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Re-Envisioning Materials Science Education Through Atomic-Level Computational Modeling

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Abstract: This paper presents a re-designed introductory materials science and engineering (MSE) course that uses computational atomistic modeling for nearly every topic. Computation is becoming ubiquitous in MSE, and it can help dramatically improve understanding of how macro-level behavior *emerges* from atomic behavior. Just three modeling techniques—molecular dynamics, Monte Carlo, and random walk—can be used to model most topics in an introductory MSE course, and understanding conceptually how these techniques work is not very difficult. After providing background on computation in MSE and in education, we describe the structure of the course as a whole, provide detailed descriptions of two units in the course to illustrate how computational models can be used to teach core MSE concepts, and discuss how this approach differs from the traditional approach.

1 Background: computation in MSE, ABM in education, and learning theories

1.1 Computation in MSE

Computational materials science and engineering (MSE) dates to at least the 1980s, and in the past 20 years the MSE community has begun to recognize the crucial importance of computational tools in accelerating the development, discovery, and design of new materials. There is widespread consensus among academics, national labs, and industry that computation will play an increasingly important role in MSE and that both undergraduate and graduate education should reflect that change [1], [2], [3]. This commitment to a shift in the educational approach within MSE departments is highlighted in the strategic plan of the National Science and Technology Council's Materials Genome Initiative, which posits that the next generation of the MSE workforce will need to master three competencies: experimentation, data management, and *computation* [4].

MSE educators have worked to construct educational offerings that develop competencies in the areas identified by the Materials Genome Initiative. Several departments have developed computational courses or add-on computational modules for existing courses [5], [6], [7], [8], [9], [10]. However, while inroads have been made in MSE curricula at upper-level undergraduate and graduate courses, introductory courses are still largely taught with traditional diagrams and formulae approaches, leaving computational thinking, exploration, and modeling for later. This traditional approach misses an opportunity to leverage computational modeling as a core teaching and learning tool when students begin their study of MSE. According to the Open Syllabus project [11], which has collected over 230,000 engineering syllabi, the most popular introductory MSE textbook, authored by Callister and Rethwisch [12], is the second most assigned textbook across *all* engineering disciplines. This textbook has been through many editions, but it was originally written in 1985 and does not include any computational approaches.

To maximize student learning, the integration of computation into introductory courses should use tools designed specifically for education. The existing computational MSE initiatives in upper-level courses focus mostly on using computational tools designed for research and industry to solve problems [5], [6], [7], [9], [10]. The value of this approach is that students learn to use tools they may encounter in professional settings. However, these tools are designed for efficient problem solving and do not usually help students to better understand the underlying phenomenon being modeled, making them suboptimal for an introductory setting.

Here, we describe an introductory MSE course grounded in computational modelling from a *complex systems* perspective in which the interactions of large numbers of atoms lead to the *emergence* of larger-scale properties. Models showcasing emergence fit perfectly with the classic MSE paradigm which emphasizes that a material's properties emerge from its structure which emerges from the processing the material undergoes. The course utilizes computational agent-based or atomistic models (ABMs[1]) designed specifically for educational purposes. Beyond providing computational skills that students will need in their careers, these models will leverage a truly transformative aspect of computation in education: the ability of the computer to represent scientific phenomenon in new, powerful, and intuitive ways.

1.2 ABM in Education and Restructurations

Representing content in new ways can dramatically improve learning. For example, with the use of modern Hindu-Arabic numerals, elementary school children routinely learn to do long division and long multiplication. Using Roman numerals, these operations were considered so difficult that only trained professional were able to do them [13]. Similarly, the notation of algebra radically changed the difficulty of kinematics. It took Galileo, who did not have algebraic notation, a full page of text to prove simple relationships between distance, speed, and time, such as "if two objects travel at the same speed, then the ratio of their distances traveled equals the ratio of their times travelled," but with algebraic kinematics, we can simply write, $d = s \times t$ for each object, (where d is distance travelled, s is speed and t is time travelled) and divide them to see this result in one line of algebra: $\frac{d_1}{d_2} = \frac{s \times t_1}{s \times t_2} = \frac{t_1}{t_2}$ [14].

Wilensky and Papert call this kind of dramatic transformation in thought due to a new representational form a "restructuration" [13], [15]. They offer several criteria for evaluating a restructuration. For one, a successful restructuration can be more powerful than the old structuration, either by enabling new things to be done that weren't possible under the old structuration or by bringing different phenomena, previously viewed as unconnected, under a shared framework. A restructuration can also have cognitive properties that make it easier to learn and reason with than the old structuration. Additionally, it might make learning more engaging, or accommodate different learning and thinking styles.

By the above criteria, ABM can serve as a restructuration for a large swathe of MSE content. While traditional equation-based modeling techniques naturally treat more simple material systems, such as perfect crystals, computational techniques that model large number of atoms allow scientists to model "real, complex materials as they are" [16]. This powerful property of atomistic modeling results from the fact that the basic entities of the model are individual atoms

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[1] We will use ABM to refer to all computational modeling techniques that model individual entities, including atomistic techniques such as Molecular Dynamics and Monte Carlo methods. Although the "A" of ABM usually represents "agent," in the context of MSE it should perhaps be interpreted as "atom."

which can interact to produce complex aggregate patterns. In contrast, traditional equations usually represent aggregate quantities directly and require simplifying assumptions about the material system to be tractable, often to the point that they do not represent any real material system at all. Atomistic models can also help researchers “to gain insight into a physical system and then obtain a new theoretical understanding” [17], showcasing their cognitive properties.

Bringing restructurations to educational settings can have a profound impact. No amount of improved pedagogy would have improved children’s ability to do arithmetic as much as switching from Roman to Hindu-Arabic numerals. Similarly, bringing computational ABM to students can profoundly impact their learning about complex systems of all kinds, including materials systems studied in MSE [13], [15]. First, the rules that individual agents follow are often more intuitive to learners than equations representing aggregate quantities, giving students a solid grasp of the mechanisms from which scientific phenomena emerge. Second, ABMs are usually much easier to adjust and modify than equation-based models, allowing students to engage in authentic modeling practices. Students are very good at plugging values into equations but adjusting the equation itself to model a different phenomenon is much more difficult. Third, with the right software, ABMs can produce rich visualizations to help learners interpret and learn from the output of a model.

