Touch on Chemistry: Interaction System

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Acknowledgments

I would like to start by referencing a portuguese expression that is often told among universitary students, which is “O curso não se faz sozinho”. While this is usually used as a means to say one should work to conclude its studies, I prefer the irregular interpretation that it will not be possible to complete alone, you are going to need help. And in that since, I fully empathise with the expression.

If not for my friends who worked, played, carried, supported and above all, had lots of meaningful and meaningless discussion with me in the past years, I would not have managed to reach where I am today.

Next, I would like to acknowledge the support of all the teaching body, be it in the university, as before, since without all the knowledge their partook in me, I would not have managed all I have until today.

Last, a special thank you to my family. I may not always demonstrate it, but I could not be more thankful for all the support I have been receiving ever since I was born.

Abstract.

The enjoyment players can get from an immersion in a virtual environment is directly related with how interactive the system is. Virtual Reality becomes more common in games and other applications, pointing for the need to improve the use of this technology especially for teaching and learning purposes. The game “Touch on Chemistry” is a game for teaching Organic Chemistry, a field combining high number of theoretical concepts with difficulties on its visualization. By employing Virtual Reality, the game facilitates the visualization of those concepts originating a fun and interactive way of learning Organic Chemistry. We aim to improve the interaction system for “Touch on Chemistry” by implementing a model where hand figures and gestures are used to perform actions such as moving, rotating, linking, or grabbing objects, with the use of a Leap Motion device in a virtual environment. These new actions were defined based in data collected from testing users/players and from interviews providing information on the needs felt to increase the interactivity of the system. In order to do so, this dissertation focus on the development of an interaction system that makes use of the Leap Motion capacities of recognizing the hands of the users along with the gestures and hand figures they make. The actions the users can make were catalogued in separated interaction modes. The activation of those modes was mapped with the hand figures and gestures the users can make, creating three interaction models: Two-hands activation model, One-hand activation model and Buttons Model. The model One-hands activation was through the execution of 9 different tasks developed. The results on performance and execution time indicated that this model allows the users to perform the necessary actions and complete the tasks required of the interaction system, improving the immersion experience. Further research on the developed interaction models and the difference between them should be done to create new ways to interact with the system.

Keywords

Virtual Reality; Organic Chemistry; Game; Learning; Hand-Free Manipulation; Leap Motion; Interaction System.

RESUMO

O aproveitamento que os jogadores podem obter da imersão num ambiente virtual está diretamente relacionado ao quão interativo ele é. Como o uso da Realidade Virtual é cada vez mais comum em jogos e outras aplicações, torna-se necessário melhor o uso desta tecnologia. Ao mesmo tempo, os novos métodos de ensino consistem na utilização de questionários e jogos para aumentar a qualidade e interatividade do processo de aprendizagem dos alunos. A partir destes conceitos surgiu o jogo "Touch on Chemistry", um jogo para o ensino de Química Orgânica, área com um elevado número de conceitos teóricos de difícil visualização. Ao utilizar a Realidade Virtual, torna-se possível ao jogo facilitar a visualização desses conceitos.

Enquanto o jogo apresenta uma forma divertida e interativa de aprender Química Orgânica, testes e entrevistas com utilizadores forneceram informação de que o jogo poderia ser melhorado aumentando a interatividade do sistema. Como tal, esta dissertação foca-se no desenvolvimento de um sistema de interação que faz uso das capacidades do Leap Motion de reconhecer as mãos dos utilizadores juntamente com os gestos e figuras que eles fazem. As ações que os utilizadores podem realizar foram catalogadas em distintos modos de interação. A ativação destes modos foi mapeada com as figuras e gestos que os usuários podem fazer, criando três modelos de interação. Cada modelo de interação faz um uso diferente das capacidades do Leap Motion em um ambiente virtual, no entanto, apenas um desses modelos foi testado. Os resultados indicaram que o modelo permitia os utilizadores realizarem as ações necessárias e concluíssem as tarefas que seriam exigidas do sistema de interação. É necessário fazer mais pesquisa para ter informação concreta sobre qual dos diferentes modelos de interação apresenta a melhor maneira de interagir com o sistema.

PALAVRAS CHAVE

Realidade Virtual; Química Orgânica; Jogo; Apredizagem; Manipulação a Mãos Livres; Leap Motion; Sistema de Interação.

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Acronyms

VR	**Virtual Reality**
IT	**Information Technology**
3D	**3 Dimensions**
HMD	**Head-Mounted Device**
UI	**User Interface**

1

Introduction

1.1 Motivation

The number of students applying at national contest of access (CNA) for higher education is increasing almost every year with 62 561 applying for the first call of 2020, an increase of 23% in comparison to the 51.291 that applied to the first call of 2019, according to the Portuguese's governmental institution Direção-Geral de Ensino Superior (DGES) [1]. The area of Chemistry is no exception. Considering the programs of integrated master's degree of Chemistry (MEQ) and Biology (MIEB) of the Instituto Superior Técnico's (IST), the data on Figure 1 indicates that the number of applications is approximately five times of the availability, according to the data from the official DGES website [2] [3] .

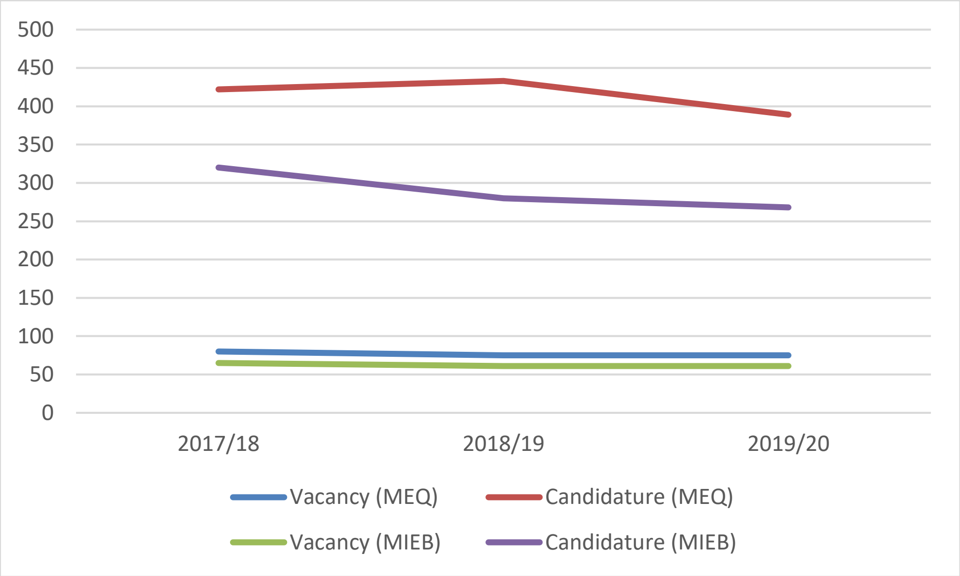

Figure 1 - Comparison between the candidatures and the vacancies for the courses of MEQ and MIEB in the last three academic years in Portugal [1]

The growing number of students justify the need of new methods for teaching and learning, mostly using IT technologies applied to scientific domains.

Organic Chemistry also presents a challenge in terms of visualization, since most of the contents would benefit from 3D perception, which is absent from common teaching methods.

At the same time, with the VR technology, all sorts of tests are being made to validate its possible benefits in education, where there are reports of it having a more positive effect, including in the chemistry area, where the results it achieved are better than with some of the most frequently used techniques. While previously, VR immersion would depend on visual and auditory stimulation however, new tools are being developed to improve the immersion experience, by implementing more senses to it, like touch and smell.

In this context emerged the game "Touch on Chemistry", which the interactive system it possesses will be updated in the present project, with the improvement to the use of Leap Motion, in order to adjust

[1] Imaged adapted from the data in [2] and [3]

it according to the needs of the program of Organic Chemistry in IST namely, as a better and more interactive 3D perception tool. This project will then focus on improving the interaction by making use of the capabilities of the Leap Motion sensor to capture and register the hands of the users in a virtual environment, to better captivate the players and possibly increase the effectiveness of the learning process.

1.2 Objectives

The main goal of this dissertation is the development of an interaction system that can improve the Hands-Free Manipulation within the game “Touch on Chemistry”, where the player will be able to directly manipulate atoms and molecules. This will be achieved by increasing the quality of the interaction between the player and the virtual environment, along with its components. The immersion experience is obtained from using VR technology paired with a Leap Motion sensor to capture the hands of the users in the virtual environment.

2

Project Background

2.1 Organic Chemistry

2.2 Definition

Organic Chemistry is a chemistry subdiscipline focused on the study of the structure, properties, and reactions of organic compounds (chemical compounds that contain carbon) [4]. The study of these factors contributes to know and to understand the compound's chemical composition, its formula, its physical and chemical properties, the chemical reactivity and its behaviour [4]. Organic compounds constitute most known chemicals, having diverse structures and a large range of applications, being crucial to life on planet Earth [4].

2.3 Nomenclature

Chemical nomenclature is a process that dates back from the times of alchemy, with a huge growth in organic chemistry since the XIX century as seen by the number of Nobel prizes in chemistry. The nomenclature is based on the work of chemists such as Fischer, Liebig, Dumas and Werner, being essential to distinguish each compound according to its chemical properties (functional groups). The Nomenclature of Organic Chemistry can be systematic or semi-systematic, follows the recommendations of the International Union of Pure and Applied Chemistry (IUPAC) and uses preferred IUPAC names, although there are still many nonsystematic (commercial) names in use [5].

2.4 Structural drawings

The most common way to represent organic molecules is by drawings or structural formulas of the carbon skeletal [4]. In fact, this method is used for more than 150 years [6] and its main objective is to convey information about the identity of the molecule/compound, be it from person to person, or as input of computer programs ensuring that all participants are able to understand each other [7]. This results in different ways to represent the molecules, as seen in Figure 2, available in [4].

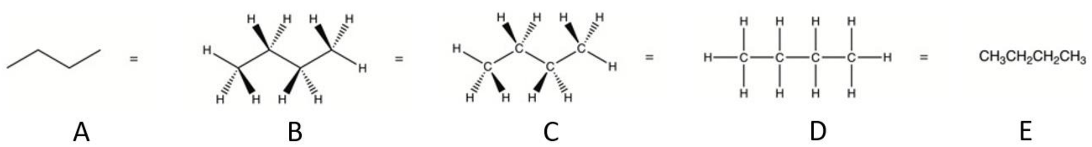

Figure 2 - Different ways of drawing butane (C4H10), using Line drawing (A), Bond-line formula (B, C and D) and Condensed formula (E) [2]

2.5 Programs

Nowadays there are several programs, academic or commercially available, applied to organic chemistry. They can estimate names according to the nomenclature systems, draw formulas, predict physical-chemical properties and interactions and all the possible information related to each known compound. Doing an overall evaluation of the market is out of the scope of this project.

For the present project, we will consider just the programs used by the group of interest, the teachers and students of Organic Chemistry at IST, in order to include the main features in our game.

2.6 Virtual Reality

VR technology dates back from the 60's (since even the meaning of virtual as in "something not physically existing but made to appear by software" dates back from only 1959 [8], however, due to the lack of processing power at the time, there was a huge decline of interest. Only in recent years has the interest in the area of VR resurfaced in the consumer market, with the development of devices capable of providing a full immersion in a digital environment, such as the Oculus Rift, a Kickstarter project in 2012, with the purpose of providing an affordable high-quality Head-Mounted Display (HMD) to the public, looking for funding and achieving the goal of $250 000 in less than 24 hours [9]. It is this reawakened interest that contributes to a better understanding of what is being called the "second wave of VR development", where a vast amount of products, like the ones seen in Figure 3, are emerging and flooding the market, trying to implement aspects of the vision of the Ultimate Display [9].

[2] Image from https://en.wikipedia.org/wiki/Organic_chemistry

Figure 3 -. HTC Vive Pro (Left) and Oculus Quest (Right) [3]

These devices now have better software, better hardware and new technology, like good haptics, eye tracking programs and better HMD's, along with new applications, such as in training, learning, immersive collaboration, data visualization, retail and gaming [10].

[3] Images respectively from https://www.pccomponentes.pt/htc-vive-pro-full-kit-realidad-virtual and https://www.pccomponentes.pt/oculus-quest-128gb-gafas-de-realidad-virtual

3

Related Work and State of Art

3.1 Previous version of the project "Touch on Chemistry"

The current version of the game "Touch on Chemistry" was developed using Unity Version 5.6.5f1 and consists of a VR environment simulating a chemistry classroom. For the user to be able to play it needs an HTC Vive with Leap Motion and the setup made through SteamVR.

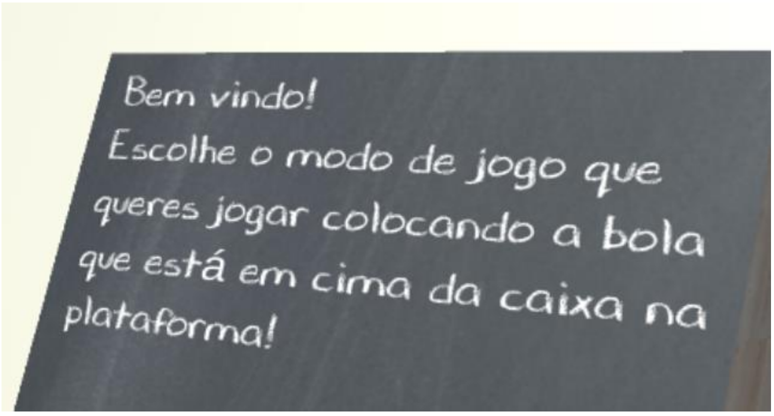

Figure 4 - Welcoming board from the game "Touch on Chemistry" start menu interface

3.1.1 Features

The game main components are objects that represent atoms and bonds. The molecules are the junction (parent) made of the atoms and the bonds between them.

The principal interaction happens when user grabs an atom, which highlights the atom, to make it easier for the player to understand that he is now holding it. The user can grab up to two atoms at a time, one in each hand, since it is not possible to have two atoms held at the same time in just one hand or, an atom being grabbed by both hands at the same time.

Each atom has the number of bonds it can have defined and according to its number of electrons (which is the number that defines the amount of bonds an atom can have [11]). A molecule can be infinitely built by adding more atoms to it, however, two molecules could not be joined together. In the same way, it is not possible to have a circular bond, rings, in the molecule (if an atom A is connected to an atom B, and an atom B is connected to an atom C, it will not be possible to make a direct bond between A and C). An illustration of this scenario can be seen in Figure 5, where the user is unable to unite both molecules and to join the ends of the molecule on the right.

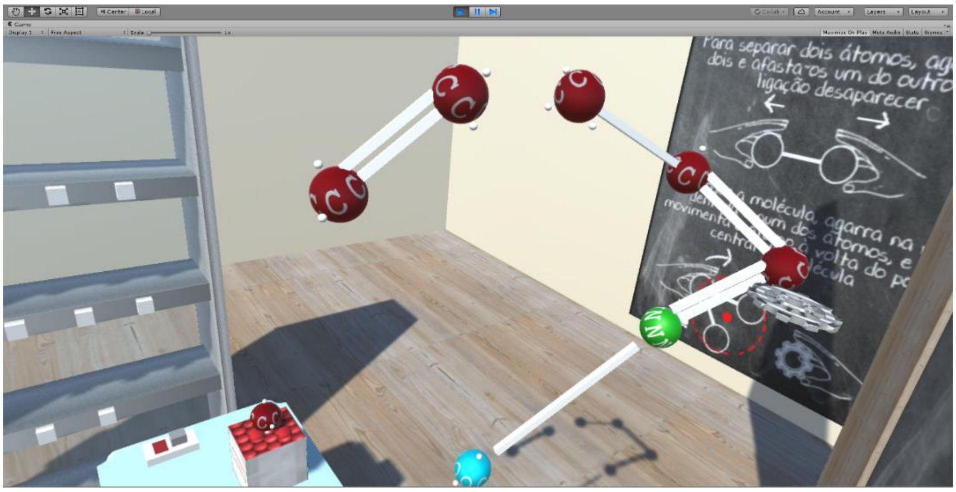

Figure 5 - In game view of two molecules

The game has different game modes implemented, and also the possibility to implement even more. At the present, the ones already implemented are the Normal Mode and the Speed Run Mode. In Normal Mode, players go through the levels by completing the challenge in each of them and trying to get as high of a score as possible. In Speed Run Mode, the purpose is to complete the levels as quickly as possible. Some additional modes that can be implemented are the Building Mode (for the player to creatively build the molecules he wants), the Complete Mode (where the player is given an incomplete molecule and he needs to complete it to pass the level), Transform Mode (a mode for the player to transform one molecule into another) and Multiple Choices Mode (in this mode, the player needs to choose a correct answer based on the provided possibilities). The game also has implemented a Scoring Board (Figure 6), in other to give scores to the performance of the players.

The levels of the game are not hardcoded, but instead are written in a text file. While this gives more options for the teachers to design specific level, the edition of the files must be precise, otherwise, the game will not load the levels.

Figure 6 - Scoreboard after completing a level [4]

[4] Image from [43]

3.1.2 Users Interview and Problems

To foresee the expectations of the target audience, we conducted a semi-structured interview with two teachers and one researcher from the area of Organic Chemistry at IST. Both teachers had previously played the actual version of "Touch on Chemistry", while the researcher did not.

All interviewed mentioned the importance of having the ability to rotate the molecules. Although it was mentioned that the size of the bonds between the atoms are fixed, it was also pointed that could be useful to stretch the bonds, as such, further inquiry is required for this aspect. Considering the size of the atoms, all the participants mentioned that hydrogen should be smaller than the other atoms but, there is no need to create further size distinction, since all atoms also have colours to differentiate them. The importance of the geometry in each molecule was mentioned, so additional research should be considered for this matter. Both professors noted the impossibility to join two different molecules and make rings with the atoms (as it was mentioned above and shown on Figure 5) as a problem and something that is essential to do.

It was noted that the game should be able to read molecules data from specific files, similar to what they have in other programs frequently used, such as ChemDraw. In the current version, only the levels of the game are reed from a file.

3.2 Learning process and VR

The development of Virtual Reality technology is allowing for an increased diversity of experiences in different areas like entertaining [12] [13], training [14] and education [15].

For education, there is research made that came to the conclusion that "Learning is Not a Spectator Sport" [16], and how we tend to get better at a given task after practicing it several times, and thus improving our proficiency [15, 16]. This type of practice can be achieved in the real world, but for some tasks, a VR environment can prove to be useful [14], 17, 18]. In 'Virtual and augmented reality as spatial ability training tools' [21], a study is performed to verify if VR and AR can improve spatial ability, one of the main components of human intelligence. By giving the participants different geometry tasks, created using Construct3D, they are to try to solve them, although, as it can be imagined, only students with geometry education were eligible for the training, since previous knowledge was necessary. The main conclusions indicate that augmented reality can be used to develop useful tools for spatial ability training and how traditional spatial ability measures probably do not cover all skills that are used when working in 3-D space. The study also notes how individual differences could be an aspect to consider when evaluating spatial ability.

More specifically, using VR has advantages like encouraging learners to experiment by interacting with the environment, providing a multimodal interface to resources supporting learning and allowing the learners to actively participate in the creation and organization of their learning environment [22].

3.3 Hand-based object manipulation in VR

This advance of technology and VR techniques is accompanied with newer and better devices, has can be seen with the addition of touch, which became a possibility after the boost in the development of haptic interfaces in 2016 [23].

3.3.1 Devices

The increased development brought new supports, mostly for the hands, like the ones described in 'Three Haptic Shape-Feedback Controllers for Virtual Reality' [24], where there is an analyses of three hand controllers: CLAW, Haptic Revolver and Haptic Links.

The CLAW (Figure 7) is based on force feedback and actuated movement to the index finger, designed as a multi-purpose controller, to provide the expected functionalities of a VR controller while enabling a variety of haptic renderings for the most expected hand interactions.

