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A Multi-level Diffusion Unit: Connecting Submicro- and Macro-levels with Computational, Graphical, and Mathematical Representations

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Abstract

This paper describes an undergraduate unit for teaching diffusion as an emergent phenomenon using computational models. Previous research has shown that students have difficulties in understanding the role of randomness in diffusion and the connection between the micro- and macro- level properties. Analysis of learning outcomes from the first version of this curriculum showed that the computational representations helped students understand the random-walk behavior underlying diffusion, but students still struggled to connect this understanding to the macro-level relationships encoded in Fick's laws. This paper describes the revised curriculum that was developed to address this conceptual gap. Future work will analyze learning outcomes of students using this revised curriculum.

Introduction

Diffusion is one of the most important mechanisms of change at the atomic and molecular level. It is a central process in materials science and engineering (MatSE) as well as in chemistry, chemical engineering, molecular biology, and any other science dealing with atomic scale phenomena. Therefore, all students of atomic-scale sciences ideally should acquire a deep understanding of diffusion, but such understanding has proven difficult to achieve across age-groups and subjects [1]–[5]. One core reason for the difficulty is that it is not obvious how the macro-scale behavior—net movement of particles from regions of high concentration to regions of low concentration—emerges from random-walk behavior at the submicro-scale. This leads to "levels-slippage" [6] in which a person assumes the behavior at the submicro-level applies at the macro-level or vice versa. In the context of diffusion, downwards levels-slippage means incorrectly imputing the behavior at the macro-level onto the micro-level, resulting in a belief that atoms move deterministically from areas of high concentration to low concentration. Upwards levels slippage can result in confusion as to how random behavior at the micro-scale can result in the (approximately) deterministic behavior at the macro-scale. In prior work, we have found both examples of levels slippage among undergraduate MatSE majors after taking courses on diffusion [5]. The difficulty of understanding diffusion across length-scales can be viewed as a microcosm of MatSE as a whole in which the core paradigm is to understand how macro-level material properties emerge from micro- or submicro-structures. Accordingly, a core goal of our curriculum is to help students develop understanding of emergent behavior across length-scales.

Various science education researchers have employed computational models and simulations to help students understand physical phenomena from the lens of "emergence." In contrast to equation-based models, which generally describe the macro-level behavior of a system directly, agent-based or atomistic models can encode the behavior and interactions of individual elements of the system from which macro-level behavior emerges. Such an approach has been successfully used across the physical sciences, including chemistry, physics and MatSE [7]–[12].

In addition to helping students understand systems from an emergent perspective, computational atomistic approaches also expose students to computational materials science techniques. There is a widespread consensus among academics, national labs and industry that computation will

play an increasingly important role in MatSE and that both undergraduate and graduate education should reflect that [13]–[15]. There are multiple ways to integrate computation into MatSE education. One approach taken by several departments is for students to solve problems using computational tools designed for research and industry [16]–[21]. The advantage of this approach is that students learn to use tools they are likely to encounter in professional settings. A second approach is to have students use tools designed for education and/or to have them implement computational techniques themselves [8], [22]. The advantage of this approach is that students are more likely to gain fundamental understanding of computational models and techniques. The two approaches are both valuable and can be complementary, but we opt for the second in this curriculum in order to focus on foundational understanding.

This paper describes a diffusion curriculum originally reported on in [5], now updated in accordance with the findings of that paper. We recently implemented this updated version but have not had time to analyze learning results, as the course is still ongoing. The next section describes the theoretical framework guiding the design of the curriculum and summarizes results from the first version of the curriculum that motivated changes to this version. This paper represents work in progress, and future work will report on student learning outcomes with these learning activities.

Theoretical Background: Emergence, Restructurations and Active-Learning

The theoretical framework for our curriculum design revolves around three big ideas. The first, already discussed in the introduction, is the focus on emergence and thinking across levels. Our goal is for students to understand diffusion behavior at both the submicro-level and the macro-level and how the latter emerges from the former.

The question of how to help students gain a multi-level understanding leads to the second big idea: the external forms we use to represent ideas have a huge impact on how we think and what we can do. For example, it took Galileo a full page of text to prove an idea in kinematics that we can now prove in a single line using algebra [23]. Without the representational form of algebra, it took a scientist of Galileo's stature to prove things that middle school students can prove with algebra. Similarly, the advent of Hindu-Arabic numerals allows elementary school students to do calculations like long division that required expert training in the era of Roman numerals [24], [25]. Wilensky and Papert use the term "restructurations" of knowledge to refer to such fundamental changes in representational form, and these historical examples raise the question as to whether we can intentionally design new representations with equally profound effects on thinking and learning about subjects that are currently challenging for students [24], [25]. They argue that computational, agent-based models have the ability to "restructurate" knowledge about emergent phenomena. In agent-based models, the behaviors of individual components (micro-level) are programmed explicitly, and macro-level patterns emerge from these behaviors, allowing the learner to explore the connection between micro-behaviors and macro-patterns.

