Computational Science 101 - Towards a Computationally Informed Citizenry

Victor Winter[1[0000−0002−3264−624X]]

University of Nebraska at Omaha, Omaha NE 68182, USA
vwinter@unomaha.edu

Abstract. This article gives an overview of CSCI 1280, an introductory course in computational science being developed at the University of Nebraska at Omaha. The course is intended for all students, regardless of major, and is delivered in a fully asynchronous format that makes extensive use of ed tech and virtual technologies.

In CSCI 1280, students write programs whose excution produce graphical block-based artifacts. This visual domain is well-suited for the study of programming fundamentals and also aligns well with scientific simulations based on cellular-automata. An overview of CSCI 1280's simulation framework for percolation theory and the spread of infectious diseases is given.

Keywords: functional programming · patterns · computational science

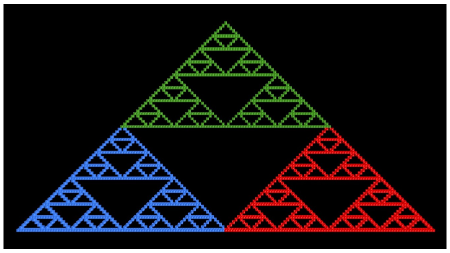
1 Overview of CSCI 1280

At the University of Nebraska at Omaha (UNO), *CSCI 1280 - Introduction to Computational Science* is a freshman-level gen ed science course that embraces the domain of computational science as a means to provide a gentle and engaging introduction to programming.

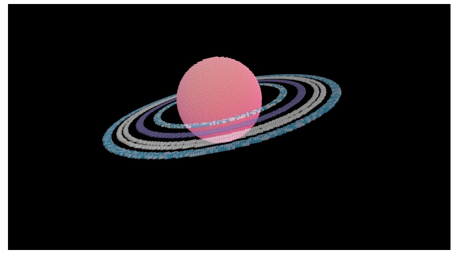
All programs in CSCI 1280 are written in a freely available programming environment called *Bricklayer* [9][8] which extends the functional programming language SML with a collection of graphics and computational science libraries. Using these libraries, programs can be written to construct block-based artifacts (AKA pixel art) like the ones shown in Figure 1.

In addition to enabling the creation of art, Bricklayer's block-based infrastructure is also suitable for scientific exploration. A variety of scientific models and simulations are based on cellular automata [3]. For example, diffusion models and simulations can be used to study heat-diffusion, spreading of fire, ant behavior, and biofilms [6]. Cellular automata have also been used to model and study the formation of biological patterns (e.g., molds), Turing patterns, as well as adhesive interactions of cells [1].

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55



(a) A Sierpinski triangle.



(b) An artist's rendition of Saturn.

Fig. 1: Examples of 2D and 3D Bricklayer artifacts.

1.1 Contribution

CSCI 1280's curriculum provides a gentle introduction to programming as well as computational science. The visual domain used allows concepts to be covered in a fashion that is not math intensive and therefore suitable for all majors (STEM majors as well as non-STEM majors). This visual domain is also enables instructional design to heavily leverage interactive technology to achieve educational goals.

2 Patterns

CSCI 1280 begins with an informal study of patterns, a concept the National Science Teachers Association (NSTA) has classified as crosscutting all the sciences[5].

The first assignment in CSCI 1280 asks students to use a Bricklayer web app, called the *Grid*, to create a pattern. A link to the Grid is provided below.

https://bricklayer.org/apps/CSCI_1280/Grid_CSCI_1280/grid.html

A key question in the *create-a-pattern* assignment is whether students understand the patterns created by their peers. A thought experiment students are asked to perform is the following:

Ask yourself whether you could continue working on (i.e., increase the size of) a pattern created by another student?

To enable students to engage in such thought experiments, the patterns created by students are shared online in a 3D interactive art gallery. A link to such a gallery is provided below.