1.3 Learning Theories: Model-Based Learning

Model building is at the core of scientific practice [18], [19]. Modeling theory itself began as an investigation of how science works and has since grown into an educational theory of its own with many taking the stance that modeling should be at the core of science education [20]. The goal is for students to learn disciplinary knowledge while also gaining procedural knowledge of how to use, create and assess models.

Our discussion of modeling in science refers to the creation of external, sharable models. There are many kinds of external models including visual representations (e.g., a map is a model of a place), mathematical models that relate various observable quantities together, and emergent models in which some aspect of a system emerges from the interactions of modeled objects [21], [22]. A long history of research has investigated the use of computational tools to help students engage in various types of modeling and learn through model-based inquiry (for reviews see [23], [24]).

One class of learning environments known as *microworlds* [25] use interactive computational environments to enable students to actively explore a topic. Dynaturtles, an early microworld, allowed students to “kick” computational objects following Newton’s laws of motion to gain a more intuitive understanding of Newtonian motion [26]. In an *emergent systems microworld*, many computational agents (or atoms) interact to produce a phenomenon which students can explore [27]. For example, interactive molecular dynamics models have been used to help middle and high-school students inquire into how the phases of matter emerge from atomic interactions [28]. Similarly, microworlds of gas molecules have been used to help students understand how the ideal gas laws emerge from the aggregate behavior of many particles [29]. Explorations of microworlds can constitute an authentic modeling activity. After all, a large part of the work of a computational scientist is experimenting with their computational models to understand their behavior.

Emergent systems sandboxes (ESS) are an approach to engaging students in model *construction* without having to write code [30]. In an ESS, the learner can construct models from ready-made entities that already follow rules governed by a core scientific model. For example, students could add particles of different sizes to a molecular dynamics model to see how they interact. In this way, students can construct the initial conditions of a model and run experiments, even if they are not coding the micro-level behaviors themselves.

With the right tools, it is also realistic for students, even at an introductory level, to engage in computational modeling through writing code. NetLogo [31] is an agent-based modeling environment designed specifically to have a “low threshold” to make it easy for novices to start modeling, while still having a “high ceiling” of what is possible [32]. To start, students can engage in inquiry through modifying small amounts of code in existing models. This can either be a form of open-ended “tinkering” with the code to explore what happens, or more directed modifications to model a new phenomenon [33]. There have been many successful examples of high school and college students learning to use NetLogo and successfully building incisive models in subjects such as biology [34] and MSE [35], [36].

Prior research has shown increased student understanding of core concepts in MSE through the use of computational models [36] as well as in related fields of chemistry and physics [29], [37], [38], [39]. As discussed above in the context of restructurations, starting with the micro-picture is a qualitatively different way of thinking about these phenomena compared to equation-based approaches and often leads to deeper conceptual understanding.

Prior work on computation in MSE education analyzed the way MSE phenomena are traditionally represented and then compared student understanding under the traditional approach with an ABM-based approach [35], [36]. Most traditional class time was spent on deriving and analyzing equations. These derivations usually start with a qualitative description of atomic behavior paired with a schematic picture of atoms. Then, multiple simplifications and assumptions are made to transform the qualitative picture into a statement about aggregate level, continuous patterns that can be handled by differential equations. Because of the complexity of MSE phenomena, multiple equations and derivation steps must be related to one another to model a single phenomenon, and students can easily get lost in the math without gaining conceptual understanding [36]. Additionally, the final equations no longer refer directly to atoms, hiding the mechanisms which give rise to the phenomenon in the first place. This results in an “epistemological gap” between the equations and conceptual understanding of the phenomenon [36].

In contrast, a single computational model of atomic interactions can exhibit multiple emergent properties. For example, a molecular dynamics model of atoms exerting forces on one another and moving according to Newton’s laws can exhibit crystal structure, thermal expansion, phase transformations and more. The “one-to-many” [36] property of many computational models, in which a single model can represent many phenomena, helps students gain deeper understanding of core MSE ideas, because multiple phenomena are connected by a small number of principles, such as atoms moving stochastically but tending towards lower energy positions.

2 The Structure and Delivery of the Course

Our course surveys the standard topics covered in an introductory MSE course. Approximately one broad topic is covered each week. There are two 80-minute class periods on Tuesdays and Thursdays and one 50-minute TA section on Mondays. Over the course of the design, we have authored our own interactive textbook hosted on a website[2] designed and created by the first author which can contain interactive models, diagrams, and questions for students to answer within the website. Before each class, students are assigned pre-lecture exercises that typically take between 30-60 minutes. These pre-lecture questions usually consist of interacting with one or more computational models and answering questions. Tuesday and Thursday class periods usually consist of three segments of 20-30 minutes: a lecture on the topics covered in pre-lecture exercises, an active-learning period in which students explore another model and answer questions on the website, and a final short lecture on the topics covered.

2.1 The MSE Topics Covered

Table 1 lists the main modules of the course and the computational techniques used in them. Brief conceptual descriptions of these modeling techniques are included in Appendix 1. There are a few topics covered in the course which currently do not have computational models accompanying them: composite materials, biomaterials, materials selection, and broader impacts.

Table 1: List of topics and the computational techniques used to model them.

Module	**Computational technique(s)**
Interatomic potentials and bonding	MD (molecular dynamics)
Crystal structure	MD
Energy of Point defects	MD
Diffusion	Random walk
Energy Distributions and Vacancy Concentrations	MC (Monte Carlo) on lattice
Polymer structure	Random walk
Phase diagrams	MC
Mechanical properties (including dislocations)	MD
Electronic properties – metals & semiconductors	MD

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[2] https://www.morfli.com/ - if the full course is unavailable at the time of reading, contact the first author for access.

3 Example Units

Due to space constraints, the entirety of even a single unit cannot be fully described in this paper. Instead, the focus will be on describing the computational models used in each unit and the activities students engage in using the models. Appendices 2 and 3 include the complete text of the questions students answer in these units. It should be assumed that there is some amount of lecture and explanation following each student activity with a model.

