Dynamical modeling of complex systems: a microscopic approach

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Introduction

The purpose of this note is to discuss how the microscopic approach, successfully used for the physical systems, can be extended to complex systems. The first difficulty we face is a universally accepted definition of complexity. Dictionaries refer to complexity as the result of many connected parts or elements, to complex as a synonym of complicated. The first definition applies to any macroscopic system, which has a large number of interacting elementary components. The emergent large scale properties are related to the microscopic dynamics even though its details are not relevant. Certainly these systems are complicated because they are non linear and exhibit a weakly or strongly chaotic behaviour.

I will restrict the denomination complex to the the living systems and to the artificial life systems. This is a personal viewpoint because I could not find a consensus on the subject, wandering in my library or navigating in the web. In the absence of a reliable selection criterion to sort the vast amount of information on the subject, it is reasonable to look back at the classics, namely to those authors, whose ideas have strongly influenced the development of science during the last half century and even further away in the deep past, since most of the funding ideas in science have ancient roots [1]. If this claim holds for physics it is especially true for complex systems, where the philosophical speculation has been active for thousands of years. A generally agreed feature of complexity is its trans-disciplinary character. Several aspects of complexity related to life and human societies have been extensively investigated by specific disciplines. What is really missing is a common language and a common theoretical approach. Physics and information science can provide a conceptual framework suitable to take into account, in a rigorous and synthetic language, the phenomenology developed by the disciplines dealing with specific aspects of complex systems. The forties and the fifties have been the golden age in which this process was initiated and solid basis were established by eminent scientists like Von Neumann [2], Wiener [3] and Turing. They have built a bridge between hard and soft sciences by providing the mathematical foundations of the information science. The increase of performances of computing devices has been exponential henceforth but the conceptual design of hardware architecture and software structure has not changed significantly. The steady progress of computation capabilities and the development of nanotechnologies have boosted the development of modern life science from biochemistry to molecular genetics, from systems to synthetic biology. Information science emerged in the forties from joint research in neurophysiology, mathematics, control theory and electrical engineering and is in many respects complementary to physics, whose goal has been the search of the elementary units of matter and the discovery of the universal laws governing their interaction. As a consequence reductionism has been the key-word and the driving force of any experimental and theoretical investigation. Combined with a rigid determinism of the time evolution laws it leads to some apparent paradoxes related to reversibility which emerged when the statistical-mechanics interpretation of thermodynamics was proposed. These paradoxes are easily resolved by importing within the physical framework the notion of information content. The framework of real analysis is suitable to formulate Newton’s laws or Maxwell equations, but assumes that an infinite information content is accessible, since we deal with real numbers. For weakly or strongly chaotic systems simple
conceptual experiments produce results conflicting with common sense and every-day’s experience. The paradoxical results of any mathematical theory where the access to an infinite information content is implicitly assumed are also known in economics where the agents are infinitely rational and capable of making at any step the optimal choices. As a consequence they make the optimal move in a game where this is known to exist even though cost to find it can be incredibly high. In addition there are equilibria, on which the system can accommodate permanently, because no random disturbance capable of driving it away is allowed. Physical systems like the atmosphere have limited predictability due to their internal instabilities and the limited amount of information on their initial state. An extremely accurate determination of the microscopic state would interfere with it just as for a quantum system because the amount of required energy is macroscopically relevant. In the case of biosystems the existence of several scales of organization, where the constituents form a network with metastable equilibria and emergent properties, prevents a strongly reductionist approach. The research is focused on the detection of the elementary components, at the molecular level, and on the measure of their interactions. The reconstruction of the global pattern allowing to explain the functioning of a cell and to simulate it is one of the present challenges. The dynamic modeling of the nervous and immune systems taking into account the cells repertoire, their interactions and connections is another undertaking. The selection of the basic rules defining the interactions of living creatures among themselves and with the environment and their simulation is a preliminary step to understand a variety of phenomena ranging from the dynamics of herds or swarms, to urban mobility, social behaviour and economics.

