

Energy-based Artificial Chemistry Simulator

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Abstract

We present a new artificial chemistry simulator based on simple physical and chemical rules. The simulator relies on a simplification of bonding and internal energy concepts found in chemistry to model simple, large scale, chemical reactions without delay between computation and visualization. Energy introduction and removal can be controlled in the simulations in order to modulate reaction rates. The simulations demonstrate that with this simplified model of artificial chemistry coupled with the concept of energy, it is possible to see the emergence of specific types of compounds, similar to real molecules.

Introduction

The origin of life and the transition from non-living state to living state are fundamental questions that humans have pondered for many centuries. The auto-assembly and self-organization of molecular structures, in particular in biochemistry, are a continuing source of questions and study. The field of artificial chemistry aims to answer these questions. Of course, there are still many longstanding challenges in artificial chemistry. One of them is to demonstrate a model in which the transition to life occurs in Silico (Bedau et al., 2000). The simulator presented in this paper aims at taking a novel route to achieve this goal.

The field of artificial life revolves around simulations to explain phenomena related to the origin of life like emergence, evolution, self-replication and adaptation. Some researchers (Chaumont et al., 2007; Lassabe et al., 2006; Sims, 1994) have developed techniques to create creatures that evolve and cooperate. Using genetic algorithms and neural networks, they created virtual organisms that reproduce intelligent behaviors and execute various tasks. Other researchers are interested in the phenomenon of self-replication (Hutton, 2002; Tominaga, 2005; Hutton, 2007). Using artificial chemistry, these researchers were able to simulate simplified cells that reproduce themselves (Hutton, 2007). They were also able to reproduce biochemical pathways like the fatty acids oxidation (Tominaga et al., 2009). Other researchers went further and made evolving biochem-

ical pathways (Ono and Suzuki, 2003; Hintze and Adami, 2008).

One of the key properties of all living organisms is their ability to reproduce. Researches show that it is possible to obtain simple auto replicative molecules or organisms from artificial chemistry (Tominaga, 2005; Hutton, 2002, 2003, 2005). Dittrich et al. (2001) gives a definition of such artificial chemistry that is a triple $\langle S, R, A \rangle$ where S is the set of particles, R is the set of reactions and A is the algorithm that apply the reactions. Using this definition of an artificial chemistry, it was demonstrated that rules can be specified that allow the replication of some molecules and simple cells (Hutton, 2002, 2007). However, as explained in the third experiment of Hutton (2007), it is necessary to randomly modify the state of the atoms to eventually obtain a cell that could use the defined set of chemical rules to replicate. The property of replication is explicitly defined within the different reactions, thereby limiting the possibility of evolution for the molecules. Emergence is hard to achieve, even if the rules are generic and mutations possible. In order to find the right rules to achieve replication in his chemistry, Hutton created a simulator in the form of a game (Hutton, 2009). The artificial chemistry used in this simulator is based on the same principles used in his previous works. The possible reactions are defined by the user in each level to achieve a specific goal. Even if this method works well to resolve specific problems, the fundamental concept of energy found in physics and chemistry is missing.

However, the simulation of actual chemistry and physics is computationally taxing. Numerous theoretical models exist to describe molecular structures and properties. For example, force fields exist to rapidly describe structural and conformational properties of molecules. These methods can be used on fairly large (i.e. biochemical) systems and molecular dynamics calculations (Van der Spoel et al., 2005). They cannot however describe the electronic properties of the molecules, and reactions cannot be readily modeled. On the other hand, numerous quantum chemistry software packages exist to model electronic properties of molecules with

varying degrees of precision (Schmidt et al., 1993). They are computer intensive, and usually used to obtain single molecule properties. It is clear that formal computational chemistry software cannot be used to rapidly model and study dynamic reactions and emergent phenomena.

Simulating simplified concepts of molecular dynamics and reaction processes of organic chemistry and living organisms is actually more interesting for real-time applications. There are simulators that use this approach. Some of them are based on computer code (Rasmussen et al., 1990; Ray, 1991; Adami and Brown, 1994). Computer code forms programs in the core. When executed, these pieces of code can erase parts of other programs, changing them, thus developing different functional properties. The initial parameters of these simulations allow experiments on different conceptual environment like desert and jungle (more or less resources) and on different type of organisms. Even if these organisms have no equivalent in reality, their behaviors and their properties on the other hand, do. Our goal is to devise a new artificial chemistry simulator that will result in the emergence of dynamic chemical behaviors, through the use of very simple models.

A key concept of our system is to use simple forms of energy to define the chemistry. In Gerlee and Lundh (2010a,b), the energy is used in relation to entropy to determine if an organism can replicate after processing a chain of bits. In our simulator however, a reaction between two atoms will occur if enough energy is involved during the collision. The energy drives and controls the reactions and the evolution of the system. Explicit consideration of energy is in contrast to most rule-based simulators, where reactions occur when two atoms have the right type and a rule to link them.

