Computer Simulations as a Bridge between Different Representation Levels of Scientific Concepts

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Abstract

Chemical phenomena can be represented on three modes: macro, sub-micro and symbolic. These representation modes are often referred to as representation “levels”, but lack a precise definition of what kind of levels are meant. This ambiguity results in distinct meanings to the concept of “representation level”. The present work suggests referring to these levels as levels of complexity.

Through interviews of faculty members, graduate and undergraduate students, we have shown that faculty members think of system properties as emerging from mechanistic interactions between particles at the sub-micro level. Students’ understanding of the relation between these levels often deviates from that of the faculty members. One deviation is the consideration of a system representation level only, either in the macro or symbolic modes. The other deviation is thinking about system properties as the reason for particle behavior, rather than the other way around. Students often use their familiarity with macroscopic properties of the system or with a symbolic equation relating system properties (such as the ideal gas equation) as the starting point of a thought process which leads them to impose mechanistically unwarrantable behavior upon the particles. Being the reverse of the ‘emergent’ perspective on scientific phenomena, we designated those as a ‘submergent’ perspective. Such a perspective allows students to avoid confronting their misconceptions about particle behavior, and leads them to incorrect conclusions when solving conceptual problems.

Based on these inferences we designed and developed two computer simulations which emphasize the emergent nature of several chemical concepts, and the emergent direction of the connections between the different representation modes. Through interviews of undergraduate students we discerned three distinct types of students’ behavior: Students who show a consistent tendency to emergently connect different representation modes, students who show a consistent tendency to ‘submergently’ connect them, and students who do not show a consistent tendency to form neither emergent nor submergent connections. We have shown that these students’ behaviors are in agreement with their cognitive styles, and affect both the way they solve conceptual problems, as well as the way they interact with and interpret a computer simulation of emergent phenomena.
Students with a consistent tendency to emergently connect different representation modes tend to learn from simulations which present the emergent nature of concepts they are familiar with, but question the emergent mechanisms presented in the simulation of advanced topics. However, after being confronted with a demand for a mechanistic explanation which undermines their confidence in their previous knowledge, most of them accept and are able to correctly employ these emergent mechanisms while solving conceptual questions. In turn, students with a consistent tendency to ‘submergently’ connect different representation modes have difficulties in learning from simulations which present the emergent nature of subjects they are familiar with, but apparently have no problem in accepting the emergent mechanisms presented in simulations of advanced topics. Students without a consistent tendency either to the emergent or submergent perspectives tend to confuse system and component levels behavior, and have difficulties both in successfully answering conceptual questions and in following and learning from computer simulations of emergent phenomena.

It is suggested that both the discrimination between the system and component levels behavior, as well as the directionality of connecting particle behavior to macroscopic system properties, should be emphasized in teaching. If the emergent directionality is not explicitly addressed, students often tend to implicitly assume a submergent directionality. Nonetheless, when the emergent directionality is explicitly addressed, students who previously tend to assume a submergent directionality become able to recognize and use emergent thinking processes.
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1 Introduction and Theoretical Background

The teaching and learning of chemistry have been the focus of innumerable research works for decades. Researches and teachers have been asking different questions of distinct natures, trying to understand, change and improve both the way chemistry is being taught by teachers, as well as the way it is being learned by learners. Many obstacles were found in students’ route to mastery. One of them, which has been repeatedly quoted, stems from the threefold manner of representing chemistry.

1.1 Introduction

1.1.1 The Threefold Manner of Representing Chemistry

When addressing chemical phenomena, there are three modes of representation that can be employed: macro mode – description of tangible and visible properties; sub-micro mode – explanation in terms of invisible and untouchable particles; and symbolic mode – representation by a formula or an equation (Johnstone, 1991). This threefold manner of representing chemistry has been identified as a main obstacle to learning chemistry, because students often experience difficulties in connecting the different representation modes (e.g. Dori and Hameiri, 2003; Gabel, 1999; Johnstone, 1991; Treagust, Chittleborough and Mamiala, 2003). When teaching, teachers constantly move between multiple representation modes, each time using the one (or a combination) that is most appropriate for the situation. However, learners have difficulties both in understanding the role of the representation that is assumed by the teacher, as well as in properly switching between different representations.

The ability to use multiple representations for the same concept, and the ability to easily switch from one representation system to another, is essential for successful scientific thinking. These factors have been found to be the main distinction between novices and experts (Kozma and Russel, 1997), and between unsuccessful and successful students (Bodner and Domin, 2000). In addition, many misconceptions in chemistry are attributed to students’ difficulty in understanding and integrating different representations of chemical concepts (e.g. Abraham, Williamson and Westbrook, 1994; Haidar and Abraham, 1991; Nicoll, 2003; Novick and Nussbaum, 1981; Williamson and Abraham, 1995).
1.1.2 Students’ Difficulty in Connecting Different Representation Modes

A closely related problem is that of conceptual vs. algorithmic problem solving, which was described in several studies (Nurrenbern and Pickering, 1987; Sawrey, 1990 and Nakhleh, 1993). In these studies, undergraduate students were given pairs of questions with similar content, one expressed as an algorithmic question (solvable by manipulating a symbolic formula), and the other as a conceptual question (requiring consideration of sub-micro diagrams). They all found that while most of the students were able to solve the algorithmic question, only a small part succeeded in solving the conceptual one. In other words, there was a large mismatch between students’ abilities to solve these two kinds of problems.

One possible explanation for this mismatch is that many students fail to connect the symbolic representation of a system with its sub-micro representation. Therefore, their successful utilization of one representation mode does not give them any advantage when dealing with the same question presented using a different representation. An alternative explanation is that students do make connections between the symbolic and sub-micro modes of representation, but these connections are inappropriate, or non-scientific, and lead them to an incorrect conceptual conclusion. Such inappropriate connections between representation modes have been documented for the macro and sub-micro modes. It was shown that middle school students tend to attribute macroscopic properties to sub-micro particles, such as ice molecules being colder than molecules of liquid water (Lee et. al, 1993), atoms having the color of the substance they compose (Albanese and Vicentini, 1997), or oxygen and carbon dioxide molecules intentionally moving towards an area of lower concentration (Chi, 2005).

We propose that undergraduate students often make inappropriate connections between the symbolic and sub-micro modes, analogous to the connections between the macro and sub-micro modes made by middle school students. Such inappropriate connections lead students to misapply their symbolic algorithmic knowledge when formulating sub-micro conceptual explanations.

This research is comprised of two stages. In the first one we have used a qualitative approach to probe the way experts and novices represent scientific concepts and move between different representation modes. The questions that guided this part of the research were: Which representation modes do students use when solving
conceptual problems? How do they connect between different representation modes, if at all? Our findings demonstrate that both explanations suggested above (no connection vs. inappropriate connection) are viable: there are cases in which students fail to make any meaningful connection between the symbolic and sub-micro modes, and there are cases where inappropriate connections are made between these two modes. Following these results we defined the questions that guided the second research stage: Does the way in which students connect different representation modes change as a result of the interaction with a computer simulation, and if so, how?

1.1.3 Computer Simulations in Chemistry Teaching and Learning

Computer simulations are computer generated, dynamic models of the real world and its processes (Smetana and Bell, 2007). They are flexible tools which present theoretical and simplified models of chemistry phenomena, and thus can provide many advantages to support chemistry teaching and learning. Indeed, computer simulations have been successfully used for different purposes in chemistry education, for example as a visual aid during chemistry classes, as assigned activities in computer laboratories, and as part of the assessment of conceptual questions, or of classes, prior to formal instruction (Hargrave and Kenton, 2000; Sanger, Campbell, Felker and Spencer, 2007; Williamson and Abraham, 19951). In addition, computer simulations can provide dynamic visualization of both macroscopic phenomena and sub-micro atomic and molecular behavior.

Based on this characteristic, several visualization tools were developed to improve students’ ability to connect different representation modes of chemical concepts, and to translate information expressed in one representation mode to another (e.g. ChemSense by Schank and Kozma, 2002; CMM by Barnea and Dori, 1999; eChem by Wu, Krajcik and Soloway, 2001; 4M:CHEM by Russel et. al., 1997). These tools can provide either a single view or simultaneous views of multiple representation modes, such as molecular animations and graphs or diagrams of macroscopic properties or structures. The simultaneous views are displayed in a separate frame.

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1 Some of these works describe the use of computer animations. As in the eyes of the end user most of the time there is no difference between computer animations and computer simulations of scientific phenomena, we decided not to differentiate between them in the context of this study. Computer animation is the art of creating moving images via the use of computers, and is not necessarily based on scientific models of the real world phenomena, like computer simulations.
each, and are simultaneously updated when the user performs an action in one of the frames. This provides explicit links between different representation modes.

We designed and implemented two computer simulations, with the purpose of guiding students in constructing appropriate and meaningful connections between different representation modes of several chemistry concepts. The design of the computer simulations was based on our previous findings: We first characterized the connections between different representation modes (the first research stage), then applied this characterization to computer simulations (the second research stage).

1.1.4 The Efficiency of Computer Simulations

Promising results were described regarding the use of such ‘multiple linked representations’ tools. For instance, Schank and Kozma (2002) concluded that ChemSense facilitates representational ability and chemical understanding of sub-micro mechanisms; Wu, Krajcik and Soloway (2001) found that eChem facilitated the development of translation abilities. Similarly, most of the studies investigating the use of computer simulations in chemistry education describe promising results (e.g. Geban, Askar and Ozkan, 1992; Hargrave and Kenton, 2000; Sanger, Campbell, Felker and Spencer, 2007; Williamson and Abrahm, 1995). In a comprehensive review of literature about the use of computer simulations to support science instruction and learning, Smetana and Bell (2007) found that over the 40 studies reviewed, 32 demonstrated positive impacts.

Nonetheless, there are studies which present different conclusions: several reviews of literature on dynamic visualizations, such as computer animations and simulations, failed to show a clear advantage of dynamic displays over the static ones (e.g. Hegarty, 2004; Tversky, Bauer-Morrison and Bétrancourt, 2002). A possible explanation proposed is that simulations were often found to be too complex or too rapid for accurate perception (e.g., Hegarty, Kriz, and Cate, 2003; Schnottz, Bockheler, and Grzondziel, 1999). In addition, computer simulations were found to be quite ineffective when used in isolation, rather than in conjunction with other instruction methods (Cavin and Lagowsky, 1978; Hsu and Thomas, 2002).

In the light of these contradictory conclusions, we decided to use a qualitative approach in order to probe deeper and gain a better understanding of the effects of the interaction with a computer simulation. Moreover, this approach enabled us to deal
with an important question that has not been addressed by most previous works: What sets back those students who did not show improvement? Our findings demonstrate that the inappropriate way students make connections between the symbolic and sub-micro representation modes leads them not only to incorrect conclusions while solving conceptual questions, but also to incorrect interpretations of computer simulations.
1.2 Theoretical Background

1.2.1 From Representation Modes to Representation Levels

The three modes of representation are often referred to as ‘levels’, which implies that there exists a hierarchy or order between them. However, there are different criteria that can be used to order the levels, resulting in different meanings to the concept of ‘representation level’. The common use of the names ‘macroscopic level’ and ‘microscopic level’ may suggest that these two are levels of observation, and that the ordering criterion between them is one of magnification. Such a view is problematic, as it may lead to the misconception that the only difference between the sub-micro particles and the macroscopic substance is one of size, while all other properties remain the same (Wilensky and Resnick, 1999). The popular (but misleading) definition of a molecule as the smallest division of a compound that still retains or exhibits all the properties of the substance, is an example of this view.

When Johnstone (1991) first introduced the three modes, he addressed them as ‘levels of thought’, and used a triangle to graphically represent the relations between them. He put the submicro and symbolic modes at the base of the triangle, and the macro mode at the apex. Johnstone was concerned about the lack of students’ familiarity with abstract concepts (associated with the submicro and symbolic modes), and that over-reliance on such concepts in teaching creates a cognitive overload on students’ working memory (Johnstone, 1993). In both of these papers, he emphasized the cognitive difference between concrete concepts that arise from everyday macro-level experience and the abstract nature of concepts that arise from the sub-micro and symbolic levels.

![Figure 1: Johnstone’s “levels of thought” classified into levels of abstraction.](image-url)
This suggests a classification of the modes into **levels of abstraction**, with sensory experience as an ordering criterion (see Figure 1).

A very different meaning of levels comes from the science of complexity, which deals with systems of interacting components, and their emergent properties. An **emergent property** is a property of a system that is not a direct sum of the properties of its components. The emergent view describes properties at the system level as arising from interactions between objects at the component level (Penner, 2000; Wilensky and Resnick, 1999). Within this view, we can explain phenomena at the macro level as emerging out of the mechanical interactions of numerous ‘agents’ at the submicro level, like atoms or molecules, rather than directly reflecting the properties of these agents. For example, while individual gas particles do not have a ‘tendency’ to expand in all directions, a macroscopic sample of gas acquires this tendency from the random collisions between its constituent particles. Understanding of a macro-level phenomenon is realized by describing a submicro-level mechanism that produces it. This view classifies the representation modes into **levels of complexity**, with emergence being the ordering criterion.

The levels of complexity view emphasizes the following:

1. Objects at the submicro level act differently and have different characteristics from the macro-level phenomena; for instance, the atoms comprising a motionless piece of solid gold are neither motionless nor gold colored.
2. There is a distinct direction for relating the levels — the submicro particles do not inherit the macro-level properties of the substance, but rather the properties of the substance arise from interactions of the particles.

How does the symbolic mode fit into this classification? The symbolic mode is used to represent both the macro and the submicro levels (Gabel, 1999), and in general cannot be classified as a distinct level of complexity. However, in the context of algorithmic problem-solving, the symbolic mode is mostly associated with relations between observable properties of substances (e.g., the relation between temperature and pressure in a gas, or between the masses of reactants and products in a stoichiometric reaction), and rarely describes interaction of particles. In such a context, the symbolic mode should be classified as a system-level representation, at the same level as the macro mode of representation (see Figure 2).
1.2.2 Connecting Representation Levels: Emergent vs. 'Submergent' Connections

When solving conceptual questions, a student is expected to specify how the behavior of submicro particles produces the macro-level properties and symbolic relations. The ability to explain system-level properties and relations as arising from the interaction at the component level requires an emergent perspective. Unless explicitly taught, this perspective is often beyond the intuitive reach of students (Wilensky and Resnick, 1999). For example, middle school students are likely to base their thinking on what they experienced at the macro level (Johnstone, 1991, 1993). This explains why many students at this stage tend to confuse levels of complexity with levels of observation (Albanese and Vicentini, 1997; Chi, 2005; Lee et al., 1993). Starting from what they see or feel at the macro level (e.g., coldness, color, or direction of flow), they project these properties or behaviors onto the intangible sub-micro particles. They expect the components to act as small copies of the observable system, or to intentionally move in a direction that fulfills the goal of the system (e.g., particles moving deterministically from an area of high concentration towards an area of low concentration).

This is the exact opposite of the emergent perspective. To emphasize that in this view properties of the high complexity level (system) are imposed on a lower complexity level (component), we call this view a submergent perspective (see Figure 2). In addition, at the undergraduate level one would expect students’ thought processes to also involve symbolic representations. Since, in the context of this study, the symbolic mode is considered a system-level representation, projecting system-level symbolic relations onto their components is also considered a submergent perspective.
Another example of submergent perspective can be seen on teleological explanations. In general, explanations are answers to ‘Why?’ questions and often include conjunctions such as ‘because’, ‘therefore’, ‘in order to’ and so forth (Taber and Watts, 2000). Teleological explanations are answers to ‘Why?’ questions in which the properties and behavior of objects at the component level are explained as deriving from, or directed to, a desired goal at the system level. In such explanations the ends are used as causes for the way certain functions are built, and objects at the component level are considered as having purposes or functions (e.g. “Each group of valence electrons around a central atom is located as far away as possible from others in order to minimize repulsions”, or “The intestine of vegetarian animals is longer than that of meat eating animals in order to be able to digest larger volumes of food which are needed for normal functioning of the vegetarians” (Keil, 2006; Talanquer, 2007; Tamir and Zohar, 1991). This is in contrast to emergent explanations, which are built in terms of the properties of objects at the component level and their interactions (e.g. ‘each group of valence electrons around a central atom repels the other groups, therefore the minimum energy configuration is one where each electron group is located as far away as possible from others’, or ‘vegetarian animals can digest larger volumes of food than meat eating animals because their intestine is longer’).

1.2.3 Emergency within Visualization Tools

Computer animations and simulations have been widely used in chemistry education. Among other goals, they have been used to improve students’ ability to connect different representation modes. Many visualization systems were designed and developed with this purpose in mind (e.g. Schank and Kozma, 2002; Barnea and Dori, 1999; Wu, Krajcik and Soloway, 2001; Russel et.al., 1997). The fact that different representation modes are often treated as representation levels is also salient within these systems, and the hierarchy according to which the representation levels are ordered is implicit in the design of the system. For example, Wu, Krajcik and Soloway (2001) designed eChem to support what they called ‘multiple linked representations’. They enable students to make connections between molecular models at the “microscopic level” (molecular structures) and their collective behaviors at the “macroscopic level” (chemical and physical properties derived by their position in the periodic table).
Wu, Krajcik and Soloway (2001) defined macro representations as those referring to macroscopic observable phenomena and sub-micro representations as those referring to the sub-microscopic nature, arrangement, and motion of molecules. Nonetheless, within this view it is difficult to place the symbolic representation, which can represent concepts at both the macroscopic and the microscopic levels. They then referred to the different representation modes as ‘levels of abstraction’: “Learning microscopic and symbolic representations is especially difficult for students, since these representations are invisible and abstract while students’ understanding of chemistry relies on sensory information”. Overall, the definition of representation levels is not clearly stated, and sometimes gives rise to ambiguities.

This situation is not unique to eChem. It is present in most visualization systems which enable multiple linked representations. Such characteristic is problematic, as it may lead to misconceptions which can either make it difficult for students to make connections between the different representation modes, or induce them to make inappropriate connections. In addition, there is no guidance on how to connect the different representation modes, and no reference as to how the structure and behavior of submicro particles produces macro level properties and symbolic relations. This requires an emergent perspective, within which representation levels are seen as levels of complexity.

ChemLogo (Stieff and Wilensky, 2002) is one of the few visualization systems designed to focus on the emergent nature of chemistry concepts. It is a chemistry modeling and simulation package that teaches chemistry from the perspective of emergent phenomena. ChemLogo consists of a number of particular computer-based models within which thousands of objects at the component level draw themselves on the screen. By that, the overall behavior of all these component objects’ constitute the behavior at the system level, and macro level patterns in chemistry result from the interactions of many particles at a submicro level. For example, students can observe how the collisions between two nitrogen dioxide molecules can result in the formation of one dinitrogen tetroxide molecule and, as a result, the macro level concentrations of each chemical species change as reactions occur (Stieff and Wilensky, 2002). Similarly, the emergent aspect of chemical concepts is emphasized also in the two computer simulations we developed in the framework of this research.
ChemLogo is written in the multi-agent modeling languages StarLogoT and NetLogo (Wilensky, 1997; Wilensky, 1999; Wilensky, 2000). Within these languages system level characteristics emerge from the properties of thousands of agents at the component level. This results in computing demanding simulations, and it is difficult for the user to concentrate on the behavior of an individual agent. We thus decided to implement our simulations in Java. With only dozens of agents we developed two simulations which run fast on every computer platform, without the need for special software installation. They enable the user to see the emergent nature of several chemical concepts, as well as to focus on the behavior of specific agents. The simulations show the user how changes in the behavior of submicro particles (agents) produces changes at macro level properties (such as temperature and pressure) and symbolic relations (such as PV=nRT).

1.2.4 Designing Computer Simulations

The language in which a computer simulation is written and how many particles are simulated are only two of the many parameters to be chosen when designing and implementing a computer simulation. The overall process of determining the principles and characteristics that guide the design of a visualization tool is a difficult task, and it has been the focus of numerous research works (e.g. Chandler, 2004; Mayer, 2003; Rieber, Tzeng and Tribble, 2004; Wu and Shah, 2004). In most of these, the high cognitive demands of learning from dynamic visualizations are pointed out, and the importance of basing the design of dynamic visualizations on existing theories of learning has become a central issue.

