POLITECNICO DI MILANO

Scuola di Ingegneria dell'Informazione

POLO TERRITORIALE DI COMO

Master of Science in
Computer Engineering

Usability Evaluation of a Haptic-based Framework for Chemistry Education

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Academic Year 2010/11

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Corso di Laurea Specialistica in

Ingegneria Informatica

Valutazione di usabilita di un framework aptico per la didattica della chimica

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Anno Accademico 2010/11

ABSTRACT

The use of haptic technologies in molecular analysis is an emerging trend and several applications have been developed so far for educational and research purposes including the one from Politecnico di Milano considered in this thesis. However there are very few formal usability evaluations available for those.

The mentioned haptic-based framework from Politecnico di Milano is a “virtual environment, where the considered molecule to be analyzed is shown to the user and a probing charge is associated with a haptic device. The interaction between the molecule and the electric charge is felt via the haptic device and allows one to explore the electrostatic surface of the molecule” [1]. In terms of this thesis the usability evaluation for this framework was designed and performed. The usability questionnaires and usability tests using *thinking aloud* protocol were used. The qualitative analysis of the obtained results has been done. One of interesting observations includes that the haptic feedback was indicated as the most useful feature while having also the highest number of the identified problems related to it. Overall the participants showed a great excitement about the tool and readiness to use it during a chemistry course. Some future study directions are discussed as well.

The results of this work can be used as a basis for future evaluations once the framework is introduced in a chemistry course or transformed into recommendations for the development of similar tools.

SOMMARIO

L'uso della tecnologia aptica per l'analisi molecolare è un trend emergente e diverse applicazioni sono state sviluppate fino ad oggi per scopi di ricerca, quali lo strumento sviluppato al Politecnico di Milano e considerato in questo lavoro. Esiste tuttavia un numero molto limitato di valutazioni di usabilità riguardanti tali strumenti.

In questo lavoro di tesi, è stata progettata ed eseguita la valutazione di usabilità per framework chimico sviluppato, che fa uso di uno dispositivo aptico come strumento di interazione. Sono stati progettati questionari di usabilità usati in opportune sessioni di test per la rilevazione dei feedback dell'utente, utilizzando il protocollo thinking aloud. Dall'analisi qualitativa dei risultati ottenuti, è emerso che il feedback aptico è utile per gli scopi del tool, nonostante non sia esente da problemi d'uso da parte dell'utente. Tutti i partecipanti hanno mostrato un enorme interesse nei confronti dello strumento utilizzandolo con solerzia durante un corso di chimica.

I risultati di tale studio possono essere usati come base per future valutazioni di strumenti simili, o per la stesura di raccomandazioni per lo sviluppo di strumenti analoghi.

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1. INTRODUCTION

The word 'haptic' derived from the Greek word *haptesthai* or 'to touch' [2] refers to the sensing and manipulation through touch. Nowadays it is extended to the concept of "*information acquisition and object manipulation through touch by humans, machines, or a combination of the two; and the environments can be real, virtual or teleoperated*" [3]. The cost of the haptic technologies is decreasing and therefore the use of these technologies in different applications is becoming more widespread. They are exploited in number of fields including chemistry and molecular analysis where the latter has acquired a great importance in recent years.

Trying to address the emerging needs of molecular analysis, the haptic-based framework for exploration of the electrical surface of molecules was developed at Politecnico di Milano. The main feature of the tool is that it integrates not only the visual representation of a molecule and its related force potentials, but also a haptic device with an associated charge which allows to explore electrostatic fields of molecules through the haptic force feedback. The tool is intended to be used for learning and/or research purposes [4].

Even though similar tools to afore described haptic-based framework do exist in the field there is very few information available in the literature about the usability evaluations of these tools. In fact the author found only one explicitly described investigation performed by P. Bivall Persson [5] – [6] which was more concentrated on studying the learning gains of the students using this tool during the course than on finding the usability problems.

It is important to note that the usability feature of any application is its key to success and one can find several examples where improvement of application's usability has raised the work efficiency and decreased the number of errors made by users, the time spent per task and even the time necessary for a user training [7]. Indeed if one does not follow the usability principles designing the applications' interface it can create unnecessary problems for the users of this application [8].

1.1. Research goal

Therefore the main goal of this work was to evaluate the usability aspects of the developed haptic-based framework using the formal usability evaluation methods. It was expected that usability evaluation results would reveal the possible improvements that can be made for the framework or aspects to cover during user trainings as well as the readiness of the framework to be introduced in the chemistry courses. The following tasks were performed in order to achieve the goal:

- literature review about usability concept, usability evaluation methods and haptics concept;
- review of the similar haptic-based chemistry applications and their usability evaluations (if available);
- designing the usability evaluation process (choosing methods, defining measurements etc) for the haptic-based framework for chemistry education developed at Politecnico di Milano;
- analyzing and summarizing the results of the evaluation and preparing the recommendations and relevant conclusions.

1.2. Outline of this thesis

The first chapter includes the related work performed in the related fields. It discusses the usability concept, usability evaluation methods, haptics and haptic-based systems, gives a non-exhaustive review of the similar haptic-based chemistry applications and short descriptions of their usability evaluations if such were available.

The second chapter introduces the haptic-based framework that was evaluated and lists its main features.

The third chapter describes the methodology used for the conducted usability evaluation, presents the detailed evaluation results and the recommendations for the discovered problems and discusses them.

2. RELATED WORK

The technological advances supported the interest and facilitated the development of haptic devices, interfaces and systems. The evolvement of the term 'usability' was facilitated by the fact of the appearance of personal computers and growth of their popularity.

In this chapter the author gives insights about the usability concept and its evaluation methods, the haptics concept and its application in different fields, presents the survey results about the visual and haptic based systems for inter-molecular force studies shortly describing their features as well as pointing out if any evaluations were performed for these tools.

2.1. Usability concept

There is no unique definition for the term 'usability'. The usability professionals and standardization organizations define this term very often in different ways. The first appearance of the term 'usability' goes back to the beginning of the human-computer interaction researches in 1970-1908s when the popularity of the personal computers increased and the questions how to make the computer applications and systems easier to use and to learn became more relevant [8]. Since then the 'usability' term definition and associated attributes changed, developed and included new aspects. For example, nowadays the following definitions are available in the ISO and IEEE standards for the term 'usability' [9]:

- ISO 9241-11: "*the extent to which a product can be used by specified users to achieve specified goals with effectiveness, efficiency and satisfaction in a specified context of use*" ('Efficiency' is defined as the resources expended in relation to the accuracy and completeness with which users achieve goals and 'effectiveness' as the accuracy and completeness with which users achieve specified tasks. 'Satisfaction' is defined by concerns the comfort and acceptability of use by end users) (1998) [10];
- ISO/IEC 9126-1: "*the capability of the software product to be understood, learned, used and attractive to the user, when used under specified conditions*" (2000) [11];
- IEEE Std. 610.12-1990: "*The ease with which a user can learn to operate, prepare inputs for, and interpret outputs of a system or component*" (1990) [12].

On the other hand the leading usability experts develop their own understandings and definitions of the term 'usability':

- Shackel defines the term 'usability'' as "*the artifact's capability, in human functional terms, to be used easily, effectively and satisfactorily by specific users, performing specific tasks, in specific environments*" (1991) [13];

- Nielsen defines 'usability' in terms of five attributes: "*Learnability - systems should be easy to learn, users can rapidly start getting some work done with the system; efficiency - systems should be efficient to use, when a user has fully learned the system, productivity will be possible on a high level; memorability - systems should be easy to remember, making it possible for casual users to return to the system after some period of not using the system, without having to learn everything all over again; errors - the system should have a low error rate, which enables users to make few errors during the use of the system, when they do make errors they can easily recover from them; catastrophic errors should not occur; satisfaction - the system should be pleasant to use; which makes users subjectively satisfied when using it*" (1993) [14];
- Shneiderman gives the definition as "*five measurable human factors central to evaluation of human factors goals - speed of performance, time to learn, retention over time, rate of errors by users, subjective satisfaction*" (1998) [15];
- Constantine and Lockwood considers usability as "*Learnability, efficiency in use, rememberability, reliability in use, user satisfaction*" (1999) [16];
- Garzotto and Paolini use the following definition of 'usability': "*Different attributes are usually associated to the notion of usability, such as learnability (the ease of learning the behavior of the system), effectiveness (the level of attainable performances, once the user has learned the system), efficiency (the resources expended in relation to the system effectiveness), robustness (likelihood of users error, and ease with which users can correct errors), and user's satisfaction*" (2002) [17].

One can notice that attributes such as efficiency, learnability, satisfaction and errors are not changing from one definition to another. The definition of 'usability' used in this thesis is given below.

Usability (Figure 2.1) is a feature of an application that is characterized by following attributes:

- *effectiveness* - the level of attainable performances, once the user has learned the system;
- *efficiency* - the resources expended in relation to the system effectiveness;
- *learnability* - the ease of learning the behavior of the system;
- *memorability* - systems should be easy to remember, making it possible for casual users to return to the system after some period of not using the system, without having to learn everything all over again;
- *robustness* - likelihood of users error, and ease with which users can correct errors;
- *user satisfaction* - how satisfied is the user while using this system.

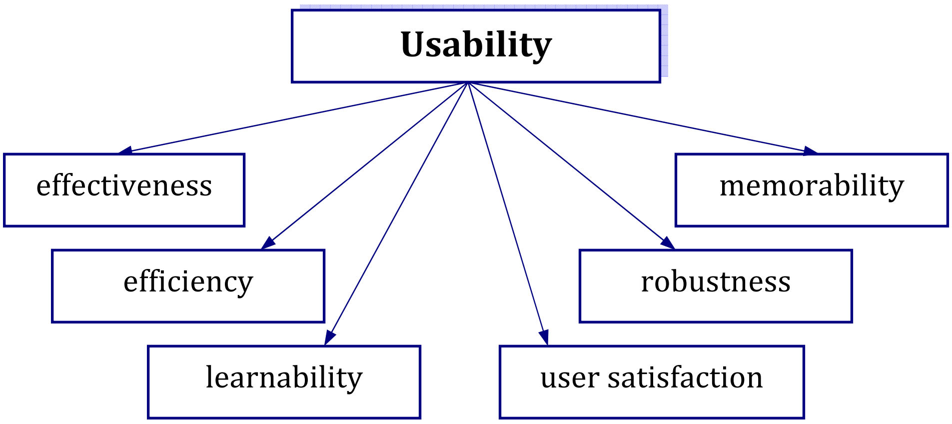


Figure 2.1. Usability attributes.

2.2. Usability evaluation

Similar to the situation with the definition of 'usability' the one unique method for the evaluation of applications usability currently does not exist. Many different methods were developed and are used depending on the different needs and aspects of the application under evaluation, namely, goal of the application, user profiles, context of use, available resources etc.

Most widely used usability evaluation methods can be subdivided in two general groups - user-based methods and inspection methods. In order to apply user-based methods the involvement of the real users is necessary, but inspection methods are usually used by the usability experts who perform the evaluation of an application and then give their feedback. Even though very often in the literature one used to find articles supporting one or another method now there appears the tendency to describe the advantages or disadvantages of one or another method and even supporting the use of several methods for evaluation. The reason for this tendency is that the different usability evaluation methods allow discovering different types of usability problems and in this way the methods are in fact complementing each other. The different usability evaluation methods are presented in Figure 2.2. [18] – [19]

2.2.1. User-based methods

As already mentioned previously the user-based evaluation methods directly or indirectly, but require the involvement of the real user in the process. Costs and time required therefore are the main disadvantage because these are higher when compared to the inspection methods.

In the following several user-based methods used in usability evaluations are described.

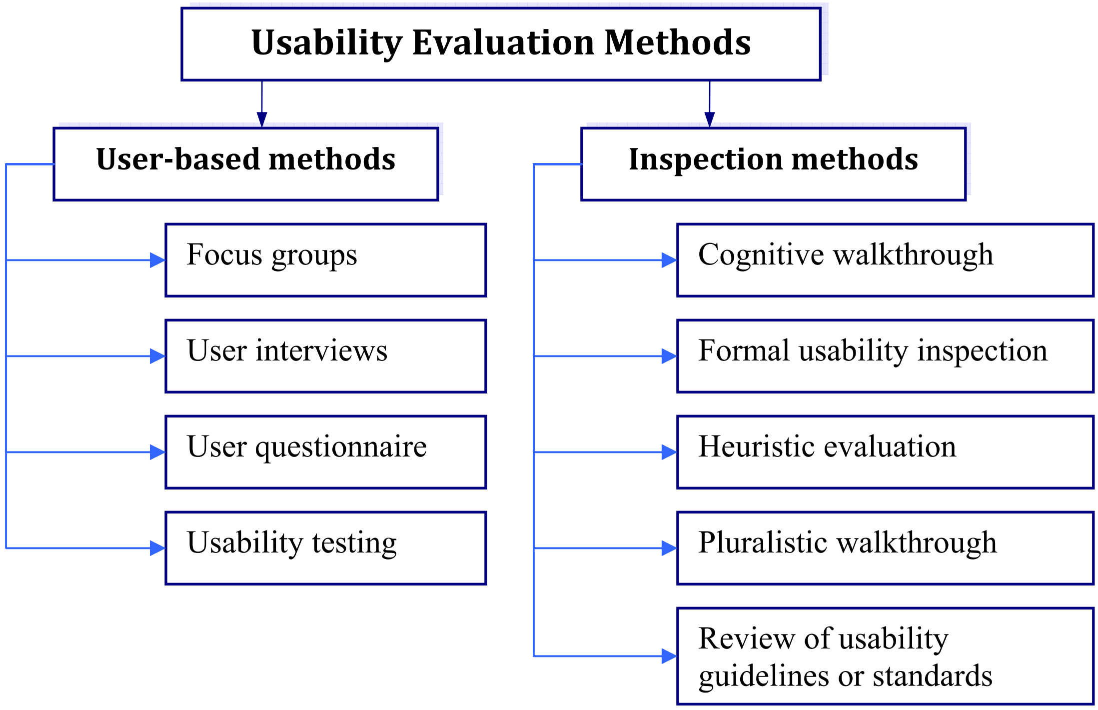


Figure 2.2. Usability evaluation methods.

2.2.1.1. Focus groups

Focus group is a concentrated discussion where a moderator leads a group of participants through a set of questions on a particular topic. The group of participants usually consists of the potential or existing application's users and through the discussion the reactions, insights, opinions, attitudes and preferences are gathered. [9], [20]

The main advantages of this method is that it is relatively inexpensive, it is possible to obtain first feedbacks from the users and the interaction between users as well as the results can be used for the basis of the future more detailed evaluations. [9], [20]

The main disadvantages are that this is not the exact user behavior observation, but rather the interpretations given by the users themselves, dominant discussion participants can influence the results obtained and no quantitative conclusions can be made. [9], [20]

2.2.1.2. User interviews

This method allows discovering the facts and opinions expressed by the users about the application under consideration. Interviews are usually conducted with a single interviewee at a time. One can distinguish the following types of interviews:

1. *contextual* – interviews that take place in a typical user's environment in order to obtain the contextual data,

2. *non-contextual* – interview that take place in person, but not in a typical user environment (in the office of interviewer etc),
3. *remote* – interviews are performed over the phone or any other communication media, but not in person. [9], [20]

The clear aim has to be defined in order to create a specific plan for an interview. It is suggested to prepare short explanations about the topics asked as well as to choose the methods for summarizing and presenting the results before the actual interview. One should keep in mind that the resulting data obtained from the interviews is not structured which creates a risk of misinterpretation or censoring. Nevertheless the risks can be mitigated if the propositions are based directly on the expressions of the interviewee without additional interpretations from interviewer. [9]

2.2.1.3. User questionnaire

Questionnaires have been widely used for quite a long time as a method to evaluate user interface of an application. As a result of the specific usability studies several questionnaires were developed as a response to the industry needs related to the costs and time resources. These questionnaires are re-usable and still exploited in the industry nowadays. The most widely used questionnaires are summarized in Table 2.1. Due to the rapid development of the communication technologies nowadays there are available online tools for conducting, managing and summarizing the results of questionnaires which makes the task even easier.

The main advantages of the questionnaire is its relatively low costs, the feedback can be obtained from wide number of users and it can be used also as one of the steps during usability tests. Nevertheless the main disadvantage of the questionnaire is that the exact usability problems faced by the users cannot be concluded from the results.

Table 2.1. Summary of usability questionnaires

Acronym	Name	Developed by	Availability	Reference
QUIS	Questionnaire for User Interface Satisfaction	University of Maryland	Free	[21]
PUEU	Perceived Usefulness and Ease of Use	IBM, MIT	Free	[22]
CSUQ	Computer System Usability Questionnaire	IBM	Free	[23]
ASQ	After Scenario Questionnaire	IBM	Free	[23]

Acronym	Name	Developed by	Availability	Reference
PSSUQ	Post-Study System Usability Questionnaire	IBM	Free	[23]
PUTQ	Purdue Usability Testing Questionnaire	Purdue University	Free	[24]
USE	Usefulness, Satisfaction, and Ease of Use Questionnaire	Sapient	Free	[25]
SUMI	Software Usability Measurement Inventory	University College Cork	Commercial	[26]
MUMMS	Measurement of Usability of Multi Media Software	University College Cork	Data exchange	[27]
WAMMI	Website Analysis and Measurement Inventory	University College Cork	Commercial	[28]
SUS	System Usability Scale	Digital Equipment Corporation	Free	[29]

Considerable amount of research is done using SUS questionnaire and about it, for instance, in [30] SUS is being compared to other six usability questionnaires (ASQ, CSUQ, PSSUQ, SUMI, USE, WAMMI), where several advantages of SUS over mentioned questionnaires are listed, namely, it is:

1. "*flexible enough to assess different user interfaces of different technologies*,
2. *relatively quick and easy to use for both - participants and administrators*,
3. *providing single score which is easy to understand by wide range of people*,
4. *non-proprietary, which makes it cost effective tool*". [30]

SUS questionnaire uses Likert scale and consists of 10 statements where respondents are asked to indicate the degree of dis/agreement with the statement on a 5 point scale. The result of a conducted SUS questionnaire is a single score 0 to 100 which can be compared to the previous evaluations done using SUS [29]. In [31] are summarized the results of more than 3500 different usability evaluations performed using SUS questionnaire. In this study the 11th statement asking a respondent to indicate the user-friendliness of a product on an adverb scale was added to SUS to associate the interpretive adverb with an obtained SUS score. The resulting adverb scale's relation to the score intervals and the score acceptability ranges were summarized [31] and are shown in Figure 2.3 below. The example of the latest SUS questionnaire used in the research described before is included in ANNEX 1.

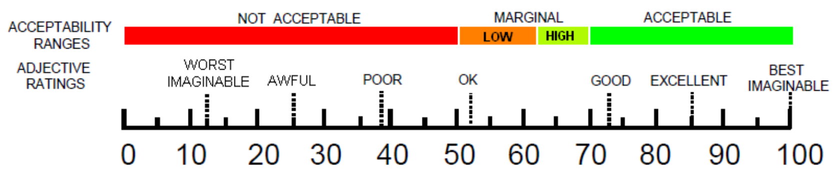


Figure 2.3. SUS questionnaire score acceptability ranges.

2.2.1.4. Usability testing

Usability testing (also called user testing) deals with the real users of an application, their behavior during the use of an evaluated application or its prototype. Usually the representative group of users is asked to perform a set of tasks that are prepared in advance. Tasks can be also prepared taking into account the specifics of the user group chosen and the testing can be performed just for a part of an application corresponding to these specifics and prepared tasks. During this process the moderator is observing how the users accomplish the tasks. The observation can be passive where moderator is only observing and not interfering with the user actions or active where moderator can ask additional questions while a user is performing the tasks. One of the additional methods which can be used during usability testing is the *thinking aloud* protocol when users are asked to express their thoughts out loud while using an application and trying to accomplish the assigned tasks. The *thinking aloud* allows discovering *why* the users do something and in this way getting closer to the use of the system in practice. [32] - [34]

In [34] it is recommended to perform the necessary preparations for the usability testing in order to increase the reliability of the results and the following preparation steps are suggested:

1. *Define the goals of the test* – for instance, to determine the most common user problems while using the interface of the application.
2. *Define the user sample to participate in the test* – the sample should be representative of the end users of the application tested. The number of the users to be involved in the tests usually varies, for instance, Nielsen and Molich suggests that three users are enough in order to discover up to 50% of the most important usability problems [35], but Virzi in his research came to the conclusion that around 80% of the problems are found after tests are run with five users, nevertheless he also suggests that the number of users should not fixed prior to the testing and the tests with the users should be performed until the number of new usability problems discovered is starting to decrease [36]. Faulkner in more recent study argues that widely accepted five user assumption is not very reliable and suggests increasing the number of the users in order to gain more confidence in the acquired testing results [37].

3. *Select the tasks and/or scenarios to be tested* – the tasks and/or scenarios should replicate the ones which users would normally do with the application.
4. *Define how to measure usability* – the measures can be qualitative (user satisfaction, difficulty of use etc) or quantitative (task completion time, number and typology of errors etc).
5. *Prepare the material and the experimental environment* – the place where the tests will be conducted should have all the necessary equipment (computer, any other required additional equipment) and the necessary materials (manuals, pencils, paper), the plan how the tests will be actually performed should be clear at this point, one should also decide the way to record the results of the evaluation (taking notes, recording a video or a computer screen etc).

2.2.2. Inspection methods

User-based methods very often are too time consuming and involve considerable costs which often turns out to be the main reason why usability evaluations for applications or products are not always performed. Nevertheless the usability aspect of any product or application is an important factor of success and therefore a cost-effective alternative to the user-based methods evolved called inspection methods.

The inspection methods are used by experts who perform usability evaluations based on generally accepted usability standards, principles and their own experience in usability issues. Their main goal is to discover potential usability problems. The evaluation result is usually a set of recommendations for the design improvements.

Some studies argue that the inspection methods should be used by usability experts, but the other studies on the contrary show that some of these methods are relatively easy adopted also by novices [38]. However these methods can not replace the user-based methods entirely because the studies show that some problems are discovered only while exploiting the user-based methods, on the other hand the best suggested approach is to combine both – user-based and inspection methods. [34], [38] - [39].

In the following the author gives a description of several inspection methods that are used by practitioners.

2.2.2.1. Cognitive walkthrough

In [40] the cognitive walkthrough method is defined as "*a usability inspection method that evaluates the design of a user interface for its ease of exploratory learning, based on a cognitive model of learning and use*". The method is based on an assumption that users prefer to learn an application in an exploratory way while performing their usual tasks rather than participating in special trainings or going through user manuals. An application's interface is evaluated in the context of one or more user tasks. The evaluation process consists of the following steps:

1. defining inputs to the walkthrough (potential users, sample tasks, action sequences to complete the tasks, description or implementation of the interface),
2. organizing a meeting with analysts,
3. walkthrough the action sequences for each task using the action sequence developed by Lewis and Polson [41]:
    a. the user sets a goal to be completed within the system.
    b. the user determines the currently available actions.
    c. the user selects the action that they think will take them closer to their goal.
    d. the user performs the action and evaluates the feedback given by the system.
4. record critical information,
5. revise the interface to fix the problems. [38], [40]

During the walkthrough it is possible to determine whether an interface facilitates the choice of right steps in order to complete the task. If during any of the steps there is tendency for the wrong choice or user's confusion about how to proceed it is necessary to do a revision of an interface. [40]

2.2.2.2. Formal usability inspection

The method uses a formal procedure consisting of six-step framework to perform an inspection of a set of tasks that users might perform with a system under evaluation in order to discover usability problems that users might face. The inspection is carried out by a team where each of the members has a predefined role. Usually these roles are the following:

1. *moderator* – responsible for the organizational aspects of the inspection,
2. *owner* – designer of the product, usually a person who fixes the problems discovered during inspection,
3. *recorder* – logs the problems discovered during the inspection,
4. *inspectors* – inspect the application and report any problems found.