Figure 7 - Hand holding the Haptic device CLAW[5]

[5] Image from [24]

Figure 8 - Haptic Revolver in contact with the user finger[5]

For the Haptic Revolver (Figure 8), its most notable feature is the actuated wheel underneath the fingertip, which allows the user to feel like he is touching the virtual surface. Since this is a reconfigurable handheld device, it would be expected for it to allow different sensations, and so it does; the device is virtually tracked and the wheel rotates below the finger, to change its outer surface, positioning the correct texture on the user's finger at the correct moment. Considering that the wheel rotates without coming into contact with the finger during that movement, it's possible to understand another very interesting characteristic of this device, which if that it can selectively touch the finger, unlike other devices that are making permanent contact with it.

Lastly the Haptic Links (Figure 9), this device goes outside the norm in terms of virtual controllers, but that is because it is not supposed to be one in the first place. Haptic Links was designed as a haptic connector between controllers, with an electro-mechanically actuated physical connection capable of rendering variable stiffness between two commodity handheld VR controllers. This allows this device to make the linked controllers feel and behave like a two-handed tool or weapon, as seen in the Figure 10

Figure 9 - Haptic links connection two virtual devices[6]

[6] Image from [24]

Figure 10 - Player using Controllers connected by Haptic Links and how it is perceived in the virtual environment (Gun on the Left, Bow on the Right) [7]

The haptic devices can be applied to scenarios such as in a virtual classroom, where interactive gloves are used for teaching organic chemistry, in an immersive learning environment, with a game-like approach to learning [25]. The results of such project allowed to conclude that the system in use was highly rated for multisensory learning, motivation, engagement, adequacy of system as an instructional tool for chemistry and a high support for haptics. On the other hand, there was also data on how the system could provide more feedback to the uses on their actions and have better precision and sensitivity to support the grasping action. The biggest problem of the system is related to all the wires need for it to work properly, since almost all participants suggested a lighter, wireless glove system to support free movement.

With the importance of a good haptic device that possess great precision and freedom of motion becoming more evident, different developers are working on possible solutions and some results can be seen in the latest year of 2019, be it a holdable devices focused on the greater freedom of motion and larger workspaces [26], or on high-dexterity finger interaction [27], both cases report of precise manipulation for virtual objects. On a different scenario, a Robot was used as a Haptic Device [28], for the training of hip replacement surgeries, showing how some devices can be adapted to fit emergent necessities.

A very well developed device is Dexmo Force Feedback Gloves [29], with full hand motion capture, high stiffness, variable force and realistic haptic feedback, all this points in a wireless device.

3.3.2 Leap Motion

A different type of hand-based object manipulation device is Leap Motion. So far, all previously listed devices evidence the need to hold a physical equipment in the hands to interact with the virtual environment. However, the interaction provided by the Leap Motion tracks the hands of the person, allowing the user to input the movements and figures of the hands into the virtual environment [30].

Since this device is based on tracking the hands, it is possible for these readings to not always be as precise as it would be intended, which has been verified in several system. Figure 11 shows a virtual

[7] Image from [24]

environment where through a finger-based recognition system, the Leap Motion sensor is compared to a video camera in terms of tracking accuracy [31].

Figure 11 - Virtual Environment developed to test the recognition of a Leap Motion device

On the other hand, this also opens doors to the development of fun and interactive games, with a much deeper degree of immersion, and interactivity. A system that can capture simple hand figures like a closed hand, and open hand and a hand with only two fingers extended, is actually capable of mapping those actions to develop a game for playing Rock-Paper-Scissors with a Robot (Figure 12) [32].

Figure 12 - User playing Rock-Paper-Scissors with a Robot

Another example is a game featuring virtual blocks manipulation, created using Augmented Reality to explore the freehand movements provided by Leap Motion [33]. While the system we are developing is in VR, much of the functionalities that this game uses can serve as base and inspiration for our project.

3.3.3 Challenges

Apart from being very powerful, hand-based manipulation deals with different types of issues, as described in the previous sub-sections (3.3.1 and 3.3.2).

One problem that affects the user experience is precision. Whatever be the purpose, either training or gaming, there is a need for the devices and the experience to provide a clear precision of position of the virtual elements, as to not break the illusion provided by the immersion in the environment. An example of a precision error would be the user seeing his hand much more to the left than it actually is.

Another point that needs to be attended is recognition. If precision refers to position, recognition is about the figure. With a tracking devise, if the readings are not correct, this could lead to a mismatch between what the user is doing and what the user is seeing. An example of a recognition error would be the user seeing is hand closed when it is opened.

The use of wire also needs to be minimal, as it can easily disturb the user and ruin the experience.

3.4 Games of Chemistry

Nowadays there are games for all types of people and purposes. This holds true for games in chemistry. A good example would be MOL [34], a game designed to serve as an educational tool regarding player engagement, fun, learning of higher-order thinking skills in the context of organic chemistry, and fostering a cycle of experiential learning. To test the game, it was implemented from 12th grade to university's Organic Chemistry I and II classes, allowing for a good range of test subjects and feedback. The data collected by this study pointed how the students expect educational games to be boring and too heavily focused on the learning materials, but that after playing the game, those predefined expectations were overthrown, since the game proved to be fun and engaging. Moreover, in terms of pedagogical relevance, is that the game can be effectively used as a teaching tool from high school to higher education.

The benefits of playing dedicated games in class is presented in 'Playing with chemistry' [35]. This study verifies the direct effectiveness of games and defends how both gamification and game-based learning approaches have a place in an active learning classroom environment.

Starting with Chirality 2 [36], an app presenting a gamified approach to reviewing stereochemical concepts, this game practices concepts such as functional groups, different types of isomers and the recognition of chiral carbons. The main interaction is done using drag and drop or multiple-choice interface, and the answer to the questions can be revealed afterwards. With this combination of components, the game allows for a built-in assessment as they play and review.

The next game mentioned in the paper is Backside Attack [37], another app available for iOS to teach the concepts of the SN2 reaction, where players must first learn to shoot a molecule from a syringe into a beaker to unlock a reaction activity. After managing so, they then proceed to drawing the mechanistic curly arrows for attack of a nucleophile on an electrophile and then for cleavage of a leaving group. The game presents a novel approach to understanding energy and reaction coordinate, by using a tapping mechanism, where the players repeatedly press the screen to add energy, thus helping the molecule over the transition state.

Then we have Labster, a collection of laboratory simulations that use storylines and missions to keep students interested and involved and by using the GearVR interface, it becomes possible to create an immersive laboratory experience in Virtual Reality.

A different type of setting is presented in SuperChemVR, where the player is in a space station and must perform specific chemical reactions correctly in order to survive. This game simulates experiences, that could be hard to perform, in a safe fully immersive VR system, like the Oculus Rift or HTC Vive.

It finishes by presenting us Mechanisms, a game that aims to transform curly arrow notation from a pen and paper activity to an interactive experience for both touch- screen and web. It includes game levels appropriate for introductory courses in organic chemistry, while also using machine learning algorithms to make the game 'smarter' and personalize the experience for each user. The data platform will map student progress in real- time and compare these mechanism maps with those of subject matter experts, predicting when and how a student understands a concept, providing it afterwards to the student in gameplay, and to instructors through a dashboard.

Another board game on organic chemistry, is React! [38], a multiplayer based on the buying and trading of chemicals (Figure 13). The objective is to discover and perform reactions, however, in order to do so, the players must draw and transform chemical functional groups to create new molecules, which puts in practice the contends they learned on the course.

Figure 13 - Board of the game React! [8]

A good example of how simple games can also be adapted to fit the needs is in the "Spot the differences" Game [39], where students must identify the differences between two images, as seen in Figure 14. Not only this attest for the knowledge the students have on the concepts, but also prompts them to pay close attention to the details on the bonds between each atom and molecule.

[8] Image from https://www.kickstarter.com/projects/345110877/react-the-organic-chemistry-board-game

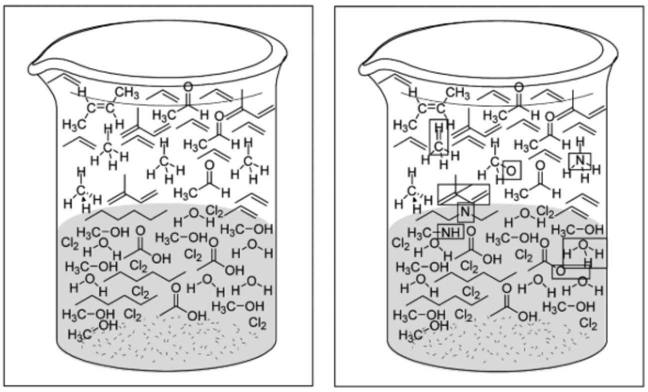

Figure 14 - An activity from the game "Spot the Differences" [9]

All presented games show how games brought engagement, collaboration, and a spirit of joy, which is difficult to attain with a more traditional teaching method.

3.5 Tools used in the teaching of Chemistry

A large variety of tools is used by Chemistry professor to help the student's comprehension of the subject.

In 'Personal Experience with Four Kinds of Chemical Structure Drawing Software: Review on ChemDraw, ChemWindow, ISIS/Draw, and ChemSketch' [40], a deep analyses of some chemical structure drawing software is made, in particular, on the four mentioned in the title, ChemDraw, ChemWindow, ISIS/Draw, and ChemSketch, since these were the most popular chemical drawing software at the given time. This comparison allows us to understand how the programs differ from one another. The analyses done categorizes and differentiates the features that are the most important for the people in this area of work: Installation, Free-Hand Drawing of Chemical Structure, Drawing with Templates and Pre-setting, Drawing of Glassware and Chemical Process Chart, Structure and Nomenclature, Three-Dimensional Structure, Management of Spectral Information and some Other Usages. From those topics, the paper highlights an easy installation process, without many complications; the free-hand drawing is essential in the finishing and detail modifications after templates are used, supported by a high availability in types of bonds between the atoms; user-friendly templates of molecules with possibility to add custom templates, that are easy to use; operations of selection, move, duplicate, paste, rotate, reflection, flip, and alignment are indispensable; containing glassware templates for chemical equipment and units drawing; an easy to use interface; the supply of different nomenclature modules, to allow the naming of different compounds; displaying the structures in 3D, for easier visibility and understanding; possibility to do spectral management; supporting many files format and doing some calculations for molecules properties.

[9] Image from [39]

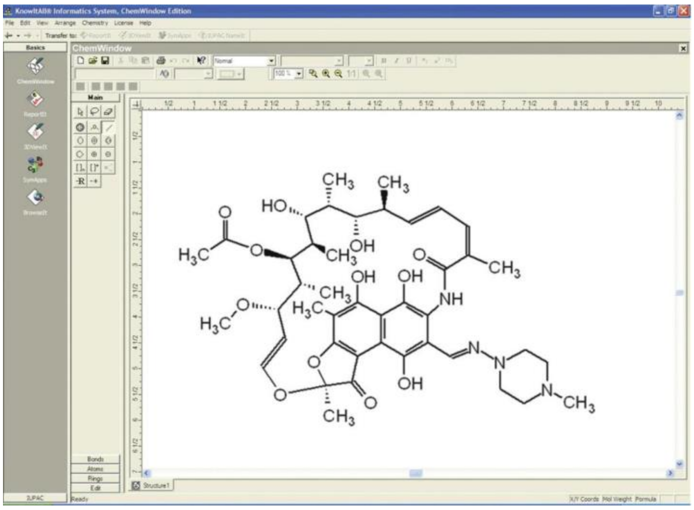

Figure 15 - Interface of ChemWindow [10]

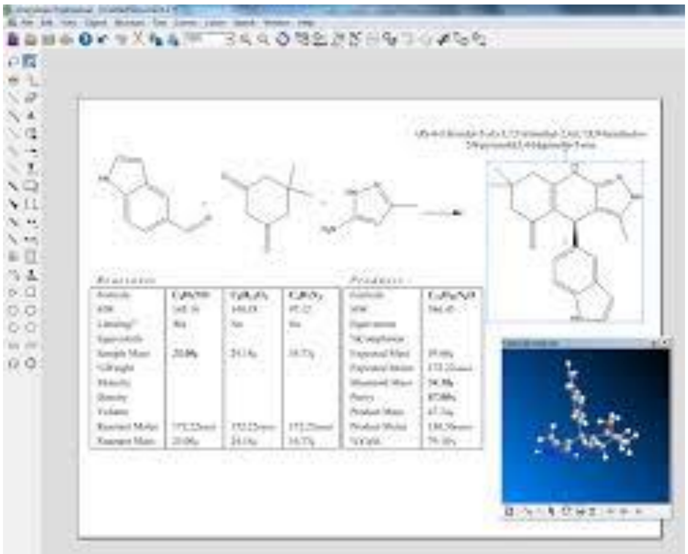

Figure *16 - Interface of ChemDraw* [11]

Another similar tool, although not focused in Chemistry, but on Biology, is described in 'BioVR: A platform for virtual reality assisted biological data integration and visualization' [41]. Using Unity3D it was possible to build the VR-enabled desktop application, based on the software package called UnityMol.

The focus of this work is to facilitate the viewing of DNA/RNA sequences and protein structures in aggregate, leading to a novel workflow for researchers. This is achieved by utilizing an Oculus Rift and Leap Motion hand detection, resulting in intuitive navigation and exploration of various types of biological data.

In the development of this work, it was possible to conclude that VR is a ground-breaking medium with major advantages over traditional visualization and that animated simulations can be made to help

[10] Image from https://docplayer.net/52664662-Knowitall-chemwindow-edition.html
[11] Image from https://www.additive-net.de/en/software/produkte/perkinelmer/chemdraw

users visualize temporal datasets. The interesting point of this conclusions is that, although the focus here was in Biology, it is possible to extract some information for my work, like the use of animations, and the importance of making good use of the advantages of having a VR environment for the display.

4

Methodology

4.1 Overall approach

To reach the defined objective of implementing an improved version of the interaction system of the game “Touch on Chemistry”, this project focuses on developing and exploring different ways of interaction between the users and the virtual environment.

The overall approach of present project will essentially follow an experimental methodology organized in 3 major steps:

STEP 1: Analysis of the pre-existing version of “Touch on Chemistry”; Identification and assessment of needs of the users for the new implementation

STEP 2: Development and Implementation of the System

STEP 3: Validation of the System

The diagram in Figure 17 indicates all Steps of the Methodology and what each of them will be subdivided into.

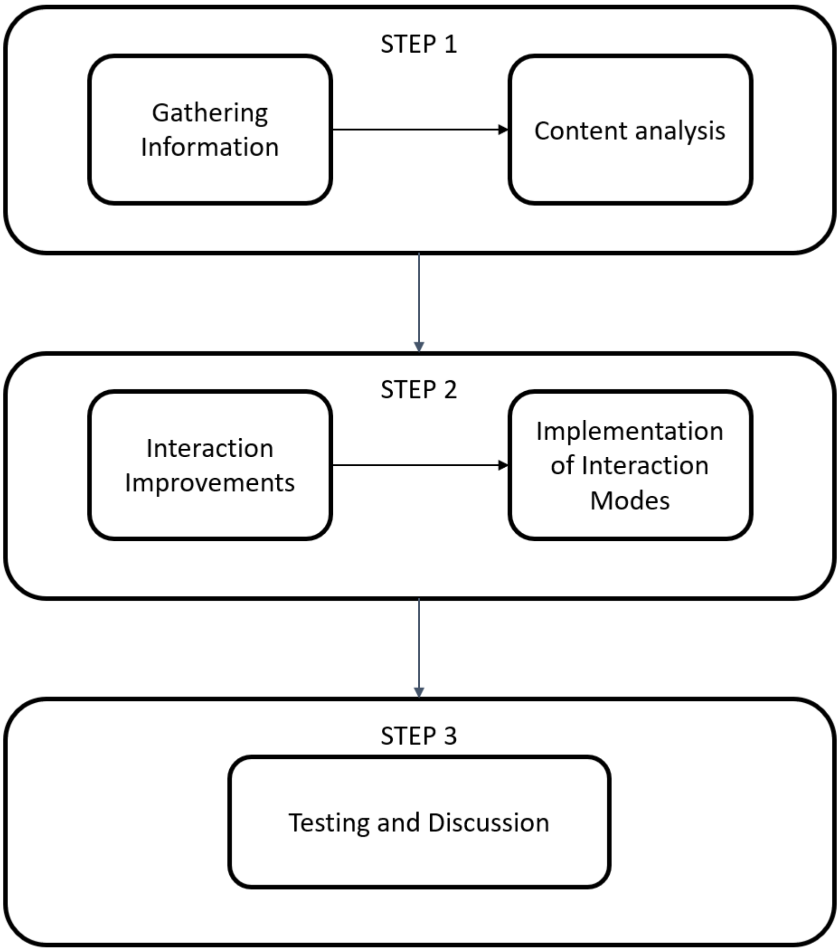

Figure 17- Flowchart of the Methodology

For the Step 1 we start by gathering information. The samples are of convenience with volunteers being recruited at the University or online, and when applied, the volunteers signed an informed consent

(Annex A). We will realize tests of the current version of the system with users from high schools since they are a target audience of the game. This will allow us to gather data on the current performance of the game. We will also conduct an interview with teachers and researchers of chemistry at university, to know what type of interaction this system is expected to provide and how they would expect this interaction to happen. To better define the interaction possibilities of the system a new set of tests were carried out online with others volunteers.

After gathering the data, it is necessary to analyse its contents in order to identify the aspects that can be improved in the system and its interaction.

Step 2 starts based on all the information previously obtained, by designing possible ways of interaction. We then develop and implement new interaction models of the system. When the implementation of such models is over, we will proceed to test the system and discuss the data collected from such tests.

For this Step 3, users to test the new system are volunteers and will also sign an informed consent. This validation will be based on time and performance metrics, so the results will evidence if the interaction is fulfilling the defined objectives or not.

Having finished all the testing and discussion, we will present the conclusions reached by this project.

4.2 Virtual Reality

The virtual immersion can be achieved by using a HMD with VR Sensors (Figure 18).

Figure 18 - HTC Vive Equipment [12]

For the software, we will use Unity3D, Version 2019.1.11f1 (Figure 19) on Windows to create the virtual environment and the SteamVR packages to allow the connection between the HMD and Unity.

[12] Image from: https://ifworlddesignguide.com/entry/199745-htc-vive

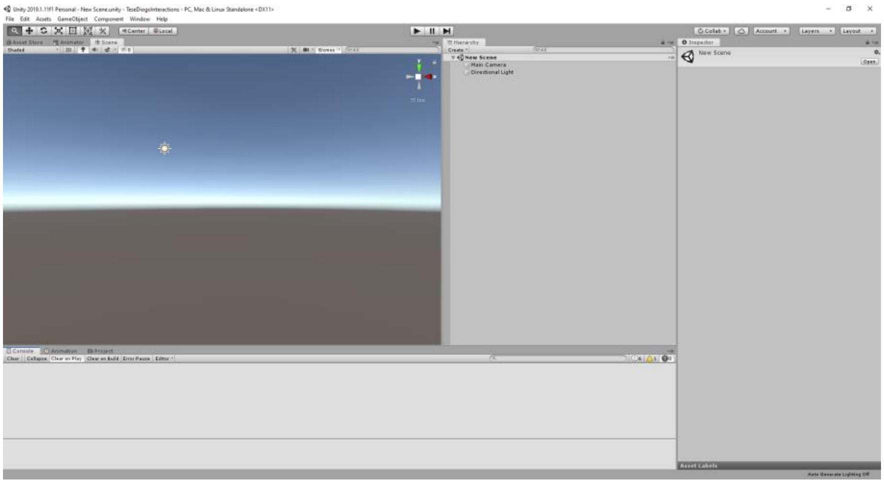

Figure 19 - User Interface of the software Unity version 2019.1.11f.1

4.3 Leap Motion

For the hands recognition, it is used the Leap Motion device from Ultraleap (Figure 20) with the Orion software version 4.0.0 of its Developer Kit and the package of Leap Motion Unity Modules version 4.5.0.