Agent-based models usually include multiple representations of the phenomena being modeled at different levels. In general, it is almost always necessary to use and coordinate multiple representations to understand complex scientific phenomena, including verbal, visual, graphical and symbolic representations. Three edited volumes address the importance of multiple

representations in physics, chemical and biological education [26]–[28]. Our curriculum combines computational agent-based representations created in NetLogo (a language and modeling environment for agent-based modeling) [29] with more traditional graphical and mathematical representations to help students understand the different levels of diffusion and their linkages. Figure 1 shows these various representations, including Fick's 2nd Law (the classic differential equation describing diffusion), graphical representations of concentration, a computer code representation of random-walk behavior written in NetLogo [29] and a visual representation of random-walk behavior. However, simply including multiple representations does not ensure that students will actually make links between them [30]. So, our curriculum includes activities to help students actively make connections between the various representations.

The third big idea guiding our design is that students actively construct their own knowledge and understanding. As a result, we try to maximize the amount of time that students are interacting with models and discussing with one another to build their understanding. Class time is used for these active explorations when instructors can answer questions, and any lecture material is delivered via video outside of class time.

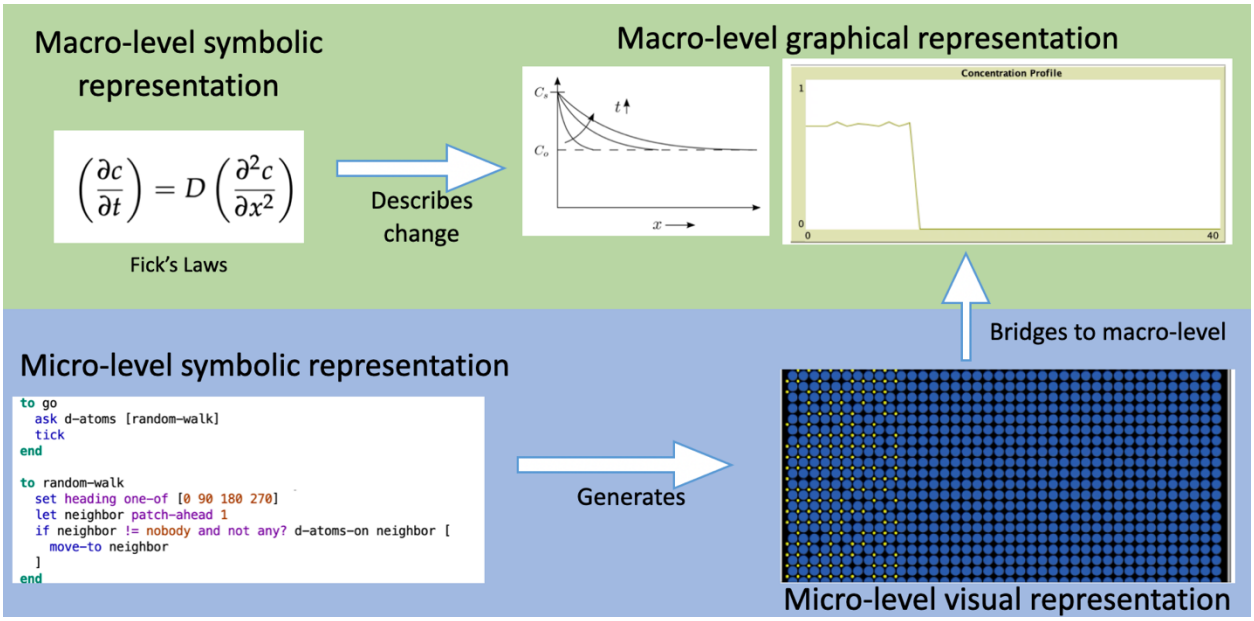


Figure 1: The multiple representations used in our diffusion unit. In the lower blue region are micro-level representations: (left) a symbolic representation of random-walk behavior written in NetLogo code and (right) the visual representation of lattice and diffusing atoms generated by NetLogo. The concentration of diffusing atoms is represented at the macro-level by a concentration profile, a graphical representation. Fick's Laws are a mathematical representation of the dynamics of how the concentration profile changes in time.

Setting and Summary of Findings from the First Iteration of the Curriculum

The setting for this study is a sophomore-level MatSE course on thermodynamics and kinetics at a private research university. It is the third course taken by MatSE majors after an introductory MatSE course and a first course in thermodynamics. Student have also taken a year-long

chemistry sequence and an introductory physics course. We do not assume students have any prior computer programming experience, although most have at least a little.

In the first version of the curriculum, students explored initial versions of the random-walk and interstitial diffusion models (described below), but these explorations occurred after the traditional lectures on Fick's laws and were not intimately linked to them. We found that exploring the models helped students understand random-walk behavior better, but they still had difficulty connecting random-walk behavior to macro-level behavior through either graphical or symbolic representation (Fick's Laws) [5]. As a result, we've rearranged the curriculum so that students start by learning about the submicro-level using computational models and then build on this understanding to bridge to the macro-level. In an entirely new activity since the first version, students use a graphical representation to qualitatively derive Fick's laws themselves. We hope that this will help students better understand the links between the different levels.