The next section of this article will give a description of the simulator with the different components and the chemical and physical rules of the system. Results that demonstrate the functionality and viability of the system will be presented in the third section following by a discussion on further development of the simulator.

System description

The system developed can simply and quickly simulate dynamically a large quantity of various atoms. To achieve this, the system is based on an artificial chemistry to simplify calculations. The atoms collide with each other, based on the simple principles of kinematics. They can bind together or break the bonds between themselves by releasing or absorbing energy. The artificial chemistry is simulated onto a two-dimensional grid divided in rows and columns. The borders of the grid can exchange energy with atoms and molecules that collide with it to represent heating and cooling processes. An editor was developed to change the shape of the grid. It allows the specifications of properties for the borders of the container, such as their capability to release or absorb kinetic energy.

Components

The fundamental units of the system are the atoms. They are the components that allow all the interactions and the evolution of the chemistry. As with real atoms, our model atoms possess intrinsic properties: *type* (or element), *mass*, *radius*, and *valences*. The *types* are named after existing atoms \in {Hydrogen, Carbon, Nitrogen and Oxygen}; the *mass* and *radius* are also defined to correspond to the actual atomic values. Finally the number of *valences*, which is the number of possible bonds that an atom can do with other atoms, is also defined from known atomic properties. In addition to these immutable properties, the atoms possess *energy*. The energy of the atoms varies throughout the simulation, but remains constant for the entire simulated system in accordance with the principle of conservation of energy. In other words, energy variation on the atoms only occurs through exchange during collisions and chemical reactions.

Group of bonded atoms are called molecules. In the system, a molecule is not a defined entity, it is simply the result of atoms bonded together. Each atom contains its bonding information with other atoms. Molecules do not have any intrinsic properties, besides mass and molecular energy (sum of atomic masses and energies, respectively). These properties are calculated and taken into consideration in the event of collisions. However, since collisions always occur between atoms, either part or not of molecules, the term particle will be used throughout the paper to avoid ambiguities.

The energy of an atom is divided into three categories. *Kinetic energy* represents the energy associated with the motion of an atom in the simulation. It is directly related to its velocity. *Internal energy* represents a crude simplification of the internal vibrational and rotational energies of an atom. In conjunction with the kinetic energy, they are the available energy that an atom can transfer during a collision to break bonds. The last type of energy is the *bond energy*. It represents the electronic potential of an atom. It is the abstraction used to represent the energy stored in electrons to form bonds.

Chemistry and physics

Since we wanted a simulation without delay between calculation and visualization for a large number of atoms, a simplified physics was implemented. Two basic concepts of classical physics are used in the simulation, which are the energy and the momentum conservation.

When simulations start, atoms are positioned randomly onto the grid. To ensure motion in the simulation, they are assigned random velocities. This initialization influences the different collisions scenarios that happen throughout the simulation.

A collision between two atoms will occur only if these atoms are not already bonded together and their centers are at a distance less or equal to the sum of their defined radii, that represents their zones of interaction. Since bonding only

occurs if the two atoms are not already bonded, there are some restrictions on the possible shape a molecule can take. These restrictions will be discussed later.

Energy is a key concept in our simulation. Each atom possesses different kinds of energy. Bond energy represents a simplification of the behavior of electrons involved in chemistry. Bond formation involves pairing of two electrons located on two different atoms. When these two electrons pair to form a bond, they get stabilized, and thus release energy. This energy is transformed into internal energy. Each bond possesses a specific strength that can be defined as *dissociation energy*. It represents the energy required to break that bond and it corresponds exactly to the amount of energy released and transformed into internal energy during bond formation. All the dissociation energies are taken from empirical chemistry tables (Cottrell, 1958). The energy available during a collision thus needs to be sufficient in order to break a bond. The way the atoms collide changes the energy available for a reaction to occur, which is different from a rule-based artificial chemistry.

Using this simple concept, there are four possible scenarios that can occur during inter atomic collisions. Independently of the scenario, there is always a transfer of internal energy between the colliding particles. This transfer is calculated with

$$E_{transfer} = \frac{(E_1 - E_2)}{2} F_{transfer} \quad (1)$$

where E_1 and E_2 are, respectively, the internal energy of the first and second colliding particles and $F_{transfer}$ is a constant transfer factor. This transfer factor represents the ratio of internal energy between the particles. A factor of one means the energy is distributed equally. It is the default value used by the simulator. The internal energy of each particle is then distributed with

$$E'_1 = E_1 - E_{transfer} \quad (2)$$

$$E'_2 = E_2 + E_{transfer} \quad (3)$$

where E'_1 and E'_2 are the new internal energies of each particles following the collision.