The team can consist of different representatives related to the system – design engineers, customer support representatives and sometimes even customers themselves. The results of the inspection include a list of the usability problems discovered during evaluation and help the design engineers and developers to acquire a better user perspective. [38] - [39], [42]

2.2.2.3. Heuristic evaluation

This method was introduced by Nielsen and Molich in 1990. This method determines a group of usability experts who analyzes an application and evaluates its interface based on recognized usability principles known as heuristics. Several studies have shown that the heuristic review is an effective method in terms of cost efficiency and ability to predict usability problems in an application. The perfect case scenario is to have a group of specialists who represent knowledge and expertise in both: the usability field and the field of an evaluated application. Usually this group consists of three to five experts. The usability evaluation is performed individually by each of the group members and the results are compared, discussed and summarized after that. [34], [39] - [44]

Several sets of heuristics were developed and introduced by different researchers since introduction of this method. The most widely used are summarized in Table 2.2. These lists of heuristics are generalized which makes it possible to use them for different types of interfaces - internet-based applications and websites, mobile phone applications etc.

Table 2.2. Summary of most common heuristic lists used in heuristic evaluation

Name	1st time published	Year of last update	Reference
Nielsen’s 10 heuristics	1990	1994	[45]
Schneiderman’s 8 golden rules of interface design	1987	2004	[46]
Muller’s and McClard’s 15 heuristics	1995	1998	[47] – [48]

2.2.2.4. Pluralistic walkthrough

The pluralistic walkthrough method can be described in terms of five characteristics:

1. it incorporates in the process representative users, product developers, members of the product team, and usability experts,
2. a scenario is defined and interface screens are showed to participants in the order as they would appear while conducting this scenario,
3. participants are asked to assume the role of the user and
4. to write down actions how they would try to achieve the goal of the scenario reviewed going through the interface screens,
5. after writing down the actions the discussion is started where the users speak first followed by usability experts and product team members. [49]

During the process it is very important to keep the discussion productive. All the comments, recommendations and critique logged during the discussion can serve for the interface and design improvements. Also a level of usability can be established if before the discussion respective usability parameters are defined. [49]

2.2.2.5. Review of usability guidelines or standards

The review of an application interface is conducted based on usability guidelines or standards and carried out by specialists that can be usability experts, developers, advanced users etc. The formulations of recommendations in usability guidelines or standards can be both very precise and also very vague therefore the required expertise level of the reviewer can vary as well. Very often the recommendations from standards need to be adopted and changed into lists in order to make them usable for the review process.

After the review the conformity level to the respective guidelines or standards is established. If it is necessary to increase the conformity level the necessary interface improvements and fixes can be done. More widely guidelines and standards are adopted for the web site usability reviews where the most widely known are: ISO 9241-151 standard [50] and „Research-Based Web Design & Usability Guidelines" developed by U.S. Department of Health and Human Services [51]. [52]

2.3. Haptics concept

The word 'haptic' is derived from the Greek word *haptesthai* or 'to touch', which describes the feeling as a tactual perception [2]. So the haptics concept refers to the sensing and manipulation through touch. This tactual sensory information which is sent from the hand to the brain when the hand touches an object can be divided into tactile information (referring to the sense of the nature of contact with the object) and kinesthetic information (referring to the sense of position and motion of limbs along with the associated forces). [3]

In the early part of the 20th century the term was mainly used in psychology for studies on the active touch of real objects by humans, but in the late 80s when the work started on the new technologies related to the touch the scope of the term 'haptics' was enlarged to include machine touch and human-machine touch interactions. More generally the term '**haptics**' nowadays refers to "*information acquisition and object manipulation through touch by humans, machines, or a combination of the two; and the environments can be real, virtual or teleoperated*" [3].

Therefore in [3] the author also suggests the subdivision of haptics into three areas: *human haptics* – the study of human sensing and manipulation through touch, *machine haptics* – the design, construction, and use of machines to replace or augment human touch, *computer haptics* – algorithms and software associated with generating and rendering the touch and feel of virtual objects (analogous to computer graphics).

Burdea in [53] describes **haptic feedback** as a "*group of the modalities of force feedback, tactile feedback, and the proprioceptive feedback*" where:

1. the *force feedback* "*provides data on a virtual object hardness, weight, and inertia*",
2. the *tactile feedback* "*provides a feel of the virtual object surface contact geometry, smoothness, slippage, and temperature*",
3. the *proprioceptive feedback* "*in the sensing of the user's body position, or posture*".

Concept of haptics in human-computer interaction is usually very closely related to the areas of teleoperations or telerobotics, Virtual Reality or Virtual Environment and simulation where the haptic feedback is widely used and consequently the relevant research in haptics is done. For instance, the first use of haptic feedback was performed by Goertz at Argonne National Laboratories who developed a teleoperator to handle radioactive materials and he used the force feedback [54]. The first researches in the area of tactile feedback were conducted at MIT – Patrick's project of "Dextrous Hand Master Exoskeleton" [55]. Since then the research in haptics is significantly progressed and several commercial haptic interfaces are currently available for affordable cost.

2.4. Haptic-based systems

Haptic technology provides feedback for the senses of touch in a similar way as the computer graphics does it for the vision. Haptic technology allows creating computer generated 'haptic virtual objects' which can be touched and manipulated with a hand or a body. This is achieved through application of forces, vibrations and/or motions to a user. [56]

Haptic interfaces are devices that enable manual interactions with virtual realities or teleoperated remote systems by receiving force and/or tactile feedbacks. These interfaces are used for the tasks where hands are used in the real world like exploration or manipulation of objects. [3]

2.4.1. Types of haptic interfaces

Haptic interfaces differ a lot – starting from pen-type devices and ending by full body force feedback interfaces. Therefore development of one general classification approach for whole variety of haptic interfaces is a challenging task. Author found the most relevant to be the one proposed by Hayward and Astley in [57]: device classification based on **degrees of freedom** (**DOF**). Degrees of freedom in [58] are defined as "*the number of parameters needed to specify the configuration of a mechanism, in terms of the number of links and joints and the freedom of movement allowed at each joint. This number is the degree of freedom or mobility of the mechanism*". For instance, using as example a robot arm - its degrees of freedom would be a number of different ways in which the arm can move; the human arm has seven degrees of freedom:

three in the shoulder, one in the elbow, and three in the arm below the elbow [59]. Based on DOF Hayward and Astley distinguishes Low DOF, High DOF and Very High DOF devices [57]. For the easier understanding of the concepts the author proposes the following metaphors for the mentioned terms: Low DOF haptic devices – desktop basic haptic devices, High DOF haptic devices - desktop advanced haptic devices, Very High DOF haptic devices – body haptic devices.

2.4.1.1. Desktop basic haptic devices

This category includes the devices that do not intend to emulate a task literally during actual performance [57]. For instance, in some cases 2 or 3 DOF are already sufficient for a high level of usefulness. Usually these devices are used for penetrating or touching virtual objects, exploring and/or manipulating a planar world. The following popular devices can be listed as examples in this group:

1. Phantom Premium haptic devices that provide 3 DOF for positional sensing and are used in wide range of different simulations and researches (Figure 2.4a) [60].

(a) Phantom Premium 1.0 and 1.5 [60]

(b) Pantograph Mk-II [61]

(c) Phantom OMNI [60]

Figure 2.4. Desktop haptic devices.

2. Pantograph Mk-II – a 2 DOF haptic device that was presented for the first time in 1994 ACM SIGCHI conference and redesigned in 2005. The device is able to apply tactile sensations to a fingertip (Figure 2.4b) [62].

2.4.1.2. Desktop advanced haptic devices

Devices from this category try to recreate a task entirely. Here one could include devices designed around a hand and that apply arbitrary forces and torques. Usually it would require having 6 DOF for devices in this category, but here fall also devices that are literal in their use even having less DOF [57]. Several example devices are listed below:

1. Teleoperations devices – 6 DOF devices, for instance, Jet Propulsion Laboratories' FRHC teleoperator [63],
2. Game controllers - Logitech G27 Racing Wheel for racing simulators, Griffin's The Strike Rod Controller for fishing game simulators [64],
3. Phantom OMNI device – 6 DOF which is claimed in [60] to be one of the most cost-effective haptic devices today (Figure 2.4c) and is used in wide range of different applications in medicine, graphics, design etc.

2.4.1.3. Body haptic devices

This category includes devices that try to recreate a task in its actual form and in combination with body motions – with a complete arm, shoulder or leg etc. It usually includes more than one body-device interfaces and needs to be worn on the operator's body. [57]

This category is represented by the following devices:

1. Hand exoskeletons (Figure 2.5a) [65],
2. Arm exoskeletons (Figure 2.5b) [66], [67], [68],
3. Leg exoskeletons (Figure 2.5c) [69],
4. Full body exoskeletons serving as human body amplifiers to carry/move heavy loads [70], also used in locomotion – active motion – interfaces in virtual environments (Figure 2.5d) [71, 72].

(a) CyberGrasp [65]

(b) Exoskeleton Prototype 3 (EXO-UL3) [66]

(c) Powered Legs from Sarcos Research Corp. [73]

(d) Sarcos Treadport [72]

Figure 2.5. Body haptic devices.

These are just few examples for the haptic devices; there exists many more that are specific or adopted to the related research or application needs.

2.4.2. Current applications

Enriching virtual realities and teleoperations with haptic feature creates exciting possibilities for applications in different fields, the costs for development of haptic devices is also decreasing therefore a lot of applications are already brought to use in real life. Below are listed the examples of the applications in different fields nowadays [3].

Robotics.

Used for teleoperators which are remotely controlled robotic tools that reproduce the contact forces to the operator, one of the first tools was developed by Goertz to handle radioactive materials in 1950s, later the concept was employed for attempts to develop space robotics, for underwater manipulations and dispatching of explosives, for instance, for mines [54], [74].

Science.

Used for data display, for instance, molecule docking, multi-dimensional maps, data mining in geology (or in related, applied fields such as oil and gas prospecting), remote sensing, and the display of fields and flows, for instance, the systems developed by Nanoscale Science Research Group at the University of North Carolina: “nanoManipulator”, “Nanometer Imaging and Manipulation System”, “3-Dimensional Force Microscope” [75], or interactive 3D browsers for large topographic maps [76].

Medicine.

The haptic-based systems are widely used in different fields of medicine, namely, manipulating micro and macro robots for minimally invasive surgery (in the source [77] information about researches conducted is collected in this area, one of the available commercial examples is the Da Vinci Surgical System [78]), remote diagnosis for telemedicine, aids for rehabilitation (one of the examples is “Rutgers Ankle” interface which is used for orthopedic rehabilitation [79]), aids for the disabled such as haptic interfaces for the blind (the multimodal haptic mouse [80]), educational simulators for students (the virtual haptic back – simulator of a human back for training in palpatory diagnosis [81]).

Education.

The haptic-based systems are used to give the students the feel of phenomena at nano, macro, or astronomical scales; “what if” scenarios for non-terrestrial physics; experiencing complex data sets, for instance, Multi User Virtual Interactive Interface (MUVII) project with the aims to develop two haptic feedback devices with accompanied educational prototypes that would exploit these devices [82] - [83].

Design and engineering.

Integration of haptics into CAD systems such that a designer can freely manipulate the mechanical components of an assembly in an immersive environment, for instance, 3D Design & Modeling systems from Sensable [84].

Entertainment.

On of the popular applications is in video games and simulators that enable the user to feel and manipulate virtual solids, fluids, tools, and avatars, for instance, the first commercial products were force-feedback joysticks with some basic haptic application that now advanced till more sophisticated products, like “Logitech Driving Force GT” [85].

Culture.

Virtual art exhibits, concert rooms, and museums in which the user can login remotely to play the musical instruments, and to touch and feel the haptic attributes of the displays; individual or co-operative virtual sculpturing across the internet, possibility for visitors to feel rare and fragile artifacts, for instance, several projects for enhancing museum experiences with haptic technologies were run by Glasgow University where one of the projects was "Senses in Touch" [86] or the project "Museum of Pure Form" developed at PECRO in Pisa, Italy [68].

2.5. Examples of haptic-based systems in chemistry education and their usability evaluations

The described technological advances and the decreasing costs of the haptic devices have opened new application opportunities for chemistry and molecular analysis related education and research. The haptic force feedback and visualization technologies can be used to model a virtual interactive environment for inter-molecular force simulations and offer to the users the interaction possibilities. Currently there are a lot of studies conducted in this field and different tools, systems and applications developed.

The visualization expert Mario Valle in 2005 started a survey of the non-commercial tools that are used in chemistry and crystallographics [87]. This survey served as a starting point for developing the following non-exhaustive list of interactive tools and systems used for modeling inter-molecular forces. The list includes only the tools that meet the following criteria:

- have haptic and visual features that convey information about inter-molecular forces;
- for desktop use;
- are non-commercial or started as non-commercial projects.

The short overview of the tools reviewed are given in Table 2.3., but further in this section the author presents a short description of each tool, their visual and haptic features as well as the short descriptions of the evaluations of these tools if such were conducted and these results were published.

Table 2.3. Summary of visualization and haptic based systems for chemistry education

Name	Suggested use by the authors of the tool	Visual features	Haptic device	Year
VMD [88] – [89]	Display, animate and analyze large biomolecular systems	3D graphics with rich molecule visualization options and possibilities	PHANTOM haptic device and 3D tracker (currently in development)	1996 (haptic feature in development)

Name	Suggested use by the authors of the tool	Visual features	Haptic device	Year
CFF [5] – [6]	Higher education	3D graphics with possibility to integrate stereo graphics environment via Reachin Display, van der Waals molecule visualization	6DOF haptic device	2003
MV [90]	Undergraduate chemistry studies	3D graphics with possibility to integrate stereo graphics environment via Reachin Display, several molecule visualization options	PHANTOM Desktop haptic device via Reachin API	2005
HMolDock [91] - [92]	E-learning in multi-user virtual environment	3D graphics , van der Waals molecule visualization	PHANTOM 1.5A/6DOF haptic device	2009
Nano-Manipulator [93]	Examining mechanical and electrical surfaces at nanoscale	3D Visual SPM Display and Controller	PHANTOM Desktop haptic device	1992
MyPal [94]	Molecular dynamics simulation with interaction possibility	Navigation of scene using Spaceball device	PHANTOM Omni or Premium 1.5A haptic device, 3D tracker	2010

2.5.1. Visual Molecular Dynamics

Short description.

Visual Molecular Dynamics system (VMD) is continuously developed since 1996 being an extensive molecular visualization tool for displaying, animating, and analyzing large biomolecular systems. It can be run under most widespread OS systems - MacOS X, UNIX and Windows - and is distributed free of charge including its source code. The main feature of the tool is variety of methods to render and color a molecule while supporting over 60 molecular file formats and data types (including PDB). There are also available many VMD tutorials and user manuals describing how to install and use the tool. Many plug-ins and tutorials are developed by the research community that uses this tool for their specific needs. There is also a dedicated website

[88] that collects and has the most explicit information about this tool as well as the possibility to download it.

Visual features.

VMD facilitates the creation of different molecular visualizations and scenes using 3D graphics, built-in scripting and developed plug-ins for the specific needs. It offers different molecular coloring styles, material properties and transparency features. User can also control the rendering techniques used and lighting parameters of the molecular scenes.

The VMD offers both graphical and text-based user interfaces. The graphical user interface is XForms based menuing environment.

Haptic features.

The haptic feedback was not the primary feature of VMD. In fact the support for the 6-DOF 3-D trackers (e.g. Polhemus FastTrak) and for the devices with haptic feedback (e.g. Phantom) is in continuous development. Currently this feature can be integrated in VMD using VRPN (Virtual Reality Peripheral Network). It can be used, but not required instead of mouse in interactive molecular dynamics simulations. According to lead developer of VMD J.E. Stone the main problems related to integration of this kind of technologies arise from lack of skills configuring and maintaining them by the direct users of the tool – scientists and researchers [89].

Evaluation.

There were no particular usability evaluations of the VMD haptic features found.

However there were conducted user surveys tri-annually in order to examine the user satisfaction, the impact of the software on work quality, and user ratings of existing and planned features. The latest user survey was conducted in 2006 [95]. The main findings of the survey were:

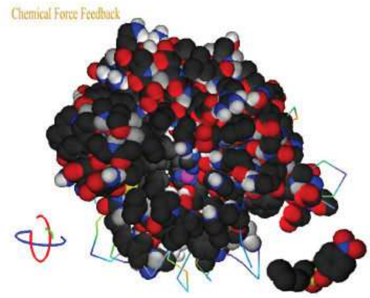
- around 90% of VMD users were related to academic institutions and use it for research purposes;
- most users also indicated that they are satisfied with VMD and it improved their quality of work;
- around 60% of the users used VMD tutorial;
- most of the users also indicated that they are using VMD because it is free and useful in their work.

2.5.2. Chemical Force Feedback

Short description.

Being a multi-sensory system and having combined the visual and haptic feedbacks it is in development since 2003 at the department of Science and Technology at the Linköping University by P. Bivall who started that as his master thesis. It allows examining the forces between a protein and a substrate in real-time. It is possible also to manipulate the substrate while placing it into the docking site using the "*molecule-on-a-stick type of interaction*". This tool can be also integrated with the stereo graphics environment providing the depth to the visualized molecules. The .pdb files are used as an input and to generate the grid is used the AutoGrid software, the rotational bonds analysis is performed by AutoDock in order to determine which bonds in a ligand can be rotated. The tool was deployed in education two subsequent years during its evaluation. The main accent of the research was the use of the tool in higher education. [5, 6]

(a) Example of the molecule-on-a-stick type of interaction in CFF [5]



(b) Screenshot of CFF where the protein (center), the ligand (lower right) and torque visualization (lower left) [6]

(c) Student working with CFF within the stereo graphics environment [6]

Figure 2.6. Chemical Force Feedback (CFF) application in use and its screenshots.

Visual features.

Representation of the proteins and ligands is performed with 3D visualizations and possibility to integrate the stereo graphics environment that adds depth to the rendered image (Figure 2.6).

Haptic features.

The tool supports 6DOF devices and provides the "*molecule-on-a-stick type of interaction*" that allows moving the ligand molecule around the protein molecule discovering the attraction/repulsion forces. The ligand is moved around using the haptic device. The main problem described by the evaluation participants was related to the feedback of the weak interaction forces – this feedback was not adequate enough. The History Dependent Transfer Function was developed for this purpose [Chapter 4.2. in 5] that "*adjusts depending on the level of the previously translated forces*" nevertheless the further evaluation results did not show significant improvements.

Evaluation.

P. Bivall in [5] describes the extensive evaluation of the developed CFF tool with the goal to evaluate learning, performance and usability aspects. The first evaluation was performed in 2005 which led to several evaluation process refinements, improvements and the second evaluation in 2006.

The tests were performed with the university students in a cross-over mode: the same group of students performed the tests in both modes – with and without haptic force feedback, but for both groups the 3D visualization of the molecules was available. Both evaluations included the following:

1. Background survey – collecting the demographic information about the students and their knowledge,
2. Tasks and conditions (with/without haptic feedback) related tests
    a. Pre-tests – open-ended questions about biomolecular interactions with the aim to compare the answers with the post-tests,
    b. Pre-haptic exercise (only for the group that had haptic force feedback available),
    c. Tasks – the actual laboratory tasks to perform related to substrate, inhibitor and transition state,
    d. Post-tests – open-ended questions about biomolecular interactions,
3. Experience survey – designed to evaluate the usability aspects of the tool,
4. Interviews – semi-structured interviews with a smaller representative group of students to understand better their knowledge about proteins and ligand docking problem and conducting the *thinking aloud* session.

The second evaluation was enriched with the spatial test and final exam consideration.

The main results of the evaluation were the following:

- "*the system effected learning regardless of condition*" – with/without haptic feedback,
- learning gain was dependent on the task,
- the reasoning of a student was more force-based when the tasks for performed with haptic force feedback available,
- the interviews revealed that the haptic force feedback "*supported the connection of knowledge (..) in the students' conceptions of molecular recognition*",
- the docking accuracy did not improve regardless of the condition however the time to complete the task was lower for the students with the haptic force feedback,
- "*a van der Waals representation for the ligand (..) caused visual occlusion as the ligand covered the view of the binding site during docking*".

2.5.3. Molecular Visualiser

Short description.

Molecular Visualiser (MV) is a Web3D technologies based tool for visualization of molecular systems, potential energy surfaces, and wavepacket dynamics. The development of this tool was started in 2005 at the University of Wales by the leading researchers R.A. Davies and N. W. John.

The main features of this tool are the possibilities:

- to use it for molecular visualization via web browsers having a suitable plug-in VRML 97 (ISO-standard Virtual Reality Modeling Language);
- to integrate it with the Reachin Display environment offering the molecular visualization and the usage of the haptic feedbacks.

The potential use suggested by the authors is for undergraduate chemistry students. It supports the file formats of Cartesian coordinates e.g. .pdb. [90]

Visual features.

The tool allows different molecular visualization options: ‘stick’, ‘balls-and-stick’, ‘tube’, and ‘space-filled’. The colors of the most common elements are compliant with other widely used chemistry modeling software. The change of the molecular visualization options is achieved via menu buttons. The Reachin Display allows the stereoscopic projection of the molecule.

Haptic features.

These features are added via the Reachin API and the haptic features are not explicitly discussed in [90].

Evaluation.

No formal usability evaluations were found, but the testing of the tool is shortly discussed in section 5 of [90] claiming to obtain good results.

2.5.4. Haptic-based Molecular Docking

Short description.

Based on the related biomolecular docking studies in drug design the development of Haptic-based Molecular Docking (HMolDock) started in 2008 at the Nanyang Technological University primary for a Transmembrane helix docking problem modeling. The tool is using the Protein Data Bank (PDB) files for input, other file formats as per suggestion of the authors can be converted into this format using the dedicated conversion tools. A user can assign the haptic device to a probe or to a molecule and interact in context of probe-molecule or molecule-molecule discovering the related attraction/repulsion forces. In [92] the stabilization method is discussed for the haptic force feedbacks in order to avoid the strong vibrations of the haptic device. The authors are discussing the possibility to integrate the tool in the e-learning process and multi-user virtual environments. [91, 92]

Visual features.

For 3D visualization the coordinate grid is used in order to facilitate the manipulations with probes and/or molecules in 3D space (Figure 2.7). The visualization of the molecules is performed with van der Waals surfaces.

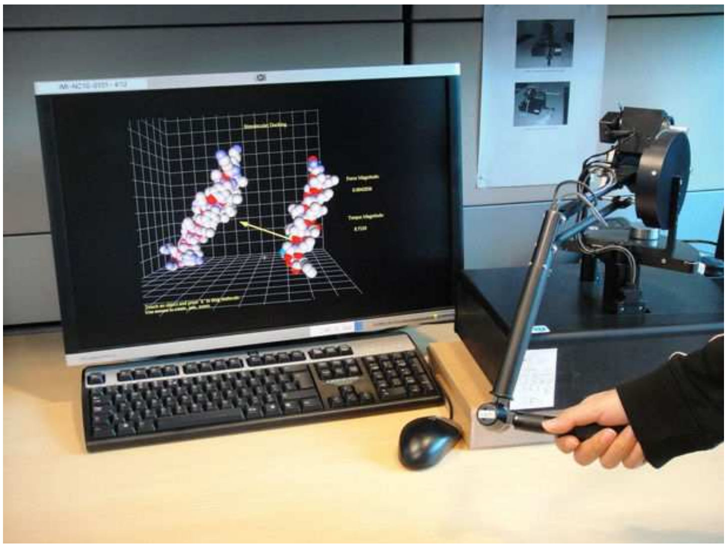


Figure 2.7. Haptic-based Molecular Docking (HMolDock) application in use [92].

Haptic features.

The PHANTOM Premium 1.5/6DOF haptic device made by SensAble Technologies is used during manipulations. There is possibility to connect two haptic devices in order to model a ligand and a receptor docking process as an interactive process in a multi-user environment. More than one device adds complexity to the developed tool due to stability issues of the haptic devices when the forces are applied. The vibration problem occurs when there is a change of the intensity of the forces and the relevant *Linear smoothing method* for solving it is given in [92].

Evaluation.

No formal usability evaluation results were found published, but [92] suggests that the initial tests of the developed tool were performed and the results show that tool is useful for education.

2.5.5. NanoManipulator

Short description.

The development of the tool is ongoing since 1992 through the collaboration between the departments of Computer Science and Physics of the University of North Carolina at Chapel Hill. This Interactive Visualization and Control system adds the virtual presence interface to the Scanning Probe Microscopes (SPMs). The goal of this system is to enhance capabilities of STMs through 3D visualizations and haptic force feedback during experiments of different surface feature observations and modifications in real-time. The leading researcher of nanoManipulator R.M. Taylor in his thesis describes it the following: "*it allows the user to see, fell and manipulate matter at the nanometer scale*" [96]. The system is used for the different surface researches at nanoscale to examine their mechanical and electrical properties. The system was taken over by 3rdTech in order to create the SPMs performance enhancing product. [93], [97]

Visual features.