Figure 20- Leap Motion Equipment[13]

[13] Image from: https://www.ultraleap.com/product/leap-motion-controller/

5

System Implementation

5.1 Previous Version Data Collection

To update the system with a new version of the game “Touch in Chemistry”, it was crucial to identify users expectations, as well as to know the performance of the previous version.

Expectations were identified through an interview with chemistry teachers and researchers. To validate the performance, a first set of anonymous user tests were executed. Domains of interaction were also assessed to better define the possibilities of interaction of the system through some online tests with a third set of volunteers.

5.1.1 Interview of Chemistry Teachers

As mentioned in section 3.1.2, a semi-structured interview was conducted to 2 universitary teachers and 1 researcher of the chemistry department of the “Instituto Superior Técnico” of the Lisbon University.

From this interview it was clear that the system should be useful for both classes and autonomous study of students of chemistry. Also, the most notable aspects and features would be the possibility of rotating a molecule, having a good way to control the distance of the links between the atoms, along with the size of the link and considering the type of link (if it were a single link, double or a triple). It was also pointed by the interviewed the importance of being able to connect any atom of a molecule or even join two molecules. Both aspects were not working in the previous version.

5.1.2 First set of tests

The first set of tests was held during the activity ‘Laboratórios Abertos DEQ 2020’ [42] through the course of 3 days. A total of 120 highschool students were recruited as testers, of which 55 (45,8%) were men, 21 (17,5%) were women and 44 (36,7%) did not register their gender. Of the 120 users, 66 (55%) had some experience with VR and for the remaining 54 (45%) this test represented their first contact with this technology.

After the test, users answered three questions: “Did you have any struggle while interacting with the system? If so, what was it”, “What did you enjoy the most about the system?” and “Is there anything where you think the system could be better?”.

For the first question, over 41% of the users mentioned that the system was sometimes lagging. This hindered their performance tremendously, to the point where there would barely be any actual overlapping between the hands position in the virtual environment and their actual position in the real world. As such, this was registered as one of the most important aspects to consider for the development of the new version of the system.

It was also mentioned some difficulties with the mechanic of grabbing the atoms, being reported by over 35% of the users that sometimes the atom would be grabbed at a different point of contact than the one intended by the user. Consequently, for the new version, a special attention to the area to grab the atom was considered.

Was also reported by 2.5% some discomfort since the system was considered to be too bright.

In the second question, the most enjoyable aspect reported by 15% of the users mentioned the possibility of interaction with atoms and molecules. Thus, interaction was accepted as a key factor for the virtual environment of the new version. There were also over 10% of users that highlighted as a major advantage the interaction without the need of a controller. This is direct evidence of the importance of interaction, preferentially using their own hands. .

It was also pointed by 6% of the users as a major aspect of the system, the creativity of the idea behind the system. Considering that VR has been around for some decades and Leap Motion for a couple years, there is space for both technologies, such as in teaching purposes, increasing the proximity with younger students.

Question three was focused on ways pinpointing key factors to improve in the system to provide the user with a better experience.

Nearly 16% of the users provided feedback on how they would like the action of the grabbing atoms to be better. The feedback of 4% of the users focused on interaction but with playful purposes by the possibility of throwing atoms, for instance. Since atoms are supposed to be static in the virtual environment, so that users can grab them easily, the implementation of this suggestion would not have impact on the core gameplay but can be considered as a possible easter egg or funny feature to bring more enjoyment into the game.

5.1.3 Interaction Recordings

Considering the data collected from the interview and tests with users, interaction was defined as the part of the system requiring more attention.

Data collected also suggest that interaction includes different domains, namely the creation of molecules, movement of atoms and molecules as their rotation and even changing their connections inside molecules.

To better define the interaction possibilities of the system we prepared a group of simple tasks and asked online for volunteers, that were currently frequenting university, to record themselves performing such tasks. These tasks (Annex B) were based on simple interactions, to be performed during 5 to 10 minutes.

An example of the simplicity can be observed in Figure 21, where a user is seen showing the result of a task.

Figure 21 - User signalling that the task is completed

After a week, the request for testing was taken off and was possible to collect data from 3 videos of 3 higher education students (2 men, 1 women).

While the number of samples was not enough to retract any general information, it did allow us to improve our understanding on how some users might expect the interaction with the system to proceed, especially since some users were narrating as they performed the tasks.

5.2 System Update

Since the development of the previous version of the system, much of the used software had already been updated by their respective developers, and some of the issues seen in the tests could be solved by updating the modules and components of the system, in particular the components related to the Leap Motion.

As such, we decided to update the Leap Motion Unity Modules to the version 4.5.0. With this new version of the Leap Motion Unity Modules, it is necessary to have a Unity version compatible with it, so, we also upgraded Unity to version 2019.1.11f.1. The SteamVR unity plugin used was the version 2.6.1.

At the same time, in order for the focus of this update to be on the interaction part, the system developed will refrain from considering the chemistry concepts.

5.2.1 Installed Software

5.2.1.1 Steam VR

For the user to be recognized in the virtual environment, it is necessary to have software that can make use of the information captured by the HTC Vive and the sensor it provides. For unity, the SteamVR plugin allow us to use this information by the use of the prefab LeapRig, which translates to the virtual world the mapping of the real-world space detected.

5.2.1.2 Leap Motion Application

The previously mentioned Leap Motion Unity Modules consist of the following unity packages: Core Module, Graphic Renderer, Hands, and Interaction Engine. For a Unity project to work with Leap Motion, it will always need the Core Module. The Graphic Renderer package main purpose is to boost the rendering of the project. The Hands package offers more hand models. The Interaction Engine allows a more natural interaction with the virtual objects and interfaces .With all this information in mind, we knew we would need the Core Module as a base, and the Interaction Engine to provide the user with a higher quality of interaction. Since the two other packages were not as essential considering the objective of this project, they were not implemented.

5.2.1.2.1 Core Module

To be able to use the information about the hands of the user, the Core Module provides scripts that allow the detection of different aspects of the hand, as the Extended Finger Detector, the Finger Direction Detector, the Palm Direction Detector, Pinch Detector, and Detector Logic Gate. There are the main scripts we will use need to process that information.

The Extended Finger Detector looks at the fingers of a selected hand and activates if the chosen ones are extended or not. The parameters of this scripts can be confirmed in Figure 22.

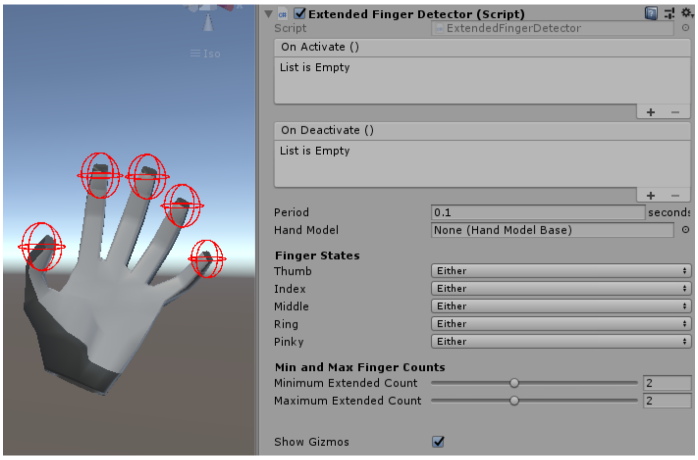

Figure 22 - Parameters of the Extended Finger Detector script and gismos representing if the parameters are true or false

The Finger Direction Detector verifies if a selected finger is pointing in the given direction. As seen in Figure 23, the index finger of the left hand is not pointing towards the y = 1 direction seen on the image, as such, the gismo is represented with red. In the Figure 24, where the Index finger is already pointing towards the desired direction, we can see the gismo at green.

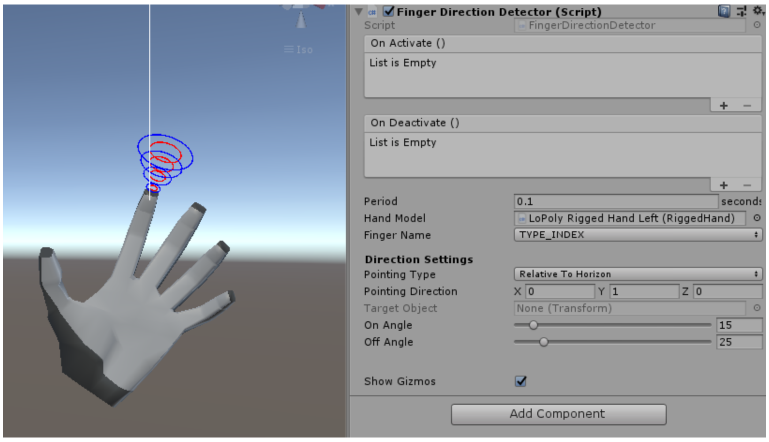

Figure 23 - Parameter of the Finger Direction Detector script

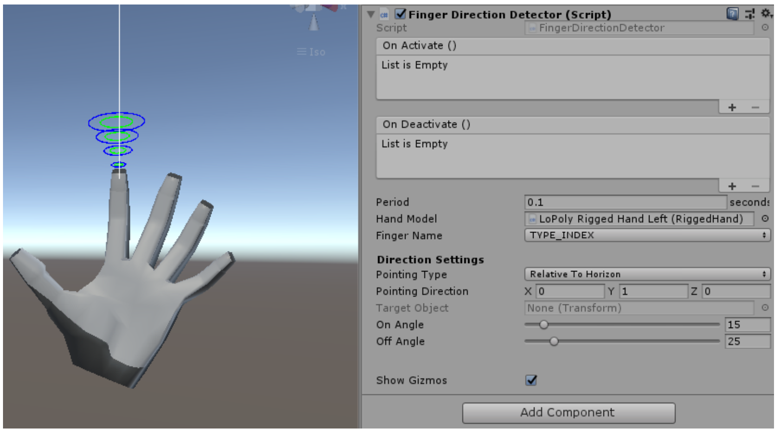

Figure 24 - Parameter of the Finger Direction Detector script and index pointing in the correct direction

The Palm Direction Detector, much like the previous script, indicates if the Palm of a selected hand is pointing in the specified direction (Figure 25)

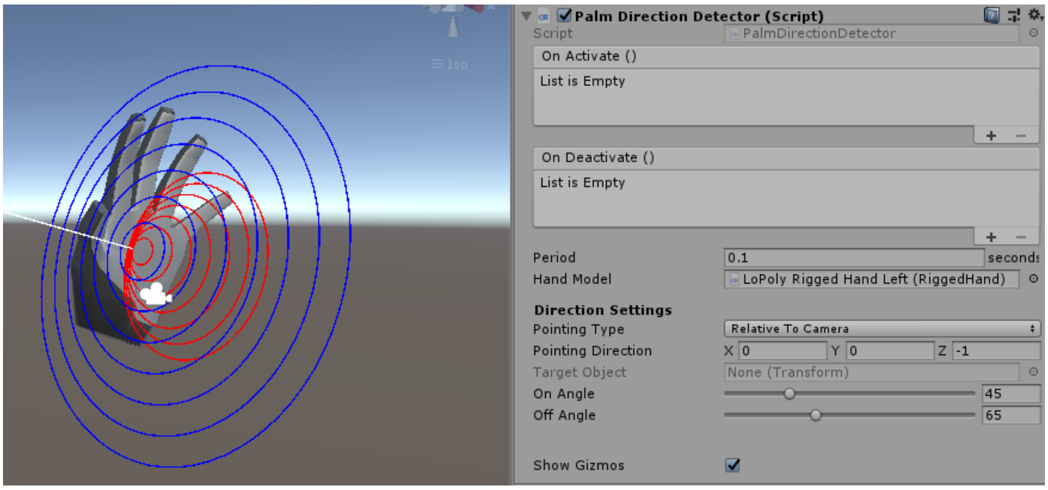

Figure 25 - Parameter of the Palm Direction Detector script

The Pinch Detector script detects if the selected hand is performing a pinch (fingertips of index and thumb fingers touching). We can see in Figure 26 the pinch not activated, and in the Figure 27 that the user successfully executed a pinch.

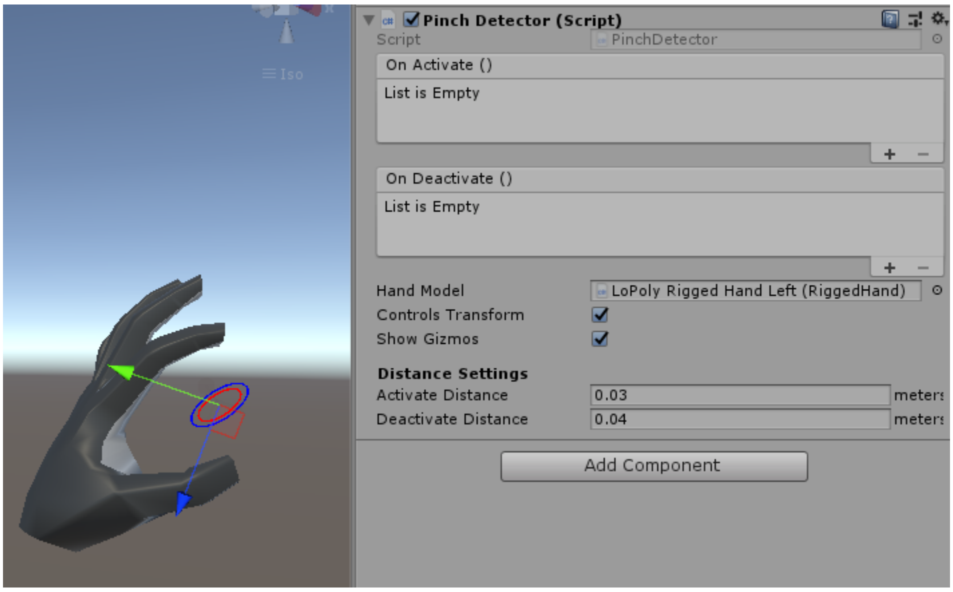

Figure 26 – Parameter of the Pinch Detector script

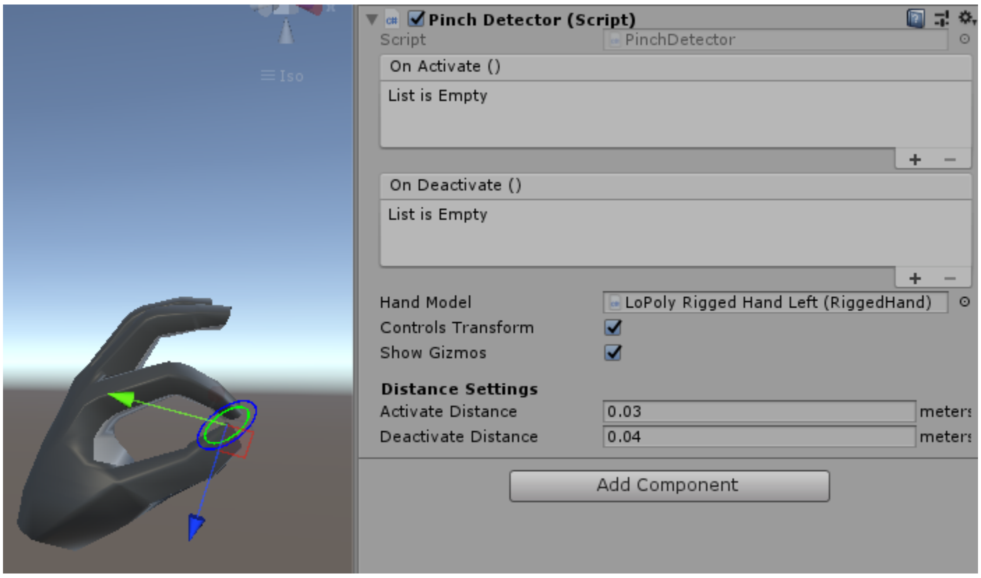

Figure 27 - Parameters of the Pinch Detector script and pinch being performed by the user

5.2.1.2.2 Interaction Engine

The Interaction Engine package gives access to a group of scripts that improve the behaviour of the virtual objects when interacted with. However, it is necessary to add an Interaction Manager unity prefab, which comes with the module, to the project scene. This prefab contains the script Interaction Manager, that will be responsible for controlling the execution of all interaction in the scene. The other necessary step is to add the Interaction Behaviour script to all objects that we want the user to interact with. It is important to note that this script cannot be used if the object does not have a Rigidbody component.

The contents of the Interaction Manager prefab and its respective script can be verified in Figure 28.

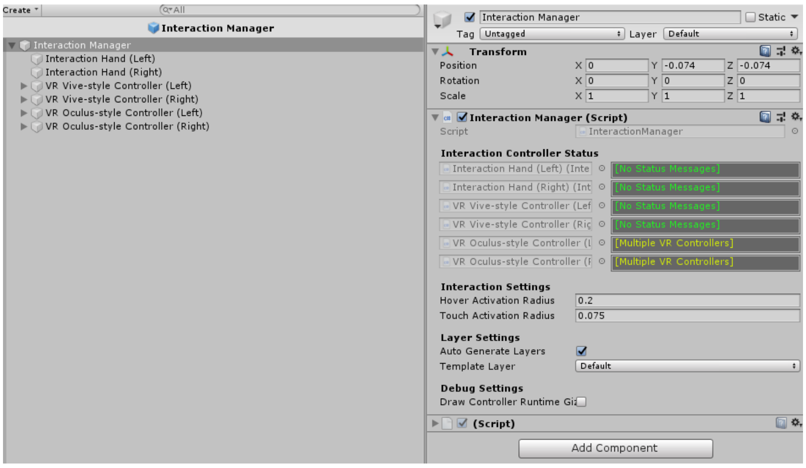

Figure 28 - Interaction Manager Prefab (left) and Parameters of the Interaction Manager script (right)

The Interaction Behaviour script added to all interactable objects is shown in Figure 29. This script also contains the possibility of adding new event types to the behaviour of the object, like the ones seen in Figure 30.

