# MaterialSim: An Agent-Based Simulation Toolkit for Learning Materials Science


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***Abstract*** *- Computer modeling and simulation is progressively penetrating the engineering workplace across a wide variety of contexts. However, their use in undergraduate engineering education lags far behind. Although there are many commercial simulation packages available, most background and "black-box" the actual mathematical and physical models used in the simulation engine, assigning a passive role to students as they do not have access to the underlying dynamics. This paper reports on a user study of MaterialSim, a Materials Science agent-based set of microworlds built in the NetLogo modeling-and-simulation environment, for investigating crystallization, solidification, metallic grain growth and annealing. Six undergraduate students enrolled in an introductory Materials Science course participated in the study, in which they could run experiments and build models. This design-based research builds on previous studies that have suggested the benefits of multi-agent simulation for understanding how a variety of complex behaviors in science derive from simple, local rules. Whereas professional simulation tools in Engineering are targeted for "modeling-for-doing", emphasizing aggregate-level simulations to predict macroscopic variables, MaterialSim was built within a "modeling-for-understanding" framework, which focuses on agent-level elementary behaviors that bring about emergent macroscopic behaviors. The rationale for the design is that the agent-based perspective may foster deeper understanding of the relevant scientific phenomena. A core feature of this design is that students can apply a small number of rules to capture fundamental causality structures underlying behaviors in a range of apparently disparate phenomena within a domain.. We present evidence in the form of excerpts and samples of students' work which demonstrate that the experience with the tool enabled them to identify and understand some of the unifying principles across phenomena and build sophisticated new models based on those.*



***Index Terms*** *—Agent-based modeling, Constructivism, Engineering education, Materials Science.*


## INTRODUCTION

Albert Einstein once said that "the secret of creativity is to hide yours sources". In a positive sense, engineers might fit perfectly into his quote. Having their scientific and intellectual traditions lying in the borders of different fields of knowledge, they are in a privileged position to be creative, integrate knowledge, and reinvent the world.

In spite of this, engineering teaching and learning have remained remarkably traditional. A fixed curriculum, assessment through exams and the "information transmission" metaphor constitute a solid and enduring triad in most engineering schools. Only very recently universities have started to implement more significant changes, introducing design-based activities and using modeling and simulation technologies [1, 2].

However, many of the tools used in such new engineering educational initiatives are typically software targeted for "doing", and not for learning. They often background and "black-box" their mathematical and physical models, which could constitute a considerable drawback for learners. As the rate of knowledge obsolescence increases, there is a greater need for flexibility and adaptation of new knowledge for new situations. In order to do that, students should master present knowledge and the fundamental principles underlying it.

Professional tools of the domain are targeted for *modeling-for-doing*, rather than for *modeling-for-understanding*. Modeling-for-doing often emphasizes aggregate-level simulations to predict macroscopic variables (e.g., time, temperature, concentration, current, pressure). To accomplish this goal, numerous equations, models, tools and heuristics have to be employed, oftentimes "mixing-and-matching" different levels of explanation to deliver the expected results. The modeling-for-understanding framework, conversely, focuses on simple agent-level behaviors (atomic-level interactions, free energy minimization) from which complex macroscopic behaviors emerge.

In this paper, we will present and discuss a user study of a system designed within this latter framework: *MaterialSim*, a multi-agent Materials Science modeling and simulation environment built with the NetLogo language [3]. We will present the work that students developed with the tool and draw some comparisons with their classroom activities, using the data

from our observations during an introductory course in Materials Science at a highly-ranked Engineering school within a liberal arts university.

## RESEARCH DESIGN AND METHODS

Six undergraduate students (volunteers) participated in the research, all enrolled in the "Microstructural Dynamics" undergraduate course in the engineering school of a liberal arts university in the spring of 2004. This class was being offered to junior year Materials Science students. They were all computer literate and had some contact with computer programming, typically in class assignments in MatLab.

The user study took place between one and two weeks after sessions that dealt with grain growth in metals (the topic explored in the model), and was divided into two parts. The first, one hour long, was comprised of the following:

- General presentation of multi-agent simulation environments.
- Exploration of two NetLogo models: fire spreading in a forest with variable densities and social segregation with varying degrees of racial tolerance.
- Oral pre-test/interview with six open-ended questions on Microstructural Dynamics.
- Exploration with MaterialSim environment, running a few simulations with different parameters.
- At least one systematic experiment using "BehaviorSpace" (a NetLogo feature which allows users to run and compare multiple simulations with different parameters). Students would choose one variable and run tenths of simulations with different values, and then plot and interpret the final curve.

The second session (2 hours), which took place one or two days later, was dedicated to:

- Brief introduction to the NetLogo programming language.
- Choice of one component of a MaterialSim's model to be modified, or a new component to be programmed.
- Programming the new/updated model, with one-to-one help from the first author.
- Running experiments with the new model.
- Final interview.

We videotaped all student sessions and recorded their computer interactions using real-time continuous screen capture software. Approximately 20 hours of video and 10 hours of screen capture were analyzed and selectively transcribed. All of the models and experiments done by students were also saved and analyzed. The first author attended three weeks of classes with the students and analyzed class materials and related literature.

Even though the MaterialSim environment is capable of simulating diverse phenomena in Materials Science, in this study we chose to work only with grain growth in metals.

## WHAT IS NETLOGO?

NetLogo [3] is an integrated multi-agent modeling environment. It includes a graphical user interface for exploring, experimenting with and visualizing models, as well as a multi-agent modeling language (MAML) used for authoring models. Such languages enable users to easily create and manipulate thousands of graphical agents, and define simple rules which govern their behavior. The NetLogo architecture has two kinds of agents: stationary, called "patches", and moving agents, called "turtles". Both kinds can have simple behaviors associated with them, such as to seek or to avoid being surrounded by other agents. Such simple rules, however, give rise to complex emergent behaviors, many of which are congruent with the traditional macroscopic, aggregate-level descriptions of the phenomenon. The NetLogo language was designed with a "low threshold" principle – that is, it was designed so that people without prior computer programming experience could quickly learn to construct their own models.

In addition to the modeling language itself, NetLogo also includes a graphical user interface with advanced visualization features. There are also some specialized tools such as BehaviorSpace, which enables users to run multiple experiments and automatically log all their data for further analysis.

The next picture shows the NetLogo environment with the "Fire Propagation" model, in which we can see the graphics window, the "Interface", "Information" and "Procedures" tabs, as well as the widgets used to build the user interface (text boxes, buttons, monitors, plots, sliders and switches).

