presents the related works that investigated MAS as a tool to support nanotechnology. In the sequence, we present Section 5 that discusses the MASPN tool, its characteristics and functionalities. Finally, the conclusions and bibliographical references are presented.

2. Computational nanotechnology

Nanotechnology can be categorised in relation to applications, structures and tools. The tools are mechanisms to assist in the measurement, manipulation and development of nanostructures, and the area of computing provides innumerable resources to contribute to both measurement and manipulation of nanomaterials. Thus, we assume that computational nanotechnology contributes to molecular modelling, nanodevice simulation, high-performance computing, etc. [1].

We believe that computation applied to nanotechnology focuses on the design and construction of tools to aid the understanding of physical and chemical phenomena occurring on a nanometric scale, for example, in electronics, logic and

computing, sensors, drugs, cosmetics and new materials with specific characteristics.

Systems and computational simulation are carried out in time and space using analytical models and physical, chemical and material science fundamentals [1, 12, 13].

Molecular modelling involves computational methods and techniques to mimic the behaviour of atomic and molecular systems. We assume that modelling is the process of extracting really relevant information from a given system, such as structural aspects (set of attributes or characteristics and their possible values) and functional aspects (operations or methods and their constraints).

3. MAS and simulation

The MAS form an area of research in distributed artificial intelligence, manipulating aspects related to distributed computing in artificial intelligence systems [14]. These systems consist of several entities (agents) that interact in a shared environment in order to achieve some individual or collective goal.

The simulation studies the modelling of the functionalities (behaviours) of a physical or conceptual system over time [12]. These same authors state that for more than 20 years, the MAS field and the simulation field were combined into lines of research.

On the one hand, agents have been used as a tool for modelling and simulation of problems; on the other hand, simulation has often been used for MAS design in a variety of application domains. Thus, Uhrmacher and Weyns [12] believe that joint research efforts promise benefits between the two research areas and their work aims to integrate and consolidate the knowledge and experience gained in both areas.

The definition of the internal architecture of the agent is related to the task type that the agent will perform and its role in the multi-agent society.

In this way, what characterises an agent and the society that it is inserted in are the interactions with the environment and the internal processes that make possible the accomplishment of these interactions [14]. The specification of what and how these internal processes are is called architecture. Different architectures have been proposed with the objective of characterising the agents with a level of intelligence and autonomy. Therefore, the architectures can be classified according to the mechanism used by the agent to select actions [15].

Once considered this, agent can be classified as [14]:

- Reactive, in which the choice of action (response) is directly situated in the occurrence of a set of events (stimuli) that it perceives in the environment, captured by its sensors or by messages sent by other agents.

- Cognitive or deliberative, because it has an explicit process to choose the action to be performed. This action can be chosen, also, through a utility function and carried out by plan and a symbolic representation of the environment. A cognitive agent is a rational agent who has some explicit representation of his knowledge and goals. An agent may be more cognitive than another, depending on the degree of explicit rationality of his behaviour [14, 16].

Cognitive agent architectures [14] can be classified into functional architectures, in which the agent is composed of modules that represent each of the functionalities necessary for its operation. The agent has knowledge, set of objectives, perception

skill, communication, decision and reasoning. There are also architectures based on mental states, which adopt a psychologically inspired perspective to define the structure of agents, which are entities in which the state consists of mental components such as beliefs, desires, capacities, choices and commitments. It may be that a mental state-based architecture also has functional aspects and vice versa [15].

Definitions and properties that characterise an agent are not meant to divide the world between entities that are and are not agents but serve as tools for analysing systems as well as specifying, designing and implementing systems whose basic elements are agents [17].

Thus, we assume all approaches to modelling and development of multi-agent systems can be classified as top-down and bottom-up. Top-down approach specifies the organisation towards the structure and behaviour of agents, while the bottom-up approach starts from the individual aspects of an agent in a way that the collective aspects emerge. This classification is very similar to nanostructure development methodologies, with the same principle, top-down and bottom-up.