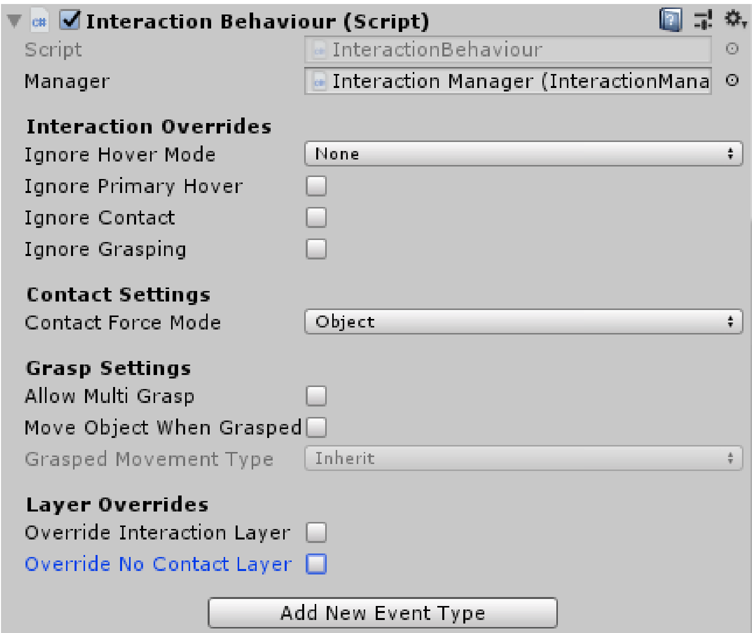

Figure 29 - Parameters of the Interaction Behaviour script

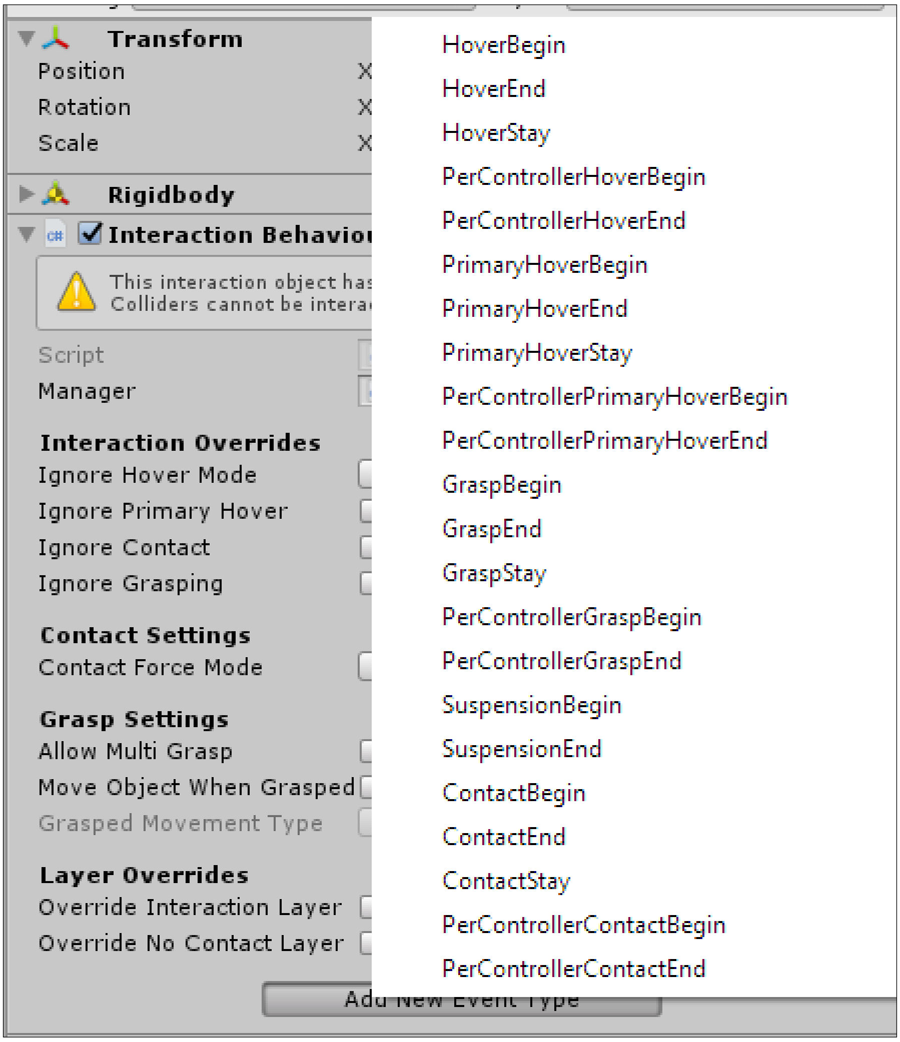

Figure 30 - All Event types that can be added to an Interaction Behaviour

5.2.2 Interactions of the System

Previous results (Section 5.1) of the previous version of the system clarify that the ways of interactions between user and virtual environment were: to grab and move an atom (Figure 31), link two atoms (Figure 32 and Figure 33), move a molecule (Figure 34), rotate a molecule and pressing buttons (Figure 35).

Figure 31 - User Moving an Atom

Figure 32 - Two Atoms before Linking

Figure 33 - Two Atoms after being Linked

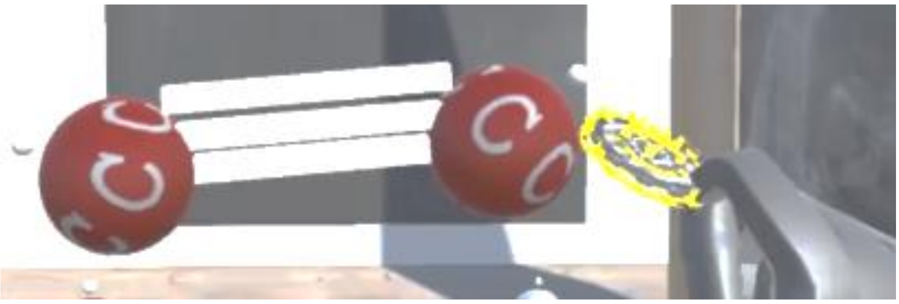

Figure 34 - User moving a Molecule by grabbing the highlighted cog wheel

Figure 35 - User pressing a Button

Furthermore, not only some of these actions were not clear for the users how to perform them, but those actions were not making use of the capacity of the Leap Motion to capture certain hand figures and gestures.

Thus, to improve the interactions of the system, we implemented more and different ways of interaction with the objects in the virtual environment. To facilitate the distinction of each interaction and their purpose, these actions were catalogued into different groups, to which we refer to as interaction modes.

An interaction mode defines the group of actions that the users are allowed to perform at a given time. The description of these modes and their corresponding interactions is presented in Table 1.

Table 1 – Modes of Interaction of the System and respective description

Mode	Description	Interactions
Free Mode	The player can grab and move the objects, as well as collide them to create new links or remove existing ones.	Grab Object Move Object Collide Objects
Selection Mode	Touching an object selects it and all the objects he is linked to it, either directly or indirectly. If the objects are already selected, they are instead unselected.	Touch Objects
Translation Mode	Translates all selected objects by moving hands.	Move Hand
Rotation Mode	Rotates all selected objects around the center of their links by rotating hands.	Rotate Hand
Link Mode	Allows the player to change the number of links between two objects or remove a link between them.	Pinch Links Cut Links

5.2.2.1 Modes of Interaction

Thus, the new version of the interaction system includes the different modes available to the users, with the possibility to alternate from one mode to another. As such, it was necessary to implement ways of controlling how to alternate between the different modes. That is to say, how the user could deactivate one mode or activate another.

Having in consideration the different purposes of each mode and how those purposes should affect the transition of one mode to another, Figure 36 represents the possible state transitions:

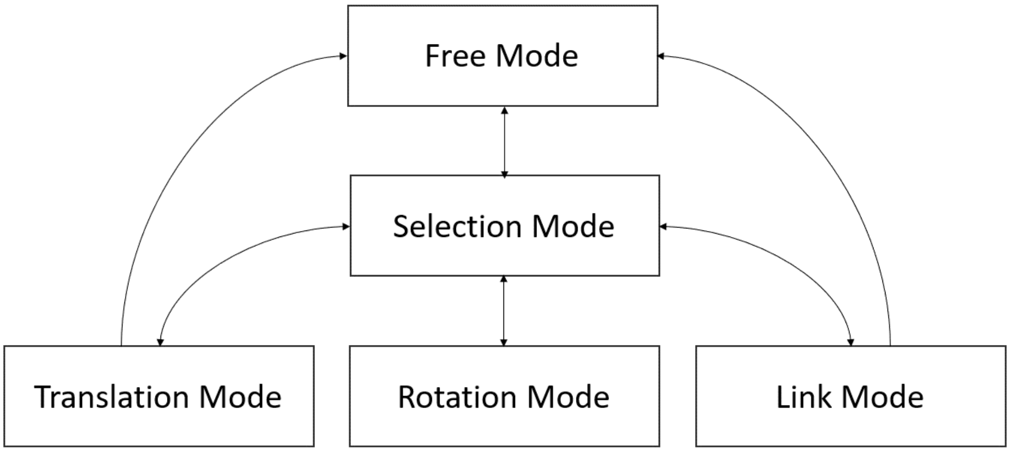

Figure 36 - Possible state transitions of the system

It is possible to activate Free Mode and Selection Mode from every other state. From the Selection mode, users can choose to activate Translation Mode, Rotation Mode or Link Mode.

After setting these transitions, it was necessary to implement their functionality (what the users could do in each mode) and an adequate interface (what the user could see in each mode).

5.2.2.2 Functionality

The Leap Motion sensor allow the capture of Hand Figures (static figures of the hands with how many fingers are extended and what direction is faced) (Figure 37) and the recording of gestures (dynamic execution of a Hand Figure) (Figure 38).

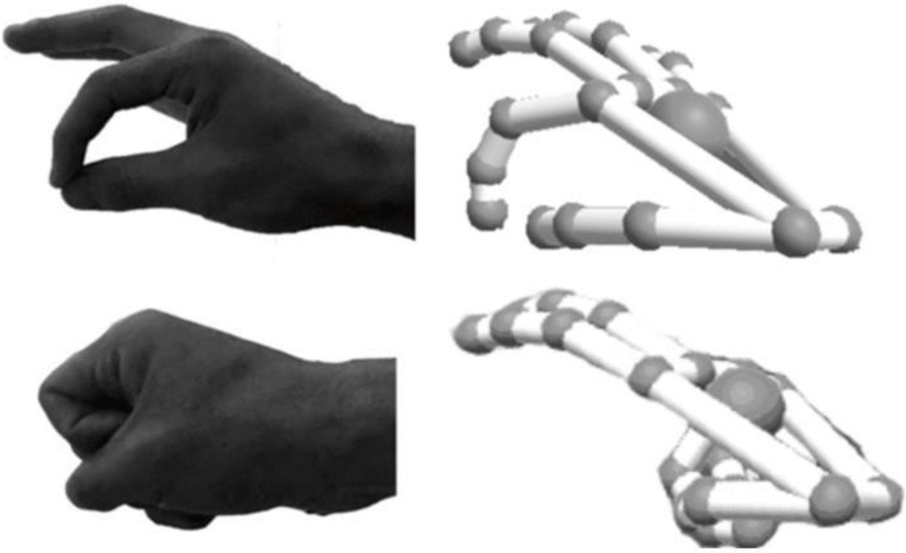

Figure 37 – Hands (left) and respective recognized Hand Figures by the Leap Motion (right) [14]

[14] Image from: https://www.researchgate.net/figure/a-Test-of-Type-1-b-Real-gesture-of-Type-1-c-Type-1-rendered-by-Leap-Motion-d-Test_fig1_322872342

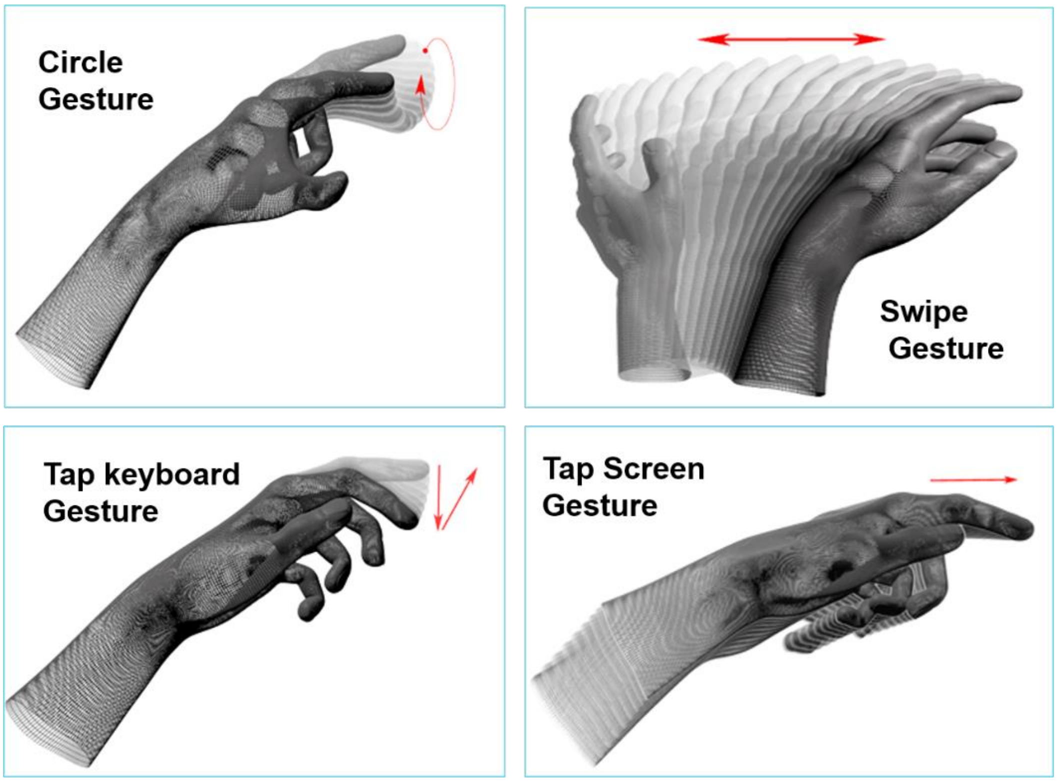

Figure 38 - Examples of gestures capture by the Leap Motion [15]

Considering how to implement the activation of the new modes by making the most use of the Leap Motion, the solution was to use the recognition of a Hand Figures as activation of a mode, and then a Gesture for performing an action of the mode.

The Gestures for the actions of each Mode will be mentioned next. The Hand Figures for the activation of the modes will be mentioned further ahead in section 5.2.3

5.2.2.2.1 Free Mode

In Free Mode the user is able to grab an object, move the currently grabbed object and collide to objects to form or remove a link.

Grabbing an object can be done with the exact same gesture a user would do to grab an object in a non-virtual environment. As seen in Figure 39, before an object is grabbed, it has no highlight at all, however, in order to give feedback to the user that an object is currently grabbed, a small highlight was programmed to appear around the grabbed object (Figure 40)

[15] Image from: https://xiaotingrunning.wordpress.com/2015/03/page/2/

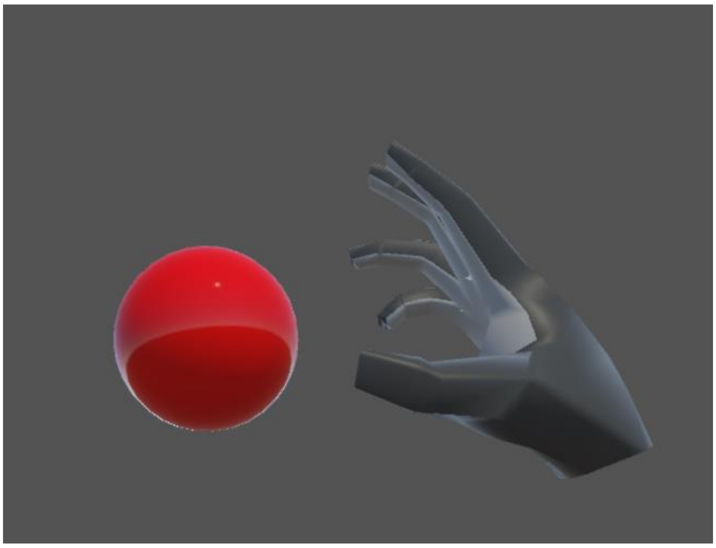

Figure 39 - An object before being grabbed by the user

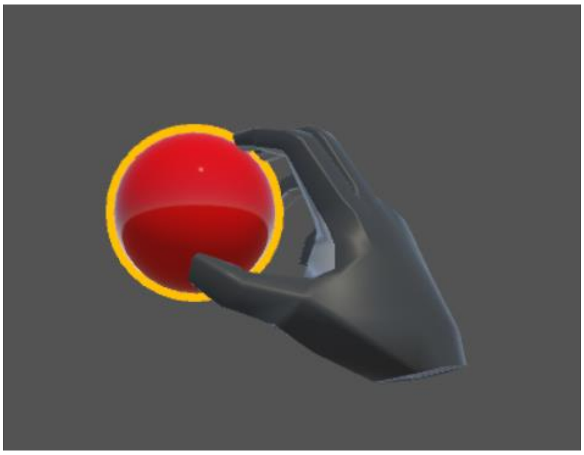

Figure 40 - User grabbing an object

To move an object, the user would only need to move his hand while the object is being grabbed (Figure 41 and Figure 42). A previous error in this action was that if the user grabbed an object with a hand, but the hand disappeared from the vision of the user, the grabbed object would remain in the place it was when the hand reappeared. However, in the developed system, once the hand reappeared, if it were still doing the gesture of grabbing an object, the object would remain grabbed, that was grabbed, when the hand appeared again, the object would remain in the position it was before the hand. To stop moving an object the user would need to stop grabbing it.

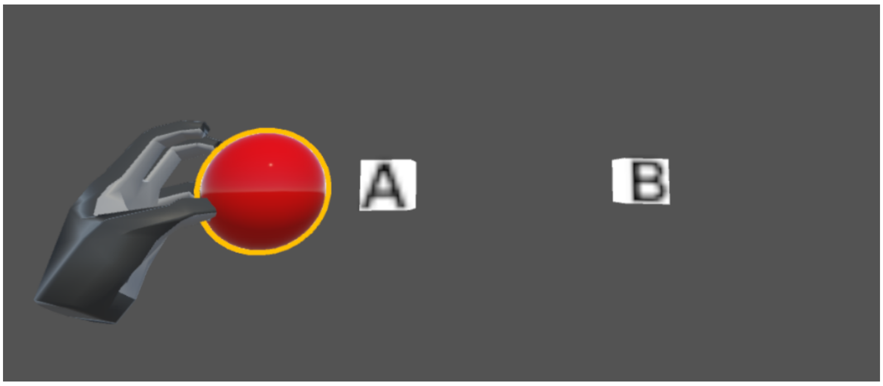

Figure 41 - User beginning to move moving an object from A to B

Figure 42 - User finishing to move an object from A to B

The collision of objects was based on the actual OnCollisionEnter event of Unity. If the user grabbed one object in each hand and approximated them close enough to trigger the event (Figure 43), a link would be formed between those two objects (Figure 44) . If the objects were already linked together, the link would be removed.

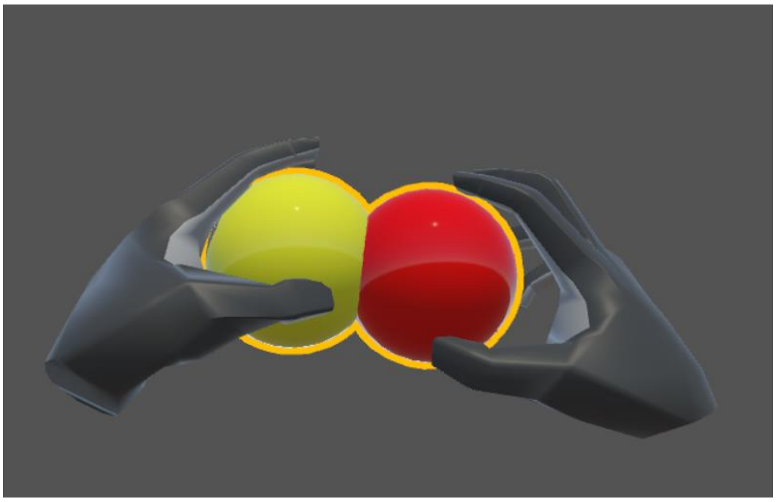

Figure 43 - User colliding two objects

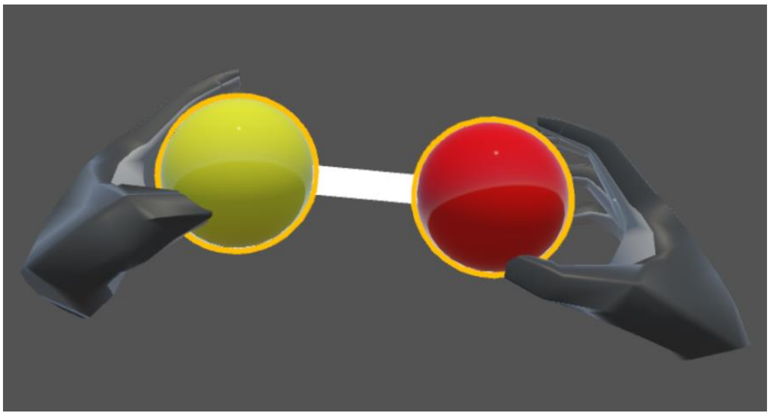

Figure 44 - Link formed after the collision of two objects

5.2.2.2.2 Selection Mode

In Selection Mode, the user is only allowed to touch an object in order to select it and all object linked to it, directly or indirectly. The user is allowed to select more than one group of objects (Figure 45).