The Learning Goals

Our primary goal is for students to gain a deep understanding of diffusion. By deep understanding we mean that they will:

1. Understand the submicro-level random-walk behavior of individual particles and be able to express this behavior computationally in pseudo-code
2. Be able to qualitatively predict the macro-level dynamics of concentration profiles (i.e. where concentration will increase/decrease) and be able to connect these predictions to the symbolic forms of Fick's Laws
3. Be able to explain *why* the macro-level dynamics emerge from the submicro-level random-walk behavior

A second goal is to expose students to computational materials science techniques and engage them in computational modeling practices by having them explore models and then write small extensions for them. We want to give students experiences with exploring, assessing and creating models of phenomena, as these are all core parts of science and engineering practice. Specifically, we want students to:

1. Feel confident exploring a model to understand a phenomenon better.
2. Understand that all models make assumptions and that their validity depends on those assumptions holding (e.g. Fick's Laws are not universally true despite being called "Laws"). This is a core aspect of scientific literacy.
3. Learn to extend and create models. In this case, students write small extensions to an existing model. This is an authentic practice, because much of real-world computational modeling consists of modifying code written by others.

These learning goals will be assessed in future work through qualitative analysis of student exams and interviews with students after the course is over.

The Updated Learning Activities

The updated unit consists of some short video lectures, three in-class exercises and a homework assignment. Each in-class exercise took place during a single 50-minute class period. Students who did not finish in that time were able to finish on their own. During in-class exercises, students worked together in groups of 2-4 students. Since the course took place during the

COVID-19 pandemic, all class meetings were conducted virtually over Zoom. Each group of students was placed in a breakout room and the instructors rotated through breakout rooms to answer questions. At the end of the week, there was also an additional 50-minute recitation period for students to ask questions pertaining to the exercises or the homework. The various components of the unit are described below.

Pre-Class Video Lectures
As most of the students have never used NetLogo before this course, the students watched a 17-minute introduction to NetLogo video before the first in-class exercise and answered a few simple quiz questions on the video. Before the second in-class exercise, they were asked to watch a 12-minute video describing the interstitial diffusion model.

In-Class Exercise 1: Exploring Random Walk
The goal of the first in-class exercise is for students to become familiar with micro-level random-walk behavior and the relationship between root-mean-square distance and time for random walkers. The exercise starts with students imagining a drunken sailor stumbling around randomly. They calculate the probability of him reaching his destination four steps away, along with his most likely end position, the total distance he will have walked and the expected displacement. These pen and paper exercises are intended to help students understand the basics of random walk and expected value. As some students have never had a course in probability, this is an important part of the exercise.

Next, students explore a NetLogo model of random walk shown in Figure 2 below. The model consists of a variable number of random walkers in one dimension. They all start at $x=0$ and take a step randomly to either the left or the right each time step. The three panels of Figure 1 show the random walkers at $t=0$, $t=4$ and $t=20$. The black square shows the position of each individual random walker (they are distributed randomly in the y-direction to make it easier to see them all). The Displacement Distribution graph shows the distribution of displacements in the x dimension and shows the characteristic binomial distribution over time. The NetLogo code used to run this model is shown in the bottom right of Figure 2. Each time step, agents are asked to face either to the left or the right and then to move forward by 0.5 units. Students predict what the distribution will look like and then run the model to check their predictions.

