Restructurations: Reformulating Knowledge Disciplines through New Representational Forms[1]

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Abstract

The goals of instruction are usually taken to be fixed, at least in their broad outline. For example, in elementary school mathematics, students progress from counting to addition, multiplication, and fractions. Given this state of affairs, the business of educational research has been to determine how the fixed instructional aims can best be reached. Education researchers have traditionally asked questions such as: What are the typical difficulties that students experience? Which means of instruction – method A or method B – is better for achieving our instructional aims?

In contrast, we will describe a line of work in which we have shifted the focus from the *means* to the *object* of learning. We are concerned with how the structure and properties of knowledge affect its learnability and the power that it affords to individuals and groups. We briefly review three agent-based restructurations of traditional science content and discuss the consequences for scientific power and learnability.

Keywords

Epistemology, representation, computer-based modeling, agent-based modeling

Introduction

The advent of powerful computation has brought about dramatic change in many areas of life, including dramatic changes in the practice and content of science. But, to a great extent, these dramatic changes have not resulted in significant change in the world of education. The authors of this paper have worked for many years in a more or less loosely coupled interaction on projects directed at bringing the benefits of these changes to students. This paper develops a conceptualization of this enterprise in historical and epistemological terms that go beyond computers and suggest broad new directions for the sciences of learning.

As a first step to presenting this conceptualization, we look back historically at changes in science that had significant benefits for both scientists and learners. The example that we have found most useful in presenting our idea is the shift from Roman to Hindu-Arabic numerals in arithmetic. This was not done with an "educational intent." But it had profound consequences for education. The new direction suggested in the paper is to study more systematically changes of this kind, to examine the practices of science in search of cases that could but have not had similar educational consequences and to consider the possibility of deliberately making such changes in thinking about scientific (and, indeed, other) topics

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[1] This is a short version of a longer working paper begun by the authors in 2005. The authors were finishing the paper in 2006, when the second author was seriously injured, so that paper has not yet been completed (Wilensky & Papert, in preparation). Many of these ideas were reflected in a proposal to the National Science Foundation, Wilensky et al, 2005.

with an educational intent. The conceptualization of our own projects developed in the paper presents it as exemplifying this direction of work.

We begin by looking more closely at the Roman to Hindu-Arabic transition through the lens of a thought experiment:

A thought experiment

Imagine a country, FOO, where people represented numbers as the Romans did, using symbols such as MCMXLVIII. Learning Science researchers in this imaginary country were very concerned with the difficulty of learning to handle numbers, and they worked hard to make these skills accessible to more of their citizens. They engaged in a number of different approaches. Some researchers collected the misconceptions and typical mistakes made by children. For example, they might have discovered that some children believed that since CX is ten more than one hundred, then CIX must be ten more than CI. Others constructed and studied computer programs that allowed students to practice numerical operations. Still others constructed specially developed manipulatives -- wooden blocks marked with the symbols C, X, V, and I— to help students learn. Members of the Fooian ministry of education called for more rigorous testing on Roman arithmetic. Yet another group tried to elucidate the problem by framing it in evolutionary terms, speculating that perhaps humans were just not wired to do multiplication and division. It is not hard to imagine, in our thought experiment, that many of these approaches brought about substantial improvement in learning. But let us now imagine that, at some point, the educators of this country invented Hindu-Arabic numerals This invention then opened up a new way to handle and think about numbers. Resulting gains in educability towards a functional numeracy would likely far outstrip any of the benefits that would have accrued from any of the improved techniques for teaching with the Roman numeral system. Before: the learning gap in arithmetic was immense; only a small number of trained people could do multiplication. After: multiplication became part of what we can expect everyone to learn[2].

This parable is not intended to show that the other approaches were wrong. They added knowledge that would likely have useful applications even after the shift in representations. But the point is that the most dramatic improvements did not come from what we usually think of as the main part of the science of learning.

In point of fact, Hindu-Arabic numerals were not invented with an educational intent. But they could have been, and that allows us to show the need for a new branch of the learning sciences with the mission of understanding, facilitating and even designing shifts similar to the shift from Roman to Hindu-Arabic numerals.