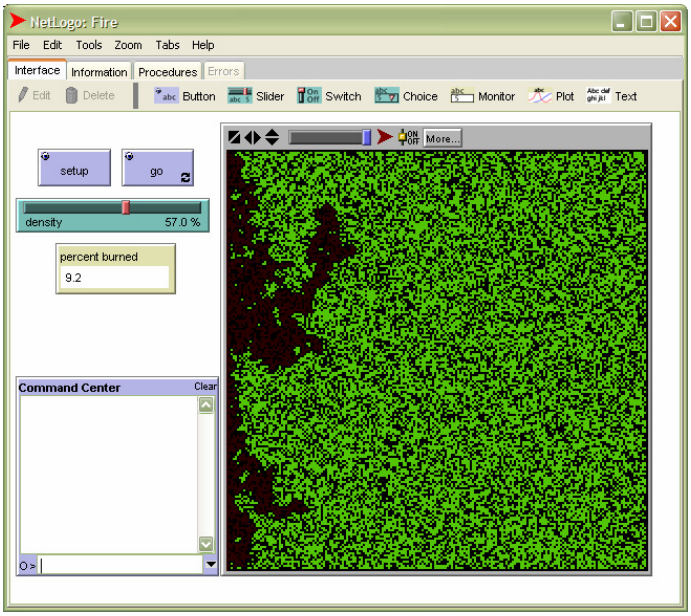



FIGURE 1
A SCREENSHOT OF THE NETLOGO ENVIRONMENT, SHOWING THE FIRE PROPAGATION MODEL.

## WHAT IS GRAIN GROWTH?

Most materials are composed of microscopic "crystals". Even though we commonly associate the term 'crystal' with the transparent raw material used for glassware manufacturing, its scientific meaning is different. A crystal is just an orderly arrangement of atoms, and materials such as metals are made up of millions of them. In Materials Science, scientists use the term **"grain"** to refer to those crystals. Although invisible to the naked eye, they are observable under an optical microscope after special chemical procedures.

Some environmental circumstances can cause the size of such a grain to change. High temperature is the most important one, which can increase the average grain size of the material. This phenomenon is known as **grain growth**, during which smalls grains disappear while bigger ones grow (the overall volume is maintained). Car engines and airplanes turbines, for instance, can reach very high temperatures in service – an incorrectly designed material can then undergo "grain growth" and suffer catastrophic failure. Moreover, different manufacturing techniques result in different grain sizes, which have to be adjusted to the correct specification. Oftentimes, the final product has to be "heat-treated" to achieve the target grain size – typically, the material is placed in a special furnace for many hours until it reaches the desired grain size. The following pictures show a metallic sample *before* and *after* being heat-treated for 20 hours at 850 ºC. Grain size, therefore, is one of the most important issues for determining materials' properties, and exhaustively studied in Materials Science.

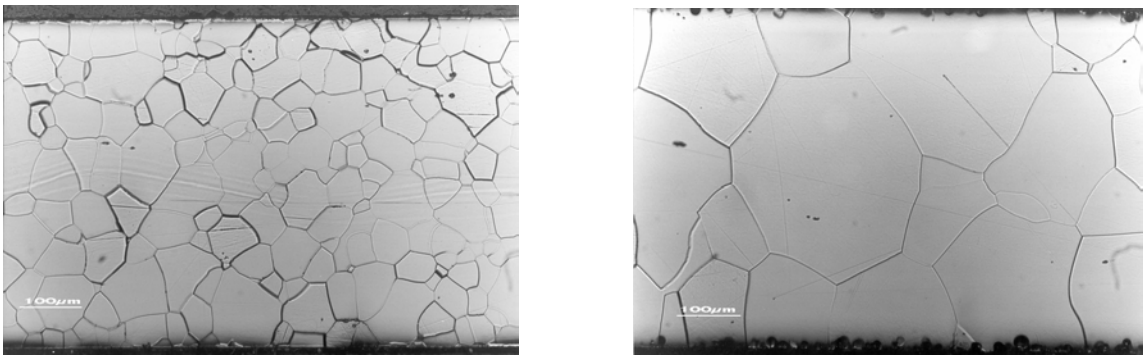


FIGURE 2
METALLIC SAMPLE BEFORE AND AFTER HEAT TREATMENT, SHOWING CONSIDERABLE GRAIN GROWTH

Among other properties, grain size determines how much a material will deform before failure, which is one of the most important issues in engineering design. Predicting grain growth is extremely important for Engineers – it is very important to

know how many hours a material needs to be heat treated to achieve the target grain size. Burke [4] was one of the first to introduce a law to calculate it. He proposed that the growth rate would be inversely proportional to the average curvature radius, and the simplified version of his grain growth equation is:

$$R = kt^n \tag{1}$$

where $R$ is the mean grain diameter, $t$ is time and $k$ is a constant that varies exponentially with temperature. The theoretical value of $n$ (rarely observed experimentally) is 0.50. This equation, however, describes only an average growth. It cannot predict, for instance, different growth rates for the different classes of grains present in the microstructure.

Over the last decade, as the processing power of computers increased, a new and promising approach has been made possible: computer simulation of grain growth [5, 6]. Anderson, Srolovitz et al. [7, 8] proposed the most widely known and employed theory for computer modeling and simulation of grain growth, using the Monte Carlo method and a cellular-automata approach. This kind of simulation not only made predictions faster and more accurate, but allowed for a completely new range of applications. Researchers were not anymore constrained by approximations or general equations, but could use the dynamics and topology which were very similar to the actual phenomenon. As mentioned by Anderson, Srolovitz et al.:

> "While it is generally observed that large grains grow and small grains shrink, instances where the opposite is true can be found. This suggests that knowledge of the instantaneous absolute or normalized grain sizes is not sufficient to predict the evolution, or even the direction of evolution, of individual grains. [...] The results indicate the validity of a random walk description of grain growth kinetics for large grains, and curvature driven kinetics for small grains." [7, p. 794]

In other words, Anderson et al. state that the classic rule-of-thumb about grain growth ("large grains grow and small grains shrink") is not necessarily valid, and randomness plays a much more important role. Given the dimensional and time scales of the phenomenon, one of the only ways to visualize this new finding is through computer simulation. The traditional methods for investigating grain size and growth, nevertheless, reflect the tools (and visualization techniques) that were available in the fifties: mathematical abstractions, geometrical modeling, approximations, and empirical data. We are remembered of a secret of science: models are just approximations of reality, and reflect the tools that were available when they were created. Engineers should be prepared to redesign new models as their tools become obsolete. Nowadays, the introduction of digital tools is radically transforming engineering practice, but engineering education still does not benefit as much as it could from the new possibilities brought about by these new tools.

## MATERIALSIM DESIGN

MaterialSim is a set of exploratory micro-worlds built in the NetLogo multi-agent-modeling environment [3]. Currently there are two modules, including models of crystallization, solidification/casting, metallic grain growth and annealing.

