Constructor of Molecular Objects: an interface for creation and visualization in computing environments[1].

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The human being has been busy with materials since its own constitution while species as his survival has been set in the interaction with the natural world which provides him with food and shelter although it also challenges him with inclemency and enemies. Being for hunting, planting, struggling or procreating, the manipulation of materials is a primary action for the species. Thus, one cannot understand the historical-cultural course of the human being without considering the role of materials in the species´ characteristic actions, fundamentally in higher cognitive structured activities and in the material basis construction for the interactions of social and technical character.

In the same way, the control over the production and transformation of the materials has been determined by the construction of knowledge about the constitution of these matters. If in the past, the human being concentrated in producing and transforming the materials having as reference only their tangible proprieties, nowadays the control over the manipulation of the matter occurs in the field of its molecular constitution. It is a fact that the access to a world of particles constituent of the matter is deeply rooted in ways of thinking and in a language

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constructed in the interactions performed in the core of communities with their own cultural and historical statutes. Therefore, one cannot understand the formation of thought and of the language of sciences that deal with the transformation of the matters without considering not only how the interactions of the matters occur but also how the actions are performed in these communities.

In this article, we deal with a specific aspect of the representation of particles by means of computing applications and how this relatively new way of representation is inserted into the scientific education of secondary school students. Firstly, we consider some general aspects of the representation in chemistry basing ourselves on the contributions of the teaching chemistry research community. Then, we discuss the representation of particles also getting support from some studies in the area of Science Education so that we can show the contributions of the studies about the use of the applications of visualization, with emphasis on the distinction between animations and simulations. In the second part, we describe the functionalities of the application in the construction of molecular objects that has been developed in our laboratory and their first use in secondary school classrooms.

On the ways of representing the chemical knowledge.

There is a certain consensus around the idea that the chemical knowledge is constructed by the combination of three dimensions of reality: macroscopic, microscopic and symbolic (Johnstone, 1993; Gabel and Bunce, 1994; Garnet et al. 1995; Dori et al., 1996; Gabel, 1998; Bowen, 1998; Ardac and Akaygun, 2004). Part of the phenomena and the chemical processes are perceptible and observable through sensorial information and measurements that are materialized in a macroscopic dimension. Within the atomic-molecular paradigm in force, in which the particle nature of the matter is the theoretical basis for the interpretation of these phenomena and processes, it is admitted another dimension of the reality in which the phenomena involving movement and interaction of particles occur. In a symbolic dimension, substances, particles and transformations are represented

by means of symbols, formulas and chemical equations, as well as by algebraic expressions, being, therefore, a semiotic materialization of the reality.

According to Hoffman and Laszlo (1991), the symbolic and microscopic representations evolved from phenomenological analogies of sensorial experiences in macroscopic level, which allow the chemists to have a common language for their joint investigation and is used for the communication among the community professional (Kozma, Chin, Russel and Marx, 2000). Also according to Hoffman and Laszlo, the chemical representations are metaphors, models or theoretical constructs of the chemical interpretation of nature and reality, with what Nye (1993) agrees upon. This author also suggests that these characteristics are determinant of the formation of a thought that differentiates chemistry from other sciences.

Teachers and researchers of chemistry teaching have done studies about how to promote the conceptual understanding of secondary school students (Wu, 2001) and of university students (Kozma and Russel, 1997) through the development of the ability of representing the three dimensions of the chemical knowledge. In these studies it was noticed that students seem to master the chemical symbolic constructions treating equations as mathematical entities instead of thinking chemical equations as representations of dynamic and interactive processes. Other researches point out the fact that the students can elaborate the correct answer to the problems in chemistry having just a limited conceptual understanding (Sawyer, 1990; Smith and Metz, 1996), without having appropriated, for example, the associated symbolical system. It is in this way that it has been defended the satisfactory resolution of problems challenging the students to appropriate the device of chemical thought, which is observed in situations that allow them to correlate the phenomenon in its symbolic dimension with the symbolic and microscopic representation.