3.1 Atomic Bonding to Crystal Structure

Atomic bonding and crystal structure are covered in three chapters in our text: (1) Atomic Bonding, (2) Modeling Interatomic and Intermolecular Interactions, and (3) Bonding to Crystal Structure. Our Atomic Bonding chapter begins with an exploration of a model of just two atoms. The student can click and drag the atoms around in 2D and see how they interact. They discover that the atoms do not interact at large distances, attract at short distances, and repel at very short distances. These three facts are then labeled “the atomic hypothesis”. In the words of Richard Feynman: “the atomic hypothesis [is] that all things are made of atoms—little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another” [40]. These facts need to be explained. To this end, the chapter introduces the electrostatic interpretation of atomic bonding [41]. This interpretation of the bond emphasizes three key similarities of *all* bonds, including secondary bonds. First, it is the attraction between the nuclei and electrons of different atoms that cause bonding. Second, this attraction leads to increased electron density between the nuclei of two bonded atoms compared to their unbonded state. One could perhaps even say that the increased electron density between the nuclei of bonded atoms *is* the bond. Third, if the atoms are squeezed too close together, the repulsion between the nuclei push the atoms apart.[3] This approach to conceptualizing bonding has been recommended by a number of chemistry education researchers because it explains *why* atoms bond in terms of fundamental physical forces, instead of heuristics like the octet rule, and unifies all the bond types under one overarching physical explanation [42], [43], [44].

This is not the approach taken in the most popular MSE textbook [12] which explains primary bonds as arising “from the tendency of the atoms to assume stable electron structures, like those of the inert gases, by completely filling the outermost electron shell” while, in contrast, “secondary or physical forces and energies are also found in many solid materials; they are weaker than the primary ones.” This explanation makes it sound like primary bonds are not due to physical forces! In reality, the reason a full valence shell is stable is because the valence electrons feel a strong attractive force from the nucleus while additional electrons only feel a much weaker force due to a combination of (1) shielding from the valence (and core) electrons and (2) necessarily being further from the nucleus since the valence shell is filled. [12] goes on to explain ionic and secondary bonding as being the result of coulombic attraction, but covalent bonding is not described as being due to any forces at all, and metallic bonding is described as a

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[3] The reason that repulsion is only described as between nuclei and not between the electrons of each atom is because electrons, being so much less massive than nuclei, move approximately instantaneously compared to the movement of the nuclei. When the atoms are squeezed together, the electrons will rearrange themselves to be in equilibrium within the whole system while the nuclei are still repelling each other [41].

sea of electrons being the "glue" that holds the ionic cores together, without explaining what physical force makes the electrons glue-like. These types of explanation are still common in chemistry education as well despite extensive chemistry education literature documenting the conceptual issues arising for students who are taught bonding in this way [45], [46].

In the electrostatic interpretation of bonding, all the bond types are due to increased electron density between nuclei but differ in how the increased electron density is distributed. For covalent bonds, it is approximately equally distributed between them. For ionic bonds, it is much denser near the more electronegative atom. For metallic bonds, it is spread out between each nucleus and all of its neighboring nuclei, rather than localized between just two nuclei. Figure 1A illustrates the difference between covalent and ionic bonds from this perspective. For secondary bonds, since the valence shells are full, the electrons of each atom cannot approach very close to the other nucleus. Nevertheless, the electron density of the full valence shells can shift slightly in between the nuclei, resulting in weak bonds. These types of bonds are illustrated in Figure 1B.

Next, our Modeling Interatomic and Intermolecular Interactions chapter introduces interatomic potentials. It begins with a review of the concepts of force and potential energy in the context of a spring. Students are then given a model in which they can draw a potential energy curve between two atoms and drag the atoms to start at different distances and then see how the atoms move as a result. They are first asked to draw a spring-like potential and then to draw a potential that will result in behavior consistent with what we know about atoms: effectively no interaction at large distances, attraction at short distances, and repulsion at very short distances. The interface with examples of both these drawings is shown in Figure 2. This corresponds to an exploration phase in the learning cycle [47], [48], [49].

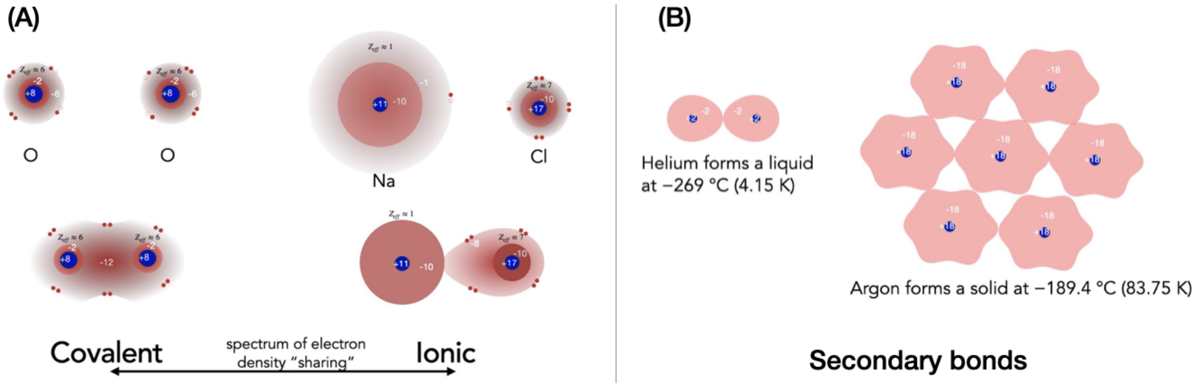

Figure 1: (**A**) Cartoon illustration of electron density shift in a pure covalent bond between two oxygen atoms and a highly ionic bond between a sodium and chlorine atom. Z_{eff} is the effective nuclear charge that valence electrons feel based on the attraction to the nucleus and the repulsion from non-valence electrons. More electronegative atoms have a higher Z_{eff}. The Z_{eff} values shown here are very rough approximations as the reality is more complex than a simple canceling out of charges from the nucleus and core electrons. (**B**) Even with noble gasses that have full valence shells, the electron density can shift slightly, resulting in weak bonds between atoms. This means that despite full valence shells, an electron near a noble gas still feels a *slight* attraction towards its nucleus. Since these bonds are so weak, noble gases only form liquids and solids at extremely low temperatures.