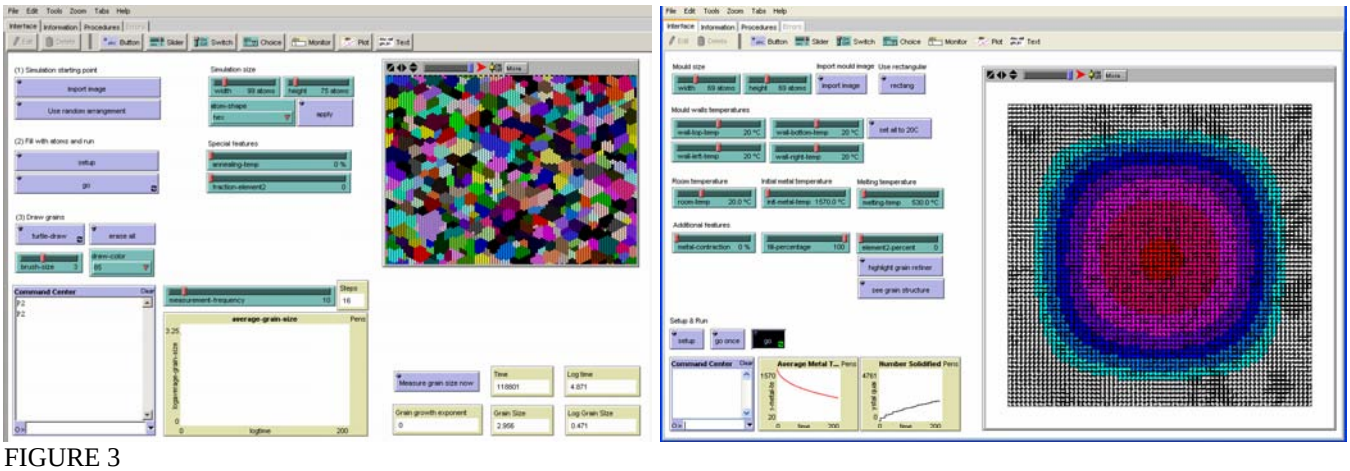


FIGURE 3
MATERIALSIM'S METALLIC GRAIN GROWTH (LEFT) AND SOLIDIFICATION/CASTING (RIGHT) MODULES

The system was conceived to allow four kinds of activities:

- **One-dimensional exploration:** users can change variables, draw microstructures or mould shapes and observe their behavior over time.
- **Multi-dimensional exploration:** students can run experiments altering multiple parameters to find out rules, mathematical relationships, and patterns in the evolution of the microstructure.
- **"Multi-world" exploration:** Students can connect real-world and virtual experiments, importing digital photos from real experiments and observing their "virtual" evolution.
- **Model building:** students can change, create or extend the system by coding their own procedures or modifying existing ones, using the NetLogo modeling language.

We chose the NetLogo modeling-and-simulation environment as a platform as it is well adapted to all of those activities. Using a constructionist design framework [9] combined with a multi-agent approach, its "low-threshold, high-ceiling" design enables learners to quickly achieve sophisticated results after a very short period of time. Moreover, its built-in visualization allows dynamic, flexible and customizable views of model results. NetLogo and other multi-agent-based simulation tools have been used in many school and research environments to investigate a variety of phenomena in Chemistry and Physics [10-15].

In the user study, we used one MaterialSim module, the metallic grain growth module, which interface has four main components:

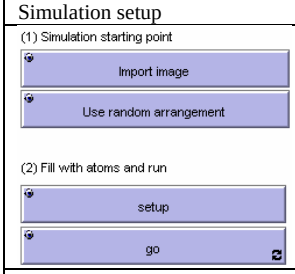
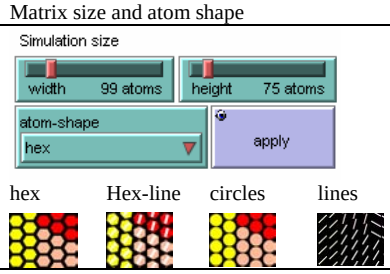
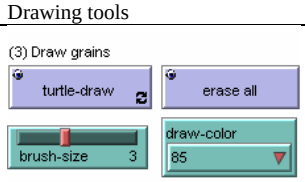
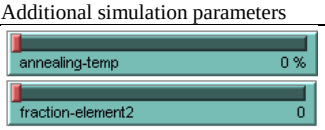
| Simulation setup | Matrix size and atom shape | Drawing tools | Additional simulation parameters |
|---|---|---|---|
|  |  |  |  |
| Users can either start from a random arrangement of atoms or from a pre-set stage, which can be drawn or imported from a bitmapped image. | The matrix size can be set by the user, or automatically when a picture is imported. The appearance of the atoms can be changed for better visualization of particular phenomena ("lines" mode was very useful to understand the differences in crystallographic orientations). | To investigate particular situations, users can "draw" their own microstructure, or retouch an existing one. | The annealing temperature slider allows for experiments with different thermal agitation, which increases the likeliness of a non-energetic-favorable orientation switch to happen. The other slider can introduce a certain percentage of solid precipitates in the sample, which can slow down or stop the evolution of the microstructure. |

TABLE 1
MATERIALSIM INTERFACE COMPONENTS (GRAIN GROWTH MODULE)

## ENGINEERING PRACTICE VS. ENGINEERING TEACHING

Grain growth is a good example of an area in which the teaching tools have not kept pace with the existing research tools. Even though the novel research tools make a deeper understanding of the phenomenon more accessible, they have not yet reached the classroom. Common practice in teaching grain growth is to think of grains as spheres (which they are not), "boundaries" as real entities (whereas they are just imaginary lines between grains), and make use of numerous metaphors and rules-of-thumb (e.g., "dislocations climb", "grains swallow others", "vacancy sink", "precipitates hold boundaries" etc.) to describe and predict changes in the grain.

This teaching practice is widespread in engineering education: traditional engineering teaching relies on a large number of ad-hoc models, approximations, metaphors, and shortcuts, which have been accumulating over decades. They constitute a web of ideas of very different natures, granularities, levels of analysis, and mathematical descriptions. Due to the applied and integrative aspect of engineering research and practice, oftentimes explanations are drawn from a variety of sources: geometrical proof, thermodynamics, algebraic deductions, and statistical mechanics. Specifically, our classroom observations revealed that at least four of these sources were employed during the classes covering grain growth:

- The *Laplace-Young equation for pressure* is commonly used to in Fluid Dynamics to calculate surface tension in liquid-gas interfaces (such as a drop of water). It basically states that the surface tension grows as the pressure difference is increased, and as the radii of curvature decreases. In other words, any small grain (with a low radius of curvature) will have high surface tension, as opposed to large grains. The equation is written as follows:

  $$p^{\beta} = p^{\alpha} + \frac{2\gamma}{R} \quad \text{and} \quad du = \overline{V_c} dP$$

  where $\alpha$ and $\beta$ are the outside and inside pressures, $R$ is the spherical particle radius, $du$ the change in chemical potential, and $\overline{V_c}$ the partial molar volume.

- *The Flux equation* (based on statistical mechanics), which states that the probability of an atom to jump to a neighboring grain grows with temperature, and therefore the mobility of a grain boundary also increased with temperature. The equation is written as follows:

  $$A_2 n_1 \nu_1 \exp\left(\frac{-\Delta G^{\alpha}}{RT}\right)$$

  where $A_2$ is the probability of being accommodated in the other grain, $n_1$ the number of atoms in grain 1 in position to make the jump, $\nu_1$ the vibrational frequency of an atom in grain 1.