Studies also show that secondary school and university students have difficulty to understand phenomena and chemical transformations in terms of the model of particles accepted nowadays (Garnet et al., 1995). Some authors have interpreted these difficulties of learning as result of the particle, abstract and non-

observable nature of chemistry and the necessity of a rapid transfer between the three levels of representation (Johnstone, 1991; Gabel et al., 1992).

There is a major difficulty faced by the students in understanding the microscopic level and in the representation of the symbolic level, because these levels are invisible and abstract. Thus, due to the fact that the students´ thought is based on sensorial information, they have the tendency in staying in the macroscopic level in their explanations about the phenomena and properties of the substances (Ben-Zvi, Eylon and Silberstein, 1987; Ben-Zvi, Eylon and Silberstein, 1988; Griffths and Preston, 1992).

Teachers, researchers and chemical professionals operate properly between the knowledge dimensions while students have difficulty in establishing connections between these levels. Thus, it seems very probable that the use of models, analogies and computing graphics in structured teaching situations is productive for students to appropriate the of chemical thought devices, as some studies have suggested. It is necessary, therefore, to consider both the epistemological basis of chemistry in the specificities of its atomic-molecular paradigm and the organization of the teaching activities when we propose to introduce a mediational means strange to the classroom and to the own concept of teaching chemistry predominant in secondary schools.

Using molecular models in chemistry teaching.

The representation of levels of knowledge through multiple means has been efficient in chemistry teaching through the use of different systems of symbols to represent information in different ways (Kozma, 1991). The superficial characteristics of each system of symbols can better represent certain characteristics of the information (Kozma and Russel, 1997).

Researchers have suggested different instructional approaches as support to chemistry teaching, such as adaptation of teaching strategies based on the model of conceptual change (Krajcik, 1991), integration of lab activities in the

classroom (Johnstone and Letton, 1990), the use of concrete models (Copolo and Hounshell, 1995) and the use of technologies as learning tools (Barnea and Dori, 1999; Kozma, Russel, Jones, Marx and Davis, 1996; Wu, Krajcik and Soloway, 2001). The use of concrete models, together with technologies as learning tools, seems promising (Wu, Krajcik and Soloway, 2001).

Studies have shown good learning results when using concrete molecular objects as a way of visualizing the model of particles and the associated chemical transformations (Copolo and Hounshell, 1995; Gabel and Sherwood, 1980; Talley, 1973). Some authors have observed a cumulative effect of long term in the students´ understanding of the phenomena when submitted to the manipulation of these concrete molecular objects (Gabel and Sherwood, 1980). This type of visualization is pointed as one of the most used nowadays once it simplifies, illustrates and allows the exploration of the structure and of the associated chemical process. However, these objects are rigid and generally in limited quantity, which restricts its use to the representation of small molecules (Barnea and Dori, 1999).

One of the functionalities of the computing applications is to show animations in the molecular level of the chemical phenomenon, which is not possible through other means of representation. The use of this technology as a teaching tool allows the visualization of dynamic animations projected tridimensionally, which has helped students to represent symbolically the chemical processes and, therefore, to interpret the phenomenology in macroscopic and microscopic dimensions (Williamson and Abraham, 1995). This support to learning provided by computing technologies has been considered as a specific and especially useful characteristic of these means to represent the three dimensions of the chemical thought, as they have the quality of disposing the information in different symbolic systems, though coordinated (Kozma, 1991). Multiple representations interconnected allow the student to visualize interactions between molecules and to understand the related chemical concepts (Kozma et al., 1996).

A problem that students frequently face is the performance of tasks that require abilities of tridimensional visualization, as well as tridimensional

visualization of molecules that are represented bidimensionally in books (Barnea and Dori, 1999). There are evidences that this type of representation, especially when animated and dynamic, might refine students´ tridimensional visualization (Seddon e Shubber, 1985; Seddon and Moore, 1986; Tuckey et al., 1991). Studies showed that the construction of concepts is closely related to the visual format the students had contact with during their learning (Clark and Paivio, 1991; Paivio, 1986). It is in this way that some authors have defended the integration between computing graphics and tridimensional representation as an effective way of refining the ability of visualization in the teaching of sciences (Kiser, 1990; Rodriguez, 1990; Wiley, 1990; Bezzi, 1991; Barnea and Dori, 1996).