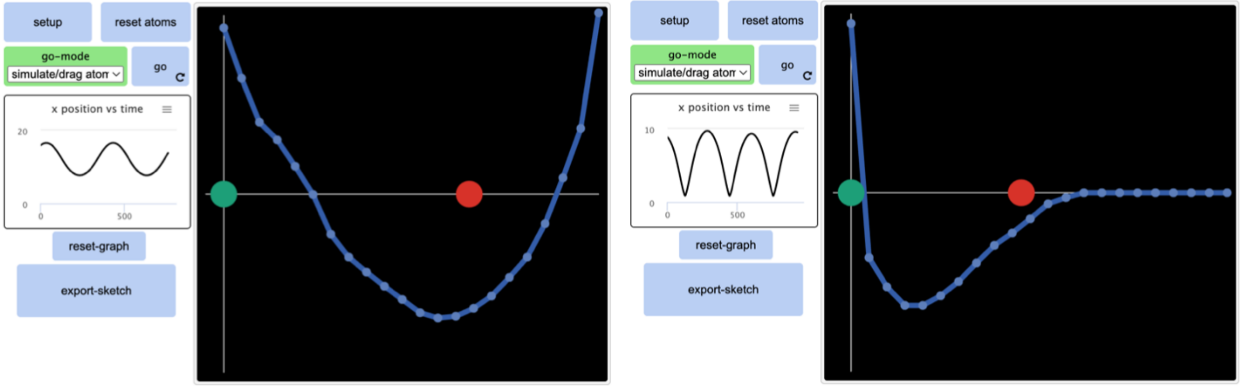

Figure 2: Interface for drawing an interatomic potential and seeing the dynamics of the atoms. **Left**: A spring-like potential results in a symmetrical oscillation as seen in the "x position vs time" graph. **Right**: an interatomic potential results in an oscillation that spends more time far from the equilibrium distance because of its asymmetry.

After the exploration phase, students are introduced to the Lennard-Jones potential as a mathematical and graphical representation of interatomic potentials, and they answer a number of questions about it. Next, they interact with a simple molecular dynamics model of two atoms in one dimension interacting according to the Lennard-Jones potential. Students can change the parameters of the potential, drag one of the atoms to different starting positions, and initialize the atom with different amounts of kinetic energy. The model is similar to the one shown in Figure 2B except that the potential is drawn for the student according the Lennard-Jones potential. Students use this model to answer a number of questions about the potential, kinetic, and total energies of the atoms in different initial conditions and under what conditions the bond will break. In contrast to our approach, the most popular MSE textbook introduces interatomic potentials before discussing bond types and then only explicitly discusses them in the context of ionic bonds [12]. The static diagrams in a textbook also cannot convey the dynamic nature of bonded atoms, i.e., that they are constantly oscillating around the equilibrium bond position (unless they are at absolute zero).

In the following chapter, students interact with MD models of many atoms interacting in two dimensions. Crystal structures emerge from these models as shown in Figure 3. These crystal structures are not explicitly encoded anywhere in these models. Atoms simply follow Newton's laws, accelerating due to interatomic forces, and crystal structures emerge as the equilibrium structures. The chapter also discusses the limitations of these models including that they cannot produce non-close packed crystal structure without significant modifications to the code to deal with directional bonds. To our knowledge, this is a novel approach to introducing crystal structure in that we first have students "discover" that crystals emerge from simple models of interatomic forces and only then introduce the ways to characterize and describe crystal structures. This focus on emergence helps connect crystal structure back to the basic physics principles underlying MD models and the ideas of bonding and interatomic potentials introduced in the previous chapters.

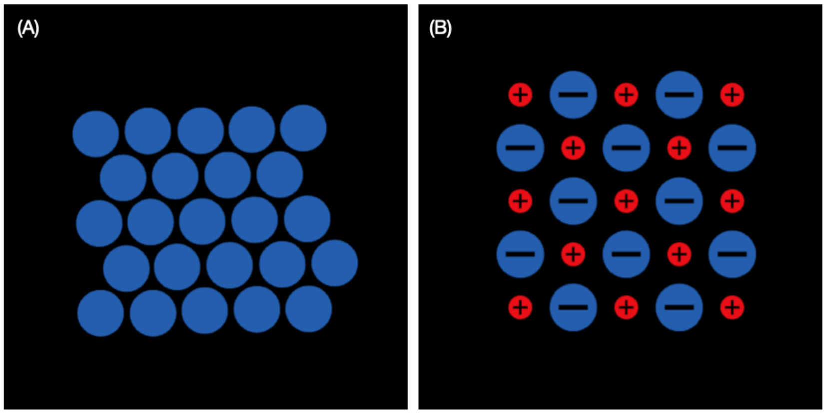

Figure 3: (A): Emergent close-packed hexagonal crystal structure from atoms interacting according to Lennard-Jones potential. (B): Emergent rock-salt crystal structure from cations and anions interacting according to an interatomic potential with an ionic attraction/repulsion term.

3.2 Diffusion

Diffusion is covered in a single chapter in our text which begins with some history: the discovery of Brownian motion in 1827, then Einstein's paper in 1905 explaining it as a result of random movement of atoms, and finally Jean Bapitiste Perrin's experimental confirmation of Einstein's predictions in 1909. This history is interesting in part because there were still prominent scientists in 1905 who did not think atoms existed, but Einstein's explanation of Brownian motion provided extremely strong evidence for their reality. The unit presents traces of the random paths of colloidal particles taken from Perrin's paper [50], and then shows a molecular dynamics simulation with one atom tracing its path to show that this type of random motion emerges naturally, as shown in Figure 4A. This is used to justify the random walk model: given that each atom follows what looks like a random path, we can drastically simplify our model by ignoring all the Newtonian physics and instead modeling each atom as simply taking a step in a random direction each time step, as shown in Figure 4B.

Students then explore a random walk model with thousands of atoms to explore how concentration profiles emerge from many random walkers. Using the model, shown in Figure 5, students can draw concentration profiles which causes atoms to populate according to that concentration. They can then run the random-walk model and see how the concentration profile evolves. Next, students are introduced to diffusion mechanisms in solids and explore one model of vacancy-mediated diffusion and one of interstitial diffusion, shown in Figure 6.