The system allows creation and update of the visual 3D model of the surface in real-time and storing for the playback later. The display has a perspective view and can be customized using rotation and scaling features as well as customizing the color maps, textures, and contour and grid lines. [93], [98]

Haptic features.

The specifications show that the Phantom Desktop 6DOF haptic device is used for force-feedback generation. With the Phantom stylus it is possible to move the displayed surface, zoom in or out, move a virtual or an actual probe and to interact with the scanned surface. [98]

Evaluation.

No formal usability evaluations published were found, but the system is successfully employed by the researchers at the University of North Carolina at Chapel Hill and Katholieke Universiteit Leuven which facilitates the new kind of experiments. [97]

2.5.6. MyPal

Short description.

MyPal is a simulation tool and stands for **M**olecular scrutin**Y** of **P**otenti**AL**s. It was developed in order to apply visual and haptic features to study and possibly discover the binding sites of metal ions in this way decreasing the costs of the process and adding the interactivity feature during simulations. The development of the tool was carried out by M. Baaden from Theorethical Biochemistry Laboratory in Paris. The paper [94] which was published in 2010 describes the application of this tool for DNase I enzyme binding sites studies and gives the following description of MyPal: "*a method for interactively locating ion binding sites by steering ionic probes into electrostatic potential maps using a haptic device*".

Visual features.

The VMD tool was used for the visualization of the molecules using van der Waals model, but according to the authors this tool had several shortcomings. Therefore they are currently developing their own simpler visualization tool using the VTK visualization toolkit. The stereo rendering feature is achieved via Crystal Eyes stereo vision device. [94]

Haptic features.

The force constraints of the simulation for the probe particles can be added by a mouse or a haptic device. These devices can be used also for the selection or movement of the particles. It is also possible to control the direction and to adjust the amplitude of the forces. According to the authors the haptic feedback adds intuitiveness to the tool and decreases the necessity for additional explanations when only the visual feedback is used. The VRPN library is used in order to generate the force feedback. Two haptic devices were used for the haptic feedback tests: Phantom Omni and Phantom Premium 1.5A. The Spaceball device was used for scene navigation. [94]

Evaluation.

In [94] are described the tests performed with the MyPal and that proved this tool to be useful for locating the binding sites. Nevertheless these tests are not explicitly described and it was also not possible to find any related formal usability evaluation results published.

2.5.7. Conclusions

The results of the survey above reveal the trend of the wider emergence of the haptic-based tools for the research and education purposes related to the molecular dynamics fields such as chemistry, biochemistry, medicine etc. The authors tend to suggest wide application options for their developed tools: for undergraduate and graduate education, as virtual environments for multi-user interaction, for molecular dynamics simulations with possibility for the user to interfere and slightly adjust the simulation process etc.

The approaches of the visual and haptic feature development also vary from one tool to another; however in most cases the existing development frameworks, libraries or modeling languages were used for the implementation of the mentioned features. For instance, MV (section 2.5.3.) considers the advances of Web3D features, but MyPal (section 2.5.6.) integrates VMD (2.5.1.) for the visualization of their simulations at the same time indicating the shortcomings of VMD. One can conclude that still a general framework, library or modeling language for developing this kind of visual and haptic based tools does not exist.

Since the description about these tools was obtained from different sources: some were more chemistry specific, but the others were more technology specific; also the language and approach used for describing these tools varied which made harder the actual comparison in terms of the used technologies and actual application for inter-molecular force studies.

The most extensive and explicitly described evaluation was performed by P. Bivall Persson for the CFF (section 2.5.2.). However the evaluation was more concentrated on the study of the learning gain of the students using this tool and one of the conclusions in [6] was that "*there was, however, no obvious advantage from the addition of the force feedback element to the system* *that could be isolated in the pre- and post-test analysis*". He also considers for the future work the improvement of the design of evaluation [6].

Using the formal usability evaluation methods might facilitate discovering usability problems and improve the overall usability of these tools.

3. USABILITY EVALUATION

The usability evaluation of the haptic-based framework was conducted using the specifically adopted user-based methods for usability evaluation. The first section introduces the haptic-based framework and describes its main features that are further referenced in this chapter. The methodology section describes in detail the approach developed for this evaluation. The process of the evaluation is described further in the third section and the final results section describes the main findings of the evaluation.

3.1. Description of the framework

The evaluated haptic-based framework was developed in Politecnico di Milano as a response to the growing need of the tools that can be used for the molecular analysis, in particular, for the studies of interactions among molecules and their attraction/repulsion forces. This framework is a "virtual environment, where the molecule to be analyzed is shown to the user and a probing charge is associated with a haptic device. The interaction between the molecule and the electric charge is felt via the haptic device and allows one to explore the electrostatic surface of the molecule". [1]

The input of the system is a geometrical representation of a molecule. There are two representations which can be used by this system – theoretical model in .PDB file format or experimental data in .CIF file format. Figure 3.1 shows an overview of the architecture of the framework.

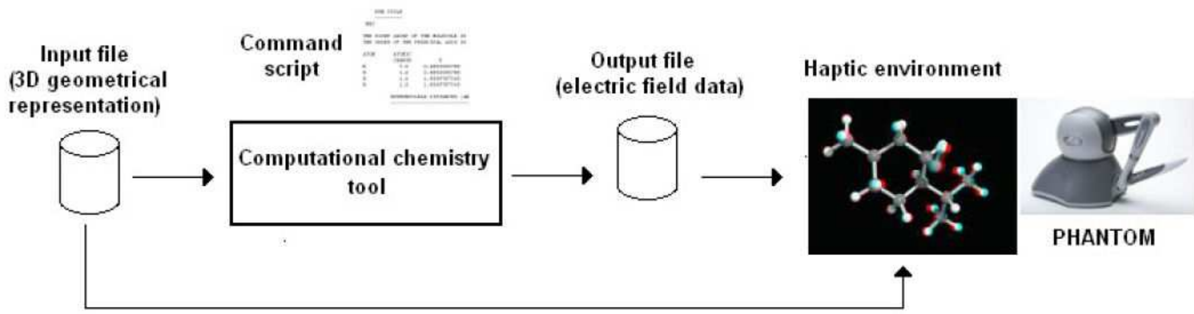


Figure 3.1. The architecture of the haptic-based framework for chemistry education [1].

The output of the system is the electric field data which is used by the virtual environment of the system which generates 3D graphical representation of the molecule and allows interaction with the forces through the Sensable Phantom® Omni haptic device.

The force field is represented in terms of quantized grid surrounding the molecule which is available only until a limited distance from the molecule. The force feedback generated by the haptic device is the one associated with the voxel of the grid within which proxy position falls in.

Depending on the situation the forces either attract or repulse, the intensity of the force feedback is very weak (nanoscale), but the proportion to the real forces is not lost. [1]

In the Figure 3.2 one can see the screenshot of the framework and the detailed description of different modes and options. The main features are:

- the haptic proxy that shows the current interaction point with the electric field in the virtual environment (Figure 3.2),
- different molecule visualization options: wireframe, ball'n'stick, covalent space fill, van der Waals space fill (Figure 3.2 and Figure 3.3),
- the plot of the electrostatic field along the direction connecting the proxy position and the center of the molecule (Figure 3.2),
- the force field of the molecule surface represented by means of different colors (Figure 3.2).

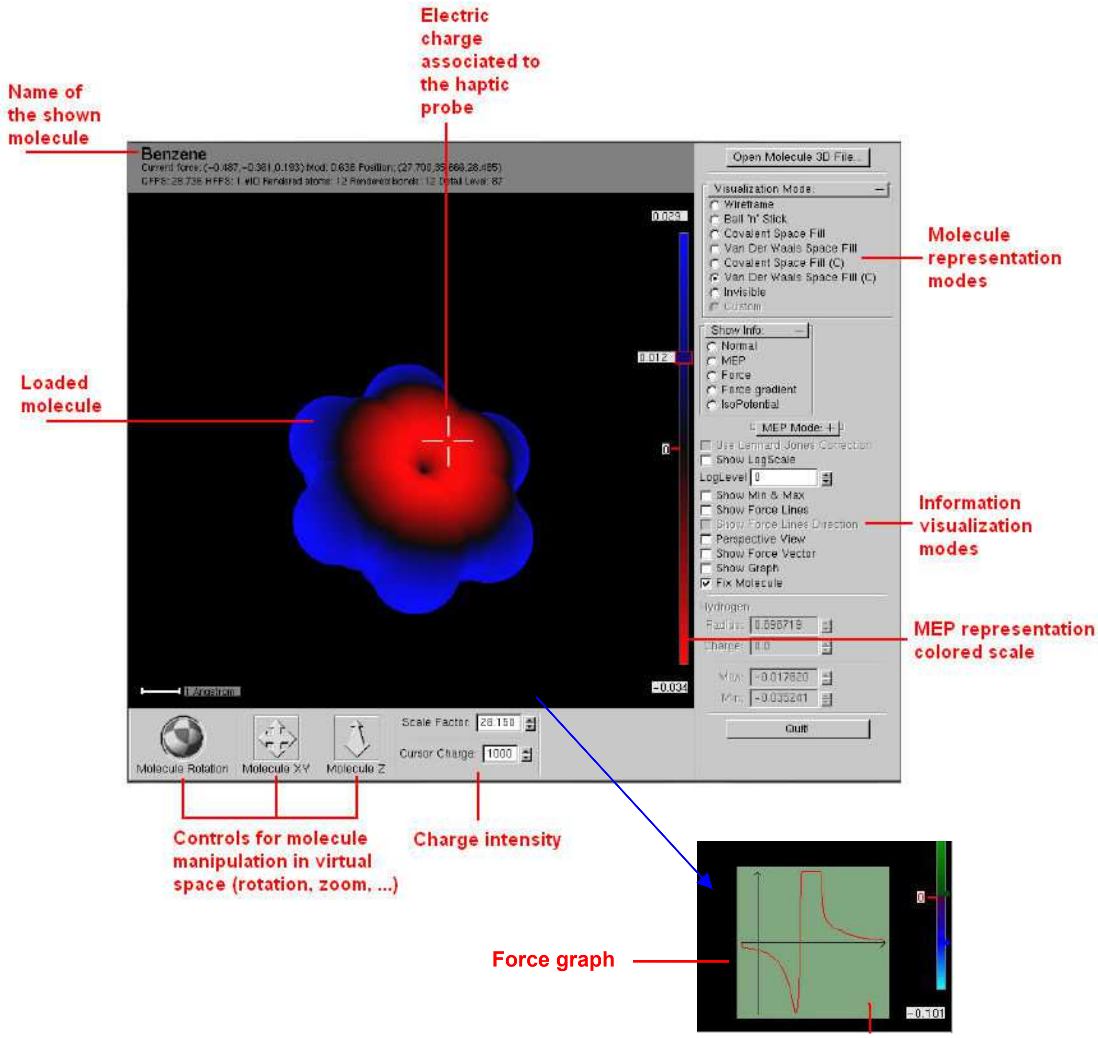
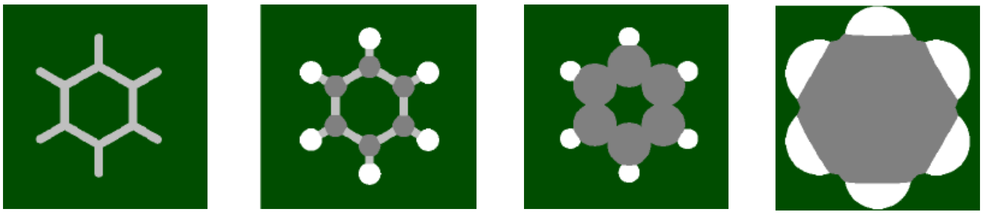


Figure 3.2. The screenshot of the haptic-based framework

The different options of the additional information (Figure 3.2) can be hidden or shown according to user preferences or to the problem under consideration, for instance, the minimum and the maximum electrostatic potential points of the loaded molecule. A user can also choose among different molecule visualization modes (Figure 3.2) and change the charge intensity value increasing or decreasing it and in this way changing also from negative to positive potential and vice versa (Figure 3.2).



(a) Wireframe (b) Ball-n-stick (c) Covalent space fill (d) van der Waals space fill

Figure 3.3. Molecule visualization options in the haptic-based framework for chemistry education [99].

In the Figure 3.4 one can see the "*ready-for-work*" setup of the framework – the haptic device and the example of the loaded molecule on in the virtual environment on the laptop.

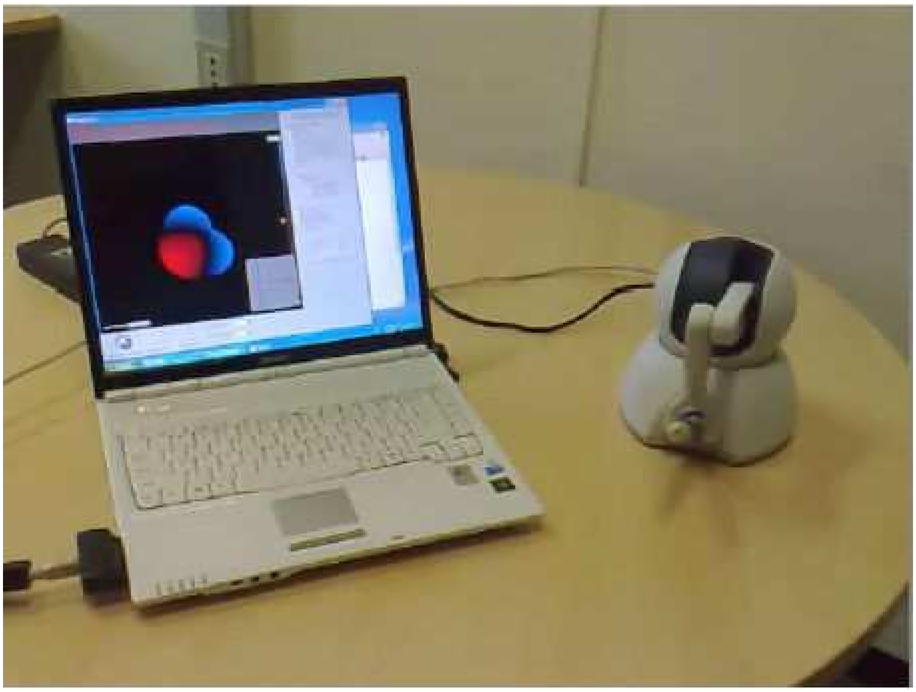


Figure 3.4. The setup of the haptic-based framework for chemistry education at work [1].

The framework is easy to setup and to start using which gives it a competitive advantage among other similar tools.

3.2. Methodology

The usability evaluation approach was developed partly following the steps described in subsection 2.2.1.4 and partly based on the practical experience of the author. The overview of the design process is given in Figure 3.5.

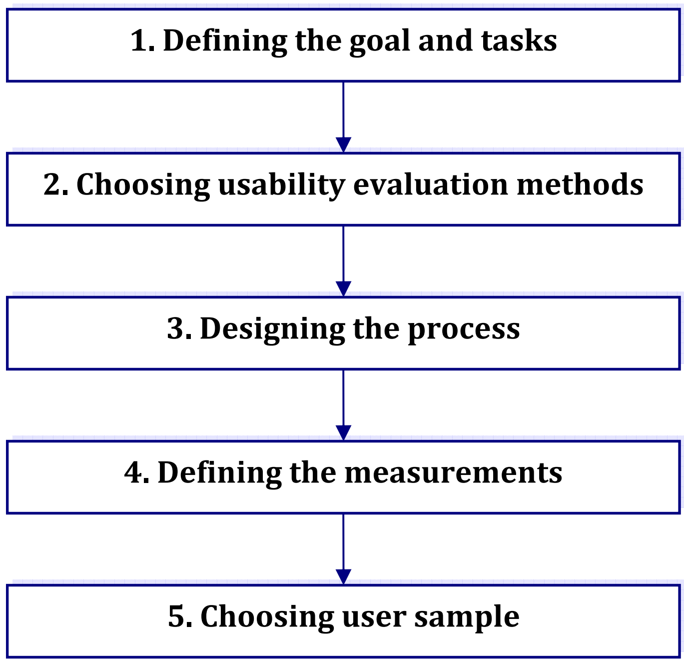


Figure 3.5. The usability evaluation preparation steps.

3.2.1. Defining the goal and tasks

The main goal of the usability evaluation is to determine through formal usability evaluation methods if the considered haptic-based framework is ready to be introduced in the chemistry courses. The following tasks were defined to achieve this goal:

1. to develop the usability evaluation procedure for the haptic-based framework;
2. to perform the usability evaluation and summarize the results according to the defined measurements;
3. to identify the main problems that users face when using this framework;
4. to recommend the solutions for the identified problems;
5. to conclude if the framework is ready to be introduced in the chemistry course.

3.2.2. Choosing usability evaluation methods

The most suitable method to achieve the goal among the methods described in 2.2. was considered to be the *usability testing* due to the following reasons:

1. user feedback that describes advantages and drawbacks of the system can be collected directly for the users;
2. observations how the user is interacting with the haptic-based framework can be used as additional supportive data for the results obtained from the user feedback.

To validate the obtained results during the usability testing two usability questionnaires (ASQ and SUS) and two additionally developed questionnaires (haptic features and final feedbacks questionnaire) were added in this evaluation.

3.2.3. Designing the process

The tasks and the questionnaires for the test sessions were prepared in advance. The special user forms for the test sessions were developed and were expected to be filled by the users. The process of the usability evaluation itself was divided into three consecutive parts (Figure 3.6).

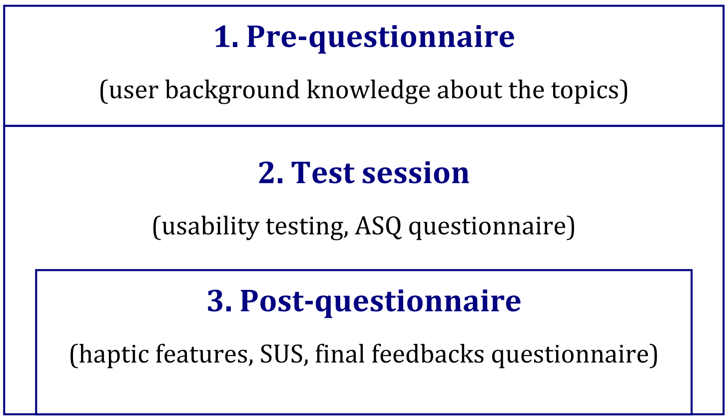


Figure 3.6. The usability evaluation process of the haptic-based framework.

Pre-questionnaire.

The goal of the pre-questionnaire was to determine users' knowledge about the topics covered during the usability evaluation such as molecular analysis, haptic devices and computer technologies. The users were asked to rate their knowledge on their own. The pre-questionnaire was sent and filled in by the users before conducting test sessions.

An example of the pre-questionnaire is included in ANNEX 2.

Test session.

The user forms were prepared for each user. These forms included the details of the three tasks to be performed by the user individually, in the end of each task there was added ASQ questionnaire. The ASQ score included the efficiency, effectiveness, satisfaction and use of haptic device usability aspects – the smaller the average score value the better evaluated are these aspects by the participants. Separate test sessions were planned for each of the invited users.

An example of the test session user form is included in ANNEX 3.

Post-questionnaire.

The post-questionnaire included the haptic features, the SUS questionnaire (general features of the application) and the final feedbacks questionnaire. The SUS score gives an overall score for the usability of the application – the higher the score the better application is evaluated. An additional haptic features questionnaire was developed based on the SUS in order to specifically evaluate the haptic features of the application – the higher the score the better application is evaluated. The final feedbacks questionnaire included the questions about understanding the purpose of the application, its attractiveness and whether the user would recommend it to his/her colleague. One additional question was about didactic/learning aspects of the application. The users were also encouraged to share their suggestions for the possible improvements and any other comments about their experiences during the session.

An example of the post-questionnaire is included in ANNEX 4.

3.2.4. Defining the measurements

During the evaluation process the following measurements were collected:

1. Number of tasks successfully accomplished by the users;
2. Problems faced by the users while executing the tasks and their typology (the grouping criteria for the problems was developed later during the summarizing process of the results);
3. Efficiency – time in minutes spent for each of the tasks;
4. Accuracy of the tasks – if the users were able to accomplish the tasks correctly;
5. ASQ questionnaire score – average (arithmetic mean) of the four items of the questionnaire [23];
6. User's feedback about framework features used during tasks execution – the results were taken into account only if the feedback was given in more than one test session and it was not contradictive with each other;
7. SUS questionnaire score - sum each item's score contributions (for items 1, 3, 5, 7 and 9 the score contribution is the scale position minus 1; for items 2, 4, 6, 8 and 10, the contribution is 5 minus the scale position) and multiply the sum of these contributions by 2.5 to obtain the overall SUS score value [29].
8. Haptic features questionnaire score - the score of the haptic features was calculated using the similar method as one for the SUS questionnaire: sum each item's score contributions (for items 1, 3, 6 the score contribution is the scale position minus 1; for items 2, 4, 5 the contribution is 5 minus the scale position) and multiply the sum of these contributions by 2.5 to obtain the overall score value.
9. Final feedbacks questionnaire – an average score of the feedbacks for each of the questions and an overall average score.

3.2.5. Choosing user sample

The haptic-based framework is to be introduced in chemistry course therefore the potential users of it are the students of Computer Engineering study programme at Politecnico di Milano who have chemistry course available as optional and who already have background knowledge in chemistry. The students were invited to apply on a voluntary basis for the test session.

3.3. Evaluation process

Each user had an individual test session that was held in a *testing lab* – an office like room equipped with the haptic-based framework and all the necessary devices - the Sensable Phanotm® Omni haptic device and a laptop with the virtual environment setup (Figure 3.4).

In each of the test sessions there were present a moderator, an observer and the user representative.

The **moderator** introduced the tool and guided the user through the test session user form. The moderator was also answering the questions of the users if s/he had any.

The **user** was asked to *think aloud* while performing the each of the tasks.

Without interrupting any interaction the **observer** was following the actions of the user and taking notes about the observations and also about user's feedbacks. The observer was also fixing the specific problems when the user encountered them while interacting with the tool.

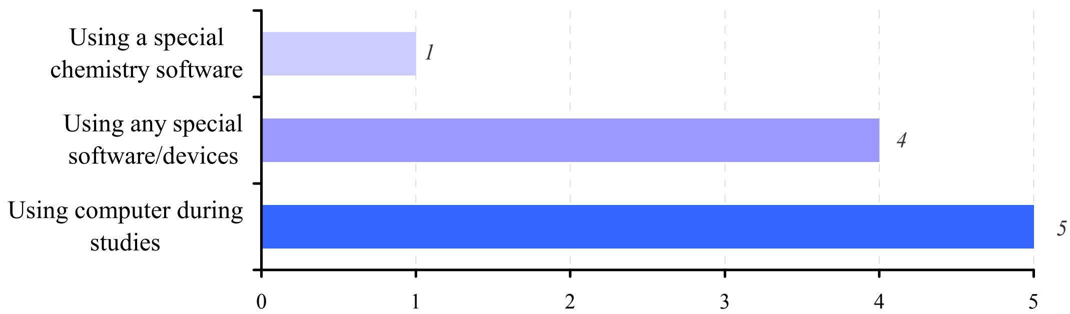
On average the length of one test session was 1.5 – 2 hours. The test session results were the user filled forms and the notes taken by the observer.

4. USABILITY EVALUATION RESULTS

There were five participants in the usability evaluation - students from the Computer Engineering programme at Politecnico di Milano: 2 females and 3 males with the average age of 21.6 years. Further in this chapter are discussed the pre-questionnaire results, the test session results and the post-questionnaire results. The related filled forms of questionnaires and tests sessions obtained from each of the participant are available in ANNEX 5.

4.1. Pre-questionnaire results

All the participants indicated that during their studies they are using computer - reading lecture slides, for applications development and compilation and for mathematical analysis (SciLab, Matlab). Only one of the participants is using a special chemistry application. The Graph 4.1 shows the summary results of the software and computer usage.



Graph 4.1. Number of participants that use computer and any special software/devices during their studies.