3.1 MAS modelling and implementation tools

In recent years, many agent-based system development tools or environments have been deployed (or released). Each environment has a variety of features and functionalities. There are some studies comparing these tools, for example, [18]. The research evaluated whether tools have some features and functionalities, such as (i) an integrated development environment, (ii) what the programming language is, (iii) the operating system, (iv) manuals and examples, (v) integration with other libraries and (vi) 2D or 3D visualisation.

The modelling and verification of multi-agent systems present many challenges, especially when it comes to reliability, robustness and visualisation of the simulated system (spatial properties) [18]. Thus, visualisation property of simulation scenarios is also an important property in the construction of simulation systems.

Multi-agent simulation environments suitable for the context of nanoparticulate systems are:

- FLAME[1] is a general agent-based model building system that generates highly efficient simulation software that can run on any computing platform, such as high-performance parallel supercomputers and GPUs. You can set up large-scale models with millions of agents.

- JASON[2] is a multi-agent system development environment with many user-customisable features. It is the interpreter for the AgentSpeak language.

- MASON[3] is a discrete event library for multi-agent simulation in Java language.

- Netlogo[4] is a simulation environment, that is, it is both a programming language and a programmable modelling environment for the simulation of multi-agent systems. It has a graphical interface for visualisation of the simulations.

[1] http://www.flame.ac.uk

[2] http://jason.sourceforge.net/wp

[3] http://cs.gmu.edu/eclab/projects/mason

[4] https://ccl.northwestern.edu/netlogo

- Repast[5] is a set of free and open-source platforms for multi-agent modelling and simulation. It has Java versions for workstations and small clusters of computers and C++ for supercomputers and high-performance computing clusters.

- SeSAm[6] is a generic environment for the modelling and experimentation of agent-based simulation. It is a tool for building complex models, which include dynamic interdependencies or emerging behaviour.

- SWARM[7] is a general-purpose simulator, mainly of social complexity based on the programming languages Objective-C and Java.

Of the tools analysed, only JASON and SWARM do not have an integrated development environment, but JASON can be incorporated (as a plugin) in other development environments. All tools run on major operating systems and have excellent developer support. FLAME and Repast are the only ones that do not have an open source, that is, they do not allow you to change the source code of the tool. The NetLogo tool stands out because it also has the integrated simulation execution environment. FLAME and Repast can be executed in computational clusters or in graphic cards, allowing the large-scale simulation of many agents.

We did not investigate issues of performance and robustness of the analysed tools.

4. Related works

In this section, we will present some works in the context of nanotechnology that used MAS as an evaluation or simulation tool.

4.1 Multi-agent system simulation of nanorobotic drug delivery in tumours of body tissues

The paper discusses the simulation of specific drug delivery in tumour tissue through MAS simulation [19]. The simulation was designed, implemented and evaluated with reference to some initial requirements, such as energy consumption, drug loading capacity and the perception of some agents. The work has simulated the behaviour of nanorobots, the agents responsible for drug delivery. The use of nanorobots was proposed as a hypothetical situation, and the main characteristics were biocompatibility, minimum energy for operation, communication and navigation skills (e.g., target search) and decentralised and cooperative coordination. The proposal of the nanoparticle simulation experiment was recognition and binding to the target, with the release of the drug and with biodegradation protective surface. For this, three types of nanorobots were designed: searcher, digger and killer (drug delivery).

Due to the complexity of the biological system, it was necessary to apply layers of abstractions and to focus on some parameters and functionalities. For example, the way nanorobots are injected has been disregarded. However, blood flow (velocity) and obstacles in blood (macromolecules) were taken into account.

[5] http://repast.sourceforge.net

[6] http://130.243.124.21/sesam

[7] http://xenia.media.mit.edu/nelson/research/swarm

The limitations of the simulation tools for time, size, density, viscosity, size of nanorobots in relation to body cell size and energy resources by the nanorobots were all considered in the simulation.

The NetLogo simulation platform was used for the construction and execution of the simulation. The results obtained were the visualisation interface generated and the analysis of some situations, as if the tumour was eliminated, if there was failure to eliminate the tumour or failure to complete the experiment. For this, 500 simulations were executed for each experiment, with the following parameters: number of searcher type agents, number of load capacity and radius of diggers, number of load capacity and energy of killers and agents and agent collaboration.