An atom with at least one free valence, called a radical, is a highly reactive atom. The first scenario occurs when each of the atoms involved are radicals. When they collide, a bond is automatically formed. There is a release of bond energy representing the bond formation and the electronic stabilization of the atoms. All this released energy is converted into internal energy and distributed to each atoms of the newly formed molecule as a function of their masses and the total mass of that molecule (Fig. 1). Since a bond is formed between the atoms, the resulting velocity of the newly formed molecule must be the velocity of the center of mass of the two particles colliding. This fact is explained by Koenig's theorem, which states that the total kinetic energy

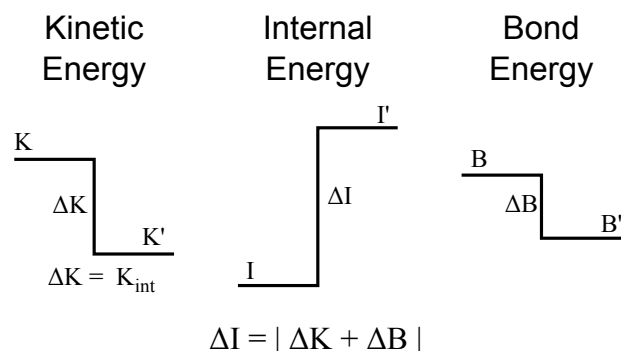


Figure 1: Energies transfers on bond formation. The energies are represented for the whole system in collision. The kinetic and bond energies decrease and are transformed into internal energy.

K_{tot} of a system is the sum of the kinetic energy of the center of mass with the kinetic energy of that system relative to its center of mass, termed *internal kinetic energy* (K_{int}). Since there are only two particles in the collision, the sum can be extended to

$$K_{int} = \frac{1}{2}m_1\vec{U}_1^2 + \frac{1}{2}m_2\vec{U}_2^2 \quad (4)$$

$$K_{tot} = \frac{1}{2}m_{tot}\vec{V}_{cm}^2 + K_{int} \quad (5)$$

where m_1 and m_2 are the masses of the first and second particle in collision, \vec{U} are their velocities relative to the center of mass and \vec{V}_{cm} is the velocity of the center of mass. This first scenario is therefore a perfectly inelastic collision. All the *internal kinetic energy* K_{int} is transformed into another form of energy, thus all the resulting kinetic energy is included completely into the velocity of the center of mass. The velocity of the center of mass can be found with

$$\vec{V}_{cm} = \frac{m_1\vec{V}_1 + m_2\vec{V}_2}{m_1 + m_2} \quad (6)$$

where m are the masses of each initial particle and \vec{V} their velocities. The *internal kinetic energy* K_{int} is transformed into internal energy. To summarize, when a bond is formed, there is a loss of kinetic energy corresponding to the *internal kinetic energy* of the Koenig's theorem and a release of bond energy representing the stabilization of the atoms. These energies are transformed into internal energy (Fig. 1).

For all three other scenarios, the available energy must be taken into consideration. The available energy is the *internal kinetic energy* (K_{int}) of Koenig's theorem (Eq. 4) for the two particles in collision. To this energy, a part of internal energy of the system in collision is added. This portion is taken in the same proportion as the *internal kinetic energy* (K_{int}) from Koenig's theorem. The energy $E_{reaction}$

required to break a bond is

$$\Delta E = F_{diss} E_{diss} \quad (7)$$

$$E_{reaction} = E_{diss} + \Delta E \quad (8)$$

where E_{diss} represents the *dissociation energy* of the bond and F_{diss} is a constant factor. In the simulator, this factor is set to 10%. This excess energy is used to transfer enough kinetic energy to the two atoms between which a bond is broken allowing them to move away from each other. When more than one bond can be broken, the one with the highest *dissociation energy* is chosen.

An atom without free valence cannot form any bond. When two atoms in that state collide, they can either bounce off each other or break one of their bonds. These are the second and third collision scenarios and are highly related. If the particles do not have enough energy available to break a bond, then the collision is modeled as a perfectly elastic one. The particles just bounce and there is no gain or loss of kinetic energy for the system in collision. Kinetic energy is however distributed normally by the principles of kinematics. The second scenario ends here.

Otherwise, if the colliding particles have enough energy to break a bond, the third scenario occurs. This process can be decomposed in two steps, the first one being a partially inelastic collision. Since the required energy to break a bond can exceed the available internal energy of the system in collision, part of the *internal kinetic energies* of the particles is used to fill the potential well of the bond. As a result, the particles will move away more slowly than before the collision. This is the case a) of Fig. 2. On the other hand, if the required energy to break the bond is less than the amount of internal energy available, the excess of available internal energy is transformed into kinetic energy, resulting in the two particles in collision moving away faster than before the collision (Case b) of Fig. 2). The second step of this scenario is the scission of the bond. Again, the Koenig's theorem is used which also states that the sum of the momentum of each particle relative to the center of mass must be null. Thus, the extra energy ΔE used to break the bond will only be transformed into *internal kinetic energy* for the particles of the scission. The speed of one of the particles relative to the center of mass can then be calculated with

$$\|\vec{U}_1\| = \sqrt{\frac{2m_2\Delta E}{m_1(m_1 + m_2)}} \quad (9)$$

where \vec{U}_1 is the velocity relative to the center of mass and m_1 and m_2 are the masses of the first and second particles. Since the calculation gives only the magnitude of the velocity, an exit angle relative to the center of mass must be set. This angle is arbitrarily set to 30 degrees in the simulation. The final velocity relative to the center of mass can be found with simple trigonometry from the exit angle and the magnitude of the velocity. To find the final velocity \vec{V}_1 of the