The use of virtual molecular objects generated by computers, besides permitting the arrangement of multiple representations which are coordinated and tridimensionally projected, also favours varied types of manipulation of these objects, such as translation, rotation, size augment or reduction. Another advantage of computing visualization is the possibility of representing molecules of, virtually, any size, depending only on the capacity of the computer processing. In this sense, the development of computing applications for teaching activities appears as a potentially transforming alternative of school practices and of knowledge construction between students, once one considers the correlation of the three dimensions of chemical knowledge in the organization of activities and one investigates the rules of the actions mediated by the applications that are fundamentally different from those performed in teaching situations anchored in the experimentation or any other way of access to the phenomenology; this is so because the statute of the phenomenon alters radically when it is shifted from the bench to the computer screen (Giordan, 1999).

Simulation, animation and visualization of molecular objects through the computer.

Let us consider some specificities of the representation of molecular objects in the computer taking into consideration two distinct ways of visualizing them: the animation and the simulation.

Computing animations are generated from general graphic edition applications, without necessarily including empirical values of properties of the substances or of the transformations obtained in scientific research, and they intend to emphasize certain superficial macroscopic or microscopic characteristics without obeying time or size scales. On the other hand, the computing simulations are generated from specific applications for the study of properties of the substances and chemical transformations, and are closely related to the environment of scientific research. To perform these simulations, theoretical or empirical values of chemical properties, such as angles and bond distances, are used, and time and size scales are parametrized in mathematical equations, which satisfy the physical laws that describe the phenomena.

In any case, the molecular object is an imagetic representation of the molecular entity and can be conceived as a metaphor of what we suppose to occur in the microscopic dimension of the matter and not as a portrait of the reality. We call molecular objects the representations of microscopic particles, whose means of dissemination can vary from paper, going through plastic sets - expanded polystyrene and wood - to the computer screen or the holographic projection (Giordan, 2004). The environment and also the ways of representation are varied, aiming at putting in evidence one or the other property of the molecule. And so, the molecular object is an iconographic entity that serves both for indexation and reference objectives and for mimetizing certain molecular property, having it the possibility of being simulated by means of a system of equations when the object is screened in computer.

The fact that the simulations have taken into consideration the properties of the system under study, they can be visualized as virtual dynamic molecular objects, once it is possible to simulate the variation of properties as distance and bond angles. From these simulations it is possible to generate films simulating the joining movement of atoms in molecules and in molecular systems.

An important outcome of the manipulation of several ways of representation is the possibility of creating a linking effect between the variable - theoretical nature - and the way of representing the property - imagetic nature. The visualization of molecular objects mediated by computer seems, therefore, to promote the linking between the simulation of a property of the molecule and its representation in the same environment. This is a situation of high didactic value capable of mobilizing the students´ actions in the manipulation of objects, in the discursive elaboration and also in the meaning construction, as we have discussed somewhere (Giordan, 2004).

In spite of the fact that there are several tools for the visualization and construction of virtual molecular objects aimed at researchers, such as the mechanic and dynamic molecular applications, the use of these tools by secondary school students and even by university freshmen in chemistry is hindered due to the depth of knowledge involved in the calculus and in the control of variables. In some cases, the students have to supply values to variables such as force constants of chemical bonds, to know details about the process of minimizing the energy or else details about the organization of output information produced by the applications. Thus, having access to the applications of molecular visualization based on simulations, it is necessary to develop tools that simplify data transfer between input and output interfaces, and simultaneously make it possible to students to take control over variables that affect visualization.

Some groups have been devoted themselves to the development of interfaces to provide the students with computing tools that allow the visualization of virtual molecular objects. Russel and Kozma (1994) use a prototype software environment (4M: Chem) that incorporates simultaneous and synchronizedly multiple representations of chemical phenomena. The use of module with animations about gaseous equilibrium indicated an increase in the students´ knowledge on the characteristics of the systems in the equilibrium and the effect of the temperature in these systems. Evaluations about the use of this system indicated a decrease of wrong statements about the chemical concepts.