The purpose was to estimate the ideal parameter values for the possible experiments (qualitative analysis). The conclusions were as follows: it is possible to have a combination of values in the parameters that eliminate the tumour; large numbers of diggers do not eliminate the tumour; the amount of drug loading influences tumour clearance rather than the radius of perception; mean values in the parameters cause tumour elimination; and the greater the energy allocated to the agents, the greater chance of elimination of the tumour.

Finally, the authors conclude that drug delivery through nanostructures is a promising area, as nanotechnology is more widely used, be it in the development of structures to coat pharmaceutical substances and proteins or in the design of chemical sensors and structures with "stealth" property (are not detected by the immune system).

4.2 Agent-based modelling of stem cells

Here, MAS was used for biological simulation of complex system (modelling and simulation) known as haematopoietic stem cell (HSC) system in adults [20].

Biological systems have reactive and complex behaviour, such as self-regulation and self-organisation, and it is a challenge to understand the mechanisms and processes of interaction. Therefore, in the use of MAS, as they are recognised for modelling and simulation of these complex systems [20], since they explicitly represent the environment, the cells are modelled as agents containing the physical, chemical and biological properties, and there is facility in changing experiment parameters.

The haematopoietic stem cell system in adults has limitations, such as difficulty in tracking stem cells in adult human bodies, making it impossible to observe the behaviour of the system. The alternative presented is to use modelling and simulation to understand both individual and collective behaviours (prediction). In the research, a framework was proposed containing the base structure of the simulation environment, agents representing the cells, stochastic processes of the simulation system, etc.

For the experiment, the MASON library was used. The main components of the structure were modelled and implemented separately. Cellular agents were used to model the individual cells of the system. The environment represents the physical, biological and chemical environment where the cells meet. The simulation mechanism promotes the "movement" of the simulation of a cell system. This is done by updating the environment in response to agent requests and signals.

An important point to note in the work is environment initialisation that includes chemical and topological information that reduces the need to resort to stochastic processes. In addition, it is possible to model the physical movement of cells to ensure self-organisation in stem cell systems.

4.3 Coordinating microscopic robots in viscous fluids

In [21], the multi-agent control (by simulation) is discussed that provides strategies to agglomerate microscopic robots (named in the text as nanorobots) in environments of fluids relevant for medical applications. Unlike larger robots, viscous forces and Brownian motion tend to dominate behaviour. Examples range from modified microorganisms (programmable bacteria) to robots used in the development of molecular computing, sensors and motors. Controls were evaluated for the location of a cell of specific size by emitting a type of chemical signal in a moving fluid. Parameters corresponding to chemicals released in response to injury or infection in small blood vessels were also considered.

These authors state that robots, with sizes comparable to bacteria, could provide new skills through their ability to feel and act in small-scale environments. Robots could be useful in a variety of biological and medical research contexts. For example, robots and nanoscale materials inside the body can improve the diagnosis and treatment of diseases [21]. However, making these robots is beyond the capacity of current technology, but progress in nanoscale engineering devices could eventually allow the production of such robots.

In that paper, they affirm that it is possible to evaluate control methods, before constructing the robots, by means of simulation, thus guaranteeing an environment with chemical signals, movement of cells and robots according to the characteristics of the fluid. Robots could act independently, for example, by detecting specific patterns of chemicals. Such coordinated action would produce an agglomeration effect, necessary for a rapid and adequate response to infection [21]. The agglomeration of small-scale robots differs significantly from larger robots in several respects. First, the physical environment is dominated by the flow of viscous fluid and requires movement in three dimensions. Second, thermal noise is significant for sensors, and Brownian motion limits the ability to follow precisely specified paths. Third, targets are recognisable through chemical signatures rather than visual markings or specific forms. Fourth, tasks involve a large number of robots, each with limited capabilities in sensing, communication and computing.

Thus, these characteristics suggest that control by multi-agent simulation with reactive architecture is particularly well suited for robots on a very reduced scale.