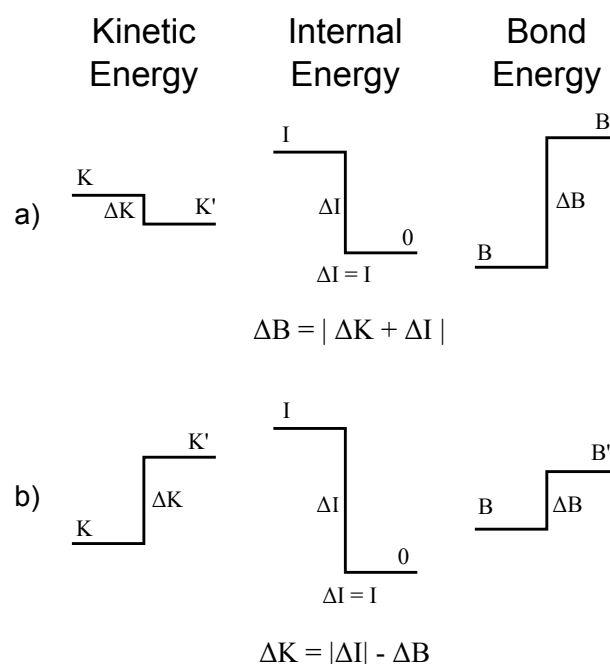


Figure 2: Energies transfers on bond dissociation. The energies are represented for the whole system in collision. There are two possible cases. Case a) occurs when the bond dissociation energy is larger than the internal energy. The remaining energy needed comes from kinetic energy. Case b) occurs when the bond dissociation energy is smaller than the internal energy. The excess is transformed into kinetic energy.

particle back in the simulation frame (instead of the center of mass frame), the result of the elastic collision previously calculated (the bounce between the particles before breaking the bond) that represents the velocity of the center of mass of the molecule that is cleaved must be added to the internal velocity of the particle. Since the momentum must be conserved, \vec{V}_2 can easily be found with

$$\vec{V}_2 = \frac{(m_1 + m_2)\vec{V}_{cm} - m_1\vec{V}_1}{m_2} \quad (10)$$

It is possible for a radical to collide with a stabilized atom. This corresponds to the fourth scenario of collision. When this scenario happens, the simulator breaks a bond from the stabilized atom (scenario 3), freeing a valence. This case can occur only if there is enough energy in the system in collision to break that specific bond (Eq. 8). The newly formed radical is then bonded with the initial radical (scenario 1), stabilizing both atoms again. The atom previously bonded becomes the new radical since it has a free valence. The result is an exchange of atoms between the two molecules. This mechanism keeps the amount of radicals to a reason-

able level. Fig. 1 and Fig. 2 summarize the change in energy for the dissociation and the bonding of two particles.

Molecular Geometry

The way the atoms are positioned around each other will have an influence on their reactivity (i.e. how accessible atoms are for collisions). There are many possible methods to arrange bonded atoms in space. For example, the atoms could simply bond at the position they collide. However, the resulting shape of the molecules in the system could lead to collisions between atoms that should not be possible. Moreover, in reality, atoms bond together in well-defined energy-efficient configurations. To ensure a more uniform representation, all atoms that bond to or break from another are rearranged to represent these energy-efficient configurations. The heaviest atom bonded is used as a reference to decide which one must remain fixed in space and the others are moved according to that position. So, when an atom at the end of a big molecule gains or loses a bond, only the atoms that form the lighter part of the molecule are repositioned. Repositioning the atoms this way facilitates the recognition of molecules from visual information. Two molecules with the same bonded atoms will be represented identically; the only possible difference is the orientation of the molecule in space. Since atoms are not permitted to move relative to each other to simplify calculation, the repositioning is necessary. This also implies that rotational degrees of freedom are not currently implemented.

In the simulator, the carbon and nitrogen have each three valences and oxygen has two. Carbon valences were reduced, instead of the four naturally found, to avoid overlapping problems in the two-dimensional representations. However, to ensure a different reactivity for the carbon atom, the dissociation energies of bonds with the latter are different from the nitrogen atom.