There are many learning theories of distinct natures; however, when addressing learning through multimedia and visualization tools the Dual Coding Theory (Clark and Paivio, 1991) occupies a primary role. It is an empiric theory based on a major assumption called The Dual Channel Assumption. According to this assumption humans possess separate information processing systems for visual and verbal representations. This assumption has been supported also by cognitive science researches about the nature of human learning (e.g. Baddeley, 1992; Kozhevnikov, Hegarty and Mayer, 2002; Mayer, 2003). The Dual Channel Theory defines two different kinds of links between the visual and verbal systems: referential connections, which join verbal and visual codes allowing operations such as imaging.
words and naming pictures; and **associative connections**, which join representations within verbal and nonverbal systems. Furthermore, it predicts that more and effective learning should result when information is encoded both visually and verbally, and connections are made between the visual and verbal codes (referential processing).

This prediction was reinforced by several further studies, which emphasize the crucial role of relating verbal and visual information (e.g. Clement, 2005; Mayer, 2003; Wu and Shah, 2004). Following these studies Rieber, Tzeng and Tribble (2004) investigated the role, timing and structure of explanations during an interactive computer-based simulation. They looked for “the right mix” between verbal and visual information to maximize referential processing and learning. Their results show that explanations should be on one hand brief enough so that they do not interrupt the interactive nature of the simulation, and on the other hand wide enough to provide sufficient guidance and opportunity for reflection.

We added explanations to our computer simulations through two learning activities. The learning activities were designed to accompany the simulations, and had two main purposes: guide students about what they are seeing in the simulation on every step, and encourage them to reflect about possible reasons which explain the mechanistic nature of the simulation. Since in the context of this study the learning activities were applied through individual interviews, this was done through personal explanations. A special emphasis was put on one hand on the individual pace of each student, and on the other hand on the continuity of the computer simulation based activity.

The way we designed and applied the learning activities also goes in accord with other principles which were found to improve students’ learning while interacting with a computer simulation. For example, students were found to learn more deeply when words are presented personally, in a conversational manner, rather than in a formal style (Mayer, 2003). In addition, the learning activities are designed according to the Predict-Observe-Explain (POE) model purposed by White and Gunstone (1992). Students are first asked to **predict** what will happen in the simulation if some existing parameter or condition will be changed, and explain the reasons for such prediction. They then **observe** what happen in the simulation as a consequence of the change, and finally **explain** what they saw, whether or not it was in accordance with what they predicted, and why they think it happened. This approach was shown to significantly
improve the effectiveness of computer simulations (e.g. Tao and Gunstone, 1999; Zacharia, 2003).

The process of asking students specific questions about the simulation also aims to help them overcome other difficulties, for example difficulties in interpreting chemical equations as a process rather than as a composition of letters, numbers and lines (Wu, Krajcik and Soloway, 2001). We guided students on how to connect between symbolic equations and submicro representations through questions like: How is each parameter of the equation PV=nRT represented in the simulation (through the behavior of particles)? How has the change in particles’ velocity affected the relation described in the equation? Students working with molecular dynamic simulations were also found to have difficulties in relating the visual representation of particles (moving spheres or circles) with the concept they represent (atoms or molecules) (Jones, Jordan and Stillings, 2005). Again we included in the simulation based activity specific guiding and clarifying questions such as: According to particles’ distribution and behavior, can you recognize which physical state we are seeing in the simulation? Why do you think so?

1.2.5 The Visualizer and Verbalizer Cognitive Dimension

Asking students questions while interacting with a computer simulation adds verbal information to a primary visual information system. Parallel to this classification of information as visual and verbal and to the Dual Channel Assumption, there is The Visualizer-Verbalizer Hypothesis. According to this hypothesis some people are better at processing visual data, such as pictures and animations, while others are better at processing verbal data, such as words (Mayer and Massa, 2003).

A great effort has been invested for decades to quantify and classify the visualizer-verbalizer individual differences (e.g. Bodner and Guay, 1997; Borich and Bauman, 1972; Hegarty and Kozhevakin, 1999; Lean and Clements, 1981; Leutner and Plass, 1998; Mayer and Massa, 2003; Price and Eliot, 1975; Richardson, 1977). However, a major obstacle in understanding these differences concerns how to conceptualize and measure the visualizer-verbalizer dimension. Different studies decompose it into distinct factors, and technical terms are not used consistently in the literature. Among these, there are three distinct but related terms that are further referenced in the present study: cognitive ability, cognitive style and learning style.
Cognitive abilities are brain-based skills and mental processes that are needed to carry out a task (Massa and Mayer, 2006). For example, a person possesses either high or low spatial abilities. Such abilities refer to the proficiency in creating, holding, and manipulating spatial representations. On top and based on these cognitive abilities, cognitive styles are defined: Similarities in mental abilities among individuals define tendencies to process information in certain ways. These tendencies are cognitive styles. “They are consistent and stable over time, regardless of content information” (Jonassen and Grabowsky, 1993). Individuals with a tendency to process information verbally are called verbalizers, while those with a tendency to process information visually are called visualizers. Verbalizers thus have good verbal abilities, such as good communication skills and rich vocabulary. Visualizers in turn have good imagery abilities, such as the ability to perform complex spatial transformations or to remember detailed and vivid images.

A term that is tight related to the individuals’ cognitive style is their preferred learning style (sometimes called learning preferences). While cognitive style is the tendency to use visual or verbal modes of knowledge representation and thinking, learning style is the preference for receiving instruction involving pictures or words. These two terms were found to be highly correlating, i.e. individuals who tend to use visual representations of knowledge prefer to receive instruction which involves primarily pictures, while individuals who tend to use verbal representations prefer to receive instruction which involves primarily words (Massa and Mayer, 2006). Therefore, although the exact terms to characterize different individuals according to their learning style are ‘visual learners’ and ‘verbal learners’, they are generally called visualizers and verbalizers in the literature. In this research we characterize students according to their cognitive style.

There are innumerable tools, instruments and tests designed to assess the verbal-visual cognitive style dimension (e.g. Kit of Factor-Referenced Cognitive Tests by Ekstrom, French and Harman, 1976; The Perdue Visualization of Rotation Test by Bodner and Guay, 1997; Verbalizer-Visualizer Questionnaire by Richardson, 1977). These tools evaluate, among other factors, the extent to which different people habitually use imagery. Nonetheless, there is controversy concerning the nature of imagery and which factors should be evaluated. Kozhevnikov, Hegarty and Mayer (2002) believe that imagery is “not general and undifferentiated but composed of
different, relatively independent visual and spatial components”. Visual imagery refers to a representation of the visual appearance of an object, such as its shape, size, color, or brightness. Spatial imagery refers to a representation of the spatial relations between parts of an object, the location of objects in space and their movements, and is not limited to the visual modality. Based on this assumption they suggest revising the visualizer–verbalizer cognitive style dimension to include two types of visualizers: those whose imagery is primarily pictorial (called object imagers) and those whose imagery is primarily spatial (called spatial imagers). These are the terms used further in this study to discuss the relation between students’ cognitive styles and the ways they interpreted the computer simulations and solved the conceptual questions.
1.3 Research Objectives

This research is comprised of two stages. In the first we characterized the connections between different representation modes. In the second stage we used this characterization to design, implement, apply and check the influence of two computer simulation based learning activities. In both stages we have used a qualitative approach. In the first stage we probed the way experts and novices represent chemistry concepts and move between their different representation modes. The questions that guided this part of the research were: Which representation modes do students use when solving conceptual problems? How do they connect between different representation modes, if at all? In the second stage of the research we used inferences from the first stage to design and implement two computer simulations and two computer simulation based activities respectively. We then probed the way students interact with the computer simulation based activities. The questions that guided this stage of the research were: Does the way in which students connect different representation modes change as a result of the interaction with a computer simulation, and if yes how?

Due to the qualitative nature of the research, the theoretical framework of the second stage was defined only after the full analysis of the first stage. Therefore, I will describe the methodology and results of each stage in a separate chapter. Each chapter will briefly describe the specific research objectives and questions, followed by a detailed description of the relevant research tools, population, methods used for data collection and analysis, as well as the analysis results. At the end of each chapter I will include a Discussion section, were the meaning of the results presented will be discussed by contrasting our findings with previous work.
2 Characterization of the Connections between Different Representation Modes

During this stage of the research we aimed to characterize the way experts and novices represent scientific concepts and move between different representation modes. We used students’ difficulties to solve conceptual problems as a trigger to highlight the differences by which students and experts explain and use different representation modes of chemistry concepts. The questions that guided this stage were: Which representation modes do experts and students use when solving conceptual problems? How do they connect between different representation modes, if at all? To answer these questions we applied a qualitative approach based on clinical interviews, as described below.

2.1 Methodology

An interview protocol was designed to expose which representation modes students use when solving conceptual problems, and how they connect between them. We first used the protocol with senior faculty members, to test the instrument and see if it reveals the modes we expect experts to use and the connections we expect them to make. After verifying that we can identify these modes and connections with experts, we used the same protocol with students. To increase sample variance, we used both undergraduates and graduates as our student population.

2.1.1 Participants

A total of 16 participants took part in this research: 6 senior faculty members, 4 graduate and 6 undergraduate students. Three of the senior faculty members specialize in organic chemistry and three in physical and theoretical chemistry, all of them at a large research university. The graduate and undergraduate students were all chemistry majors at the same university. The undergraduate students were either in their first or second year of study, and all had completed a course in general chemistry before being interviewed.
2.1.2 Data Collection

A think-aloud protocol interview was conducted with each participant, encouraging them to verbalize their thoughts as they discuss scientific concepts and solve conceptual problems. The interviews were semi-structured, i.e. the primary questions were pre-planned and standardized in order to minimize interviewer effects (Patton, 1990), but the course of the interviews varied depending on student responses. The interviews lasted from 25 to 60 minutes. Most of the interviews with scientists and graduate students lasted about 30 minutes, while most of the interviews with undergraduate students lasted about 45 minutes.

The interview was comprised of two topics: the effect of temperature on pressure in gases, and heat conductance via a solid vs. via a vacuum. The questions in the first topic focused on the concepts of gas pressure, gas volume and temperature. First, the ideal gas equation \((PV = nRT)\) was presented. The interviewees were asked to explain what meaning they find in the equation, what is its domain of validity, and if and how they have used it in the past. This was followed by a conceptual problem (see Appendix A) depicting a particulate level diagram representing the distribution of gas molecules in a tank. The interviewees were asked how this distribution would change if the temperature of the gas was reduced (Nurrenbern and Pickering, 1987; Sawrey, 1990). The second topic focused on the concepts of heat capacity, heat conductance and temperature. The equation relating heat to temperature change \((Q = mc\Delta T)\) was presented\(^2\), and the interviewees were asked about its meaning. This was followed by a conceptual problem (see Appendix B) depicting two glass\(^3\) pots filled with water, one with a partially hollow base. The interviewees were asked which pot will conduct heat faster from an external heat source into the water.

In both topics, the equation that was presented related only macro level concepts, while the correct solution of the conceptual question required consideration of the interactions between sub-micro particles. The diagram in the first topic explicitly

\(^2\) Newton’s law of heat transfer might have been a more appropriate equation for this topic. However, this equation is not a part of the undergraduate chemistry curriculum in Israel. We resorted to use a more ubiquitous equation which deals with heat and temperature change.

\(^3\) Metal pots seem to be a more natural choice for this question. However, heat conductance in metals and crystals is a collective quantum phenomenon, which is well beyond the scope of undergraduate studies. In glass, heat conductance can be adequately explained in classical terms, as the interaction between the vibrational motion of neighboring atoms.
portrayed the particles, while in the second it only illustrated the experimental setup on the macro level.

In addition to these pre-planned questions, the interviewer also asked clarification questions, which varied according to the interviewees’ responses. Through these questions, the interviewer encouraged the interviewees to expose their internal representation of the concepts. All interviews were audio-taped, transcribed, and analyzed with Narralizer©, a qualitative data analysis software program.

2.1.3 Data Analysis

We chose the multiple-case narrative approach to analyze how chemistry students and experts represent scientific concepts. The multiple-case narrative is a qualitative strategy that can deal with a large number of narratives, assisting the researcher in identifying similar or distinct characteristics that have become apparent from comparing many case narratives. This method facilitates bringing order and structure to the collected data, and thereby arriving at an understanding of its meaning (Shkedi, 2005).

Data analysis involved breaking down the transcripts of the interviews into building blocks (short text segments that convey a single specific meaning), labeling each segment, and then grouping conceptually related segments into categories. This process is called categorization, and was the main tool used to analyze the data. During the categorization process, different categories are created, which range from descriptive to more general conceptual categories (Shkedi, 2004). The initial categories emerged from comparison between segments, identifying common features and differences in the way different informants addressed the same scientific concept. After these content categories were formed, we tried to find relations between categories, based on the concept of representation levels. We expected that a view of levels of abstraction would fit well with data, but the data proved us wrong. Going back to the literature, we found that the views of levels of observation and levels of complexity better represent the relations between categories. These new theoretical concepts have allowed us to incorporate our initial content categories into an evolved structure of conceptual categories. During the whole process, categories were constantly checked against the original data, to ensure any changes made to the emerging structure still fit the data. In addition, we compared our categories to relevant data in the literature (such
as descriptions of representation modes used by middle school students). This iterative process continued until all of the data fitted logically in a coherent structure, which is in agreement with, but extends upon, previous research.

The end result of the categorization process is an explanation of observed student behavior, generated by coupling together collected data and relevant literature. We thus combine the words of our informants with theories of representation of scientific concepts, to construct a consistent picture of the distinct ways in which university students internally represent scientific concepts, and how they connect between these representations.
2.2 Results

The repeated process of comparison, grouping, and differentiation results in a tree-like structure (Figure 3). This “categorization tree” graphically illustrates the relationships and hierarchies between the categories. The content categories (light gray) are the “leaves” of the tree, and hold the basic building blocks (text segments). The conceptual categories (in white), are more general and abstract – they group categories rather than text segments. The names of the content categories indicate the specific scientific concept the informant was explaining or using in the text segment; the names of the conceptual categories reflect the relation between different modes of representation used for the same concept. Where the same name for a content category appears under different conceptual categories, it means that the same scientific concept has been verbalized in different ways by different informants.

Figure 3: Categorization tree.
The content categories are specific to the scientific concepts we deal with in this research (rectangular leaves), and to the relations between them (oval leaves). However, we believe that the conceptual categories are not restricted to these specific concepts and can be generalized to other scientific concepts as well.

The tree is presented “upside-down” (“root” up and “leaves” down), to reflect the generalization hierarchy of the categories. The higher the category in the tree (the closer to the “root”), the more inclusive it is. At each branching point, the left branch represents the more advanced scientific view, and the right branch represents a less sophisticated view. All the text segments of faculty members reside in the leftmost branch.

In the following sub-sections, we will explore each branch in the categorization tree. The specific branches will be illustrated in each sub-section. We encourage the readers to use them and figure 3 as a roadmap to guide them through the process, as we illustrate the meaning of the conceptual categories with representative text segments. The names of the interviewees in the examples have been changed to protect their privacy.

2.2.1 System Only vs. Connected Representation Levels

We found two major ways of representing a scientific concept, each of which corresponds to a different branch of the main category, representation of scientific concepts: either by using only a system level representation or by connecting the system and component levels (see Figure 4).

![Diagram of representation categories](image)

*Figure 4: Sub tree which focuses on the two major ways of representing a scientific concept.*
We did not find any representations that were restricted to the component level alone—sub-micro particle representations were always connected to other representation modes.

The content category that showed the most distinct differentiation between system level and connected representations was explaining the relation between concepts in an equation. All faculty members explained the meaning of the equations by integrating all three representations modes:

Q: What is the meaning of $PV = nRT$?

A: If you think about the [thermal] expansion of gases, you have a linear graph of expansion, or $PV/T$ is a constant for ideal gases. And then you get to a discontinuity at 0, and the graph looses its physical significance. The molecules don’t just vanish; there is no zero volume; very small, but not zero. […] But when you consider the kinetic explanation, you take $mv^2$, the kinetic energy of molecules. […] The velocity can go down to zero, and then the temperature is zero. Then you understand the connection between molecular velocity, or kinetic energy of molecules, and temperature. (Jacob, faculty – organic chemistry)

In contrast, all undergraduate students and three of the four graduate students focused on the relations between system level variables, without any mention of the underlying structure of the system. They considered the equations as describing mathematical relationships between variables:

This is an equation for ideal gases that can tell a lot about a substance. For example, that there is an inverse relationship between pressure and volume, which is a very important thing. N is the number of moles, R is a constant, the gas constant, and T is temperature. I can learn about the relationships between pressure, volume and temperature. Pressure and temperature are directly related, and so is volume, but pressure and volume are inversely related. (Lea, undergraduate)

or for calculating one unknown variable from other given variables:

This is the ideal gas equation. Pressure times volume equals number of moles times the gas constant times the temperature. From this you can derive all the changes in one variable from all the others. (Shawn, undergraduate).
Another content category that set apart system level from connected representations was that of heat conductivity. When solving the second conceptual problem, all faculty members associated the bulk thermal conductivity of a solid with the motion of its constituent particles:

We need matter to conduct heat because heat conduction is a motion of molecules. If it was a complete vacuum in here, there was nothing to conduct the heat from the heat source to the water. (James, faculty – theoretical chemistry)

In contrast, there were undergraduate students who exclusively referenced the system level when first approaching the same problem. Since no equation was associated with the concept of thermal conductivity, they only used the macro mode of representation. They partially confused thermal conductivity with heat capacity:

The higher the pot’s heat capacity, the stronger it will resist [the conduction of heat]. At some point it won’t be able to resist anymore, and then it will continue to heat the water. (Robert, undergraduate)

and considered thermal conductivity as an inherent property of the system, rather than a process of interaction between its components:

Q: Which pot will heat faster?
A: The vacuum will not allow the heat to come in.
Q: Why?
A: Because it isolates. So it will be easier to heat the solid cooking pot than the one with the vacuum. The solid pot will heat earlier and this will heat the water faster.
Q: Why does vacuum isolate?
A: Hmmm… it repels… it doesn’t let the heat to come in.
Q: Why doesn’t it let the heat come in?
A: It has this property, it repels… it doesn’t accept the heat. (Suzan, undergraduate)

Suzan was finally able to arrive at a sub-micro representation after some more prodding from the interviewer, who asked her to describe a mechanism for heat conduction. Robert referenced the component level only after he was explicitly prompted by the interviewer to consider what happens to the molecules upon heating.

In fact, Robert prevalently used the macro and symbolic modes throughout the entire interview. For example, he initially defined pressure in terms of its relation to other system level variables (symbolic mode):
Q: What is the definition for pressure of a gas?
A: It has to be in a container. Essentially, it comes from this equation. We know the volume of the container, we know the temperature and how many moles of gas we put in, then we calculate the pressure that the gas exerts on this container.

He later explained pressure as the effect of compressing a large object into a small container (macro mode):

Q: How does the gas exert pressure on the container?
A: Usually, if we take a gas under standard conditions, […] if we take the same volume and push it into a smaller container, then it will exert a certain pressure, because the volume of the gas is greater than the volume of the container. Then it has to be compressed in a certain pressure.

His use of the sub-micro mode was very limited. Even when he was explicitly prompted by the interviewer to consider gas molecules, he immediately reverted back to the system level representation:

Q: If I increase the temperature of a gas, what happens to its molecules?
A: The gas expands. But there is an inverse relation between pressure and temperature – if we raise the temperature, then the pressure decreases.

Robert was an extreme case in this regard. The other students did not show such persistence in avoiding using sub-micro mode representations, but most of them still required some prodding before they evoked component level representations. This shows that forming connections between the system level and component level is not a trivial task. In the next section, we will demonstrate that even when students did relate these two levels, the relations many of them formed were quite different from what was expected of them.