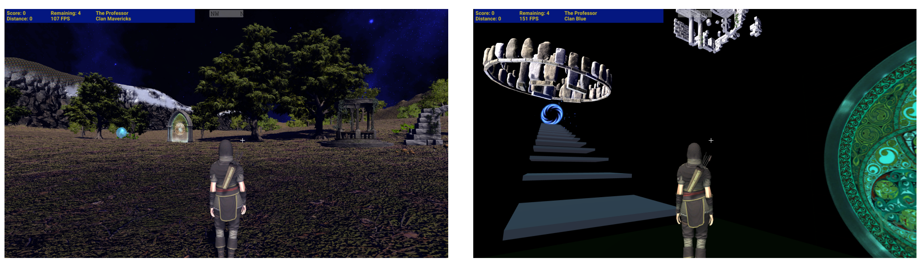
https://mygame.page/csci1280-create-a-pattern-art-gallery-02

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55

These art galleries employ PlayFab leaderboards allowing players (i.e., students) to rate the patterns of their peers using a Likert scale. A painting can be rated by "shooting" (i.e., positioning the crosshair and pressing the left mouse button) the desired circle below the painting. Players can report their ratings and visit a ratings summary page to view how the paintings in a gallery have been rated by the class as a whole.

To strengthen students' understanding of pattern the create-a-pattern assignment is followed by a discussion of several forms of symmetry that a grid-based artifact can possess. Specifically, vertical and horizontal reflection symmetry is discussed as well as 2-fold and 4-fold rotational symmetry. To help develop a students understanding of these symmetries, a web app called *Mystique* was developed. A link to Mystique is provided below.

http://mystique.bricklayer.org



(a) A Celtic forest with a blue will-o-the-wisp off to the left.

(b) The Upside Down - Portals to various lands.

Fig. 2: Triskelion.

To encourage a more sustained and hopefully enthusiastic engagement with the study of symmetry, a third-person game, called Triskelion, was developed. Triskelion interleaves gameplay with solving Mystique puzzles. The goal of gameplay is to cast magic spells in order to collect will-o-the-wisps which are moving orbs randomly spawned at various locations on a map. When a player collects a will-o-the-wisp they are teleported to a puzzle realm where they must solve a symmetry puzzle in order to return to gameplay. When all the will-o-the-wisps in the first map have been collected, the player is teleported to *The Upside Down* where they encounter two parkour-based pathways. Each pathway ends in a portal that transports the player to a distinct final map. Thus, when playing a game of Triskelion only two of the three maps are visited. The hope here is that curiosity alone will result in students exploring all maps. Screenshots highlighting Triskelion are shown in Figure 2.

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55

Triskelion supports clan-based competition in which the score a player receives is based on the speed and accuracy with which they solve puzzles. During a match, the score for a clan is the average score of the players in the clan. Educators have access to leaderboards that track a variety of engagements metrics such as: (1) how many games an individual has played, (2) the total time devoted to solving puzzles, and (3) the total time devoted to gameplay.

3 Bricklayer's Percolation Library

Percolation theory [2][7] involves the study of clustering in graphs. In practice, percolation theory has applications in numerous fields of study including: chemistry, biology, statistical physics, epidemiology, and materials science.

An example of a question fundamental in percolation theory is the following: *If a liquid is poured on top of some porous material, will it be able to make its way through the pores in the material and reach the bottom?* If so, the material is said to *percolate*.

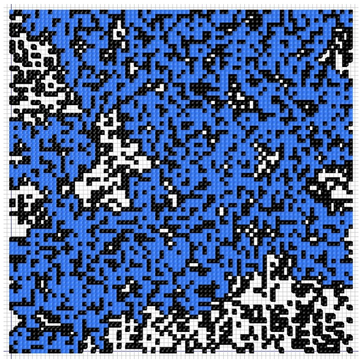
When studying percolation, a density known as a *percolation threshold* is of central importance. This threshold represents the material density above which the material almost never percolates and below which the material almost always percolates. While approximate values for percolation thresholds can be determined through simulation, no mathematical solution has yet been discovered for calculating such values. For this reason, percolation theory provides an interesting domain highlighting an important role that computers can play in scientific inquiry.