A first step is to name the sort of innovation associated with the shift from Roman to Hindu-Arabic representations of number. This sort of transformation has no name in the standard educational discourse. It is not sufficient, for example, to say that we have a new "curriculum" or a new "instructional approach." Even in this simple case, the algorithms that are taught, students' mental representation, their sense of systematicity in the field, psychologically important landmark values, and even social embedding ("who can do what," e.g., scribes for the emperor vs. modern carpenters or business people) changes. In our terminology, we will say that we have a new *structuration* of a discipline. The main thrust of this paper is to flesh out this term through concrete examples. But, for now, we introduce a preliminary formal definition: By structuration we mean the encoding of the knowledge in a domain as a function of the representational infrastructure used to express the knowledge. A change from one

[2] This parable, of course, is based on the historical change in number representations. For a history of the transition from Roman to Hindu-Arabic numerals in Europe (which took 400 years!), see Ball, 1960; Cajori, 1919; Kline, 1972.

structuration of a domain to another resulting from such a change in representational infrastructure we call a *restructuration*.

Our Roman-to-Arabic example is just one of many examples we could have chosen. in his book *Changing Minds* (2000), DiSessa describes the historical restructuration of simple kinematics from a text-based to an algebraic representation. He illustrates the restructuration through a story of the 16th century scientist Galileo. He describes Galileo struggling to handle a problem involving the relationship between distance, time and velocity without being able to appeal to algebraic notations such as d=vt. The central new idea in his book is exemplified by this representation of algebra as an *epistemological* entity capable of transforming what was a complex and difficult idea for as powerful an intellect as Galileo's into a form that is within the intellectual grasp of every competent high school student. The vista opened to the imagination is dramatic: if the problems with which we struggle today could be so transformed, think of the new domains we could enter and conquer! As educators, we might take the prospect in a different slant: if algebra could make accessible to students what was hard for Galileo, our holy grail should be whatever can similarly transform what is hard for them today. This is the quest on which we, and diSessa, have embarked. A subtext that is left implicit in his description, perhaps out of politeness to his colleagues, is the relative puniness of what mainstream educators would have brought to bear on helping students understand Galileo's thinking: design a curriculum, introduce manipulables, create a learning community, embed it in a computer game. Surely bringing all the machinery of *How People Learn*[3] to bear on teaching Galileo's students would have resulted in improved understanding of kinematics, but inventing algebra did better by a long shot.

You can imagine the reply of our Fooian learning scientists if somebody proposed to develop Hindu-Arabic numerals to solve the social problem of the low proportion of the population that could pass the multiplication tests. The funders of the Fooian Learning Science Foundation and the chairpeople of the Learning Science departments said: “That's not learning science”. Some might say: “It's not learning science, it's mathematics”. Others would say: “It is not science research, it is design.” From our perspective, they are caught in a dilemma: either they expand their conception of the learning sciences discipline to include such restructurations or they exclude a dramatic improvement in learning from the province of learning sciences and give it up to, for example, the mathematics department. The mathematics department of FOO might recognize this restructuration as research, but their criteria for whether this is important research is whether it addresses the set of problems currently regarded as important by professional mathematicians and not whether it addresses problems in education.

This dilemma is not just confined to our imaginary country of FOO. In the contemporary world, the science of structurations has no natural home. It requires deep disciplinary knowledge, creativity in the design of representations and sensitivity to the epistemological and learning issues. The structure of academic departments, funding organizations, etc. does not have a place for such work. We would like to see the fact that a few researchers including ourselves have found places in the University and funding system as a manifestation of the trend we noted at the beginning of the paper, and we believe that this trend would be accelerated by the development of the new branch of Learning Sciences.

It is the argument of this paper that computation-based restructurations are poised to make a significant impact on knowledge domains. The Learning Sciences is thus presented with an opportunity to study the process of restructuration and to direct it for the benefit of learners.

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[3] The most widely used text on improving education by changing *how* children learn in a child-centered way without changing *what* they learn, Bransford, 2000.

Ways to evaluate restructurations

From our current perspective, it is obvious that the Hindu-Arabic restructuration leads to better results in being able to handle numerical relationships than the Roman structuration. However, to the people of Foo and to Foo's evaluators and test-makers, it was not obvious. In our thought experiment, students who learned the new Hindu-Arabic system would likely not be able to pass the standardized tests developed using the old Roman system. Suppose they were asked: Which is the largest, CIX, XCI, or CXI? A student of the Hindu-Arabic system might not even understand this question, yet they would still be much better prepared to deal with real-world arithmetical problems. The same set of difficulties may be anticipated today. To overcome this difficulty, the Learning Sciences must strive to create evaluation measures that go beyond the specifics of a representation that is a means to an end and instead devise measures for the ends themselves.

