Bringing Simplification Assumptions to the Forefront in Chemical and Biological Physics: Research-Based Development of an Introductory Computational Science Curriculum.
Abstract

In the world of contemporary research and technology, the boundaries between the disciplines have become blurred. For example, simplified models in physics are used to conceptualize phenomena in multi-particles systems that are of interest to chemistry, biology and material engineering and can be solved with analytical or numerical tools. However, the current high school science curriculum does not engage students in simplifying complex phenomena, nor does it equip them with the conceptual foundation and numerical tools they need to analyze phenomena in multi-particle systems. Thus, it fails to provide students who are interested in science and engineering with key pillars of their intellectual foundation that they are likely to need in their professional future. Central position papers have called for introductory level science curricula to better reflect the growing interest in contemporary science, interdisciplinary work, scientific modeling and computational tools.

The "Interdisciplinary Computational Science: Chemical and Biological Physics" (ICS) program developed as a collaboration between the Department of Science Teaching, the Department of Chemical and Biological Physics, and the Davidson Institute for Science Education in the Weizmann Institute for Science responded to this call. This novel three-year program (10th to 12th grade) is oriented toward capable motivated high school science students who are interested in interdisciplinary, project-based work. It takes place as a regional class at the Davidson Institute and at the University of Haifa (for the Arab sector), and grants matriculation credit for an advanced science course.

How can instruction help introductory level students construct physics-based models for phenomena involving multi-particle systems? A number of educational programs in the literature have addressed this challenge in the context of introductory courses in physics, some of which have been successfully implemented in several universities. These programs include an introductory statistical thermodynamics course, some even provide computational tools, but they do not emphasize the process of modeling, or in particular the simplification assumptions of complex phenomena in a multi-particle system such as structure formation in materials. The ICS program was based on these pioneering programs, in order to address the missing aspects.

This dissertation describes the design-based research accompanying the curricular design of the first unit of the ICS program, entitled "Particle Dynamics", that lasts one year (10th grade). The Particle Dynamics unit engages students in constructing a series of computational models intended to explain Brownian motion and diffusion. Analysis of the development in time of the particles' trajectories at different time scales serves to justify the shift from the Newtonian model of the particle motion in a vacuum (anchored in students' prior knowledge of Newton's laws) to a Random Walk model for colloidal particles in a solvent, with fine-grained and coarse grained-modeling. Instruction explicates the simplification methods, and challenges naive perceptions of simplification and modeling that are widespread among high school science students. The use
of computational tools allows the students to explore the behavior of “messy” phenomena in multi-particle systems that cannot be treated analytically.

The study consisted of both a formative evaluation of the curricular design leading to refinements of the curriculum during three consecutive cycles, as well as an investigation of the students’ perceptions of modeling that emerged as the result of their participation in the program. In particular, the ways in which the students integrated and differentiated the scientific principles of the discipline from the programming procedures, and their conceptions of the simplification assumptions were explored in the context of two-particle and multi-particle systems.

This dissertation makes a methodological and theoretical contribution to the study of students' conceptualizations of simplification assumptions in the modeling process. The methodological contribution includes a category system that was formulated to serve as an analysis tool, which specifies the extent in which students portray expert-like motivations for simplification and consider the components of simplification assumptions that are used by physicists. The theoretical contribution relates to the data analysis collected from the midterm exam, and to the two case-studies investigated in the context of students' final projects. The analysis characterizes students' perceptions which were shaped through their exposure to the Particle Dynamics unit combining knowledge in physics, programming and scientific modeling. The findings showed that at least half of the students developed rich and complex views of the simplification process: they perceived the goals of modeling in relation to the phenomena measured, discussed timescales to characterize models, and understood the key characteristics of coarse-grained modeling. These results suggest that interested and capable high school science students can develop expert-like simplification approaches to coarse-grained and fine-grained modeling.
In the world of modern research and technology, the boundaries between fields of knowledge are becoming increasingly blurred. Physics, in particular, serves as a tool for analyzing complex phenomena in multi-particle systems relevant to chemistry, biology, and materials science, acting as simplified models, and predicting their behavior using analytical and computational methods. Statements of position emphasize the need to reflect a better understanding of the study program of introductory science courses, the growing interest of contemporary science in bridging fields of scientific thought, especially in models that integrate computational tools. Against this backdrop, the current study program in secondary schools does not aim to simplify complex phenomena, nor does it provide students with the scientific foundation and computational tools necessary to analyze phenomena in multi-particle systems; therefore, it does not provide the intellectual foundation for students interested in a variety of scientific and technological fields in the future.