Results

Several simulations were done with the current version of the simulator to evaluate its similarities with respect to classical physics and chemistry, as well as to explore emergent phenomena. The first experiment demonstrates that the system can reach equilibrium in terms of the kinetic energy distribution. The second experiment shows that it can also attain dynamic chemical equilibrium and adapt to a chemical perturbation. The third experiment demonstrates that the simulator enables flexible energy modulations that influence the behavior of the system. Finally, the fourth experiment shows that different molecules can dynamically emerge from the chemistry. The first three experiments use 800 molecules of dihydrogen (H_2), for a total of 1600 atoms. For the last experiment, the number of atoms is set to 800 distributed with 40% of carbon, 20% of nitrogen and 40% of oxygen. Each valence of all atoms is bonded with hydrogen, for a total of 2898 atoms.

First experiment: Statistical distribution of particle speeds

The simulator uses Koenig's theorem to compute kinetic energy distribution between moving particles during a collision. Upon equilibration of a simulation, the distribution of particle speeds should thus obey Maxwell-Boltzmann statistics (for more informations on Maxwell-Boltzmann, see Levine (2008)). For a two-dimensional system, the normalized probability density function is derived as

$$f(v) = \frac{mv}{kT} e^{-mv^2/2kT} \quad (11)$$

where k is the Boltzmann's Constant (defined as 1 in Eq. 11) and T is the virtual temperature of the system. Speed (v) is defined as

$$v = \sqrt{v_x^2 + v_y^2} \quad (12)$$

The average speed $\langle v \rangle$ is

$$\langle v \rangle = \sqrt{\frac{\pi kT}{2m}} \quad (13)$$

The first experiment was designed to confirm this behavior. For the simulations, chemical reactions were deactivated. Simulation was run using 800 H_2 molecules. Molecules were initially given random velocities, but identical speeds. Four simulations were done with initial speeds of 5, 10, 15 and 20. The simulations were each run for 20000 iterations. It takes approximately 1000 iterations to attain stabilization of the speed distribution. At thermal equilibrium (iterations 1000-20000), the speed distribution obeys perfectly Maxwell-Boltzmann statistics, as illustrated in Fig. 3. A theoretical distribution was plotted for an initial velocity of 15. For the simulated distribution, the temperature was defined using the average speed relation

$$T = \frac{2m\langle v \rangle^2}{\pi k} \quad (14)$$

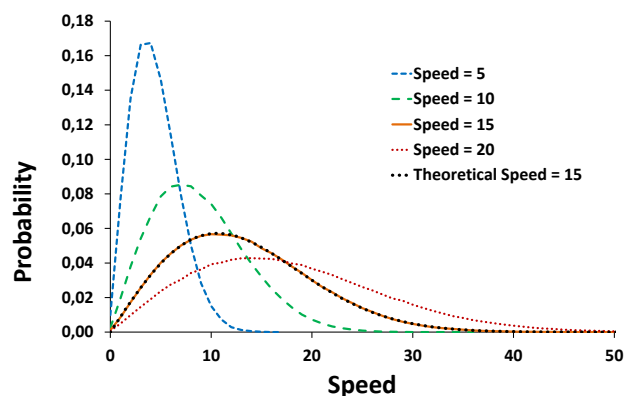


Figure 3: Molecular speed probability distribution. Only one theoretical result is shown to simplify the graph.

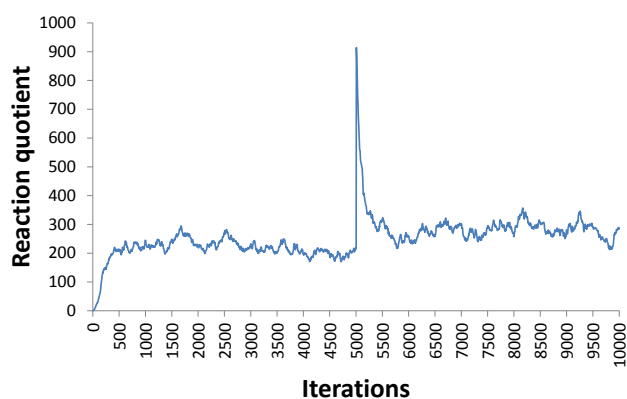


Figure 4: Equilibration of the reaction $2H \rightleftharpoons H_2$. At 5000 iterations, 400 hydrogen atoms were added.

where $\langle v \rangle$ was defined as

$$\langle v \rangle = \sum_i \frac{n_i v_i}{N} \quad (15)$$

where n_i are the relative occurrence of the speed v_i and N the total number of particles.