In order to study and evaluate restructurations, we have found it useful to focus on five core properties of structurations:

a) *Power properties.* By definition, a restructuration of a domain must be able to do what could be done before and, as in the cases we describe here, preferably more as well. A new structuration can, in some respects, have the effect of broadening a discipline, in some cases by bringing what were regarded as essentially different phenomena into a common framework, and in other cases by encompassing phenomena that could not be treated at all. An example of the former kind will be seen in our use of formalism for multi-agent models to treat phenomena in physics and in biology. An example of the other kind is chaotic dynamics, which is famously intractable with algebra and calculus, yet is readily amenable to simulation and study with computers.

b). *Cognitive properties.* We are interested in restructurations that are more easily learned while preserving or augmenting the power of the old. Some factors that make for learnability are traditionally classified as cognitive. For example, the sheer "complexity" of the tasks to be performed surely affects ease of learning. A more subtle dimension is the fit of knowledge to be learned with pre-existing knowledge (whether it is learned or innate), as in diSessa's theory of p-prims (1988) or in Chomsky's theory of linguistics (1957).

c) *Affective properties.* A restructuration can make the knowledge more or less engaging, holding or simply likeable. Computational media offer especially rich opportunities to make use of this fact to increase engagement of the learner (Turkle, 1984).

d) *Social properties.* Richard Dawkins (1976) has used the concept of "meme" in analogy with gene to describe how ideas can spread in an evolutionary manner through a society, social niche or culture. Restructurations generate memes that can have varying evolutionary fitness in the social landscape. Ecology is an example of a meme that has spread quite rapidly from science into the general culture. The presence of ecology as a common meme enables some of the restructurations we present below to more easily spread through the culture. This is an example of interactions between properties of structurations. The presence of the ecology meme is affected by and affects the response of individuals and creates knowledge elements that are good cognitive fits with systems-based restructurations.

e) *Diversity properties.* One way in which structurations of a discipline can differ is in their match with a diversity of learning styles and ways of thinking. How does the learnability of the new structuration differ for learners with different backgrounds and learning styles? How does a learner's or a teacher's culture, ethnicity, gender, cognitive or emotional style affect their interaction with the properties of a structuration? Howard Gardner (1993) has shown how learning is served by an appropriate match between the learner's kind of "intelligence" and the material being learned. However, the situation in schools where matching means choosing among given domains limits the power of this idea. The prospect of restructuring domains offers dramatically greater scope: instead of characterizing people in terms of their match with subject domains (mathematical, musical, literary, etc.), we look for restructuration of domains to match people's styles.

We now turn to giving concrete examples of restructurations. We have chosen as domains core representative topics in the areas of mathematics, science and engineering. All of the examples we will give make use of computational objects as their representational infrastructure. In these examples, the computational object replaces a more traditional mathematical representation such as geometric, algebraic or calculus-based. As we will see in the examples, the computational object, or agent, has power properties that make it attractive to scientists and has cognitive, affective, social and diversity properties that make what we currently think of as advanced topics learnable by a much wider and younger population. Just as the advent of Hindu-Arabic numerals enabled a democratization of numerical facility, we suggest that computational agents will enable a democratization of STEM knowledge, particularly so for understanding the evolution of systems over time.

Our examples are framed by a large story with two plot lines. One is about the development of science through three major restructuring phases; the other is about how these restructurations enter (or fail to enter) the learning lives of children.

We introduce the scientific restructurings by looking at a number of ways to think about a circle.

For Euclid, a circle is defined by the fact that all its points are at the same distance from a certain point called its center. An aspect of this that has to be kept in mind is that the decision about whether a point is on the circle requires access to a point that is not on the circle: an ant crawling on a path could not use this definition to decide whether the path is circular.

The second view of the circle is its definition by an equation such as $x^2 + y^2 = K$. This was made possible by a major restructuration of geometry, due to Descartes, by representing geometric entities in algebraic form.

The third view will be presented anachronistically in terms of a computational object known as "the turtle" or "the Logo turtle" (Papert, 1980). Think of this as an entity that has two essential "state properties." In Euclid's geometry the fundamental element is a point defined by the fact that it has position *and no other properties*. As a mathematical entity it has no color, size or shape, although the geometer may represent it as a small, black dot. The turtle is much like the point except that its has position and ONE other property, called its heading. Again, on a computer screen it is represented as something with shape, color and size but these are not properties of the pure mathematical turtle. A turtle in motion has two velocities: its linear velocity is the rate of change of its position; its angular velocity is the rate of change of its heading.