2.2.2 Emergent vs. Submergent Perspective

The ability to connect system level and component level representations was not the main contribution to the significant difference between faculty members and students. It was the direction of these connections that most distinctly differentiated

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4 He probably thought about the inverse relation between pressure and volume, and followed the (incorrect) reasoning path: T increases → V increases → P decreases (as described in Rozier and Viennot, 1991).
between the two groups. We found that all text segments of faculty members demonstrate an **emergent** perspective, while many of the students’ segments can be characterized as **submergent**. These distinct approaches define the two branches of the **Connecting the System and Component Levels** category (see Figure 5).

![Figure 5: Distinct directions of the connections between different representation modes.](image)

**Emergent Perspective.** An emergent perspective of phenomena is characterized by deducing system level behavior from interactions at the component level:

Let’s say the gas is comprised of particles; the particles collide with the walls; the collision with the walls creates pressure. […] The moment I looked at the diagrams, I immediately thought ‘particulate model’. According to this approach, it should be divided to the smallest particles that are still relevant to the problem. In this case, the fact that we have H$_2$ is not relevant. The molecular structure of the gas does not change at all. Therefore we can simplify H$_2$ to be a sphere, a particle, does not matter what. Then I asked myself: which particulate theory is relevant to the problem? We can use a theory of motion, a basic mechanistic theory. (John – faculty, theoretical chemistry)

In this case, the sub-micro particles are the components, and the sample of gas in the container is the system. The macroscopic property of the system, the pressure, emerges from the interactions of the sub-micro particles with the walls of the container.

In addition to the faculty members, there were also a few instances where students managed to define and use concepts by connecting the two representation levels in an emergent way. This required some prodding by the interviewer, asking them to give causal explanations:
Q: What does pressure measure?
A: The pressure… it is the force applied outwards…
Q: What is outwards, the container?
A: Its definition, as I remember, is force per unit area. So… yes, towards the container.
Q: How is the force applied?
A: Through their [the molecules’] kinetic energy, they collide with the wall.
Q: So pressure is…
A: The force by which they collide with the walls of the container. (David – undergraduate)

Submergent Perspective. In contrast to the emergent perspective, a submergent perspective is characterized by deducing the behavior and properties of the components from the behavior and properties of the system. We found that many students repeatedly demonstrated a submergent perspective of the presented phenomena, which was guided either by macroscopic properties or by symbolic equations. These form the two branches under the submergent perspective category (see Figure 6).

Figure 6: Submergent connections between system and component levels representation modes.

In the macro → sub-micro branch, macroscopic properties of a substance are taken as known from experience, and then reflected on its particles, giving the particles the same properties as the substance. We found very few examples of this kind of behavior. In one such example, Julia associated the transfer of heat from high to low
temperature (a macro representation) with the flow of hot particles (a sub-micro representation):

Q: How is heat transferred?
A: It moves from the hot place to the cold place by diffusion, by the flow of particles.

This created a conflict with another system level observation, that solids show no observable motion (a macro representation):

Q: How do the particles move?
A: In effect, the heating causes them to move.
Q: Even if it is a solid?
A: The… [long pause]
Q: What is the conflict? I see that on one hand you want to say ‘yes’, but on the other hand there is something that tells you ‘no’.
A: The molecules in the pot, it doesn’t make sense… molecules in a solid…
Q: What doesn’t make sense – that there is motion in molecules of a solid?
A: Yes.
Q: And why do you want to say yes?
A: Because the heat is transferred into the liquid itself [through the pot].

Julia tried to impose her macro representations of heat and solids on the particles, but didn’t know if she should attribute the particles with the stationary character of the solid, or with the ability of heat to move from one place to another. She never considered the possibility that the particles can be vibrating in place, and that the flow of heat emerges from the transfer of motion through interactions between the particles.

The second branch, symbolic $\rightarrow$ sub-micro, is richer than the first. It holds both undergraduate and graduate students’ segments, especially those associated with the first conceptual problem (see Appendix A). In this branch, macroscopic properties of the substance are taken as known from the mathematical equations that describe their relations. In this case, particles acquire specific properties because the system level laws need to be satisfied. For example, when Leo (an undergraduate student) was asked to describe how the distribution of gas particles would change when the temperature is lowered, his first answer was:
OK, I’ll go with (b) [gas particles are concentrated in the middle of the tank], since the product PV should decrease, because you lowered the temperature, and P remains the same.

In his answer, he first considers the ideal gas equation, and gets to the (incorrect) conclusion that the volume of the gas should decrease. This in turn leads him to impose this conclusion on the sub-micro representation, and consider the particles as concentrated in a smaller volume. Later on, he uses macro and symbolic representations to explain how pressure arises from a decrease in volume:

Q: If I reduce the volume of a gas, what happens to its pressure?
A: If you reduced the volume, the pressure will increase.
Q: Why?
A: Both by common sense, and according to the equation – in order to keep the other side of the equation being the same magnitude. This makes sense, if we take something and decrease the volume, the pressure will increase, and vice versa.

He then tries to impose this logic on the behavior of gas molecules:

Q: What makes the pressure increase? What is the pressure of a gas? What happens to the molecules?
A: The repulsion between molecules. After all, the molecules also move, they have kinetic energy, so they collide. I presume that it is all sorts of repulsions that happen between molecules. All the energy is more concentrated now.
Q: But you said there are no forces between molecules in an ideal gas?
A: Ah… [silence]
Q: I want to hear your reasoning. […] What is pressure?
A: Intuitively, I’d say that it is a kind of proximity between molecules. The more crowded they get, the higher the pressure. But this is not really mathematical reasoning…

So even though he knew about all the basic elements needed for an emergent representation (molecular motion, kinetic energy, collisions), he chose to describe pressure as a result of a decrease in volume on the molecular level. This led him to change his initial answer, after he realized that the volume of the container is constant:

If the container stays the same, something on the right hand side was reduced [the temperature in the equation], so something on the left hand side has to be reduced to
keep the relationship. The only thing that can be reduced here is P, since V is a constant. 

[…] Maybe it is (d) [molecules spread out closer to the walls], because if the pressure was reduced, there is more spreading out of the molecules, and this one seems more spread out.

Once again, Leo first assesses the effect of temperature change from the equation (symbolic representation), and then imposes this effect on the behavior of the particles (sub-micro representation).

Elizabeth (a graduate student) used a similar structure of reasoning when answering the same question:

I go straight to the equation, and I say the temperature is directly proportional to the volume and pressure. […] If I reduce the temperature, my pressure will be reduced. What does it mean that the pressure is reduced? The pressure is… hmmm… the number of collisions of the molecules with the walls, and with themselves, OK? […] So if the pressure is low, it means less collisions between the molecules; and if there are less collisions between the molecules, I would expect them to be as far as possible from each other, and therefore the best diagram is (a) [molecules evenly spread throughout the volume].

Even though she basically views pressure as emerging from interactions on the component level, she still exhibits a submergent reasoning perspective overall. She starts her reasoning process with the system level equation, to assess the effect of temperature change on the pressure, and then imposes this effect on her sub-micro representation. The sub-micro representation does not explain the system’s behavior, but rather the other way around.
2.3 Discussion

2.3.1 The Shortcomings of a Submergent Perspective

Our data shows that most of the explanations categorized under submergent perspective involved misconceptions. In the above examples, Julia thought that heat is always conducted via the translation of particles; Leo thought that gas pressure is a result of the proximity of particles; Elizabeth thought that pressure is a result of collisions between particles. If such misconceptions regarding the component level were used as the mechanistic basis for an emergent perspective thought process, these students would arrive to a contradiction with known behavior at the system level. If Julia’s concept had been correct, heat would not have flown through solids; if Elizabeth’s concept had been correct, the ideal gas equation should have included another term associated with molecular size, to account for the increased rate of collisions between larger molecules. Conversely, such component level misconceptions can endure under a submergent perspective without leading to any conflict, because the consequences of going from the component to the system level are never checked. The submergent perspective doesn’t provide a way for students to assess their component level explanations as they form them. Chi (2005) claims that such misconceptions are robust, because their correction requires a conceptual shift in perspective.

Moreover, we found that most of the students using a submergent perspective were unaware of incoherencies or contradictions in their thought process. Only after prodded by the interviewer to make a causal argument justifying their explanation, many of them became aware of the shortcomings in their reasoning. Like Leo said: “This is actually the first time I think about that. I find it hard to define what ‘pressure of a gas’ is.” Until they were confronted with their inability to give causal explanations, these students were sure they understood the scientific concepts under consideration. They became embarrassed and frustrated with the fact that the interview highlighted these shortcomings in their understanding. Many of them said that they are even more surprised because they had performed well on exams. This is in agreement with previous work (Nurrenbern and Pickering, 1987; Sawrey, 1990; Nakhleh, 1993), which showed that the ability to correctly solve numerical problems, typical of exams,
is not necessarily a good indication of the ability to solve conceptual problems. Our research suggests that the difference lies in the fact that while the first requires one to reason only at the system level, the latter requires arguing causally from components to system. Whereas a submergent perspective is sufficient for success with the first, it is inadequate for the latter.

2.3.2 The Central Role of the Symbolic Representation

Previous work (Lee et. al., 1993; Albanese and Vicentini, 1997; Chi, 2005) indicates that middle school students’ thought processes depend on macro representations, which relate to their direct experience with matter. However, our results show that the symbolic representation and symbolic $\rightarrow$ sub-micro branches are much more populated than the macro representation and macro $\rightarrow$ sub-micro branches (see Figure 3). This suggests that in a tertiary level student population, the symbolic representation takes over the role that the macro representation plays with younger students, and exerts more influence on the way they interpret chemical systems. We found that most of our students depended on symbolic equations when they tried to solve conceptual problems, and used them as their trustworthy starting points for a submergent thought process.

The obvious explanation for this would be the difference in cognitive development between the populations, which allows university students to operate more freely with symbolic terms. In addition, it might be that the situations dealt with in university courses are less familiar, and do not lend themselves to representations based on personal experience:

Q: Why was it intuitive for you to use the equation for the gas problem, but not for the pot problem?

A: I can imagine how a pot behaves when you heat it up, I cannot imagine how a gas behaves inside a container. I never saw it. (Robert)

Furthermore, modern science often seems to discourage intuition based on everyday experience:

It is very convenient that there are equations, in the modern world. [Lecturers] are trying to astound us again and again with something that altogether contradicts our intuition. Both in physics and in chemistry, it happens a lot. So we learned pretty fast that usually
our intuition is wrong, and it deceives us. [...] Maybe by graduation intuition will be annulled altogether [laughs]. (Leo)

This leads to a dependency on equations that can sometimes become overwhelming, and the students might not find a way to think about the problem if they don’t have an equation with the relevant variables:

Time, which is generally appears in equations as $t$, does not appear [in the equation $Q = mc\Delta T$]. So I cannot tell you physically, or scientifically, or mathematically how long it will take [to boil the water]. I can tell you that if the mass is changed, the heat will change accordingly, but I cannot say anything about the time because there is no parameter here that tells me this. [...] I am not good at imagining things, that’s the reason I came to do chemistry and not literature! I need an equation: if $t$ equals this and this, and I have this and this, I will tell you that $t$ is faster over here. But here I cannot tell you, it is hard for me to know. (Elizabeth)

The situation reverses again when we examine the faculty members’ answers. Most of them ignored the equations when solving the conceptual problems, and based their answers either on personal experience (via macro representations) or particle theory (via sub-micro representations). They always confirmed their answer by tying these two together, along with the symbolic representation, in an emergent way. These findings support Wilensky (2001), who claims that understanding concepts as emergent phenomena, rather than as results of equations, is a more accurate picture of science.

2.3.3 *Levels of Abstraction vs. Levels of Complexity*

The symbolic and sub-micro representation modes are often treated on the same level, and contrasted against the macro representation mode as being two extreme levels of thought – the abstract vs. the concrete (Johnstone, 1991; Treagust, Chittleborough and Mamiala, 2003). Our data exposes many similarities between the symbolic and macro modes, while drawing sharp distinctions between these two and the sub-micro mode.

In conceptual problem solving, both the symbolic and the macro modes served as anchors for a submergent perspective. They determined the behavior of the system, which was then imposed on its components. In the emergent perspective, both were the
target of thought process, which showed how the system’s behavior (represented either in symbolic or macro modes) can be deduced from the interactions of the components (represented in the sub-micro mode).

In terms of the major representation used in discussing chemical systems, the symbolic mode replaced the macro mode as the population changed from middle school to university students. The difficulties in relating these two modes to the sub-micro mode remained the same, regardless of population.

When students failed to connect different representation modes, the only modes they used were either macro or symbolic. We did not encounter any instance in which students made do with a sub-micro representation, without connecting it to either one of the system level modes.

The opposing roles that symbolic and sub-micro modes played throughout, as well as the similar roles of symbolic and macro modes, indicate that a levels of complexity view offers a better interpretation of our data than levels of abstraction (see Figure 2).

In the next chapter I will describe the second stage of the research, in which we use the levels of complexity view of representation modes and their directed connections to design, implement and check the influence of two learning activities, each based on a distinct computer simulation.
3 Characterization of the Connections between Different Representation Modes Applied to Computer Simulations

During this stage of the research we aimed to characterize whether and how students change the way they connect and move between different representation modes as a result of interaction with a computer simulation. In order to do that we designed and implemented two computer simulations, and developed two computer simulations based learning activities. We then used a qualitative approach to apply and check the influence of these learning activities.

3.1 Methodology

During this stage of the research we used two main research tools – clinical interviews and two learning activities, each one about a different subject matter. The interviews comprised two parts of four consecutive sections each: a pre-activity interview, a macroscopic demonstration, a learning activity based on an interactive computer simulation and a post-activity interview (based on the same questions as the pre-activity interview). Each part dealt with a different subject matter.

3.1.1 Participants

A total of 14 undergraduate chemistry students took part in this phase of the research. They were interviewed during the second semester of their first year of study, and all of them had completed a course in general chemistry before being interviewed. The interviewees learned at a large research university, and were part of a large number of students registered at the same year. We thus looked for some criteria to help us choose which of these students will take part of this research. The aim of this stage of the research was to check the way students interact and interpret two computer simulations, and how these influence the way students connect between different representation modes. Therefore we hunt for a criteria related to students preferences and ability to learn through a computer simulation, and found students’ cognitive style suitable.

Following this decision, we looked for a validated questionnaire through which we could characterize the students’ cognitive style. Maria Kozhevnikov developed at the Rutgers University, Newark, a Mental Imagery and Cognitive Style (MICS)
questionnaire. The MICS questionnaire was designed to distinguish between three different types of people: object imagers, spatial imagers and verbalizers. This is the instrument we use in this research.

It consists of 45 self-report questions with equal number of questions on object imagery ability (the ability to construct vivid, concrete and detailed images of individual objects), on spatial imagery ability (the ability to schematically represent spatial relations among objects and to perform complex spatial transformations), and on verbal ability (the ability to use verbal-analytical tools to solve cognitive tasks) (15 each). It is a computerized questionnaire, taking approximately 15 minutes. Like other self-report questionnaires, it is based on studies which found that self-rating spatial ability and preferred learning styles strongly correlate with ‘hands-on’ time consuming instruments (e.g. Bryant, 1991; Hegarty et.al., 2002; Mayer and Massa, 2003). It was originally written in English, but to minimize the effect of a foreign language on Israeli students we translated it to Hebrew\(^5\).

In the end, not many students volunteered to participate in the research. Consequently, we did not use this tool to select students, but we did use it to characterize their cognitive style and check its influence on students’ behavior throughout the interviews. From the 14 (random) volunteer students, 6 were characterized as verbalizers, 4 as spatial imagers, and 4 as object imagers (see Table 1). The characterization is according to the student’s highest cognitive ability score (verbal, object or spatial). It is important to note that students characterized as spatial imagers showed low object abilities, as predicted by Kozhevnikov, Hegarty and Mayer (2002). Their mean object ability score was much lower than that of students characterized as object imagers, and lower than the mean score Kozhevnikov found\(^6\) among scientists and engineers (3.28). In contrast, students characterized as object imagers showed also high spatial abilities. These were both similar to those of students characterized as spatial imagers, and above the mean spatial ability of scientists and engineers as described by Kozhevnikov (also 3.28). Possible reasons for such contradictory results will be suggested in the Discussion section.

\(^5\) Maria Kozhevnikov, the author of the MICS questionnaire, did her Ph.D. at the Technion - Israel Institute of Technology. She thus knows Hebrew and validated our translation. She is now at the psychology department of Rutgers University.

\(^6\) According to the values described by Kozhevnikov in The MICS Questionnaire Manual.
<table>
<thead>
<tr>
<th>Name</th>
<th>Verbal Ability</th>
<th>Object Ability</th>
<th>Spatial Ability</th>
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<tr>
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<td>2.20</td>
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<td>Jacob</td>
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</tr>
<tr>
<td>Object imagers (with high spatial ability)</td>
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<td>------------------------------------------------</td>
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<td>Andrew</td>
<td>Verbal Ability: 3.4</td>
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<td>Spatial Ability: 3.47</td>
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</tbody>
</table>

Table 1: Categorization of students' cognitive style.

3.1.2 Data Collection

A think-aloud protocol interview was conducted with each participant. During the interviews students were encouraged to verbalize their thoughts as they discuss scientific chemistry concepts, solve conceptual problems, and interact with a computer simulation. The interviews were semi-structured, containing both pre-planned and spontaneous clarification questions. The clarification questions encourage students to expose their internal representation of concepts and differ from student to student, according to their responses. In contrast to them, the pre-planned questions are fixed and equal to all interviewees, in order to minimize interviewer effects (Patton, 1990).

The pre-planned questions of the pre and post activity interviews are identical to those used in the previous research stage interviews. Between the pre and post activity interviews, the student saw a macroscopic demonstration and interacted with a computer simulation through a learning activity specifically designed for this purpose. The learning activity defined the sequence of the interaction with the simulation, and the pre-planned questions of this part of the interview. As a consequence of the semi-structured nature of the interviews, in spite of the primary pre-planned questions, the
course and duration of the interviews varied depending on students’ responses. The full two parts interviews lasted from 70 to 110 minutes. The first part lasted from 25 to 45 minutes, and the second part lasted from 45 to 70 minutes. Most of the interviews lasted about 100 minutes. In addition to this time, immediately after the interview or between the two parts, as a short break, the students answered to the MICS questionnaire. All interviews were audio-taped, transcribed, and analyzed with Narralizer©, a qualitative data analysis software program. Some interviews, when students consented to, were also video-taped.

The First Part. The pre and post activity interviews dealt with the effect of temperature on pressure in gases. Throughout the pre activity interview each student was first asked to explain the meaning of the ideal gas equation and its parameters, then solved a related conceptual question while thinking aloud (for a full description see Methodology section, Chapter 2). After that the student saw a macroscopic demonstration. We first showed him/her a big glass syringe with an open tip, and asked to explain why the piston inside the syringe falls down when we leave it. We then closed the tip, and asked the student to try to push the piston. After realizing how hard it is, we asked the student to explain why it is so hard, what prevents him/her of being able to push it, and if s/he can explain in terms of particles what happens inside the syringe. Following this demonstration, the student engaged in a learning activity based on the simulation of a gas in a container. The simulation emphasizes the emergent aspect of macroscopic properties of the gas, like temperature, volume and pressure, as well as their relationship. Immediately after the simulation based activity, the post activity interview took place: the student was asked again to solve the same conceptual question and explain the meaning of the ideal gas equation and its parameters (the post activity interview). The pre and post activity interviews were designed to have the same pre-defined questions in order to emphasize the influence of the simulation based activity on student’s perspectives. In the whole course of the interview the student was constantly encouraged to think aloud.

The first learning activity is based on a simulation of gas particles moving in a closed container, under constant pressure. The container has a piston on top, loaded with a weight which symbolizes the downward gravitational pull (see Figure 7).
The piston constantly moves up and down, reflecting the dynamic balance of gravity vs. the upward force applied on it by the collisions of gas particles. Particles are simulated by hard disks, moving according to Newton laws. Some parameters can be interactively changed during simulation, like gas temperature. When the gas temperature is increased, the particles start moving faster, collide more frequently and more forcefully with the walls, pushing the piston up. As the piston moves up, the volume of the gas increases, and the frequency of collisions decreases. The piston finally achieves a certain height where the total upward force applied by the particles is balanced by the weight of the piston.