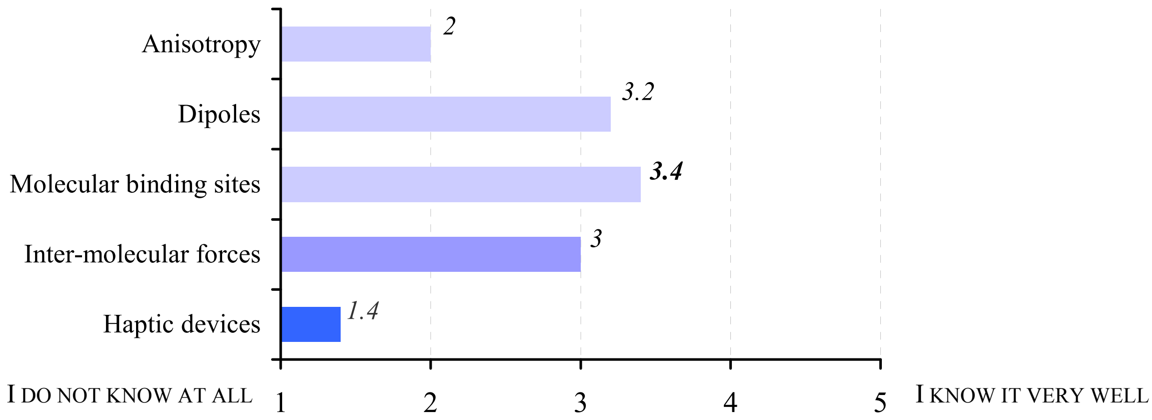
The Table 4.1 presents the detailed information about each test session's participant: his/her usage of computer and software as well as the demographic information.

Table 4.1. Pre-questionnaire results - general information about the evaluation participants.

				Usage of computer/software		
Test session Nr.	Age	Sex*	Year of studies	using computer for studies**	using any special software/devices**	using a special chemistry software**
Test1	20	1	3	1	0	0
Test2	26	1	>5	1	1	1
Test3	20	1	3	1	1	0
Test4	21	2	3	1	1	0
Test5	21	2	3	1	1	0
Average	**21.6**	**n/a**	**n/a**	**1**	**n/a**	**n/a**

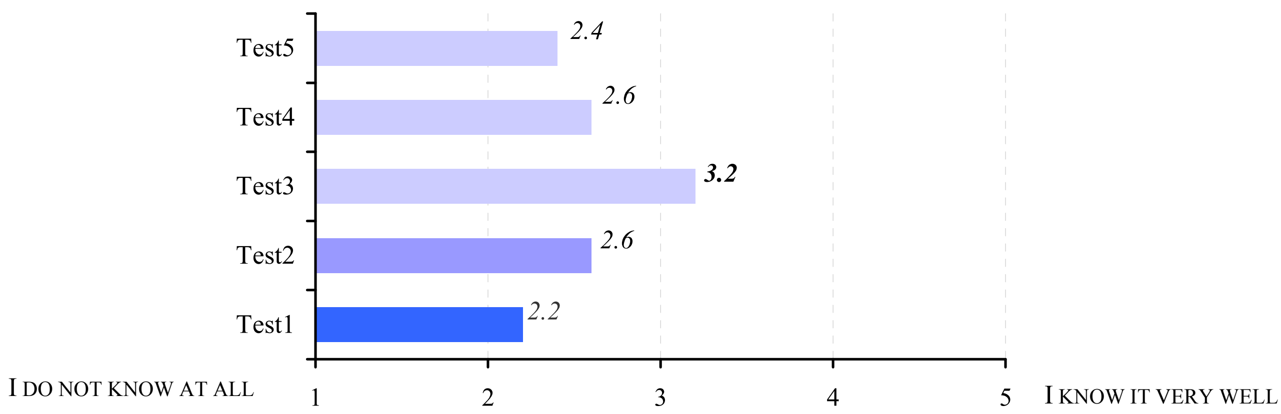
** 1 – Male, 2 – Female;*
*** 1 – Yes, 0 – No*

The participants were also asked to rate their knowledge about chemistry concepts and haptic devices on the scale 1 (I do not know at all) to 5 (I know it very well). The results showed that participants have very little knowledge about haptic devices. They rated their knowledge about chemistry concepts on average better; however it was not rated as very good either. They gave the least scores to their knowledge about anisotropy concept which was considered in the Task3. The Graph 4.2 presents the average scores among all of the participants.



Graph 4.2. Pre-questionnaire results - average concepts knowledge scores grouped by the related haptic and chemistry concepts.

The Graph 4.3 presents each participant's average score for all rated concepts. The score of the Test3 participant is on average higher when compared to the others, but the Test1 participant's score is the least.



Graph 4.3. Pre-questionnaire results – average concepts knowledge scores grouped by the participants.

The Table 4.2 shows the detailed scores for each of the test session participant.

Table 4.2. Detailed participants' knowledge rates about related haptic and chemistry concepts

Test session Nr.	Inter-molecular forces*	Molecular binding sites*	Dipoles*	Anisotropy*	Haptic devices*	Average
Test1	2	2	3	2	2	**2.2**
Test2	3	3	3	3	1	**2.6**
Test3	4	4	3	3	2	**3.2**
Test4	3	4	4	1	1	**2.6**
Test5	3	4	3	1	1	**2.4**
Average	**3**	**3.4**	**3.2**	**2**	**1.4**	
** rated on the scale: 1 – I do not know at all .. 5 – I know it very well*						

4.2. Test session results

The results are presented by the tasks that were used during usability tests. The observations and the users' feedback were collected for several visualization and haptic features of the application. Based on this feedback the most useful features were highlighted and the problematic ones were identified. The obtained problems were categorized in the following groups:

1. *cognitive* – cognitive effort of the user while using the tool,
2. *graphics* – problems related to the graphical choices of the tool,
3. *haptic* – problems related to the haptic features of the tool including spatial problems and the haptic device itself,
4. *semiotic* – problems related to the meanings of the messages of the tool.

Each task's results subsection presents the related problems according to their groups; the whole list is available in the ANNEX 7.

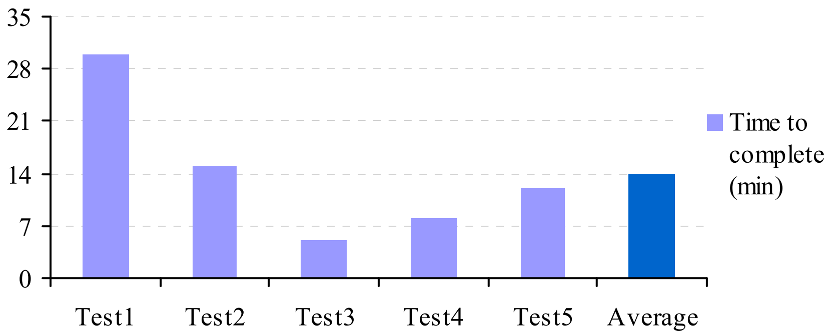
4.2.1. Results of Task 1: Critical points detection

Topic of the task: Critical points detection on the molecule of benzene.

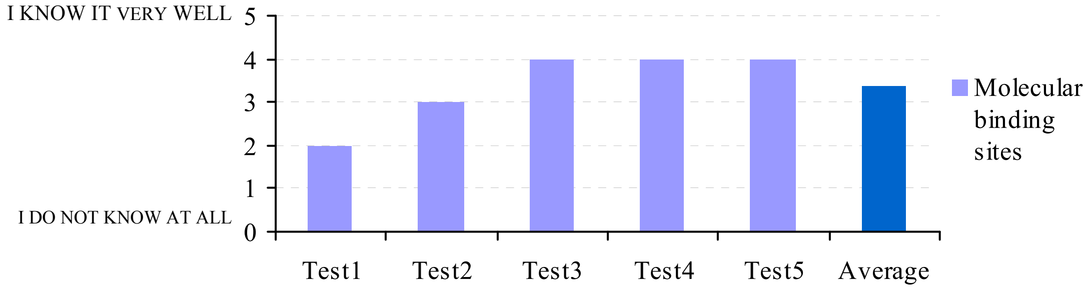
Completion of the task: All the participants were able to complete the task and find the critical points.

Time to complete: The mean of the task completion time was 14 minutes with standard deviation 8.69. Some of the participants used this task to explore and to get accustomed with the haptic device and the virtual environment therefore the time spent on the task is on average higher compared to the subsequent tasks (Graph 4.14). For the consecutive test sessions the demo application was used so that participants could get acquainted with the device. Also the evaluation process itself was adjusted. Therefore the time to complete this task considerably decreased for the consecutive test sessions after Test1 (Graph 4.4).

The results also show that for the students with better concepts' knowledge it took on average less to complete the task: the Graph 4.4 and Graph 4.5 show respective measurements once the rated knowledge is higher the time to complete is below the average completion time and the Test3 participant has the least completion time.

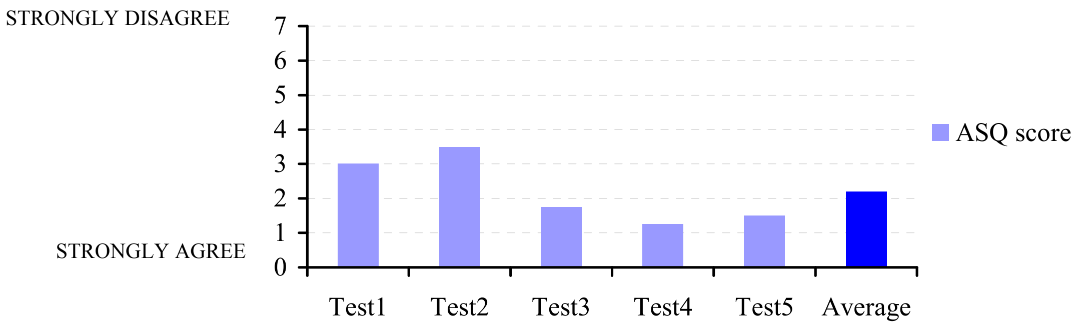


Graph 4.4. Time to complete (min) Task 1 for each test session and average for all sessions.



Graph 4.5. Participant's knowledge scores for molecular binding sites.

ASQ score: The mean ASQ score is 2.2 with standard deviation 0.89 which is a good overall indicator (Graph 4.6), however it is higher than the one for the consecutive tasks. Compared to the time to complete (Graph 4.4) and concept's knowledge (Graph 4.5) the ASQ scores tend to be lower (better) for the participants with better knowledge and less time to complete the task.



Graph 4.6. Average ASQ scores of the Task 1.

The Table 4.3 shows the detailed results of the above described measurements – ASQ score, Time to complete and shows whether the task was completed or not.

Table 4.3. ASQ score, Time to complete and 'Completed?' results of Task 1.

Description	Average	Test1	Test2	Test3	Test4	Test5
ASQ score	**2.2**	3	3.5	1.75	1.25	1.5
Time to complete (min)	**14**	30	15	5	8	12
Completed?*	**1**	1	1	1	1	1
** 1: yes, -1: no, 0: partially*						

Observations:

The Graph 4.15 based on the Table 4.4 gives users feedback overview about the visual and haptic features of the framework. For this task all of the users found very useful the "van der Waal's" molecule visualization, the "Force graph" and the haptic feedback. This figure also indicates that the problematic features were colors of the molecule and the "Force lines".

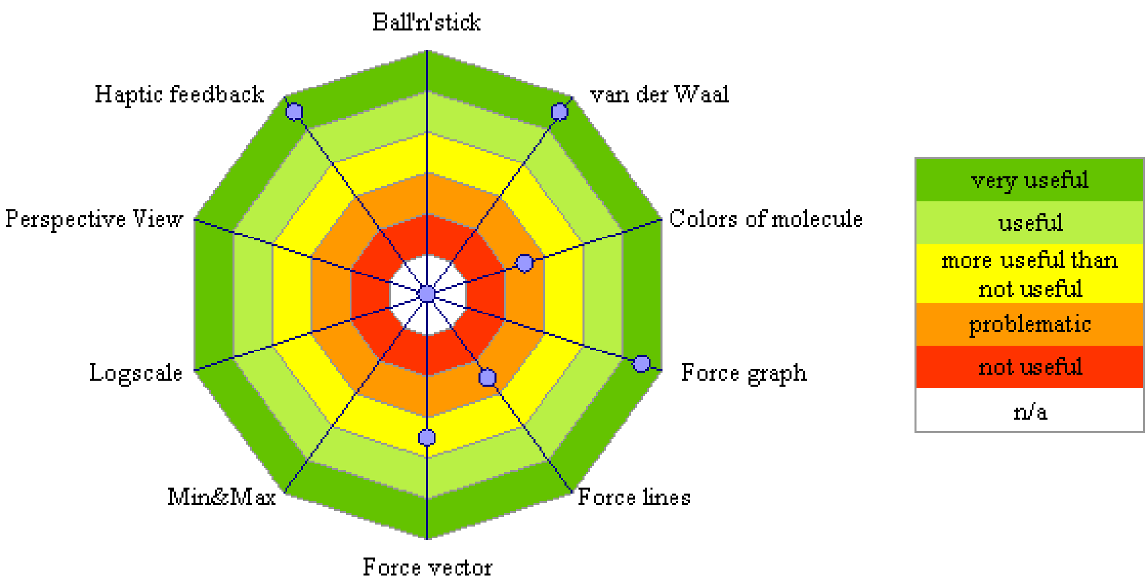


Figure 4.1. Feedback of the users about haptic-based framework features for Task 1.

The detailed feedback is summarized in the Table 4.4. where relevant user comments are included as well. For some of the features though there was no feedback from the users since they were not used during the task.

The comments of the participants were regarding the colors of the molecules which according to them were misleading, but the "Force lines" were mainly not useful or difficult to understand.

Table 4.4. Feedback of the users about haptic-based framework features – results for Task 1.

	Test 1	Test 2	Test 3	Test 4	Test 5	Average
Molecule visualization						
Ball'n'stick	not used	not used	not used	not used	not used	n/a
Van Der Waal	useful	useful (forms the idea of the structure of the field)	useful	useful	useful	very useful
Colors of the molecule	no feedback	misleading	no feedback	no feedback	misleading	problematic
Show Info						
Force Graph	useful	useful	useful	useful	useful	very useful
Force Lines	not useful	not useful	useful (if explained)	not useful (difficult to understand)	useful	problematic
Force Vector	useful (first few minutes)	useful (helps to understand direction)	not useful	useful	not useful	more useful than not useful
Min & Max	useful	no feedback	no feedback	no feedback	no feedback	n/a
Perspective view	useful	no feedback	no feedback	no feedback	no feedback	n/a
Haptic feedback						
	useful	helps to find the region only, but not the specific points	useful (mostly relied on this feedback)	useful	useful	very useful

Main problems:

The problems observed and mentioned by the users while performing the first task are presented in the Table 4.5 below. Most of the problems were related to the spatial location of the haptic device proxy and the usage of the device even though it was indicated as a very useful feature, too. Several semiotics related problems were discovered: meaning of the points in the graph, which is the charge of the tip, colors of the molecule etc. The haptic feedback was not fully reliable as well for some of the users - too far from the molecule might become misleading as if it is the critical point.

Table 4.5. Problems indicated by the users during Task 1.

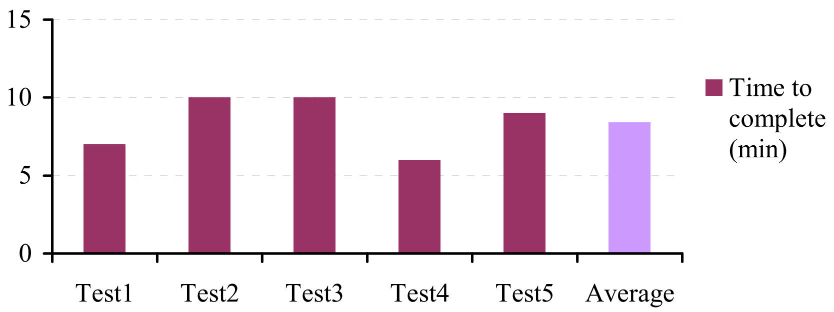
Category	Problem description
Cognitive	C1: Too much information at once (haptic feedback and all the visual elements).
Graphics	G1: Force lines are difficult to understand.
Haptic	H1: Difficulties to understand location in a 3D space. H2: Hard to understand the direction of 3D arrow of the force vector. H3: The user was mostly behind the molecule (not seeing the tip), not straight forward understandable how to move the tip to the front of the molecule. H5: User is expecting to use buttons on Phantom to move/rotate molecule. H6: Difficulties to adjust the haptic device after changing the location of the molecule. H7: In some cases appear the strong vibrations of the haptic device changing the force intensities or when approaching the molecule closer.
Semiotics	S1: Not obvious the meaning of the points in the graph (yellow and green). S2: Not obvious which is the charge of the tip. S3: Not obvious the meaning of the colors of the molecule. S4: When tip is too far from the molecule user inquired why she cannot see the graph. S5: Being too far from the molecule can be misleading as if it is a critical point.

4.2.2. Results of Task 2: Dipoles

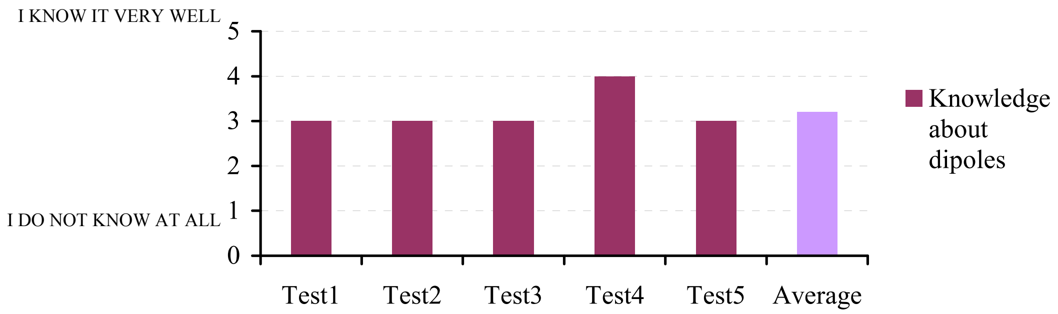
Topic of the task: Dipoles using molecule of water.

Completion of the task: All of the participants completed the task successfully.

Time to complete: The average of the task completion time was 8.4 minutes with standard deviation 1.62 (Graph 4.7) and it is almost a half of the average time to complete the first task (Graph 4.14). The least time it took for the participant Test4 who also rated the knowledge about the concept slightly higher compared to others. The participant Test3 had the average performance, but Test1 had a good performance in this task when compared to the previous task.

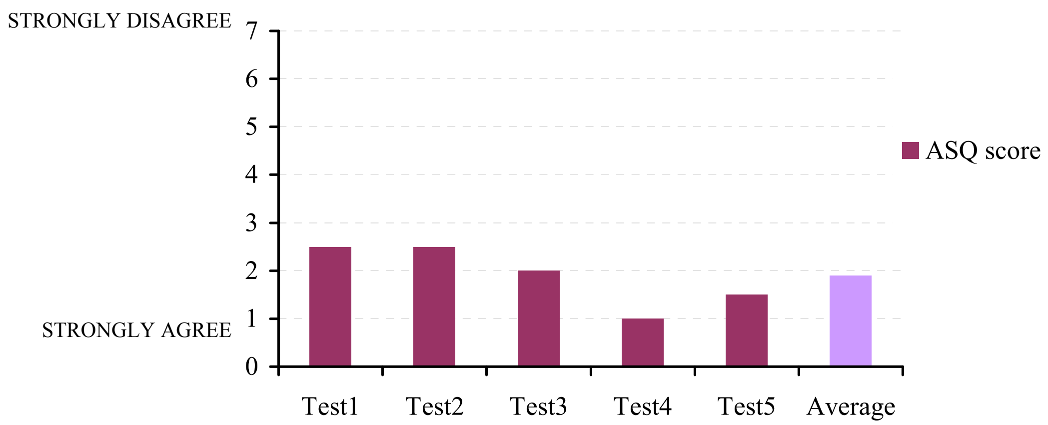


Graph 4.7. Time to complete (min) Task 2 in each test session.



Graph 4.8. Participant's knowledge about dipoles.

<u>ASQ score</u>: The average ASQ score 1.9 with the standard deviation 0.58 is smaller than for the first task indicating on average higher user satisfaction with different aspects of the framework (Graph 4.9). Similar to the first task when observing the results of the participant Test4 they show that the higher knowledge (Graph 4.8) about the related chemistry concept seems to decrease the time to complete the task and gives lower (better) ASQ score.



Graph 4.9. Average ASQ scores for Task 2.

In the Table 4.6 the detailed results of the above described ASQ score, Time to complete and the task completion indicator are summarized.

Table 4.6. ASQ scores, Time to complete and 'Completed?' results of Task 2.

Description	Average	Test1	Test2	Test3	Test4	Test5
ASQ score	**1.9**	2.5	2.5	2	1	1.5
Time to complete (min)	**8.4**	7	10	10	6	9
Completed?*	**1**	1	1	1	1	1
** 1: yes, -1: no, 0: partially*						

Observations:

The Figure 4.2 based on Table 4.7 summarizes user's feedback about different framework features which shows that in this task the most useful ones were the haptic feedback, "van der Waal's" visualization and the "Force lines" even though in the previous task they were indicated as being problematic.

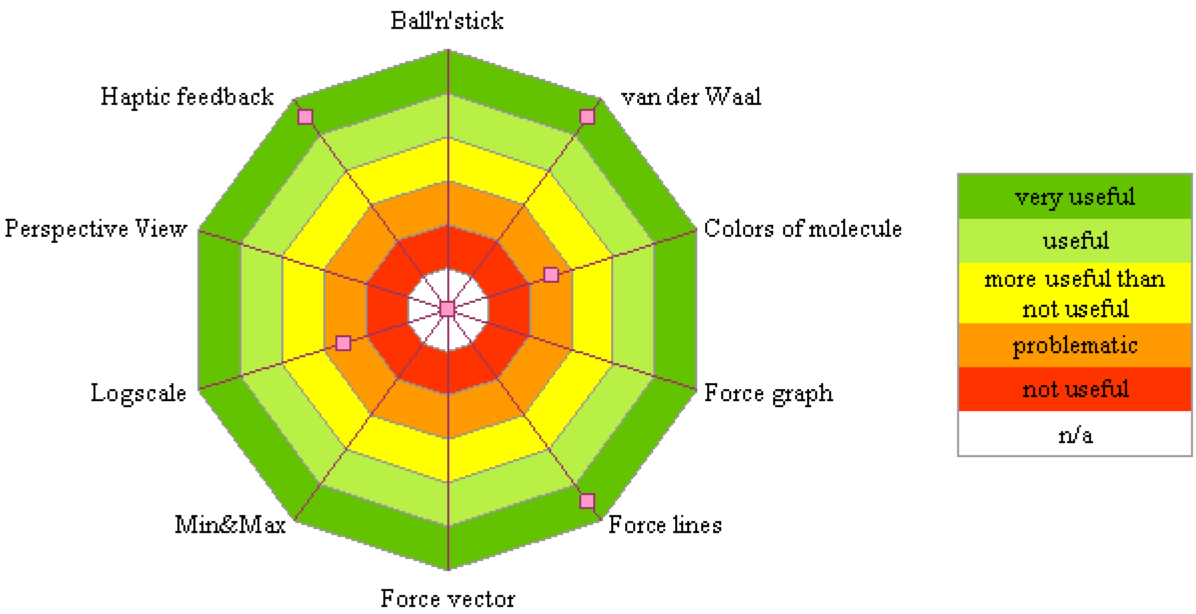


Figure 4.2. Feedback of the users about haptic-based framework features for Task 2.

The Table 4.7. gives more detailed summary of users' feedback with detailed comments for the problematic features – "Logscale" and colors of the molecule. The main problem related to "Logscale" was the considerable decrease in the force feedback which was not expected and confusing for the user. For the "Force Graph", for instance, the feedback from two different participants was the opposite. The colors of the molecule still remained misleading or not so useful.

Table 4.7. Feedback of the users about haptic-based framework features – results for Task 2.