Wu, Krajcik and Soloway (2001) used a simplified version of professional student centered tools (eChem) to help secondary school students to construct models, to visualize multiple tridimensional models and to compare macroscopic representations. Instead of offering ready built models, the software offered the opportunity for the students to construct their own models and so to externalise their representation. In this software each molecule to be visualized must be constructed atom by atom and bond by bond, and the type of bond must be specified.

Ardac and Akaygun (2004) developed a tool of chemical visualization (Chemical Change) about chemical transformations which emphasizes the macroscopic, symbolic and microscopic representations. Through the use of animations the software offers the three types of representation simultaneously to the students. Besides, the software proposes situations in which it is necessary the interaction with a folder of instructional support material as it is required from the students drawings and written answers as final results.

We have not heard so far of any applications of molecular visualization that allows students to produce their own representations of molecular systems by means of simplified interfaces that do not require deep knowledge of the theories of molecular modelling. Due to this gap, that has probably hindered the use of computers in situations of teaching and learning chemistry, we have developed a project that, in its phase of production of applications, has two stages, the creation of the user communication interface with the applications of simulation for building molecular objects and the development of the interface for disseminating the molecular object in the computer screen. Then, we will describe the functionalities of application for the construction of molecular objects.

Construtor

Construtor is a tool for the creation of virtual molecular objects that use the hypertext transfer protocol (http) to perform the communication of the Client with the Server. Through this interface the student can build animations of

bidimensional molecular models, and also build and visualize simulations of these models tridimensionally projected from the condensed structural formula by means of a *plug-in*. The animations and the simulations are disposed on the same screen so that the student has the opportunity to compare his own representations with the representations associated with the model scientifically accepted. The simulations are done using a molecular modeling program Tinker (Ponder and Richards, 1987), and visualized with a *plug-in* Chime®, both applications of public domain and highly used in the scientific field.

The environment of graphic animation was written with the help of the application Flash®, from Macromedia, which is an application of general use in the construction of graphic animations. In this application, bidimensional designs can be created from simple geometric figures. The tools provide options in which the draws can simulate the visual sensation of tridimensionality. The draws are created in a varied quantity of pictures with different dispositions, so that the overlap of pictures creates a visual sensation of movement. The possibility of creating different draws in separated layers as part of the same animation, favours an environment of organized and planned edition.

The program running in the Server, which interacts with the user environment of tridimensional simulation and provides appropriate files for visualization was written in C language ANSI pattern to be run in the Server with the environment GNU/Linux, from RedHat 9.0 distribution. This part of the environment provides an input box for the user to send to the Server, through the communication protocol via the Internet hypertext, a sequence of letters and numbers correspondent to a condensed structural formula of an organic molecule, such as CH3CH2CH3, CH3CH2CHO, CH3CH2COCH3 or CH3OCH2CH3 [2], including branched, unsaturated and cyclic chain. Until the present moment the Construtor program has recognized sequences correspondent to hydrocarbons, halide compounds, alcohols, aldeids, cetones and ethers. The Construtor program running in the Server, receives a sequence of letters and numbers, and sends back to the user browser the file, which corresponds to the geometrically optimized

[2] The interface is not yet adapted to work with sub-indexes.

tridimensional structure of the molecule. The necessary time for the construction of the file in the Server depends on the quantity of atoms. For molecules with until 20 atoms the processing time does not exceed 1 second in a CPU with Celeron 333 MHz processor. The answering time will for sure depend on the speed of user's connection to the internet. The user can visualize the file automatically in his browser if he installs in his computer a visualization *plug-in* highly known and used in the academic field[3].