4.4 Related work considerations

In nanoscience investigations, nanostructured drug delivery research is conducted in a number of research centres and can be considered one of the most promising.

In [19], the drug delivery and MAS areas were combined. The relation with this work happens through the use of the simulation tools, statistical model for the evaluation process and the layers of abstractions. In relation to the work presented in dinverno:2009, this research also specifies, performs and evaluates the behaviour of interacting particles obeying a dynamics of self-organisation. Another relation is there is the possibility of changing the values of the input parameters.

A contribution in [21] is how groups of robots were collectively controlled (individual vs. collective behaviour in response to the environment and other agents).

Generally, computational studies of controlling groups of robots complement the studies to control individually. And this can be extended to a system with particles that exhibit coordinated behaviour in response to different stimuli, for example, the agglomeration effect generated by physical-chemical properties of the environment, as ionic strength of the environment.

5. MASPN: multi-agent system for polymeric nanoparticles

Finally, we present MASPN simulation environment [3, 4, 17], an environment built with the Java language that integrates JASON and the *algs4* simulation package. The *algs4* package contains the entire implementation of equations of the Brownian model that guarantee elastic and inelastic collisions. MASPN has been developed according to the feature-driven development methodology of software design and the methodology of multi-agent systems.

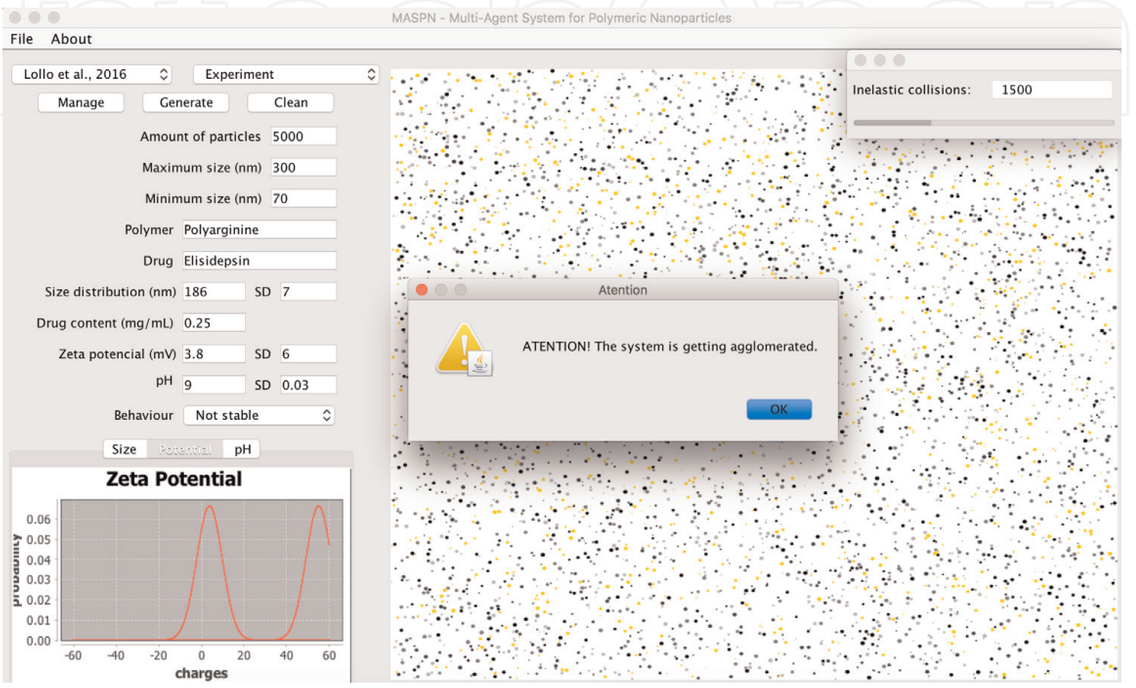

Figure 1.
MASPN tool interface.