- Geometrical approximations is a common technique used to calculate grain size an also the effect of second-phase particles in grain growth. Here, the force (P) is applied by the particle to grain boundaries. The model assumes the particles as spheres and boundaries as lines or surfaces.

  $$P = \pi r \sin(2\theta)\gamma$$

  where P is the force, $\theta$ is the angle with the grain boundary, $r$ is the particle radius.

## AGENT-BASED GRAIN GROWTH SIMULATION

The agent-based simulation of grain evolution, on the other hand, offers a very different perspective on the process of grain growth. Its principle is both simple and fascinating: the thermodynamics of atomic interactions. The first step is to represent the material as a 2D (or 3D) matrix, in which each site corresponds to a surface (or volume) element and contains a value representing its crystallographic orientation. Contiguous regions (containing the same orientation) represent the grains. The grain boundaries are fictitious surfaces that separate volumes with different orientations, but they have no physical existence in the simulation. In MaterialSim, the algorithm for updating grains is as follows:

a) Each element of the matrix calculates its free energy ($G_i$) based on its present crystallographic orientation ($Q_i$) and its neighborhood (the more different neighbors, the higher the energy). Figure 4 shows an example of such a calculation: the central element has five different neighbors, hence a value for its free energy of 5.

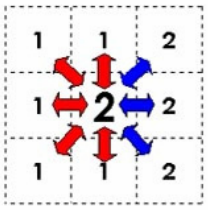



FIGURE 4
CALCULATIONS OF FREE-ENERGY IN THE ELEMENT'S PRESENT STATE. THE CENTER CELL BASES IT S NEXT STATE ON THE CURRENT STATE OF EACH OF ITS 8 NEIGHBORS.

b) One new random crystallographic orientation is chosen for that element ($Q_f$), among the orientations of the neighbors. In this case, the only possible choice is to flip the element from "0" to "1".

c) The element calculates its free-energy again ($G_f$), now with the new proposed crystallographic orientation ($Q_f$=2). Figure 5 shows such situation, in which and $G_f$=3

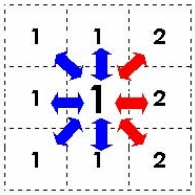



FIGURE 5
CALCULATIONS OF FREE-ENERGY IN THE ELEMENT'S PRESENT STATE AND A RANDOMLY CHOSEN STATE

d) The element compares the two states. The orientation that minimizes the energy is chosen. In this case, $G_i$=5 and $G_f$=3, so the latter value is lower and constitutes a state of greater stability, and is therefore maintained.

## PRE-TEST MODELS AND EXPLANATIONS

The pre-test consisted of two activities: first, students were asked to identify, in a printed picture of a metallic microstructure, grains that would grow or shrink. Then, they were asked the five questions in **Error! Reference source not found.**.

| *A friend missed two weeks of classes. Now she/he is back and wants to catch up. How would you explain to her/him the following ideas?* |
|---|
| 1) What is a grain? |
| 2) What is a grain boundary? |
| 3) What is grain growth? |
| 4) What is the driving force for grain growth? |
| 5) What is effect on grain growth of dispersed particles? Why? |

TABLE 2
QUESTIONS ASKED DURING THE PRE-TEST

The hypothetical situation ("a friend who missed classes") was an effective "ice-breaker" to start the conversation, and enable the students to feel that they were not being tested on content. Below we have a commented transcription of some pre-test excerpts (the names of the students were changed). The findings were consistent with the hypothesis that the multiple descriptive models used in their classroom instruction resulted in the students generating a large diversity of explanations for the phenomena they were asked about: The excerpts below illustrate this diversity.

**Interviewer:** Imagine that a friend of yours missed class for a week, and you need to explain some ideas from the course to him. How would you explain what a grain is?

**Bob:** A grain is just an orientation of a crystal structure, a group of atoms in a crystal structure, a specific orientation, and [pause] you know, and it is just molecules aligned [pause] in one direction and then you have various grains and each grain has its own directions and when they meet [there is a] grain boundary [pause] and if for some reason if they were the same direction they would be considered one grain, and since they are lined up there would be no boundary anymore.

**Betty:** If you have a metal and you are looking at it under an optical microscope, at the surface of the metal, where [pause] different [pause] what I call grains grow, and these grains are just areas where the atoms collect and the boundaries in between the grains are [pause] sinks and sources for dislocations and [pause] vacancies and so.

**Liz:** It is so hard to explain... When I think of grain, you know, those kinds of pictures that we see, what comes to [my] mind... just one of those grains [pause] I feel that it is a word that we use in the English language and you always associate with something small, that is individual, you can see its limits and stuff like that. So when you use it in class, you just associate it with... like... I mean, a grain of rice... it is just one, out of many, that you can see right now. So I suppose that is how I associate it with things.

In these first answers to the question we can already observe how diverse the understanding of the three students was – which might be surprising given the fact that they are all Materials Science majors and have just attended a class about the topic a few days before. Bob offers a reasonably complete explanation, based on crystallography, but says that when two

grains had "the same direction they would be considered one grain", and mixes atoms with molecules. Betty, on the other hand, bases the explanation on a visual model, and integrates models from other topics in a vague way. Liz uses yet another explanation path, utilizing her previous knowledge about the morphology of a "real-world" grain to understand the Materials Science meaning of the word. Thus, students recourse to a variety of metaphors and explanations for characterizing a grain: visual (surface under the microscope), analogical ("grain of rice") or geometrical (atoms with same orientation). The responses to the second question bring some further information:

***Interviewer:*** *How would you explain what grain growth is?*
**Bob:** Grain growth is just when a grain, when more molecules [pause] come into one grain and line up that same direction. The driving force is [pause]...
***Interviewer:*** *Why don't they stay the way they are?*
**Bob:** Well, [pause] I mean [pause] I know the method of it, it is diffusion.
***Interviewer:*** *What is the reason they grow?*
**Bob:** Well, I mean, grains grow through diffusion, through vacancy diffusion, and atomic diffusion, for one, it is all over the place, temperature increases, molecules move around faster and they just... [pause] but the reason that they would grow [pause] I guess they grow... the driving force is to lower the free energy, overall, there is excess free energy due to dislocations and impurities in the grains, so by growing out, they can get rid of those and thus lower the free energy.

**Betty:** So when you heat-treat a metal, so when you deform a metal first the grains shrink and become compacted, you get all sorts of dislocations then, like twin boundaries, stuff like that, so if you do a high temperature anneal, then the grains all grow because you increase the energy of the system when you heat it and so it tends to decrease its internal energy so the grains become bigger and anneal out the dislocations because [pause] there is a high mobility for the atoms to move and so they move to the lower energy positions which is into the grains and the grain decrease.... ahn... the grain size increases, and the total area of the grain boundaries decrease, which decreases to decrease the overall energy of the system.

**Liz:** It is because, it wants to be more energetically stable, or have less energy in the crystal, so it will grow, just to form one big grain, because that's the least energy configuration, and it does this because, by the whole radius of curvature idea, where it starts shrinking.