Second experiment: Dynamic Chemical Equilibrium

The first experiment demonstrates that the simulation, from the point of view of kinetic energies, can attain thermal equilibrium that obeys Maxwell-Boltzmann statistics. The second experiment was thus devised to validate that the simple model for bonding and internal energies, defined in the simulator, could reproduce dynamic chemical equilibrium, as expressed by the Le Chatelier's principle. This principle states that if a chemical system in dynamic equilibrium is disturbed by changing the conditions, the position of the equilibrium moves to counteract and to dissipate the effects of the perturbations (for more informations about Le Chatelier's principle, see Levine (2008)). This simulation was again run with 800 initial H_2 molecules, but with the chemical model activated. The simple dihydrogen dissociation reaction ($H_2 \rightleftharpoons 2H$) was thus studied. The reaction quotient for this reaction is defined as $Q_r = [H]^2/[H_2]$ where $[H]$ and $[H_2]$ are, respectively, the number of hydrogen atoms and the number of dihydrogen molecules. The simulation was run for 5000 iterations. The results (Q_r vs time) are illustrated in Fig. 4. The system reaches chemical equilibrium after 750 iterations, as the reaction quotient becomes stable. To perturb the system, free hydrogen atoms were added after the 5000th iteration and the simulation was resumed. Initially, a drastic increase in Q_r is observed. As the simulation progresses, the system evolves towards a new equilibrium to counteract the perturbation. After 10000 iterations, the system has shifted to a new equilibrium near the

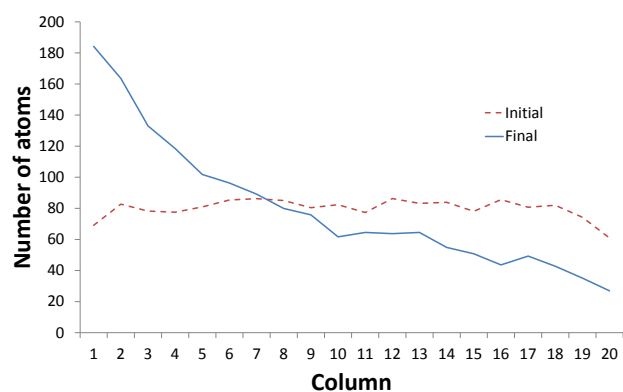


Figure 5: Partitioning of atoms in each column of the simulator grid. The grid has 20 columns and 20 rows. The left column cools the system, the right column heats it.

initial one.

This experiment clearly demonstrates that the system can reach dynamic chemical equilibrium and adapt to perturbations. The simple chemistry model defined in this simulator thus reproduces the Le Chatelier's principle, even if it has not been explicitly defined. It is a result of all the interactions combined with the energy driving the system to a stable equilibrium and it demonstrates, with the results of the first experiment, that the chemistry model is self-consistent and coherent.

Third experiment: Energy influences on the system

As explained previously, the artificial chemistry defined in the simulator is driven by energy (kinetic, internal, bonding) constraints. Modifying the total energy of the simulation should influence the kinetic and chemical behaviors of the atoms and molecules. To show the flexibility of the grid editor and demonstrate that the energy has an influence on the system, the third experiment uses a grid with a side that cools atoms (decreases their kinetic energy) bouncing on it and the opposite side that heats them (increases their kinetic energy). Simulation was run ten times using 800 H_2 molecules with deactivated chemistry. Since the atoms are randomly and uniformly positioned on the grid, the number of atoms by row and column in the grid is initially evenly distributed. After 5000 iterations, a condensation phenomenon is observed on the side that cools atoms. Fig. 5 shows the average initial quantity of atoms per column into the grid and the average quantity after 5000 iterations. The results show clearly that the majority of the atoms are positioned into the left columns.

Fourth experiment: Emergence of molecules

For the final experiment, the simulation involves all atom types defined in the simulator (i.e., H , C , N , and O). The simulation is initiated with predefined proportions of these

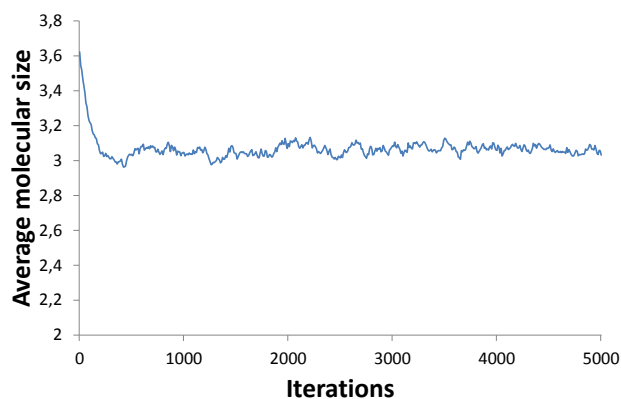


Figure 6: Average molecular size over time. As collisions occur, molecules are broken apart until chemical equilibrium is attained.