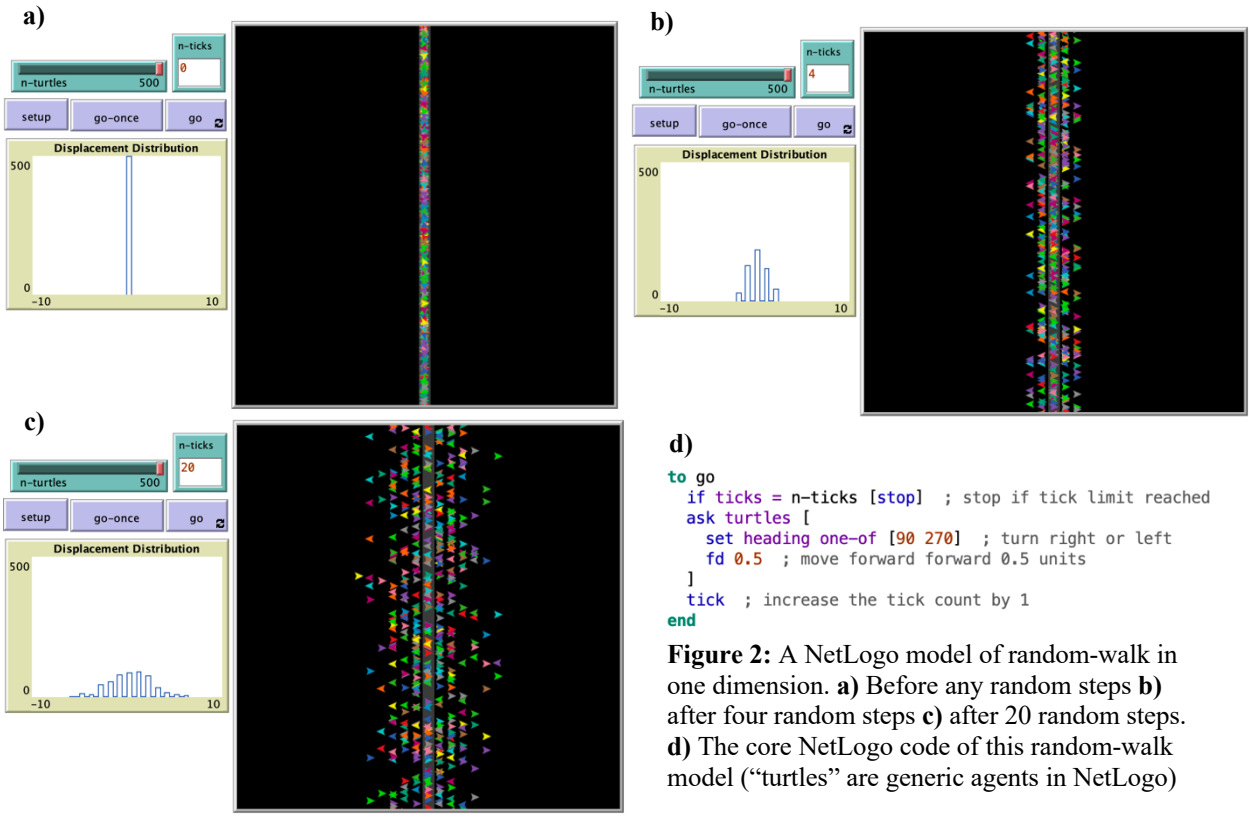
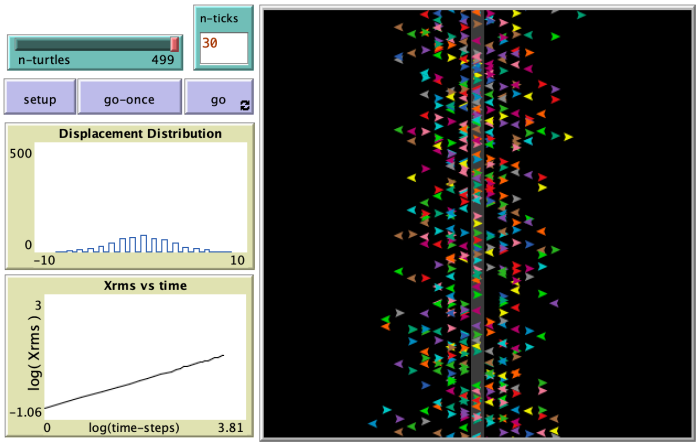


Figure 2: A NetLogo model of random-walk in one dimension. **a)** Before any random steps **b)** after four random steps **c)** after 20 random steps. **d)** The core NetLogo code of this random-walk model ("turtles" are generic agents in NetLogo)

Next, students are asked to think about a single number that could be used to describe the distribution. Students are meant to realize that mean displacement will not work for this purpose, because it is always zero. The students are then introduced to the concept of standard deviation as a way to describe the width of the distribution and root-mean-square (X_{rms}) distance as the special case when the mean position is zero. They are then given the formula for X_{rms} and asked to program it in NetLogo and plot the result in such a way as to reveal a power law relationship. As NetLogo is new to the students, they are given all the commands they will need to calculate X_{rms}, but they have to figure out how to put them together. The result, both the code and the graph, are shown in Figure 3 below. On the homework (see below) students are asked to adapt this code so that the turtles randomly walk in two dimensions and to see how the X_{rms} vs time graph changes.




```
to-report Xrms
  report sqrt mean [xcor ^ 2] of turtles
end
```

Figure 3: (above) the code for calculating $X_{rms.}$ (left) The log X_{rms} vs log time graph is shown on the bottom right of the interface. The linear relationship reveals a power-law.

In-Class Exercise 2: Exploring Interstitial Diffusion

The goal of the second exercise is for students to become more familiar with random-walk at the micro-level and to connect this behavior to the emergent macro-level behavior of concentration profile evolution using both graphical representations and Fick's laws. This section will first describe the model students used and then the learning activities they engaged in. The students were given the interstitial diffusion model shown below in Figure 4. Blue circles represent lattice atoms (e.g., iron) and yellow circles represent diffusing atoms (e.g., carbon). For simplicity, we use a square lattice. Above the atomistic representation is a concentration profile of the diffusing atoms aligned in the x-dimension. In the center, where there are few diffusing atoms, the concentration is low. Near the boundaries, where there are many diffusing atoms, the concentration is high. The buttons and switches on the left side of the interface allow the student to control various parameters of the model. The core NetLogo code of the model is also included in Figure 4.

The "draw-profile" button allows the user to draw the concentration profile as shown in Figure 5. The lattice atoms disappear, and a second concentration profile appears on the atomistic view which the user can change by clicking and dragging the mouse. The concentration of diffusing atoms adjusts accordingly. This allows the student to explore how arbitrary concentration profiles will evolve instead of just a limited set of pre-programmed conditions. The initial concentration in Figure 4, shown by the grey line on the concentration profile, is the same as that drawn in Figure 5. The yellow line in Figure 4 represents the current concentration profile after some diffusion has occurred. Since "constant-left-surface?" switch is set to "true" and the "left-surface-concentration" slider is set to 1.0, concentration at the left boundary remains at one. On the right boundary, the concentration has decreased because the surface is not held at a constant concentration. Everywhere else, concentration has changed as would be expected from Fick's 2nd law (with some noise).