Bricklayer's Percolation library provides a variety of functions for exploring the basics of percolation. One function can be used to create rectangles having a desired size and density. Another function allows "water" to be "poured on the top" of such a rectangle. Figure 3 shows 2 Bricklayer squares having similar density. One square percolates and the other does not.

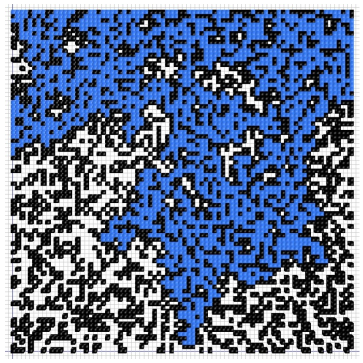
Using these two functions students can explore the roles played by rectangle size and density in percolation. Such experimentation is labor intensive and motivates the need for another function, also provided by the Percolation library, which is able to perform numerous tests automatically and summarize the results (e.g., 6540 rectangles out of 10000 rectangles percolated). Through automated testing of this kind it becomes possible to obtain information that could not realistically have been obtained through manual experimentation. This provides students with a concrete and compelling example of the importance of computational power in scientific inquiry.

By varying the density of a fixed size rectangle, automated testing can be used to manually search for the percolation threshold. However, in order to estimate the percolation threshold in a manner that is fairly accurate, a large number of automated tests will need to be performed. To support the search for accurate percolation thresholds, Bricklayer provides a function that performs a Monte Carlo search. This significantly increases the computational complexity of the simulations being performed, which now can take minutes or even hours

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55



(a) A randomly generated Bricklayer 2D cell structure that percolates.



(b) A randomly generated Bricklayer 2D cell structure that does not percolate.

Fig. 3: Pouring water on 80×80 squares whose density is approximately 59%.

to complete. However, the information obtainable through Monte Carlo search significantly exceeds the information that can be obtained through manual search based on automated testing. The hope is that through this sequence of ever more computationally demanding experiments and simulations students will gain an understanding of how computational power can meaningfully contribute to scientific exploration.

4 Bricklayer's Infectious Disease Library

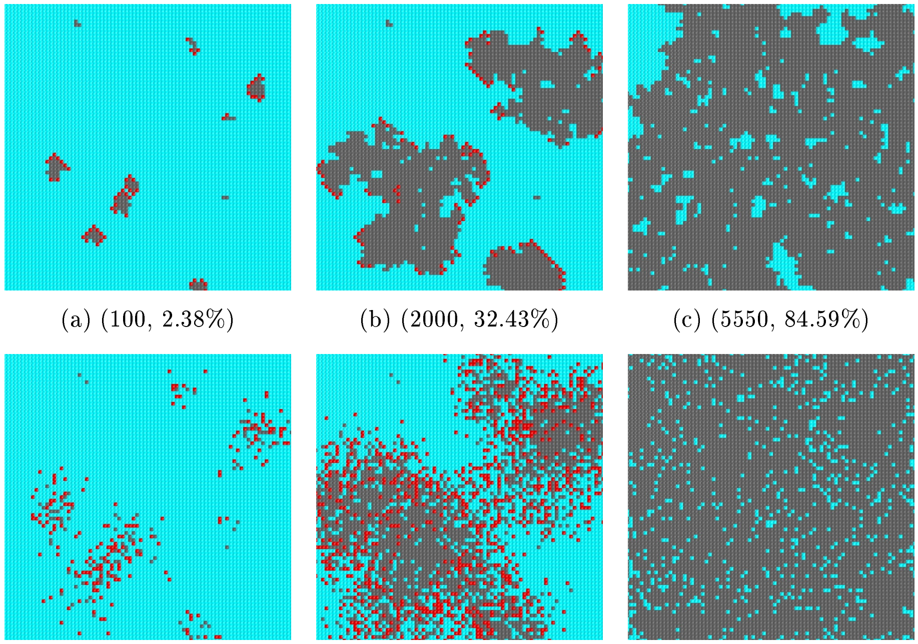
Bricklayer's infectious disease library (IDL) implements a fairly straightforward variation of a susceptible, infected, recovered (SIR) transmission model. Though not of medical grade, for questions with known (i.e., non-politically contentious and scientifically agreed upon) answers, Bricklayer's simulations align closely with scientific findings. An example of such a question is: "Given the R_0 value for the measles, what percentage of the population needs to be vaccinated in order to achieve heard immunity?"