The other parameters which can be interactively changed are piston weigh and particles’ size (for snapshots of these changes see Appendix C). These specific parameters were chosen according to the main misconceptions that were identified during the previous stage interviews with undergraduate students. In addition, these changes emphasize the emergent nature of the macro level concepts and relations defined by the ideal gas equation. The pre-planned questions asked during this simulation based activity (see Appendix D) are based on these parameters’ changes. Before each change students were asked to predict its outcome, and only after that to describe what happened as a consequence of the change. If there was a conflict
between their prediction and observation, the interviewer guided the student to reconcile it.

Second Part Interviews. The pre and post interviews dealt with heat conductance via a solid vs. via a vacuum. The same four steps process was then repeated for the second subject matter. This time during the pre activity interview the student was asked to explain the equation \( Q = mc\Delta T \), as well as the meaning of each one of its parameters (for a full description see Methodology section, Chapter 2). We then started macroscopic demonstration, along with the student saw a glass thermometer with its base inside an aluminum cube. The aluminum cube is fixed a few centimeters above a candle. Initially the candle is not lit. We asked the student to say which temperature the thermometer is marking. After that we lit the candle, and asked him/her to say what happens with the thermometer, both macroscopically and in term of submicro particles: how the heat is transferred from the fire to the aluminum cube, through the air, how it spreads inside the cube and how it raises the gas inside the thermometer. Finally, we blew off the candle and asked the student again to explain macroscopically and in terms of particles what s/he sees and what s/he thinks is happening inside the thermometer.

Following this demonstration, the student starts the learning activity based on the simulation of two solids and a gas in a very big container. The simulation shows the particulate behavior within a narrow window in this container. We again highlighted emergent aspects of the chemistry concepts we are interested in, such as heat transfer and thermal equilibrium. Once more, the post activity interview comprised the same pre-defined questions as the pre activity interview, and was conducted immediately after the simulation based activity was finished.

The second part simulation based activity is based on a simulation of three different kinds of particles: a gas – argon (in purple), and two solids – gold (in yellow) and aluminum (in gray), moving in space (see Figure 8).
Initially, the gas and solids particles are separated by a thermal isolating partition, with gas particles on top and the gold and aluminum particles on the bottom. All particles are simulated through soft disks affected both by gravitational force, as well as by attraction and repulsion forces according to Lenard Jones Potential Function.

Similar to the previous simulation, some interactive changes can be performed during the simulation. One of them is the removal of the partition. When this occurs, gas particles start colliding with particles of the solids, and energy starts to be transferred between them. As the mean kinetic energy of gas particles is initially higher, most gas particles transfer energy to solids particles when colliding with them. At some point the probability of a particle to transfer energy becomes the same as its probability to gain energy. This stresses the emergent nature of the macro level concepts such as thermal equilibrium. In addition, students can then realize, and are guided by the interviewer to do so, that this is a continuous process: the interactions between particles of the same and/or different substances continue all the time, and energy is constantly either transferred or received by particles. The only difference is the probability at which this occurs.
To emphasize the process of energy transfer, as well as the temperature as a measure of particles’ kinetic energy rather than particles’ velocity (commonly confused by students), we implemented three distinct rendering modes.

Figure 9: Particles displayed in velocity (left) and kinetic energy (right) mode.

In one of them we ‘show atoms’ according to the substance they comprise. Atoms of distinct substance are differently colored (see Figure 8). In another mode we ‘show velocities’. Faster particles are displayed in red, slower in blue, and particles with in-between velocities are displayed in in-between colors (like distinct tones of purple). Similarly, we can ‘show kinetic energy’. Within this mode more energetic particles are displayed in green, less energetic in blue, and in-between tones (like darker greens) are used to display in-between energies (see Figure 9).

This figure depicts gas particles (at the top) and solids particles (at the bottom) in a system at thermal equilibrium. The three substances: argon, aluminum and gold are at the same temperature. We can see that in this situation, as expected, the kinetic energy (right picture) is homogenous distributed among particles of the three substances. However, velocities (left picture) are not. The mean velocity of the Argon (at the top) and aluminum (at bottom left) particles is much higher (more red particles) than that of gold particles (at bottom right). This is due to the difference in their atomic masses.
The kinetic energy, mathematically represented by \( \frac{mv^2}{2} \), depends both on the velocity and on the mass of particles. To highlight this fact we chose the solids to be aluminum and gold, because their atoms are approximately the same size but have very different masses. The molar mass of gold is more than 7 times the molar mass of the aluminum. Therefore when gold and aluminum atoms have the same mean kinetic energy, aluminum atoms are much faster than gold atoms. The gas was chosen to have an in-between molar mass: Argon particles have a mass that is approximately 1.5 times the mass of aluminum particles, but it is still much smaller than that of gold particles.

To emphasize the even more the difference between kinetic energy and velocity, and its relation to temperature, we can keep the overall kinetic energy of the gas constant and reduce either the mass of all gas particles or their number. In the first case the system remains in equilibrium. Gas particles become faster but remain with the same mean kinetic energy. Consequently, the temperature of the gas remains the same. In the second case the equilibrium of the system is broken, as the same amount of energy was given to less gas particles. Each particle becomes more energetic, rising the temperature of the gas (for snapshots of these changes see Appendix E). These changes emphasize the emergent nature of a macro level concept: temperature, and its relation to particles’ motion. The pre-planned questions that guide this and other learning objectives comprise the second simulation based activity (see Appendix F).

3.1.3 Data Analysis

The process of analyzing data was very similar to the one performed in the previous research stage. Data analysis involved breaking down the interview transcriptions into building blocks and then rearranging them according to conceptual categories (Shkedi, 2004). This process, called categorization, was done according to the multiple-case narrative strategy: a qualitative strategy which assists the researcher in identifying similar and distinct characteristics which become apparent from comparing many case narratives (Shkedi, 2005). We used this strategy to identify similar and distinct characteristics on the way students connect different representation modes, and how it influences and/or is influenced by the computer simulation based learning activities.

The categorization process is an iterative process throughout which we constantly reconsidered existing categories according to the emergent and submergent
direction of the connection between different representation modes. Categories were constantly checked against the original data, to ensure the validity and reliability of the process. In addition, we compared our categories to relevant data in the literature (such as the difficulties of students in understanding emergent phenomena), until we reached a coherent structure. This structure is called a grounded theory (Shkedi, 2005). It emerges from data and is both in agreement with, but also extends previous works and theories, offering an explanation of the observed behavior of students which is generated by coupling together collected data and relevant literature.
3.2 Results

The results of the data analysis process will be graphically illustrated through a categorization tree, like in previous chapter. Similarly, the hierarchy is defined according to the height of the category in the categorization tree: the higher the category (the closer to the “root”), the more inclusive it is. The content categories (in light gray) are the “leaves” of the tree, and hold informants’ text segments; the conceptual categories (in white) are the “nodes” of the tree, and are more general and abstract categories (see Figure 10).

The connections between multiple representation modes of scientific concepts were still classified as either emergent or submergent. However, during this stage we refined these definitions and both the emergent and submergent concept categories split in two different branches. Each branch reflects a distinct way to perform an emergent or a submergent connection. In addition, we found useful to define the situation and the context within which the connections were encountered – either during the simulation based learning activities, or during the pre and post-activity interviews; either related to the gas or to the solids subject matter. This classification defines four very similar sub-trees. Each one contains the relevant content categories classified according to the context and the situation they appeared. For simplicity of the illustration we fully describe only one of them in Figure 10. Nonetheless similar sub-trees would appear also under the other three branches of the emergent and submergent categories, where denoted by broken lines.
Figure 10: Categorization tree.
Each text segment in the categorization tree is fully characterized by its path. A path in the tree starts in the root and goes down through specific nodes, until it reaches a leaf. This path “tells the story” of the text segments in the leaf. For example, the path highlighted in Figure 11 characterizes text segments containing emergent connections between multiple representation modes. These emergent connections included misconceptions, which appeared during the simulation based activity of a gas in a container. More specifically, it appeared during interviewees’ explanations regarding what happens to the gas when we change the size of its particles. Each text segment presents a different explanation of either the same or different situations within this event.

Figure 11: Example of a path in the categorization tree.
In the following sub-sections I will describe the meaning of each conceptual category with representative text segments, in which the names of the interviewees will be changed to protect their privacy. The specific branches of Figure 10 will be illustrated in each sub-section. I encourage the user to use these illustrations as a roadmap.

3.2.1 Theoretical Framework

One of the conclusions that arose from previous stage results is that the main contribution to the significant difference between faculty members and students did not come from the ability to connect system and component level representations, but from the direction of these connections. We found that most of the students managed to connect between system and component level representations, but they did it differently from faculty members. While faculty members demonstrate a consistent emergent perspective, many of the students’ demonstrated a submergent perspective. Therefore we chose to:

1. Focus on the way students connect between multiple representation modes, the root of the categorization tree.
2. Keep the same theoretical framework to characterize the distinct approaches to connect between different representation modes: emergent vs. submergent. These are the two branches of the root category (see Figure 12).

![Figure 12: Two distinct approaches to connect multiple representation modes.](image-url)
3.2.2 Submergent Perspective

During the previous stage of the research the submergent perspective was characterized by deducing the behavior and properties of the components from the behavior and properties of the system. We found that many students repeatedly projected system level properties and behavior to particles. They were guided either by macroscopic properties, taken as known from experience, or by symbolic equations, taken as known from the mathematical equations that describe relations between macroscopic properties. These macroscopic properties and system behavior were then projected on particles, giving the particles the same properties and behavior of the system. This kind of perspective contradicts both emergent premises:

1. Objects at the component level act differently and have different characteristics from the system level phenomena;
2. There is a components → system direction for relating the levels – the properties and behavior of the system arise from random interactions of sub-micro particles.

It actually can be described as having opposite characteristics:

1. Objects at the component level reflect system level characteristics and/or behavior;
2. There is a system → components direction for relating the levels – the sub-micro particles inherit system level properties and/or behavior.

This perspective was found also during the present research stage. For example, when I asked Anthony during the pre-activity interview to describe what happens to gas particles when we cool the gas, he considers the relation between two system level properties: gas temperature and gas volume. According to his acquaintance with the ideal gas equation, he gets to the (incorrect) conclusion that if the gas temperature was decreased, also the volume of the gas should decrease. This leads him to project this conclusion on the sub-micro representation, and consider the particles as concentrated in a smaller volume:

Q: In general, when we cool a gas, what happen to its particles?
A: The volume gets smaller

...
Q: Let’s talk by means of particles. We were at a determined temperature, then we decreased it. What happened to the particles?
A: They got closer.

This submergent perspective appeared throughout the computer simulation based activity too. Anthony expected particles to behave in the simulation according to the same system level rules. For example, in the beginning of the simulation Anthony conceives the simulated particles as gas particles because they occupy the whole space inside the container. I then probed him to explain why is it different from the situation presented in the conceptual question, where he assumed gas particles to become concentrated in the middle of the tank after decreasing the temperature of the gas. Even though he had no idea at which temperature is the gas in the simulation, he claimed gas particles will behave the same way – concentrate in a specific region, if we would reduce the temperature of the gas:

Q: Which state of matter do you think we are seeing in the simulation?
A: Gas
Q: Why do you think it is a gas?
A: Because particles are far away from each other, and they occupy the whole container.
Q: So do you think gas molecules occupy the whole container?
A: Yes
Q: But here [in b option of the interview questionnaire] molecules are not occupying the whole container [they are concentrated in the middle of the tank]…
A: Because here [in the conceptual question] the temperature of the gas was reduced.
If you reduce the temperature of the gas in the simulation, particles will become closer as well.

Moreover, Anthony was very troubled when the simulation did not match the macroscopic behavior he expected to. For instance, the piston depicted in the simulation constantly oscillates, in contrast to the behavior of the glass syringe he just observed in the macroscopic demonstration:

A: The weight [loading the piston] is not enough… if you remove this weight, it should stand…
Q: Are you trying to think why is the piston oscillating?
A: Yes
Q: Why do you think it happens?
A: Because the weight loading the piston is too light, compared to the force applied on it.

I then clarified and reinforced his assumption with specific information about simulation parameters:

Q: You are right. The weight loading the piston is very small compared to the mass and number of particles. The mass of the weigh is just 100 times the mass of particles, compared to the glass syringe which is much, much more heavy. In addition, we have here only 50 particles, instead of $10^{23}$ times the number of moles. Therefore the piston in the simulation is always oscillating.

Nevertheless, when afterwards I asked Anthony to predict what we will see in the simulation if I would double the weight loading the piston, he expected to see a static piston:

A: If it [the weight] will be enough, the piston will stop oscillating
Q: What do you think that raises the piston?
A: The collisions [between the particles and the piston].
Q: Do you think we could reach here [in the simulation] the conditions within which the piston will be stable?
A: Yes
Q: And if the weight won’t be enough to stabilize the piston, what do you think will happen?
Q: It will keep oscillating
A: In the same place?
Q: Yes, but may be slower.

After I inserted another weight, I asked him to tell me what he sees. Although the piston height decreased to its half, he still concentrated on what he expected to see, according to system level phenomena:

The question is if it oscillates less now

I needed to probe him to pain attention on the simulation behavior, but he again tried to project on particles a system level behavior. This time based on his answer to the conceptual question, where he concluded that the volume of the gas decreases:
Q: This is the only change you see? Can you see any other change?
A: No… I see also a concentration of the molecules; like in the b drawing option
[molecules are concentrated in the middle of the tank]

Throughout the pre and post-activity interviews Anthony showed difficulties in discerning the mechanical causality of the system level phenomena behavior; throughout the computer simulation based activity he showed difficulties in discerning the mechanical causality in the simulation. Matthew presented similar difficulties. For example, during the simulation Matthew was unable to discern that gas particles have energy and are in constant moving. He thought that the weight loading the piston was a magnet which attracted particles and caused them to move. Furthermore, he thought that if we remove this magnet force, particles will become static:

Q: What do you think the weight on top of the piston indicates?
A: The weight? Oh, now I can see it, it’s a magnet!
Q: Why do you think it is a magnet?
A: Just a minute, I’ll tell you… no, it’s not a magnet.
Q: It is very interesting. Why did you think it is a magnet?
A: It seems that when it [a circle] gets close, it accelerates, like it is being attracted […]
Q: But there are no attraction forces here.
A: I see… Are you asking what does the weight do? What’s its influence?
Q: No, I am asking what it indicates. Why do we have this weight here? What would happen if we remove it?
 […]
A: They [the particles] might not move. First of all the question is: what makes them move?

Like Anthony, Matthew focused on system level representations when trying to explain the changes in simulation parameters, and was unable to coherently connect them to a particulate mechanism:

A: [After witnessing the effect of increasing the temperature under constant pressure] the piston rose. I’ll tell you more than that, the volume increased but the pressure decreased, because P is inversely proportional to V.
Q: Why does the pressure decrease? The particles are moving faster … Are they colliding less with the walls now?
A: There are more collisions in every second [...] but the piston rose, so the volume increased and therefore the pressure decreased… There are many dependent variables here, you know…

Anthony and Matthew presented a submergent perspective similar to this defined during the previous research stage. In general, students who presented this perspective tend to confuse the component level mechanism and the system level phenomena behavior. They tend to project system level properties and behavior to particles. Therefore, we characterized such submergent perspective as system projection.

System projection submergent perspective. Within this perspective the sub-micro representation is defined according to the system level properties and behavior. Therefore the connections between the component level sub-micro representation and the system level macro and/or symbolic representation modes, when existent, are directed from the system level representations to the sub-micro representation. Moreover, as in the great majority of the cases particles do not have the same properties and do not behave the same way the system does, most of this explanations involved misconceptions. Like Anthony who thought that after we increased the weight loading the piston the volume of the gas should decrease, and thus expected gas particles to concentrate in the middle of the tank; or Matthew who thought that some external force should drive particles to move, otherwise they will become static or have “negligible movements”.

This perspective appeared both throughout the computer simulation based activities and throughout the pre and post-activity interviews (see Figure 13). Similarly, misconceptions were encountered both in students’ answers during the pre and post activity interviews, and in their explanations during the simulation based activities. Furthermore, in most cases the misconceptions presented during students’ answers to the pre activity interview guided what they expected to see in the simulation.
Figure 13: The “System Projection” branch of the submergent perspective category.

For example, when I asked Jacob to define what temperature is, he answered “the velocity of particles”. He then expected to see this one-to-one relation also in the simulation. When he saw that the relation between the average velocity of aluminum, gold and argon particles is not the same even though they are supposed to be at the same temperature, he got confused:

Q: [After the system reaches an equilibrium state, and particles are colored according to their velocity] what do you think is the relation between the velocities of particles?  
A: Aluminum is faster, then the gold, and the argon has some of this [faster particles] and some of that [slower particles]  
Q: What does it mean “it has some of this and some of that”? There are faster and slower particles also in the aluminum and in the gold…  
A: But in the argon it is more… I think argon is the slowest. Actually, they all should be the same!  
Q: Why?  
A: Because the temperature is the same.  
Q: Temperature of what?  
A: Of all of them, of the whole system.  
Q: But you said the aluminum is faster, the gold is slower than the aluminum…  
A: The average… I don’t know. […] I am confused right now.
I then probed him to explain why he sees different velocities for different substances if the system is in equilibrium and all its components are supposed to be at the same temperature. He turned to a system level property (heat capacity) to try to find an explanation:

Q: Why do you think the aluminum is faster than the gold, if you think they are at the same temperature?
A: Because its [the aluminum] heat capacity is smaller.

Nonetheless, by saying this he explains that the aluminum is actually at a higher temperature, and therefore its particles should move faster.

In contrast to Jacob, where misconceptions appeared both throughout the interviews and throughout the simulation based activities, there were cases where misconceptions appeared only throughout the simulation based activities. For example, when I asked Elizabeth (during the macroscopic demonstration) to describe how the thermometer standing on the aluminum cube base becomes hot after I light the candle, she hesitated but managed to (correctly) explain it by means of energy transfer between the aluminum particles:

Q: How does the heat reaches the thermometer?
A: It heats it from outside. … It first heats the aluminum cube, then it heats the gas inside the thermometer.
Q: How the heat reaches the cube?
A: It heats the air and then … they [air particles] collide with the cube.
Q: So what they transfer to the metal that heats it?
A: Energy.
Q: And then, what happens to the metal?
A: It gets hot…
Q: What happens to its particles?
A: Its particles… collide with the thermometer?
Q: And then, what happens?
A: They transfer energy to the thermometer.

Nevertheless, during my explanation of what we are seeing on the screen in the beginning of simulation based activity, she got confused. Elizabeth could talk about solids as a collection of particles, like she was taught, but she didn’t see it that way. She could see it for gases, where the system (the gas) behaves similarly to its
components (as moving particles), but not in solids, where the system does not seem to move and looks uniform:

A: I didn’t “see” it this way…
Q: Which way?
A: That it is solid…
Q: That the moving circles here represent a solid?
A: Yes.
Q: I am trying to understand what disturbs you…
A: It seems natural when we are talking about gases, but it is hard to me to think about aluminum as particles, as a collection of particles…

Like Elizabeth, most of the misconceptions found in students who presented a system projection submergent perspective can be characterized by lacking a clear distinction between the component level mechanism and the system level phenomena behavior. This “slippage” between levels is characteristic of the system projection submergent perspective, but this is not characteristic of all submergent perspectives, as we will see in the next section.

Teleological submergent perspective. Within this perspective sub-micro particles acquire a specific behavior because macroscopic and/or symbolic laws need to be satisfied. Students using teleological explanations answer to “Why” questions in terms of the consequences of the event, instead of in terms of the antecedent conditions that are necessary for an event to occur (Talanquer, 2007). For example, when I asked Isabella to explain why particles collide more with the walls of the container when we double the piston weight, she said:

Because they have less space to move; and also because this is what they are expected to do, from a physical point of view. […] When you insert another weight [on the top of the piston], the gas has to apply force in the opposite direction. It is not due to incidental collisions, […] there is a cause for such behavior. […] Particles collide because the system has to reach an equilibrium state; because all system components aspire to reach an equilibrium state, then it happens. This is how I believe things work.”
Like the system projection submergent perspective, also this submergent perspective appeared both throughout the computer simulation based activities and throughout the pre and post-activity interviews (see Figure 14).

