From Molecular Dynamics to Random Walks: Students Construct Computational Models in an Interdisciplinary Science Program (Poster)

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Abstract

Recent position papers have called to reform introductory science curricula to reflect contemporary scientific practices such as computational thinking (States NGSS Lead, 2013) and interdisciplinary research (AAMC-HHMI, 2009). For example, phenomena of interest to chemists, engineers or biologists, in which molecules organize themselves into stable structures at the micro level (e.g. liquid crystalline ordering in LCD screens, or change in form of cell membrane), are analyzed by physicists in terms of "competition" between the molecules' random, thermal motion and the inter-molecular interactions.

The literature points out that instead of viewing these processes as emergent from the collective interactions of the many-particle constituents of the system, students often explain them as the product of direct causal processes (Chi, Roscoe, Slotta, Roy, & Chase, 2012). It was therefore suggested that computational models that relate the macroscopic properties of the system to the constituents of the system can help develop students' understanding of emergent phenomena (Levy & Wilensky, 2008). Computational modeling enables students to picture phenomena microscopically and dynamically in a step by step manner (Chabay & Sherwood, 2008).

In high-school physics the focus is on Newtonian mechanics - predicting trajectories of point particles subjected to interactions with other objects. This deterministic approach might result in the erroneous explanation of emergent phenomena in terms of direct processes. We hypothesize that bridging deterministic mechanical laws, governing the local, short-time behavior of the constituents of the system, with a higher level (both temporally and spatially) view of the effectively random motion of particles in a many-body system, will allow students to develop a more coherent understanding of emergent phenomena.

To examine this hypothesis we designed a curricular sequence in which students construct different computational models for phenomena such as diffusion: a deterministic molecular dynamics model, an intermediate model and a random walk model, and justify the validity and appropriateness of each approach. The sequence was implemented in an experimental program for scientifically oriented excelling 10th grade students at a regional science center (School for Contemporary Science, the Davidson Institute of Science

Education, Weizmann Institute.). As part of evaluation of a pilot implementation of the program we asked students to draw concept maps portraying the sequence of ideas that were introduced. We found that the students focused on the phenomena (i.e. diffusion, osmosis) rather than the assumptions underlying different models (e.g. molecular-dynamics, random-walk). A 2nd version of the program is currently designed to respond to the above findings.

Keywords: Interdisciplinary, Micro-macro, emergent phenomena, computational modeling.

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