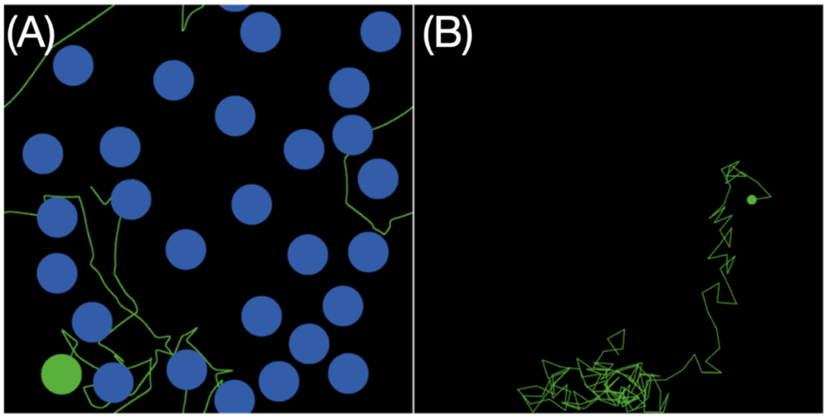

Figure 4: (A) A Molecular dynamics simulation with one atom colored green and tracing its trajectory, which results in what looks like moving in fairly straight lines with periodic random changes in direction. (B) A random walk model in which the atom turns a random direction and takes a step forward each time step.

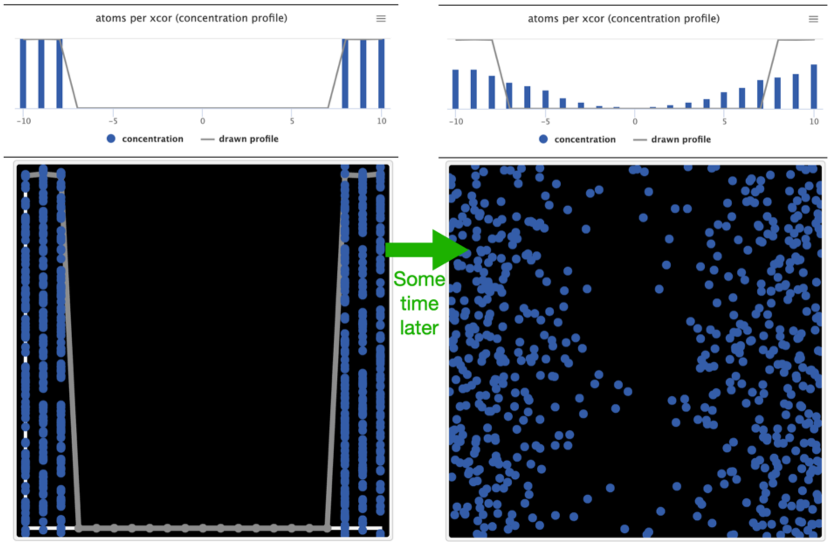

Figure 5: Students are able to click and draw a concentration profile (grey line) and the concentration of atoms (blue circles) is updated accordingly. **Left:** right after drawing a concentration profile with high concentration near the edges and zero concentration in the middle. **Right:** The same model after running it for several time steps. The graph above the atomic view shows the initial concentration profile with the grey line and the current concentration profile with blue bars.

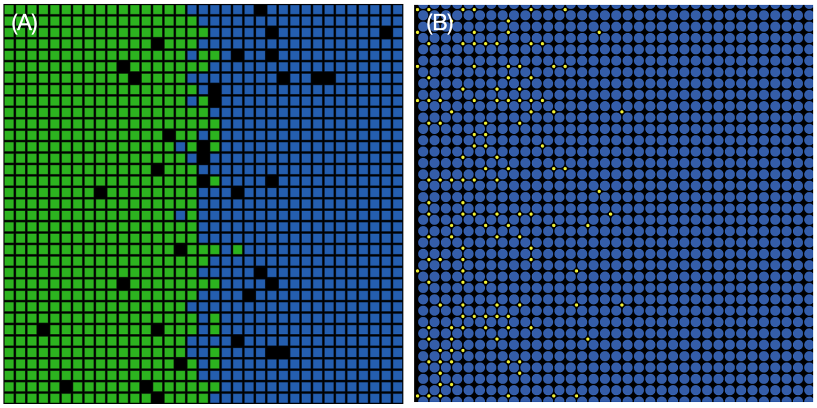

Figure 6: (A) Random-walk model of vacancy-mediated diffusion. (B) Random-walk model of interstitial diffusion. The yellow dots are interstitial atoms and the blue lattice atoms are just for visualization.

The next section of the unit helps students to understand why the macro-level concentration profile dynamics they observed in the previous models emerge from random walk. This entails a qualitative derivation of Fick’s laws of diffusion starting from a random walk. The students are given the diagram shown in Figure 7 and are first asked to fill in the black boxes with the expected number of atoms jumping in each direction and the blue boxes with the resulting expected flux between columns. They are instructed to explain what feature of the concentration profile determines the flux (the slope) and then to try to invent a mathematical rule for what the flux will be at each position. After spending a few minutes on this, they are shown the standard answer, which is Fick's 1st Law.[4] We ask students to first try to invent an equation before introducing Fick's 1st Law based on research that when students first try to invent a mathematical formula, it prepares them better for future learning [51].

This process is then repeated for Fick's 2nd law. The students first fill in the green boxes shown in Figure 7 with the expected concentration change at each x-position based on the fluxes in/out of that position. Then they are asked to explain in words what determines the rate of change in concentration at each position. Finally, they are asked to invent a mathematical rule for the rate of change of concentration after which they are shown Fick's 2nd law.[5] After these derivations, students are given some questions to qualitatively predict how concentration profiles will change over time and some quantitative questions using the mathematical form of Fick's laws.

Apart from the interactive models which support active learning, this approach to diffusion at the introductory MSE level differs from the traditional approach [12] in two important ways. First, we spend more time justifying and exploring the random walk model, including introducing NetLogo code for it. This is important for students to develop a clear understanding of the atomic-level behavior and avoid the misconception that individual atoms move deterministically from areas of high concentration to low concentration [52]. Second, we have students qualitatively derive Fick's laws instead of simply introducing them without any derivation. This aids in conceptually understanding Fick's laws and in connecting them with the underlying atomic behavior from which they emerge.

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[4] Fick's 1st law is: $J(x) = D\frac{dC}{dx}$, where $J(x)$ is the flux at position x, D is the diffusion coefficient, and $\frac{dC}{dx}$ is the spatial derivative of concentration with respect to x.