We search the paradigms of complexity in the living systems, trying to detect, at any level of organization, the elementary units with their essential physical and cognitive (information processing) properties. The existence of many levels with specific space-time scales suggests a hierarchical organization in a sort of hypernetwork where the organized emergent structures at one level become the elementary units at the next one. A similar organization occurs in the aggregation of letters of an alphabet to forms words and sentences, of sentences to form paragraphs, chapters and books, of books to form a library. Having fixed the level, the basic properties of the corresponding elementary units and the rules of their interactions, it is difficult to describe mathematically the coherent structures resulting from a self organization and the evolutions towards quasi equilibrium states. The mean field equations, obtained in the continuum limit, describe the collective phenomena but their solution may also require sophisticated numerical procedures. Adopting physical models such as spin systems or charged particle systems, for which mathematical results are available, implies drastic or unjustified simplifications. The alternative to the analytical description is simulation. After a statistical analysis of the results it may provide the basis for a theoretical understanding and a formal theory. The simulation is a way of approaching a complex system by imitating it in a simplified form. Any artifact having the properties of life, such as a computer simulation or an assembly of robots, is a form of artificial life [4]. A literary text or an artistic work are also a forms of artificial life since they recreate life to communicate feelings and emotions. Knowledge is the only goal of a computer simulation and in this respect it is similar to the process we develop in our mind mirroring the real world we perceive.
1 Physics and complexity

Every material system, we perceive with our senses, amplified by our instruments, can be subject of physical investigation. The process of knowledge is based on reproducible experiments and on the reduction of the observations to simple and universal laws. This was achieved by looking at the elementary constituents of matter, after the discovery of the gravitational law which governs the behaviour of the celestial bodies. Later the laws of thermodynamics provided a satisfactory description of the changes of state and of the energy balance including heat. The theoretical nature of physics, even though this science is based on experiments, was already pointed out by Aristotle [5]

Therefore, if any rational knowledge is either practical (political) or poietic (engineering) or theoretical, physics shall be a theoretical knowledge not separated from matter......

The search of the ultimate elementary components, quarks and leptons, eventually strings, and of the final law governing all the interaction of matter is powered by an implicit belief that, once this process is achieved, we shall have the key to explain the whole universe from the smallest to the largest scale, from its first instant after the big bang, to the last instant of its existence. This strongly reductionist viewpoint implies that the final unified theory of fundamental interactions, known as TOE (theory of everything), would explain cosmology on one side, nuclear and atomic physics on the other [6]. Since chemistry, is a consequence of the laws governing the atoms and biology is reducible to the chemistry of some polymeric chains, one might extend the argument to conclude that that TOE finally is the key to explain sociology, psychology, human sciences and beyond. Following the chain from the top to the bottom would be a mere computational problem. From the epistemological viewpoint this is very similar to Laplace’s claim: given the initial conditions and a sufficiently powerful computer, the future of the whole universe can be predicted and its past can be reconstructed. This program fails even if we deal with much simpler systems like a variable pendulum or a few balls in a billiard, because these systems are not regular and consequently predictable on a long time scale. A plausible argument to contrast the strongly reductionist viewpoint is the following: if a TOE exists there is absolutely no reason why it should be integrable, except in some asymptotic limit, very far from ordinary conditions of matter, which allow the atoms to form, the large polymeric chains to be assembled and so on. Some theoretical physicists claim that once TOE is found physics will die [7], coherently with an irreducible reductionism. Certainly the physics of the extreme scales, the physics of simple and universal laws will reach its terminal point. On the contrary the physics of all the phenomena at intermediate scales, the physics of complex systems will grow and flourish, since number of open questions is endless. Possibly it will take a long time or forever before anything as general, simple and elegant as Newton’s laws or Maxwell’s equation will pop out from the physics of complex systems. Nevertheless the physical approach based on the Newton’s and Boltzmann’s paradigms, jointly with Von Neumann’s paradigms of information science and Darwin’s paradigm of evolution will provide the theoretical frame to approach the complex systems and the technical tools to simulate them.
Order and chaos The systems at intermediate scales have usually a complicated behaviour. Regular motions occur only in presence of a complete symmetry and the system is equivalent to a collection of clocks running at different speeds, eventually masked by some distorting transformations. This is the case of the planetary motions, as long as mutual interactions can be neglected. The system without symmetry or with partial symmetries are by far more frequent; they are generic, using the correct mathematical terminology. They exhibit chaotic motions in the extreme case or an interplay between regular and chaotic motions visible on an arbitrarily small scale. A strongly chaotic system becomes simple from the statistical viewpoint.