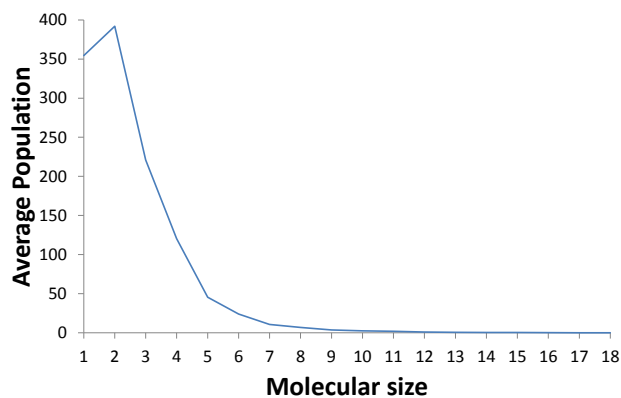


Figure 7: Average molecular population. Smaller molecules tend to accumulate more in the system than bigger ones.

atoms with their valences completely filled with hydrogen atoms (i.e., CH_3 , NH_3 and H_2O). At first, as collisions occur, these initial molecules are broken apart into smaller fragments. From these simple portions, larger, more complex molecules arise. Bigger molecules are inherently more collision prone and therefore, their chance of being broken apart increases, producing more building blocks for others, more stable molecules. With the results of the third experiment, when condensing molecules, the available energy reduces their chances to be broken. After 750 iterations, an apparent chemical equilibrium is attained, and the molecular average size appears to be constant (Fig. 6) which is coherent with the second experiment. Fig. 7 shows the average distribution of molecules with respect to molecular size, regardless of atomic composition. The size of a molecule is represented by its number of atoms. Fig. 8 shows a portion of a simulation. Bigger molecules emerged from simple initial molecules. Dihydrogen molecules have naturally

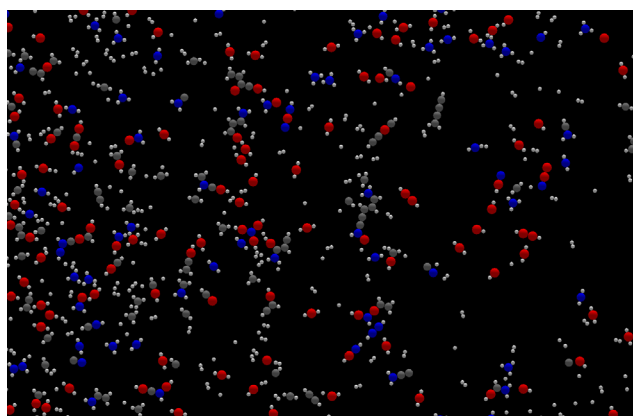


Figure 8: Emergence of complex molecules. Bigger and more complex molecules emerge from simple initial conditions. Hydrogen (white), Carbon (gray), Nitrogen (blue) and Oxygen (red).

appeared from free hydrogen atoms as a result of prior collisions.

Discussion

The simulator and the artificial chemistry described in this work represent a simple, yet reasonable approximation of reality. As demonstrated in the four experiments, realistic physical and chemical behaviors, not explicitly defined, emerged from this simulator. In relation to actual chemistry, properties emerged and were observed. Molecules spontaneously appear from the original blocks and patterns do emerge. The artificial chemistry is therefore constructive.

The transition from simple molecules to self-replicating ones could eventually be achieved with the presented artificial chemistry. At the present moment, there are some restrictions on the type of molecules that can emerge. As explained previously, an atom can only bond to another if they are not already bonded together, directly or indirectly, thus preventing formation of cyclic molecules. This restriction is only due to the current implementation of the control of geometry of the molecules in the simulator, not the chemistry itself. Although cycle formation is interesting, it is not mandatory to observe emergent phenomena; it simply has not been implemented yet in order to speed up the simulator development. It is a feature that will be added in a future version of the simulator.

The simulator currently uses a hard sphere scheme for collisions between atoms. This model is an excellent approximation in the context of the simulator. There are some other schemes that exist to simulate collisions on an atomic scale, like quantum mechanics. Unlike Newtonian mechanics (and thus hard sphere collisions), quantum mechanics is more complex and more computer intensive. Furthermore, there is no need for such precision with the presented arti-

ficial chemistry, because it is only an approximation of the reality, not the reality itself. Another interesting scheme for collision and motion that is valid with Newtonian mechanics is a force-driven simulation. A force-driven simulator could bring interesting add-ons to the artificial chemistry. For example, partial charges could be added on molecules and atoms to influence their motions and positions. With partial charges, surface tension could be modeled as well as hydrophobic phenomenon. This change in the way the atoms move does not, however, influence the specification of the artificial chemistry. Moreover, partial charges could lead to additive non-covalent (non bonding) attractive interactions between molecules, and lead to self-assembly phenomena, bridging the gap between small molecules and biochemical systems.

The actual implementation of motion uses simply the product of velocity and time to move atoms. Since acceleration is null, this method gives excellent results and is accurate. The need for a better integrator will appear only if acceleration changes, for example when forces will be added. However, modification of the simulator will not affect the artificial chemistry and its underlying simple rules.