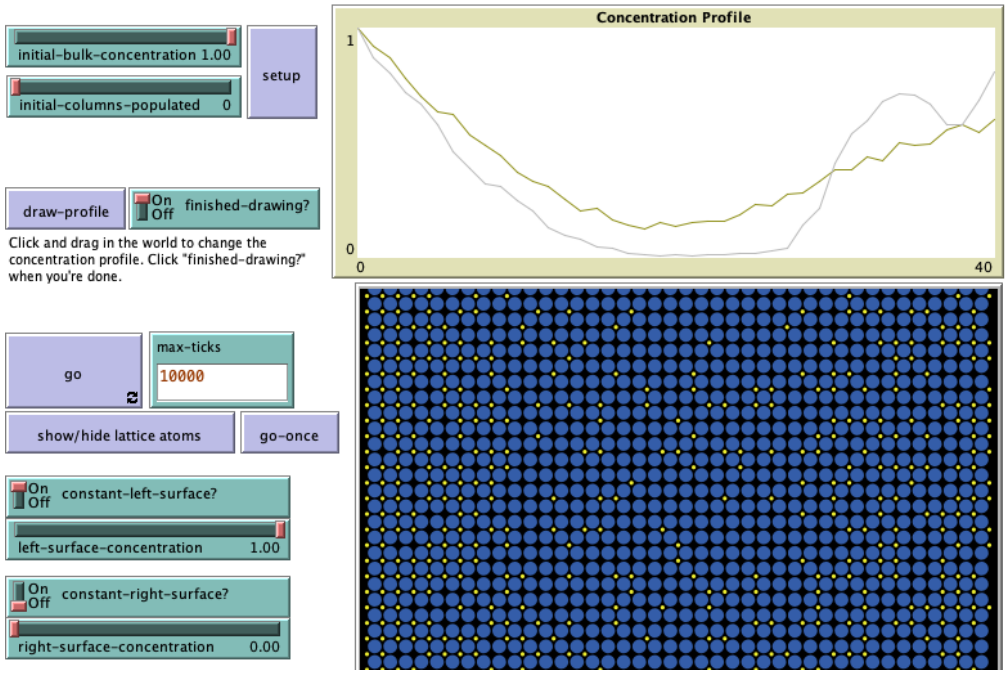


Figure 4: A NetLogo model of interstitial diffusion. Blue circles represent lattice atoms and yellow circles represent diffusing interstitial atoms. Above the atomistic visualization is a concentration profile aligned with the x-coordinates of the atomistic visualization so that moving upward from a column of atoms you can read off the concentration at that x position. The grey line shows the initial concentration profile, and the yellow line is the current concentration profile after some diffusion. Various settings and controls are on the right.

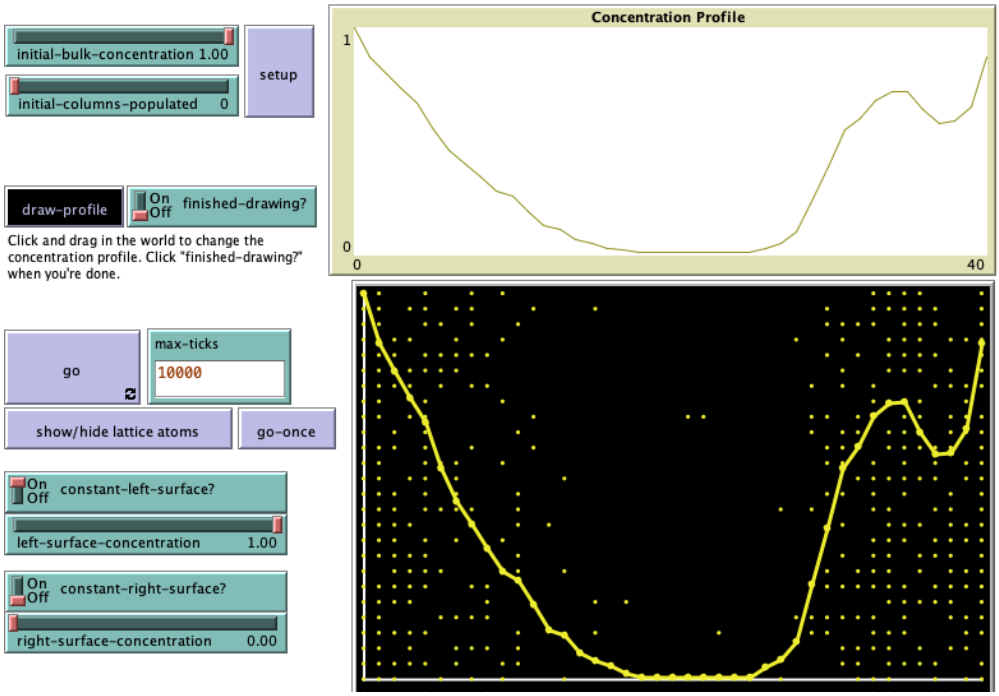


Figure 5: The model during "draw-profile" mode. Students can click and drag on the concentration profile to set an arbitrary initial condition. When they are satisfied with the initial condition, they click the "finished-drawing?" switch and press "go".