	Test 1	Test 2	Test 3	Test 4	Test 5	Average
Molecule visualization						
Ball'n'stick	no feedback	no feedback	no feedback	no feedback	useful	n/a
Van Der Waal	useful	useful	useful	useful	useful	very useful
Colors of the molecule	misleading	no feedback	not so useful	no feedback	no feedback	problematic
Show Info						
Force Graph	no feedback	no feedback	less useful than lines	useful	no feedback	n/a
Force Lines	no feedback	useful	useful	most useful	useful	very useful

	Test 1	Test 2	Test 3	Test 4	Test 5	Average
Force Vector	no feedback	no feedback	no feedback	useful	no feedback	n/a
Logscale	useful, but problematic due to weaker force feedback	useful, but problematic due to weaker force feedback	no feedback	no feedback	problematic due to weaker force feedback	problematic
Haptic feedback						
	useful	useful (only haptic is enough to understand the forces)	useful	useful	useful	very useful

<u>Main problems</u>:

The main problem highlighted by most of the participants during this task was related to the force feedback change with the "Logscale" visualization – it became weaker and therefore harder to detect. Also the information conveyed by colors in the "Logscale" visualization was not straight forward understandable for several participants (Table 4.8.).

Table 4.8. Problems indicated by the users during Task 2.

Category	Problem description
Semiotics	S6: The colors of the "Logscale" visualization seem to indicate repulsion/attraction areas therefore they are not so intuitive.
Graphics	G2: Black color in the molecule makes association with the transparency in the molecule due to black background.
Haptic	H8: The "Logscale" visualization of the molecule changes also the force feedback – it becomes weaker and therefore harder to perceive. H9: Determining the position of the cursor in the space.

<u>Comments from the participants:</u>

"*It is easier to understand the force field by repulsion instead of attraction nevertheless the attraction areas are easier to find since you are guided to them/attracted immediately.*"

"*The "Force lines" are like ways to attraction/repulsion and makes easier discovery of the force field.*"

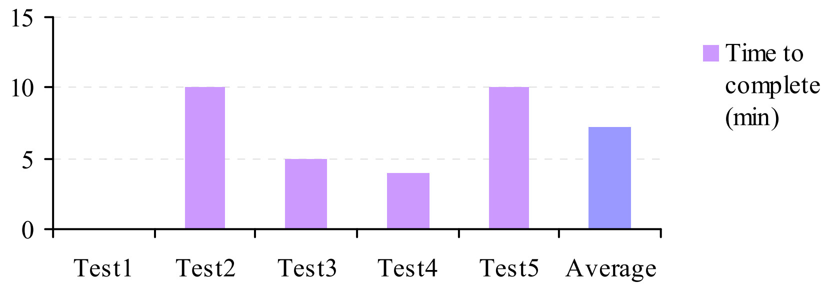
4.2.3. Results of Task 3: Anisotropy

Even though during this task there were discovered the problems with the molecule visualization (the colors were not fully correct) several considerable points were made by the users and some of the participants managed to complete the task mainly using the haptic feedbacks.

Topic of the task: Anisotropy using the molecule of Carbon Dioxide.

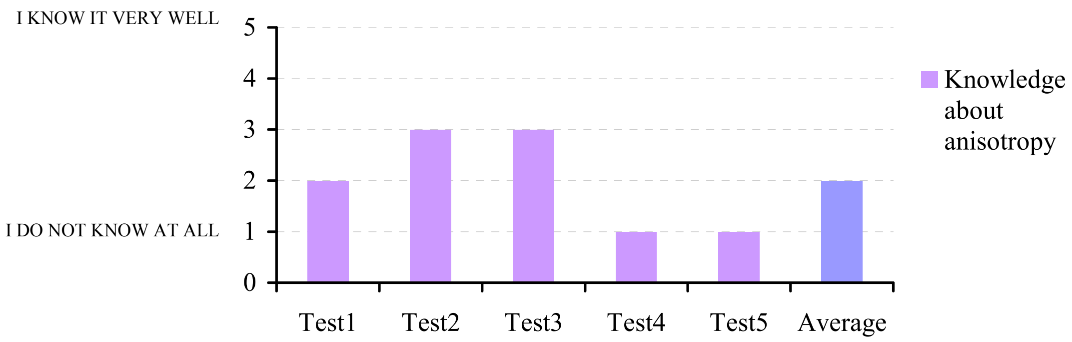
Completion of the task: 4 out of 5 participants managed to complete the task, one of the participants completed the task only partially.

Time to complete: On average it took around 7.25 minutes with standard deviation 4.08 to complete the task (Graph 4.14) which is the least time compared to the previous tasks in spite of problems with the molecule visualization. The least time to complete was for the Test4 participant (Graph 4.10). The Test1 participant's time to complete was not considered since the task was completed only partially.



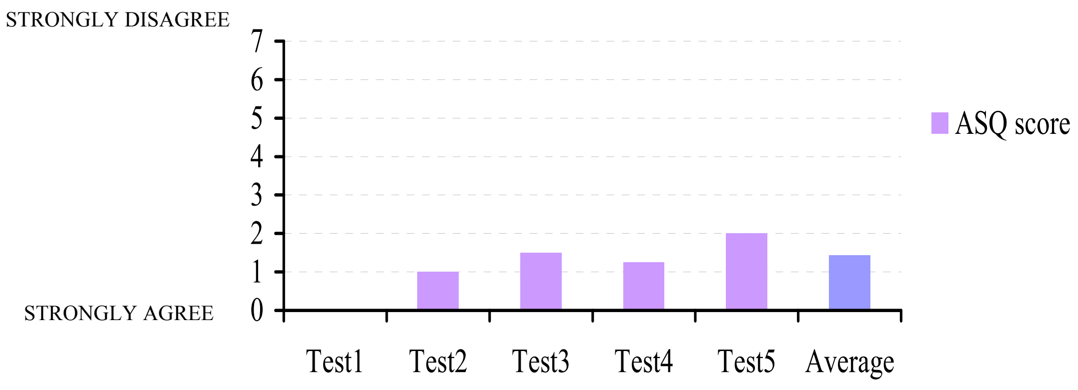
Graph 4.10. Time to complete (min) Task 3 in each test session.

Comparing the completion time to the knowledge about the related concept (Graph 4.11) there is no particular dependency observed: Test2 has higher completion time, but also the score of the knowledge is comparatively higher, nevertheless for Test4 participant both the completion time and knowledge scores are low (comparing Graph 4.10 and Graph 4.11).



Graph 4.11. Participant's knowledge about anisotropy.

ASQ score: The average ASQ score (Graph 4.12) is 1.44 with the standard deviation 0.37 was smaller compared to the previous tasks (Graph 4.15).



Graph 4.12. Average ASQ scores for Task 3.

The Table 4.9 shows the detailed results of the completion time, ASQ scores and whether the task was actually completed.

Table 4.9. ASQ scores, Time to complete and 'Completed?' results of Task 3

Description	Average	Test1	Test2	Test3	Test4	Test5
ASQ score	**1.44**	n/a	1	1.5	1.25	2
Time to complete (min)	**7.2**	7	10	5	4	10
Completed?*	**1****	0	1	1	1	1
** 1: yes, -1: no, 0: partially* *** here the average is rounded to the nearest integer value*						

Observations:

This summary does not include the results of the first test session since the task was completed only partially and there was not enough feedback to summarize.

The Figure 4.3 based on Table 4.10. summarizes user's feedback about different framework features which shows that for this task the most useful ones were again the haptic feedback and the "Force lines", but the "Logscale" was again indicated as being problematic and "Force vector" features was not useful.

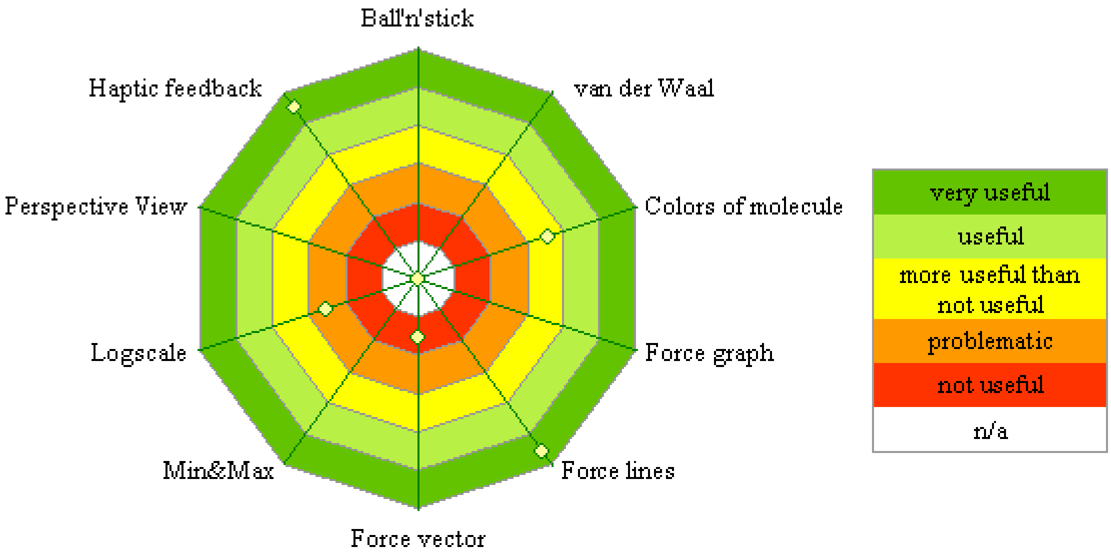


Figure 4.3. Feedback of the users about haptic-based framework features for Task 3.

The Table 4.10. shows more detailed information about users' feedback and for some cases where applicable also the comments of the users.

<u>Comments from the participants:</u>

Force lines attract the main attention since they are in the middle of the screen and therefore are used in order to discover the force field.

It is easier to understand the forces if the cursor is visible (not behind the molecule).

Table 4.10. Feedback of the users about haptic-based framework features – results for Task 3.

	Test 2	Test 3	Test 4	Test 5	Average
Molecule visualization					
Ball'n'stick	no feedback	no feedback	useful	no feedback	n/a
Van Der Waal	no feedback	no feedback	no feedback	useful	n/a
Colors of the molecule	confusing	attracts attention to discover their meaning	useful	useful	more useful than not useful
Show Info					
Force Graph	no feedback	only for extra information	useful	no feedback	n/a
Force Lines	no feedback	useful	useful	useful	very useful
Force Vector	no feedback	not useful	not useful	no feedback	not useful
Logscale	colors are confusing	no feedback	useful	no feedback	problematic
Haptic feedback					
	useful	useful	useful	useful	very useful

Main problems:

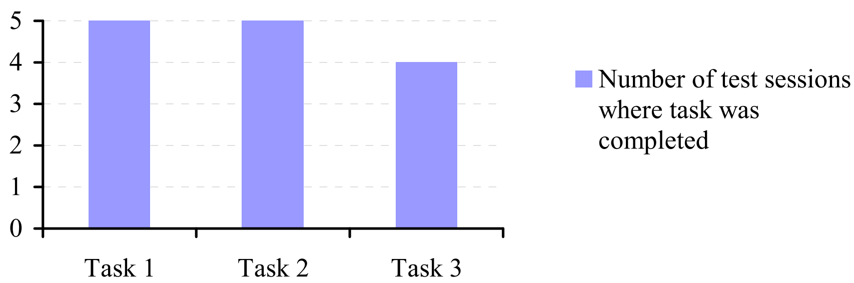
The Table 4.11. gives the summary of the problems discovered after the Task 3. The problems from the previous tasks are not included here. This task revealed one more problem related to graphics and two the haptic feature related problems. An interesting observation was that the user tried to overcome the repulsion feedback using force which could cause the damage of the haptic device.

Table 4.11. Problems indicated by the users during Task 3.

Category	Problem description
Graphics	G3: Arrows of the Force lines are not enough visible and therefore makes it harder to understand the actual direction.
Haptic	H10: Difficult to perceive the distance from the cursor to the molecule this makes it difficult also to perceive the force field. H11: The repulsion feedback in some cases might invite the user to try to resist it till the extent that can cause the damage of the haptic device.

4.2.4. Summary

Completion of tasks: Only during the first test session the Task 3 was completed partially due to technical issues with the framework, during all the other test sessions all the tasks were completed successfully (Graph 4.13).



Graph 4.13. Number of test sessions where tasks were completed.

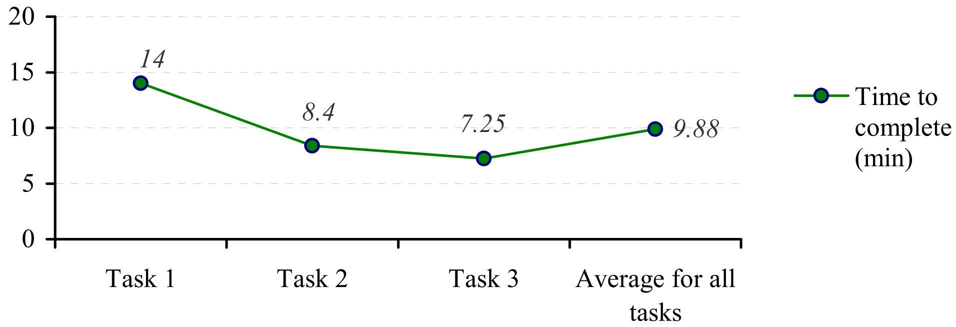
The details for each of the test session are given in Table 4.12.

Table 4.12. Summary of test sessions results

	Task 1			Task 2			Task 3		
	ASQ score	Time to complete (min)	Comp-leted?*	ASQ score	Time to complete (min)	Comp-leted?*	ASQ score	Time to complete (min)	Comp-leted?*
Test1	3	30	1	2.5	7	1	n/a	n/a	0
Test2	3.5	15	1	2.5	10	1	1	10	1
Test3	1.75	5	1	2	10	1	1.5	5	1
Test4	1.25	8	1	1	6	1	1.25	4	1
Test5	1.5	12	1	1.5	9	1	2	10	1
Average	**2.2**	**14**	**1**	**1.9**	**8.4**	**1**	**1.44**	**7.25**	**1**
SD**	0.89	8.69		0.58	1.62		0.37	4.08	
Average Time to complete for all tasks:				9.88 (SD=2.95)					

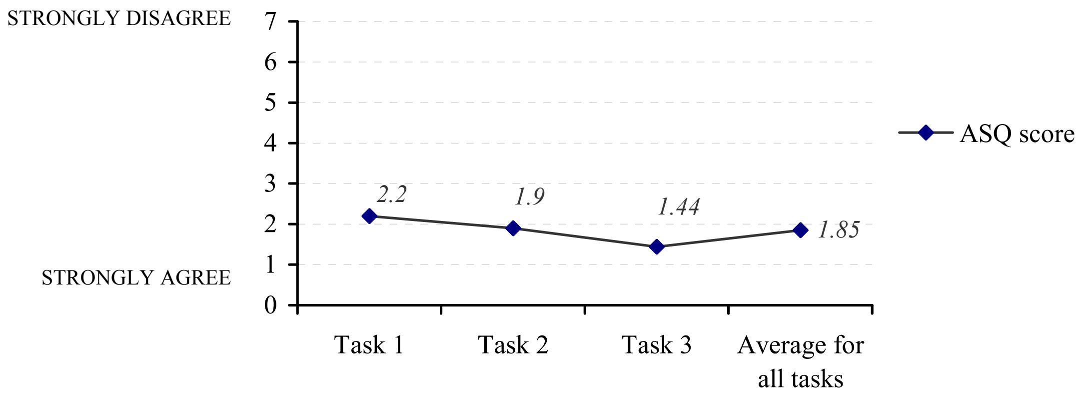
** 1 – Yes, -1 – No, 0 - Partially*
*** - SD – Standard deviation*

Time to complete: As it was already discussed before – it took on average more time to complete the Task 1 because it was used to get acquainted with the framework. Nevertheless the average time to complete decreased with each consecutive task which indicates that users are becoming more efficient with the framework (Graph 4.14). The average of all tasks is 9.88 with standard deviation 2.95. The detailed results are included in the Table 4.12 the results of Test1 for the Task 3 are excluded from the evaluation.

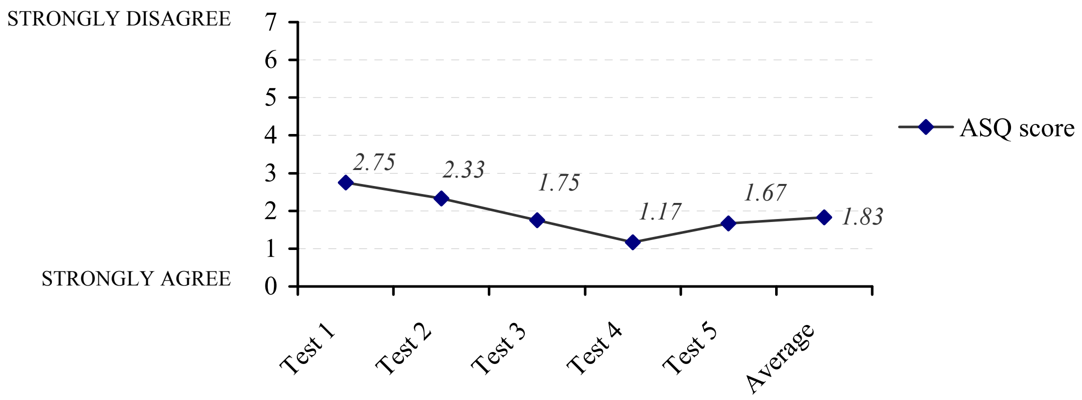


Graph 4.14. Average time to complete (min) grouped by tasks.

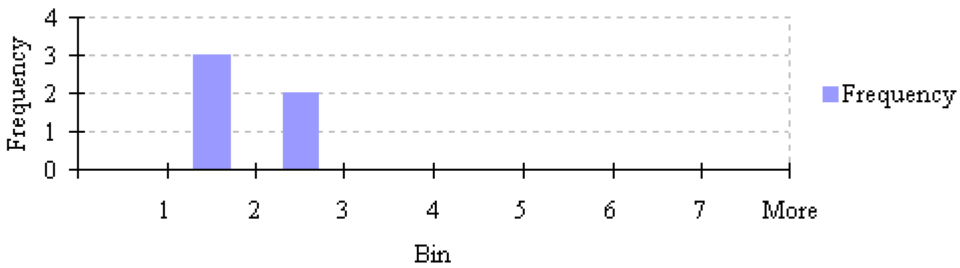
ASQ score: Also the average ASQ score decreases with each of the task showing that users are becoming more satisfied with different aspects evaluated by ASQ. The average ASQ score for all tasks is 1.85 with standard deviation 0.31 (Graph 4.15). The result of Test1 for the Task 3 is excluded from the evaluation. The Graph 4.16. Average ASQ scores for the tasks by test participants.Graph 4.16 presents the average ASQ scores for all tasks grouped by test participants and the Graph 4.17 gives the histogram of these score results which shows that all ASQ scores fall into interval [1; 3].



Graph 4.15. Average ASQ scores by the tasks.



Graph 4.16. Average ASQ scores for the tasks by test participants.



Graph 4.17. Histogram of average ASQ scores for the tasks by test participants.

The summary users' feedback about different framework features (Figure 4.4) show that the most useful was haptic feedback, "van der Waal's" molecule visualization, "Force lines" and "Force graph". In most of the cases the "Logscale" and the colors of the molecules were indicated as problematic. The "Force vector" in some cases was not useful, but in Task 1 it was indicated as problematic.

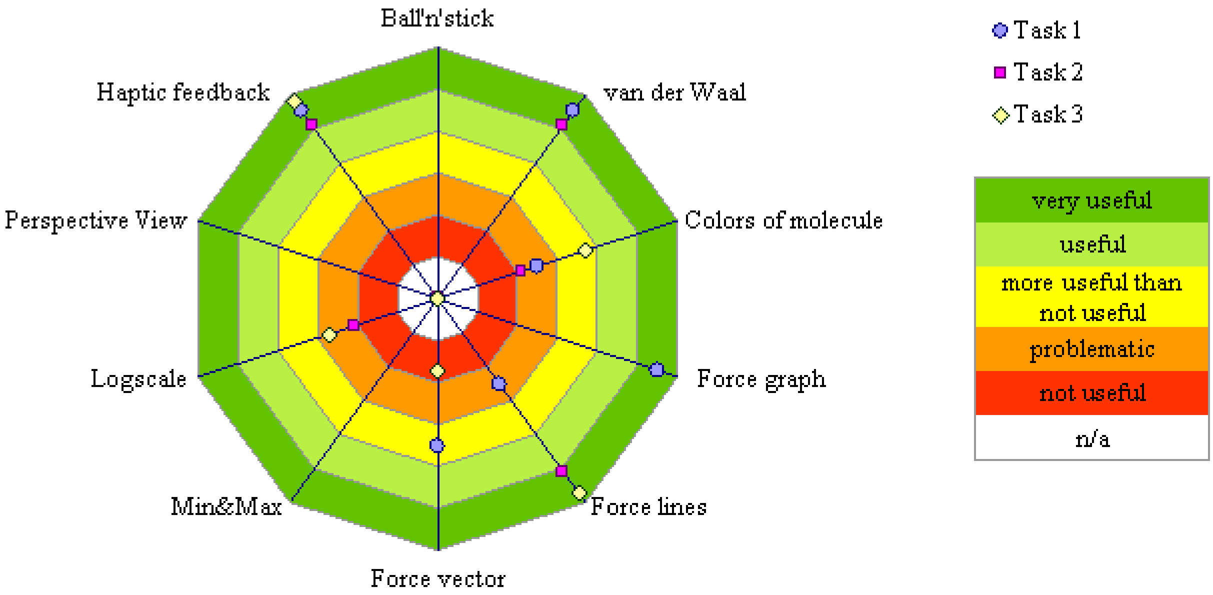
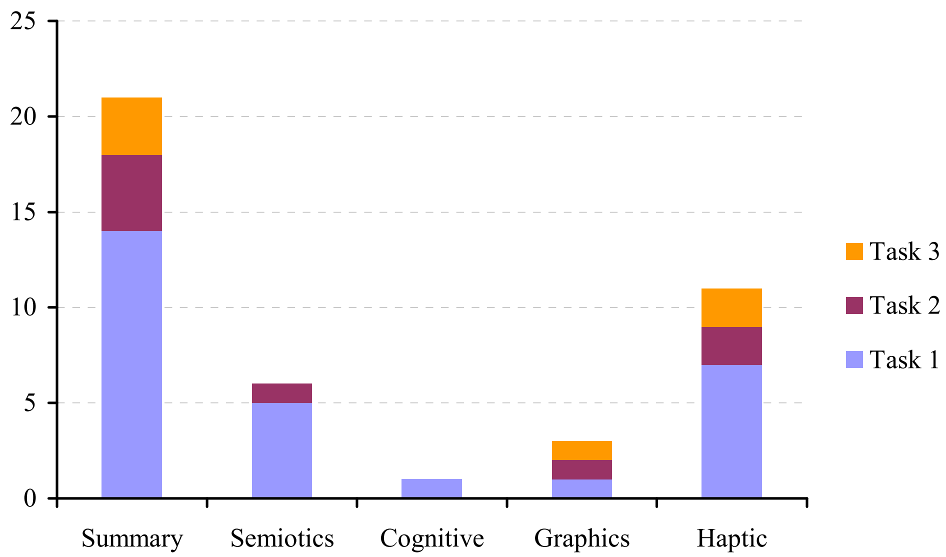


Figure 4.4. Summary users' feedback about haptic-based framework features.

Overall 21 different problems were discovered during usability testing. The Graph 4.18 gives the summary counts of the problems that were discovered during all of the tasks. The major part of the problems was discovered during the first task when compared to the subsequent tasks. Most of the problems are related to semiotics and haptic feedback even though the haptic feedback was indicated as very useful feature of the framework.

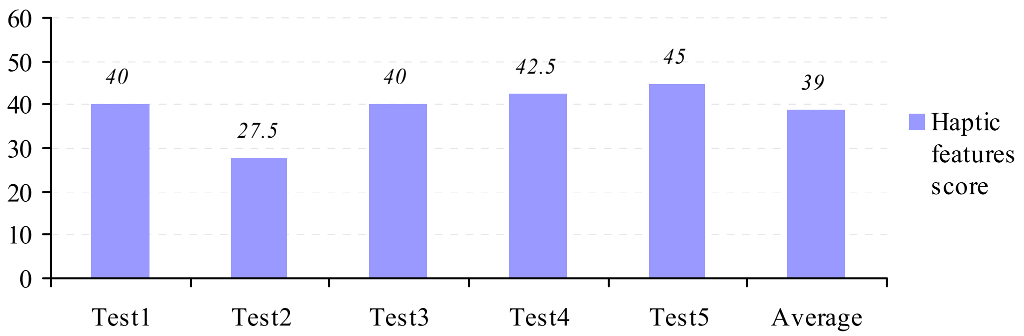


Graph 4.18. Number of problems discovered by groups and by tasks.