Once the objects are selected, it would be possible to observe around them the same highlight as when the objects were grabbed.

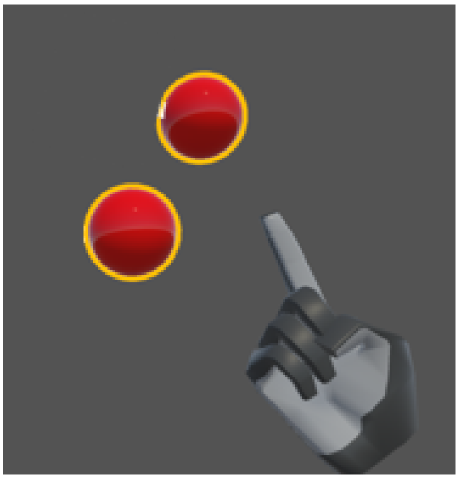

Figure 45 - User selecting two different objects

5.2.2.2.3 Translation Mode

In Translation Mode, the only gesture necessary is that of the movement of the hands. By moving a hand, the selected objects would move in the same manner (Figure 46). The highlight of the selected objects would change to blue.

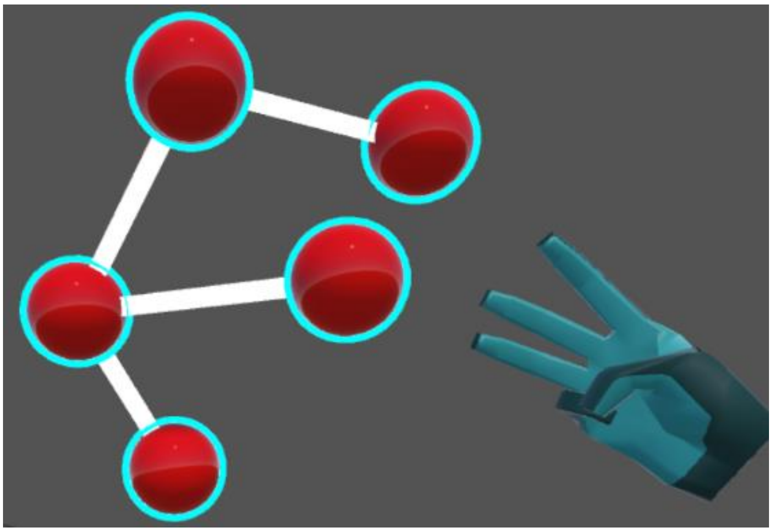

Figure 46 - User moving a group of objects

5.2.2.2.4 Rotation Mode

Rotation Mode works in a similar way to Translation Mode, however, instead of the group of objects moving in the same way as the hand, they would rotate around the center of their link in the same way the hand would rotate (Figure 47). In Rotation Mode the highlight of the objects would change to dark blue.

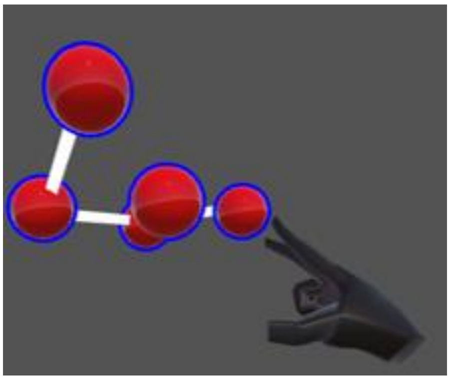

Figure 47 - User rotating a group of objects

5.2.2.2.5 Link Mode

In Link Mode, the user can cut or change the size of a link in the selected group. While in Link mode, the highlight of the selected objects would be green.

To change the size of a link (to a maximum of 3), the gesture necessary is to move the hand to the location of the link and pinch it (Figure 48). If it was a single link, it would become a double link, then a triple, and if a triple link were pinched, it would reset to being a single link.

To cut a link, the user would need to move his hand and as if it were scissors and cut the link (Figure 49).

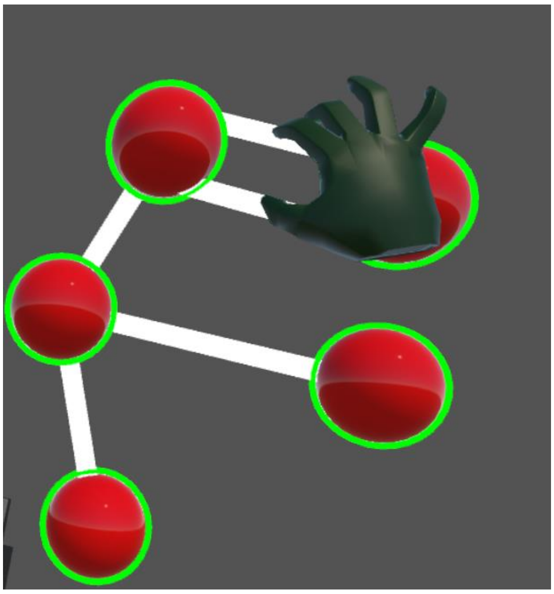

Figure 48 - Single Link becoming a Double Link after being pinched

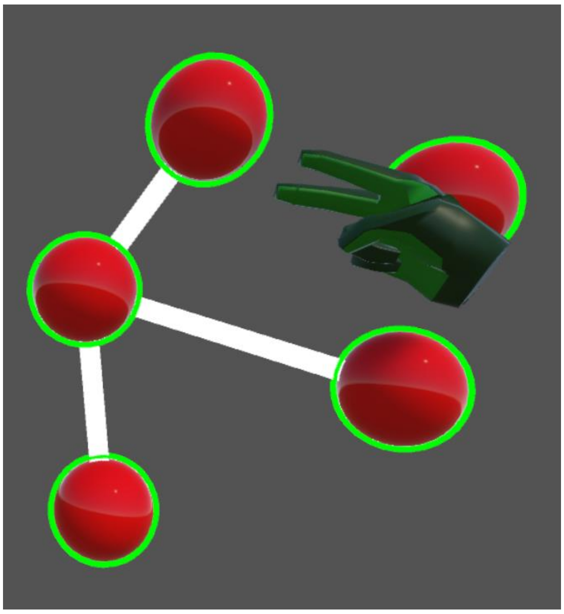

Figure 49 - Link removed after being cut by the user

5.2.2.3 Interface

Designing user interfaces assume as relevant to give feedback to the user about the actions executed. In our interface system, the feedback is assumed as a change of colour of the hands whenever a mode is being activated. By deactivating a mode, the colour returns to the previous one.

The Figure 50 through Figure 54 demonstrate the corresponding hand colour of each mode. When the

Figure 50 - Free Mode Hand Colour

Figure 51 - Selection Mode Hand Colour

Figure 52- Translation Mode Hand Colour

Figure 53 - Rotation Mode Hand Colour

Figure 54 - Link Mode Hand Colour

This colour change is not made immediate but is made in a smooth transition between the current colour and the colour of the mode that is being activated. Just before a mode finishes activating, the hand would blink in a black colour (Figure 55) and then permanently change to the colour of the activated mode.

Figure 55 - Hand color when changing Mode

5.2.3 Interaction Models

Three different interaction models were developed in the upgraded version of the interaction system. All the models assume a comfortable feeling during interaction aiming to potentiate the advantages of a VR system combined with Leap Motion. These Interaction Models are responsible for mapping the Hand Figures the user does to do the activation of Mode of Interaction.

5.2.3.1 Model 1: Two-Hands Detection Activation

The first interaction model is based on having both hands in a certain position while doing a specific figure in order to activate a mode. Each mode has a combination of Hand Figure for each hand with a position of the hands in relation to each other. The combination for the activation of Selection Mode can be seen in Figure 56, Translation Mode in Figure 57, Rotation Mode in Figure 58, Link Mode in Figure 59 and Free Mode in Figure 60.

When the combination of the figures of both hands is executed for a small period of time it would activate the desired mode.

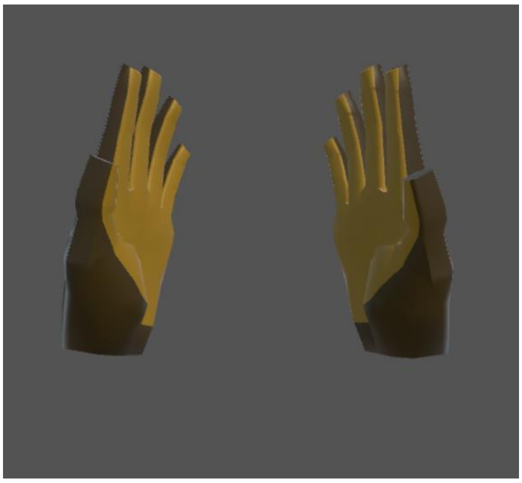

Figure 56 - Hand Figure for the Activation of Selection Mode using 2-Hands Interaction Model

Figure 57 - Hand Figure for the Activation of Translation Mode using 2-Hands Interaction Model

Figure 58 - Hand Figure for the Activation of Rotation Mode using 2-Hands Interaction Model

Figure 59 - Hand Figure for the Activation of link Mode using 2-Hands Interaction Model

Figure 60 - Hand Figure for the Activation of Free Mode using 2-Hands Interaction Model

5.2.3.1.1 Advantages and Disadvantages

The biggest advantage of this model is taking full advantage of the virtual environment around the user to map the selection of the modes.

When immersed in a virtual environment, surrounded by virtual objects with which we can interact, the most natural action is the use of our hands to do so, since it is how we act it in a non-virtual environment where our hands are the first controllers and input devices. Consequently, this model creates a feeling of similarity for the user, facilitating the learning process of the correct hands combination for the activation of the desired mode.

Another advantage of this interaction model is that the activation of the modes can be done as a toggle. Allowing toggle means that the activation can function in two different ways. With toggle on, once the system captures the Hand Figure the user is doing, the user does not need to keep the hand in the same figure while performing the action. If toggle is off, the user needs to maintain the same Hand Figures for the mode to remain active, otherwise the system would have no way of knowing what mode was active.

At the same time, it is necessary to consider that this model needs to interpret the Hand Figure of both hands correctly, as such, it can be more frequent for an activation process to stop midways because the Leap Motion misreads the hand figure of one hand.

5.2.3.1.2 Implementation

Each activation is based on the figure of both hands and the position in relation to themselves.

The figure of the hands could be with fists and the position facing each other (Figure 60) or one hand opened facing the other hand, with this other hand facing the camera without having all fingers extended (Figure 57). However, it should never be with both hands touching each other since that could cause incorrect readings from the sensor of the Leap Motion (Figure 61 and Figure 62).

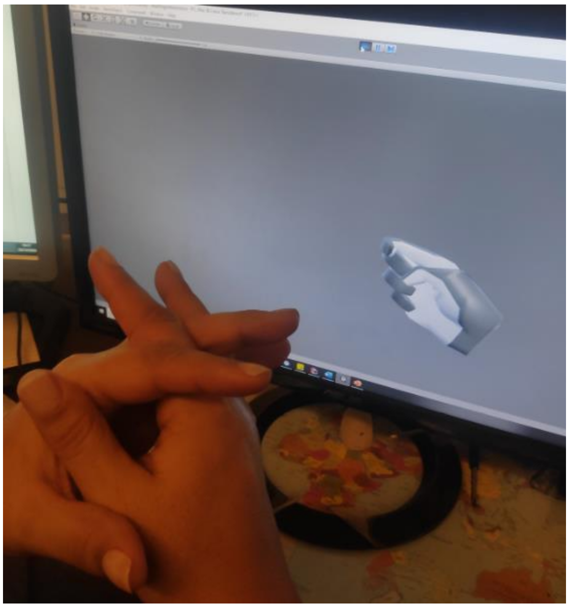

Figure 61 - Leap Motion not correctly reading two hands meshing together

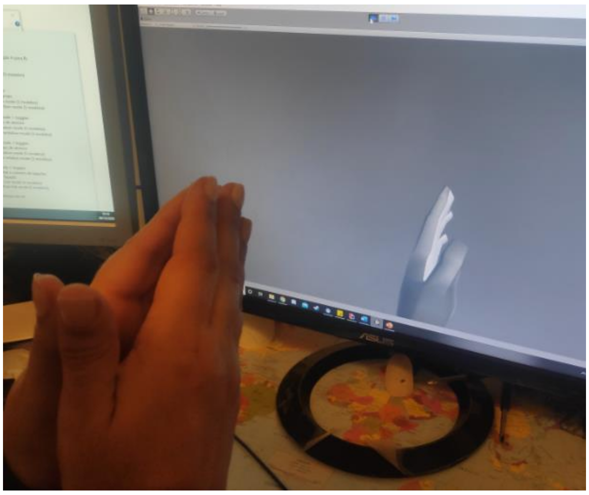

Figure 62- Leap Motion not detecting both hands when they are touching each other

The position would consider if the hands were facing each other or the camera. Lastly, the hand figure of both hands would also be a factor for the activation of the desired mode.

These combinations are not based on symmetric or mirrored figures of the hands. For each combination, one hand could be facing the other hand and doing a certain figure, while the other hand is facing the camera doing another figure (as previously seen in Figure 58).

For the use of the toggle feature, if toggle were on, the moment the user did the combination, he could change the position of the hands and the respective Hand Figure, and the mode would remain on (Figure 63) until he did the same combination for the activated mode. If the toggle were off, one of the hands figures would work as a control for the mode activation and if the user changed that hand figure, the mode would be turned off (Figure 64).

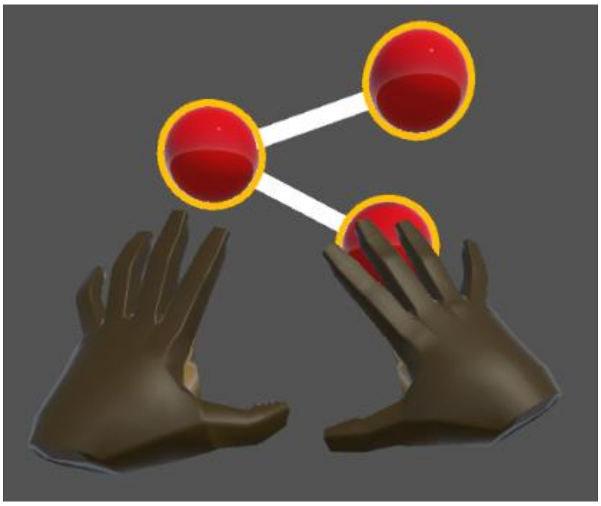

Figure 63 - User freely selecting objects with both hands in Selection Mode (Toggle On)

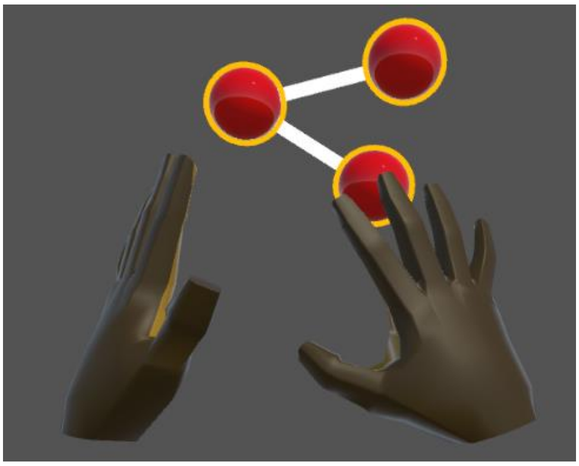

Figure 64 - User maintaining his Left Hand figure as control, while using his Right Hand to select objects (Toggle Off)

5.2.3.2 Model 2: One-Hand Detection Activation

This interaction model implemented is based on executing a Hand Figure with only one hand for a small period of time. It is similar to the previous interaction model, but only considering the Hand Figure and the direction that one hand is facing.

The figure for the activation of the Selection Mode is shown in Figure 65, Translation Mode in Figure 66, Rotation Mode in Figure 67, Link Mode in Figure 68 and Free Mode in Figure 69.

Figure 65 - Hand Figure for the Activation of Selection Mode using 1-Hand Interaction Model

Figure 66 - Hand Figure for the Activation of Translation Mode using 1-Hand Interaction Model

Figure 67 - Hand Figure for the Activation of Rotation Mode using 1-Hand Interaction Model

Figure 68 - Hand Figure for the Activation of Link Mode using 1-Hand Interaction Model

Figure 69 - Hand Figure for the Activation of Free Mode using 1-Hand Interaction Model

5.2.3.2.1 Advantages and Disadvantages

This interaction model is based on usability and simplicity.

By making full use of the aspects of being in a virtual environment with a Leap Motion sensor, using only one hand allows as a controller makes it easier for the user to learn the system controls and the necessary Hand Figures to activate the modes he wants.

At the same time, it is to note that the use of only one hand for the activation of a mode is simpler than needing both hands for the same process.

This model also features the use of toggle in the same way as .mentioned for the Two-Hand Detection Activation model.

5.2.3.2.2 Implementation

For this interaction model, whenever the user wants to activate a mode, it is required to look at the palm of the hand in which he wants to activate it. Since the interaction is based only on one hand at a time, once the user starts activating a mode using any given hand, that hand becomes the currently interactable hand, and the user can no longer activate any mode with the other hand until the currently activated mode is deactivated and back to being Free Mode.

Something necessary to consider while implementing this interaction model is that, due to the possibility of the Leap Motion incorrectly reading the Hand Figure at a given time, this could activate a mode when such is not intended. To correct those misreadings from the Leap Motion, it was necessary to implement some extra factors. One of those factors is the previously mentioned need to look at the palm of the hand when activating the mode, since this ensures a higher chance of correctly reading the Hand Figure. The other factor is the time the user needs to be doing the hand figure for the mode to activate, this will guarantee that the user does not mistakenly activate a mode while doing a different action with his hand other than the intended one.

For the toggle feature implementation, it was made similar to the Two-Hand Detection Activation model. When toggle was on, the user needed only to make the correct figure with his hand for the given period of time and the mode would activate, allowing the user to then change the Hand Figure while the mode was active (Figure 70), and to deactivate the mode by doing the same Hand Figure he used to activate it, for the same period of time. When toggle was off, the moment the user stopped doing the Hand Figure associated with the mode, it would deactivate the mode (Figure 71).

