Motivating Computational Science with Systems Modeling

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ABSTRACT

This paper describes introducing rate of change and systems modeling paradigms and software as tools to increase appreciation for computational science. A similar approach was used with three different audiences: freshman liberal arts majors, junior math education majors, and college faculty teaching introductory science courses. A description of the implementation used with each audience and their reactions to the material is discussed, along with some example problems that could be used in a variety of courses.

Keywords

Rate of Change, Systems Modeling, Computational Science

1. INTRODUCTION

The concepts of rate of change and modeling are addressed at many levels in the K-14 mathematics curriculum. Some example student learning outcomes include:

- "Interpret the rate of change and initial value of a linear function in terms of the situation it models" – Eighth Grade (Common Core Math Standards) [1]
- "Calculate and interpret the average rate of change of a function" – High School (Common Core Math Standards) [2]
- "Find a derivative interpreted as an instantaneous rate of change" – AP Calculus (ETS) [4]
- "Analyze growth and decay using absolute and relative change" – Content Learning Outcome for Quantitative Reasoning (New Mathways Project) [5]
- "Apply the mathematics they know to solve problems arising in everyday life, society, and the workplace" – High School (Common Core Math Standards) [2]
- "When making mathematical models, they know that technology can enable them to visualize the results of varying assumptions, explore consequences, and compare predictions with data" – All Levels (Common Core Math Standards) [3]
- "Apply simple mathematical methods to the solution of real-world problems" – Quantitative Reasoning for College Graduates (MAA) [6]

Meeting these learning outcomes provides opportunities to introduce computation as a modeling tool to students as early as middle school. In addition, these students can be acclimated to the notion that computation is an important part of doing science, hopefully paving the way for more students to move into HPC.

In this article an outline of steps for introducing a systems modeling paradigm is presented, along with results from using software packages to investigate modeling change with three different audiences: college freshmen through a quantitative literacy course; pre-service high school teachers through a junior level mathematics modeling course; college faculty in summer workshops. In all three situations, one of the main goals was to raise the awareness of the importance of computation in doing science by modeling and solving non-trivial problems without first teaching the syntax of a standard programming language. First, consider an example modeling problem to provide some context.

2. A MOTIVATING EXAMPLE

Suppose rabbits are invading an asparagus patch, and we wish to investigate how the rabbit population affects the asparagus patch over time. What assumptions might be made? While not the only approach, we can start by thinking about what might cause increases and decreases in the number of rabbits and amount of asparagus. Some reasonable assumptions might be:

1. Rabbits are born, and how many are born depends upon the number of rabbits present to have offspring and amount of asparagus present to provide energy from food.
2. Rabbits die, and more rabbits means more competition for food, space, etc.
3. Asparagus grows steadily.
4. Asparagus is eaten by rabbits when the rabbits can find asparagus to eat.

The next step in the process is to "mathematize" these assumptions about the rates of growth and consumption of

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asparagus and the rates of birth and death of the rabbits. Refining the assumptions:

1. When the number of rabbits or the amount of asparagus increase, so do the rabbit births.
2. When the number of rabbits increases, so does competition and hence rabbit deaths.
3. Asparagus grows steadily, so the growth rate is some constant amount.
4. When the number of rabbits or the amount of asparagus increase, more asparagus gets eaten.

What are some mathematical expressions that capture these ideas? A very simple proportionality argument yields the following components of the model. Let $R(t)$ represent the number of rabbits and $A(t)$ represent the amount of asparagus at a particular time t.

1. Rabbit births: proportional to both R and A implies that the increase due to births can be modeled by $r_b \times A \times R$, where the proportionality constant r_b can be interpreted as the factor controlling the rabbits' rate of reproduction.
2. Rabbit deaths: proportional to R implies a model of $r_d \times R$, where r_d can be interpreted as the fraction of the rabbit population that dies in a given time period.
3. Asparagus growth: constant a_g.
4. Asparagus consumption: $a_c \times R \times A$, where a_c can be interpreted as the fraction of interactions between rabbits and asparagus that results in a unit of asparagus being eaten.

Using these expressions we can build a mathematical formulation for our model, which can take several forms depending on the audience. Working with students who have calculus backgrounds, the model can be presented as a system of differential equations:

$$\frac{dR}{dt} = r_b AR - r_d R$$

$$\frac{dA}{dt} = a_g - a_c RA$$

$$R(0) = R_0; A(0) = A_0$$

where R_0 and A_0 represent initial quantities of rabbits and asparagus. While this approach works well for calculus-ready students, consider how to approach the problem recursively: "The quantity at a later time $(t+1)$ is the quantity now (t) $\pm$ what changed."