The loss of regularity is associated with the appearance exotic (fractal) geometric structures and the exponential behaviour in time typical of unstable equilibria. In this case a small change in the initial conditions causes important deviations in a short time. The loss of memory of initial conditions is exponentially fast, whereas it is linear for the regular systems. Moreover in the latter the linear change concerns the phases, because the orbits belong to very close invariant manifolds. The appearance of chaos is not a feature of systems with many degrees of freedom like a gas or a plasma, but can be be observed in a pendulum whose suspension point oscillates or in the asymptotic dynamics of a reduced model for the atmosphere like the Lorenz system, see figure 2.

Even in presence of chaos the evolution preserves its deterministic character if the state of system at any time is expressed by real numbers, that is infinitely long binary (or decimal) strings. In this case by reversing the speeds at any time \( t \) we are back to the initial state at time \( 2t \). If the accessible information is finite, that is we know the velocities with a finite accuracy, the return to the initial state will by be possible only up to a time \( t \) shorter than
the time required to lose memory of the initial conditions. As a consequence reversibility will be observed only for short time intervals, the same time intervals on which the system is predictable [8].

**Complex systems** We define complex the living systems and artificial life systems. The essential properties are: self organization, perception and memory, self-replication. Complex system are characterized by a variety of space time scales corresponding to different levels of organization: macromolecules (DNA, proteins), cells, organs, individuals, ecosystems [8]. The elementary components interact and can self organize as networks. By drawing a line between two connected components, we obtain a pattern which illustrates the organization structure, whereas a quantitative information is provided by the statistics of links [9]. The frequently observed scale free networks are intermediate between random and hierarchical networks and achieve a good compromise between robustness and efficiency. A network becomes the elementary unit at a higher level so that a hierarchical structure on many levels is defined. The network is the crudest description of many interacting units. The description as a dynamical system is limited by our ignorance of the interaction laws and by unavoidable internal and external randomness. The elementary component of a complex system can be represented by a Von Neumann automaton. It has a physical space and cognitive properties, which might be implemented with bistable systems [10], neural networks, or by assigning the probabilities of possible choices. The hardware obeys physical laws. As a consequence the automaton moves in a given environment avoiding the obstacles perceived by its sensors. The software processes the information received from the environment, stores it and takes decisions. The self replication is the most subtle aspect, because it requires a reservoir providing the necessary components and a directive to carry out the process. If during the self replication process random mutations are allowed, a selection based on fitness insures a Darwinian evolution of the automata. The theoretical possibility of the entire replication process was proved by Von Neumann.

**Figure 3** Microscopic model for a physical system: the gas of hard spheres. The DNA helix (center). The gas of automata in a urban environment (right)

The basic difference between a physical system like a fluid or a crystal and a complex system is the structure of the elementary units and consequently the kind of organization they achieve. In the first case the elementary unit is an atom, a molecule, or an aggregate, described as a mechanical system with a few degrees of freedom (point mass or rigid body). In the second case the elementary unit has a hardware and a software capable of information processing and of coding the project for the self replication. Von
Neumann itself first pointed out the correspondence between the hardware and software of an abstract automaton with the proteins and the nucleic acids, which are essential for the metabolic processes and the self replication. The appearance of molecules capable of coding the information required for self replication and for assembling the proteins, which allow the metabolic functions, was a necessary condition for the emergence of life. Life has progressively taken an increasingly large number of forms. Inert matter also exhibits a huge variety of shapes, classified, since the presocratics, into four different categories. They correspond to the four aggregation states of matter: plasma, gas, liquid, solid whose transitions are governed by pressure and temperature. The elementary constituents are electrons and ions for the plasma, atoms or molecules for the the remaining three states. The atomic hypothesis, underlying the structure of matter, which reduces the aggregation states to emergent properties of the same material substrate, was first proposed by the Greek philosopher Democritus, who also had the intuition that the atoms might follow chaotic trajectories. Even though to interpret life as a fifth state [11] might be questionable, certainly its appearance is a huge jump a sort of discontinuity with respect to inert matter, in any of its states. The theoretical description and modeling of any living system requires a new approach based on the key paradigms and techniques of physics, information science and biology.