[5] Fick's 2nd law is: $\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2}$, where $\frac{\partial C}{\partial t}$ is the partial derivative of concentration with respect to time, D is the diffusion coefficient, and $\frac{\partial^2 C}{\partial x^2}$ is the second spatial derivative of concentration with respect to x.

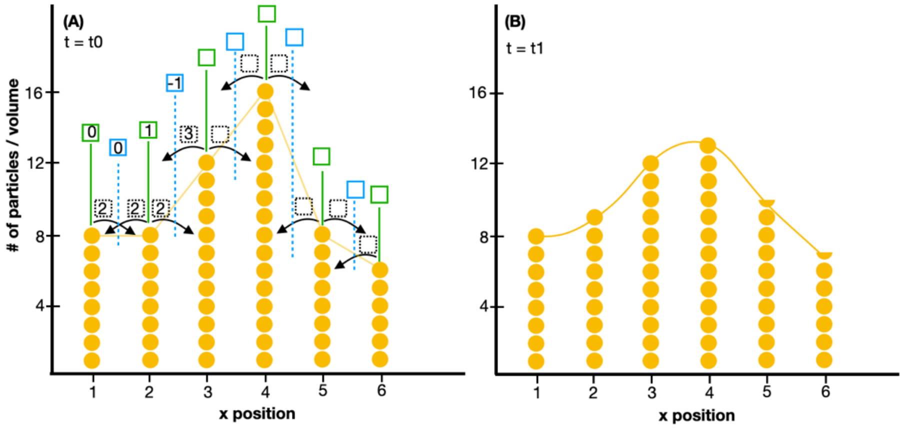

Figure 7: Students were given the graph on the left to qualitatively derive Fick's Laws and then produce a graph like the one on the right. Each yellow circle represents a diffusing atom at a certain x position. Each atom has a 25% of jumping in either direction. Students first fill in the black boxes with the expected number of atoms that will jump from that column in the indicated direction. Next, they fill in the blue boxes with the expected net Flux across the dotted blue lines between each column (Fick's 1st Law). Finally, they fill in the green boxes with the expected change in concentration at each x-position (Fick's 2nd Law). The first few boxes are filled in with the correct numbers for illustration.

4 Conclusion

The educational potential of computational representations matches perfectly with the increasingly computational field of materials science and engineering. Atomistic computational modeling techniques are "one-to-many" [36], meaning that one modeling technique can address many MSE phenomena. This is because atomistic techniques are based on fairly basic atomic behavior from which larger-scale properties emerge. One-to-many models have advantages both scientifically and educationally. Scientifically, they enable the modeling of real complex materials without needing to make overly simplistic modeling assumptions. Educationally, they help students grasp the underlying mechanisms of MSE phenomena and connect them with more basic physical principles.

Rather than being seen as advanced topics, computational techniques should be introduced at the introductory level—as presented in this paper—to help students develop conceptual understanding of MSE. With the right tools, such as NetLogo, computational models can be made easily interactive to engage students in active model-based learning, leading to understanding of many MSE topics from the perspective of emergence, starting with atomic behavior and ending with macro-level phenomena.

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Appendix 1: The Computational Modeling Techniques

Molecular Dynamics (MD)

Molecular dynamics (MD) is the first atomistic modeling technique we will use in the course and the most frequent. In MD, atoms are modeled as Newtonian point masses. Since all the MD models used in the course are in two dimensions, the atoms in our MD models have a mass and four state variables: x position, y position, x velocity and y velocity. In an MD model, atoms exert forces on one another according to an interatomic potential/force function. The details of the interatomic potential depend on the atoms being modeled, but the general shape is always like that shown in Figure 8. The potential energy approaches zero at long distances, decreases to a minimum at a relatively short distance (the equilibrium distance), and then increases towards infinity if the atoms are squeezed together. Force is defined as the negative derivative of potential energy, with a positive force being repulsive and a negative force being attractive. So, the atoms feel a repulsive force when they are closer together than the equilibrium distance and an attractive force when they are further apart than equilibrium distance.

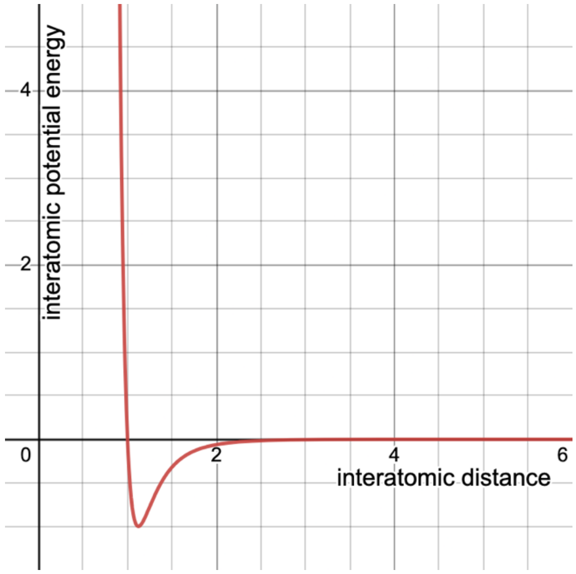

Figure 8: An interatomic potential function plots the potential energy due to the interaction of two atoms as a function of their distance. It is defined such that potential energy is zero at infinite distances. The distance with minimum energy corresponds to the bond length at absolute zero. When atoms are further apart that this, they attract and when they are closer together, they repel.

The interatomic potential is an abstraction, treating each atom as a unified whole. In reality, the protons and electrons in each atom interact with the electrons and protons in other atoms. The particles of opposite charge (protons in one atom and electrons in the other) attract and the same-charged particles repel. At close distances, the repulsion is stronger than the attraction and atoms exert a net repulsive force on each other. At long distances the attraction is stronger than the repulsion and the atoms exert a net attractive force on each other. In most MD simulations these details are abstracted away, and atoms are treated as the fundamental entities of the model.

The core of an MD model, from the perspective of an atom, consists of calculating the forces it feels from other atoms, accelerating, and then moving. This takes place in two steps:

1. Each atom calculates the force it feels from all other atoms within a cutoff distance and sums them together. It then updates its velocity (i.e., it accelerates) based on this force.
2. Then, each atom moves (updates its position) based on its velocity.