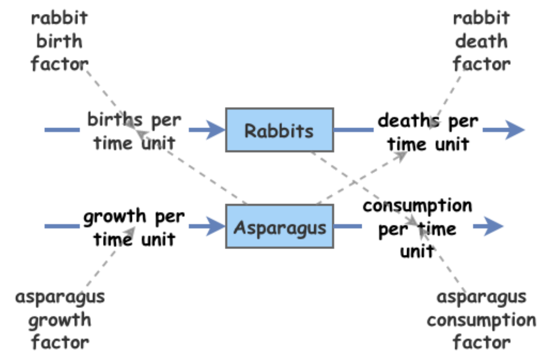
$$R(t+1) = R(t) + r_b A(t)R(t) - r_d R(t)$$

$$A(t+1) = A(t) + a_g - a_c R(t)A(t)$$

$$R(0) = R_0; A(0) = A_0$$

If the goal is spreadsheet use, these equations can be implemented a spreadsheet such as Microsoft Excel, producing a table of values documenting the changing quantities over time. Alternately, systems modeling tools allow for

Figure 1: Rabbit-asparagus model in Insightmaker



easy construction of the change formulas. Stella (iseesystems.com/), VensimPLE (vensim.com/), and Insightmaker (insightmaker.com/) all begin with construction of a diagram as in Figure 1.

All of these systems modeling software environments include primitives similar to those illustrated in Figure 1: The changing quantities are represented by rectangles ("stocks"), rates of change are represented by thick arrows ("flows"), and interdependencies ("links") are represented as thin or dashed arrows. Other inputs, such as parameters, are represented by plain text or circles.

Once the diagram is completed, each primitive can be initialized for the specific model. Flows require a formula for the increase or decrease in each full time step. For example, in Figure 1 the flow labeled "consumption per time unit" that represents the rate of decrease of the asparagus contains the expression:

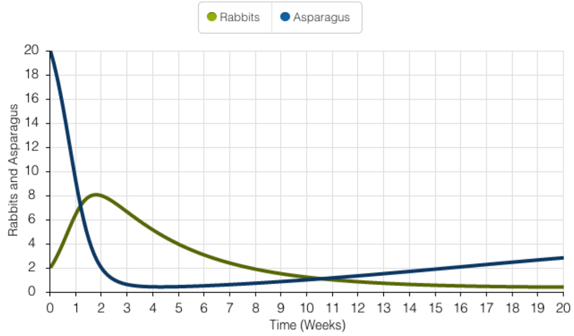
[asparagus consumption factor]*[Asparagus]*[Rabbits]

This expression is a wordier version of the proportionality description of asparagus consumption arrived at above, and all of the software packages use a "clickable list" interface to build these formulas. Stocks require initial values, which can be input as constants or as mathematical expressions involving other elements of the model. Parameters also can be modeled as constants or expressions.

After entering the relevant mathematics, the systems packages produce solutions in either tabular or graphical form. Figure 2 shows the output generated by Insightmaker for the rabbit-asparagus model with parameters: initial quantities of 2 rabbits and 20 acres of asparagus; a rabbit birth factor of 0.1; rabbit death factor of 0.3; asparagus growth factor of 0.4; asparagus consumption factor of 0.2.

One other important consideration for the systems approach to the solution is selection of the time-step. If the goal is to mimic change that happens more frequently than once per unit time (e.g., continuous change), all of the software environments allow the time-step to be set to a fraction smaller than one. In the Rabbit-Asparagus model simulation output (Fig. 2), the time-step is set to 0.125 (i.e., $1/2^3$) to approximate the continual growth of asparagus. All of the systems modeling software environments adjust the flow calculations appropriately for time-steps other than one so that growth and decay parameters do not have to be recalculated by hand.

Figure 2: Graphical solution from Insightmaker



3. IMPLEMENTING SYSTEMS MODELING IN THE CLASSROOM

The same general outline for introducing systems modeling can be used with many types of students:

1. Introduce a scenario, such as the rabbit-asparagus model. Choosing population growth allows most audiences to contribute to the discussion.