![Diagram](image)

**Figure 14:** The “Teleological” branch of the submergent perspective category.

Nonetheless the great majority of the cases were encountered during the simulation based activities. As a result, the simulation branch of the teleological submergent subtree is richer. This is for example the case of Isabella. The teleological perspective was not prominent in her responses throughout the pre and post activities interviews. However, throughout the simulation based activities, specially the first one, related to a gas in a container, this was not the case. In order to predict and explain the particulate behavior she saw on the screen, Isabella needed a system level rule. Like in the example cited above, where she explains that particles collide more with the walls of the container (when we double the piston weight) because physical laws impose particles to apply a force in the opposite direction. She does not believe and does not accept it happens through incidental or random collisions.

Similarly, when she does not find such system level rule, she has difficulties in predicting and explaining what she sees in the simulation. Isabella can only predict the behavior of “creatures” when she knows them and the physical rules which guide their behavior:
Q: I’ll now abolish the particles-particles collisions. Do you think it will cause any change?
A: I don’t know. I can’t think about...
Q: Let’s see: what did we say about the motion of particles?
A: They move in several directions.
Q: Randomly?
A: I don’t know if they all move upwards, downwards or in a line…
Q: What do you think? [All particles move to random directions, there is no rule ordering their motion]
A: I don’t know how you did it, the software
Q: I now just abolished the particles-particles collisions. It means that the spheres we see on the screen move straight forward and if they touch another sphere in their way, they keep moving in the same direction, instead of changing direction.
A: Ha, as they can pass through each other!
Q: Exactly!
A: I don’t know how this creature behaves. You’re inventing here creatures which I don’t know them. I don’t know how they behave.
Q: Why?
A: Because this is not the way gas particles behave.

In addition to cases like Isabella, where the teleological submergent perspective was eminent only throughout the simulation based activities, there were a few cases where it appeared also in students’ answers to the conceptual questions. For example, Mary showed this perspective both during the simulation of a gas in a contained and in her answer to the conceptual question during the pre activity interview. In the course of the simulation she mentioned expressions such as:

Q: [After witnessing the effect of inserting another weight loading the piston] why the molecules collide more with the walls now, if they don’t move faster?
A: Because we dropped the volume.
Q: OK, we dropped the volume, why do they…?
A: Because they [molecules] must do that in order to balance the equation. The ideal gas equation, now you increase the pressure.
During her answer to the conceptual question Mary described a particles tendency to be ordered and closer to each other as the temperature decreases, “looking forward” to the structure of particles in a liquid:

A: If we decrease the temperature [of the gas] so particles will be ordered, this is the way to get a liquid, […] or is hydrogen already a liquid at this temperature [-20°C]?
Q: No, it is far from that.
A: So they [the molecules] will be just more ordered, closer to each other.
Q: Is this a linear process? As we cool the gas molecules become closer and ordered until it becomes a liquid?
A: Yes

I then checked if she projected the relation lower temperature → lower volume to particles, but she didn’t. She knew that gas particles occupy the whole volume of the container until the gas becomes liquid. Nonetheless, she was worried that particles must be ordered and close to each in the temperature the gas liquefies. She thus assigned them a tendency to assemble as the temperature decreases:

Q: When a gas is cooled, does it occupy a smaller volume?
A: No, I think it still should occupy the whole volume [of the container] … so I think it is b) […]
Q: Why?
A: Because on one hand molecules are still in motion, but on the other hand they have a tendency to assemble.

Both Isabella and Mary used many times, explicitly or implicitly, the word **must**: particles are expected to (must) behave like that, from a physical point of view; something must change - if we change particles’ size; molecules must balance the equation; if we lower the temperature particles will (must) be ordered because this is the way to get a liquid. Like Isabella and Mary, students who showed a teleological submergent perspective defined the sub-micro representation as directed to a certain goal, or to fulfill a certain function at the system level. Therefore, on one hand this submergent perspective is different from the system projection submergent perspective, where macroscopic properties and behavior are reflected on particles, giving them the same properties and behavior from the substance. In this case particles can have, and in the great majority of the cases indeed had, different properties and
behavior from the substance. Yet, on the other hand, the properties of sub-micro particles at the component level were still determined based on macroscopic properties and behavior occurring at the system level. Hence both the system projection and the teleological perspectives are different kinds of Submergent Perspectives (see Figure 10).

3.2.3 Emergent Perspective

In contrast to the submergent perspectives, an emergent perspective of phenomena is characterized by deducing system level behavior from interactions at the component level. Similar to faculty members and some students during the previous research stage, during this research stage there were also cases where students described macroscopic phenomena by means of interaction between sub-micro particles. For example, when I asked William during the first simulation based activity (of a gas in a container) to predict what will happen if I double the weight loading the piston, he based his answer on the interaction between particles and their interaction with the piston:

The piston will descend while colliding [with gas particles], until it will get balanced… now [an equilibrium state with one weight loading the piston] it also ascends and descends all the time.

William understood the particulate mechanism behind the simulation, within which the piston is pushed up by the force applied by gas particles when colliding with it. The relation between the number of particles, their mass and the piston weight is such that the piston always oscillates, even when in an equilibrium state. In this case, the piston makes small oscillations without changing its mean height. When I inserted another weight on top of the piston, I asked him: why does it get balanced at all? And: why it doesn’t continue descending until the bottom of the container? He again based his answer on particulate behavior:

A: Because they [the particles] raise it [the piston]
Q: So why don’t they raise it more? When does it stop?
A: It is related to the particles’ concentration. When the particles are very sparse in the container, there are fewer collisions, and fewer particles collide upside and raise the piston. If
we increase the weight [loading the piston], more collisions are needed to raise it. Then the pressure increases.

This was also the way he thought when solving the conceptual question during the pre and post activity interviews. William correctly related gas temperature with particles’ velocity, and deduced the decrease in gas pressure from particles behavior. He then chose the diagram that better depicted his prediction, even though he saw it looks surprising when it is depicted in two dimensions:

A: It may look surprising, but I think it is (a) [the diagram which is similar to the one in the question, before the change in temperature]. They [particles] move slowly on lower temperature, but there is no reason for the distance between them to change.

Q: So what was changed? The temperature changed, particles move slower…

A: Then there are fewer collisions […] so the pressure is smaller. Because particles are moving slower, they less collide with the walls.

Andrew also presented an emergent perspective when answering to several questions throughout the pre and post activity interviews and throughout the simulation based activity. However, in contrast to William, Andrew did not deduce system level behavior from the interactions at the component level, but he explained system level behavior via interactions at the component level. For example, when I asked Andrew about the relation between the temperatures of the argon, gold and aluminum before and after I remove the partition separating the gas and solids particles in the simulation, he answered by relating thermodynamics rules to particles’ behavior:

A: [After witnessing the removal of the partition separating gas and solids particles] the collisions stimulate the solids, giving them energy through the collisions; the collisions stimulate metals’ particles.

Q: So what was the relation between the temperatures [before I removed the partition]? Can you say that now? Was the gas hotter or colder than the metals? (I asked the same question before I removed the partition and he said we haven’t enough information to answer the question).

A: OK, if we think about it by a thermodynamic point of view, so a thermodynamic equilibrium should take place; a thermal equilibrium. If there is a substance at a given temperature, and another substance at a different temperature, so one will transfer heat, and the other will receive it. Then we’ll get to an equilibrium state. As the gas’ particles became slower [he earlier defined heat as a kind of energy], it means that they
transferred heat [through gas-solids particles’ collisions]. If it transferred heat, it means that it was at a higher temperature than the solids, and in this way they got to a thermal equilibrium.

William and Andrew presented a different kind of thinking throughout the simulation based activity. While William focus his thinking process first on particles’ behavior and then use it to predict and explain system behavior, Andrew focus his thinking process first on the system behavior, and use system level rules to predict future system behavior. Nevertheless, he uses the interactions between particles to explain such behavior. In both cases the two emergent premises take place:

1. Objects at the component level act differently and have different characteristics from the system level phenomena;
2. There is a components → system direction for relating the levels – the properties and behavior of the system arise from random interactions of sub-micro particles.

Therefore both William and Andrew responses were characterized as emergent. In addition, their description of particles and system behavior contained no misconceptions.

Emergent perspective without misconceptions. Students responses within which the sub-micro representation was emergently connected to the macro and/or symbolic representations, and were free of misconceptions, were characterized as emergent perspective without misconceptions (see Figure 15).

![Connection between Multiple Representation Modes](image)

Figure 15: The emergent branch which contains explanations free of misconceptions.
This perspective, like previous ones, appeared both during the computer simulation based activities and during the pre and post-activity interviews. Moreover, in many cases students that presented an emergent view of events in the simulation, tried to expand it to the situation presented by the conceptual question in the post-activity interview. For example, Michael tried to associate the situation presented in the conceptual question with the particles behavior he saw during the simulation of the process of heat transfer between gas and solids particles. The question asks about the relation between the temperatures of two solid bars, therefore he focused on the relation between temperature and particles’ velocity. However, this relation didn’t help him to answer the question:

A: The temperature of the copper will be higher than that of the lead.
Q: Why?
A: Like we saw in the simulation, more kinetic energy… it was the same energy but…
Q: But what?
A: But different velocities… [Silence, he understands that something is wrong]
Q: […] what do you think we can see here [in the diagrams] that can give you a hint regarding their [copper and lead] temperatures?
A: More particles mean less weight to each one. The copper molar weight is smaller, so the velocity of each copper particle will be higher than the mean velocity of lead particles.
Q: And does it change the temperature?
A: No…

He needed some probing to find the specific particulate mechanism he looked for:

Q: So what do change the temperature? Is there any other parameter here that can help you to say something about their temperatures?
A: [Silence]
Q: What do we said temperature is?
A: Energy
Q: Per what?
A: Per… Ah! Per particle!

Once he found it, he correctly predicted the system level behavior, the change of the copper and lead bars’ temperature, based on the interaction between particulates at the component level:
Q: So what does it mean?
A: That if there are more particles, the temperature will be lower.
Q: Why? What happens to the energy if we have more particles?
A: Per particle or per bar?
Q: Per particle.
A: Here [in the copper bar] will be less [energy per particle].
Q: And what does it mean?
A: That the temperature of the lead bar will be higher

This kind of thinking typifies an emergent perspective. In addition, the mechanism Michael described contained no misconception, therefore we characterized it under the emergent perspective without misconceptions branch (see Figure 15). Nonetheless, the examples of Michael, William and Andrew do not cover the whole characterization tree of the emergent perspective. There were students who presented an emergent perspective, but their description of either particles or system behavior, or even both of them, contained misconceptions.

Emergent perspective with misconceptions. Students' responses within which the sub-micro representation was emergently connected to the macro and/or symbolic representations, but contained misconceptions, were characterized as emergent perspective with misconceptions (see Figure 16).

![Connection between Multiple Representation Modes](image-url)
This perspective was less common than the emergent perspective without misconceptions. Consequently, this branch of the emergent sub-tree is sparser. Moreover, most of the cases of this perspective were encountered during the simulation based activities (the left most branch of the emergent perspective \textbf{with misconceptions} category). For example, during the simulation of a gas in a container I asked Mary to predict what will happen in the simulation if I change the behavior of the simulated particles so that they won’t collide with their selves anymore, but only with the walls of the container (as assumed in ideal gases). She (incorrectly) predicted that gas pressure will rise. On one hand Emily correctly described gas pressure as arising from the collisions between gas particles and the walls of the container. However, on the other hand she incorrectly assumed that a particle moving straight to a wall will always get to the wall before than it would get if its direction would be changed as a result of a collision with another particle. This incorrect assumption about particles behavior causes her to incorrectly predict the system behavior – an increase in gas pressure, instead of staying constant:

Q: I will now change the behavior of particles so that they will behave like an ideal gas. The circles will not collide with each other anymore, but will be able to pass through each other. There will be no interaction between particles; therefore there will be no collisions inside the container anymore. Do you think will it cause any change?
A: Yes, the pressure on the wall of the container will be much higher.
Q: Higher? Why?
A: Because they [particles] won’t collide with each other anymore, so they won’t change direction as a consequence of [internal] collisions. Therefore more particles will get upside, to the blue line [the piston].
Q: Because they don’t change direction, will they collide more with the blue line?
A: Yes.

I was very surprised with her prediction, as it contradicted all other answers I got until then. Mary’s prediction was the opposite of the more common and intuitive mistaken prediction, in which gas pressure becomes lower. In this case the misconception is generally on the particulate definition of gas pressure as both the collisions of particles with the walls and the collisions with themselves. Therefore the conclusion is that if there are two factors affecting gas pressure and we leave only one of them, gas pressure should decrease. Nevertheless my surprise only emphasizes the emergent
aspect of Emily’s answer. She concentrated exclusively on particulate behavior, and used her (incorrect) assumption about it to predict future system behavior. She believed in it so much that even after I implemented the change in the simulation, and she saw her prediction was wrong, she tried to reconcile the system behavior she was seeing on the screen with the one she expected to see:

Q: OK, so let’s see. You can concentrate on the green circle. Right now it changes its direction as a consequence of collisions with other particles. Now I’ll change to ideal gas mode, and you can see it goes straight until it collides with a container wall. Do you think there are few collisions now?
A: No. The truth is that it seems they [particles] are colliding more or less the same... May be a bit more... […] They don’t change direction... I think there are just a few more collisions.

The conceptual question branch of the emergent perspective with misconceptions sub-tree (see Figure 16) is very sparse. In addition, this branch is almost entirely related to the conceptual question which asks students to predict the relation between the temperature of the lead and copper bars after heated for the same amount of time, by an equivalent heat source. For instance, when I asked Christopher this question during the post activity interview, he based his answer on the (incorrect) assumption that temperature is a measure of the rate of particles collisions. According to this particulate inference he got to the (incorrect) conclusion that the temperature of the copper bar will be higher. Christopher thinks that lighter particles mean higher temperature because if the molar mass of particles is smaller, then they move faster and therefore have more collisions:

Q: When I turn on the heat source, what happens?
A: The kinetic energy of the copper is higher than the lead.
Q: Why?
A: Because its [the copper] molar mass is smaller.
Q: And what does it mean? That copper particles move faster or have more energy?
A: There will be more collisions between particles, and in this way the temperature will raise more.
Q: So lighter particles mean higher temperature?
A: Yes
This conclusion contradicts what has been shown in the simulation, but this is the way he remembers it:

Q: How can you correlate this conclusion with what we saw in the simulation?
A: Hamm
Q: The aluminum moved faster, was its temperature higher?
A: Yes (No, it wasn’t - and he said that although the aluminum moves faster, it is at the same temperature as the gold)

3.2.4 Similarities and Differences between the Perspectives

We defined four types of perspectives, two emergent and two submergent perspectives. According to these perspectives we characterized students’ responses throughout the entire interview. In order to be able to perform such categorization, as well as to compare different students’ responses, it is important to highlight the similarities and differences between these perspectives.

Emergent vs. submergent perspectives: a main difference. The emergent perspectives are characterized by the presence of a mechanism at the component level, throughout which the properties and behavior of the system can be explained and predicted. For example, let’s look at the first subject matter, where the system is represented by a gas in a container. When I asked William what happens if the temperature of the gas (a system level property) decreases, he answered: “particles move slower […] then there are fewer collisions so the pressure is smaller.” He both explained and predicted system level behavior (T↓, P↓) through a causal mechanism:

\[ T↓ \equiv \text{particles move slower} \implies \text{there are fewer collisions with the walls} \equiv P↓. \]

This is in contrast to the submergent perspectives, where the properties and behavior of the system define the behavior of components. The mechanism (when it exists) is a result of system level behavior and properties. For instance, when I asked Sophia the same question, she answered: “the temperature decreased, so the pressure on the container decreases, and this means particles will move slower [and collide less with the walls]”. She deduced the mechanism according to system level behavior:

\[ T↓ \implies P↓ \equiv \text{particle move slower [and collide less with the walls]}. \]

The emergent perspectives. We thus defined the emergent perspectives as fulfilling two basic premises:
Objects at the component level act differently and have different characteristics from the system level phenomena;

There is a components \(\rightarrow\) system direction for relating the levels – the properties and behavior of the system arise from random interactions of sub-micro particles.

Students’ responses, in which the connections between the sub-micro representation (at the component level) and the macro and/or symbolic representations (at the system level) meet the two premises described above, were characterized as emergent. Within both emergent perspectives the system level behavior and properties can be explained by a causal mechanism at the component level. Moreover, the two emergent perspectives are very similar to each other and have the same characteristics. They are distinguished only by the presence or absence of misconceptions in this mechanism, or in its connection to system level representations. Therefore we called them emergent perspective with misconceptions and emergent perspective without misconceptions.

The submergent perspectives. In contrast to the emergent perspectives, the submergent perspectives are characterized by the contradiction of either both emergent premises, or the second one only. In both cases the connections between the sub-micro representation and system level representations has a system \(\rightarrow\) components direction for relating the levels. Therefore within both submergent perspectives particles behavior is defined according to macroscopic properties and symbolic relations. Nonetheless, besides this common faculty, the two submergent perspectives have very different characteristics. Within the system projection submergent perspective macroscopic properties and symbolic relations are projected to sub-micro particles, such that particles either act or have the same properties as the system, or both of them. For example, if the gas volume (a system property) decreases, students expect gas particles to shrink together, to be concentrated in a smaller region. Therefore this submergent perspective contradicts both the first and the second emergent premise.

Within the teleological submergent perspective the sub-micro representation is defined directed to a certain goal or to fulfill a certain function at the system level. For example, if we insert another weight to the one loading piston, the volume of the gas decreases. Within this perspective particles are not expected to shrink together, but
to collide more with the piston. However, they do it “because this is what they are expected to do, from a physical point of view. [...] Particles collide because the system has to reach an equilibrium state; because all system components aspire to reach an equilibrium state, then it happens” (Isabella). Therefore this perspective generally does not contradict the first emergent premise. However, it does contradict the second one.

**Emergent and submergent perspectives: similarities.** Besides the differences between the emergent and the submergent perspectives, as well as the differences and similarities between the two emergent and submergent perspectives, there are also similarities between them. For example, misconceptions were present both in students responses characterized as emergent perspective with misconceptions, and in students responses characterized as system projection submergent perspective. Nonetheless, they differently affected students thinking processes, leading them to different conclusions. For instance, both Christopher and Jacob think that temperature is equivalent to the velocity of particles (instead of a measure of particles’ energy). Both of them expect to see in the simulation the same distribution of velocities to substances at the same temperature. Moreover, they both think that after enough time all the three substances simulated - gold, aluminum and argon, will be at the same temperature. Nevertheless, when Christopher and Jacob saw in the simulation that aluminum particles move much faster than gold particles, even after the system reaches a thermal equilibrium, they reached distinct conclusions. Christopher analyzed the situation through an emergent perspective. He concentrated on particles behavior: given that particles move at different velocities, he tried to find an alternative explanation to the temperature of the system – the three substances may not really be at the same temperature:

Q: So you say that the aluminum particles move faster, then argon particles, then gold particles?
A: Yes
Q: And what about their temperatures? You told me before that they are all at the same temperature…
A: They are at the same temperature; the whole room is at the same temperature. The particles themselves may be different…
Q: What do you mean?
A: [...] May be the average temperature is the same, but per molecule…
Q: Is the temperature of gold and aluminum the same?
A: According to the simulation, not really.
Q: Why?
A: Because the velocity here (within aluminum particles) is much higher

As opposed to Christopher, Jacob analyzed the situation through a submergent perspective. He concentrated on his assumption about the system behavior: gold and aluminum are at the same temperature. He then tried to find an alternative explanation to why aluminum particles move faster than gold particles, and (incorrectly) found the answer in a macroscopic parameter – again, the heat capacity:

A: In theory it all [the distribution of particles’ velocity] should be the same.
Q: Why it all should be the same?
A: Because the temperature is the same.
Q: […] and why do you think the aluminum is faster than the gold, if you think they are all at the same temperature?
A: Because its heat capacity is smaller…

Similarly, students responses characterized as teleological submergent perspective where generally free of misconceptions, like the ones characterized as emergent perspective without misconceptions. However, as described above, besides this similarity there is a main difference in such responses: the direction of the connections between the component level sub-micro representation and the system level macro and symbolic representations. These connections and their directions are the heart of the characterization of students' responses throughout the entire interview.