This second question brings about at least three different ways to explain grain growth. Bob uses the metaphor of willpower ("molecules come into the grain and line up"), and employs ideas about diffusion, dislocation and impurities in a contradictory way. He does not recourse to the Laplace-Young equation, for instance, to explain the process of decreasing free energy by simply increasing the curvature radius. To him, excess free energy is due to impurities or imperfections in the crystal structure (known as dislocations). "Purity" is taken as a synonym for low energy, whereas the equation seen in class stated a very different idea. Impurities are not eliminated by grain growth, and growth can exist in 100% pure materials. Interestingly, he also states that temperature causes molecules to "move faster", which would be a "driving force", confusing causality and mechanism. Apparently, he imagines that grain growth drives impurities to the outside of the materials, "cleaning" it of impurities and dislocations. Betty goes even further searching for explanation ideas. The phenomenon she describes (deformation and recrystallization), was taught in a previous series of classes, but is not totally related to grain growth. During the pre-test, when presented with a printed picture of grains, she incorrectly indicated that the small ones would grown (which is what happens in recrystallization, but not in grain growth). She also had a hard time making the distinction between driving force and mechanism. A. Interestingly, when explaining the phenomenon in his own words, she mentions that "atoms move to the lower energy positions which is into the grains and the grain decrease", correcting his own conclusion just seconds later.

Liz's explanation is more coherent, relying on the idea of having "less" energy in the crystal being correlated to the "whole radius of curvature idea" (which is correct) but without demonstrating how those things connect. This analysis suggests that, in fact, students are picking different explanations fragments from models of different granularities, and having difficulty identifying the driving force behind the phenomenon.

The fourth question also raised an important point, and made the model "mix-and-match" even clearer.

***Interviewer:*** *What is the effect of second-phase particles on grain growth?*
**Bob:** I think that... I feel that particles [pause] precipitates constrict grain growth and when a grain boundary meets a precipitate it bends around it, it kind of moulds around it, it will slow it down, it

won't make it stop completely, but it will slow it down, it hits the particle, it goes around the particle, as it happens, there is a pull on the opposite a force direction that the grain the grain boundary is moving. They slow... every time the grain boundary is moving out it slows down the growth.

***Interviewer:*** *Is it good?*

**Bob:** It depends of how big you want your grain. You know, more particles, the closer they are together, the smaller the grains will end up being, in that case it will be a harder and strong material

**Betty:** If you have a lattice around the impurity and that increase the energy of the system, and then that is bad, but if you have a lattice and you add particles of similar grain size, or, similar atom size, you can strengthen, get strong materials, because this small grains or atoms they act to stop dislocation movement in the material, and so it becomes harder and harder to push dislocations through so the plastic deformation becomes harder. The more particles you put [pause] in a system, the harder it is, [pause] the closer the spacing, the harder it will be to put dislocations through, so the harder the material will be.

**Liz:** Basically, if there is an impurity, the grain boundary will just go around it so it will just do like this, viewing it from a top angle, this will be a grain boundary [showing a drawing]

***Interviewer:*** *Do you think more particles will affect grain growth?*

**Liz:** [looks at the notebooks for several seconds] As for now, I don't think it does anything to grain size.

Again, the students tried to employ a variety of models: a "force-feedback" model, where particles pull boundaries away, and slow grain growth (Bob), a dislocation movement model (Betty), and a purely geometrical one, with no consequences for the behavior of the material (Liz). Betty's explanation is clearly drawing from another set of models from dislocation theory (another topic explored in class weeks before), but not addressing grain growth; Liz does not see any relationship between grain size and precipitates; Bob only see it as a factor to decrease speed, but never to "stop it completely".

The excerpts above, extracted from the videotapes of the pre-test interviews, demonstrate the model "cross-breeding" that was present in students' explanations. Different topics (recrystallization, dislocations, grain growth) were mixed together with a weak sense of their interconnectedness, whereas in fact they all describe different aspects of atomic movement. Constructivist theory would describe students as trying to accommodate the new knowledge into existing structures and representations. Indeed, as most knowledge in Materials Science is removed from everyday experience, students are very sensitive to the first models and explanations they come across in class.

## FISRT SESSION: INTRODUCTION AND MODEL EXPLORATION

As described in the Research Design and Methods section, the first session of the user study was dedicated to basic manipulation of the environment and of the model. The first activity was very simple: observe and reflect on of curvature as a driving force for grain growth. Students knew that large grains consume small ones, and also that grains grow toward their center of curvature, and high-curvature boundaries tend to disappear. However, those concepts appeared to be isolated ideas, separate phenomena, and hardly connected to the Laplace-Young equation. This activity consisted in drawing two grains divided by a curved surface and observing their behavior. The pictures below are snapshots of what students observed.

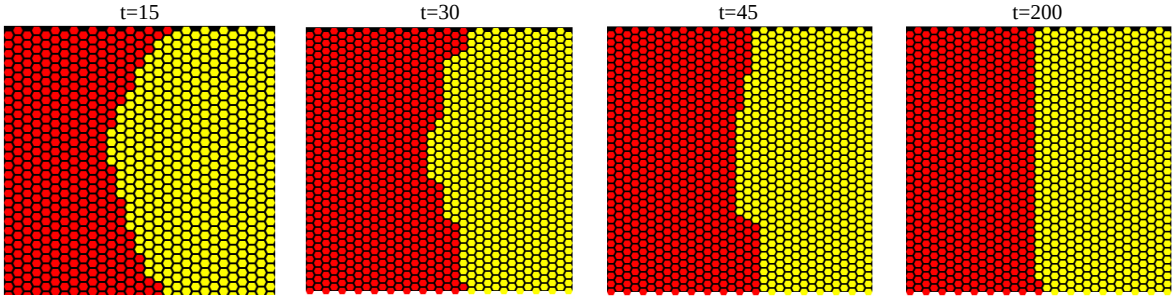



FIGURE 5
THE EVOLUTION OF A CURVED SURFACE

Before the simulation, most students were unsure of what would happen. As they saw grains growing toward their centers of curvature, they also observed random flipping of atoms. The following excerpt suggests that visualizing this evolution sparked some changes in Liz's understanding:

| | |
|---|---|
| ***Interviewer:*** | *Can you describe what you see?* |
| **Liz:** | Just because one grain has a concave side and the other has a convex side, so it comes in towards the concave, because... [pause] does line tension apply in this situation? |
| ***Interviewer:*** | *Line tension?* |
| **Liz:** | That might be from dislocations... I might be mixing them up. Just because... when you have something... part of the grain is like, curving in, mostly likely other parts of the grain are curving in, so the tension of the grain boundary lines, so the force outside is greater than the force inside, so it will like shrink, it looks like that probably be like straight in the middle, rather than entirely red... just because if the red part also have some concave thing that is off the screen it will just like go together. |

Liz is apparently mentioning the results of the Laplace-Young equation, which relates surface tension and curvature. However, she cannot yet think in the "micro" level: to visualize what is happening on the computer screen, she has to imagine a large circle going off-screen – which is probably a consequence of what she remembers from class, in which grains were always approximated as spheres. She cannot yet think of the local interactions along the curved interface as a driving force, but only the "macro", aggregate level effect of curvature.