With these preliminaries we can state our third view of the circle. If a turtle moves with both velocities constant it will draw a circle! What is remarkable about this is that the turtle draws the circle without reference to any external entity such as Euclid's "center" or Descartes "coordinate axes." Another way of saying this is that with this definition an ant walking on the circle can know that it is a circle. Yet another is that someone with a tiny field of view can tell whether a figure is a circle by looking at all parts of it confined at each instant to the tiny field of view – and this is true no matter how tiny the field. We recall that using Euclid's definition the observer's field of view would have to be big enough to include the center as well as points of the circumference.

We used a computational object to define a way of thinking about the circle for the reason that underlies the second plot line of our story: the turtle enables us to explain the concept in a simpler and more concrete way than the one used by the pioneer of this way of thinking two centuries before the computer was invented. The pioneer was Isaac Newton, and the concept is the core of what is now known as “calculus,” although most contemporary students who are required to undergo school courses with this name would probably not recognize any connection. Newton’s great achievement was to deduce a global property (such as being a circle or an ellipse) from local properties (such as having constant curvature or the force of gravity at each point.) This achievement gave rise rapidly to a restructuring of large areas of science. But – and one might say that this is the main theme of this paper – this restructuration could be appreciated and used only by people who had already acquired a rather complex body of prerequisite skills and knowledge, until the computer enables us to restructurate the restructuration and so make it accessible to many more people including, particularly children considered too young to learn “calculus” in its pre-computational form.

This last assertion will be elaborated shortly, but first we introduce our fourth way of thinking about a circle. Place a large number of turtles at the same place. Give each one a random heading. Make them all move forward (i.e. in the direction of their headings) by the same amount. They will form a circle. In some ways this goes back to Euclid’s definition, but it has a new slant: the circle *emerged* from the behaviors of a large number of agents. What will emerge in this case is “obvious.” But we shall see how the interaction of large numbers of agents, each following a very simple rule, can give rise to complex, scientifically interesting and by no means obvious emergent effects.

The view of the circle as an emergent property of a large number of agents captures in a very simple form the second plot line of our story of scientific restructurings. Newton’s breakthrough led to the understanding (“Newtonian mechanics”) of the behavior of individual physical objects such as the earth or moon in orbit. It did not take long before scientists tried to apply mechanics to large populations of entities, especially the molecules of a gas. But it was not until the nineteenth century that the necessary mathematical methods were developed to create the systematic theory now known as statistical mechanics which led to a deep restructuring of the understanding first of gas laws and later of liquids and solids as the aggregate behavior of large numbers of molecules. Here again, representing these situations as collections of computational agents allows us to make accessible to young students a level of understanding that in the past has been very difficult even for much older students.

We now turn from this outline to the actual chapters of our story. The first example is about individual (or small groups) of entities matching the original Newton restructuration, the next is about gas laws and the last shows the beginnings of an extension of the ideas to understanding solids.

Turtle Geometry and Beyond

We show in this section how the introduction of the turtle opens the possibility of far-reaching restructuring of early mathematics education. But first we want to counter in advance the justified skepticism about the idea that we have an overly grandiose obsession with our turtle as a “silver bullet” or “panacea.” Our response has two opposite parts. On one side, we point out that what is at play here is not an idea that we invented: what we are doing is showing that the computer can make available to children the essence of one of the most important ideas of all time made by one of the scientific geniuses of all time. This goal is surely worthy of a few lifetimes of obsession. We are not being overly grandiose in expecting that this idea, which has deeply transformed science, could have deep consequences for learning as well. On the other side, although we believe that many very different innovations will come as more people join the search for restructuration, we also believe that the best way to serve this goal is not to spread ourselves thin by trying to go in too many different directions, but rather to bring out the depth and variety of the one we have opened.

Example 1: The Tick model - Newtonian Physics and Beyond

In chapter two of *Changing Minds (2000),* diSessa describes the "tick model" of motion. It is a computational model of motion whereby an imaginary clock repeatedly ticks at a fixed interval and an object moves in the interval between ticks. The tick model is fundamental to a computational restructuration of kinematics. diSessa argues that the tick model is marvelously adapted to representing kinematics content. It is both very expressive as well as precise. It reveals the essential components of motion: its repetitiveness and its differential components accumulating over time. Indeed, the tick model has become essential not only for describing motion but also for describing any system that changes over time.

Our first example uses a single turtle agent or a small number of agents to restructurate traditional kinematics. In the next two examples, we will employ large numbers of agents and the methodology of agent-based modelling. We use an extension of the Logo language, NetLogo (Wilensky, 1999a), that allows thousands of turtles, We will claim that computational agents form a new computational infrastructure that is already restructurating scientific disciplines, and that careful thought is needed in order to both understand the impact of these restructurations on learning of the knowledge domains and to design a restructurated curriculum that takes advantage of the properties of the restructuration. We take a brief digression to introduce agent-based modelling.