2 Particles dynamics and thermodynamics

After the foundation of modern mechanics by Newton and Lagrange, a mechanical explanation for most physical process was systematically looked for. Along this way the possibility of obtaining from mechanics the laws of thermodynamics was explored by Boltzmann and Gibbs. They succeeded and founded the statistical mechanics, which establishes the connection between the microscopic dynamics of a system and its large scale properties, by using the probability theory. Assuming molecular chaos, for which we presently have theoretical support and numerical evidence, Boltzmann wrote an equation from which the local relaxation to the thermodynamic equilibrium can be proved and the continuum mechanics with its constitutive equations can be derived. Its derivation is rigorously justified for a dilute gas of particles with short range interactions. More precisely for a gas of \( N \) hard spheres of radius \( R \) per unit volume Boltzmann’s equation holds in the limit \( N \to \infty \) provided that the product \( R^2 N \) is kept constant. In such a limit the collisionality is preserved since the mean free path remains constant. The short range repulsive forces cause a very rapid relaxation to the equilibrium state, also in presence of an external field, which just changes the space distribution at equilibrium. In the absence of collisions each particle moves under the action of the external field only. The collisionless limit, known as the mean field limit, describes a perfect gas: the momentum of each particle or its norm is preserved depending on the boundary conditions (periodic or reflecting), see figure 4. The initial momentum distribution is preserved and if it is smooth a uniform space distribution is reached by filamentation. The equation of state \( PV = N k_B T \) holds as a consequence of the virial theorem. In order to reach the Maxwell-Boltzmann equilibrium distribution for the momenta the collisional randomization is needed. The collisions cause a rapid loss of memory of the initial conditions. The reason is that each collision causes a divergence of
the orbits. This is exactly what happens when a beam of particles or light rays is reflected by a convex mirror, see figure 3. Since the problem of $N$ colliding spheres can be treated only numerically, a phenomenological description is obtained by considering a point mass moving in a viscous medium, subject to a random impulsive force $\xi(t)$ (white noise) and eventually the external field. Letting $H = p^2/2m + V_{\text{ext}}(r)$ the equations of motion read

$$\frac{dr}{dt} = \frac{\partial H}{\partial p} \quad \frac{dp}{dt} = -\frac{\partial H}{\partial r} - \beta p + \gamma \xi(t) \quad (1)$$

![Figure 4 Divergence of trajectories after reflection on a convex surface (left). Trajectories of the particles of a perfect gas in a box with reflecting (center), periodic (right) boundary conditions.](image)

The probability density function satisfies the Fokker-Planck equation, whose equilibrium solution is the Maxwell-Boltzmann distribution where the temperature $T$ is given by $k_B T = \gamma^2/(2 m \beta)$, having denoted by $k_B$ the Boltzmann’s constant.

When the interactions have a long range the picture changes considerably since all the particles interact. In this case the field acting on a particle can be split into two distinct contributions: the near field, due to the particles within a sphere of small radius (Debye’s sphere), the far field generated by all the remaining particles. Nearby particles collide, whereas the far field is obtained by replacing the point charges with a continuous charge distribution. As a simple example we consider a system of $N$ parallel charged strings which are confined by an elastic potential and repel each other according to Coulomb’s law, see figure 5. Letting $m$ and $q$ be the mass and charge per unit length of each string the Hamiltonian reads

$$H = \sum_{i=0}^{N} \left( \frac{p_{x_i}^2 + p_{y_i}^2}{2} + \omega_0^2 \frac{x_i^2 + y_i^2}{2} \right) - \frac{\xi}{N} \sum_{i<j} \log(r_{ij}) \quad (2)$$

where $\omega_0$ is the elastic oscillations frequency of the neutral strings, and $\xi = 2 (Nq) (q/m)$ is repulsive strength of the charged strings. These parameters do not change if we very $N$ keeping fixed the total mass and change per unit length. The limit $N \to \infty$ corresponds to a continuous charge distribution, and the mean field theory holds since the collisional effects vanish [12] The single particle phase space density $\rho(x, y, px, py)$ satisfies the Liouville equation for an Hamiltonian $H_1$ which includes the potential of the electric field generated by the corresponding charge distribution.