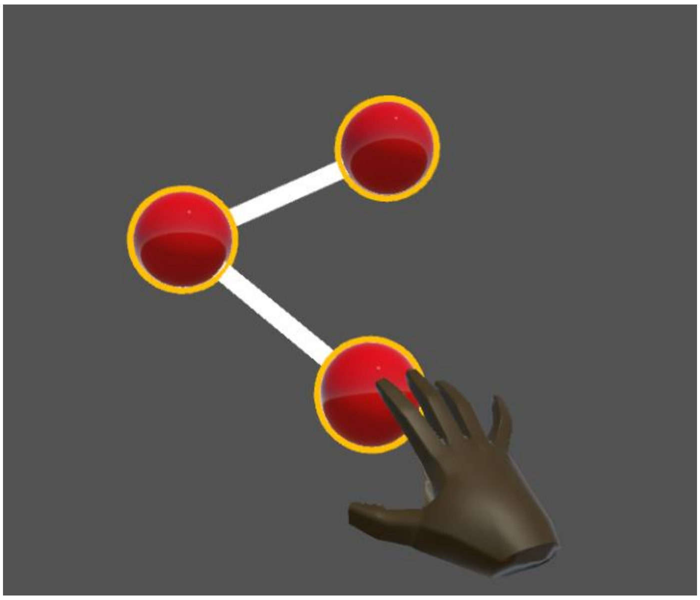

Figure 70 - User freely selecting objects in Selection Mode (Toggle On)

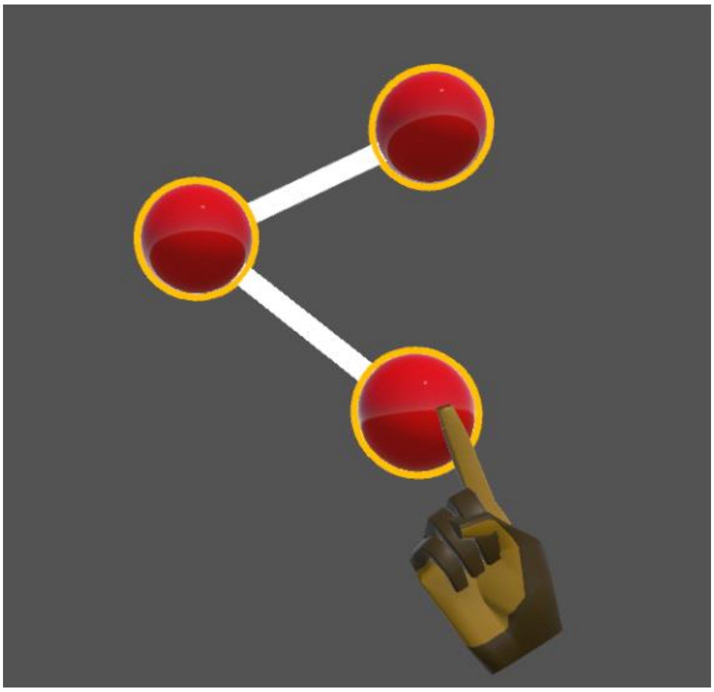

Figure 71 - User selecting objects in Selection Mode while maintaining the necessary Hand Figure (Toggle Off)

5.2.3.3 Model 3: Buttons

The last interaction model implemented was based on buttons.

As previously stated, the Leap Motion does not always make the best capture and reading of the hands. As such, in this model, the activation of modes involves pressing a button in a UI panel next to a hand(Figure 72).

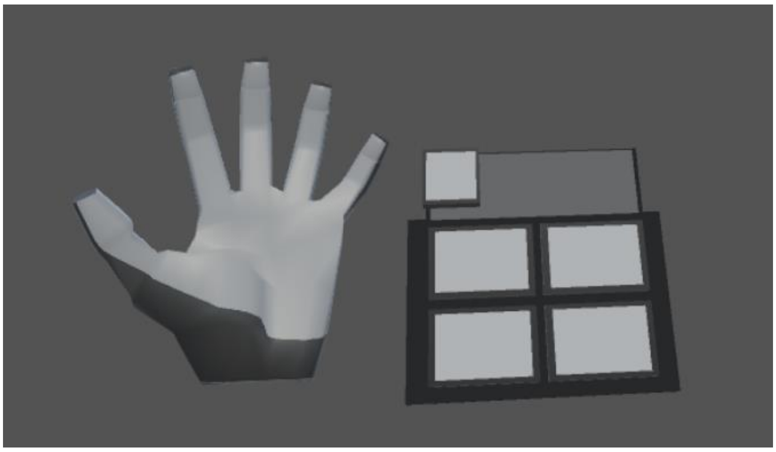

Figure 72 - UI Panel next to the left hand of user

After a button was pressed, the user would need to put one of his hands in the specific Hand Figure associated with the desired mode activate it. The Hand Figure are the same ones used in the previous model (Figure 65 – Figure 69).

Thus, this interaction consists of two factors for the Activation of a mode: pressing the button and then execution of a Hand Figure.

Since the Translation Mode, Rotation Mode and Link Mode are all based on the Selection Mode, the activation of this mode is done with a different button. To activate Selection Mode, the user needs to slide the topmost button to the right (Figure 73). To activate any of the Translation, Rotation or Link Mode, this topmost button needs to be on the right, and then press the adequate button on the other part of the UI panel for the desired mode. That would be the top-left button for the Translation Mode (Figure 74), the top-right button for Rotation Mode (Figure 75) and the bottom-left for the Link Mode (Figure 76).

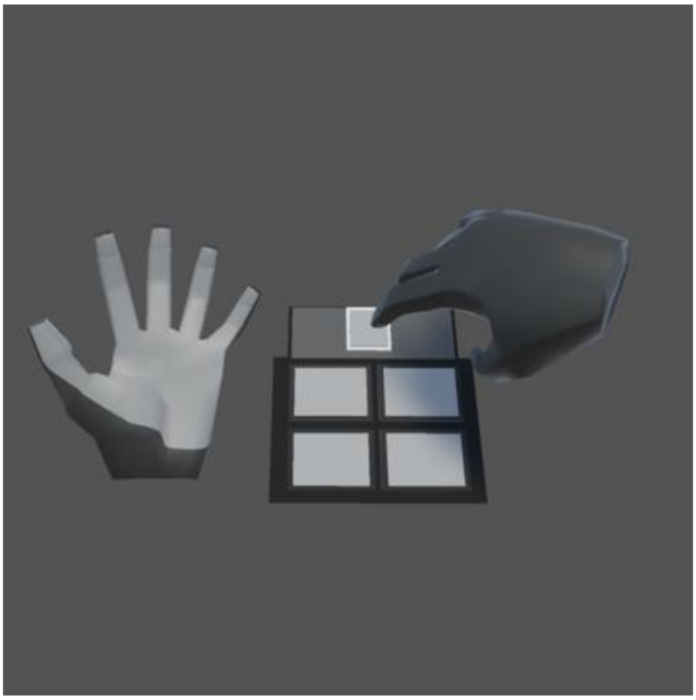

Figure 73 - User in the process of moving topmost button to the right to activate Selection Mode

Figure 74 - User pressing the top-left button to activate Translation Mode

Figure 75 - User pressing the top-right button to activate Rotation Mode

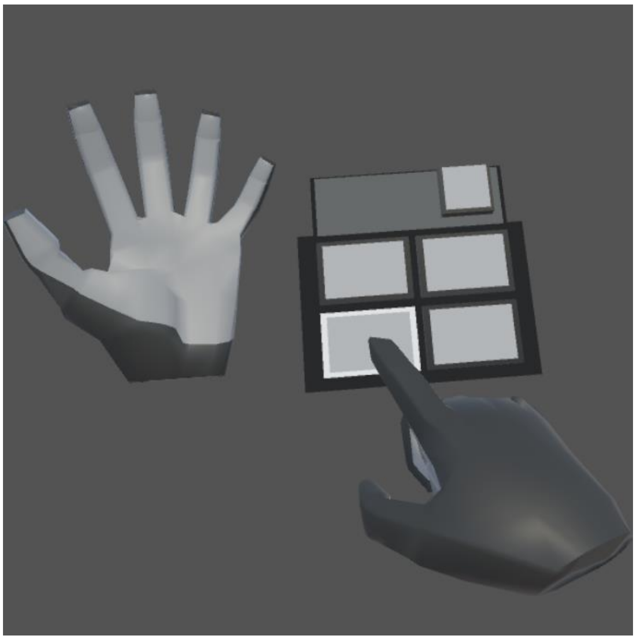

Figure 76 - User pressing the bottom-left button to activate Link Mode

5.2.3.3.1 Advantages and Disadvantages

Pressing buttons are actions with large familiarity and infallibility in the perspective of the individuals, due to social technological advancements from computers, cell phones and other equipments, with either virtual or physical buttons.

As such, by using a model based on buttons, it would be clear for the user what action is needed, and in that way, the system makes use of the past experience that the user has with keyboard, be it in desktop or mobile, and improves his experience in the virtual world.

As previously mentioned, the Leap Motion hand detection capacity is not perfectly accurate, existing the possibility of not capturing the adequate position of the fingers and not inferring the correct figure of the hand .

The combination of buttons and hand figure capture increases the accuracy of this model to activate modes, avoiding the chance of a mode activation being triggered by accident from an incorrect detection of the hands figure.

5.2.3.3.2 Implementation

By having the palm of one hand in front of the camera, a UI panel would appear next to it, with buttons for the different modes (Figure 72).

Using the other hand and pressing one of the buttons would indicate the intention to activate the mode associated with the pressed button. Since the pressing of a button only demonstrates the intention of activating a mode, if after 5 seconds an incorrect Hand Figure or no Hand Figure is performed, it would be necessary to press the button again.

After pressing the button, the user would need to execute the corresponding Hand Figure of that mode to perform the action (Figure 77). The Hand Figure was not associated with any hand in particular, so it could be made using either the left or right hand.

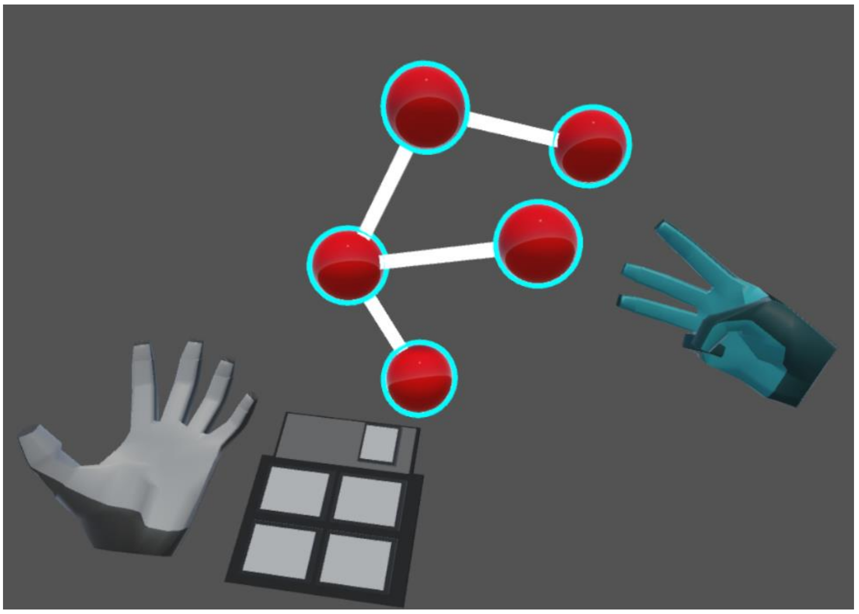

Figure 77 - User moving his hand while doing the Hand Figure of the Translation Mode to move a group of objects

The mode would deactivate once the user stopped doing the Hand Figure. To reactive the mode, he would need to press the same button again.

The UI panel would disappear as soon as the palm of the hand stopped facing the camera.

5.2.4 Testing System

5.2.4.1 Concept

In order to prepare the system for the realization of tests, it was necessary to implement Scenes in the Unity project for the tasks that were to be performed, along with some way to change between them.

This testing system could be implemented so that we could have control over the completion of a task and the selection of the next one. However, since one purpose of the system is to be used to teach chemistry, it was decided to develop this testing system in a way that the user could control the passing and submission of each task, as if they were a student completing the questions given by a teacher.

5.2.4.2 Implementation

To have the testing system be fully operational and as autonomous as possible, it was necessary to introduce the tasks into the system. These tasks were a custom data type that required only a name and a description of the tasks (Figure 78).

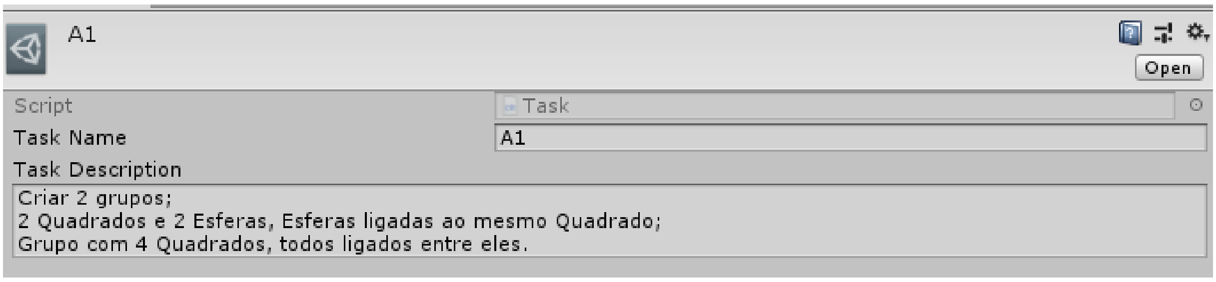

Figure 78 - Task data type created in Unity

Having the tasks introduced into the system, the user would need a way to go from one to another. Since the functionality of this system is not directly based on any of the interaction models previously mentioned, we opted for using hand figures.

Considering the video recordings mentioned in section 4.1.3, and the Figure 21, where a user is seen doing a “thumbs-up” to indicate the completion of a task, it was decided that such a hand figure could easily be accepted as a way of showing the completion of a task (Figure 79). To guaranteed that this figure was not read when not desired, we made it so that the thumb would need to be pointing upwards.

Figure 79 - 'Task Complete' Panel after a user did a "thumbs-up"

At the same time, not only the user needs to submit a task, but he will also need to start a new one. This action also required a hand figure. This hand figure needed to be a figure hard for the user to make unwillingly but at the same time related to the meaning the gesture would portray, of being ready to start. With that in mind, we decided to use the gesture of a hand fully opened and pointing upwards (Figure 80).

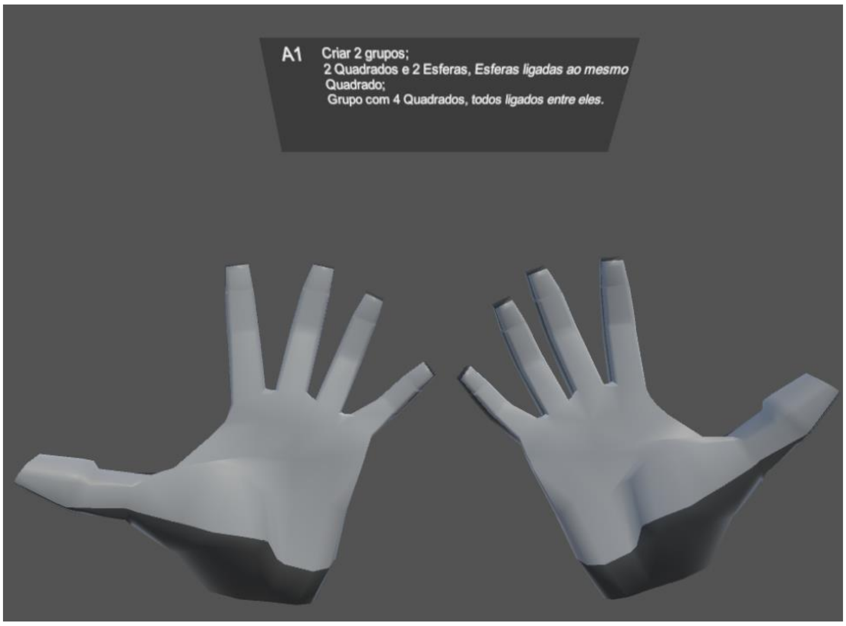

Figure 80 - User opening his hands to start the task and UI panel of the task instructions

To guarantee that those actions would hardly be triggered unless the user wanted to clearly execute them, we also decided to make it so that the hand figures would need to be performed by both hands at the same time.

So that the user could keep track of the task at any time while performing it, we also added a UI panel element, showing the description of the current task to the user.

Since this testing system was first to be used to test the quality of interaction and improvements made to the system before actually being used for teaching purposes, no data was recorded by the system about what the user was doing, the system would only count the time from the start of the task until its submission.

Given that while performing tests there is always a chance of the question not being performed in the same order by all testers, the testing system did not implement a way for the user to choose the next task, it was necessary for the investigator observing the test to input the name of the next task after the submission of the current one.

6

System Analyses

6.1 Testing

To test the quality of the implemented interaction system we organize a set of tests. While all three interaction models previously mentioned (Section 5.2.4) had their advantages and disadvantages, the testing phase was held just for the second interaction model: One-Hand Detection Activation. This model was tested with the toggle feature on, to simplify the interaction.

To ensure minimal intervention between the investigator and the tester as possible, it was also added to the scene an instruction board (Figure 81) clarifying the instructions about the fingers to activate each mode.

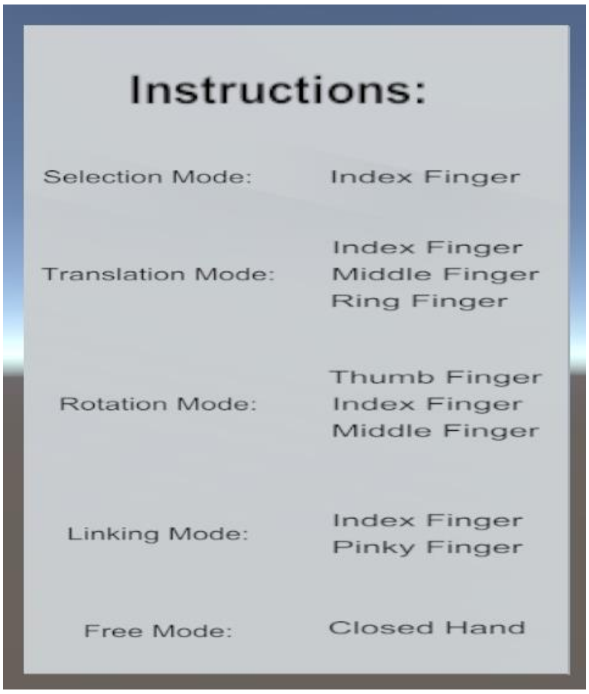

Figure 81 - Instruction Board present in the testing scene

The choice of this model as the only one to be tested is justified by its simplicity and usability assuming as it is a simplified version of the first interaction model (Two-Hands Detection Activation). Depending on the amount of observed and registered misreads by the Leap Motion, it might not be justified to have an interaction model featuring buttons (third interaction model).

6.1.1 Metrics

The evaluation of the data obtained from the tests focus on metrics to verify if the interaction is being performed as expected.

The first metric considered was the quality of the performance of each of the 9 tasks, assessing if the task was successfully executed without mistakes, successfully executed with mistakes, or not successfully executed.

The execution time spent on each task is another metric considered. The information on how long each user took while performing a task, gives information about if the interaction is being carried out as expected.

The balance between performance and the time spent to execute each task is crucial to the evaluation since there are no time limit defined. Just the quality of performance of the task does not allow us to know how well the interaction was implemented, since a user could perform everything without mistakes by doing every process with a much higher execution time than expected. On the other hand, the execution time spent alone is not enough to the evaluation since it is possible that the users executed the tasks quickly with poor quality or without performing the instructions correctly.

Only by knowing if the task is being correctly performed at the expected time, will the results be strong enough to analyse and draw conclusions from.

6.1.2 Sample

The tests were performed with a convenience sample, composed by 8 volunteers, acting as users, 7 men and 1 woman (Figure 82), ranging ages from 20 to 27 years old (Figure 83).

These volunteers, students at the university or already graduated (Figure 84), signed an informed consent and have different levels of chemistry knowledge ranging from middle school to university level (Figure 85). Six users had experienced Virtual Reality before, while for the other 2 this was the first contact with this technology (Figure 86). Of all users, 3 have a weekly use of 3D modelling tool, 1 has used it in the past 6 months and 4 are not aware of the last time they have been in contact with this type of equipment.(Figure 87).