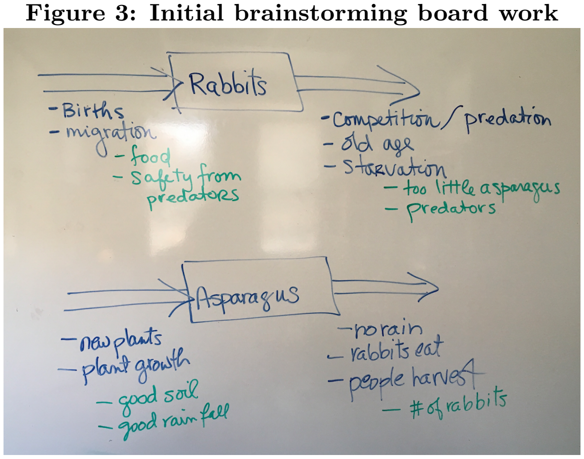
2. Draw a diagram similar to one that would be produced by the software on the board, soliciting suggestions for what might cause the populations to grow and to shrink, recording ideas on the diagram (Fig. 3).

3. Encourage the group to identify the most important components to include in the model, adding arrows to represent the interdependencies (Fig. 4).

4. Determine values for the parameters. In the absence of scientifically produced estimates for the parameters, a reasonable first attempt is to set all growth and decay parameters to be the same (e.g., 0.1). In addition, the model requires initial values for each of the populations and also a value for the time step.

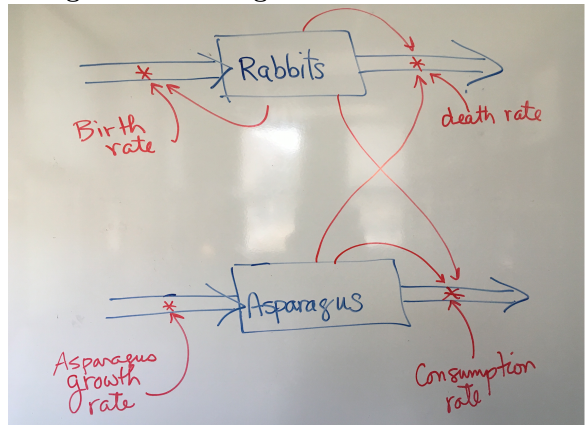
5. Build and run the model in the systems software.

Figure 3: Initial brainstorming board work



Once a working model is produced, ask students to discuss whether the model and the output makes sense. What does

Figure 4: Refining the model board work



the software appear to be doing? What do the parameters really represent? Does it make sense that the rates are all the same? Where should parameter values really come from? Where do scientists get them? What happens to the solution if we change them? What time-step is most meaningful? Why is using a power of two as the time step important computationally?

Since the goal is often for the students to build their own models, it is helpful to make available a video of building the same model; a simple approach is to use screen sharing with *Hangouts on Air* (via youtube.com/live_dashboard) during the class to capture the entire conversation. That way students can view the video again anytime they need to be reminded of the intricacies of using the software.

This same approach to introducing systems modeling has been used with a variety of audiences. Sections 3.1, 3.2, and 3.3 provide detail on how systems modeling was introduced to three different audiences. Several common themes emerged from observations and discussions with these groups after the modeling activities were completed.

- Computational tools are crucial for solving problems in science.

- Mathematical formulas can be used to model real situations.

- Tools that minimize programming allow more students to experience using computation to solve problems.

- Tools that incorporate diagrams illustrating individual model components are more engaging and help students to focus on individual components of the model in the construction process.

3.1 Quantitative Literacy Course

As described in the introduction, students in a quantitative literacy (QL) course should have exposure to solving real-world problems. Systems modeling environments provide opportunities for students who are not calculus-ready to explore interesting models and gain experience with using computational tools.

3.1.1 Implementation

The approach outlined above was used in a one-week unit on modeling change in a freshman QL course, after which the students were given a week to work in groups of three on creating and analyzing a model for the "Pollution in a Chain of Lakes" problem (see Section 5). This problem does not entail much in the way of background scientific information for the students, and so all of the students could participate in conversations about how pollution might disperse in a lake and whether the assumption of immediate mixing of pollution throughout the water in a lake would lead to unreasonable solutions.

Prior to this unit, students had significant experience with building formulas in a spreadsheet for projects in personal finance and consumer statistics; the spreadsheet was discussed as an alternate method for finding solutions to the chain of lakes problem, but students were required to use the simulation software (Stella in this particular class).

3.1.2 Reactions

During a class debriefing discussion at the completion of the project, students were asked to submit a reflection on what they learned from working on the project. Their responses indicated that they understood better how mathematical expressions could be used to model real situations and how computers are an important tool in solving problems. The students also indicated that they liked working in the visual, simulation environment more than building formulas in a spreadsheet; the process helped them to "see" the parts of the model and work on one part at a time.