The next activity was to draw a microstructure with many grains, but one of them a lot smaller than the others, as we can see in Figure 6. Liz continued with her line of reasoning.

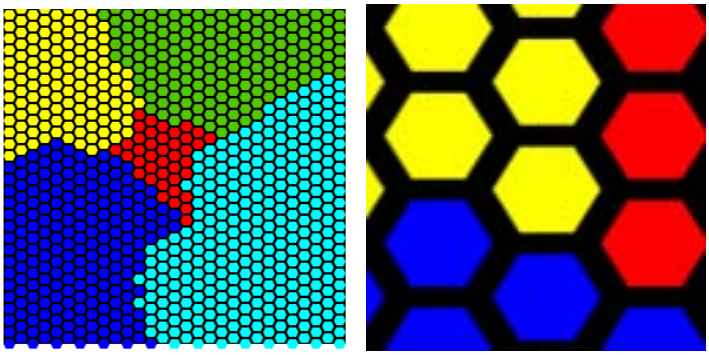


FIGURE 6
FIVE GRAINS WITH A SMALL RED ONE, WHICH IS BOUND TO DISAPPEAR (LEFT) AND A TRIPLE POIINT, WHERE THREE GRAINS MEET AND THE PROBABILITY OF THE FLIPPING TO YELLOW, RED OR BLUE IS EQUAL (RIGHT)

Watching the evolution of this simple microstructure was a key experience for Liz. She started to move from rote memorization and a topic-specific model to more general, principled knowledge. This excerpt took place when she was observing a triple point, a region where three grains meet and the flipping probability is the same for all the grains (as there are two atoms of each grain around the central element).

| | |
|---|---|
| Liz: | Right here there is an equal position for red, yellow and blue, but it just happens to be that blue won, it keeps winning. |
| ***Interviewer:*** | *How would you explain that?* |
| Liz: | Because... it you look at one of those points, either of the three colors, they all have the same number of other colors around it, so it is not really more favorable to choose one or the other... |
| ***Interviewer:*** | *What angle is here?* |
| Liz: | Oh, so this is the 120 degree angle between the... [pause] |
| ***Interviewer:*** | *Did you talk about it in class?* |
| Liz: | Briefly. He [the professor] said that when you reach a triple junction, it will become 120 degrees. |
| ***Interviewer:*** | *So you are saying that there is an equal probability?* |

Liz: Well, I just don't understand why blue is doing so much better, in general. Eventually just one has to become bigger, because this is the most energetically favorable thing, so maybe... blue was bigger, but now yellow is coming back, so maybe next time blue gets bigger again, and they will just keep going. Maybe it will just be like that for a long time.

***Interviewer:*** *So what happens to growth speed?*

Liz: Eventually they will get like... two big ones... and then it will take forever.

***Interviewer:*** *So what could be the law?*

Liz: Isn't it like... it will eventually taper off... to some point... because if you have a lot or grains then you will... the rate of increase will be faster, but when average grain size increases it gets harder and harder to increase the rest of them, so it just goes...

***Interviewer:*** *Why is it harder and harder?*

Liz: Just because there isn't a distinct... [pause] being in this orientation is more favorable than this other one so you have to pick and choose... the grains are doing that, but it is not happening quickly just because you know, either one can happen.

In this very short time, working with MaterialSim, Liz was able to understand and generate hypotheses about two essential (and complex) ideas: triple points and the time dependency of grain growth. Without realizing it, she understood the reason for the triple point to be considered a "low-mobility" point in a microstructure. The central atom has two atoms of each of the surrounding grains as neighbors, so they probability of switching to any of those grains is the same (1/3), and there is no preferred growth direction. In addition, she realized that the time dependency is not linear, and that growth speed decreases over time, and eventually "tapers off". The additional importance of this discovery is that, rather than being told, Liz got to this conclusion on her own, observing the dynamics of the simulation and changing variables.

Generally, most students knew that the small grain was going to disappear. From their reactions while observing the simulation, it was apparent that they were expecting a unidirectional animation of a grain being "eaten" or "consumed" by the surrounding ones. This was consistent with both the heuristics and the kind of results of aggregate tools, animations and equations

However, what they observed was different: behaviors emerge from local interactions, which take place with some degree of randomness. At times, the small grain would grow, but most of the times it would shrink. Some of them wanted to slow down the simulation and use the "zoom" tool to see the process in more detail. Then, students could only see the micro-level phenomenon (atoms jumping to positions where they have less different neighbors). By zooming out again, they could observe the emergent behavior: curved surfaces tend to disappear, as the Laplace-Young equation would predict. There is a qualitative difference in this process: not only students are observing an expected outcome, but they are able to see the process. There is a qualitative difference between MaterialSim and other modeling environments in that the processes which students observe are visually and functionally similar to the actual phenomenon. This is dramatically different from purely numeric simulations in which what students can compare are the outputs, not the processes. In addition, words commonly used in the classroom, such as "shrink", "consume", and even "growth" acquired a new meaning. Those metaphorical terms, as our pre-test data suggested, can lead to misconceptions and misunderstandings about the actual phenomenon taking place in the material, and limit how much they could extend the models seen in class. Therefore, students realized that no grain was being "consumed" or "shrinking", but actually atoms were just switching places.

The last activity of the first day was the "BehaviorSpace" experiment. This NetLogo feature allows users to automatically run tenths or hundreds of simulations with different parameters, having all the resulting data stored in a file. Students ran at least one experiment, charted the data, and came up with theories to describe the phenomenon. Most students chose to model the influence of second-phase precipitates. Figure 6 has a sequence of images at the same time step for different percentages of precipitates, as well as the individual NetLogo plots and the Excel chart done by one of the students (note the very good fit with the theoretical data, in pink, superimposed on the chart). By doing this, they could even further generate their own hypotheses and equations, having not only the dynamic visualization but actual numerical data on the evolution of the microstructure.