Students were first asked to explore the main code of the model (some of which is shown in Figure 6) and write in English what one of the sub-procedures inside of the "go" procedure does. Next, they ran the model to explore how different concentration profiles change over time. They did this by drawing profiles as shown in Figure 5 and then watching the model evolve. They were asked to explain what influences the rate of change of the concentration profile and why. They were also asked to determine what happens at long times and to explain why. Next, students explored changing the boundary conditions by turning constant surface concentrations on and off. They again had to describe how this influences the rate at which the concentration profile changes and determine the long-term behavior.

After using the model to explore diffusion behavior at the micro-level and connect it with the macro-level, students were asked to qualitatively derive Fick's laws using the diagrams shown in Figure 7. The students are meant to fill in all the boxes to determine how the concentration profile will change, assuming each particle has a 25% of jumping to the left, a 25% of jumping to the right and a 50% of staying put (75% for those on the boundaries). The black boxes represent the expected number of particles to jump in each direction. The blue boxes represent the expected flux between each x-position and the green boxes represent the expected change in concentration at each x-position at the next time step. The first few boxes are filled in on Figure 7a and the concentration profile at the next time step is shown in Figure 7b, which the students were asked to draw themselves. Through this exercise, students qualitatively derive Fick's first law with the blue boxes (flux is proportional to the slope of the concentration profile) and Fick's second law with the green boxes (the change in concentration is proportional to the curvature of the concentration profile). The students are then directed to watch a video lecture of a more formal derivation of Fick's laws.

```
to go
  if ticks >= max-ticks [stop]

  ask d-atoms [random-walk]

  if constant-left-surface? [set-constant-left-surface]
  if constant-right-surface? [set-constant-right-surface]

  calc-concentration
  tick
end

to random-walk
  ; turn to one of 4 neighbors
  set heading one-of [0 90 180 270]
  ; if on boundary & facing outwards, neighbor will be nobody
  let neighbor patch-ahead 1
  if neighbor != nobody and not any? d-atoms-on neighbor [
    move-to neighbor
  ]
end
```

Figure 6: The main NetLogo code for the interstitial diffusion model. In the "go" procedure diffusing atoms are asked to random walk and then if there is a constant surface concentration on the right or left, it gets set. The random-walk procedure defines a 2D random walk on a square lattice: pick one of the four cardinal directions and then if there is an empty interstitial site there, jump to it.

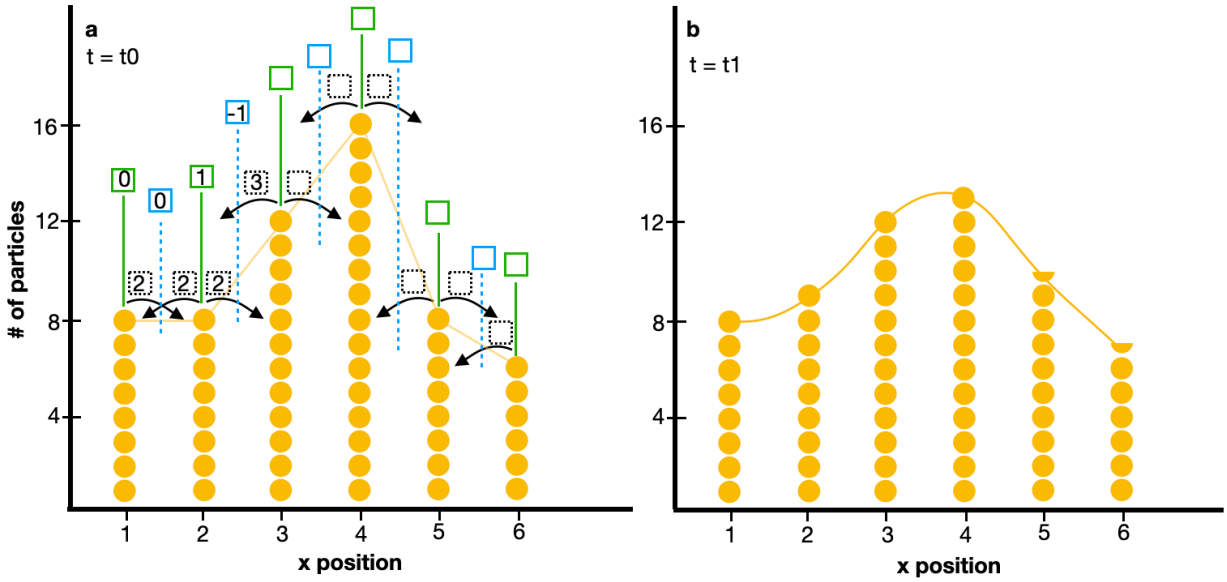


Figure 7: The graph on the left was given to students to qualitatively derive Fick's Laws and then produce a graph like the one on the right. Each yellow circle represents a diffusing atom at a certain x position. Each atom has a 25% of jumping in either direction. Students had to first fill in the black boxes with the expected number of atoms that would jump in that direction, then fill in the blue boxes with the expected flux between two columns (Fick's 1st law) and finally fill in the green boxes with the expected change in concentration for that column (Fick's 2nd law). The first several boxes are filled in with the correct numbers to illustrate what students are meant to do.