3.2.5 Students’ Behavior throughout the Entire Interview

I will now describe, for each student, which perspective he/she showed throughout the entire interview. We individually interviewed each one of the 14 undergraduate students participating in this stage of the research. As previously mentioned, we focus on the way students connect between multiple representation modes. As most of the connections appeared during students’ answers to the conceptual questions (in the pre and post interviews) and during students' predictions and explanations throughout the simulation based activities, these are the situations we concentrate in during the analysis of the data. These are also the two branches under
each emergent and submergent nodes in the categorization tree (see Figure 10), and the situations throughout which I summarize students’ perspectives (see Table 2).

Each row of the table comprises two paragraphs: the first describes student’s behavior during the first part of the interview, related to a gas in a container; the second describes student’s behavior during the second part of the interview, related to heating solids. Each paragraph briefly describes the perspectives the student showed throughout the simulation based activity, as well as the way he/she answered to the conceptual questions in the pre and post activity interviews. To give some additional information, I also state whether the student answered the conceptual questions correctly or incorrectly, from a scientific point of view.

<table>
<thead>
<tr>
<th>Matthew</th>
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<tbody>
<tr>
<td><strong>Ideal Gases</strong></td>
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</table>
| During most of the simulation Matthew clearly shows a system projection submergent perspective. However, there are a few situations where he explains what he sees in the simulation through an emergent perspective. The system projection submergent perspective was also predominant throughout the pre and post activity interviews, particularly when answering the conceptual question. Matthew concentrated on the ideal gas equation (PV=nRT) and concluded: “If I change the temperature, and R and the number of moles [n] do not change, so between P and V ... Let's say that the pressure stays constant, inside the same container, so the volume should change. The volume decreases, therefore they [particles] will be like this [concentrated in the middle of the tank], because this way their volume is smaller”.

**Conceptual question:** Pre – Incorrect
  
  Post – Incorrect |

| **Heating Solids** |
| Matthew is very confused during the simulation, and hardly follows the activity. He cannot connect the particulate behavior he sees on the screen neither with macroscopic properties of the system, nor with the equation. Matthew has difficulties in discerning what he is seeing on the screen, and describes it in contradictory ways until he gets a positive feedback from the interviewer. During the pre activity interview he tries to |
deduce the answer to the conceptual question from the equation and looses his way. Matthew did not even try to answer the conceptual question in the post activity interview; he just asked me to tell him the answer.

*Conceptual question: Pre -- Incorrect
Post – Incorrect

Mary

*Ideal Gases*
Mary explains most of the simulation through an *emergent* perspective, but there are situations where she shows an *submergent* perspective which she is very convinced of (can even see it). For example, she is convinced that particles slow down after collisions “*because according to the constant energy rule, particles have a slow natural velocity which they should return to*”. We asked her several times to concentrate on the (constant) motion of particles between two collisions and describe what she sees. Mary repeatedly saw that particles slow down. During the pre and post activity interview she also ‘sticks’ to some *submergent* ideas (which lead her to incorrect conclusions). Nonetheless, in the post activity interview she shows a more *emergent* perspective than in the pre activity interview.

*Conceptual question: Pre -- Incorrect
Post – Incorrect

*---------------------------------------------------------------

*Heating Solids*
Mary doesn’t show any predominant perspective throughout the simulation. She predicts and explains what she sees either by an *emergent* perspective without misconception, or by a *submergent* perspective – both *system projection* and *teleological*. However, she is again very convinced of certain rules like “*the lighter (the object or particle) the more energy (it has)*”. During the simulation based activity on one hand Mary manages to understand that many times these rules don’t take place, but on the other hand she gets lost and starts answering according to what she thinks I am expecting to hear. In the pre and post activity interviews she answers the conceptual question based on *submergent* considerations. For instance, in the pre activity interview she showed a *system projection submergent* perspective when
concluded the lead will be at higher temperature: "Heat capacity is how much heat a substance can absorb without emitting it to the environment, [... and] temperature is how much heat is emitted to outside. The more heat is emitted, the more the temperature increases. [...] The bigger spheres [representing lead particles] have more force to hold each other closer, thus they will emit less heat to outside". When probed during the post activity interview to consider what she saw in the simulation, Mary found a way to reconcile things such that they strengths her submergent assumptions.

Conceptual question: Pre -- Incorrect

Post – Incorrect

<table>
<thead>
<tr>
<th>Emily</th>
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**Ideal Gases**

During most of the simulation Emily sees and explains things through an emergent perspective. Sometimes emergent with misconceptions. She a priori doesn’t know well the subject matter, thus many of her predictions are incorrect. However, most of the time she sees they were wrong. Except in one case, where she expects (and sees) that the volume of the gas (which stays constant) increases when we change particles’ behavior to be as in ideal gases. Her preconception of gas volume determines also her answer to the conceptual question both in the pre and post activity interviews. However, after many guiding questions, she managed to correctly answer the conceptual question in the post activity interview.

Conceptual question: Pre -- Incorrect

Post – Correct -

**Heating Solids**

Emily shows an emergent perspective throughout most of the simulation, sometimes emergent without misconceptions and sometimes emergent with misconceptions. She thinks temperature is equivalent to particles’ velocity, what confuses her many times during the simulation. She even says that what she sees “contradicts my assumption that temperature is equivalent to particles’ velocity”. By the end of the simulation it seems that Emily manages to relate temperature to kinetic energy and not just to
velocity of particles. However, in the post activity interview she becomes very confused and turns to a submergent perspective to answer the conceptual questions: 'the same mass + same energy to both bars = same temperature'.

Conceptual question: Pre -- Incorrect

Isabella

Ideal Gases

Isabella has very strict opinions about how things work, and she fully believes on them. During the great majority of the simulation she shows a clear teleological submergent perspective, which derives from these opinions. Nevertheless, there are some situations where she didn’t form a strict opinion yet, as in the case of ideal gases: “you fabricate here new creatures that I don’t know them, I don’t know how they behave... this is not the way gas particles behave”. During the pre and post activity interviews she correctly answered the conceptual questions, and the clear submergent perspective which she showed throughout the simulation didn’t become prominent.

Conceptual question: Pre -- Correct

Heating Solids

Isabella doesn’t show any predominant perspective throughout this simulation. She predicts and explains what she sees either by an emergent perspective without misconception, or by a submergent perspective – both system projection and teleological. She uses every day experience to predict and explain both the behavior of the system and the behavior of particles. As in the previous simulation, Isabella is very convinced of her opinions: “I don’t think so, I really don’t think so. And if you’ll say it is true I’ll prove you that it is not true, because I don’t think so”. She gets lost by the end of the activity, what makes her feel very frustrated. In the pre activity interview she answer to the conceptual question through a submergent perspective based exclusively on the equation, and got stuck. In the post activity interview she tries also to apply what she saw in the simulation, but fails to do that.

Conceptual question: Pre -- Incorrect
**Ideal Gases**

Emma doesn’t show any predominant perspective throughout the simulation. Although she concentrates on particulate behavior, she can’t connect it to any macro or symbolic representation. Most of the time she feels lost and embarrassed. Emma felt embarrassed also during the pre activity interview, when she had difficulties to answer the conceptual question: “it erodes my knowledge about $PV=nRT$”. Nonetheless, in the post activity interview she applies what she saw in the simulation and successfully answers the conceptual question through an *emergent* perspective: "It is a) [the diagram in which particles are distributed in the whole cross section], because it [the decrease in temperature] won't affect the distribution of particles, but their velocity. [...] Particles move slowly and therefore the pressure decreases, because there are fewer collisions [with the walls]".

**Conceptual question: Pre -- Incorrect  
Post – Correct**

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**Heating Solids**

Emma doesn’t show any predominant perspective throughout the simulation. Sometimes she shows an *emergent* perspective, but has difficulties in connecting the particulate behavior to system level representations. Sometimes she shows a *system projection submergent* perspective, and if it is not consistent with the behavior shown in the simulation, Emma feels embarrassed and gets lost. As the simulation progresses this situation becomes more and more frequent until she feels completely lost by the end of the activity. In the pre activity interview Emma answers to the conceptual question through a *submergent* perspective. In the post activity interview she starts answering it through an *emergent* perspective, trying to project what she saw in the simulation, but reaches a vague (and incorrect) conclusion. When I asked her if it fits also the equation she said “no...” She then asked me to tell her the answer.

**Conceptual question: Pre -- Incorrect  
Post – Incorrect**
Ideal Gases

Throughout most of the simulation Jacob predicts and explains the simulation through an emergent perspective. However, he is convinced of a system projection submergent rule: the bigger the volume and/or temperature, the more particles become organized in distinct groups. He also sees it in the simulation (although it does not happen at all). This rule guides him also when answering to the conceptual question in the pre and post activity interviews.

Conceptual question: Pre -- Incorrect
                         Post – Incorrect

Heating Solids

Jacob is very confused and has difficulties in following the activity throughout almost the entire simulation. He predicts and explains most of the simulation through a system projection submergent perspective, but sometimes he also show emergent explanations – both with and without misconceptions. Jacob uses the heat capacity to 'explain' almost everything he does not understand, both during the simulation and during the pre and post interviews. In the pre activity interview he again applies the same submergent argument and says the heat capacity of copper is lower so its temperature is higher. In the post activity interview he chooses to ignore the emergent view presented in the simulation and go back to his submergent assumptions “I’ll ignore everything we did (in the simulation); I still think that copper will be hotter”.

Conceptual question: Pre -- Incorrect
                         Post – Incorrect

Michael

Ideal Gases

Michael shows a very predominant teleological submergent perspective throughout the entire simulation. All his predictions are correct, everything runs as he expects and he claims he doesn’t saw anything new in the simulation. Michael also answers
(correctly) the conceptual question, both in the pre and in the post activity interviews, through a teleological submergent perspective: “The pressure [of the gas] decreases, therefore [...] there will be less collisions with the walls of the container. ... There is no reason for the diagram to change [to be different from the one depicted in the question]. It does not shrink - the volume stays constant, it is the pressure that changes. [...] The volume stays constant, R is given, n doesn't change, it is a closed container, so the only think that can change is the pressure”.

Conceptual question: Pre -- Correct

Post – Correct

Heating Solids

Michael predicts and explains most of the simulation through a teleological submergent perspective, but many times he shows also an emergent perspective without misconceptions. During the simulation Michael sees things that contradict his previous knowledge. In these cases he is open to listen and learn. Michael also promptly applied what he learned in the simulation to solve the conceptual question in the post activity interview. He successfully solved it through an emergent perspective. This is in contrast to the submergent line of thought he applied to solve it in the pre activity, based exclusively on equations.

Conceptual question: Pre -- Incorrect

Post – Correct

Ideal Gases

Sophia predicts and explains most of the simulation through a submergent perspective – sometimes teleological and sometimes system projection. Particles behave according to the PV ~ T relation. Sophia has a problem in discerning the difference between the situations presented in the simulation, where both the pressure (P) and the volume (V) can change if the temperature changes, and the situation presented in the conceptual question, where the volume stays constant after changing the temperature. She thus applies the same submergent considerations and reaches to incorrect conclusions when solving the conceptual question, both in the pre and post activity interviews.
Conceptual question: Pre -- Incorrect
Post – Incorrect

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Heating Solids

Sophia predicts and explains most of the simulation through an emergent perspective without misconceptions. When the particulate behavior shown in the simulation contradicts her predictions, she is open to change her mind and learn new things. In the pre activity interview Sophia does not know how to use the diagrams to help her solving the conceptual question, and (incorrectly) answers it through a submergent perspective which derives from the equation only. In the post activity interview she immediately applies what she learned in the simulation and successfully solves the conceptual question through an emergent perspective: "In the simulation, when the number of particles was bigger, the energy was smaller [...], so the lead will be hotter than the cooper. [...] Because we said [temperature is a measure of the energy] per particle. Both the lead and the copper got the same amount of energy, but in the copper it was divided among more particles than in the lead".

Conceptual question: Pre -- Incorrect
Post – Correct

Anthony

Ideal Gases

Anthony shows a predominant submergent perspective throughout the simulation. He tries to see in the simulation macroscopic relations, so if the temperature of the gas changes, he expects the pressure and volume to change accordingly. In addition, Anthony expects particles to behave according to system behavior – particles should stabilize the piston so it will stop oscillating (like a real syringe), or get closer if the volume decreases. Most of the time he sees his predictions were wrong and tries to understand why. The same happened in the interviews. When answering to the conceptual question in the pre activity interview, he applied a system projection submergent perspective and expected particles to get closer when thought that the volume of the gas should decrease. In the post activity he changed his answer interview to an emergent one, according to what he learned in the simulation.
**Conceptual question: Pre -- Incorrect**

**Post – Correct**

Heating Solids
Anthony doesn’t show any predominant perspective throughout this simulation. He has some difficulties in accepting that two substances on thermal equilibrium have the same temperature, but use it when solving the conceptual question in the post activity interview. Moreover, in the post activity interview Anthony promptly applied what he saw in the simulation and successfully solved the conceptual question through an *emergent* perspective. This is in contrast to the pre activity interview, where he (incorrectly) solved the question using a *submergent* perspective.

**Conceptual question: Pre -- Incorrect**

**Post – Correct**

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Olivia

Ideal Gases
Olivia predicts and explain most of the simulation through a *teleological submergent* perspective. Almost all the time her predictions are correct, she is not surprised of anything and it seems that she also doesn’t learn anything from the simulation. Olivia answers to the conceptual question in the pre and post activity interviews exactly the same way, through a *teleological submergent* perspective.

**Conceptual question: Pre -- Correct**

**Post – Correct**

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Heating Solids
Throughout this simulation Olivia doesn’t show any predominant perspective. She thinks about temperature as velocity of particles, and it is difficult for her to see that it is also related to the mass of particles. This difficulty appears also when answering to the conceptual question. Nonetheless, in the post activity interview she answered it through an *emergent* perspective. This is in contrast to the pre activity interview, where she answered the same question through a *submergent* perspective based exclusively on the equation.
Conceptual question: Pre -- Incorrect
Post -- Incorrect

William

Ideal Gases

William predicts and explains the entire simulation through an emergent perspective without misconceptions. When necessary, he connects the particulate behavior shown in the simulation both with the system level macro and symbolic representations. William solves the conceptual question through an emergent perspective, both in the pre and post activity interview.

Conceptual question: Pre -- Correct
Post -- Correct

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Heating Solids

William predicts and explains the entire simulation through an emergent perspective without misconceptions. Nonetheless, he had difficulties in answering the conceptual question both in the pre and post activity interviews. In the pre activity interview William shows a submergent perspective when he tries to base his answer exclusively on the equation, but sees it is not enough. He then ‘guesses’ it is may also based on the size of the particles. In the post activity interview William knows he should answer it by using what he saw in the simulation, but as these are different situations it takes many tries until he understands how to do it. When he finally manages to do it, he hesitates “According to the model you presented [in the simulation], if it is correct, if we divide the same amount of energy to less particles, the temperature will be higher”.

Conceptual question: Pre -- Incorrect
Post -- Correct

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Andrew

Ideal Gases

Andrew shows a predominant emergent perspective throughout the simulation, accompanied by a constant necessity to connect everything he sees with an equation - either the ideal gas equation or another familiar equation. The ideal gas equation also
guided him when solving the conceptual question in the pre activity interview, and led him to incorrect conclusions. In the post activity interview he successfully solved the conceptual question through an emergent perspective.

Conceptual question: Pre -- Incorrect
    Post – Correct

Heating Solids

Andrew predicts and explains the entire simulation through an emergent perspective, sometimes with and sometimes without misconceptions. During the simulation he raised objection to the emergent explanation of some system level behavior, but in principle accepted them in the course of the simulation. Nonetheless, when solving the conceptual question in the post activity interview, Andrew first turns to submergent considerations. After I probed him to consider the diagrams and try to use what he saw in the simulation, he manages to give an emergent answer. However, this answer contradicts his previous assumption that the heat capacity (c) of the lead is higher than the heat capacity of copper. He thus decides to reject the emergent explanation and adopt his initial (submergent) explanation: “No, I don’t accept it. It doesn’t fit... because if we look at the heat capacity, the heat capacity of the lead is higher”.

Conceptual question: Pre -- Incorrect
    Post – Incorrect

Christopher

Ideal Gases

Christopher predicts and explains the entire simulation through an emergent perspective. When necessary, he connects the particulate behavior to the macro and/or the symbolic representations. Nevertheless, sometimes he is not aware of these connections and finds it difficult to explain them - “I don’t know why... it is just intuitive”. In the pre activity interview Christopher answers to the conceptual question through an emergent perspective, but he is not sure about it and tries to look for other possible answers. In the post activity interview he gives the same emergent (and correct) answer, but this time he is sure about it.

Conceptual question: Pre -- Correct
Post – Correct

Heating Solids
Christopher predicts and explains most of the simulation through an emergent perspective, sometimes with and sometimes without misconceptions. The most prominent misconception he shows is in the way he connects between particles collisions and temperature. Christopher thinks that the more collisions the more temperature because: “the collisions increase the temperature, change the energy”. This misconception appears also in the post activity interview, when Christopher solves the conceptual question. He answers it through an emergent perspective, but reaches incorrect conclusions.

Conceptual question: Pre -- Incorrect
Post – Incorrect

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Elizabeth

Ideal Gases
Elizabeth explains most of the simulation through an emergent perspective, although in general she had difficulties in explaining herself. She makes many incorrect predictions throughout the simulation, but promptly sees that she was wrong and corrects herself. In the pre activity interview she chooses the correct diagram (a) when answering the conceptual question, but cannot explain it because she doesn’t know the particulate meaning of gas pressure. In the post activity interview she chooses the same diagram, but now she explains her answer through an emergent perspective.

Conceptual question: Pre -- Correct
Post – Correct

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Heating Solids
Elizabeth predicts and explains most of the simulation through an emergent perspective without misconceptions, but sometimes shows also an emergent perspective with misconceptions. She does not feel comfortable at the beginning of the simulation based activity “it is difficult for me to see solids as a collection of particles”. Nonetheless, she very fast overcomes her confusion and follows the
activity until its end. Elizabeth is never sure of her answers, both throughout of the simulation and throughout the interviews. In the pre activity interview she answers the conceptual question through a *submergent* perspective. In the post activity interview she changes her answer and answers it through an *emergent* perspective, by projecting to the conceptual question what she saw in the simulation. However, she again emphasizes she is not sure about her answers.

*Conceptual question: Pre -- Incorrect  
Post – Correct*

| Table 2: Students perspectives throughout the entire interview. |

### 3.2.6 An Outline of Students’ Behavior throughout the Activity

When observing students’ behavior throughout the entire interview we can discern three general types of behavior. To emphasize that, we arranged the table (see Table 2 above) such that students who showed similar behavior are described in consecutive lines.

The first type of behavior we discerned was showed by the first six students described in the table: Matthew, Mary, Emily, Isabella, Emma and Jacob. All of them predicted and explained both the first and the second simulation sometimes through a *submergent* perspective, and sometimes through an *emergent* perspective. They did not show any preference or tendency to any one of the perspectives throughout the simulations. Nonetheless, during the first part of the interview, related to a gas in a container, we can find among most of them very clear submergent expressions, such as “*particles behave this way because this is the way they are expected to behave, from a physical point of view*”. Such expressions were generally accompanied by clear ideas about the way particles should behave, as defined by symbolic rules or macroscopic properties of the system. These ideas were prominent throughout the interview, both during the simulation based activity, as well as during the pre and post activity interviews. In some cases these ideas were so strong that students claimed they see them on the screen, although it does not fit the simulated behavior of particles.

During the second part of the interview, related to heating solids, all of them got lost at some earlier or later stage of the simulation based activity. This was obvious
also in their answers during the post activity interview. In addition, all of them incorrectly answered the conceptual question both in the pre and post activity interviews.