4.3. Post-questionnaire results

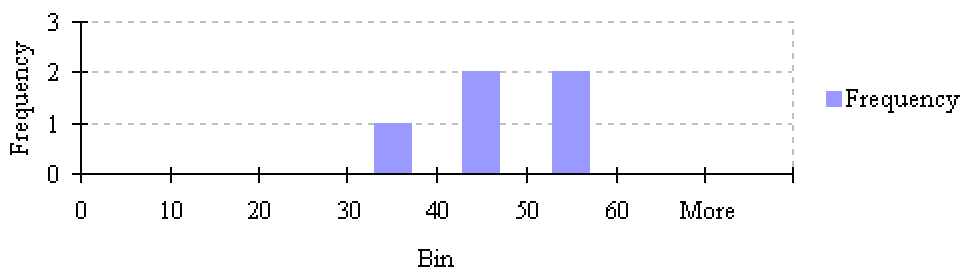
4.3.1. Haptic features of the framework

The average score of the haptic features is 39 which is above mean score and shows that the participants found the haptic features of the framework useful (Graph 4.19). The least score was given by the Test2 participant. It took for him on average longer to complete the tasks. He was also the only participant who in the pre-questionnaire results indicated using chemistry related software. The scores given by other participants do not differ considerably. Interesting to note the highest score was give by the participant Test5 whose average completion time was also above average for each of the tasks. The ASQ scores of the participants Test2 and Test5 differed for the Task1 and the Task2: for the Test5 those were considerably lower (better) than the average among all participants.



Graph 4.19. Post-questionnaire results - haptic features score.

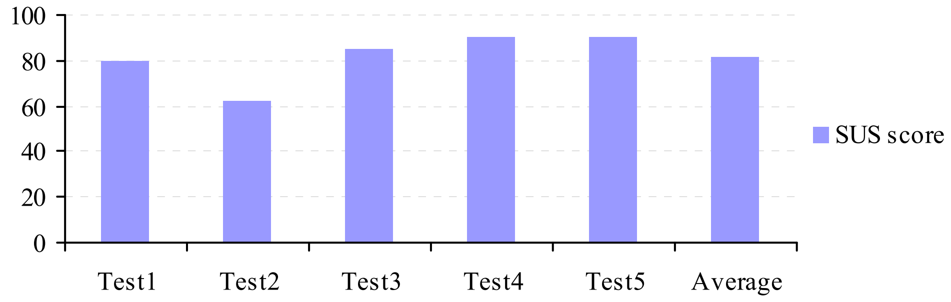
The Graph 4.20 presents the histogram of the haptic features scores and shows that the distribution does not hold the normality condition.



Graph 4.20. Histogram of haptic features scores.

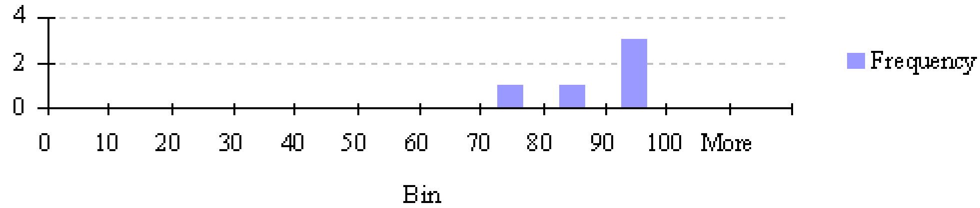
4.3.2. General features of the framework

The Graph 4.21 shows the SUS score of each participant. Again the least score was given by the participant Test2, but the highest by the participant Test5.



Graph 4.21. Post-questionnaire results - SUS scores by participants.

In the Graph 4.22 the histogram of the SUS scores is presented – all of the scores are between 70 and 100.



Graph 4.22. Histogram of the SUS scores by participants.

The overall SUS score is 81.5 which falls into the acceptability range of the usability of applications and it is even higher than the mean score (76.2) of graphical user interfaces [31] that were evaluated by SUS (Figure 4.5).

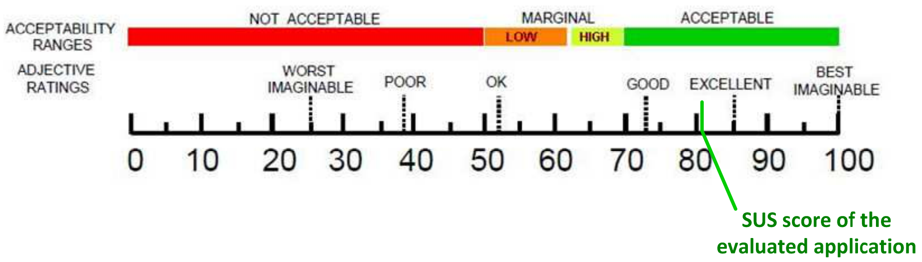
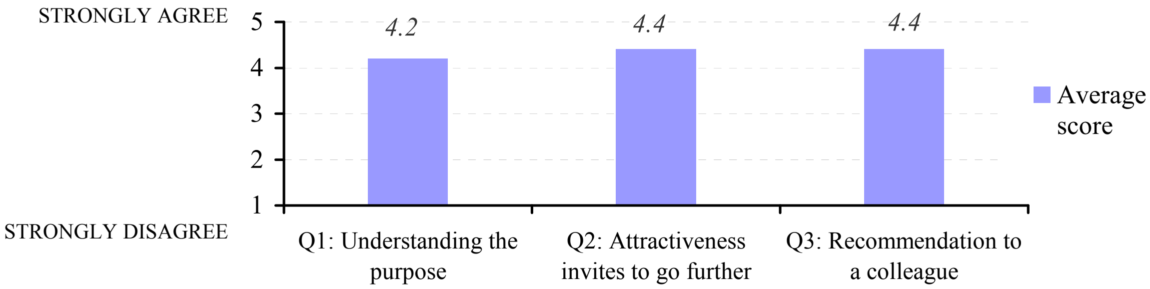


Figure 4.5. Post-questionnaire results - SUS score on the Acceptability ranges scale.

The participants rated the user-friendliness of the framework on average *Good*, too, which corresponds to the results of the SUS score.

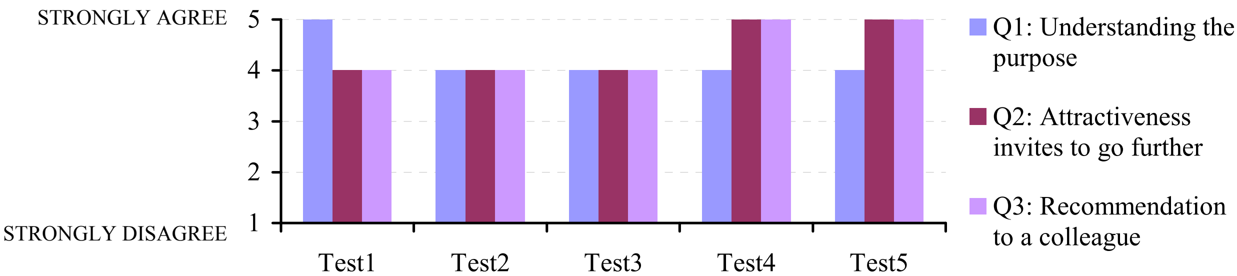
4.3.3. Final feedbacks

Also the average score of the final feedbacks is very high (4.3/5) which shows that the users have understood the purpose of the application, it was attractive for them and they would even recommend it to the colleagues. The detailed average scores by the questions are shown in the Graph 4.23, but the detailed scores by participants are included in Graph 4.24.



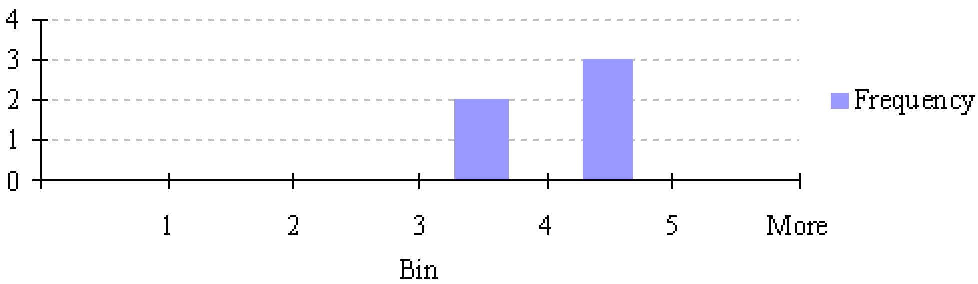
Graph 4.23. Post-questionnaire results - average scores of final feedbacks by questions.

Even though the haptic features and SUS scores were comparatively lower for the Test2 participant the final feedback scores did not considerably differ from those given by other participants (Graph 4.24).



Graph 4.24. Post-questionnaire results - average scores of final feedbacks by questions and participants.

In the Graph 4.25 the histogram of the final feedbacks scores is presented – all of the scores are between 3 and 5.



Graph 4.25. Histogram of final feedbacks detailed scores by participants.

The Table 4.13 shows the detailed haptic features and SUS score of the test sessions and the respective average scores, the score of the user friendliness is included as well. The participant Test1 gave the least user friendliness rating. He also rated his concepts' knowledge the least and during the Task 3 the technical issues with the tool were experienced which might have affected this given rating.

Table 4.13. Post-questionnaire results – detailed scores by participants.

	Test1	Test2	Test3	Test4	Test5	Average
Haptic features score	40	27.5	40	42.5	45	**39**
General features of the application (SUS score)	80	62.5	85	90	90	**81.5**
Overall rating of user friendliness	Poor	Good	Good	Excellent	Excellent	

The Table 4.14 gives an overview of the final feedbacks scores and their averages. All the answers of the participants were close to 'Strongly Agree' (5).

Table 4.14. Post-questionnaire results – final feedbacks detailed scores by participants.

Final feedbacks questions:	Test1	Test2	Test3	Test4	Test5	Average
Q1: understanding	5	4	4	4	4	**4.2**
Q2: attractiveness	4	4	4	5	5	**4.4**
Q3: recommendation	4	4	4	5	5	**4.4**
Final feedbacks average scores	**4.33**	**4**	**4**	**4.67**	**4.67**	**4.33**

4.4. Discussion and recommendations

The initial evaluation with the users shows good results. The students were very excited to use the tool and for some of them it helped to understand better the molecular force field topic by integrating both visual and haptic perceptions. In the task where the visualization of a molecule had some problems the users completed the task relying more on haptic feedback of the application. This points out that the haptic feedback is very useful in such applications, but since this haptic device started to be produced only recently it still causes some uncertainties in how to use it.

The valuable features of the application are the molecule visualization options and the available additional information options (Figure 3.2). The molecule visualization options give to the user the possibility to choose the most useful option for each of the tasks; for instance, - even though "van der Waal's" option was indicated as most useful one - in some cases it can create visual occlusions (section 2.5.2.), but in such cases the visualization can be changed to another.

During the analysis of the pre-questionnaire data it was observed that the participants can be grouped by gender (male, female) and by prior knowledge average scores (>2.5 and <2.5) in order to further analyze the haptic and general features scores (Table 4.13), ASQ average scores for all tasks (Graph 4.16) and final feedbacks score (Table 4.14) using the ANOVA method [100]. Nevertheless the normal distribution of the results was not achieved which is shown in the histograms of the respective scores (Graph 4.17, Graph 4.20, Graph 4.22 and Graph 4.25) and therefore the ANOVA analysis was not performed for the collected data.

Some aspects of the tool need improvements in order to provide better user experience and to avoid wrong conclusions. The whole list of the problems that were discovered during this evaluation is included in ANNEX 7, but the most common problems and the possible solutions for them are discussed further in this section.

1. The 3D space visualization problem.

The main problem related to the space visualization is: it is hard for a user to understand the spatial location of the proxy of the haptic device. This problem seems to appear mainly due to the black background in the application's virtual environment where the 3D molecule is shown (Figure 3.2).

During the usability evaluations while discussing with the users as a solution appeared the idea of enhancing the application with the virtual 3D background instead of the current black one.

The developers of HMolDock were facing the similar problem and solved it through creation of 3D coordinate grid in the 3D space (Figure 2.7). Nevertheless the author was not able to find information whether this solution facilitates the usability of the application.

Another example of successful 3D space implementation is Google SketchUp [101] –the application for 3D modeling. An example screenshot of Google SketchUp is in Figure 4.6, where one can distinguish the ground from the sky, but the red, blue and green axes create a metaphor of 3D space making it easier to perceive the position of the mouse pointer.

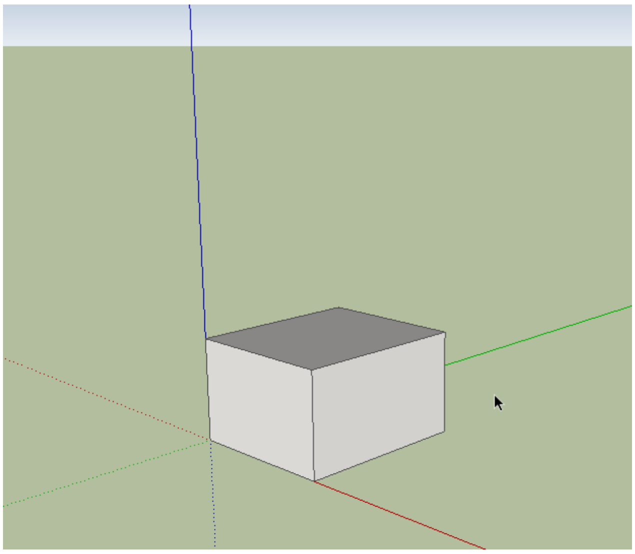


Figure 4.6. Screenshot of Google SketchUp.

2. The force information conveyed through colors.

The color information was not straight forward to the users mainly due to the fact that the explanation bar of the colors on the right of the application's window remained unnoticed.

The possible solution for this problem can be a short video demonstration of the application that explains the main features and metaphors of the application. In more detail this solution is discussed further.

3. The '*Logscale*' feature.

The wider variety of the colors and the decrease of the force feedback confused the users and they were not sure how exactly to use this feature.

The possible solution for overcoming this problem can be the same as for the problem above – a short video demonstration describing this feature.

4. The accuracy of the force feedback information.

Some of the users thought that being far away from molecule and not feeling any force is also a critical point.

This problem can be solved by giving a warning message to the user that s/he is situated outside of the force field.

5. The haptic related problems.

Most of the problems can be solved with user tutorials explaining better the haptic metaphors used.

The "Logscale" feature problem can be solved with the prompt message about the force decrease; it should have the "Do not show this message again" as well in order to avoid annoying the user each time she chooses the "Logscale" feature.

The problems related to 3D space location were discussed earlier in this section in point 1.

The strong vibration of the haptic device is a common problem of haptic-based applications for molecular force studies when there are changes in intensity of forces and at the same time considering the weak and the strong force feedbacks. This problem is also discussed in [5] and [92]. In [5] the '*History Dependent Transfer Function'* is described which was motivated by "*the challenge of delivering good force feedback for the full range of interactions*": from weak to strong force feedback, but in [92] the '*Linear smoothing method'* is discussed in order to solve the vibration problems. Both of these methods can be considered in order trying to solve the force feedback problems discovered in terms of this evaluation.

Short video tutorials as a user guide.

Nowadays one of the successful approaches of the user manuals is short video tutorials that are used to show the main features of the applications through their usage and explanations. That helps a user to quickly understand the main features of the application and to start using it for the scenarios that users have in mind. The examples of the similar videos can be found in the Internet where such approaches are used for wide range of application, for instance, already mentioned above Google SketchUp has training through video tutorials [101]. These tutorials are usually short – not more than 10 minutes.

As the results of the evaluation indicate - some of the features for the particular tasks were more useful than the others and on the contrary some of the features caused the confusion in the users. Therefore the author suggests creating the short video demonstrations for each of the tasks from usability evaluation. That could help also during the chemistry courses once the application is introduced. One of the video tutorials could introduce all the main features of the application, but the consecutive tutorial could should the approaches for critical point detection using 'Van Der Waal' visualization and information conveyed through 'Force Graph' and 'Force Vector' and the dipoles feature study using 'Van Der Waal' molecule visualization and 'Force Lines' (these settings were found most useful during the usability evaluation).

According to the users feedback the introduction of this application would be beneficial in the chemistry course and would facilitate the understanding of the molecular force interactions. The suggested improvements are not major and can be easy implemented.

Future directions.

During the qualitative analysis of the results some interesting correlations were observed, but further more specific investigation is required to ascertain the related hypothesis. Some of those are discussed here further.

For instance, the participant of the Test2 according to pre-questionnaire results is the only one who indicated to be using the special chemistry software and at the same time gave the least ratings in the post-questionnaire for the haptic features (Graph 4.19) and SUS (Graph 4.21). Therefore the further evaluation can be performed inviting the participants that are using other chemistry related software in order to determine if their prior experience affects the usability evaluation results of the considered haptic-based framework.

The other observed tendency: the participants with the higher rated concepts knowledge scores were also giving better ASQ scores and it took for them less time to complete the tasks. The further evaluation might be designed as well with the goal to distinguish the effect of prior knowledge of the related concepts on the actual usability evaluation results.

In many cases the participants of the evaluation were commenting favorably the visual features of the tool therefore the further studies can distinguish the students also by their learning styles, for instance, according to Fleming's VARK model [102] that distinguishes visual, auditory and tactile learners. The tactile learners might give more favorable evaluation feedbacks compared to the other style learners.

5. CONCLUSIONS AND FUTURE WORK

The usability and haptics concepts, several usability evaluation methods and the non-exhaustive list of visual, haptic-based applications for chemistry education and research were presented and discussed, furthermore where were available the related usability evaluations of these applications were reviewed as well. Based on the described research the usability evaluation for the haptic-based framework for chemistry education developed at Politecnico di Milano was designed and conducted. The main problems faced during the evaluation design process were related to the choice of the most suitable methods and adapting them to the current case due to novelty of this type of applications, very little information available about the relevant usability evaluations and in general one specific method for usability evaluation does not exist.

Methodology.

The usability testing and user questionnaire methods were chosen as the most suitable and adapted to the current evaluation. The most relevant and explicit results were obtained during usability testing using *thinking aloud* protocol. The obtained data was not applicable for the ANOVA analysis [100] due to invalidity of the normal distribution condition.

The obtained questionnaires' results corresponded to the comments and feedback of the users in most cases, but did not reveal the usability problems that were faced while using the framework. In fact some of the questionnaire results were contradictive to the results of usability testing: the haptic feature of the application was indicated as very useful, but at the same time it had the highest number of problems. This shows that even though the questionnaire is a cost-effective method the results can be biased when the users are excited about the application. The obtained questionnaire results can serve as a baseline for further evaluations and indicate the presence of the usability problems if the scores obtained in subsequent evaluations decrease significantly.

The usability testing is a time consuming activity – on average each test session took around 1.5 – 2 hours. It is recommended to video/audio record the test sessions because the written feedback obtained from the users not always reflects all details discussed during the test session. Nevertheless having one more person to take notes during the session is also beneficial and most of the problems can be written down using this approach.

In the future evaluations it is suggested to add more application's feature specific questions in order to obtain more detailed users' feedback about each, for instance, the users can be asked to rate them according to their usefulness while performing the task and to comment their choice.

Usability evaluation results.

The average time to complete the test tasks decreased with each task especially when the first and the second tasks are compared. So with each subsequent task the users learned to use it in more efficient way which is also justified with the ASQ scores given by the participants for each task. The average time to complete a task was around 10 minutes. This result can serve as an indication while planning to integrate the framework in chemistry courses and preparing the tasks for laboratories. One should take into consideration that it is better to design first tasks using as many features of the framework as possible so that users get acquainted with them and can use further in the course, for instance, the Task 1 of the test sessions is a good example. Only the Task 3 in Test1 session was partially completed other tasks were successfully completed.

The results showed also that the very useful features of the framework were molecule visualization, additional information ("Force graph" and "Force lines") and the haptic feedback. The problematic features were "Logscale" due to force decrease and colors of molecules being in some cases misleading. In total 21 different problems were discovered – most of them haptics and semiotics related. The haptic force feedback related problems (force intensities, giving feedback of very strong and very weak forces) are common for this type of applications nevertheless the author did not find a general approach for solving them, only the application specific approaches are discussed in the section 2.5.

The learning gain was not explicitly evaluated in terms of this work; however it is proven to exist according to the results of P. Bivall Persson in [5]. Furthermore the students showed great excitement about the framework and would be ready to start using it during the lectures and laboratories.

Future work.

The qualitative analysis of the results showed interesting correlations among data, but it requires further more exhaustive checks in order to prove these observations with relevant data. For instance, designing the evaluations where participants have wider differences in prior chemistry concepts knowledge or distinguishing them by learning styles (visual, audio or haptic) or a prior experience with other chemistry related software.

This work can be used as a basis for designing the future usability evaluations of the haptic-based frameworks for chemistry education. Furthermore the obtained results can be transformed into the recommendations for developing this type of applications.

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ANNEXES

ANNEX 1

SUS QUESTIONNAIRE EXAMPLE

	Strongly Disagree				Strongly Agree
1. I think that I would like to use this product frequently.	1	2	3	4	5
2. I found the product unnecessarily complex.	1	2	3	4	5
3. I thought the product was easy to use.	1	2	3	4	5
4. I think that I would need the support of a technical person to be able to use this product.	1	2	3	4	5
5. I found the various functions in the product were well integrated.	1	2	3	4	5
6. I thought there was too much inconsistency in this product.	1	2	3	4	5
7. I imagine that most people would learn to use this product very quickly.	1	2	3	4	5
8. I found the product very awkward to use.	1	2	3	4	5
9. I felt very confident using the product.	1	2	3	4	5
10. I needed to learn a lot of things before I could get going with this product.	1	2	3	4	5

11. Overall, I would rate the user-friendliness of this product as:

☐ Worst Imaginable	☐ Awful	☐ Poor	☐ OK	☐ Good	☐ Excellent	☐ Best Imaginable

From [31].

ANNEX 2

PRE-QUESTIONNAIRE

Your ID: ____

E-mail (optional): ____________________________________

Age: ____

Sex: ____ Male ____ Female

Study program: _______________________________________

Year of studies: ___ 1st ___ 3rd ___ 5th

___ 2nd ___ 4th ___>5th

1. Do you use a computer for your study process? _____ Yes _____ No

If – Yes. Please specify how you use it (for example, reading lectures, using special chemistry applications etc):

____

____

2. Do you use any special device and/or software during your study process?

_____ Yes _____ No

If – Yes. Please specify which device and/or software do you use and for which purposes:

____

____

3. How would you rate on the scale 1- 5 your knowledge about the topic of the inter-molecular forces?

I do not know at all 1 … 2 … 3 … 4 … 5 *I know it very well*

4. Rate on the scale 1 - 5 your knowledge about following concepts *(mark an X in the appropriate box)***:**

	1 *I do not know at all*	2	3	4	5 *I know it very well*
Molecular binding sites					
Permanent and instant dipoles					
Molecular anisotropy					

5. How would you rate on the scale 1- 5 your knowledge about haptic devices?

1	2	3	4	5
I do not know at all				*I know it very well*

ANNEX 3

USER'S TEST SESSION FORM

Please complete the following tasks using our tool. Take the notes about any difficulties that you have faced while completing the task.