Figure 1: Organogram of the functionality of the Construtor application

We shall now describe the functionality of the Construtor application, as well as its interface with receiving and sending files by the internet. The hypertext page, from which Construtor can be accessed, displays a field where the user writes a sequence of letters and numbers corresponding to a condensed structural formula of an organic molecule. Near this field there is a button, which function is to send a written sequence to the Server. The hypertext page through a POST method sends a sequence of letters and numbers to a script of the type CGI, written in Perl language, present in the Server in an appropriate directory. When receiving this sequence, the script is run in the Server, and then it processes commands and runs programs, and finally sends the file back to the user browser as an answer. Initially the script processes a sequence of letters and numbers so that this sequence is properly arranged to be recognized by the next commands and programs. The arranged sequence is sent by the script to a program, written in C language pattern ANSI, called CONSTRUTOR. The program Constructor generates from the received sequence a file with the tridimensional coordinates and also a matrix of suitable connectivity that indicates which atoms are bonded together. The corresponding file is generated in a format to use a package of molecular mechanics and molecular dynamics programs -Tinker, freeware for academic use and available in the internet[4]. The program Construtor, after the

[3] Available at: *http://www.mdl.com*
[4] Available at: *http://dasher.wustl.edu/tinker*

generation of the file with the tridimensional coordinates corresponding to the received sequence, submits this file to have the molecular geometry optimised by a method of energy minimization.

The adequate parameters to be used automatically in the optimization of geometry were selected to offer a suitable optimised geometry, and not to demand too much processing time in the Server, as well. This latter file is sent back by the script to the user browser, through the communication protocol via hypertext, as well, ending the work done by the Server computer.

Interfaces with the user

Animation

The animation interface of the Construtor program is able to generate bidimensional static animations that do not perform movement after being constructed. The program does not present the option of movement of atoms and molecules, once it is used by students in a beginning level of knowledge soon after the manipulation of concrete molecular objects and register of molecular structures in paper. In figure 2, there is a screen of the Construtor application and also of the interface of visualization produced by the Chemie *plug-in*.

Figure 2: Graphic interface of the Construtor application.

In the environment of graphic animation, the students have a tool bar in the lower part of the screen. In this tool bar there are bidimensional geometric figures that operate as virtual objects, handled by the user in quantity and disposition. The geometric shape of these objects mimetize the format of concrete molecular objects of the type ball-stick, as there are virtual ‘balls’ and ‘sticks’ in unlimited quantity, as well as a bidimensional space, available to the students, where the objects can be handled. Firstly, we selected to offer the students an area of bidimensional work, as well as bidimensional molecular objects, to avoid learning

obstacles, once the manipulation of objects in an environment with tridimensional projection requires the handling of a major quantity of commands, as well as more sophisticated commands, such as those that produce texture, shadow and depth in objects.

The virtual balls that symbolize the atoms are presented in different colors in CPK pattern to offer the students different atomic types. We have chosen this coloured pattern due to the fact that it is used by a majority of the visualization systems applied to books and to softwares. The own concrete models of the type ball-stick used in classroom situations were produced based on this pattern of colours, which favours the correlation between the concrete and virtual molecular objects. The molecular objects that represent the virtual chemical bonds are sticks of identical sizes, however, they are spacially displayed in four different positions. Any of these chemical bonds can be rotated in three-hundred and sixty degrees, as to take the appropriate disposition according to the students´ point of view. We have chosen to offer these objects in four different dispositions to allow the student to select the one that approaches more to the position that he needs to construct his representations. We have also chosen to restrict these objects to a unique size because the objective of the activity during the use of this environment is focused in the visualization of the relative positions of the atoms, as well as of the bond order.

The manipulation of these virtual molecular objects through graphic animations retains the simplicity and convenience of the manipulation of the concrete molecular objects already used, with the advantage of the possibility of constructing molecules of any type. In this interface the students can freely move each one of the objects that symbolize the atoms and chemical bonds throughout the computer screen. In spite of this, as the students have already manipulated the concrete molecular objects, they have the tendency of grouping the bidimensional objects that symbolize the atoms and chemical bonds in a way close to that that mimetizes the relative tridimensional disposition.

Simulation

The construction of virtual molecular objects through the simulation environment is operationally simple, as it requires that the student types only a sequence of letters and numbers corresponding to a condensed structural formula of an organic molecule, and to choose a format of representation between the ones available (ball-stick, space-filled, trace, skeleton and electronic cloud). Then, the student must press the left button of the mouse on the option “build”, offered right below the field where he types the condensed structural formula of the molecule in question. This sequence of letters and numbers is sent to the server computer, which generates a file having the tridimensional coordinates geometrically optimized of the molecule in question. The Server sends this file to the user browser that can visualize the molecular object in the case there is a *plug-in* for visualization.