The next four students: Michael, Sophia, Anthony and Olivia (see Table 2) show a different overall behavior. Although they also used both emergent and submergent perspectives when explaining and predicting things throughout the simulations, they showed a strong tendency to use the submergent perspectives. This tendency was more prominent throughout the first part of the interview, where the submergent perspectives were very predominant both throughout the simulation based activity, as well as throughout the pre and post activity interviews. Nonetheless, these students were much more aware of the separation between the component and system levels than the previous ones. Even though they expected particles to behave according to system level properties and behavior, they did not believe that such behavior is dictated by macroscopic properties or symbolic rules. Therefore, they did not use expressions such as “[particles collide more with the walls] because they must do that in order to balance the equation”. They know particles move randomly and incidentally collide with the walls, but they expect these random motions and incidental collisions to converge according to macroscopic and symbolic rules. Therefore, they do say expressions such as “the volume [of the gas] gets smaller, [thus particles will] get closer”. In addition, these students did not claim they see specific particles behavior during the simulation, unless it fitted what was being shown on the screen.

Another main difference between the behavior of these and previous students was their capability to follow up the second part of the interview. All four students follow the simulation based activity until its end, and tried to apply what they learned there when solving the conceptual question in the post activity interview. Moreover, although during the simulation based activity they still tended to use submergent perspectives, during the post activity interview they applied what they saw in the simulation through an emergent perspective.

The last four students described in the table (see Table 2): William, Andrew, Christopher and Elizabeth showed an even distinct overall behavior. In contrast to previous ones, they had a tendency to explain and predict the situations presented both in the simulations based activities and in the pre and post activity interviews through
an emergent perspective. This tendency was prominent in both parts of the interview. Nevertheless, these students resisted in accepting some properties of the particulate model presented in the second simulation based activity. Similarly, they had difficulties and even refused to use such properties when solving the conceptual question during the post activity interview. They tended to answer it based on the knowledge and assumptions they had before the simulation based activity. Only after probed by the interviewer they referred to the data presented in the simulation based activity, but always with skepticism and even lack of confidence.

The interpretation of the results presented here, as well as their relation to the existing literature will be described in the next section.
3.3 Discussion

3.3.1 The Refined Definition of the Emergent and Submergent Connections

In the previous research stage we characterized the connections between different representation modes as emergent or submergent. In the present research stage we applied such characterization to learning through computer based learning activities. The different nature of tasks asked during the computer based activities revealed distinct facets of the emergent and submergent connections. Such facets led us to refine previous definitions to emergent connections with or without misconceptions, and submergent teleological or submergent system projection connections.

Two of these connections, one emergent: emergent without misconceptions and one submergent: submergent system projection, are very similar to the emergent and submergent connections described in the previous research stage. During this research stage they were observed both in the pre and post activity interviews, as well as throughout the computer based activities. The other two connections: emergent with misconceptions and submergent teleological, appeared mainly throughout the computer simulation based activities.

The emergent connections with misconceptions become apparent when the particulate behavior shown in the simulation was different from what students expected to see, or from what they had in mind. The computer simulations were an effective tool for revealing and challenging students’ misconceptions by promoting cognitive dissonance (Smetana and Bell, 2007; Gorsky and Finegold, 1992). In these cases some students had difficulties in explaining the particulate behavior displayed on the screen, and in discerning the mechanical causality of system level phenomena. On one hand they saw the emergent nature of the phenomenon being simulated; on the other hand their predictions and explanations of such behavior and/or its connections to system level representations contained misconceptions, and conflicted with the one shown in the simulation. Moreover, during the pre and post activity interviews (where students did not have to cope with conflicts between the particulate behavior they had in mind and the one they see on the screen) these misconceptions were much less prominent.

The other connections which appeared mainly throughout the computer simulation based activities were the teleological submergent connections. These
connections rely mainly on students' beliefs. Students believe that particles at the component level act as directed to a certain goal, or to fulfill a certain function defined at the system level (Keil, 2006; Talanquer, 2007). Such beliefs hardly appeared during the pre and post activity interviews, where students were requested to answer specific questions. Nonetheless, the questions asked during the computer based activities requested them to describe what is happening in the simulation, predict what will happen, and explain why they believe so. This constituted a fertile ground for revealing students beliefs:

Maybe what I am saying is wrong, but I believe so. There is a reason for such behavior, it does not happen accidentally because a molecule collides with the wall. No! It collided because [...] all system components aspire to reach an equilibrium state; then it happens. This is how I believe things work. (Isabella)

3.3.2 From Connections to Perspectives

The way students connected different representation modes at the component and system levels, especially the direction of the connections, affected both the way they solved conceptual problems as well as the way they interpreted the computer simulations. Moreover, we could classify students as having a consistent tendency to use either emergent or submergent connections. We can thus say that the emergent and submergent connections indicated an overall perspective; a general line of thinking which we called emergent and submergent perspectives.

Students who presented an emergent perspective concentrated mainly on sub-micro representations. When answering questions or predicting the simulation behavior they used random interactions of sub-micro particles to define the properties and behavior of system. This is a critical step for understanding emergency (Penner, 2000; Wilensky and Resnick, 1999). For example, William connected the mean kinetic energy of particles to temperature to solve the conceptual question related to heat transfer:

A: The same amount of energy scatters between less particles [inside the Lead bar], therefore its temperature will be higher.
Q: Why?
A: Because [...] the mean kinetic energy per particle will be higher in the Lead bar.
William based his answer on an emergent definition of temperature (a measure of the mean kinetic energy per particle), as presented in the computer simulation based activity.

In contrast to them, students who presented a submergent perspective concentrated mainly on macro and symbolic representations. They first reached a conclusion at the system level. After that, and sometimes only after being probed by the interviewer, they defined particles behavior to match macroscopic or symbolic rules and properties. Therefore, even when they were conscious about components and system level relationships they were found to ascribe causal primacy to the system level of the system, and showed difficulties in discerning system level behavior from the interactions that produce those behaviors at the component level (Jacobson and Wilensky, 2006; Penner, 2000). Like Matthew when solving the gas related conceptual question: He first concluded the system level behavior: the pressure of the gas decreases. Then he tried to project it to the sub-micro representation:

Now the question is: given that pressure decreases, I wonder if it causes particles to crowd together and press less [the walls of the container], or the opposite, to spread out [and press less on each other].

Matthew also tended to explain changes in the simulation parameters in terms of macro level relations, instead of in terms of particles. He therefore had difficulty in discerning the mechanical causality in the simulation. In addition, as in the simulation it is difficult to project macro level relations to particles (because particulate behavior is shown on the screen and particles act different and have distinct characteristics from the macro level ones), Matthew was many times unable to coherently connect macro level changes to a particulate mechanism:

A: [After witnessing that the piston decreased to half of its previous height after we double the weight loading the piston] it means that particles actually do not affect how much the piston decreases. How many particles we have almost does not influenced…
Q: We did not change the number of particles
A: Exactly! Therefore if it [the piston] decreased almost twice its previous height, and you added almost twice the weight loading the piston, particles did not add any factor.

Matthews’ tendency in determining particles behavior according to predefined rules, as well as his difficulty in understanding the randomness in the mechanical
causality in the simulation is called in literature ‘a deterministic mindset’ (Jacobson and Wilensky, 2006; Willensky and Resnick, 1999). Like Matthew, students showing a deterministic mindset miss the key role that randomness plays in the mechanisms of emergence, and have difficulty in believing that randomness at the component level could lead to a desired behavior at the system level.

When observing students’ behavior throughout the entire interview we saw that, like Matthew and William, students who presented an emergent perspective behave very different from those who presented a submergent perspective. Moreover, distinct perspectives influenced students differently in the first and the second learning activities. These differences and their possible reasons will be discussed in the next section.

3.3.3 Distinct Behaviors throughout the Entire Interview: Who and Why

When observing students’ behavior throughout the entire interview we discerned three distinct types of overall behavior.

The first type characterized students who did not show a consistent tendency to any specific perspective. Throughout the computer simulation based activities Matthew, Mary, Emily, Isabella, Emma and Jacob predicted and explained both simulations sometimes through a submergent and sometimes through an emergent perspective. Nonetheless, there was a major difference in their behavior throughout the first and second parts of the interview: In the first one, related to a gas in a container, they felt much more comfortable with the subject matter. They felt they know the ideal gas equation and its relation both to the behavior of a gas as well as to the behavior of gas particles. Therefore during this part of the interview we could find among most of them very clear submergent expressions, within which they either projected gas properties and relations to particles, like Matthew, or saw them as the mandatory cause of particles behavior, like Mary when explaining "they [molecules] must do that in order to balance the equation". These inappropriate connections between the system-level macro or symbolic representations and the component level sub-micro representations are analogous to those described by Lee et. al. (1993), Albanese and Vicentini (1997) and Chi (2005), where middle school students projected macroscopic properties or behaviors of substances onto particles (e.g. coldness, color, or direction of flow).
In contrast, during the second part of the interview, related to heating solids, Matthew, Mary, Emily, Isabella, Emma and Jacob felt very uncomfortable with the subject matter. They felt their knowledge about the equation \( Q = mc\Delta T \) was pretty vague, and therefore they had difficulty in projecting or dictating particles behavior according to macro level rules they don't feel comfortable with. Consequently, during this part of the interview we did not find many submergent expressions, but more emergent ones.

We thus on one hand cannot characterize these students as having any tendency, neither to a consistent emergent nor to a consistently submergent perspective. On the other hand we can characterize the situations in which they tended to use the emergent or the submergent perspectives: in general, the emergent perspective was observed when students talked about a subject matter they didn't know well in advance, and didn't feel comfortable with. The subject matters they felt they know were almost always described through a very clear submergent perspective. This explains why the submergent perspective was much more prominent throughout the first part of the interview, which deals with a more accessible subject matter than the second one.

This students' tendency to understand, explain and use the knowledge they feel comfortable with through a submergent perspective affected also their capacity to learn from the simulation based activities. Matthew, Mary, Emily, Isabella, Emma and Jacob had a great difficulty in understanding the value of randomness in the simulation. They expected rules and properties at one level (system level) to lead a desired behavior on another level (component level), and saw randomness as something that destroys order and interferes with goals. Such behavior was found to be a major obstacle which interferes with students’ understanding of emergent phenomena. (Jacobson and Wilensky, 2006; Penner, 2000; Willenski and Resnick, 1999). Indeed, Matthew, Mary, Emily, Isabella, Emma and Jacob were able to follow the simulation based activities only when they felt comfortable enough with the subject matter to interpret what is emergently shown on the screen through a submergent perspective. Otherwise they gradually felt lost until they could not connect the simulated behavior of particles to any system level representation; their predictions and explanations became a mixture of unfounded guesses and straight forward descriptions of the images depicted on the screen.
As a result, the influence of the computer based activities on the way these students connect different representation modes was minimal. During the first part of the interview the same submergent ideas appeared both in the pre and post activity interviews, even though they were emergently presented in the simulation. During the second part of the interview all of them got lost at some earlier or later stage of the activity, and none of them was able to use the information provided in the simulation to answer the related conceptual question. All of them incorrectly answered the conceptual question both in the pre and post activity interviews.

The second type of overall behavior characterized students who showed a strong tendency to use the submergent perspectives throughout the entire interview. However, Michael, Sophia, Anthony and Olivia were conscious of the separation between system and component levels. They were able to distinguish between the behavior of sub-micro particles at the component level, and the macroscopic properties and symbolic relations at the system level. This, on one hand, did not persuade them to see the emergent nature of the simulated phenomenon if they felt they can already explain it through a submergent perspective. On the other hand it enabled them to discern the mechanical causality in the simulation, and emergently predict and explain simulated events they didn't feel familiar with. These findings support Keig and Rubba’s (1993) conclusion that students’ ability to connect different representation modes is strictly related to their domain-specific knowledge of the three representation modes.

It is then not surprising that, like in previous case, the submergent perspectives were more prominent during the first part of the interview, where we deal with a basic subject matter. The emergent perspectives were more prominent during the second part of the interview, where we deal with more advanced subjects. Nevertheless, in contrast to previous students, Michael, Sophia, Anthony and Olivia could follow the simulation based activity until its end. They were able to emergently connect the simulated behavior of particles with system level representations such that they inferred the necessary knowledge to understand following steps. Furthermore, they felt they learned much more from the second part of the interview than from the first one. This was reflected in their responses both throughout the simulation based activities and throughout the post activity interviews: In the first part of the interview we can hardly notice some change between students’ answers to the conceptual question in the pre
and post activity interviews: in both cases they comprise mainly submergent connections and almost the same expressions. Like Michael which answers in the post activity interview: “I still think that it is a), due to the same reasons I told you before [in the pre activity interview]”. In contrast, in the second part of the interview all of them tried to apply what they saw in the simulation based activity to answer the conceptual question. Moreover, they did it through emergent considerations, by recognizing the particulate mechanism of heat transfer and connecting it to changes in system level properties.

Nonetheless, it is important to notice that these students accepted the conclusions inferred during the simulation based activities without questioning them. Even in cases where these conclusions were very surprising for them, like temperature being a measure of the amount of energy per particle instead of a measure of the overall amount of energy in a substance. Such behavior may derive from the difference between the way things were presented in the simulation, emergently, and the way they are used to think: 'submergently'. Michael, Sophia, Anthony and Olivia are not used to question particulate behavior, as it generally derives from system level behavior, nor it contradicts their previous knowledge, which concentrates mainly on system level properties and rules. They thus had no problem in accepting the particulate behavior and its inferences as it was presented to them, without questioning, and had no problem in applying them while solving the conceptual question in the post activity interview.

Such behavior is in agreement with the two kinds of conceptual change defined by Posner et. al. (1982). They used Piaget’s terms ‘assimilation’ and ‘accommodation’ to define two distinct types, or phases, of conceptual change that can take place during learning process. Assimilation occurs when students can use existing concepts to deal with new phenomena, without needing to change the way they define problems, the strategies they use for dealing with them, or the criteria they use for what counts as solutions. Accommodation in turn occurs when students’ current concepts are inadequate to allow him to grasp new phenomena successfully. In these cases students must replace or reorganize his central concepts. This is a more radical and complex type of conceptual change, for which several important conditions must take place. One of them is dissatisfaction with existing conceptions (sometimes called cognitive conflict or dissonance). Michael, Sophia, Anthony and Olivia didn’t experience any dissatisfaction with existing conceptions or cognitive conflict. They could assimilate
the particulate behavior they saw in the simulation to the system level concepts they are used to deal with, without needing to change the way they define problems, or the criteria they use for what counts as solutions. In addition, although they needed to use an emergent strategy to successfully solve the conceptual problem, it didn’t change the strategy they are used to, but complemented it.

The third type of overall behavior characterized students who showed a strong tendency to use the emergent perspective throughout the interview. William, Andrew, Christopher and Elizabeth, in contrast to previous students, presented an emergent perspective also during the first part of the interview. Such perspective helped them see things the same way they were presented in the simulation, emergently, and although they felt comfortable with the subject matter, they all learned something new during this simulation based activity. For example, Raphael saw that when we change the simulation parameters such that we simulate ideal gas particles instead of real gas particles, the piston's height decreases a bit. He immediately realized that, and by asking a few guiding questions the interviewer led him to understand that the volume of the container decreases because we now neglect the volume of the particles their selves. After that, during the post activity interview, William was again asked to define what the volume of a gas is. He then promptly asked:

A: The volume of a real gas or an ideal one?
Q: Both of them
A: Like I said before (in the pre activity interview), it is the volume of the container. But if we are talking about the volume of an ideal gas we should neglect the volume of the particles their selves. Although it makes only a small difference, it still affects a bit [the overall volume of the gas].

For William, Andrew, Christopher and Elizabeth the main difference between the first and second parts of the interview was not the perspective they showed throughout them, but how much the behavior of particles in the simulation contradicted their expectations. In both cases they emergently predicted and explained the simulations, but during the first part of the interview the particulate mechanism simulated, as well as its effect on system level behavior, seemed to correspond their expectations. They thus had no problem in accepting them, learning from the simulation based activity and mentioning what they learned during the post activity interview. Nonetheless, during the second part of the interview it was different. Even
though these students followed the simulation based activity until its end, the simulated behavior of particles and the way they connected to macroscopic and symbolic parameters seemed to contradict many times their expectations. In these cases they had difficulties and even refused to accept the simulation inferences and conclusions. Their current concepts appeared to be “inadequate to allow them to grasp new phenomena successfully”, requiring accommodation (Posner et. al., 1982).

A possible explanation for such observation may lean, paradoxically, on the emergent nature of these students’ thought. William, Andrew, Christopher and Elizabeth, in contrast to previous students, appeared to be used to think about macroscopic properties and symbolic relations as emerging from the behavior of particles. Therefore, they are used to concentrate on particles behavior. This may be the reason for their behavior in cases where those were very ‘surprising’ for them, contradicting their previous knowledge or expectations about the mechanical causality of phenomena. In these cases they first tried to neglect simulation inferences and tended to ignore them while solving the conceptual question in the post activity interview.

This kind of behavior appeared also during the pre activity interview. When William, Andrew, Christopher and Elizabeth saw they can’t answer the question based on particles’ behavior, either because they don’t have enough knowledge (like in the pre activity interview) or because such knowledge contradicts their current knowledge (like in the post activity interview), they decided to ignore the mechanistic nature of the phenomena and turn to a submergent ‘safer’ strategy. Nonetheless, they didn’t feel comfortable with such strategy, and were aware that something is wrong with their answers. Therefore, when probed by the interviewer, and after they failed to answer the conceptual question in the post activity interview, most of these students accepted to take into account the simulation inferences. Once they did it, they emergently applied them and successfully solved the conceptual question, like William: “According to the model you presented [in the simulation], if it is correct, if we divide the same amount of energy to less particles, the temperature will be higher”.

This students’ behavior goes in accord with the cognitive change process as described by Posner’s et. al. (1982): disagreement between the new and old ideas and dissatisfaction with previous concepts, followed by the understanding of the new concept (intelligibility), including its plausibility and fruitfulness. Nonetheless, it is
important to notice that we did not try follow Posner’s model, nor any other model of conceptual change during the computer simulation based learning activities. Moreover, the purpose of this research was not to teach students specific subject matters, but to characterize the connections between different representation modes and check if and how they change as a result of the interaction with a computer simulation.

3.3.4 Students' Perspectives and Students' Cognitive Styles

Students' perspectives reflect the way they tend to connect different representation modes. Students' cognitive styles reflect the way they tend to process information, verbally or visually. By comparing the perspectives each student presented throughout the interview with his/her cognitive style, we found a direct relationship between students' cognitive styles and their overall behavior throughout the entire interview. In the following paragraphs we will describe this relationship by comparing the characteristics of different perspectives with those of distinct cognitive styles.

When analyzing the overall behavior of students throughout the entire interview we discerned three main distinct types of behavior, as described above. The first type comprised mainly students which were classified as verbalizers: Matthew, Mary, Emily, Isabella, Emma and Jacob. All other students (who presented a different type of overall behavior throughout the learning activities) were classified as imagers.

When comparing these students' behavior with their cognitive style we can see that their behavior suits some general characteristics of verbalizers, such as good verbal skills and difficulties in processing image based information. For example, when they felt comfortable with the subject matter they communicate their thoughts very clearly, using a rich vocabulary (Atkinson, 1999; Ekstrom, French and Harman, 1976; Richardson, 1977). In these cases they clearly expressed their selves, through very convinced submergent expressions. Moreover, such expressions included many times very 'naive', or even 'poetic' explanations, such as "[particles behaves like that] because this is the way it is written they should behave" (Jacob), or "I can't define temperature; asking me to define temperature is like asking me to define love" (Isabella). However, when they didn't felt comfortable with the subject matter and had to predict and explain what is being shown in the simulation, they had difficulties in
processing the (image based) information presented. They got lost and could not follow the computer simulation based activity until its end.