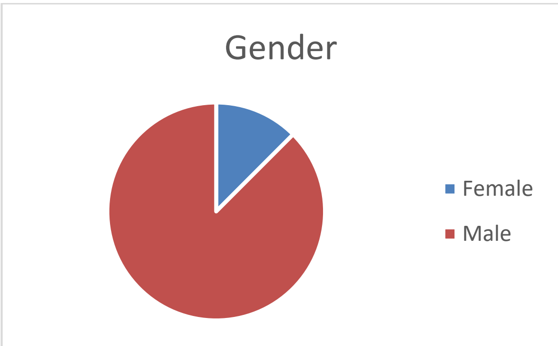

Figure 82 – Distribution of participants according to gender

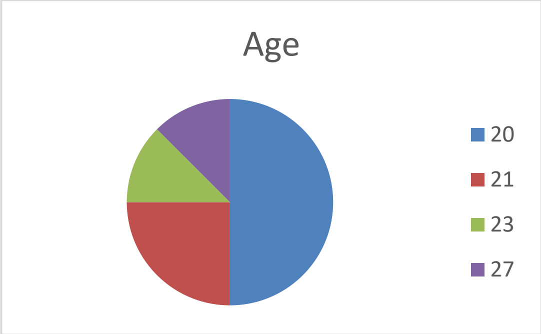

Figure 83 - Distribution of participants according to age

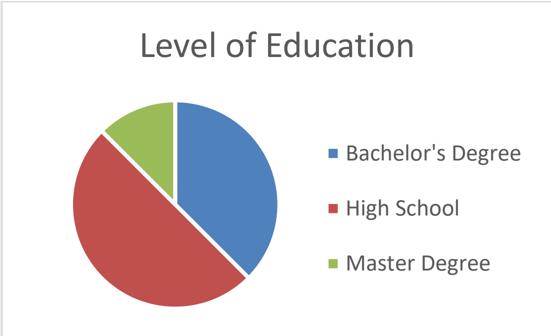

Figure 84 - Distribution of participants according to their Level of Education

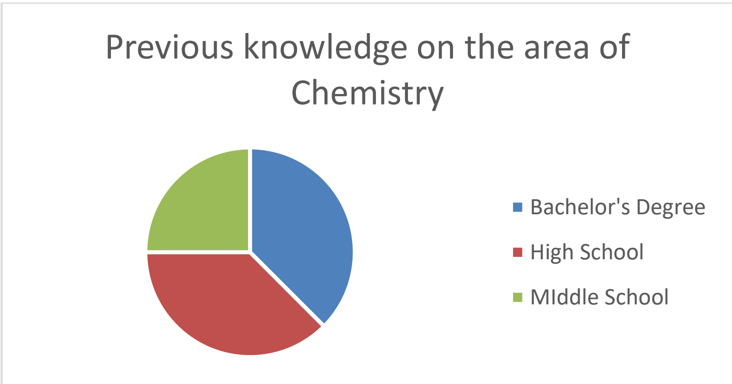

Figure 85 – Distribution of participants according to their previous knowledge on the area of Chemistry

Figure 86 - Distribution of participants according to their experience with Virtual Reality

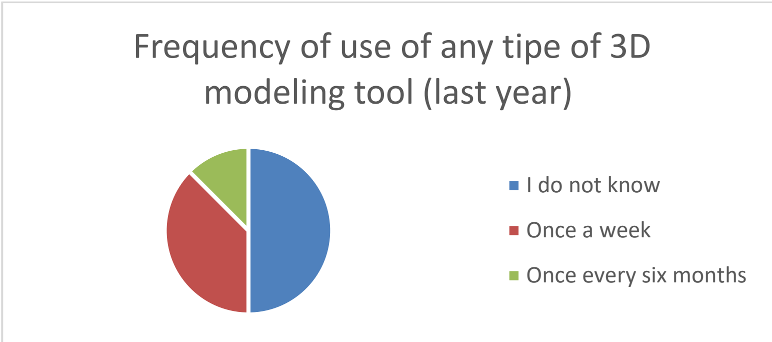

Figure 87 - Distribution of participants according to their frequency of use of 3D modelling tools in the last year

6.1.3 Tasks

To test the Model each user was asked to execute 9 tasks, shown in Table 2. All tasks were tested in a random order, with the exception of the last one that was always Task 9, the more complex allowing to test all the previous features. It should also be noted that not all users tested all tasks.

Table 2 - Tasks tested and respective description

Task	Description	Mode
1	Select 2 groups	Selection Mode
2	Select groups based on objects	
3	Move while avoiding obstacles	Translation Mode
4	Swap positions of groups	
5	Turn the group around	Rotation Mode
6	Rotate the group on an axis	
7	Remove links in a group:	Link Mode
8	Remove specific links in a group	
9	A mix of all the above tasks	All Modes

Tasks 1 and 2 tested the selection of groups (Selection Mode), Tasks 3 and 4 tested the moving of groups (Translation Mode), Tasks 5 and 6 tested the rotation of groups (Rotation Mode), Tasks 7 and 8 tested the removal of links (Link Mode). As previously mentioned, Task 9 include instructions that would lead the user to change between all modes, testing all the features. Before the users started any of the tasks, they were allowed to practise in Free Mode to get used to the system until they felt they were ready for the execution of the tasks. The users were asked to perform all tasks as best as they could without time spend concerns.

The tests start with the users seat in front of a computer and place the HDM with the Leap Motion attached to it on their head and then the investigator started the Unity application.

The execution of the tests was made using the testing system implemented (implementation previously explained in Section 5.2.4).

After each task is completed, the investigator registered the time used to perform it, and if there were mistakes or incorrections during execution.

Due to the pandemic situation, all the tests were performed following sanitary rules. All the devices were protected with plastic film that was replaced between users. The hands of the users and of the investigator were washed with alcohol before and after the test.

6.2 Results

For each task it was recorded if the task was correctly executed or not, as well as the time spent to complete the task.

Table 3 shows the average results of performance for execution of each task expressed in percentage, considering the 8 users.

Table 4 has the average results, expressed in seconds, of the time used to perform each task.

Table 3 - Average rates of the success types by task

Tasks	Successful	Successful with Errors	Not Successful
1	25.0%	75.0%	0.0%
2	50.0%	50.0%	0.0%
3	83.3%	16.7%	0.0%
4	83.3%	16.7%	0.0%
5	71.4%	28.6%	0.0%
6	28.6%	57.1%	14.3%
7	85.7%	14.3%	0.0%
8	83.3%	16.7%	0.0%
9	62.5%	37.5%	0.0%

Table 4 - Average time used in the execution of each task

Task	Min. Time (s)	Max. Time (s)	Average Time (s)	Standard Deviation (s)
1	51.00	187.00	122.50	55.89
2	35.00	107.00	63.00	27.60
3	35.00	266.00	97.00	84.54
4	44.00	259.00	101.71	69.09
5	41.00	209.00	80.71	54.36
6	42.00	460.00	217.71	135.70
7	35.00	157.00	80.29	37.75
8	45.00	169.00	103.50	39.62
9	107.00	286.00	179.00	54.97

While performing the tests it was observed that sometimes users had troubles when performing the "thumbs-up" to indicate that the task was completed.

After the end of the test, the users were asked to answer a questionnaire about their experience when using the system (Annex. C), composed by 10 questions about the usability of the system based on the System Usability Scale (SUS), 1 choice question and 2 open ended questions.

The 10 usability questions assume as answers the scale "Strongly Agree", "Agree", "Neutral, "Disagree" and "Strongly Disagree" and questions and results are shown in Figures 76-85.

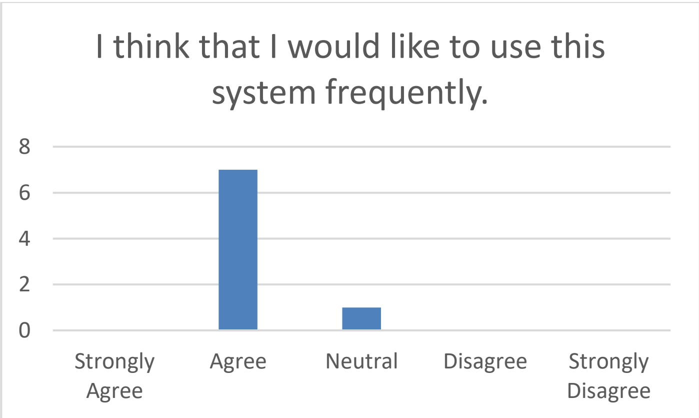

Figure 88 – Answers to the first question*: "I think that I would like to use this system frequently."*

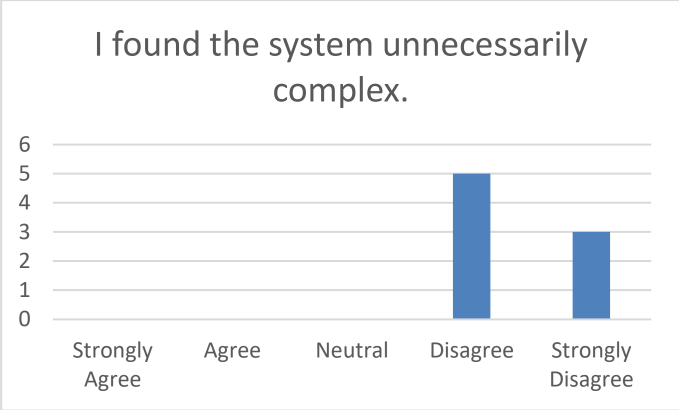

Figure 89 – Answers to the second question: "I found the system unnecessarily complex."

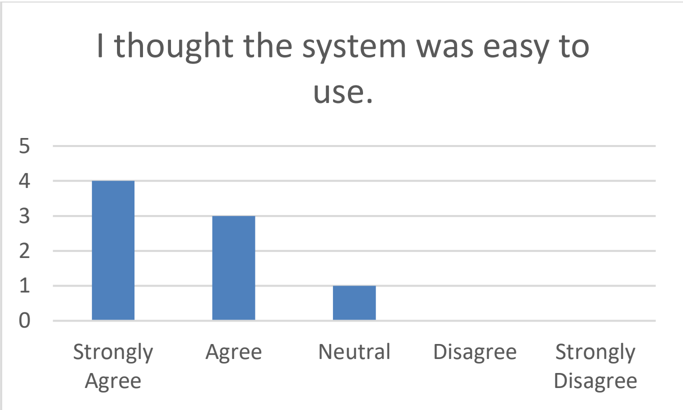

Figure 90 – Answers to the third question: "I thought the system was easy to use."

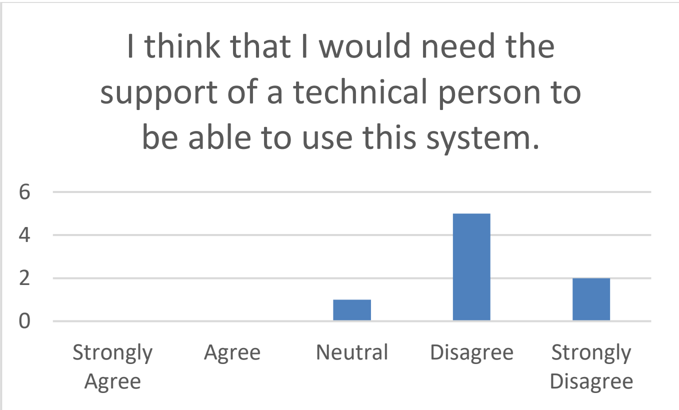

Figure 91 – Answers to the fourth question: "I think that I would need the support of a technical person to be able to use this system."

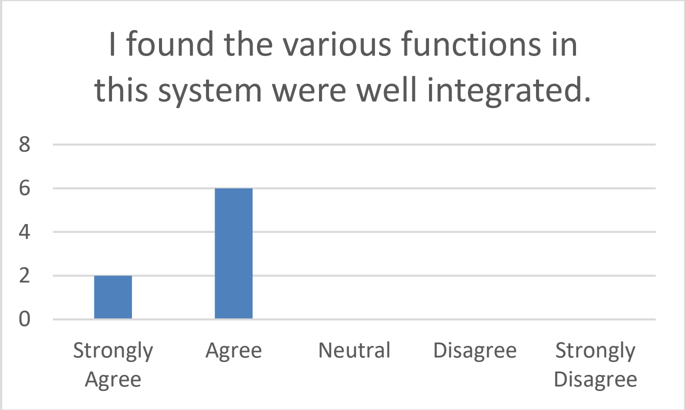

Figure 92 – Answers to the fifth question: "I found the various functions in this system were well integrated."

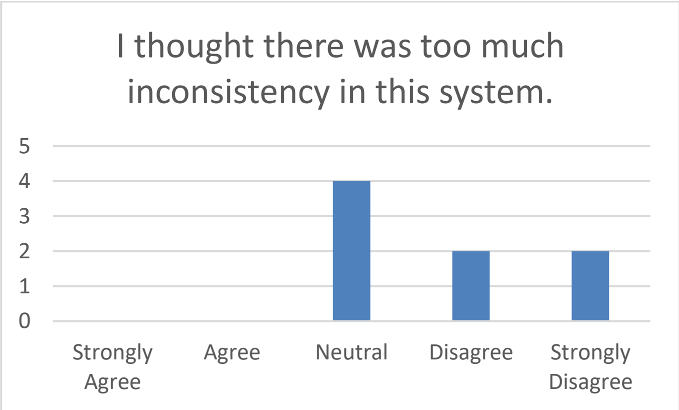

Figure 93 – Answers to the sixth question: "I thought there was too much inconsistency in this system."

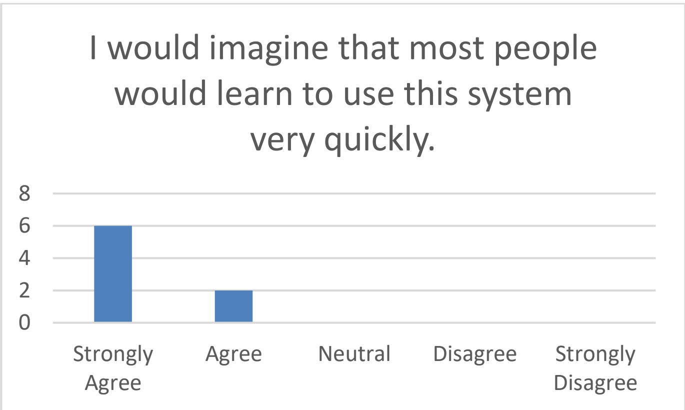

Figure 94 – Answers to the seventh question: "I would imagine that most people would learn to use this system very quickly."

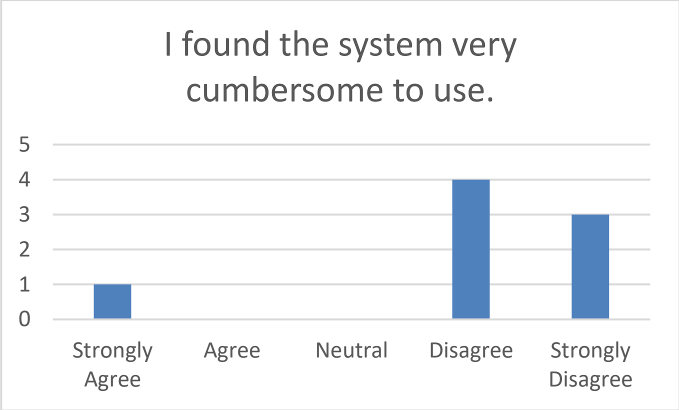

Figure 95 – Answers to the eighth question: "I found the system very cumbersome to use."

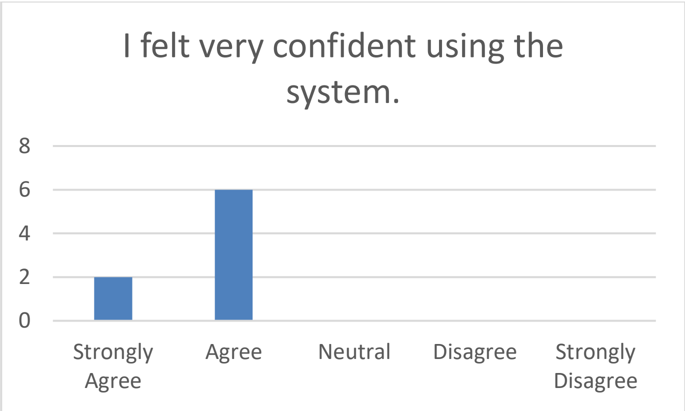

Figure 96 – Answers to the ninth question: "I felt very confident using the system."

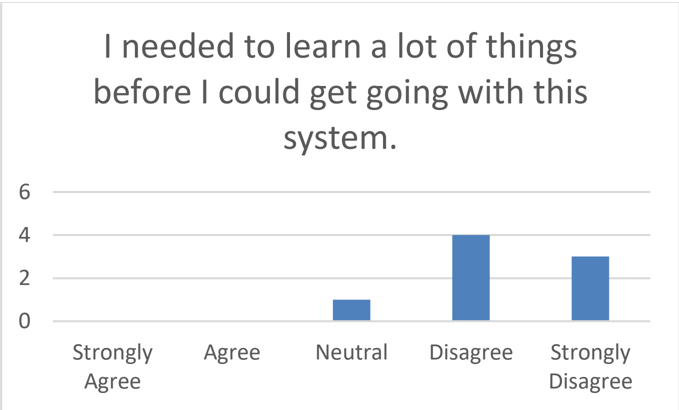

Figure 97 – Answers to the tenth question: "I needed to learn a lot of things before I could get going with this system."

The choices question was "Out of all the following modes, which one seemed more useful?" and allowed the user to choose between the Translation Mode, Rotation Mode and Link Mode. Since these new modes point to new interaction concepts that differ from the previous version of the interaction system of the game "Touch of Chemistry", it was important to know the opinion of the testers. Results are shown in Figure 98.

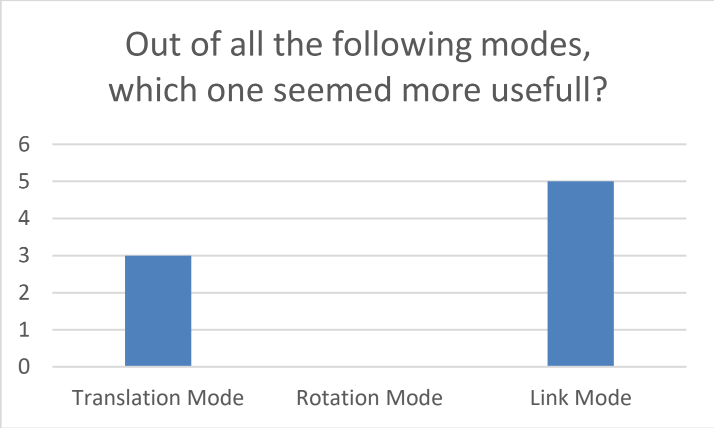

Figure 98 -Distribution of the opinion of the users about the most useful mode

The 2 open ended questions were "Of all the experience with the system, what aspect surprised you the most?" and "Of all the experience with the system, which feature did you find most useless?". The first question allows us to know if there was anything in our implementation presenting unexpected interactions (being it positive or negative aspects) and the second allow us to know what features the users consider useless.

We verify that most answers to the first question were related to the capability of the system to recognize the hands and use that recognition to command the modes of the game. Other comments were related with the hand figures necessary for the activation of the modes.

For the second question the opinions differ even more. Some users mentioned how there was no need to have a transition directly to Free Mode, since it was possible to redo the last hand figure to cancel the mode and go back. Other indicate the possibility to cut links in Link Mode, since it is possible to remove the links by colliding the objects once again. There were also a few users that did not identify any particular aspect, indicating that all features were elementary and necessary.

6.3 Data Analyses

The evaluation of the interaction system developed and its ability to provide the user with satisfying ways of interaction with the virtual environment and its components originated the group of data presented before. This data are metrics and usability regarding the execution of users along the tests, and we analyse it in the present section.

6.3.1 Metrics Evaluation

The resume of the analyses of the results obtained from the metric data of the tests can be consulted at the end of each of the following sub-sections, in Table 5. (Performance Metric) and Table 6 (Time Metric).

6.3.1.1 Performance Metric

Performance metric assessed as percentage of data is shown in Table 5 for each Mode developed. The fact that 8 out of 9 tasks present 100% of success rate (with and without errors), corresponding to tasks of Selection, Translation and Link Modes indicates that testers were able to per-form most of the tasks.