Your ID: ________________

Task 1: Critical points detection

1. Load the molecule *Benzene*

____

____

____

2. Find the critical points of the electric field that surrounds the molecule

____

____

____

3. Find which parts of the molecule take part in binding

____

____

____

Completed the task: _____ Yes _____ No

After the task:

Please complete the following after performing the task *(for each of the statements below, circle the rating of your choice)*

1. Overall, I am satisfied with the ease of completing this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

2. Overall, I am satisfied with the amount of time it took to complete this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

3. Overall, I am satisfied with the support information (help, messages, documentation) when completing this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

4. Overall, I am satisfied with the use of the haptic device during this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

5. Please, describe which visual elements and information better helped you to perform the required task

6. How such visual elements have been really helpful? Which features of them you really appreciated?

7. Do you think that visual elements helped you in better detecting the force? How?

Task 2: Dipoles

1. Load the molecule *H2O*.

____

____

____

2. Please try to describe its effect when a positive charge is moved around the molecule using our application.

____

____

____

3. Please try to describe its effect when a negative charge is moved around the molecule using our application.

____

____

____

Completed the task: _____ Yes _____ No

After the task:

Please complete the following after performing the task *(for each of the statements below, circle the rating of your choice)*

1. Overall, I am satisfied with the ease of completing this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

2. Overall, I am satisfied with the amount of time it took to complete this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

3. Overall, I am satisfied with the support information (help, messages, documentation) when completing this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

4. Overall, I am satisfied with the use of the haptic device during this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

5. Please, describe which visual elements and information better helped you to perform the required task

6. How such visual elements have been really helpful? Which features of them you really appreciated?

7. Do you think that visual elements helped you in better detecting the force? How?

Task 3: Anisotropy

1. Load the molecule *C2O*.

____
____
____

2. Please try to describe how you can feel the anisotropy of interaction using our application.

____
____
____

Completed the task: _____ Yes _____ No

After the task:

Please complete the following after performing the task *(for each of the statements below, circle the rating of your choice)*

1. Overall, I am satisfied with the ease of completing this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

2. Overall, I am satisfied with the amount of time it took to complete this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

3. Overall, I am satisfied with the support information (help, messages, documentation) when completing this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

4. Overall, I am satisfied with the use of the haptic device during this task

STRONGLY AGREE	1	2	3	4	5	6	7	STRONGLY DISAGREE

5. Please, describe which visual elements and information better helped you to perform the required task

____

____

6. How such visual elements have been really helpful? Which features of them you really appreciated?

____

____

____

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____

7. Do you think that visual elements helped you in better detecting the force? How?

____

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ANNEX 4

POST-QUESTIONNAIRE

Please fill this questionnaire about your experiences with our application. *This input will be* ***invaluable*** *for improving and making our application more useful for the chemistry studies.*

Thank you *for dedicating your time and participating in our usability evaluation!*

We hope that you had an interesting and enjoyable experience during this evaluation!

Haptic features of the application

For each of the statements below, please circle the rating of your choice:

		Strongly Disagree				Strongly Agree
1.	I found it easy to start using the haptic device for this application	1	2	3	4	5
2.	It took some time before I could start using the haptic device in this application	1	2	3	4	5
3.	I think the haptic device is very well integrated with the functionality of this application	1	2	3	4	5
4.	I found it complex to understand how the haptic device works in this application	1	2	3	4	5
5.	I was not sure how to use the haptic device while performing the tasks	1	2	3	4	5
6.	I can easily control how fast I move though the 3D world	1	2	3	4	5

Visual features of the application

For each of the statements below, please circle the rating of your choice:

		Strongly Disagree				Strongly Agree
1.	The use of graphics is appropriate for the software	1	2	3	4	5
2.	The visual elements are not annoying or distracting	1	2	3	4	5
3.	The amount of information shown through visual elements is not excessive	1	2	3	4	5
4.	Visual details are easily understandable	1	2	3	4	5
5.	The information presented is accurate and clear	1	2	3	4	5
6.	Colors are meaningful	1	2	3	4	5
7.	Graphical information is helpful to navigate the space around the molecule	1	2	3	4	5
8.	Someone without any knowledge about this application could easily find how it works	1	2	3	4	5
9.	The software has a navigationally efficient layout	1	2	3	4	5
10.	Menus and GUI widgets are appropriate (i.e., well-designed and easy to use)	1	2	3	4	5

General features of the application

For each of the statements below, please circle the rating of your choice:

		Strongly Disagree				Strongly Agree
1.	I think that I would like to use this application frequently during respective chemistry studies	1	2	3	4	5
2.	I found the application unnecessarily complex	1	2	3	4	5
3.	I thought the application was easy to use	1	2	3	4	5
4.	I think I would need the support of a technical person to be able to use this application	1	2	3	4	5
5.	I found the various functions in the application were well integrated	1	2	3	4	5
6.	I thought there was too much inconsistency in this application	1	2	3	4	5
7.	I imagine that most people would learn this application very quickly	1	2	3	4	5
8.	I found the application very awkward to use	1	2	3	4	5
9.	I felt very confident using this application	1	2	3	4	5
10.	I needed to learn a lot of things before I could begin using this application	1	2	3	4	5

11. Overall, I would rate the user-friendliness of this product as *(mark with X the appropriate box)*:

Worst imaginable	Awful	Poor	OK	Good	Excellent	Best imaginable

Didactic / learning purposes

12. Do you think to have understood some new / better knowledge about the simulated phenomena (molecular interactions) that you were not aware of before using the application? Please, specify which new notions and which better notions you have learnt:

____

____

____

____

Final feedbacks

For each of the statements below, please circle the rating of your choice:

		Strongly Disagree				Strongly Agree
1.	I understand the purpose of the software	1	2	3	4	5
2.	The software's attractiveness invites me to go further into this software	1	2	3	4	5
3.	I would recommend this software to a colleague student	1	2	3	4	5

13. Suggestions for the improvements of the application:

____

____

____

____

14. Any other comments about the application (optional):

____

____

____

ANNEX 5

DETAILED RESULTS BY TEST SESSIONS

Test1 Results

	PRE-questionnaire					
	ID:	Test1				
	E-mail	********				
	Age:	20				
	Sex:	1				
	Study program:	Ingeneria Informatica				
	Year of studies	3				
		YES (1)	NO (0)	COMMENTS		
1	Do you use a computer for your study process	1		reading lectures, notes, programming etc..		
2	Do you use any special device and/or software during your study process		0			
		I DO NOT KNOW AT ALL (1)	2	3	4	I KNOW IT VERY WELL (5)
3	knowledge about the topic of the inter-molecular forces		2			
4	knowledge about Molecular binding sites		2			
	knowledge about Permanent and instant dipoles			3		
	knowledge about Molecular anisotropy		2			
5	knowledge about haptic devices		2			

	Test session							
	Date:	10/19/2010						
	Start time:	16:00:00						
	End time:	18:00:00						
	Short description of the session:	The student was shortly introduced with the goal of the usability test and was asked to think out loud while executing the tasks in order to explicitly capture the thoughts, impressions and opinions. In order to get the user accustomed with the Phantom haptic device he was asked to try the Dice demo for around 5 minutes. During the session user was introduced step-by-step with the different visual clues that might be useful for completion of the certain task and after completing the respective task was asked to reflect whether and how the visual clues were helpful.						
	Task 1	**Critical points detection**						
	Start time:	16:20:00						
	End time:	16:50:00						
	Observations:	Difficulties to locate molecule with haptic device in 3D space; Not obvious whether the charge is positive or negative; The possibility to rotate a molecule is not obvious; Hard to use together moving molecule and a haptic device; Not straight forward understandable what do the points in the graphic mean (yellow and green); Haptic device associates with a pen; What does mean the line from the cursor?; Too much information (haptic + all screen elements (molecule, force vector, graph, force lines)).						
1	Load the molecule Benzene	n/a						
2	Find the critical points of the electric field that surrounds the molecule	Easy with a positive charge, but difficult with the negative charge						
3	Which haptic and visual elements enabled you to detect the critical points?	n/a						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the			3				

	ease of completing this task	
2	Overall, I am satisfied with the amount of time it took to complete this task	2
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	5
4	Overall, I am satisfied with the use of the haptic device during this task	2
5	Please, describe which visual elements and information better helped you to perform the required task	Perspective view, graph very useful, maybe a bit too useful (it tells where the minimum is)
6	How such visual elements have been really helpful? Which features of them you really appreciated?	Perspective view makes it look more real, natural (you have a true perspective - "punto do fuga") graph and Min&Max useful, but obvious - they tell where the min and max is
7	Do you think that visual elements helped you in better detecting the force? How?	Maybe the force vector could be useful for the first few minutes then the user should be accustomed enough with the phantom and not need the force vector. Useful for direction not intensity (maybe if it were longer). Should be overlaid upon cursor (and it should be transparent not to interfere), not at the top of the screen

	Task 2	**Dipoles**
	Start time:	17:15:00
	End time:	17:22:00
	Observations:	Logscale changes also force feedback intensity (it becomes lower and therefore harder to perceive and understand); The colors in logscale seem to indicate attraction/repulsion therefore not so intuitive and need to be introduced then; Black color indicates transparency because the background is black
1	Load the molecule H2O	the cone is problematic because it only reacts on the vertex, you wouldn't expect this. Also the Van Der Waals representation is easier to interact with (less slippery)
2	Please try to describe its effect when a positive charge is moved around the molecule using our application	the positive-positive interaction is good because repulsion gives you an accurate perception of the shape of the force field. It is easier to understand the shape of an object touching (repulsion) it rather than being attracted.
3	Please try to describe its effect when a negative charge is moved around the molecule using our application	on the other hand negative-positive interaction (attraction) is easier to spot (you are guided towards the attraction point), but it is more difficult to discover the shape of the field (the lines of force)
		YES (1) NO (-1) PARTIALLY (0)

	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task		2					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task				4			
4	Overall, I am satisfied with the use of the haptic device during this task		2					
5	Please, describe which visual elements and information better helped you to perform the required task	Logscale is very useful if the scaling is applied to the phantom, too, it helps you to find the "center of attraction" with ease. The logscale colors are not very useful they are misleading.						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	n/a						
7	Do you think that visual elements helped you in better detecting the force? How?	n/a						

	Task 3	**Anisotropy**		
	Start time:	17:45:00		
	End time:	n/a		
1	Load the molecule CO2			
2	Please try to describe how do you feel the anisotropy of interaction using our application	The distance from the molecule is difficult to perceive and therefore the shape of the field is also difficult. To improve that could: walls with shadows, use the fog to perceive the z-axis		
		YES (1)	NO (-1)	PARTIALLY (0)
	Completed the task			0

		Strongly Agree (1)	2	3	4	5	6	Strongly Disagree (7)
1	Overall, I am satisfied with the ease of completing this task	n/a						
2	Overall, I am satisfied with the amount of time it took to complete this task	n/a						
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	n/a						
4	Overall, I am satisfied with the use of the haptic device during this task	n/a						
5	Please, describe which visual elements and information better helped you to perform the required task	n/a						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	n/a						
7	Do you think that visual elements helped you in better detecting the force? How?	n/a						

POST-questionnaire

	Haptic features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)	Scores
1	I found it easy to start using the haptic device for this application				4		3
2	It took some time before I could start using the haptic device in this application		2				3
3	I think the haptic device is very well integrated with the functionality of this application			3			2
4	I found it complex to understand how the haptic device works in this application		2				3
5	I was not sure how to use the haptic device while performing the tasks		2				3
6	I can easily control how fast I move though the 3D world			3			2

	Visual features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)
1	The use of graphics is appropriate for the software	1				
2	The visual elements are not annoying or distracting		2			
3	The amount of information shown through visual elements is not excessive			3		
4	Visual details are easily understandable		2			
5	The information presented is accurate and clear			3		
6	Colors are meaningful				4	
7	Graphical information is helpful to navigate the space around the molecule		2			
8	Someone without any knowledge about this application could easily				4	

	find how it works							
9	The software has a navigationally efficient layout			3				
10	Menus and GUI widgets are appropriate (i.e., well-designed and easy to use)			3				
	General features of the application	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)	SCORES	
1	I think that I would like to use this application frequently during respective chemistry studies			3			2	
2	I found the application unnecessarily complex		2				3	
3	I thought the application was easy to use				4		3	
4	I think I would need the support of a technical person to be able to use this application		2				3	
5	I found the various functions in the application were well integrated				4		3	
6	I thought there was too much inconsistency in this application	1					4	
7	I imagine that most people would learn this application very quickly					5	4	
8	I found the application very awkward to use		2				3	
9	I felt very confident using this application				4		3	
10	I needed to learn a lot of things before I could begin using this application	1					4	
		WORST IMAGINABLE (-3)	AWFUL (-2)	POOR (-1)	OK (0)	GOOD (1)	EXCELLENT (2)	BEST IMAGINABLE (3)
11	Overall, I would rate the user-friendliness of this product as			-1				
	Didactic/learning purposes							
12	Do you think to have understood some new / better knowledge about	n/a						

	the simulated phenomena (molecular interactions) that you were not aware of before using the application? Please, specify which new notions and which better notions you have learnt:					
	Final feedbacks	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)
1	I understand the purpose of the software					5
2	The software's attractiveness invites me to go further into this software				4	
3	I would recommend this software to a colleague student				4	

13	Suggestions for the improvements of the application:	Mainly the UI friendliness and the spatial representation
14	Any other comments about the application (optional):	n/a

Test2 Results

PRE-questionnaire

ID:	Test2
E-mail	********
Age:	26
Sex:	1
Study program:	Biomedical Engineer graduate, student of Computer Science
Year of studies:	>5

		YES (1)	NO (0)	COMMENTS
1	Do you use a computer for your study process	1		Reading lectures, using special chemistry application, development software
2	Do you use any special device and/or software during your study process	1		IDE for Java, special chemistry software

		I DO NOT KNOW AT ALL (1)	2	3	4	I KNOW IT VERY WELL (5)
3	knowledge about the topic of the inter-molecular forces			3		
4	knowledge about Molecular binding sites			3		
	knowledge about Permanent and instant dipoles			3		
	knowledge about Molecular anisotropy			3		
5	knowledge about haptic devices	1				

Test session

Date:	10/21/2010
Start time:	9:00:00
End time:	11:00:00
Short description of the session:	The user did not use dice demo in order to get accustomed with the haptic device but was asked to use the application in order to get accustomed with the haptic device, but it was not effective enough.

	Task 1	**Critical points detection**						
	Start time:	9:26:00						
	End time:	9:41:00						
1	Load the molecule Benzene							
	Observations:	Using the buttons on haptic device the user was expecting to be able to rotate or move the molecule, Problems adjusting the phantom after changing the position of the molecule.						
2	Find the critical points of the electric field that surrounds the molecule							
	Observations:	The colors are misleading, It is not possible to find critical points just with the use of haptic device, it just helps to understand the direction, The force vector visual element makes more clear the direction of the vector, the line from cursor to the molecule is misleading as if it is a force vector,						
3	Which haptic and visual elements enabled you to detect the critical points?	With the haptic device it is hard to find the critical points, the region is identified.						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the ease of completing this task			3				
2	Overall, I am satisfied with the amount of time it took to complete this task			3				
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task				4			
4	Overall, I am satisfied with the use of the haptic device during this task				4			
5	Please, describe which visual elements and information better helped you to perform the required task	Graph and force vector were useful, Force lines and colors were not so useful.						

6	How such visual elements have been really helpful? Which features of them you really appreciated?	Positions of critical points were determined by graph and from min Vector is easy concept to understand in terms of force.
7	Do you think that visual elements helped you in better detecting the force? How?	Force vector - yes, Lines and color - no. Molecule visualization helps to form an idea about the field and its structure

	Task 2	**Dipoles**
	Start time:	10:00:00
	End time:	10:10:00
1	Load the molecule H2O	The process of loading the molecule sometimes gives an impression that the software is not responding
2	Please try to describe its effect when a positive charge is moved around the molecule using our application	It is easier to understand the forces (minimum points), also repulsion is straight forward, only haptic device gives enough information. The force lines are helpful. Logscale helps by visualizing Force feedback is not strong enough, maybe the slower movement is necessary in order to detect the forces.
3	Please try to describe its effect when a negative charge is moved around the molecule using our application	

	Yes (1)	No (-1)	Partially (0)
Completed the task	1		

		Strongly Agree (1)	2	3	4	5	6	Strongly Disagree (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task		2					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task				4			
4	Overall, I am satisfied with the use of the haptic device during this task		2					

5	Please, describe which visual elements and information better helped you to perform the required task	no need for visual elements, haptic feedback only was very useful logscale visualizes different areas, but not as good as haptic force feedback
6	How such visual elements have been really helpful? Which features of them you really appreciated?	n/a
7	Do you think that visual elements helped you in better detecting the force? How?	n/a

	Task 3	**Anisotropy**
	Start time:	10:24:00
	End time:	10:34:00
	Observations:	Quickly started to use widgets for increasing/moving the molecule
1	Load the molecule CO2	
2	Please try to describe how do you feel the anisotropy of interaction using our application	Haptic tool helps to understand by repulsive forces Easier to understand when actually the tip is seen and after getting accustomed with the haptic device

		Yes (1)	No (0)	Partially (0)
	Completed the task	1		

		Strongly Agree (1)	2	3	4	5	6	Strongly Disagree (7)
1	Overall, I am satisfied with the ease of completing this task	1						
2	Overall, I am satisfied with the amount of time it took to complete this task	1						
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1						
4	Overall, I am satisfied with the use of the haptic device during this task	1						

5	Please, describe which visual elements and information better helped you to perform the required task	With logscale the colors are more confusing compared to H_2O, Mainly relied of the haptic device.
6	How such visual elements have been really helpful? Which features of them you really appreciated?	n/a
7	Do you think that visual elements helped you in better detecting the force? How?	n/a

POST-questionnaire

	Haptic features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)	Scores
1	I found it easy to start using the haptic device for this application				4		3
2	It took some time before I could start using the haptic device in this application				4		1
3	I think the haptic device is very well integrated with the functionality of this application				4		3
4	I found it complex to understand how the haptic device works in this application			3			2
5	I was not sure how to use the haptic device while performing the tasks			3			2
6	I can easily control how fast I move though the 3D world	1					0

	Visual features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)
1	The use of graphics is appropriate for the software				4	
2	The visual elements are not annoying or distracting			3		
3	The amount of information shown through visual elements is not excessive			3		

4	Visual details are easily understandable				4			
5	The information presented is accurate and clear				4			
6	Colors are meaningful			3				
7	Graphical information is helpful to navigate the space around the molecule			3				
8	Someone without any knowledge about this application could easily find how it works		2					
9	The software has a navigationally efficient layout				4			
10	Menus and GUI widgets are appropriate (i.e., well-designed and easy to use)				4			
	General features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)	Scores	
1	I think that I would like to use this application frequently during respective chemistry studies				4		3	
2	I found the application unnecessarily complex			3			2	
3	I thought the application was easy to use			3			2	
4	I think I would need the support of a technical person to be able to use this application		2				3	
5	I found the various functions in the application were well integrated				4		3	
6	I thought there was too much inconsistency in this application		2				3	
7	I imagine that most people would learn this application very quickly			3			2	
8	I found the application very awkward to use			3			2	
9	I felt very confident using this application			3			2	
10	I needed to learn a lot of things before I could begin using this application		2				3	
		Worst imaginable (-3)	Awful (-2)	Poor (-1)	OK (0)	Good (1)	Excellent (2)	Best imaginable (3)

11	Overall, I would rate the user-friendliness of this product as					1
	Didactic/learning purposes					
12	Do you think to have understood some new / better knowledge about the simulated phenomena (molecular interactions) that you were not aware of before using the application? Please, specify which new notions and which better notions you have learnt:	Topological structure of force field of molecules in particular 3D structure of force field. Feedback in terms of force from tool very useful.				
	Final feedbacks	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)
1	I understand the purpose of the software				4	
2	The software's attractiveness invites me to go further into this software				4	
3	I would recommend this software to a colleague student				4	
13	Suggestions for the improvements of the application:	n/a				
14	Any other comments about the application (optional):	When cursor is behind it is hard to understand the location and force field, Possibility to realign the reference space				

Test3 Results

PRE-questionnaire

ID:	Test3
E-mail	********
Age:	20
Sex:	1
Study program:	Ingegneria Informatica
Year of studies:	3

		YES (1)	NO (0)	COMMENTS
1	Do you use a computer for your study process	1		Lettura di slide e dispense dei docenti
2	Do you use any special device and/or software during your study process	1		Dev-C++, Matlab

		I DO NOT KNOW AT ALL (1)	2	3	4	I KNOW IT VERY WELL (5)
3	knowledge about the topic of the inter-molecular forces				4	
4	knowledge about Molecular binding sites				4	
	knowledge about Permanent and instant dipoles			3		
	knowledge about Molecular anisotropy			3		
5	knowledge about haptic devices		2			

Test session

Date:	10/22/2010
Start time:	16:30:00
End time:	17:40:00

Task 1	**Critical points detection**
Start time:	16:40:00
End time:	16:45:00

1	Load the molecule Benzene	n/a
2	Find the critical points of the electric field that surrounds the molecule	When the user is too far behind the molecule can be misleading as a critical point since there is no force associated and the haptic device is stable The force vector is not really understandable (hard to understand direction of the arrow in 3D space) Graph is more understandable The force lines are helpful, but hard to start to use without extra explanation
3	Which haptic and visual elements enabled you to detect the critical points?	plot of MEP and force lines, no help from force vector

	YES (1)	NO (-1)	PARTIALLY (0)
Completed the task	1		

		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task	1						
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task		2					
4	Overall, I am satisfied with the use of the haptic device during this task		2					

5	Please, describe which visual elements and information better helped you to perform the required task	Mainly the force graph
6	How such visual elements have been really helpful? Which features of them you really appreciated?	with the graph it is easy to understand where the attraction points are, molecule is also very useful
7	Do you think that visual elements helped you in better detecting the force? How?	not so much attention is paid to visuals, more concentration is on haptic feedback from Phantom (more relied also on this feedback)

Task 2	**Dipoles**
Start time:	17:00:00

	End time:	17:10:00						
1	Load the molecule H2O							
2	Please try to describe its effect when a positive charge is moved around the molecule using our application	Easier to find attraction by haptic feedback, no force feeled from positive						
3	Please try to describe its effect when a negative charge is moved around the molecule using our application	repulsion is not easy detectable approaching to red zone initial repulsion and then immediate attraction molecular visualization helps, but not so much colors LOGSCALE: attraction is different, no repulsion easy detectable, visualization without forces does not really help, Force lines: more helpful than graph - help more to find force fields						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task		2					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task			3				
4	Overall, I am satisfied with the use of the haptic device during this task	1						
5	Please, describe which visual elements and information better helped you to perform the required task	The force lines help to understand where attraction and repulsion areas are situated. even the color of the molecule helps						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	At the beginning the colors because they let you understand where the positive and the negative charges of the dipole are situated. also the force lines are very useful to detecting areas of strong repulsion and the "roads" to strong attraction						
7	Do you think that visual elements helped you in better detecting the force? How?	yes, because if I follow the force lines I can better feel the charge interaction						

	Task 3	**Anisotropy**						
	Start time:	17:25:00						
	End time:	17:30:00						
1	Load the molecule CO_2							
2	Please try to describe how do you feel the anisotropy of interaction using our application	Force lines - simple thing to look at - center of the screen (not a graph or arrow). Without force lines color attracts attention and looking at graph for extra information, the force arrow does not give any meaning.						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task		2					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1						
4	Overall, I am satisfied with the use of the haptic device during this task	1						
5	Please, describe which visual elements and information better helped you to perform the required task	At the beginning I watch the force lines because they are the central elements they help me to find a way to stronger attraction/repulsion. When I feel a strong force I take a look at the graph in order to confirm what I feel.						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	I appreciated most the colors which detected the strong points. then the force lines that help me follow the "force ways" to get to the critical points. At least the graph which show me I'm definitely in a critical point						
7	Do you think that visual elements helped you in better detecting the force? How?	Yes because they make you understand where to move. If you see the force lines you will try to follow them in order to discover the ways to get to the critical points. The same is for the colors - you want to understand what they mean so you go near them and then feel the force.						