In spite of the fact that it is operationally simple, the use of the simulation environment requires mental operations more sophisticated than the environment of graphic animation, once the student must master the symbolic representation, as the interface of the construction demands correct sequences of letters and numbers, that is, which corresponds to a molecule within the patterns accepted nowadays. Once using this environment, the student is challenged to visualize molecules from their names in the pattern IUPAC[5], as they have the opportunity to drill the representation of the structural formula from the name, and also they have the opportunity to check if its representation corresponds to the accepted model.

When manipulating tridimensional virtual molecular objects the student might explore the molecular object under several perspectives with the help of the *mouse*, mimetizing the way the concrete molecular objects are manipulated. This leads students to create a correlation between the concrete and the virtual world, which might make tighter the correlation between their mental images and the symbolic representations and the concrete and virtual molecular objects. Besides visualizing the structural formula in three dimensions, it is possible to measure the angles and bond distances in the virtual molecular object. So, the student might compare, for instance, the bond lengths of the simple and insaturated bonds, which

[5] It refers to the International Union of Pure and Applied Chemistry.

is not possible in an environment of graphic animation or with concrete objects. Besides, the student might also compare the different atomic volumes of the atoms and atomic groups present in the molecule, which also is not possible with other forms of representation.

Thus, environments that make it possible for the student to contact with simulations favour to deepen concepts that can be introduced from less sophisticated representations, such as the chemical bonds.

Initial uses and future perspectives

A simple test of usability of the Construtor program was done with 32 year eleven school students of a public school in the State of São Paulo, aiming at collecting information to improve the present version. The students had access to the Construtor program using an Organic Chemistry Tutorial (OCT) as instructional supporting material, which was used as class guidance activity. Besides the written answers, students were requested to perform the activities of construction, manipulation and visualization of virtual and concrete molecular objects. The concrete molecular objects were made available to the students in commercial models of the type ball-stck, while the virtual molecular objects were shown to the students as examples, or constructed from the interfaces of animation and simulation.

The students were arranged in 16 pairs with the objective of stimulating the verbalization and socialization of ideas. During the classes with the Construtor program the students had the aid of the teacher who was consulted whenever there were doubts about the enunciation of the questions and the proposed activities, or whenever they disagreed among themselves with the answer to be given.

In these classes, which were performed in a room with 18 computers, the students had positive attitudes both towards the material and the activities, even those who did not actively participate in similar activities without the use of computers. The students´ answers to the activities and proposed questions

brought forth evidences of mastering the symbolical systems for the model of particles when interpreting the macroscopic phenomena and properties.

In general, the students showed good performance when using the interfaces and no operational difficulty with the animation and simulation interfaces was observed. More refined usability tests are been planned from the data of screen register, simultaneously with their audiovisual register of the students.

Another phase of the project centres in the development of an interface for visualization based on the Java 2 platform and using a API JOGL (*Java bindings for OpenGL*), in order to incorporate movements that mimetize the movement of atomic vibration besides the functionalities already available in *Chimie*®. We now study the possibility of converting the bidimensional data from representations of molecular objects, drawn in the animation interface, into input data to the simulation interface. This will offer an option for the creation of objects to manage the input data without information on the condensed structural formula. This interface of direct conversion might be used by university students who have already mastered chemical symbolical systems in high degree.

The development of computing interfaces for the visualization of molecular objects gives rise to such an old and new discussion of how the human being acts with the matter to transform the world. One of the most intriguing contemporary themes, besides the digital means and the internet, is the manipulation of the matter in nanoscopic scale. Creating devices in molecular scale is a new frontier of the manipulation of materials by the species. Producing substances of pharmacological interest from selected enzymatic plants is also part of the agenda of the chemical industry. The nanotechnology and the molecular biology are knowledge frontiers that will know rapid expansion in the beginning century.