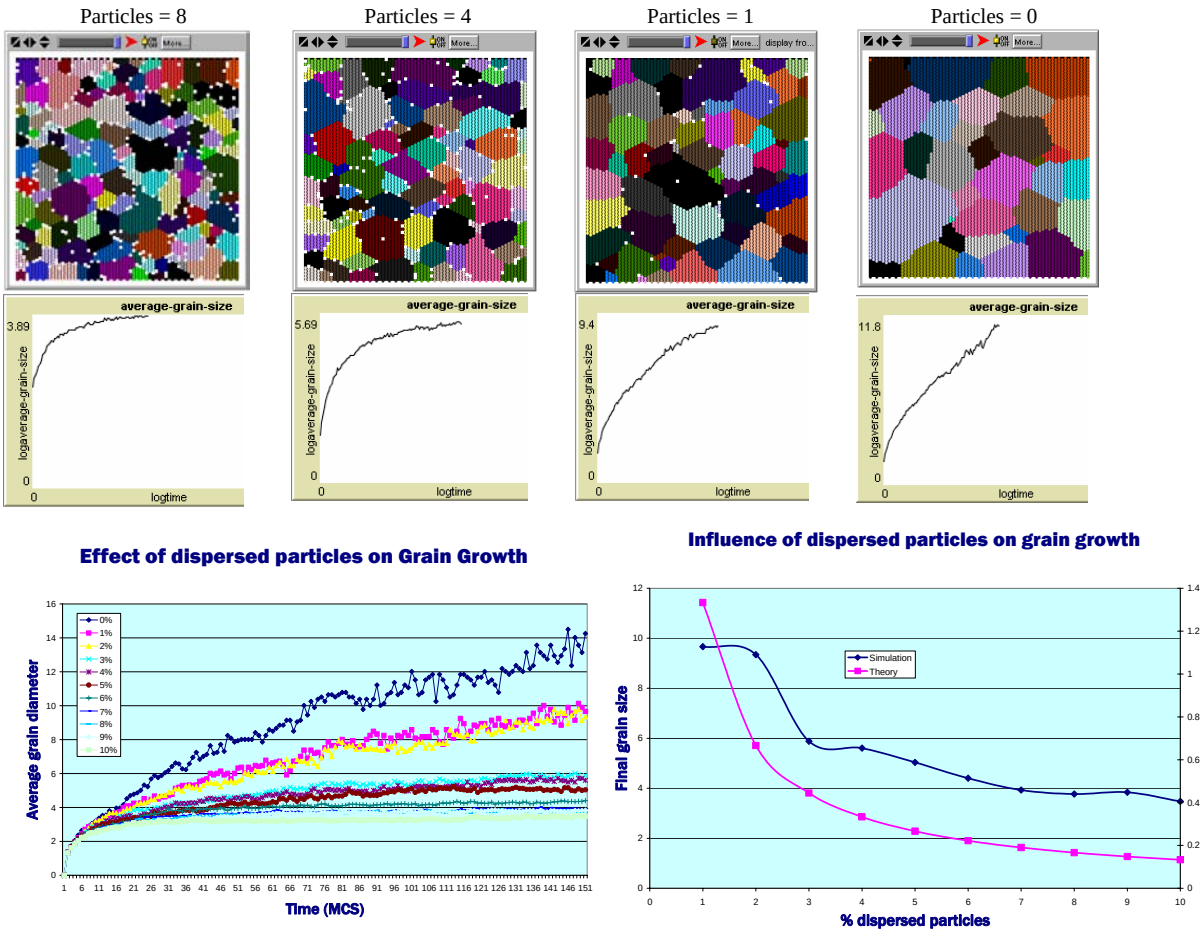



FIGURE 6
SEQUENCE OF SCREENSHOTS FROM THE STUDENTS' EXPERIMENTS. ABOUT THE EFFECT OF DISPERSED PARTICLES ON GRAIN GROWTH

## SECOND SESSION: BUILDING THEIR OWN MODELS

The main task of the second day was model construction. The first activity was to discuss the students' ideas for the new model. Next, the first author briefly introduced students to NetLogo, showing the main procedure of the grain growth simulation and explaining the basics of the language syntax and the main primitives. Students would then start coding on their own, with one-to-one assistance. Whenever possible, instead of teaching the language directly, the first author would go to the help file together with students and locate the commands of interest. They all had some contact with programming, as many of their class assignments are done in MatLab. At the end of the 2-hour session, students constructed their own working models. They pursued questions of their own and authored novel models that helped them elaborate and understand the answer their questions. This was a very impressive achievement.

The comparison between the pre-test data, when students would rely on ready-made statements about the phenomenon, and their performance on the last day of the study, when they built their own models relying just on fundamental thermodynamics, suggests that the contact with an agent-based environment made a significant difference. Even more than exploring the existing models, constructing their own ones was a transformative experience for most.

Betty built a model for taking into consideration the misalignment between the grains: the more misaligned, the harder it would be for an atom to jump from one to the other. The construction of this model presented Betty with many challenges. The first was to convert the grain orientation, which could lie in any of the four quadrants, to a useful measure independent of the quadrant. The pair 359º / 1º should be equivalent to 179º / 181º, and thus she realized that simple angle subtraction would not work. Betty's solution, after a lot of thinking and drawing, was to use the arc-sine. The following picture shows some of her reasoning (the NetLogo code is in the Appendix). From her drawing, we can observe that she was using ideas from geometry, but now in a "micro" level, taking into consideration the orientation of individual atoms.

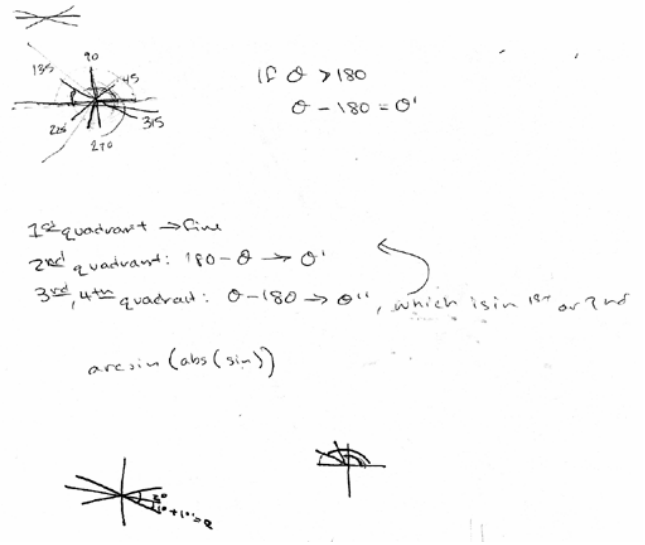



FIGURE 7
BETTY'S REFLECTION ABOUT ANGLES, SINES AND ARCSINES.

The probability of an atom to jump to the next grain was not only anymore a function of the number of different atoms around it, but the average misorientation among them. The higher it is, the harder it will be for that atom to move to another grain. Very low misorientation, on the other hand, would promote easier growth. It seemed intuitive for her – however, using aggregate and macroscopic models, it would be hard to enable the model to take it into account and explore how that would affect the growth of grains. The agent-based approach, conversely, provided a "low-threshold" entry point for her to implement her ideas and construct models. Betty's model was very consistent with known theory; despite she herself did not know it beforehand. The idea of including misorientation in the model was hers, as well as the concrete implementation.

Bob had a different problem in mind. He wanted to include a new parameter in the simulation: the size of the second-phase precipitates. The idea was to allow users not only to change their percentage, but also the radius. What seemed to be a simple problem turned into a very complex endeavor. First, he realized that given a certain percentage (in mass) of precipitates, their number had to be adjusted to compensate for the increased mass of each of them. That involved the calculation of the area of each particle (in a hexagonal grid) and the total area of the sample, to finally determine how many hexagon seeds would be necessary for a specific mass percentage. The first problem involved the conception of a formula for calculating the area of polygons placed in the hexagonal grid, which turned out to be an interesting mathematical exercise. First, Bob calculated by hand the area of particles of radius 0, 1, 2 and 3. Next, he realized that a recursive procedure would be adequate, as new layers were being added after each iteration. After concluding model, he started to investigate the influence of particle size on grain growth: maintaining the same percentage in mass, how is growth affect by changing individual particle's size? Again, he was able to run large batches of simulations in BehaviorSpace, chart the data, and find out explanations (excerpts of the Bob's code are in the Appendix).