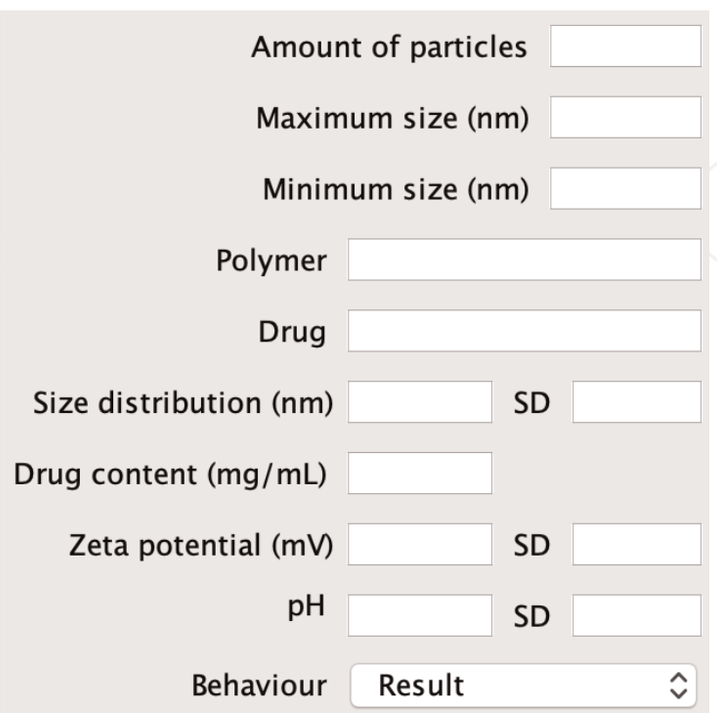

Figure 2.
Simulation parameters in MASPN.