Depending on the numerical integration scheme being used, these two steps might be done in the opposite order, but they are the two steps repeated every time step of the model.

MD can be used to model many phenomena in MSE. For example, different phases of matter can emerge from MD simulations at different temperatures. The main downside of MD is that it is computationally very expensive. Conventional MD can only be used to model processes that take tens to hundreds of nanoseconds in the real world (Pierce et al., 2012). Perhaps surprisingly, this short time scale is still useful for modeling many phenomena, but some phenomena obviously require longer time scales.

Monte Carlo (MC)

Monte Carlo (MC) simulations enable modelling phenomena over longer time scales—up to seconds with certain techniques—by giving up some of the detail of MD. MC uses probabilistic algorithms that only deal with energy and position. As such, atoms in an MC simulation only have state variables pertaining to position, not velocity. The potential energy (PE) of atoms is calculated based on their distances from other atoms using interatomic potential functions like the one shown in Figure 8. Atoms make random moves probabilistically weighted by how they change PE.

Two core insights underly MC simulations. First, when looked at over a long period of time, an atom is equally likely to be moving in any direction (assuming it is interacting with a lot of other atoms). This allows us to model the movements of atoms as taking steps in random directions. However, not every step is equally likely. The probability of a step depends on how it changes the potential energy (PE) of the system. The second core insight underlying atomistic MC simulations is that the kinetic energy (KE) of atoms in a real system follow a probability distribution, known as the Boltzmann distribution, of the form $p(E) \propto \exp\left(-\frac{E}{kT}\right)$, where $p(E)$ is the probability of having KE equal to E, T is the temperature of the system, and k is Boltzmann's constant. This distribution can be derived analytically, as Boltzmann did, and it also emerges from MD simulations. As atoms move around, energy is continuously converted between kinetic and potential energy (PE). An atom can increase its PE by giving up KE. For example, when an atom runs into another atom, it slows down, thereby losing KE, but gains PE.

The general algorithm for an MC simulation is that each time step an atom:

1. Calculates its current PE due to its interactions with other atoms (usually only those within a cutoff radius to reduce the number of calculations)
2. Makes a random move (within one atomic radius of its current position).
3. Calculates its PE in the new position.
4. If the new PE is lower than the old PE → accept the new move
5. If the new PE is higher than the old PE → accept the new move with a probability equal to $\exp\left(-\frac{\Delta E}{kT}\right)$, where ΔE is the change in PE from the old to new position and the temperature, T, is an externally set parameter. This is the probability, from the Boltzmann distribution, that the atom would have enough kinetic energy to move to the new position of higher potential energy.

MC simulations give the same spatial distribution of atomic positions over long time scales as MD simulations. This means that MC simulations can be used to simulate the equilibrium behavior of system, but they cannot be used to simulate the dynamics of how a system will change moment to moment over time.

Random walk

Random walk simulations can be viewed as a simple subset of MC simulations. In a random walk simulation, atoms are modeled as taking random steps, often on a lattice. In the simplest version, an atom is equally likely to move to any neighboring lattice site. In more complex versions, the probability of jumping to different directions or to certain types of lattice sites can be changed to model different material systems. Probability of jumps can also be weighted based on changes in PE as in Monte Carlo simulations.

Appendix 2: Questions in the Bonding to Crystal Structure Chapters

This appendix includes the exact text of the questions students answer in the chapters on atomic bonding, interatomic potentials, and the beginning of the crystal structure chapter summarized above in section 3.1.

Questions students answer using a simple MD model of two atoms free to move in 2D which students can click and drag to rearrange in space:

1. What happens when the atoms are placed far apart (greater than 10 atomic radii, $10r_0$, where r_0 is half the diameter of the atom) and are initially not moving?
2. What happens when the atoms are a small distance apart - perhaps closer than $3r_0$ apart - and not moving initially?
3. What happens when the atoms are very close together, that is, the edges of the atoms are nearly touching?

Questions students answer using a model that shows electron density shifting between two nuclei and the resulting net forces on the nuclei:

1. How does the electron density of the atoms shift (the red cloud) as the atoms are brought closer together up until the overall interaction is balanced?
2. Consider the charge present in the electron cloud and at the nucleus of the atom. Try to explain why the atoms attract each other when they are far apart, why they repel when they get very close, and why there is a distance when the overall interaction is balanced, i.e. the net force is zero.
3. Based on the answers to the above questions, explain what an atomic bond is.

Questions students answer using the model shown in Figure 2:

1. First, construct a spring potential like that on the previous page (parabola). When you have one you like, click the export-sketch button and upload your sketch here (you can drag a file onto the "choose file" button or click it and find the file). Make some observations about how the atoms behaves in this potential. Which features does the spring model have that fits atomic hypothesis (Section 3.4)? What is it missing? Would this be a good model for simulating atomic bonding?
2. Now, construct an interatomic potential that more accurately models the atomic hypothesis. When you have one you like, click the export-sketch button and upload your sketch here. Explain what the main difference is between your new potential and the spring potential? Make some observations about the atomic pair in this potential.

Questions students answer using an interactive Desmos graph of the Lennard-Jones (LJ) potential along with its equation $U_{LJ}(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$:

1. What happens to U_{LJ} when you change ϵ? What do you think we might be able to model in a two-atom system by changing ϵ?
2. What happens to U_{LJ} when you change σ? What do you think we might be able to model in a two-atom system by changing σ?
3. What happens to the interatomic potential energy as the distance between the atoms gets very large ($r \to \infty$)? Show this mathematically. What does this value at $U(r \to \infty)$ mean?
4. What happens to the interatomic potential energy U_{LJ} as the distance between the atoms gets very small ($r \to 0$)? What does this mean?

5. The LJ potential (and indeed other interatomic potentials) are constructed such that the potential energy is positive at short distances at very short interatomic separation distances r, becomes negative as r increases and reaches a minimum. Then, it increases and approaches zero at $r \rightarrow \infty$. What does the value of the negative potential energy minimum $U_0 = |U(r = r_0|$ represent?
6. Find the general expression for the distance at which the potential energy is minimized. We call this the equilibrium bond distance r_0, and it is the point of at which net force in the system is zero $F = 0$.