Matthew, Mary, Emily, Isabella, Emma and Jacob almost did not learn from the simulation based activities, neither the first nor the second one. They showed difficulties in assimilating knowledge in such a “rich and complex visual environment” (Andris, 1996). Throughout the entire interview they looked to the behavior of particles through the lenses of a more explicit and perceptible behavior at the system level. Many times they even saw such 'macroscopic' behavior of particles in the simulation, although it was different of what was being displayed on the screen. They had a stronger tendency to rely on data they could process verbally, as these they already knew, and a weaker tendency to rely on image based data, as the one presented in the simulation (Leutner and Plass, 1998; Mayer and Massa, 2003). Such tendencies were sometimes so strong that these students could ignore what is being displayed on the screen, and describe what they 'see' as being what they think that should be displayed. For example, Mary thinks that according to the law of constant energy if a particle receives energy, it also should loose it. Consequently, she expects particles which start moving faster after a collision (got energy) to slow down afterwards (loose it):

A: Does the velocity of particles change when they don’t collide with anything?
Q: Yes
No, the velocity of particles is clearly constant unless they collide with another particle. The interviewer thus tries to ask again the same question:
A: Even if they don’t collide with anything?
Q: Yes
A: Let’s see now [the interviewer points a specific particle in the simulation – the green one]. What can you say about its velocity?
Q: [...] It slows down; I think it has a tendency to slow down.
A: Why?
Q: Because it’s original motion is slower. [...] It gradually returns to it’s original velocity.
A: What makes it return to its original velocity?
Q: The law of constant energy. If it [the particle] got energy, it also should loose it.
Such behavior was exclusive of verbalizers; none of the imagers behaved in such a way.

In addition, their knowledge about the subject matters was smaller and more vague than that of the other students (classified as imagers) even before we started the simulation based activities, all the more after them. This supports the strong correlation found between spatial ability (generally average or poor in verbalizers) and students’ performance in general chemistry courses (Bodner and McMillen, 1986; Carter, LaRusso and Bodner, 1987).

The second and third type of overall behavior was comprised exclusively by visualizers: Michael, Sophia, Anthony, Olivia, William, Andrew, Christopher and Elizabeth. Visualizers, in contrast to verbalizers, have a higher ability to process visual information. Indeed, in contrast to the verbalizers, the visualizers could follow the simulation based activities until their end. Moreover, they also seemed to learn from them. However, not all visualizers presented a similar behavior throughout the learning activities.

We can distinguish among the visualizers two distinct types of overall behavior: students who showed a strong tendency to use the submergent perspectives (Michael, Sophia, Anthony and Olivia), and students who showed a strong tendency to use the emergent perspectives (William, Andrew, Christopher and Elizabeth). Such contradictory tendencies are in agreement with the non-homogeneous behavior of visualizers, as observed by Hegarty and Kozhevnikov (1999), and Kozhevnikov, Hegarty and Mayer (2002). They observed that distinct visualizers interpreted kinematics graph problems through two completely different approaches: either as an abstract and schematic graphical representation, or as a pictorial representation. They thus suggested that there are two distinct types of visualizers: spatial imagers and object imagers. Spatial imagers were found to have good spatial ability but poor object ability, i.e. they are good at remembering and interpreting spatial and abstract relations, but have difficulties in remembering and imagining clear and detailed images. In contrast, object imagers were found to have poor spatial ability but good object ability.

All students which tended to use the submergent perspectives where classified as spatial imagers, with high spatial ability and low object ability (see Table 1). Such classification is in agreement with their behavior throughout the interview: Michael, Sophia, Anthony and Olivia concentrated mainly on symbolic representations,
comprised of abstract relationships, and less on particles behavior, which requires a more pictorial imagery. However, when classifying the cognitive style of the students who tended to use the emergent perspectives, we obtained distinct results. In contrast to Kozhevnikov, Hegarty and Mayer's (2002) prediction, William, Andrew, Christopher and Elizabeth were classified as object imagers, with high object ability but also relatively high spatial ability\(^7\). A possible explanation for such difference may lie in the distinct populations participating in the researches: Kozhevnikov et.al. (2002) investigated undergraduate psychology students, while we investigated undergraduate chemistry students. Similarly, the questionnaire we used to characterize chemistry students' cognitive style was validated at the psychology department of the Rutgers University, Newark. It may have not been fully validated on science students.

Besides this contradiction the high spatial and high object ability of William, Andrew, Christopher and Elizabeth matched their overall behavior. Their high ability to deal both with spatial and abstract relations, as well as with live and detailed images enabled them to work both with the macro and symbolic representations, as well as with the sub-micro representations with no preference for one or another. In this case it seems that the 'natural choice' is the emergent perspective. Such 'natural choice' matches previous chapter findings, where all faculty members show an emergent view of phenomena. It also supports Wilensky (2001) claim that “understanding concepts as emergent phenomena, rather than as a result of equations or macroscopic properties, is a more accurate view of science”.

\(^7\) Relative both to the spatial ability scores achieved by spatial imagers, as well as to the mean visual-spatial ability scores among scientist and engineers, as described in The MICS Questionnaire Manual.
4 Conclusions

This research was comprised of two phases. In the first one we characterized the connections between different representation modes. In the second one we applied this characterization to two computer simulations. The questions that guided the first phase of the research were: Which representation modes do students use when solving conceptual problems? How do they connect between different representation modes, if at all?

We found that using the levels of complexity view of representation modes, we can answer these research questions. We have shown that some students use only system level representations when they solve conceptual problems, with a preference to the symbolic mode. These students form no meaningful connection between the system level and the component level sub-micro representation of conceptual problems. Most students are able to relate system and component level, but do this in an inappropriate way – using a submergent perspective – which misrepresents the component level and does not challenge misconceptions. Both of these processes contribute to the apparent discrepancy between students’ ability to solve algorithmic questions and their ability to solve conceptual problems.

Based on these results and inferences we defined the second phase of the research. During this phase we designed and implemented two computer simulations and two computer simulation based activities which emphasize the emergent direction of connections between different representation modes. The questions that guided the second phase of the research were: If and how the way students connect between different representation modes changes as a result of the interaction with a computer simulation? We can answer these questions by using the emergent and submergent characterization of the connections between the symbolic and macro representation modes at the system level, and the sub-micro representation at the component level.

We discerned three distinct types of students’ behavior: students who tend to emergently connect different representation modes, students who tend to ‘submergently’ connect them, and students who did not show a consistent tendency.

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8 The interaction was through a computer simulation based activity. In the framework of this research we did not intent to check the efficiency of the computer simulation, nor the efficiency of the activity. Our aim was to check the influence of the computer simulation based activity as a whole on the way students connect between different representation modes.
neither to form emergent nor submergent connections. We have shown that such behavior is consistent, is in accordance with students’ cognitive styles, and affects both the way students solve conceptual problems, as well as the way they interact with and interpret a computer simulation.

Students showing an emergent perspective learn easily from simulations which present the emergent nature of subjects they are familiar with, and tend to question the emergent mechanisms presented in simulations of advanced topics. In contrast, students showing a submergent perspective do not learn from simulations which present the emergent nature of subjects they are familiar with, and have no problem in accepting the emergent mechanisms presented in simulations of advanced topics. Students who did not show a consistent tendency to any perspective showed difficulties in discerning between system and component levels’ behavior. Such difficulties severely interfered in their ability to successfully answer conceptual questions, and prevented them from following and learning from the computer simulation based activities.

The importance of forming connections between different representation levels has been repeatedly stressed in numerous manuscripts in the past. This work has brought into focus the need for a more precise definition of which kind of levels we mean when we say ‘representation levels’, and the question of directionality in connecting these levels. Our findings show the need to emphasize both the separation of distinct levels of complexity and the direction of the connections between them, where system level properties are shown to emerge from interactions between sub-micro particles.

Such characteristics should be also underlined when designing computer animations and simulations. On one hand computer based visualization tools are widely used to improve students’ ability to connect different representation modes, on the other hand very few of them show the emergent nature of scientific concepts. We propose to link multiple representation modes by guiding the user to deduce system level properties from the simulation (or animation) of sub-micro particles, instead of by displaying synchronized multiple views. In this way students are not only encouraged to create connections between different representation modes, but also instructed in how to connect them.
The **levels of complexity** view of representation modes and emergent direction of connecting them enable teachers and visualization tools to guide students on how the structure and behavior of submicro particles produces macro level properties and symbolic relations. In addition, if this emergent directionality is not explicitly addressed in teaching, students tend to implicitly assume a submergent directionality, projecting system level properties and behavior on the submicro particles. This submergent perspective is contradictory to the mechanistic, emergent thinking of modern science, and leads to robust misconceptions about the behavior of matter at the particulate level. Furthermore, when the emergent directionality is explicitly addressed in teaching, students who previously tended to assume a submergent directionality become able to recognize and use emergent thinking processes.
5 References


6 Appendices

6.1 A: Conceptual Question about Cooling Gases

The following diagram represents a cross-sectional area of a steel tank filled with hydrogen gas at 20°C and 3 atm pressure. The dots represent the distribution of H₂ molecules.

Which of the following diagrams illustrate the distribution of H₂ molecules if the temperature of the steel tank is lowered to -20°C (hydrogen is still a gas at this temperature).

(a)  
(b)  
(c)  
(d)
6.2 B: Conceptual Question about Heating Water via a Solid

The following diagram represents two glass pots filled with water. The pots have the same mass, hold the same amount of water, and the height of their bases is the same. However, one of them has holes in its base which contain nothing (vacuum). Both of them are heated by heat sources of equal power. In which pot will the water boil first?
6.3 C: Changing Parameters in the Simulation of a Gas in a Container

Changing the number of weights loading the piston

Figure 17: From left to right: one, two and three weights loading the piston.

As we change the number of weights loading the piston, its height decreases accordingly. Nonetheless, it is important to notice that the only parameter we actively change is the number of weights. The piston’s height decreases because the relation between the force pushing it up (applied by particles’ collisions) and the force pushing it down (represented by the number of weights loading the piston) changed.

Changing the Atomic Size of Particles

Figure 18: From left to right: normal, small and tiny size.

As we change the atomic size of particles, the piston’s height decreases a bit. It occurs as a consequence of smaller volume occupied by the particles themselves.
6.4 D: Learning Activity for the Simulation of a Gas in a Container

I start running the simulation of a gas in a closed container and explains that this simulation simulates the behavior of particles of a substance. I then ask:

1. At what state of matter is this substance?
2. Why it is at a close container?
3. What do you think the weight on top of the piston is?
4. If we look at the PV=nRT equation, how can we see each of its parameters in the simulation?
5. What do you think will happen if we add another weight on the piston? Why?

I then run the simulation with two weights loading the piston.
   a. Did the simulation match you prediction?
   b. When will the piston stop dropping? Why?
   c. How is the concentration related to the pressure?
   d. What is the pressure in the other walls of the container?

6. Which parameters of the equation may change if we reduce the size of the particles, but remains the mass unchanged? Why?

I then run the simulation with smaller particles.
   a. Can you see any change in the simulation?
   b. Is the concentration changed?
   c. Is there any change in the particles-particles collisions?
   d. Did the simulation match you prediction? If not, why?

7. What will happen if we raise the temperature of the gas?
   a. Which changes will we see?
   b. How it will affect the V and P parameters?

I then run the simulation with higher temperature.
   c. What changes do you see in the simulation?
   d. Did the simulation match you prediction? If not, why?
6.5 E: Changing Parameters in the Simulation of a Gas and two Solids

Changing the mass of gas particles

First of all let’s look at two snapshots of the system at thermal equilibrium, one with the ‘velocities’ rendering mode, the other with the ‘kinetic energy’ mode. The distribution of velocities (red:fast→blue:slow) varies according to the substance, while the distribution of energy (green:high→blue:low) is homogeneous among all substances:

Figure 19: From left to right: velocities and energy mode of a system at thermal equilibrium.

We then reduce the mass of gas particles. 21 shows the velocities of particles immediately after the change (left) and after a while (right).

Figure 20: From left to right: velocities just after reducing gas particles’ mass and after a while.
This in order to emphasize that there is no change in the ‘redness’ of particles over time. Gas particles become faster after their mass is reduced (as the overall kinetic energy \((mv^2)\) of the gas is remained constant), and remain faster over time. Their velocity changes, but the distribution of the kinetic energy over the system remains constant. Therefore it does not change the probability by which they receive or transfer energy when colliding with solids particles, and the system thermal equilibrium was not broken. This is in contrast to when we change the kinetic energy of gas particles by reducing their number instead of their mass. In this case the kinetic energy of gas particles increases just after the change, and changes over time (see Figure 21). Gas particles become more energetic, and thus tend to transfer energy to solids when colliding with them.

![Image](image.png)

**Figure 21:** From left to right: energies just after reducing gas particles’ number and after a while.

This can be seen in the image by the change in the ‘greenness’ of particles. Gas particles depicted in the right most image are colored by darker tones of green, and there are two blue atoms, instead of one in the left most image.
6.6  F: Learning Activity for the Simulation of a Gas and Two Solids

I start running the simulation and explain that it simulates the particles of a gas: Argon and two solids: Gold and Aluminum (displayed in yellow and gray respectively). The particles are in a very big container, which we look inside through a narrow window. In addition, I give some details about the particles: The size of Gold and Aluminum particles is approximately the same, but their molar mass differs: Gold particles are 7 times heavier than Aluminum particles. There is the same number of Gold and Aluminum particles in the simulation, and they are separated from gas particles by a thermal isolating partition. I then ask:

1. What is the relation between the temperatures of the three substances?
2. How do you see that in the simulation?
3. What will happen to particles if we remove the partition?

I remove the partition isolating gas and solids particles and ask:

e. Which states of matter do you recognize now?
f. What you see in the simulation match your prediction? How?
g. What can you say now about the temperatures of the substances? (the temperature of the gas was initialized to be much higher than the temperature of the solids)
h. How heat is transferred by particles?

4. If we look at the $Q=mc\Delta T$ equation, how does $Q$ and $\Delta T$ are represented in the simulation?
5. What do you think the relation between the velocities of the different substances particles is?

I change the rendering mode to display velocities and explain that the redder the faster, the bluer the slower. I then ask:

a. What do you see in the simulation?
b. Is every particle of the same substance at the same velocity?
c. How the velocity of a particle changes?
d. Does the simulation match you prediction? If not, why?
e. Is it ‘OK’ that most gas particles move slower than most Aluminum particles?
6. What do you think the relation between the kinetic energy of the different substances particles is?
   I change the rendering mode to display kinetic energy and explain that the greener the higher, the bluer the lower. I then ask:
   a. What do you see in the simulation?
   b. Does every particle of the same substance have the same energy?
   c. What can you say about the distribution of the kinetic energy among the three substances?
   d. How do you explain what we are seeing?
   e. Does it match you prediction? If not, why?

7. Follow 10 collisions between a high energy gas particle (green) and a particle of one of the solids.
   a. What happened to the energy of the gas particles after colliding?
   b. Did gas particles transferred or received energy on each collision?
   Now do the same for low energy gas particles (blue):
   c. What happened now to the energy of the gas particles after colliding?
   d. Did gas particles now transferred or received energy on each collision?

8. What determines the direction of heat transfer on each collision between a particle of the gas and a particle of the solids?
9. What determines the net direction of heat transfer between the gas and the solids as a consequence of a large number of collisions?
10. When the net heat transfer between the substances stops?
11. According to the simulation, what characterizes a thermal equilibrium state?

12. What will happen in the simulation if we reduce the mass of each gas particle to its half, but maintain the overall amount of kinetic energy in the gas constant?
    I change the rendering mode to display velocities, reduce the mass of gas particles (while keeping the overall kinetic energy constant), and ask:
    a. What happened to the overall mass of gas particles?
    b. What happened to their velocity?
c. Why do they remain red (fast) even after colliding with blue (slow) atoms?

d. What does it mean about the temperature of the gas?

I change the rendering mode to display kinetic energy and keep asking:

e. What happened to the kinetic energy of gas particles?

f. What happened to the probability of heat transfer from the gas to the solids?

g. Does it match you prediction? If not, why?

13. What will happen in the simulation if we again maintain the overall amount of kinetic energy in the gas, but instead of reducing the mass of each gas particle we reduce the number of gas particles?

I keep displaying the simulation in the kinetic energy rendering mode, reduce the number of gas particles and ask:

a. What happened to the overall mass of gas particles?

b. What happened to their velocity?

c. What happened to their kinetic energy?

d. What happened to the probability of heat transfer from the gas to the solids?

e. What does it mean to the temperature of the gas?

f. Does it match you prediction? If not, why?

14. What can you infer the relation between temperature, the overall kinetic energy in a substance and the kinetic energy per particles is?
תקציר

הממצאים המגנונים של יזון בוולג שלווה: היצוג המאקרוסופי - המימוץ

את גם בהלוס קונטракти - יזון התכניות - להנות ממסטרים עם התכניות התכניות והיוזון

שמוביל - המבצע היוזוןABI שימש בסטטיסטיק ומנתחון. בגוןossa המומלץ ביניהם יזון היוזון

שהות היצוג על מוגן את שנשם מכוננות של עליונם. כדי יזון, שחזור

ערוב בודא סטטוסי מדריך יזון את אתא היתות התשובה תצוג ולのために התמונות. מדידת

הতלɦים מספקת להב incr בין פיספקות לשתייה והיועדו והיום. קיים אלו

שה התכניות התכניות המкупות על התכניות ברמות. בנוסף לכל, כדי יזון אל

_personal קרובה (רומח יזון), שכח ייזון של התכל "רומח" כיライבי

מספקות למגן "רומח יזון". המסגרת המתחק הנכון רכון והזמנת עם זכויות, סטטוסים

ודעות הזמנים הם בין התוכנית לומדת באופן מרוכזות (הדברות מרוכזות רומח

מקורי(כ) יזון הקש ביבים זה הורמ liênובים ובביים של החכם כלים בין דרים

היום והנהלה.

병וזאטיות של הארגון עליה כמד את מזוזי והشبه תכניותпромית

כגעלה (מאובטראקציה) בין התכניות המכירבים הארץ. ממד שי יזון הבステטוס

סוכני זה השורה זה לbane הליטות מזז של המ nouveר.-bot באית זה התכניות ליזון יזון

ברמת המעשר בלב: יש לשוני לבונ מקאקרוסופי ווגים הסימולציה בניה. הבור לשיה

התכניות מתכונות המועברות כסבב הלנהות התכניות, לעם גונב הממענה סטטוסים

שהשתה בתוכנות עם התכניות מתכוננות במימיי, ובלשון כמו-

הוהנה מסיקモン. נחר ובהспектלא על התכניות המועברות הפוכה המהاراتים הא-ה, -(לופכ

קראה לה "submerged". סטטוסים שקורא נר רמה היוזון השון בטינוויכת "כל

לת הייס רמה של התכניות לשון התכניות רק תכנית מסקות

שנויי זבחה בטעה קומפואטליות.

הבחנה מחמדיאים או זכון מסקנה שחי סימולציה מחמוד, בשיל ניוואום שונית.

הסימולציות מדניות את האופי h של הספר המ广大市民, אז את שיinn התכניות בין

דרכי הייס יזון. בדיקתאגוניה של השפעת הסימולציה על אופי ייזון התכניות ביני

דרכי הייס יזון השון בושב תופים התכנתות שינב בסטטוסים: סטטוסים שוניים

לקשר נר רמה הייזון השון בטין -(ה淚 emergent что emergent, "submerged"

лось של הסימולציה של פעולות הקיש וינכר ייזון השון השון בין יזון

שנות. ואנץ או הסקנית התכנית של לינק בבייה את הסחבר הכותנייה של הסטטוסים,

בכביים עליי ייזון מבר מצבר התרות פעות יזון קומפואטליות ולאבד יהודה היא הזואו

ופרור את Afroטיליטליות.
After the scientific discussion, submergent metaphysics of the macroscopic world and emergent metaphysics of the microscopic world are compared. In the macroscopic world, the emergent approach is used, where the microscopic properties are derived from the macroscopic properties, but in the microscopic world, the submergent approach is used, where the macroscopic properties are derived from the microscopic properties.

Formal Definitions:
- **Emergent**: Properties of the whole that are not present in the parts.
- **Submergent**: Properties of the parts that are not present in the whole.
עבוודת והעשתה בהדרכהו של:

דר’ גיא אשכנזי
נישור בincinn רומח ייצוג שונות של מושגים מתמטיים ע"י סימולציה מחשב

חיבור לשב קבלת תואר דוקטור לפילוסופיה
מאט
לアナ טוקוס-רופרטי

הוגש לפקט האוניברסיטה העברית, ירושלים
ספטמבר 2008