The insertion of the population in this debate is a priority of scientific literacy that cannot be excluded from secondary schools. Today, the implications of these ways of manipulating the matter reach ethic dimensions that require from us a value judgement that goes beyond the limits of science, but that does not discard the understanding of how knowledge is constructed also in its material dimension.

Taking computers to schools is more than attending the demands of the work market, it means to cultivate ways of contemporary thought that are rooted in the development of the species, at least in its anxiety to control the matter.

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Figure 1: Organogram of the functioning of the Construtor application

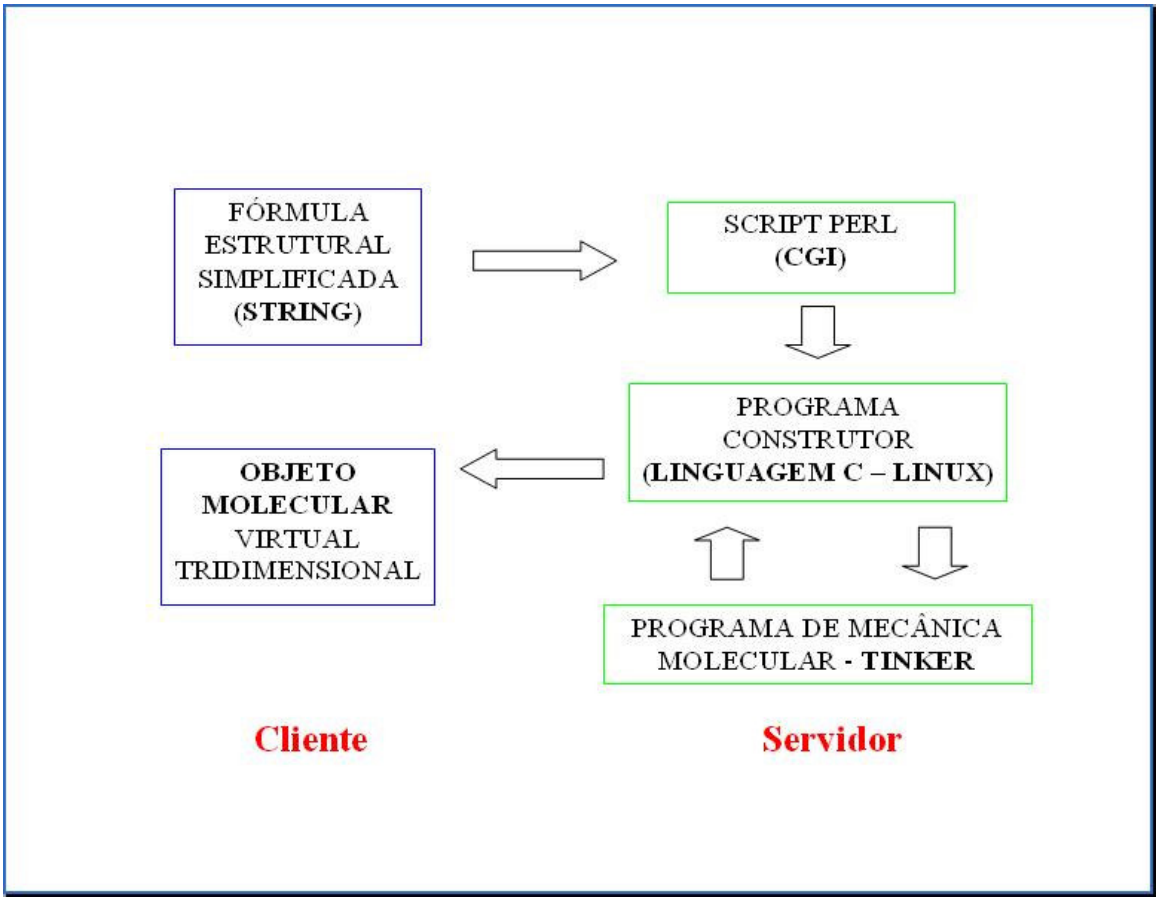

Figure 2: Graphic Interface of the Construtor application.