$$\frac{\partial \rho}{\partial s} + [\rho, H_1] = 0 \quad \nabla^2 V = -4\pi \rho_s \quad H_1 = \frac{p_{x}^2 + p_{y}^2}{2} + \omega_0^2 \frac{x^2 + y^2}{2} + \frac{\xi}{2} V(x, y) \quad (3)$$
where $\rho_s$ is obtained by integrating $\rho$ over the momenta. An equilibrium solution corresponding to a uniform charge distribution in a cylinder of radius $R$ which generates, in its interior, a quadratic electrostatic potential. The radius grows with the charge intensity $\xi$, due to repulsion, and with the average kinetic energy, due to heating. For initial distributions in a cylinder of radius close to $R$ periodic oscillations are switched on, just as any mechanical system does when it is slightly displaced from its equilibrium configuration. Other types of collective motions are observed by choosing different initial conditions and linear instabilities may occur due to the breaking of the cylindrical symmetry. The collisions are taking into account by introducing a noise in the mean field equations, according to Landau’s phenomenological theory. As a result any initial distribution relaxes towards the a Maxwell Boltzmann distribution with a self consistent electric potential. The main difference with the case of short range forces is that the system has a rich structure also in the mean field limit due to the presence of the self field. The systems with long range forces exhibit self organized structures, which are well known in the case of gravitation where the galaxies exhibit a large variety of shapes. There is a correspondence between charged strings model and a cluster of rotating stars since the centrifugal and gravitational forces are just the opposite of the elastic and electrostatic ones. The model of charge filaments describe a beam in a circular accelerator at moderate energies. When the beam is cooled symmetric structures like crystals are observed, see figure 5 and these patterns are predicted by the model. Strong and weak chaos, related to short and long range interactions, are dynamically and statistically quite different. The former triggers very rapid relaxation to the thermodynamic equilibrium, the latter allows metastable collective states slowly relaxing to equilibrium. The systems with long range forces are closer to the living systems, since they exhibit a variety of coherent structures, see figure 5, which change dynamically and slowly disappear under the action of collisions. Weak chaos and quasi integrable motions are typical of these systems and the dynamics at the edge of chaos has been proposed as a metaphor of the environment required for the emergence of life [13, 14]. As a consequence it might be appropriate to call these systems pre-complex.

Figure 5 Charge filaments (left). Coulomb crystal observed in a cold beam experiment (center). Structure of galaxies (right).

3 Automata dynamics and thermodynamics

The model we propose for the microscopic description of a complex system is based on a set of interacting Von Neumann automata [15]. Different microscopic models have been
considered have been considered in the framework of artificial life systems [16]. The aim
is to detect the key control parameters and to gather information on the global behaviour
of the system, by using the procedures of statistical mechanics. We introduce two distinct
spaces: the physical space and the cognitive space. The first one describes the physical
environment the second one the internal states of the automaton. Time is continuous
and the dynamical evolution of the automaton in the physical space is governed by the
directives issued from the cognitive space. These directives are also the result of a
dynamical process, which consists in processing the perception of the environment with a
behavioural code, which may eventually change to reach an assigned goal in an optimal
way. In the simplest models the separation between the two spaces disappears because the
directive is simply a force field depending on the kinematical state of the automata and
on the boundaries (obstacles).

Complex systems have been investigated by population dynamics models (Lotka Volterra
like equations) and reaction-diffusion equations, which may be considered the mean field
equations of an underlying microscopic model. The theory of networks has been success-
fully used to explore the statistics of links between the elementary units which often exhibit
some kind of hierarchical organization [9]. At the microscopic level the cellular automata
and the agents based models are frequently used. The former are defined on a discrete
space and time and by local interaction rules, the latter are similar to our automata which
act in a continuous space time with a decision mechanism triggered by the stimuli received
from the environment.

Our goal is not to simulate the real system as faithfully as possible, but rather to obtain
a description of its most relevant features in the simplest possible way, so that the key
variables can be detected and the large scale features are provided by a mean field limit.
We describe below some models, based on identical automata. Though many systems
exhibit vast repertoires and require a more elaborate description, our choice is motivated
by simplicity, which allows to obtain some analytical results. In addition the equilibrium
statistical mechanics, shows that the details of microscopic interactions are sometimes
irrelevant: this is the case of phase transitions governed by scaling laws with universal
exponents.