3.2 Junior Math Modeling Course

The junior-level modeling course is required for preservice secondary math teachers, an especially important audience for exposure to modeling and computation given their future interactions with high school students. This course includes modeling change as a major topic in much more depth (approximately one-quarter of the course) compared to the QL course described above. The other topics covered were data modeling, linear programming, and graph / network modeling–all of which required some use of technology for solution or visualization. At this level, the students have a calculus and linear algebra background and are proficient in the use of a computer math system and a spreadsheet.

3.2.1 Implementation

As with the QL course, the discussion of modeling change began with the process outlined above for brainstorming about a scenario and creating mathematical formulas for components of the model, after which students used both a spreadsheet (Excel) and a computer math system (Maple) to implement simulations for several problems. Then students were introduced to systems modeling software (in this case Insightmaker), and asked to implement the same problems in the new environment. For the culminating project on modeling change, groups of two or three students were assigned a project from the problems in Section 4, for which they had to produce a group poster along with individually written technical reports. They were given the option of using any of the tools they wished without any attempt to influence their choice.

3.2.2 Reactions

Over the past two years, 38 of the 52 students taking the course opted to use Insightmaker, later citing the ease of use and the ability to easily incorporate more sophisticated components in their models, such as if-then, delay, and pulse functions. Similar to the QL responses, several commented on the ability to view each component of the model individually and make progressive improvements to the model components. Eight of the remaining 14 students who decided to use a different tool for their mathematical solution still drew diagrams using Insightmaker to include as part of the explanation of their model structure in their posters and reports. Course evaluations were very positive, with several of the students volunteering comments related to the modeling change portion of the course being their favorite, also indicating that they saw the relevance of solving problems computationally and thought that tools like Insightmaker could be used in their high school classrooms once they became teachers. In comparison, no such comments were made regarding spreadsheets or computer math systems, although students also volunteered positive comments on the network analysis problems and software (another diagram-based system).

3.3 Workshops for College Faculty

For two summers, the Computing MATTERS workshops (computationalscience.net), sponsored by Project XSEDE and the National Computational Science Institute were held at several universities in the Eastern and Midwestern US. During that introductory workshop, college faculty who teach entry level math and science courses were introduced to computing software, using a context of inquiry-based learning and modeling change. Most of the participants were already motivated to incorporate computation into their freshman courses, but were not sure how to work with students who may not have any computational background.

3.3.1 Implementation

In three days, the faculty were exposed to a number of computational tools, including spreadsheets (MS Excel), systems modeling (Vensim), agent modeling (Agentcubes Online), and computer math systems (Sagemath) with approximately one-half of a day spent investigating each tool. As might be expected, many levels of computational experience were represented among the participants, but the vast majority of faculty acquired enough basic knowledge of systems modeling ideas and software to begin experimenting with problems from their own fields of study. On the third day, a portion of the morning and all of the afternoon was set aside as time for the faculty to experiment more with tools or material they thought could benefit their teaching.

3.3.2 Reactions

In the flexible time on day three, the majority of faculty opted to work more on systems modeling ideas, with agent modeling a close second (both are used to model change). In discussions with the participants at the end of the workshop, it was clear that they saw the value of exposing students in introductory courses to these tools as a way to build understanding of the role computing plays in doing science–an opinion they came to the workshop with–but now many were also more confident that they could include computation without omitting material required by their course syllabi.

The NCSI follow up survey the for the workshops, administered by Project XSEDE, revealed that faculty remained excited about computational thinking and introducing computational tools to their students even after the end of the workshop. While the likert scale questions on the survey did not differentiate between the different types of workshops offered, there were a number responses to the open-ended question, "[W]hat aspect of your experience in NCSI has most affected your work?", that could be clearly associated with participants from the Computing MATTERS workshops. All were positive, and several are reprinted below.

- I think about the classroom material more often in terms of systems and models, and think about how I might encourage my students to represent it that way.
- I was not aware of it before, and now see an entire new realm of teaching and research to explore and implement on our campus.
- After attending the NCSI workshop I have thought more about and have recognized the importance of developing activities and lessons that will introduce my students to Computational Thinking practices. I have used some of the software applications from the workshop with my students.
- Listening to Dr. Panoff discuss how to think about the processes of computational thinking made me concentrate on how I present problem solving in my classes.
- My own personal thought process on what constitutes a model and how to develop the means of creating the model using more than one computational tool. Excel, Agent Sheets, Interactive Physics, NetLogo are all programs I use in my classes.
- The use of software in my classes. I hace (sic) been using Vensim to explain physics concepts. Students enjoy this activity and they improve their concepts comprehension.