Questions students answer using a simple MD model of two atoms interacting according to the LJ potential in 1D. This model is similar to the one shown in Figure 2, but the potential is provided and students can vary the parameters of the LJ potential as well as the initial kinetic energy of the atoms and click and drag one of the atoms to different positions.

1. In previous sections, we've modeled interatomic potentials with a parabolic spring potential and a sketched potential. In this section, we'll use the Lennard-Jones equation Eq. 4.5.1 to model the interatomic interactions. Of course, to make this happen, we need to change the code! Take a look at Line 131 in NetLogo model 4.6.1 under NetLogo Code. This line asks NetLogo to report the force acting between that atoms at the so the code will accelerate the atom appropriately during the next tick. Does this line of code make sense based on your understanding of the interatomic force from the Lennard-Jones potential? Explain.
2. Set the initial kinetic energy initial-KE to zero and click the setup and go buttons. The red atom is originally positioned at equilibrium. What does it do? Why? What happens to the plots of kinetic and potential energy vs time as when you move the atom?
3. Now, let the atom go. Explain why the atom moves the way it does. Explain why the energy plots show what they show. You may want to slow the model speed down to observe this better.

Questions students answer using the model shown in Figure 3A:

1. Create a **mental** model of three atoms (represent them with circles) occupying a two-dimensional plane. Imagine that these atoms interact with each other according to a Lennard-Jones potential. First draw the atoms at an "initial" state in which they're positioned at the vertices of an equilateral triangle with sides of length $l = 4r_0$, where r_0 is the equilibrium bond distance. Then, sketch how you think the atoms will be positioned over some time Δt later at which they've reached "equilibrium". Sketch the atoms in their final equilibrium position. Upload your sketches with a short explanation of your reasoning.
2. Use the NetLogo model to validate your sketch. Make sure that settings are on the default:
    a. num-atoms is set to 3
    b. initial-config is set to "Random"
    c. Constant temp is enabled.
    d. temp is set to 0.1

    e. First, set go-mode is set to "drag atoms" and press go. Arrange the atoms as you'd like.
    f. Then, go-mode to "simulate" and press go.

Watch the system equilibrate. Describe the results. Do your results agree with your predictions above? (If they don't, explain why you see what you see now.)

Try this a few times with different initial configurations. Do you ever get any variation in your configuration - or is it always the same?

3. Repeat the previous question for 4, 6, and 30 atoms. For simulations of 4 and 6, you'll want to drag atoms so that they are close enough to “feel” each other. For 30 atoms, you can just run the simulation. What arrangements do you observe for each? Include the images and describe. For simulations of 3, 4, and 6 atoms, count the total number of bonds in each atomic assembly.

   Upload a single image showing these configurations (you can screenshot each and put them into a single image), with all the bonds indicated.

4. Comment on the trends you observed in the previous question. What patterns arise from these simulations? What can you say about the number of bonds formed in each configuration? Did you observe anything for very large assembles that differed from smaller ones?

Appendix 3: Questions in the Diffusion Chapter

This appendix includes the exact text of the questions students answer in the chapter on diffusion summarized above in section 3.2.

Question students answer using the model shown in Figure 4A:

1. Watch the green atom move around at a temperature of temp = 5.
    a. Describe its motion.
    b. Why does it change direction and velocity?
    c. Does it look like it is equally likely to move in all directions? (look at the graph as well)

Questions students answer using the random walk model shown in Figure 5:

1. What happens to the concentration profile at short times (10s of ticks)? (You may want to slow down the model for this.)

   How about long times (100s of ticks)? Should the long-term behavior depend on the initial concentration profile? Why or why not? Note - the edges (far left and far right) of the world are "closed". An atom will not pass over the edge of the world.

2. Try drawing different profiles with different types of shapes using the draw-profile button. Drag your mouse across the world to define concentrations in different regions. Try a number of different shapes.

   Which regions of your concentration profile change the fastest? Which change the slowest? (You may want to slow down the model in this case)

3. Using the random walk model, try to explain the behavior you observed in the previous question - that is, why might some regions change faster than others?

Questions using a figure similar to the one shown in Figure 7 but with only the black and blue squares:

1. Fill in all the boxes following the example for columns 1 and 2:
   a. In the black boxes, fill in the number of atoms expected to jump from the one column to the other. Assume that atoms have a 25% of jumping in either direction (unless they are at an edge, in which they can't jump in the direction of the edge). Note - you are allowed to have fractional atoms jump in this model, which has small number of atoms - in real systems there would be moles of atoms jumping around with some statistical probability.
   b. In the blue boxes, fill in the expected flux, i.e. how many net atoms will pass through the blue dotted line for the tick. If an equal number of atoms pass through in each direction, the net number of atoms passing through is zero (as shown in the example). Define atoms jumping from left to right as positive and those jumping right to left as negative. So, if more atoms are jumping through the line from the right than the left, the flux will be negative.
   c. In the written portion of your submission, explain in words what feature of the concentration profile determines the flux.
2. Based on your result in the previous problem, try to come up with a mathematical rule for what the flux will be at each point. Take 5 minutes to try to come up with something reasonable.
   a. It is okay if you feel stumped. Just do your best to invent and submit something reasonable. You'll then be able to see the canonical equation. The point of this activity is to help you practice developing mathematical models, regardless of whether you reinvent the exact traditional equation.
   b. Use $J(x)$ to represent flux at a given position. (In our discrete case, flux is only defined at values 1.5, 2.5, 3.5, ...)
   c. Make sure to define the other variables you use!

Questions using a figure similar to the one shown in Figure 7 but with the blue squares filled in and the green ones empty:

1. Fill in the green boxes with expected change in concentration at each x position based on the net flux of atoms at that position. Then, sketch a line on the graph indicating the new concentration. Upload the file.

In the written portion of the submission, explain what determines what the change in concentration will be at any given point.

2. Try to come up with a mathematical rule for what rate of change $\frac{\partial C}{dt}$ in concentration will be at each *x* position.
    a. Again, the point of this activity is intended to help you practice developing mathematical models, regardless of whether you reinvent the traditional equation. So, do your best but don't worry so much about getting it "right."
    b. Even though we are currently using a discrete representation, use $\frac{\partial C}{dt}$ to represent rate of change in concentration at a given *x* position. In the answer, we will be extending to the continuous case.
    c. Make sure to define the other variables you use!