<table>
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<th>Physical system</th>
<th>Complex system</th>
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<tr>
<td>Physical space: Newtonian dynamics</td>
<td>Physical space: non Newtonian dynamics</td>
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<td>Cognitive space: decision dynamics</td>
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<tr>
<td>Unit: point mass or rigid body</td>
<td>Unit: Von Neumann automaton</td>
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<td>Repertoire: small</td>
<td>Repertoire: large</td>
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The models for complex systems are distinguished according to the dimensionality of the
physical space. The 1D models describe animals or vehicles [17] moving on a lane. The
model of a planar network, formed by arcs and nodes connecting them, applies to the
vehicles mobility [18]. The 2D models describe a crowd or a herd moving in an open space.
The 3D models apply to swarms [19] or to cells such as lymphocytes and antigens in a lymph node.

The coordinates and velocities specifying the kinematical state of the automaton are real numbers just as for a standard dynamical system. The cognitive dynamics is governed by a processing unit whose input comes from the automaton sensors. The output consists in directives to govern the automaton actuators, and to take logical decisions. The directives to the actuators are algorithms specifying the automaton displacements in presence of other automata or of physical boundaries (obstacles) and eventually other actions if the automaton is not point-like. The decisions can be implemented by neural networks having binary outputs, by multi-stable [10] systems (landscape potentials with minima among which jumps allowed by a background noise), by probabilities assigned to a list of possible choices. The decision algorithm assigning the directives can evolve depending on the accumulated experience, in order to maximize some utility function. The time discretization is required when the automaton becomes a virtual object in a computer; the kinematical variables are represented by finite strings. The virtual world, corresponds to the mathematical world with a background noise, and is similar to reality where noise is unavoidable. The momentum uncertainty is imposed by the thermal motion, the position uncertainty by the atomic size. In addition the interference of the measuring apparatus cannot be neglected even at the classical level.

**One dimensional model** Given a sequence of pointlike automata moving on a line we impose the velocity alignment [20]. This simple rule avoids the collisions and the splitting of the column. Each automaton varies its speed by accelerating whenever it is lower with respect to the precursor and braking whenever it is higher. This operation usually has a delay $\tau$ due to the reaction time. By ordering the automata so that 0 is the leader, 1 is its follower and so on, the equations of motion are

$$\frac{dv_k}{dt} = \frac{v_k(t-\tau) - v_{k-1}(t-\tau)}{\Delta T}, \quad k = 1, \ldots, N$$

The system is a linear and its exact solution can be written. The leader, whose velocity $v_0(t)$ must be assigned governs the motion of the whole column. The mean field equation is obtained in the continuum limit. Letting $\Delta x = L/N$ be the equilibrium distance, where $L$ is the length of the column and $N$ the number of automata, we define $c = \Delta x/\Delta T$ and take the limit $N \to \infty$ keeping $L$ and $c$ fixed. Choosing the origin at the leader position and denoting by $v(x, t)$ the interpolating function equal to $v_k(t)$ at $x = -k\Delta x$, equation (4) in the continuum limit becomes

$$\frac{\partial v}{\partial t}(x, t) - c\frac{\partial v}{\partial x}(x, t - \tau) = 0$$

For a vanishing delay $\tau = 0$ the solution is a backward propagating wave $v = v_0(t + x/c)$. The presence of a delay introduces instabilities.

**Two dimensional model** The model we discuss is based based on identical point like automata of unit mass, which have a visual perception within a cone. The interaction of an automaton $A_1$ with another automaton $A_2$ falling within its sight cone is repulsive, see
figure 6, and a repulsion is exerted by the obstacles as well. The only additional attribute is memory, which allows $A_1$ to keep trace of the position $A_2$ for some time interval, after the exit from its visual cone. We have considered two scenarios: the motion in the plane with an attraction point (where the origin of the coordinate system is chosen) and the motion in a channel with two opposite flows. In the first case the origin exerts a linear attracting force whose potential is $V(r) = \frac{\omega^2}{2} r^2$. The interaction forces $F_1$ and $F_2$ acting on $A_1$ and $A_2$ are, see figure 5

\[ F_1 = -\omega^2 r_1 + \frac{r_1 - r_2}{r_{12}} f(r_{12}) \partial(C_1) \quad F_2 = -\omega^2 r_2 + \frac{r_2 - r_1}{r_{12}} f(r_{12}) \partial(C_2) \]  

(6)

where the cones $C_1, C_2$ of aperture $\alpha \in [0, \pi]$ are defined by $C_1 = v_1 \cdot (r_2 - r_1) - v_1 r_{12} \cos \alpha$ and by $C_2 = v_2 \cdot (r_1 - r_2) - v_2 r_{12} \cos \alpha$.