Agent-based Modeling

One powerful methodology that has emerged from complex systems theory is agent-based modelling (Epstein & Axtell, 1996; Grimm & Railsback, 2005; Wilensky & Resnick, 1999). In contrast to more traditional mathematical modeling, which is typically done with equations, agent-based modeling makes use of simple computational rules as the fundamental modeling elements. The equational modeling game is to observe a phenomenon and try to fashion an equation that fits the observed data. A classic example is the Lotka-Volterra equations used to model the change in predator and prey population levels over time (Hastings, 1997). In equational modeling, the core elements of the model are variables that refer to population-level descriptors. In the Lotka-Volterra equations, the core elements are L, the population level of the lynx predators; H, the population level of the hare prey; and K, the interaction constant that describes the average predation. To understand the state of the system at a future time T, you solve the equations for that time. In contrast, in the agent-based modeling game, the core elements are computational objects or "agents" that represent individual lynxes or hares. Each of these agents has state variables that describe its particular state, such as age, energy level, hunger, etc. The behavior of the agents is determined by the computational rules that tell each agent what to do at each "tick" of a clock. The rules are framed from the agent's point of view. For example, if the agent is a lynx, the rules might say: move a step in the direction you are headed; reduce your energy variable by a fixed amount; look for prey in the vicinity; if prey is found where you are, try to eat it; if not turn to face closest prey you can see, etc. To determine the state of the system at future time T, you run the system for T clock ticks. As rules typically have stochastic components, one would typically run the system many times to capture the space of possible trajectories for the system.

Increasingly, scientists are making use of agent-based models as both explanatory and predictive tools. Across a wide variety of domains in the natural and social sciences, scientists are framing their theories in terms of agent-based models (Axelrod, 1997; Gilbert & Terna, 2000; Troisi, Wong & Ratner, 2005). In the natural sciences, agent-based models have several advantages over equational approaches. Chief among these are: a) The epistemological match – rules for individual predators or molecules are closer to our intuitive notions of these "objects" as distinct individuals rather than as aggregate populations; b) The greater adjustability – equational representations tend to be brittle, that is, for some small change in environmental conditions, the algebraic forms themselves do not typically change only a little. An entire new formalism may be required to capture the new situation. In our lynx-hare example, if we discover that when hares become too populated, they start to attack each other, the changed needed to the LK equations is not straightforward. In contrast, in the agent-based approach, it is a trivial matter to give the hares an extra rule to that effect; and c) Visualization – related to the epistemological match is the greater realism afforded by visualization of individual lynx and hare and their dynamic behaviors rather than just dynamic graphs of their populations.

All three of these advantages are magnified in the educational context. Students can reason about and visualize individual animals in an ecology far better than they can population levels. They can draw on their own body and sensory experience to assess and/or design sensible rules for the behavior of individuals. They can therefore make much greater sense and meaning from the agent-based representations. Furthermore, the extensibility/adjustability of the models enables students to engage in real inquiry by asking what-if questions of the models and adjusting rules in order to get answers to their questions. While this is common practice for scientists, it is not so for students. The alternate representation, in effect, enables them to think more like scientists (Wilensky & Reisman, 2006).

In the educational context, there is one more advantage that is greatest of all: the greater ease of mastering the representations themselves. Learning to master the LK equations requires the prior mastering of an extensive algebraic and calculus-based infrastructure that is out of reach for large numbers of our students. These students are therefore shut out of the scientific exploration of most worldly phenomena that change over time. And even those students who do eventually master algebra and calculus do so late in their student "careers". Agent-based representations, in contrast, require significantly less effort to master. Research we have conducted shows that typical middle and high school students can profitably employ these representations with only a small amount of prior instruction (Levy & Wilensky, 2009; Sengupta & Wilensky, 2009; Wilensky, 2003; Wilensky & Novak, 2010). Widespread adoption of agent-based representations can therefore lead to tremendous democratization of scientific knowledge.

Our next two examples employ agent-based modeling to restructurate relatively advanced science content, making it more learnable as well as accessible to young learners.