4. FUTURE DIRECTIONS

As indicated earlier, several common themes emerged from observations and discussions with these groups after the modeling activities were completed. In particular, gains were made in students' understanding that computation plays an important role in science and that mathematics can be used to model real situations. These results have been shared in several venues: at the 2016 NCCTM State Mathematics Conference - primarily high school teacher attendees; 2017 NCMATYC Conference - primarily community college faculty attendees; 2017 ICCS - primarily university faculty attendees. In addition, several follow up activities are planned:

- The success of the material in the QL course has resulted in plans to write a more formal module that can be used by other faculty teaching the QL course as either a short (1 week) topic or a longer (3-5 week) topic.
- The modeling tools will continue to be used in the junior modeling course, and preservice teachers who took the junior modeling course will be contacted after they begin their teaching positions to inquire about the applicability of the materials to their own classrooms.

5. EXAMPLE SCENARIOS

The following are examples of situations that have been used in all three implementations. Some are more open ended than others, but all can be addressed in a manner similar to that used for the rabbit-asparagus example.

1. **Spread of Disease**: Consider an island population and suppose that some small number of people leave the island and come back, bringing with them an infectious disease. To predict the number of persons at any time who have the disease, a simple assumption would be that the change in the number of persons who catch the disease is some fraction of the number of possible encounters between susceptible and infected people. Suppose also that the disease is one for which recovery results in immunity and it just takes some set amount of time to recover. Create a model for this situation.

   Here is a data set taken from a (mythical) island of 5000 inhabitants. Do the data support your model, i.e., are there parameters that make your model come close to the data)? How long until everyone recovers and is immune?

t (days)	0	2	6	10
sick people	5	1887	4087	3630

2. **Drug Dosage**: Clinical studies have shown that a simple model for the rate at which the concentration of a drug in the blood stream is decreasing is to assume the rate is proportional to the concentration of the drug at that time; the constant of proportionality can be thought of as the "elimination rate" for the drug. In addition, it is common for the same amount of a drug to be administered at regular intervals.

   Suppose a certain drug's elimination rate is 4% per hour, the minimum effective dosage is 0.1 mg/ml, and the maximum safe dosage is 0.3 mg/ml. Determine what size initial dose to deliver via injection and then how often a repeated dosage of 0.1 milligrams per milliliter should occur.

3. **Pollution in a Chain of Lakes**: Suppose a chain of lakes connects to each other via rivers (like the Great Lakes) and that there is a pollution source in the innermost lake. Suppose we have the following information about flow rate / volume: Lake 1 is spring fed with fresh water; 20% of lake 1 flows into lake 2 each month, 18% of lake 2 flows into lake 3 each month, and 16% of lake 3 is flushed into the ocean each month. If 100 kg/month of pollutant is dumped into Lake 1 each month for five months before the leaky pipe is found, will pollution levels ever exceed 200 kg in any of the lakes? How long before the pollution is essentially washed out to sea?

4. **Harvesting in a Shrimp Farm**: Farmed shrimp are usually raised in an enclosed area, with a known a maximum sustainable quantity of shrimp given the amount of nutrients and the size of the area. Model the rate of growth of the shrimp population assuming the change in the size of the population is proportional to the number of shrimp times a limiting factor that approaches

0 as the population of shrimp approaches the maximum sustainable population. Also incorporate plans to harvest a constant amount of shrimp each month.

Suppose we have the following parameters: maximum sustainable population = 77000; initial population = 5000. Also experience indicates that for small numbers of shrimp the population doubles each month. How does the population grow if we harvest 2000 shrimp over the course of a month? Can we harvest 5000 each month without having the population crash? What if we restock with 500 shrimplets over the course of the month?

5. **Simple Chemical Reaction**: A simple chemical reaction can be thought of as follows: A "reactant" reacts with an "intermediary" compound to produce a "product." The basic ideas behind the kinetics:

   - The rate at which the reactant changes to the intermediary during the first reaction is proportional to the amount of both the reactant and the intermediary compounds – both are needed for the reaction to occur.
   - The rate at which the intermediary then converts to the product during the second reaction is proportional to the amount of the intermediary compound that is present.
   - The two reaction rates – usually referred to as k_1 and k_2 depend on the specific compounds involved.

   Suppose 1000 moles of the reactant and 1 mole of the intermediary are added to a beaker initially, with reaction rate constants of 0.005 and 0.05 per second, respectively. How quickly does the reaction occur?

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