![Figure 6](image)

Figure 6 Cone condition for two interacting automata (left). Asymptotic trajectories for the center of mass (blue) and relative coordinates (red) for two automata and with cone aperture $\alpha=0.6 \pi$ (center). Effective potential with $L=0$ for the radial motion $V_{\text{eff}}$ out of the cone and (blue) and $V_{\text{eff}} + V(r)$ within the cone (red). The first inversion point is the intersection of the purple line, and there is a jump to the green line which intersects the red curve at the new inversion point, which is an equilibrium because it is placed between the minima of the potentials (right).

After introducing the relative position vector $r = r_1 - r_2$ and twice the center of mass vector $R = r_1 + r_2$ and denoting the velocities by $v = dr/dt$ and $V = dR/dt$ the equations of motion read

\[ \frac{dv}{dt} = -\omega^2 r + \frac{r}{r} f(r) \left( \partial(C_1) + \partial(C_2) \right) \quad \frac{dV}{dt} = -\omega^2 R + \frac{r}{r} f(r) \left( \partial(C_1) - \partial(C_2) \right) \]  

(7)

The manifolds $C_1 = 0$ and $C_2 = 0$ divide the space of relative positions into four regions labelled by the signs of $C_1$ and $C_2$. In the region -- the invariant is $H = v^2/2 + \omega^2 r^2/2$, in the region ++ it is $H + 2V(r)$, and in the regions +- and -+ it is $H + V(r)$. Since the angular momentum is preserved, in the radial phase space $(r, \dot{r})$ the point moves on the line specified by the corresponding first integral until it crosses one of the cone boundaries. The problem is time dependent, but piecewise integrable. When $r(t)$ is known, $R$ is obtained by solving a linear non homogeneous equation. Choosing $V(r) = -\xi \log r$ the asymptotic orbits are ellipses in the relative and center of mass configuration spaces, see figure 5.
The explanation can be easily obtained if we consider the single automaton problem (the second automaton is fixed at the origin). The angular momentum is preserved and in the radial phase space we have two distinct energy functions, depending on the cone condition.

\[ H = \frac{\dot{r}^2}{2} + \frac{L^2}{2mr^2} + \omega^2 \frac{r^2}{2} + V(r) \vartheta(C) \quad C = -r\dot{r} - L \cot \alpha \]  

(8)

The boundary \( C = 0 \) is an equilateral hyperbola which reduces to the half line \( \dot{r} = 0 \) when \( \alpha = \pi/2 \). In this case the transition from one invariant to the other occurs at the inversion point. When the inversion point falls between the minima of the effective potential \( V_{\text{eff}} = L^2/(2mr^2) + \omega^2 r^2/2 \) and \( V_{\text{eff}} + V(r) \) it becomes a relative equilibrium and the orbit is circular. In figure 6 we plot the potentials for \( L = 0, \omega = 1, \xi = 2 \). The radial equilibrium for \( L = 0 \) becomes a relative equilibrium for \( L > 0 \), namely a circular orbit.

For a system of \( N \) automata we observe a decrease of the average kinetic energy when \( \alpha \neq 0, \pi \) and the highest rate occurs for \( \alpha = \pi/2 \). This is a consequence of the non-Newtonian character of the forces due to the cone condition. This effect is counter-balanced by memory, which allows an automaton to feel the presence of another automaton for a certain time interval after the exit of its sight cone. For simplicity the guessed trajectory is chosen to be the actual trajectory. The control parameters of the system \( \xi \) and \( \omega \) are kept fixed while \( N \) is varied so that the thermodynamic limit \( N \rightarrow \infty \) can be taken. The corresponding mean field theory is a Poisson-Vlasov equation modified to take the cone condition into account. For \( N \geq 3 \) the temperature \( \Theta \), defined by the mean kinetic energy of an automaton, \( k_B \Theta = \langle T \rangle / N \), decreases to zero. Memory counteracts the freezing and if it is long enough a thermodynamic equilibrium is reached at a finite temperature. In the case of a channel, we consider two sets of automata moving in opposite directions under the effect of two opposite force fields \( F_\pm = -\beta (v \pm v_0) \). We allow the repulsion between the two automata moving in the same direction to be weaker by a factor \( \eta \leq 1 \). The system self-organizes, in alternating rows of automata moving in opposite directions even when \( \eta = 1 \). The sight cone introduces a freezing effect, most pronounced for \( \alpha = \pi/2 \), which is balanced by introducing the memory. By varying the parameter waves, temperature oscillations and some instabilities if \( \eta = 0 \) are observed.