Example 2: GasLab - Statistical Mechanics and beyond

The GasLab package is a suite of NetLogo models of kinetic molecular theory. In the basic model, gas molecules are represented by turtle agents that bounce off each other and off their enclosing container like billiard balls with elastic collisions. Using GasLab, many groups of students have conducted experiments with the Gas-in-a-Box models (Wilensky, 1999b). They also revised and extended the model, creating the nucleus of the set of models that comprise GasLab (Wilensky, 2003). The set of extensions of the original Gas-in-a-Box model is impressive in its scope and depth of conceptual analysis. Among the many extensions students tried were: heating and cooling the gas; introducing gravity into the model (and a very tall box) and observing atmospheric pressure and density; modeling the diffusion of two gases; allowing the top to be porous and seeing evaporation; relaxing elasticity constraints and looking for phase transitions; introducing vibrations into the container and measuring sound density waves; and allowing heat to escape from the box into the surrounding container. They also reinvented various well-known thought experiments of statistical mechanics related to Maxwell's demon and second law considerations[4]. Over the course of several weeks, these high school students "covered" much of the territory of collegiate statistical mechanics and thermal physics and their understanding of it was deeply grounded in both a) their intuitive understandings gained from their concrete experience with the models and b) the relations amongst the fundamental concepts.

GasLab provides learners with a set of tools for exploring the behavior of an ensemble of micro-elements. Through running, extending and creating GasLab models, learners were able to develop strong intuitions about the behavior of the gas at the macro level (as an ensemble gas entity) and its connections to the micro level (the individual gas molecule). In a typical physics classroom, learners usually address these levels at different times. When attending to the micro level, the focus is typically on the exact calculation of the trajectories of two colliding particles. When attending to the macro level, the focus is on "summary statistics" such as pressure, temperature, and energy. Yet, it is in the connection between these two primary levels of description that the explanatory power resides.

Two major factors enable students using GasLab to make the connection between these levels -- the replacement of symbolic computation with simulated experimentation and the replacement of "black-box" summary statistics with learner-constructed summary statistics. The traditional secondary physics curriculum segregates the micro and macro levels of description because the mathematics required to meaningfully connect them is thought to be out of reach of high school students. In the GasLab modeling toolkit, the formal mathematical techniques can be replaced with concrete experimentation with simulated objects. This experimentation enables learners to get immediate feedback on their theories and conjectures. In a traditional curriculum, learners are typically handed concepts like pressure as "received" physics knowledge. The concept (and its associated defining formula) is, thus, for the learner, a "device" built by an expert, which the learner cannot inspect nor question. Learners do not come to see that this concept represents a summary statistic – a way of averaging or aggregating the behavior of many individual particles. Most fundamentally, the learner has no access to the design space of possibilities from which this particular summary statistic was selected. In the GasLab context, learners must construct their own summary statistics. As a result, the traditional pressure measure is seen to be one way of summarizing the effect of the gas molecules on the box, one way to build a gauge. The activity of designing a pressure measure is an activity of doing physics, not absorbing an expert's "dead" physics.

Example 3: MaterialSim - Materials and Beyond

Materials science and engineering has grown considerably from its roots in experimental metallurgy. It is now a fundamental part of engineering education. T*raditional* methods for investigating properties of materials reflect the tools that were available in the nineteen-fifties: mathematical abstractions, geometrical modeling, approximations and empirical data. These tools have inherent limitations both in their "power properties" for scientists but even more so in their "learnability properties" for students.

In the past two decades, massive computing power has made a new and promising restructuration possible: computer simulation of individual molecules of the materials. Practicing material scientists have rapidly adopted this new approach. However, it has not as

[4] As one example of these reinvented thought experiments, they constructed a model of a divided box with a small opening in the divider in which a propeller is embedded. They measured the work done on the propeller by the particles hitting it and the propeller's consequent motion. A version of their model is downloadable from http://ccl.northwestern.edu/netlogo/models/GasLabSecondLaw.

of yet migrated to the teaching of materials science, which still relies on the traditional methods.

As a specific example, let us consider the phenomenon of “grain growth”. Most materials are composed of microscopic “crystals”. A crystal is just an orderly arrangement of atoms, a regular tri-dimensional grid in which each site is occupied by an atom. In Materials Science, scientists use the term “grain” to refer to such an arrangement. The notion of grain is fundamental to Materials Science and Materials Engineering.

Among other properties, grain size determines how much a material will deform before breaking apart, which is one of the most important issues in engineering design. For example, a car built with steel with a wrong grain size could significantly increase the risk of serious injury for the passengers. But grain size can change, too – high temperature is the main driving force. This phenomenon, known as *grain growth*, is exhaustively studied in Materials Science: small grains disappear while bigger ones grow (the overall volume is maintained). Airplane turbines, for instance, can reach very high temperatures in flight – an incorrectly designed material could undergo “grain growth” and simply break apart. The following photographs (magnified 850x) show typical results.