POST-questionnaire

	Haptic features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)	Scores
1	I found it easy to start using the haptic device for this application				4		3
2	It took some time before I could start using the haptic device in this application			3			2
3	I think the haptic device is very well integrated with the functionality of this application				4		3
4	I found it complex to understand how the haptic device works in this application		2				3
5	I was not sure how to use the haptic device while performing the tasks		2				3
6	I can easily control how fast I move though the 3D world			3			2

	Visual features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)
1	The use of graphics is appropriate for the software				4	
2	The visual elements are not annoying or distracting				4	
3	The amount of information shown through visual elements is not excessive			3		
4	Visual details are easily understandable			3		
5	The information presented is accurate and clear			3		
6	Colors are meaningful				4	
7	Graphical information is helpful to navigate the space around the molecule				4	
8	Someone without any knowledge about this application could easily find how it works			3		
9	The software has a navigationally efficient				4	

	layout							
10	Menus and GUI widgets are appropriate (i.e., well-designed and easy to use)				4			
	General features of the application	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)	SCORES	
1	I think that I would like to use this application frequently during respective chemistry studies					5	4	
2	I found the application unnecessarily complex		2				3	
3	I thought the application was easy to use				4		3	
4	I think I would need the support of a technical person to be able to use this application	1					4	
5	I found the various functions in the application were well integrated				4		3	
6	I thought there was too much inconsistency in this application		2				3	
7	I imagine that most people would learn this application very quickly				4		3	
8	I found the application very awkward to use	1					4	
9	I felt very confident using this application				4		3	
10	I needed to learn a lot of things before I could begin using this application	1					4	
		WORST IMAGINABLE (-3)	AWFUL (-2)	POOR (-1)	OK (0)	GOOD (1)	EXCELLENT (2)	BEST IMAGINABLE (3)
11	Overall, I would rate the user-friendliness of this product as					1		
	Didactic/learning purposes							
12	Do you think to have understood some new / better knowledge about the simulated phenomena (molecular interactions) that you were not aware of before using the application? Please, specify which new notions and which better notions you have learnt:	Using the application is very useful to understand the areas of action of the forces: they are strong in particular points of the molecule - I was not completely aware of this before.						

	Final feedbacks	Strongly Disagree (1)	2	3	4	Strongly Agree (5)
1	I understand the purpose of the software				4	
2	The software's attractiveness invites me to go further into this software				4	
3	I would recommend this software to a colleague student				4	
13	Suggestions for the improvements of the application:	n/a				
14	Any other comments about the application (optional):	n/a				

Test4 Results

PRE-questionnaire

ID:	Test4
E-mail	********
Age:	21
Sex:	2
Study program:	Ingegneria Informatica
Year of studies:	3

		Yes (1)	No (0)	Comments
1	Do you use a computer for your study process	1		Uso il computer per studiare le dispense fornite dai docenti e come strumento matematico di supporto allo studio
2	Do you use any special device and/or software during your study process	1		Ho utilizzato Dev-C++ e Assembly per la compilazione di programmi. Utilizzo spesso Scilab come strumento matematico

		I do not know at all (1)	2	3	4	I know it very well (5)
3	knowledge about the topic of the inter-molecular forces			3		

		1	2	3	4	5	6	7
4	knowledge about Molecular binding sites				4			
	knowledge about Permanent and instant dipoles				4			
	knowledge about Molecular anisotropy	1						
5	knowledge about haptic devices	1						

Test session

Date:	10/27/2010
Start time:	14:00:00
End time:	15:30:00
Short description of the session:	The user has tried first a Phantom demo application (Dice Demo) in order to get accustomed with the haptic device, the brief explanation of the application was given (main features and options), and then user was asked to perform the tasks.

Task 1	**Critical points detection**
Start time:	14:11:00
End time:	14:19:00

1	Load the molecule Benzene	I think that it is very easy to use the application, and especially very useful to understand iterations. I prefer the visualization of the molecule through Ball'n'Stick and Van Der Waals space
2	Find the critical points of the electric field that surrounds the molecule	The force is minimum when I am pushed away from the molecule while it is maximum when the cursor touches the molecule. It is really interesting to sense physically what is the maximum attraction force between molecule
3	Which haptic and visual elements enabled you to detect the critical points?	To indicate the critical points the best visualization is with graph. I found very interesting also force direction vector. Instead I did not particularly liked the force lines because as for me it is more difficult to understand.

	Yes (1)	No (-1)	Partially (0)
Completed the task	1		

		Strongly Agree (1)	2	3	4	5	6	Strongly Disagree (7)
1	Overall, I am satisfied with the ease of completing this task	1						

2	Overall, I am satisfied with the amount of time it took to complete this task		2					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1						
4	Overall, I am satisfied with the use of the haptic device during this task	1						
5	Please, describe which visual elements and information better helped you to perform the required task	See 1-3						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	See 1-3						
7	Do you think that visual elements helped you in better detecting the force? How?	See 1-3						
	Task 2	**Dipoles**						
	Start time:	14:31:00						
	End time:	14:37:00						
1	Load the molecule H2O	Between the visualizations in this case I prefer Van Der Waals. I think that the tool is really helpful with this visualization						
2	Please try to describe its effect when a positive charge is moved around the molecule using our application	it is possible to sense the major attraction force especially close to H molecule						
3	Please try to describe its effect when a negative charge is moved around the molecule using our application	When I search for a negative charge it increases when I approach Oxygen.						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)

1	Overall, I am satisfied with the ease of completing this task	1						
2	Overall, I am satisfied with the amount of time it took to complete this task	1						
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1						
4	Overall, I am satisfied with the use of the haptic device during this task	1						
5	Please, describe which visual elements and information better helped you to perform the required task	The Van Der Waals visualization is very useful to understand the forces. I think also that very useful is the information of the position of the cursor in the space to understand better where you are in the space.						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	In this case I've appreciated the force lines because in this case the their idea is understandable. I think also that graph and force vector are even useful to understand the force direction and the maximum and minimum points						
7	Do you think that visual elements helped you in better detecting the force? How?	The best were the force lines with force line directions switched on. Complete vision from the forces.						
	Task 3	**Anisotropy**						
	Start time:	14:52:00						
	End time:	14:56:00						
1	Load the molecule CO2	In this case I prefer the visualization of Bal'n'stick as Van der Waals I can not see the cursor						
2	Please try to describe how do you feel the anisotropy of interaction using our application	The tool is very sensible when I move the cursor and then in this case I can understand even the smallest variation of the intensity of the forces.						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)
1	Overall, I am satisfied with the ease of completing this task	1						

2	Overall, I am satisfied with the amount of time it took to complete this task	1					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1					
4	Overall, I am satisfied with the use of the haptic device during this task		2				
5	Please, describe which visual elements and information better helped you to perform the required task	In this case very useful is the visualization of the intensity of the force by the colors. Being in the logarithmic scale is easy to represent any type of forces.					
6	How such visual elements have been really helpful? Which features of them you really appreciated?	I appreciated the force lines and also the direction. As I have already told for other molecules, the graph is very useful, also the force lines allowed immediate comprehension.					
7	Do you think that visual elements helped you in better detecting the force? How?	I think for sure that the physical feeling and seeing and the same time on the screen the intensity of the forces (through the use of colors) give the complete understanding of the forces present in the molecule					

POST-questionnaire

	Haptic features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)	Scores
1	I found it easy to start using the haptic device for this application					5	4
2	It took some time before I could start using the haptic device in this application			3			2
3	I think the haptic device is very well integrated with the functionality of this application					5	4
4	I found it complex to understand how the haptic device works in this application					5	0
5	I was not sure how to use the haptic device while performing the tasks		2				3

6	I can easily control how fast I move though the 3D world					5	4

	Visual features of the application	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)	
1	The use of graphics is appropriate for the software					5	
2	The visual elements are not annoying or distracting					5	
3	The amount of information shown through visual elements is not excessive					5	
4	Visual details are easily understandable					5	
5	The information presented is accurate and clear					5	
6	Colors are meaningful					5	
7	Graphical information is helpful to navigate the space around the molecule				4		
8	Someone without any knowledge about this application could easily find how it works					5	
9	The software has a navigationally efficient layout					5	
10	Menus and GUI widgets are appropriate (i.e., well-designed and easy to use)					5	

	General features of the application	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)	SCORES
1	I think that I would like to use this application frequently during respective chemistry studies					5	4
2	I found the application unnecessarily complex		2				3
3	I thought the application was easy to					5	4

	use							
4	I think I would need the support of a technical person to be able to use this application	1					4	
5	I found the various functions in the application were well integrated					5	4	
6	I thought there was too much inconsistency in this application		2				3	
7	I imagine that most people would learn this application very quickly				4		3	
8	I found the application very awkward to use	1					4	
9	I felt very confident using this application					5	4	
10	I needed to learn a lot of things before I could begin using this application		2				3	
		WORST IMAGINABLE (-3)	AWFUL (-2)	POOR (-1)	OK (0)	GOOD (1)	EXCELLENT (2)	BEST IMAGINABLE (3)
11	Overall, I would rate the user-friendliness of this product as						2	

	Didactic/learning purposes	
12	Do you think to have understood some new / better knowledge about the simulated phenomena (molecular interactions) that you were not aware of before using the application? Please, specify which new notions and which better notions you have learnt:	Through the usage of this tool I discovered the presence in the nature of the anisotropy and its characteristics. I think that this application can allow the user to precisely understand how and why molecule is constructed this way and especially the ties that forms it.

	Final feedbacks	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)
1	I understand the purpose of the software				4	
2	The software's attractiveness invites me to go further into this software					5

3	I would recommend this software to a colleague student	5

13	Suggestions for the improvements of the application:	I think the the application is complete. There is a lot of information and many different visualizations that allow the users change to the ones that suit the best each type of work
14	Any other comments about the application (optional):	n/a

Test5 Results

	PRE-questionnaire	
	ID:	Test5
	E-mail	********
	Age:	21
	Sex:	2
	Study program:	INGEGNERIA INFORMATICA
	Year of studies:	3

		YES (1)	NO (0)	COMMENTS
1	Do you use a computer for your study process	1		LEGGERE LE DISPENSE DEI PROFESSORI, CERCARE MATERIALE IN INTERNET
2	Do you use any special device and/or software during your study process	1		DEV C++ (PROGRAMMAZIONE), SCILAB (ANALISI MATEMATICA)

		I DO NOT KNOW AT ALL (1)	2	3	4	I KNOW IT VERY WELL (5)
3	knowledge about the topic of the inter-molecular forces			3		
4	knowledge about Molecular binding sites				4	
	knowledge about Permanent and instant dipoles			3		
	knowledge about Molecular anisotropy	1				
5	knowledge about haptic devices	1				

Test session

	Date:	10/29/2010
	Start time:	8:58:00
	End time:	10:30:00
	Short description of the session:	

	Task 1	**Critical points detection**
	Start time:	8:58:00
	End time:	9:10:00
	Observations	The user was mostly behind the molecule (not seeing the tip), probably not straight forward understandable how to move the tip to the front of molecule. Discovering and trying different visualizations and show info in order to find the best for the task. Chose the Ball'n'stick. When tip is farer user asked why she cannot see the graph. Colors were a bit misleading - expecting that red is positive potential and blue is negative - somehow user did not see the bar on the right where the meaning of the colors is indicated.
1	Load the molecule Benzene	
2	Find the critical points of the electric field that surrounds the molecule	It is easy to find maximum point of attraction because the device make you feel the force. Less easier is feeling the repulsion, but because you need to win the force - put more effort in order to feel the where the maximum repulsion is.
3	Which haptic and visual elements enabled you to detect the critical points?	In my opinion the "MEP", the "show force lines" and the "Graph" are very useful in order to detect the critical points in addition to the feeling proved with the haptic device

		Yes (1)	No (-1)	Partially (0)
	Completed the task	1		

		Strongly Agree (1)	2	3	4	5	6	Strongly Disagree (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task		2					

3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1						
4	Overall, I am satisfied with the use of the haptic device during this task	1						
5	Please, describe which visual elements and information better helped you to perform the required task	see 1-3						
6	How such visual elements have been really helpful? Which features of them you really appreciated?	I appreciated the force lines because they show where the you can feel and try more attraction or repulsion. I also appreciated even the van der waals representation because it shows how the molecule is made and the electric field that surrounds it.						
7	Do you think that visual elements helped you in better detecting the force? How?	see 1-3						
	Task 2	**Dipoles**						
	Start time:	9:27:00						
	End time:	9:36:00						
	Observations:	Logscale is not the obvious choice to complete the task, it is also harder to sense attraction/repulsion because the forces are weaker. The more senses are involved the easier it is to learn and to understand.						
1	Load the molecule H2O	It is easy to see the structure of the molecule						
2	Please try to describe its effect when a positive charge is moved around the molecule using our application	It is very easy to feel the attraction or repulsion when a positive charge is moved around the molecule and it is easier when force lines are shown						
3	Please try to describe its effect when a negative charge is moved around the molecule using our application	In my opinion when I use a negative charge is more difficult to feel attraction, but I feel more the repulsion. Using Logscale makes it more difficult to feel the forces when in a normal representation.						
		YES (1)	NO (-1)	PARTIALLY (0)				
	Completed the task	1						
		STRONGLY AGREE (1)	2	3	4	5	6	STRONGLY DISAGREE (7)

1	Overall, I am satisfied with the ease of completing this task		2	
2	Overall, I am satisfied with the amount of time it took to complete this task		2	
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task	1		
4	Overall, I am satisfied with the use of the haptic device during this task	1		
5	Please, describe which visual elements and information better helped you to perform the required task	I find very useful the "Ball'n'stick" and the "Van der Waals" visualization, the force lines and I find the natural scale better than the logarithmic one		
6	How such visual elements have been really helpful? Which features of them you really appreciated?	I find very helpful the Van der Waals visualizations because it shows the electric field and I think it's easier to understand the forces. I think that natural scale is more useful than the logarithmic scale because it makes you feel the force in a more powerful way		
7	Do you think that visual elements helped you in better detecting the force? How?	Yes because they show where maximum and minimum points are, but I also think that the haptic tool is very useful because it makes you feel the forces.		

	Task 3	**Anisotropy**		
	Start time:	9:57:00		
	End time:	10:07:00		
	Observations:	The possibility to rotate/move molecule was not obvious for the user It was hard for the user to distinguish the attraction/repulsion forces because they act with same intensity on the cursor.		
1	Load the molecule CO2	n/a		
2	Please try to describe how do you feel the anisotropy of interaction using our application	I do not know anisotropy but I feel more repulsion than attraction even that maximum point are shown. I think that the repulsion from oxygen is bigger than the attraction of the "carbonio".		

		YES (1)	NO (-1)	PARTIALLY (0)
	Completed the task	1		

		Strongly Agree (1)	2	3	4	5	6	Strongly Disagree (7)
1	Overall, I am satisfied with the ease of completing this task		2					
2	Overall, I am satisfied with the amount of time it took to complete this task		2					
3	Overall, I am satisfied with the support information (help, messages, documentation) when completing this task		2					
4	Overall, I am satisfied with the use of the haptic device during this task		2					

5	Please, describe which visual elements and information better helped you to perform the required task	I prefer the Van Der Waals visualization and the MEP because they show the molecule in a more understandable way. Also the force lines are very helpful.
6	How such visual elements have been really helpful? Which features of them you really appreciated?	I really appreciated the force lines because they show the direction of the force and if you follow them you can feel more the attraction or the repulsion, but I think that the arrows of the force lines are not enough visible.
7	Do you think that visual elements helped you in better detecting the force? How?	Yes because the force lines and the different colors in the molecule help you to see what you are feeling with the hand and the tool. They support the information obtained by the tool.

POST-questionnaire

	Haptic features of the application	Strongly Disagree (1)	2	3	4	Strongly Agree (5)	Scores
1	I found it easy to start using the haptic device for this application				4		3
2	It took some time before I could start using the haptic device in this application	1					4
3	I think the haptic device is very well integrated with the functionality of this application				4		3

4	I found it complex to understand how the haptic device works in this application		2				3
5	I was not sure how to use the haptic device while performing the tasks		2				3
6	I can easily control how fast I move though the 3D world			3			2
	Visual features of the application	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)	
1	The use of graphics is appropriate for the software					5	
2	The visual elements are not annoying or distracting	1					
3	The amount of information shown through visual elements is not excessive				4		
4	Visual details are easily understandable				4		
5	The information presented is accurate and clear				4		
6	Colors are meaningful					5	
7	Graphical information is helpful to navigate the space around the molecule				4		
8	Someone without any knowledge about this application could easily find how it works				4		
9	The software has a navigationally efficient layout				4		
10	Menus and GUI widgets are appropriate (i.e., well-designed and easy to use)					5	
	General features of the application	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)	SCORES
1	I think that I would like to use this application frequently during respective chemistry studies				4		3

2	I found the application unnecessarily complex	1					4	
3	I thought the application was easy to use				4		3	
4	I think I would need the support of a technical person to be able to use this application	1					4	
5	I found the various functions in the application were well integrated				4		3	
6	I thought there was too much inconsistency in this application		2				3	
7	I imagine that most people would learn this application very quickly					5	4	
8	I found the application very awkward to use	1					4	
9	I felt very confident using this application					5	4	
10	I needed to learn a lot of things before I could begin using this application	1					4	
		WORST IMAGINABLE (-3)	AWFUL (-2)	POOR (-1)	OK (0)	GOOD (1)	EXCELLENT (2)	BEST IMAGINABLE (3)
11	Overall, I would rate the user-friendliness of this product as						2	
	Didactic/learning purposes							
12	Do you think to have understood some new / better knowledge about the simulated phenomena (molecular interactions) that you were not aware of before using the application? Please, specify which new notions and which better notions you have learnt:	I understand what anisotropy is. I have possibility to try with my hands the force between different molecules and I think it is very important to understand all and better than only theory.						
	Final feedbacks	STRONGLY DISAGREE (1)	2	3	4	STRONGLY AGREE (5)		
1	I understand the purpose of the software				4			

2	The software's attractiveness invites me to go further into this software		5
3	I would recommend this software to a colleague student		5
13	Suggestions for the improvements of the application:	n/a	
14	Any other comments about the application (optional):	n/a	

ANNEX 6

SUMMARY OF RESULTS BY TASKS

This annex presents the usability evaluation results summarized by tasks.

In Tables 1. - 3. one can find the detailed ASQ scores for effectiveness, efficiency, haptic and satisfaction parts of this questionnaire, the time it took to complete the task expressed in minutes and whether a user has completed the task.

Tables 4 - 6 summarize the feedback of the users for different elements of the evaluated haptic-based framework. The colors of the cells identify the usefulness of the element in a particular test session: green – useful, yellow – helps to some extent, pink – not useful, white – n/a.

ANNEX 6: Table 1. Feedback of the users about haptic-based framework features after Task 1

Task description:	*Critical points detection*				
	Test1	**Test2**	**Test3**	**Test4**	**Test5**
Ball'n'stick	not used	not used	not used	not used	not used
Van Der Waal	useful	useful (forms the idea of a structure of the field)	useful	useful	very useful
Colors of the molecule	no feedback	misleading	no feedback	no feedback	misleading
Force Graph	useful	useful	useful	useful	very useful
Force Lines	not useful	not useful	useful (if explained)	not useful (difficult to understand)	problematic
Force Vector	useful (first few minutes)	useful (helps to understand direction)	not useful	useful	more useful than not useful
Min & Max	useful	n/a	n/a	n/a	n/a
Perspective view	useful	n/a	n/a	n/a	n/a
Haptic feedback	useful	helps to find the region only, but not the specific points	useful (mostly relied on this feedback)	useful	very useful

ANNEX 6: Table 2. Feedback of the users about haptic-based framework features after Task 2

Task description:	*Dipoles*				
	Test1	**Test2**	**Test3**	**Test4**	**Test5**
Ball'n'stick					x
Van Der Waal	useful	useful	useful	useful	useful
Colors of the molecule	misleading		not so much		
Force Graph	no feedback		less useful	useful	

Task description:	*Dipoles*				
	Test1	**Test2**	**Test3**	**Test4**	**Test5**
			than lines		
Force Lines	no feedback	useful	useful	most useful	useful
Force Vector	no feedback			useful	
Logscale	useful	useful			problematic due to weaker force feedback
Min & Max	no feedback	no feedback	no feedback	no feedback	no feedback
Perspective view	no feedback	no feedback	no feedback	no feedback	no feedback
Haptic feedback	useful	useful (only haptic is enough to understand the forces)	useful	useful	useful

ANNEX 6: Table 3. Feedback of the users about haptic-based framework features after Task 3

Task description:	*Anisotropy*				
	Test1	**Test2**	**Test3**	**Test4**	**Test5**
Ball'n'stick	n/a			useful	
Van Der Waal	n/a				useful
Colors of the molecule	n/a		attracts attention to discover their meaning	useful	useful
Force Graph	n/a		only for extra information	useful	
Force Lines	n/a		useful	useful	useful
Force Vector	n/a		not useful		
Logscale	n/a	colors are confusing		useful	
Min & Max	n/a				
Perspective view	n/a				
Haptic feedback	n/a	useful	useful	useful	useful

Tables 7. - 9. summarize the problems discovered during the test sessions. The problems identified are grouped by categories. The color of the cell shows the category of the problem with respect to the following notions:

Spatial	Haptic	Semiotics	Cognitive	Graphics

ANNEX 6: Table 4. Problems discovered after Task 1 by test sessions

Test1	Test2	Test3	Test4	Test5
Too much information at once (haptic feedback and all the visual elements)	User is expecting to use buttons on Phantom to move/rotate molecule	Being too far from molecule can be misleading as if it is a critical point	Force lines are difficult to understand	The user was mostly behind the molecule (not seeing the tip), probably not straight forward understandable how to move the tip to the front of molecule.
Difficulties to understand location in 3D space	Problems to adjust the Phantom after changing the location of the molecule	Hard to understand the direction of 3D arrow of force vector		When tip is farer user asked why she cannot see the graph.
Difficulties to understand meaning of the points in the graph (yellow and green)				Meaning of the colors of the molecule
The line from the cursor not understandable				
Not obvious which is the charge of the tip				

ANNEX 6: Table 5. Problems discovered after Task 2 by test sessions

Test1	Test2	Test3	Test4	Test5
*Logscale issues**	*Logscale issues**	Easier to find attraction because it attracts immediately even if trying to approach repulsion zones	The information about position of the cursor in the space would be very helpful	*Logscale issues**
The colors in logscale seem to indicate attraction/repulsion therefore not so intuitive and need to be introduced then		Lines are like "ways" to attractions/repulsions	The best are force lines with force directions	

Test1	Test2	Test3	Test4	Test5
Black color indicates transparency because the background is black				
Easier to understand the force field by repulsion instead of attraction				
Easier to spot the attraction field (you are guided to it)				

**Logscale issues - Logscale changes also force feedback intensity (it becomes lower and therefore harder to perceive and understand)*

ANNEX 6: Table 6. Problems discovered after Task 3 by test sessions

Test1	Test2	Test3	Test4	Test5
Difficult to perceive the distance to the molecule and therefore also the field	Easier to understand when the tip is visible	Force lines attract the main attention since they are in the middle of the screen	With Van Der Wall I can not see the cursor	The possibility to rotate/move molecule is not so obvious
			Tool is very sensible - easier to understand even the slightest variation of the intensity of the force	Arrows of the force lines are not enough comprehensive
			Force lines with the directions are useful	

ANNEX 7

LIST OF THE PROBLEMS DISCOVERED DURING USABILITY EVALUATION BY CATEGORIES

Category	Problem description
Semiotics	S1: Not obvious the meaning of the points in the graph (yellow and green). S2: Not obvious which is the charge of the tip. S3: Not obvious the meaning of the colors of the molecule. S4: When tip is too far from the molecule user inquired why she cannot see the graph. S5: Being too far from the molecule can be misleading as if it is a critical point. S6: The colors of the “Logscale” visualization seem to indicate repulsion/attraction areas therefore they are not so intuitive.
Cognitive	C1: Too much information at once (haptic feedback and all the visual elements).
Graphics	G1: Force lines are difficult to understand. G2: Black color in the molecule makes association with the transparency in the molecule due to black background. G3: Arrows of the Force lines are not enough visible and therefore makes it harder to understand the actual direction.
Haptic	H1: Difficulties to understand location in a 3D space. H2: Hard to understand the direction of 3D arrow of the force vector. H3: The user was mostly behind the molecule (not seeing the tip), not straight forward understandable how to move the tip to the front of the molecule. H5: User is expecting to use buttons on Phantom to move/rotate molecule. H6: Difficulties to adjust the haptic device after changing the location of the molecule. H7: In some cases appear the strong vibrations of the haptic device changing the force intensities or when approaching the molecule closer. H8: The “Logscale” visualization of the molecule changes also the force feedback – it becomes weaker and therefore harder to perceive. H9: Determining the position of the cursor in the space. H10: Difficult to perceive the distance from the cursor to the molecule this makes it difficult also to perceive the force field. H11: The repulsion feedback in some cases might create an affordance of resistance that can cause the damage of the haptic device.