**Immune system models** The cellular automata have been first used to describe the immune system dynamics [21, 22, 23]. We consider here a model of competitive exclusion for the clonal expansion by representing the T cells, APC cells and antigens as Von Neumann automata on two superimposed lattices with periodic boundary conditions, meant to describe a lymph node [16, 24]. The aim of the model was to provide a simple description of the immunological memory and to compare the simulations with the mean field equations. The basic mechanisms are the replication and apoptosis of the cells, the binding between the APC and the peptides after meeting the antigens, the formation of T-APC compounds and their dissociation with activation of the T cells, the destruction of the antigens by the activated T cells. The information exchanges between the automata occurs during the contacts and the decision processes are taken on a probabilistic base. The antigens and cells live on the the small and large spacing lattices which are superimposed, see the figure. The simulation and the mean field theory present a nice agreement in the description of
the clone expansion after a primary antigenic stimulus. The memory effect appears as a faster response to a secondary stimulus.

Figure 7 The antigens (small red squares) move on the small blue lattice. The T cells (yellow) and the APC cells (green) move on the large purple lattice (left). Antigens populations as a function of time in units of 15 minutes or $10^{-2}$ days: the red curve is the simulation, the blue one the result of mean field equations (center). The same for the T clone population (right).

Conclusions

We have proposed to define complex the living and the artificial life systems, since they have distinctive properties with respect to any other physical system, and exhibit many space time scales where distinctive structures emerge as a result of self organization. The physical systems exhibit a complicated dynamical behaviour far away from the well understood limits of regular or strongly chaotic motion. In the regions of weak chaos the long term predictability is lost and the statistical properties are intricate due to non uniformity and a slower loss of memory of the initial conditions. This is typical of systems with long range interactions, which exhibit long transients before reaching the statistical equilibrium and long lived coherent structures. This is a sort of prerequisite of complexity, which was proposed to arise at the borderline of chaos where the disorder is not too strong to allow for metastable equilibria to appear but sufficient to cause transitions. We pointed out that reversibility is always lost at a different pace because the information on the state of a system is finite, so that a background noise has to be added to any deterministic mathematical model as it happens in any numerical simulation. Modeling a complex system from the microscopic viewpoint implies the introduction of an internal structure in the elementary units. As a consequence we replace a gas of atoms with a gas of Von Neumann automata, which are characterized by having an internal space where cognitive and decisional processes take place. Their body, eventually point-like, lives in a physical space and obeys physical laws. Having chosen the scale and defined the microscopic model, its properties can be explored by numerical simulations. Whenever possible it is very convenient to write down the mean field equations, which correspond to the limit in which the number of automata grows keeping fixed some global parameters. These equations, which concern the evolution of different populations or even their space distribution, provide some information in analytic form, which is valuable also to check the numerical simulations. As an example the one lane automata model, the two dimensional model with the visual perception and
a model for the clonal expansion have been discussed. In the first two cases there is no real separation between the cognitive and physical space since the perception determines a force which causes the motion. Nevertheless a memory mechanism must be introduce to allow a dynamic equilibrium at non vanishing temperature. Recognition and duplication processes appear in the third model. More sophisticated models, where the directives are the results of a neural computation, subject to evolutionary selection, have been proposed and analyzed. As far as the models become richer and sophisticated, the analysis of the results, which depend on a large number of parameters, becomes challenging. In this case, as for most biological experiments involving genes or proteins or a repertoire of cells, the use of sophisticated statistical methods is required and the possibility of detecting the large scale properties in an intuitive way becomes remote.

References