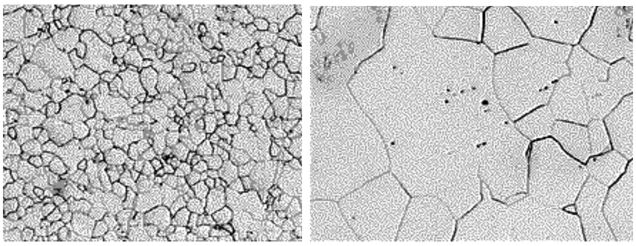

Figure 1: Metallic sample before and after grain growth (from Blikstein & Tschiptschin, 1999)

Burke (1949) was one of the first to introduce a law to calculate grain growth and proposed that the growth rate would be inversely proportional to the average curvature radius. Burke’s law states that large grains (lower curvature radius) grow, while small grains (high curvature) shrink. The mathematical formulation of Burke’s law also reveals that, as grains grow, the growth rate decreases. A system composed of numerous small grains (see Figure 1, left) would have a very fast growth rate, while a system with just a few grains (see Figure 1, right) would change very slowly. In the beginning of the century, metallurgists believed grains to have a “maximum size” for a given temperature – but that was only due to the lack of tools to detect the very slow growth rate at the end of the process. However, even Burke’s description had its limitations. In order to make the math feasible, for example, Burke was led to consider grains as spheres with just one parameter to describe their size (the radius). For most practical engineering purposes, this approximation yields acceptable results – however, its practical efficacy does not necessarily mean that this approach is the best way to understand the phenomenon, nor to build on it to understand other phenomena in materials science.

In the 1980s Anderson, Srolovitz and colleagues. (Anderson, et al, 1984) proposed the now widely used theory for computer modeling of grain growth using an agent-based approach. This kind of simulation not only made predictions faster and more accurate, but also allowed for a completely new range of applications. Researchers were no longer constrained by approximations or general equations, but could make use of more precise mechanisms and realistic geometries.

Anderson et al. state that the classic rule-of-thumb for grain growth (“large grains grow, small grains shrink”) is not always valid, and that randomness plays an important role. Given the microscopic dimensions and small time scale of the phenomenon, practically the only way to visualize this new finding is through computer simulation. As a result of these “power properties”, this approach became widely adopted for the use of professionals. But, since at first glance, it would seem that since the situations for which it is a superior approach are not the simple cases, but the advanced ones used by professionals, that there was no reason to change instruction for novices in the field.

However, an agent-based approach to grain growth has *learnability* properties that make it particularly suited for novice learners. The agent-based simulation of grain growth offers a different perspective. Its principle is the thermodynamics of atomic interactions – one of the *extensible*, *transferable*, *anchor* models. Consider the learning environment, MaterialSim (Blikstein & Wilensky, 2009), which employs the agent-based approach to teach Materials Science. MaterialSim is a set of exploratory models built within the NetLogo (Wilensky, 1999a) environment. There are models for investigating crystallization, solidification, casting, grain growth and annealing.