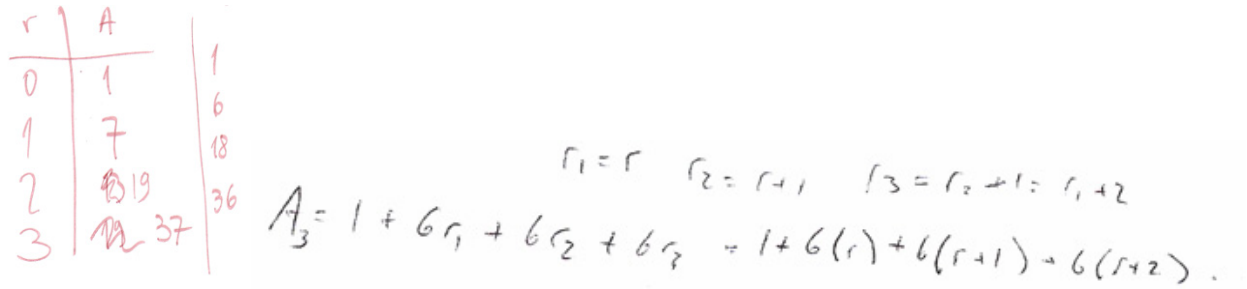



FIGURE 9
BOB'S SCRIBBLES ABOUT A RECURSIVE ALGORITHM TO CALCULATE THE "GRID-LIKE" HEXAGON AREA

Both examples were implemented in less than two hours, counting the time dedicated to learn the NetLogo language. The relative ease with which students developed their own models, even within such a short timeframe, shows that model

building is an approachable task for undergraduate students, and support one of our main claims: agent-based modeling, for some fields of engineering, offers a more principled understanding of the natural phenomena, which grants more autonomy for students when learning new content, or deriving new theories on their own. They had previous knowledge about the phenomenon from their class work. Nevertheless, during the pretest, they demonstrated difficulty in explaining related phenomena in a coherent fashion, recurring to different models and metaphors in a fragmented way. The implementation of their own model within an agent-based simulation environment, however, provided students with fewer, simpler rules closely related to the physical phenomenon, which enabled then to better understand and extend it by simply adding new proximal rules to the agents.

## CONCLUSION

Design is the new wave in many engineering schools. Starting in their freshman year, students are exposed to engineering design courses and projects. Robotics competitions, for instance, are commonplace in various institutions. However, not all of engineering is electronics or mechanical. How could we extend the powerful ideas about construction to fields such as Chemistry and Materials Science, in which the concrete products are very different than robots?

Professional tools in engineering are targeted for *modeling-for-doing*, and rich, motivating learning is often termed *learning-by-doing*. In areas such as mechanical engineering, doing and understanding could be tightly connected, as the scale of the constructions elements are visible and touchable. When a student is building a gearing system, all the components of the system are clearly laid off. However, in areas such as Chemistry, Atmospheric Science, Biology and Materials Science, that is not the case. Learners might experience or observe effects while having no clue about the causality, as the actual phenomenon it too far away from human size or time scale. As a result, technological and teaching tools in those disciplines often relied on macroscopic and aggregate descriptions. Despite their usefulness in engineering practice, are they also good learning tools?

Our user study suggested that the fragmentation of such descriptions could constitute an obstacle for learning. First, they are less extensible to new situations. Secondly, they generate "rules-of-thumb" and simple heuristics which lead to content and epistemological misconceptions. Clearly, students had a series of memorized ideas on grain growth about which they had no "feel", intuition or more general inferences. On the other hand, agent-based modeling seems to be a better fit for the content areas discussed in this paper, for four main reasons:

1) A core feature of this design is that students can apply a small number of "anchor models" to capture fundamental causality structures underlying behaviors in a range of apparently disparate phenomena within a domain. For example, free-energy minimization models enables students to understand a wide set of phenomena (grain growth, second-phase particles pinning, solidification, annealing, recrystallization, phase transformations), which are traditionally taught as separate topics, each with their own models and heuristics.

2) MaterialSim foregrounded the fundamental physical process happening in the material (atomic movement free-energy minimization), and allowed both the visualization and the computational model to have the same underlying structure (the visualization was not an animation).

3) Model building was a motivating experience for the students, an experience that is unusual in theoretical engineering classes. Students' excitement was apparent. Secondly, by creating their own models, they acquired a sense of ownership over the material.

4) Model building was a highly integrative task, putting together programming and Materials Science. Models *were selected and assembled by the students themselves.* Rather than passively receiving fragments, when building their own models learners integrate what they already know into a computational construct, what enables then to connect pieces of knowledge that were more fragmented and see their coherence.

## FUTURE WORK

At the end of the last session, Bob made a surprising statement:

> **Bob:** It is kind of hard for me to relate this [the NetLogo model] to this [his class notes]. Except for the fact that what I see overall is that grains are growing... I see overall that these grains are becoming smoother and larger and eating up small ones and that is equal to what we learned in class. And, like, the equilibrium shape and equations, and I feel that this [points to the screen] is very different, and I can't really see "oh, this makes this more obvious, or this makes this more obvious, it is because this looks more like equations, and you know, this is kind of like pictures.

This statement suggests that it is difficult for students to bridge the equations describing a phenomenon and a visualization of that phenomenon. One way to address this is to make agent-based modeling an integral part of the course, seamlessly interwoven into all the activities, classroom demonstrations, projects and assignments (similar to what is currently done in MatLab).

Another future direction is to build physical devices that could connect to NetLogo and provide students with a broader range of possibilities for experiments, as well as new ways to connect the computer simulation and real-world experiments.

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## APPENDIX

Excerpt from the NetLogo code from Betty's model:

```
to-report misorientation [angle]

  report asin (abs (sin (angle)))

end


to-report calculate-misorientation [angle1 angle2]

  report abs (misorientation (angle1) + misorientation (angle2))

end

to-report compare-misorientation

locals [i total-misorientation average-misorientation element-heading]
```

```
  set i 0
  set total-misorientation 0
  set average-misorientation 0
  set element-heading heading
  ask neighbors6 with ([heading-of] != element-heading)
    [set total-misorientation (total-misorientation +
             calculate-misorientation heading (heading-of neighbors6)
     set i i + 1]
  report (total-misorientation / i)]
end
```

Excerpt from the NetLogo code from Bob's model

```
to calculate-area-element2
locals [m]
set m 1
set element2-individual-area 1
repeat element-size
 [
  set element2-individual-area element2-individual-area + (6 * m)
  set m m + 1
 ]
end
to calculate-number-sites
locals [ white-area ]
  calculate-area-element2
  set white-area ((xmax * ymax) * (fraction-element2 * 0.01))
  set number-sites (white-area / element2-individual-area)
  set percent-sites (number-sites / (xmax * ymax)) * 100
end
```