In-Class Exercise 3: Boundary Value Problems

The third, and final, in-class exercise uses the same interstitial diffusion model as the second exercise. In this exercise, students use the model to simulate various initial/boundary conditions including:

- Steady-state diffusion: constant surface concentration on both surfaces, one high and one low
- Draining plate: initial high bulk concentration and a constant surface-concentration of zero at both surfaces
- Multi-layer diffusion: an initial periodic concentration profile
- Point-source diffusion: A finite quantity of diffusing atoms are initialized near one boundary of the material and then diffuse further into the material
- Constant surface concentration: initially low bulk concentration and one surface is kept at constant a high concentration. This models something like a carburization process (carbon diffusing into iron to create steel).

Students are asked to sketch their predictions of what the concentration profile dynamics will be in each case and then use the model to set up those conditions and test their predictions. They then use the model to extract an effective diffusion depth, X_{eff}, for the constant surface concentration condition, defined as the position at which the concentration is halfway between

the initial bulk concentration and the surface concentration. They then graph X_{eff} vs time to discover the power-law relationship between them (the same power-law as the root-mean-square distance vs time).

Homework Problem Set
After the three in-class exercises, the students are given a problem set for homework that reinforces and extends what they have learned. The first problem asks students to qualitatively determine how a concentration profile will change over time. Then, students extend the random walk model from the first in-class exercise to two dimensions instead of one, and they compare the root-mean-square distance vs time graph (log X_{rms} vs log time) for the two cases. Finally, students extend the interstitial diffusion model to simulate a new scenario. They are given the following topics as suggestions but are free to pick their own as well: anisotropic diffusion, temperature-dependent diffusion, diffusion with drift (due to an electric field). Any of these topics can be modeled with minor changes to the NetLogo code (usually between one and three lines of code). This is where the flexibility of atomistic modeling compared to continuum models is most pronounced. Modifying Fick's laws to account for one of the suggested phenomena would be extremely challenging for these students. The agent-based approach allows every student to engage in an authentic, albeit simple, model-building exercise.

Future Work

This paper describes the current iteration of our diffusion unit originally reported on in [5]. It is a work in progress, as we were not able to analyze student learning outcomes until the course finished after the writing of this paper. For that future analysis, we will use a combination of video taken during the in-class exercises, student homework, student exams, and interviews with students to assess student learning. Those outcomes will be used to determine what further changes should be made to the unit to further support students learning about diffusion from an emergent perspective, connecting across multiple levels and representations.

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References

[1] R. G. Christianson and K. M. Fisher, "Comparison of student learning about diffusion and osmosis in constructivist and traditional classrooms," *International Journal of Science Education*, vol. 21, no. 6, pp. 687–698, Jul. 1999, doi: 10.1080/095006999290516.
[2] E. A. Marek, C. C. Cowan, and A. M. L. Cavallo, "Students' Misconceptions about Diffusion: How Can They Be Eliminated?," *The American Biology Teacher*, vol. 56, no. 2, pp. 74–77, 1994, doi: 10.2307/4449757.