Conclusion

We have developed a new artificial chemistry simulator that is controlled by the energetic properties of the atoms in the system. With this initial version, it is already possible to observe the emergence of different molecules than the ones involved initially. The use of energy considerations allow a better control of the interactions between atoms than just states and type constraints, and thus represents more accurately actual chemistry. The reaction rules are simple and similar to what is found in nature. We have shown that our simulator is self-consistent, coherent and exhibits emerging behavior similar to chemistry. There are many parameters that can be modified in order to obtain different molecular results and these are what makes the richness of our simulator.

References

Adami, C. and Brown, C. T. (1994). Evolutionary learning in the 2D Artificial Life system "Avida". In Brooks, R. and Maes, P., editors, *Proceeding of Artificial Life IV*, page 377. MIT Press.

Bedau, M. A., McCaskill, J. S., Packard, N. H., Rasmussen, S., Adami, C., Green, D. G., Ikegami, T., Kaneko, K., and Ray, T. S. (2000). Open problems in artificial life. *Artificial life*, 6(4):363–76.

Chaumont, N., Egli, R., and Adami, C. (2007). Evolving virtual creatures and catapults. *Artificial life*, 13(2):139–57.

Cottrell, T. (1958). *The Strengths of Chemical Bonds*. Butterworths, London, 2nd edition.

Dittrich, P., Ziegler, J., and Banzhaf, W. (2001). Artificial chemistries—a review. *Artificial life*, 7(3):225–75.

Gerlee, P. and Lundh, T. (2010a). Productivity and diversity in a cross-feeding population of digital organisms. *Evolution*, 64:2716–2730.

Gerlee, P. and Lundh, T. (2010b). Rock-scissor-paper dynamics in a digital ecology. In *Proceedings of the Twelfth International Conference on the Synthesis and Simulation of Living Systems*.

Hintze, A. and Adami, C. (2008). Evolution of complex modular biological networks. *PLoS computational biology*, 4(2):e23.

Hutton, T. J. (2002). Evolvable self-replicating molecules in an artificial chemistry. *Artificial life*, 8(4):341–56.

Hutton, T. J. (2003). Information-Replicating Molecules with Programmable Enzymes. *Proceedings of Sixth International Conference on Humans and Computers*.

Hutton, T. J. (2005). Replicators That Make All Their Own Rules. *Proceedings Workshop on Artificial Chemistry and Its Applications*.

Hutton, T. J. (2007). Evolvable self-reproducing cells in a two-dimensional artificial chemistry. *Artificial life*, 13(1):11–30.

Hutton, T. J. (2009). The organic builder: a public experiment in artificial chemistries and self-replication. *Artificial life*, 15(1):21–8.

Lassabe, N., Luga, H., and Duthen, Y. (2006). Evolving Creatures in Virtual Ecosystems. *ICAT 2006*, pages 11–20.

Levine, I. N. (2008). *Physical Chemistry*. McGraw-Hill, 6th edition.

Ono, N. and Suzuki, H. (2003). An Approach to the Evolution of Primitive Metabolic Systems Using a Model of Artificial Chemistry. *ECAL 2003*.

Rasmussen, S., Knudsen, C., Feldberg, R., and Hindsholm, M. (1990). The CoreWorld : Emergence and Evolution of Co-operative Structures in a Computational Chemistry. 42:111–134.

Ray, T. S. (1991). An approach to the synthesis of life. In Langdon, C., Taylor, C., Farmer, J. D., and Rasmussen, S., editors, *Proceeding of Artificial Life II*, page 371. Addison-Wesley.

Schmidt, M., Baldrige, K., Boatz, J., Elbert, S., Gordon, M., Jensen, J., Koseki, S., Matsunaga, N., Nguyen, K., Su, S., Windus, T., Dupuis, M., and Montgomery, J. (1993). General Atomic and Molecular Electronic Structure System. *Journal of Computer Chemistry*, 14:1347–1363.

Sims, K. (1994). Evolving virtual creatures. *Proceedings of the 21st annual conference on Computer graphics and interactive techniques - SIGGRAPH '94*, pages 15–22.

Tominaga, K. (2005). Describing Protein Synthesis and a Cell Cycle of an Imaginary Cell Using a Simple Artificial Chemistry. *Proceedings of the Workshop on Artificial Chemistry*.

Tominaga, K., Suzuki, Y., Kobayashi, K., Watanabe, T., Koizumi, K., and Kishi, K. (2009). Modeling biochemical pathways using an artificial chemistry. *Artificial life*, 15(1):115–29.

Van der Spoel, D., Lindahl, E., Hess, B., Groenhof, G., Mark, A. E., and Berendsen, H. J. (2005). GROMACS: Fast, Flexible, and Free. *Journal of Computational Chemistry*, 26:1701–1718.