Considering our sample size, we define that the rate of tasks not successfully completed should be higher than 37% for considering a Mode with performance issues. While the rate of success with errors was also high for some tasks, such errors also include mistakes that the user did when performing the task. For example, selecting the wrong group before the correct one or forgetting to cut one link are counted as success with errors, since the user performed the task without any interaction issues.

For the purpose of this implementation, it was not necessary to have a concrete understanding of the origin of the error, but if it was due to the interaction model implemented or not, to which the selected metrics were enough, and having more unnecessary metric might bring forth other problems.

For task 9, the task expected to have more mistakes due to its complexity as explain previously, a 100% success rate was observed with zero errors. This value is better than the success rate with error (Table 4), thus indicates that after the execution of all the previous tasks, the testers feel comfortable enough with the system to make less mistakes when executing the last task.

Table 5 – Average of the Success Rate of the tasks that evaluated the same mode

Mode	Total Success Rate	Performance Issues
Selection Mode	100.0%	No
Translation Mode	100.0%	No
Rotation Mode	92.9%	No
Link Mode	100%	No

6.3.1.2 Time Metric

For the analyses of the execution time of the tasks of each Mode (Table 6) we estimate averages and standard deviations. For tasks that evaluated the same Mode, similar averages indicate that the difficulty between each task was not high, as such, the interaction of that Mode is easy to under-stand.

Small differences of standard deviations indicate that there are no discrepancies in the interaction of the mode. In contrast, if the difference is high, some incoherencies can be present in the implementation. Is also possible that some sort of detection issue is happening from one user to another, since it would mean some users had no trouble getting their hands recognized and executing the task, but the same is not verified for all of them. For both differences between averages and standard deviations, absolute values smaller than 30 seconds were considered small differences, absolute values higher than 60 sec-onds were considered high differences.

Selection mode is evaluated through Task 1 and 2. Task 2 present the lower average and minimum execution time, average of 63 seconds with the smallest standard deviation of 27.6 seconds. Since in this task half the success were with mistakes and the other half without any mistakes, we can infer that the testers did not have much trouble with the execution of the given instructions.

Task 1 present an average of 122.5 seconds and a standard deviation of 55.89 seconds.

Considering the Selection Mode, the average of the difference of execution time between the two tasks (59.5 seconds) might indicate some issues in the simplicity of the mode, the difference be-tween standard deviations (28.29 seconds) suggest that it is unlikely to exist inconsistencies in the implementation of this mode.

Rotation Mode is evaluated through tasks 5 and 6. Task 6, was the only task that did not reach 100% of success, due to the fact that one user was unable to do what was indicated in the task description. At the same time, it was also the task with the highest execution time of 460 seconds and an average of 217.7 seconds, more than 30 seconds of difference from the task with the second highest average. The standard deviation was also the highest, with 135.7 seconds, more than 1.5 times the value of the second highest deviation. This means that task 6 was the task presenting more difficulties to all users.

On the other hand, Task 5, had an average of 80 seconds (the second lowest average) with a maximum time of 209 seconds, more than half of that of task 6, and a deviation of 54.36 seconds.

With a difference of execution time averages of 137 seconds and a difference of standard deviations of 81.35 seconds, it highly indicates that the tested implementation of Rotation Mode might be more complex than expected presenting some coherence issues.

Translation Mode is evaluated through tasks 3 and 4. Task 3 had an average of 97 seconds and a standard deviation of 84.54 seconds. Task 4 had an average of 101.71 seconds and a standard deviation of 69.09 seconds.

Link Mode is evaluated though tasks 7 and 8. The average of execution times of Task 7 was 80.29 seconds, with a standard deviation of 37.75 seconds. For Task 8, the average was 103.5 seconds and the standard deviation was 39.62 seconds. This data indicated that for Link Mode, presenting a difference of averages of 23.21 seconds and a difference of standard deviations of 1.88 seconds, just as in Translation Mode, the tested implementation is of simple comprehension for the users not presenting incoherencies.

The final task, Task 9, would be expected to have the highest average time, but due to the unexpectedly high value of the average of Task 6, that is not observed. Instead, Task 9 holds the seconds highest average, with more than 50 seconds of difference from the third highest average. Since Task 9 has instructions related to all modes, its standard deviation should indicate the difference of time taken by each person to execute all modes, statistically corresponding to the sum of the standard deviations of all the modes, what is not observed. Without counting the unexpected value of the standard deviation of the Rotation Mode, the sum would be 45.62 seconds, with differs from the obtained deviation by 9.35 seconds.

A summary of the observed metrics for each implemented Mode and the corresponding interpretation is shown in Table 6.

Table 6 – Difference of Average and Standard Deviation between the two tasks of each Mode and respective assumptions

Mode	Difference of Average (s)	Simple Comprehension	Difference of Standard Deviation (s)	Possible Incoherencies
Selection Mode	59.50	No	28.29	No
Translation Mode	4.71	Yes	15.45	No
Rotation Mode	137.00	No	81.35	Yes
Link Mode	23.21	Yes	1.88	No

6.3.2 Usability Evaluation

From the data of the previous interaction system collected and detailed in section 5.1, most testers at the time mentioned issues in performance and interaction as affecting their experience.

Considering results shown in Figure 88 and Figure 90, we assume that 7 out of 8 of the testers would like to use this system frequently and found it easy to use. We can then infer that the implemented system provided them with a comfortable interaction experience, especially since 7 out of 8 users answered that they did not found the system cumbersome to use (Figure 95) with the remaining user actually agreeing with the statement and finding it cumbersome to use.

It is important to note that for some users, the Leap Motion sensor failed to correctly capture their Hand Figure of "thumbs-up", as mentioned in the results section. Since this misreadings could happened several times per user, this could explain why one user would say that the system was cumbersome to use. At the same time, it was also observed that these misreadings were happening due to the users own format of the hands. As mentioned in the implementation of the testing system, to guarantee that the task completion Hand Figure was captured correctly, it was necessary for both thumbs to be pointing upwards. For some people, when they do a "thumbs-up", due to their hand format, their thumbs would not actually point "up", but lean more towards a side. This was something not considered when developing the testing system and might be the cause for some of the misreadings observed on the "thumbs-up" figure, which was necessary to inform the system that a task had been completed.

Previously, users had also reported some issues while grabbing and interacting with atoms in the previous version, however, based on the information from Figure 94 and Figure 96 all users believe that most people would quickly get used to the system and all of them felt confident while utilizing the system, which is further supported by Figure 91, where 7 out 8 users do not think they would need the help o a technical person to use the system, with the remaining user maintaining a neutral position about the need of technical assistance.

The previous system also contained some errors related to actions performed, for example, not being able to link two molecules or join any atom of a molecule, creating a circle. Considering that the results from Figure 92 and Figure 93 indicated that all users agreed that the various features of the system were well integrated, and no user believed there were many inconsistencies in the system (with 4 disagreeing and 4 maintaining a neutral opinion), this could demonstrate that such errors were not detected in the implemented system.

Based on the responses shown on Figure 89 and Figure 97, it is seen that all users disagree that the system was unnecessarily complex and 7 out of 8 testers thinks they would not need to learn a lot of things before getting used to the system. The development of the system also considered teaching and learning purposes, as such, it is fundamental for the system to be as simple as possible since this facilitates the learning process of the user. This would be a major achievement since as simpler the system is, the easier time the user will have getting used to it.

About the usefulness of each mode mentioned in the choices question (Figure 98), 5 participants mentioned the Link Mode, 3 the Translation Mode and none indicated the Rotation Mode. The scope of the interaction system is on the building of structures, meaning that it makes sense for the Mode considered most useful to be the Link Mode, followed by the Translation Mode able to move the created structures. At the present level, in a more basic level of interaction, there is rarely the need to rotate the created structures, which justifies why the users do not considered that the most useful Mode. On another hand, from the data previously collected, especially from the interview with chemistry teachers and researchers (section 5.1.1), it was noted that such feature is crucial in a chemistry teaching context.

Lastly, both in the first set of tests as in this last one, there are always records of users enjoying the interacting with the virtual world, and in particular without needing any additional controllers, by using solely their hands. This indicates that the Leap Motion technology is still widely recognized as something new and with few occasions for people to enter in contact with it aside from specific areas of knowledge.

7

Conclusion and Future Work

7.1 Conclusion

The present work exposes the development of an upgraded version of the interaction system of the game “Touch on Chemistry”.

The idea of upgrading the interaction system arose from a set of pre-tests performed on the game. With the results from such test and the data collected from the related work, it was defined that the interactive aspect of the game would benefit the most from an upgrade. To make the most out the Leap Motion device that was being used, the improvements on the system should make use of capacity to capture gestures and figures of the hands, something that the game was not utilizing.

Feedback about the needs to improve arise from the obtained opinions of chemistry teachers/researchers and from 120 high school students of chemistry area.

New modes for the system were designed, each with a determined set of actions to be executed by the users, namely grab of objects, selection of groups of objects, translation and rotation of the groups, or linking of objects, organized in 9 different tasks. Furthermore, three interaction models were developed, each model focusing on different features that the Leap Motion has to offer. These models evidence the possibilities of gesture capture and recognition of a figure of the hand to execute each mode of the system, thus being a model of Two-Hands Detection Activation, a model of One- Hand Detection Activation or a model of Buttons.

One last set of tests was performed to verify if the proposed objective had been achieved using the Model of One- Hand Detection Activation identified as the most suitable one considering simplicity and usability features. From these last set of tests, we registered metrics of time and performance of task execution and collect data from usability questionnaires of 8 users.

Results shown that we implement an improved interaction system, showing good user acceptance considering simplicity and usability.

Having developed the system in a Virtual Reality Environment that makes use of Leap Motion we highly improved the interactivity of the system by improving the quality of the hands-free interaction assured by the Leap Motion. In this way, it was possible to increase the enjoyment of the users and their level of immersion in the virtual environment. This further supports the claim that the user should not just be a spectator in the environment, but actively interact and bring change upon it.

The Leap Motion technology is increasing in popularity, although at the present, it is still a novelty for most people. Although the Leap Motion does not present a perfect capture of the hands figures, the current state of the software and hardware are quite sufficient to allow the implementation of fun and immersive applications. On the other hand, it should be noted how the anatomy of the hands varies from person to person, exhibiting shape variations in the fingers possible explaining the difficulties on readings by the Leap Motion.

Overall, the developed system was able to achieve satisfying results in terms of interaction. The introduction of the concepts of Selection, Translation, Rotation, Link and Free Mode facilitated the process of cataloguing the actions. The interaction models implemented proved to expand the possible ways the users could interact with the system, resulting in more immersion and enjoyment experiments.

7.2 Future Work

The first point to consider for future work should be the testing of the remaining interaction models developed. Beside the satisfactory results obtained with the model tested, the amount of information and analyses that could be done by having data on the interactivity of the other two models would allow to conclude other aspects of relevance regarding Leap Motion and Virtual Reality, such as the feelings of the users towards the interaction with buttons in a virtual environment or the sensibility of the Leap Motion sensor when the modes require the caption of two hands at the same time instead of just one.

Another point to consider would be the merge between the interaction system developed and the game “Touch on Chemistry”. Since the upgraded version of the interaction was developed in a different virtual environment with a higher level of abstraction towards the chemistry concepts, the merge of both systems would definitely bring forth interesting results.

Lastly, it could be of value to see possible implementations of the developed interaction system in a different scope or area of knowledge, given that the base is a system for linking structures.

8

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ANNEX

A.

Informed Consent + Demographic Profile Questionnaire

Informed Consent + Demographic Profile

Researcher - Diogo Caria Ferreira
Advisers - Prof. Rui Prada, Prof. Dulce Simão, Prof. Daniel Lopes, Prof. Vasco Bonifácio
*Required

Informed consent

Dear Participant,

The following study has the objective of gathering information about the different ways in which it is possible to manipulate and interact with objects and relational structures in a Virtual Environment.

The participation in this test should not exceed 20 minutes, will be performed under all the health directions and recommendations for the times we live today, and requires no extra material from the participant aside from a mask.

There is no risk involved for the participant while conducting the test.

It is requested that the participant provides data regarding their age, gender and degree of education. All data will be deleted from any database of this research after a maximum period of 6 months.

All the data collected from this study will remain anonymous and will be used solely by the researcher Diogo Caria Ferreira, Student of the Master Degree in Information Systems and Computer Engineering of Instituto Superior Técnico, and the respective advisers for the purpose of Diogo MSc thesis and related publications. No third party will have access to this data.

All participation is voluntary and, at any given point, the participant can give up and request for the removal of their data from the database.

Any question can be answered along with the Researcher through the mail diogocariaferreira@tecnico.ulisboa.pt

1. I understand that the participation in this study is voluntary and I am allowed to give up at any moment, being that the data related to my experience will be removed and deleted. *

   Mark only one oval.

   ◯ Yes

2. I authorize the treatment of my demographic data in the conduct of this study. *

   Mark only one oval.

   ◯ Yes

3. I authorize the treatment of my data collected in the performance of this study. *

Mark only one oval.

- Yes

4. I understand that if I have any questions to clarify, I can do so by contacting the researcher through the mail: diogocariaferreira@tecnico.ulisboa.pt *

Mark only one oval.

- Yes

5. I agree to participate in this study and accept its conditions. *

Mark only one oval.

- Yes

By clicking on the button below, the participant is deemed to have given his consent for the tests to be carried out.

Demographic Profile

This section servers the purpose of collecting data in regards to the demographic profile of the user and will be only used in the in the realization of this study.

6. Gender: *

Mark only one oval.

- Male
- Female
- Rather not say

7. Age *

—

8. Degree of Education *

Mark only one oval.

- High School
- Bachelor's Degree
- Master Degree
- Doctorate

9. Previous knowledge on the area of Chemistry *

Mark only one oval.

- MIddle School
- High School
- Bachelor's Degree
- Master Degree
- Doctorate

10. In the last year, with which frequency did you use any tipo of 3D modeling tool (either for work of for personal use) =

Mark only one oval.

- More than once a week
- Once a week
- Once a month
- Once every three months
- Once every six months
- Once a year
- I do not know

11. Previous experience with Virtual Reality

Mark only one oval.

- ( ) I have never used it before
- ( ) I have tried it before
- ( ) I have my own virtual reality equipment

Thank you for you participation!

B.

Video Testing Interaction Tasks Document

Teste de Manipulação de átomos e moléculas

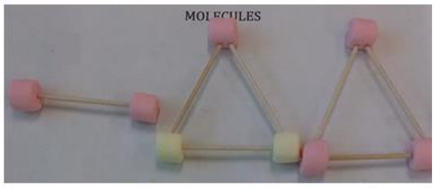
Duração: 5-10 minutos

Introdução:

Para as tarefas que vais realizar, é preciso que tenhas à tua disposição material que possa simular átomos a as ligações entre os mesmos. Em seguida tens algumas imagens de exemplos do que podes utilizar, no entanto, tens a liberdade de escolher algo que consideres mais prático. O mais importante é que o material seja algo físico e que possas manipular.

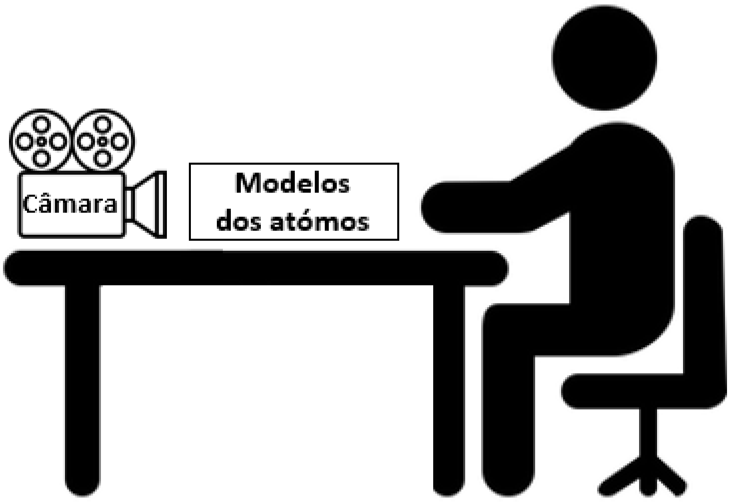
Modelos de Plástico

Esferas e Cilindros magnéticos



Modelos com Plasticina

Em seguida, arranja uma câmara para gravar a realização das tarefas. É importante gravar a manipulação dos modelos, por isso não é necessário apanhar a cara, e ideal é teres um set-up como demonstrado na imagem que se segue.

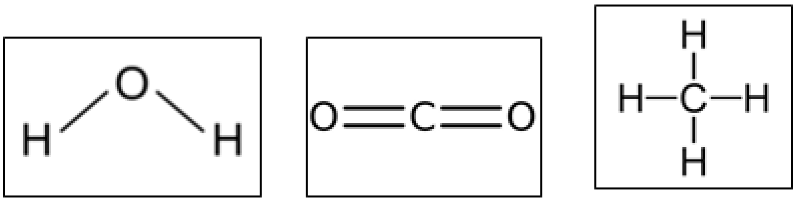


De seguida estão as tarefas que tens de realizar. Põe a câmara a gravar antes de começares a realizar e não tens de parar a gravação entre tarefas. Tens também as imagens das moléculas que são pedidas, caso tenhas alguma dúvida em como as construir.

Tarefas:

Tarefa 1:

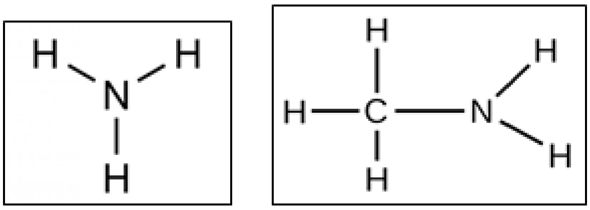
- Preparar os materiais;
- Construir molécula da água (H_2O);
- A partir da anterior, construir a molécula do dióxido de carbono (CO_2);
- A partir da anterior, construir a molécula do metano (CH_4);
- Separar e arrumar os materiais.



H_2O CO_2 CH_4

Tarefa 2:

- Preparar os materiais;
- Construir a molécula de amoníaco (NH_3);
- A partir da anterior, construir a molécula de metilamina (CH_3NH_2);
- Separar e arrumar os materiais.



NH_3 CH_3NH_2

Após terminares as tarefas, envia/partilha a gravação para o mail:
diogocariaferreira@gmail.com
Podes partilhar através de Google Drive ou WeTransfer, para simplificar o processo.

Obrigado, e uma boa quarentena!

C.

Final Test Set Usability Questionnaire

Interaction Experience Usabilibility Form

The following form serves the purpose of collecting information regarding usability of the system tested by the user.
If possible, justify your opinions and answer truthfully and with honesty.
*Required

1. About the system tested: *

Mark only one oval per row.

	Strongly Agree	Agree	Neutral	Disagree	Strongly Disagree
I think that I would like to use this system frequently.	0	0	0	0	0
I found the system unnecessarily complex.	0	0	0	0	0
I thought the system was easy to use.	0	0	0	0	0
I think that I would need the support of a technical person to be able to use this system.	0	0	0	0	0
I found the various functions in this system were well integrated.	0	0	0	0	0
I thought there was too much inconsistency in this system.	0	0	0	0	0
I would imagine that most people would learn to use this system very quickly.	0	0	0	0	0
I found the system very cumbersome to use.	0	0	0	0	0
I felt very confident using the system.	0	0	0	0	0
I needed to learn a lot of things before I could get going with this system.	0	0	0	0	0

2. Out of all the following modes, which one seemed more useful? *

Mark only one oval.

( ) Translation Mode (Move Structures)

( ) Rotation Mode (Rotate Structures)

( ) Link Interaction Mode (Cut Structures or Increase Link Count)

3. Of all the experience with the system, what aspect surprised you the most? *

4. Of all the experience with the system, which feature did you find most useless? *