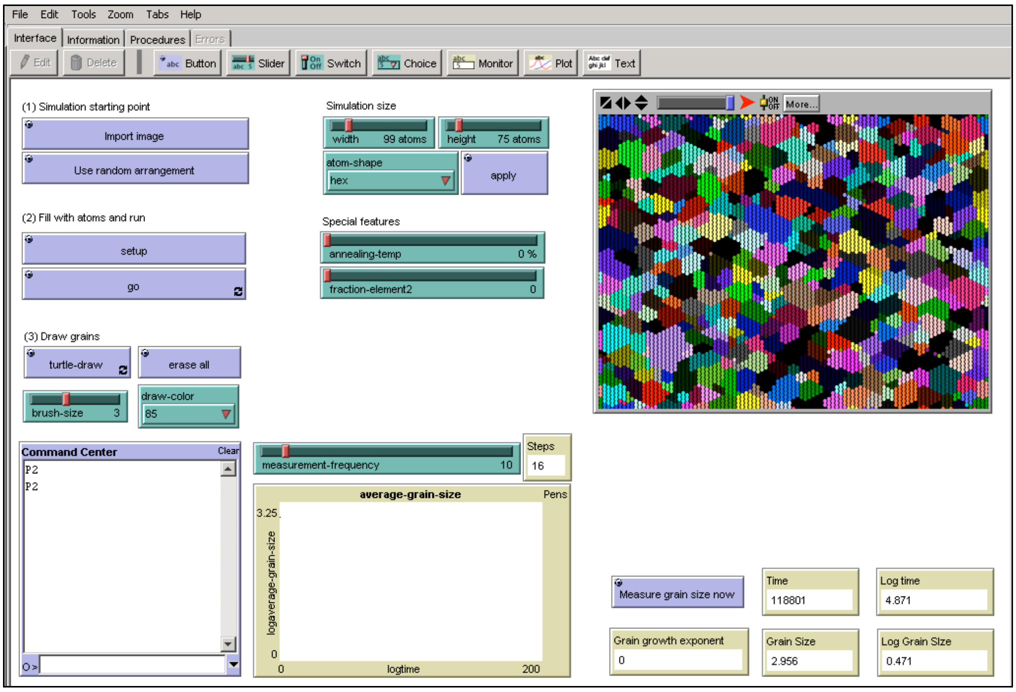

Figure 2. MaterialSim’s grain growth model (Blikstein & Wilensky, 2004)

MaterialSim represents a material as a hexagonal 2D matrix, in which each site corresponds to an atom and contains a numerical 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. MaterialSim’s grain growth algorithm is described below:

- Each element (or agent) of the matrix has its free energy (G_i) calculated based on its present crystallographic orientation (a value of 2 in figure 3) and its neighborhood (the more neighbors of differing orientation, the higher its free energy). Figure 3 (left side) shows the central agent with four neighbors with different orientations; hence the value of its *initial free energy* (G_f) is 4.

- One new random crystallographic orientation is chosen for that agent, among the orientations of its neighbors. In this case, as observable in Figure 3, the current value of the central agent is “2”, and the new transition value is “1”.

- The agent’s free energy is calculated again (G_f), with the new proposed crystallographic orientation Figure 3 (right side) shows that there are only two different neighbors in the new situation, thus the *final free energy* (G_f) decreases to **2**.

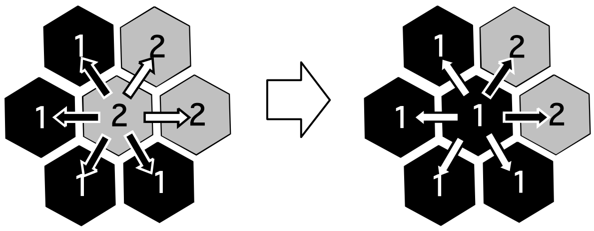

Figure 3: Initial and final free-energy calculations. Black and white arrows denote different or equal neighbors.

- The two states are compared. The value that minimizes the free energy is chosen. In this case, G_i=4 and G_f=2, so the latter value is lower and constitutes a state of greater stability. Thus, the proposed change in orientation is accepted.

From this basic model, one can understand what is going on in the material at the micro-level. Instead of having to use rules of thumb to predict what will happen to the grains, we can use this formal model to visualize and reason about the evolution of the material. For most initial conditions, we will indeed see a rule of thumb such as “large grains swallow others” obtained. But we will also see how this process develops, how it emerges from the micro-level “decisions” of the molecules, and we will see that under some conditions the traditional rule of thumb will be violated.

The greater value of the agent-based approach lies in more than understanding this particular phenomenon. Once the basic model is set up, it is easy to explore a large set of configurations and to understand possible trajectories of the system. And because the representation system is composed of simple modifiable micro-rules rather than aggregate level equations, it is easy to modify them to explore a host of other phenomena. In our implementations of MaterialSim, we have seen students adapt the basic model to explore a diversity of materials science phenomena such as recrystallization, diffusion, interfacial energy, nucleation, solidification, and phase transformations.

The agent-based restructuration of materials science enables students to reason about materials from the atom on up. Whereas traditionally they employ heuristics and formulae given to them by authority, they are now able to author their own heuristics and formulae derived from their modeling experience. Just as the restructuration of numerals enabled ordinary folks to do multiplication and division for themselves, the agent-based restructuration of materials science enables learners to set up experiments and author new models for themselves.

Conclusion

We have briefly laid out the theory of restructurations and called for careful consideration of computer-based and, in particular, agent-based restructurations of science content and instruction. We have presented three examples of such restructurations. We note that such restructurating is not confined to mathematics and natural science. Indeed, we suspect that agent-based restructurations of social science may give even greater leverage. We note that our own fields of education and learning sciences can be restructurated using agent-based approaches. To understand educational reform and phenomena such as curricular adoption, homework collaborations and the effects of educational policies, agent-based modeling can be a powerful tool. It enables us to study these phenomena as emergent from the interactions of the individuals rather than through properties of the aggregate populations.

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