The new program, "Scientific Computing Across Disciplines: Chemical and Biological Physics" (hereinafter, "SCIDisciplines") was developed in collaboration between the Department of Science Education, the Department of Chemical and Biological Physics, and the Davidson Science Education Institute at the Weizmann Institute, in order to respond to the statements of position. This is a three-year program (Years 1-3), intended for talented and interested high school students, takes place on an area basis on the campus of the Davidson Institute in Ramat-Gan, and the University of Haifa (for the Arab sector), and is recognized by the Ministry of Education as a scientific subject granting 5 academic credits. The program combines the scientific foundations needed for analyzing complex phenomena in multi-particle systems in the scientific and interdisciplinary areas, and integrates project work answering the needs of students with autonomy in dealing with complex issues. Traditionally, the foundations are presented in advanced courses for Bachelor and Master degrees. How and in what way can the program be designed to meet the needs of a course in introductory physical concepts of complex phenomena in multi-particle systems? There are several study programs whose goal is to respond to this challenge, within introductory physics courses; some of these have been successful in a variety of universities. These programs present a sequence of study for teaching statistical thermodynamics at this level, and some even provide computational tools; however, they do not emphasize the process of simplifying and modeling a complex phenomenon in a multi-particle system, and do not reach the analysis of the formation of structures in materials. The SCIDisciplines program was built on the basis of these existing programs in order to respond to the gaps.

This work focuses on the design of the first unit in the SCIDisciplines program, called "Particle Dynamics," taught over one academic year (Year 1), and relies on the limited knowledge that the students bring from junior high school. In this unit, students are engaged in constructing a series of computational models for random and diffusion movements. Analysis of the time evolution of particle trajectories is conducted in different time and space scales (grained modeling - grained and fine - coarse). Assumptions of simplification in different time and space scales help clarify and justify the move from a deterministic model for particle movement in a vacuum (which is based on the early years of students' knowledge of Newtonian mechanics), to a randomly modeled particle movement in a gas. The teaching process involves a phase of simplification in the construction of models, challenging naive perceptions of students regarding scientific models. The use of computational tools enables high school students to study the behavior of phenomena in multi-particle systems, and to build for them own computational models, since the analytical modeling of such phenomena requires advanced mathematical knowledge, which is beyond their reach.

This research consists of two parts: the first part focuses on the design developer, who accompanied the development of the study program in several versions over three operational cycles. The second part includes a design research, examining the perceptions of students regarding the modeling that was developed throughout their interaction with the implemented program. The research reveals how students distinguish between the computational, physical principles, and epistemic achievements (especially simplification assumptions), in the context of two-particle systems and multi-particle systems.
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วางו את מ Blonde כבל גזירת של סונגו מרוציפי על הנחות פיסול; מרבדר בניית התפישות; ויפוי שלן הפתרון. התורמות התיאוריות

מתיחסות לינחות ותנודות בסיסי שלהם באפשרות מבוך שמество רואית ובראשית עלי פריך Henrik שלמה. ניווטה היא פאתי או תא הפישות

החלמיים ובוור או גב הוא הת XCTAssertות התפישות ומשתמשות בבה, לאור שלם במטל랏 ושנוי תכני המשלב פיש

פיזיקלו, הנכת f בידור משקע. המנסשות מרומעות לכלヘות והחלהļיידים ושוחחות בהכובד הצלחת הכובד לשון התפישות

וזרוכבת על כל הפישות המחלאות המשנה של מרגות המודול בידס לחופשת שもらえる בטקלה ומככבי או הפישות

שקל תкратני המרכזים למודול הע对孩子. מחקר זה מתprowadzić על כר שהלמודי תכרוכ ומוכשרים מתגוננים במודיע, מכיליםзамחתות הפישות

של פיס(HWND הפיתבות לאלף של מנהמות, המחלחות הפיתות של מודול ע对孩子.)