[3] S. L. Westbrook and E. A. Marek, "A cross-age study of student understanding of the concept of diffusion," *Journal of Research in Science Teaching*, vol. 28, no. 8, pp. 649–660, 1991, doi: 10.1002/tea.3660280803.
[4] M. T. H. Chi, R. D. Roscoe, J. D. Slotta, M. Roy, and C. C. Chase, "Misconceived Causal Explanations for Emergent Processes," *Cognitive Science*, vol. 36, no. 1, pp. 1–61, 2012, doi: 10.1111/j.1551-6709.2011.01207.x.
[5] J. Z. Kelter, J. D. Emery, and U. Wilensky, "Learning About Diffusion at Two Levels: Micro-scale-computational to macro-scale-analytical," presented at the 2020 ASEE Virtual Annual Conference, 2020.
[6] U. Wilensky and M. Resnick, "Thinking in Levels: A Dynamic Systems Approach to Making Sense of the World," *Journal of Science Education and Technology*, vol. 8, no. 1, pp. 3–19, Mar. 1999, doi: 10.1023/A:1009421303064.
[7] S. T. Levy and U. Wilensky, "Students' Learning with the Connected Chemistry (CC1) Curriculum: Navigating the Complexities of the Particulate World," *J Sci Educ Technol*, vol. 18, no. 3, pp. 243–254, Jun. 2009, doi: 10.1007/s10956-009-9145-7.
[8] P. Blikstein and U. Wilensky, "An atom is known by the company it keeps: A constructionist learning environment for materials science using agent-based modeling," *International Journal of Computers for Mathematical Learning*, vol. 14, no. 2, pp. 81–119, Jul. 2009, doi: 10.1007/s10758-009-9148-8.
[9] M. Stieff and U. Wilensky, "Connected Chemistry—Incorporating Interactive Simulations into the Chemistry Classroom," *Journal of Science Education and Technology*, vol. 12, no. 3, pp. 285–302, Sep. 2003, doi: 10.1023/A:1025085023936.
[10] P. Sengupta and U. Wilensky, "Learning Electricity with NIELS: Thinking with Electrons and Thinking in Levels," *Int J Comput Math Learning*, vol. 14, no. 1, pp. 21–50, Apr. 2009, doi: 10.1007/s10758-009-9144-z.
[11] P. K. Lai, M. J. Jacobson, and M. Goldwater, "Learning nanoscience concepts through a nanoscale experience," presented at the 13th International Conference of the Learning Sciences (ICLS), London, UK, Jul. 2018, Accessed: Jun. 28, 2019. [Online]. Available: https://repository.isls.org/bitstream/1/564/1/24.pdf.
[12] U. Wilensky, "Modeling nature's emergent patterns with multi-agent languages," in *Proceedings of EuroLogo 2001 Conference*, Linz, Austria, 2001.
[13] K. Thornton and M. Asta, "Current status and outlook of computational materials science education in the US," *Modelling Simul. Mater. Sci. Eng.*, vol. 13, no. 2, p. R53, 2005, doi: 10.1088/0965-0393/13/2/R01.
[14] K. Thornton, S. Nola, R. Edwin Garcia, M. Asta, and G. B. Olson, "Computational materials science and engineering education: A survey of trends and needs," *JOM*, vol. 61, no. 10, p. 12, Oct. 2009, doi: 10.1007/s11837-009-0142-3.
[15] National Research Council (U.S.), Ed., *Integrated computational materials engineering: a transformational discipline for improved competitiveness and national security*. Washington, D.C: National Academies Press, 2008.
[16] R. Mansbach *et al.*, "Reforming an undergraduate materials science curriculum with computational modules," *J. Materials Education*, vol. 38, no. 3–4, pp. 161–174, 2016.
[17] A. Kononov *et al.*, "Computational curriculum for MatSE undergraduates," in *ASEE Annual Conference and Exposition, Conference Proceedings*, Jun. 2017, vol. 2017-June, Accessed: Nov. 04, 2018. [Online]. Available:

https://experts.illinois.edu/en/publications/computational-curriculum-for-matse-undergraduates.
[18] X. Zhang *et al.*, "Computational Curriculum for MatSE Undergraduates and the Influence on Senior Classes," Jun. 2018, Accessed: Feb. 28, 2021. [Online]. Available: https://par.nsf.gov/biblio/10093478-computational-curriculum-matse-undergraduates-influence-senior-classes.
[19] L. (Samantha) Li, "Integrating Computational Modeling Modules into Undergraduate Materials Science and Engineering Education," 2016, [Online]. Available: https://scholarworks.boisestate.edu/mse_facpubs/276.
[20] A. J. Magana and R. E. Garcia, "FiPy and OOF: Computational simulations for modeling and simulation of computational materials," in *Proceedings of the 117th Annual Conference of the American Society of Engineering Education (ASEE), Louisville, Kentucky, June*, 2010, pp. 20–23.
[21] S. P. Brophy, A. J. Magana, and A. Strachan, "Lectures and Simulation Laboratories to Improve Learners' Conceptual Understanding," *Advances in Engineering Education*, vol. 3, no. 3, 2013, Accessed: Nov. 04, 2018. [Online]. Available: https://eric.ed.gov/?id=EJ1076098.
[22] A. J. Magana, M. L. Falk, and M. J. Reese Jr., "Introducing Discipline-Based Computing in Undergraduate Engineering Education," *Trans. Comput. Educ.*, vol. 13, no. 4, p. 16:1-16:22, Nov. 2013, doi: 10.1145/2534971.
[23] A. diSessa, *Changing Minds: Computers, Learning, and Literacy*, 1st edition. Cambridge, Mass: The MIT Press, 2000.
[24] U. Wilensky and S. Papert, "Reformulating Knowledge Disciplines through New Representational Forms," presented at the Constructionism, Paris, 2010.
[25] U. Wilensky, "Restructuration Theory and Agent-Based Modeling: Reformulating Knowledge Domains Through Computational Representations," in *Designing Constructionist Futures: The Art, Theory, and Practice of Learning Designs*, N. Holbert, M. Berland, and Y. B. Kafai, Eds. MIT Press, 2020, pp. 287–300.
[26] J. K. Gilbert and D. Treagust, *Multiple representations in chemical education*, vol. 4. Springer, 2009.
[27] D. F. Treagust, R. Duit, and H. E. Fischer, *Multiple representations in physics education*. Springer, 2017.
[28] D. F. Treagust and C.-Y. Tsui, *Multiple representations in biological education*. Springer Science & Business Media, 2013.
[29] U. Wilensky, *NetLogo*. Center for Connected Learning and Computer-Based Modeling, Northwestern University. Evanston, IL., 1999. https://ccl.northwestern.edu/netlogo
[30] M. H. Wilkerson-Jerde and U. J. Wilensky, "Patterns, Probabilities, and People: Making Sense of Quantitative Change in Complex Systems," *Journal of the Learning Sciences*, vol. 24, no. 2, pp. 204–251, Apr. 2015, doi: 10.1080/10508406.2014.976647.