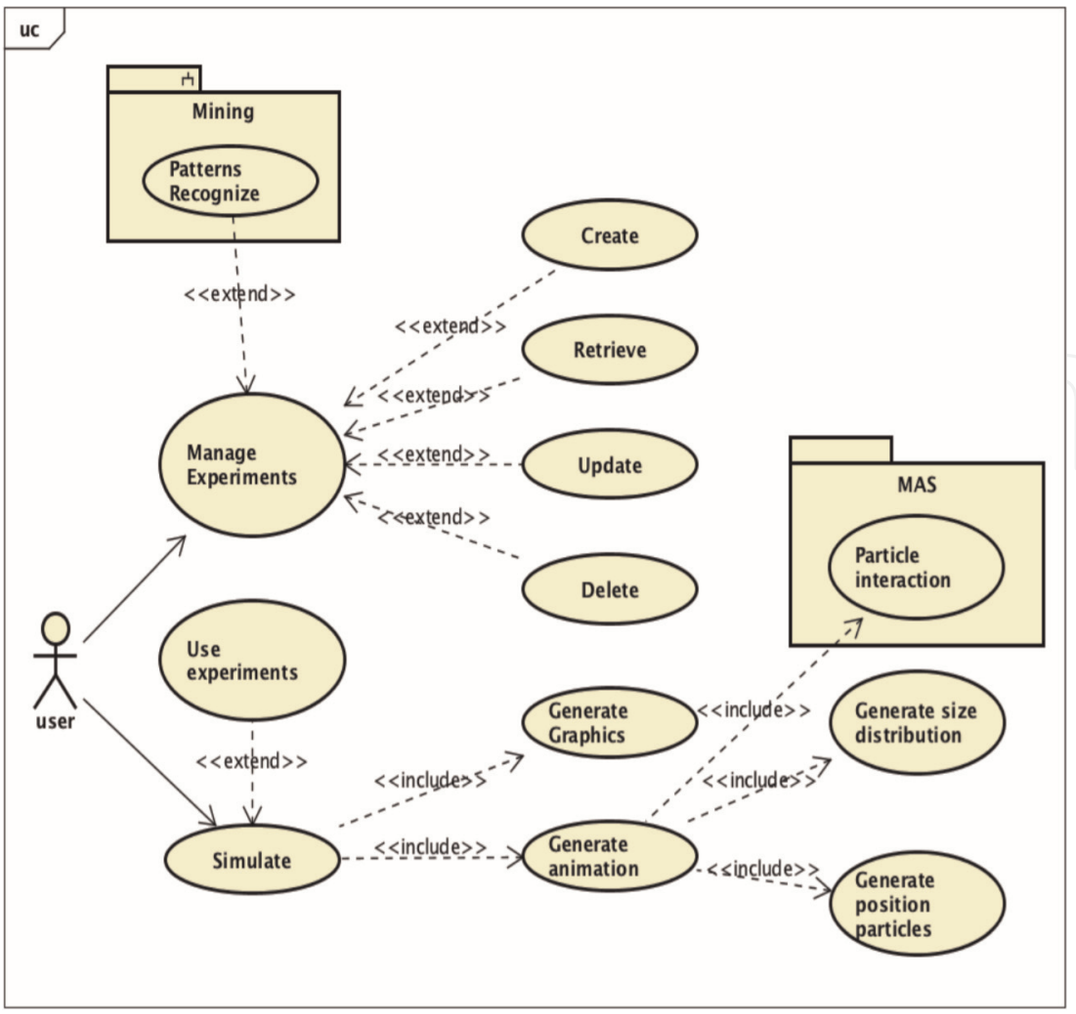

Figure 3.
Use-case diagram: MASPN main features.

The MASPN environment emerges as the main result of this research, since it is an alternative simulation tool, containing graphical interface with integrated physicochemical parameters, distribution graphs (particle size, particle zeta potential and environment pH) and particle animation under the Brownian mathematical model (**Figure 1**).

The parameters of the simulations, for evaluation of the agglomeration effect, are size, size distribution, surface electric charge, mass, drug content and pH (**Figure 2**). The simulation environment designed and built, integrating areas, methodologies and technologies can be considered a resource in the production and characterisation of polymer nanoparticles, since the simulations performed had significantly accurate results.

Figure 3 shows use-case diagram that represents all the possible functionalities of the system, for example, managing experiments and performing simulations. The results of the simulations are the interactions between the particles (agents) and the environment. The interactions obey Brownian motion of collisions, and the collisions that generate agglomeration are counted and announced in the system.

6. Conclusions

Nanostructured simulation environments can be considered reactive, ideal for reactive agent architectures. Some computing researchers would tend to indicate

the use of distributed problem-solving techniques rather than MAS. However, MAS makes it possible to design complex simulation systems in a naturally distributed and bottom-up way.

The MAS paradigm is based on natural systems, where there is emergence of intelligent behaviour from the interaction of its elements, as occurs in an anthill (the colony has an intelligent behaviour, whereas the ant does not) and in the neurons (simple cells but from their interaction and organisation emerges a complex and intelligent behaviour) [16].

The group has characteristics that cannot be reduced to its base elements. At this point, we do not say that nanoparticles have intelligent behaviour, but rather complex, once they interact with an organisation scheme and a very reactive environment.

A significant feature in an agent-oriented theory is autonomy, which also exists in scaled-down structures such as atoms and molecules, despite the strong interaction. Regarding the organisation of a reactive or cognitive multi-agent system, there are events, constraints and interactions, which also occur in a nanoscale environment.

For example (**Figure 1**), a particle is an agent that interacts with other particles and the wall of a box. The box is the environment containing the solvent (which would dissipate or not the interaction energy of the particles). In this way, the particles must perceive other particles, the walls of the box and the solvent of the environment. Next, plan your next actions (calculate the elastic or inelastic collision forces), and act (update trajectory and velocity data).

From the approaches to MAS development, the bottom-up approach is well indicated, first, because agents are designed independently of some specific problem; second, because inter-agent interaction is not built in advance but in generic situations by specifying a communication protocol for agents; and third, because there is no centralised control. Thus, there are advantages such as the feasibility of adaptive and evolutionary systems, in which MAS has the ability to adapt to new situations (inclusion or exclusion of agents or changes in the organisation).

As already mentioned, it is naturally suitable for the modelling of complex and concurrent (or distributed) systems, that is, suitable for simulations in nanostructured environments.

The MAS area is consolidated, with methodologies and tools for the design and implementation of multi-agent systems, both reactive and cognitive.

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Conflict of interest

The authors declare no conflict of interest.

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