Building upon abstractions introduced in the Percolation library, the IDL models a population as a square whose cells represent individuals. In contrast to percolation models, where cells can be in one of two states (open/closed), cells in IDL models represent individuals that can be in one of four states: infectable, uninfectable, infected, and recovered. These four states are modeled via programmatically assignable colors (e.g., individuals that are infectable can be represented as aqua colored cells).

Both uniform as well as Gaussian[1] (i.e., normal) random number generators can be used to model R_0. An additional variable is also provided to control the

[1] Research has suggested that Gaussian random number generators produce more accurate results than uniform random number generators[4] for simulations of this type.

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55



(a) (100, 2.38%) (b) (2000, 32.43%) (c) (5550, 84.59%)

(d) (100, 4.32%) (e) (2000, 43.68%) (f) (5867, 89.42%)

Fig. 4: The impact of social radius on the spread of an infectious disease.

probability of transmission (i.e., infection) when two cells interact. A variable is also introduced to model *social distancing* – the region (i.e., the population) where interaction with an infected person is possible. This integer variable denotes a radius defining a neighborhood around a cell of interest (i.e., an infected person). A radius of 0 corresponds to a Von Neumann neighborhood, a radius of 1 corresponds to a Moore neighborhood, and a radius, r, larger than 1 defines a square whose sides are $2 \times r + 1$.

The specification of an IDL simulation consists of: (1) the dimensions of the square modeling a population, (2) a color assignment denoting the state of an individual, (3) the size of the initial infected population, (4) a model of R_0, (5) the probability of infection upon contact, (6) a social radius, and (7) the number of transmission steps to be performed. A simulation stops when either (1) the number of transmission steps is reached, or (2) when the transmission opportunities have been exhausted (e.g., herd immunity is reached). Bricklayer's IDL library assumes that a person can be infected at most one time.

Figure 4 shows the results of social distancing on two otherwise equivalent simulations using a Gaussian number generator with $R_0 = 2.5$. The tuples in the captions denote (number of transmission steps, percent of the population infected or recovered). The three images in the top row were generated using a

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55

social radius of 0 while the images in the bottom row were generated using a social radius of 5.

The final assignment in this module is open ended and asks students to use the Bricklayer's IDL to explore the transmission of COVID-19 (e.g., what constitutes herd immunity for COVID-19). Students need to determine what value of R_0 they are willing to consider as well as other aspects like social distancing. The values used should be justified by citing reputable sources. The interpretation of the simulation results, should then be compared to reputable sources.

5 Conclusion

Technology is becoming increasingly intertwined in all walks of life. It's role is so significant that it is essential for all citizens to gain a deeper understanding of what technology can do as well as what its limitations and weakness might be.

A widely acknowledged goal of higher education in general (and general education requirements in particular) is to create a well-informed citizenry able to meaningfully engage in society. As a consequence of the astonishing advances in technology, the prerequisites for such engagement are changing rapidly. By targeting broad student populations having diverse backgrounds, CSCI 1280 seeks to positively contribute to the creation of a *computationally informed citizenry* - a citizenry having sufficient knowledge to participate in the technologically advanced societies of the 21^{st} century.

References

1. Deutsch, A., Dormann, S.: Cellular Automaton Modeling of Biological Pattern Formation. Birkhauser, 2^{nd} edn. (2017). https://doi.org/10.1007/b138451
2. Grimmett, G.: What is percolation? In: Percolation, pp. 1–31. Springer (1999)
3. Ilachinski, A.: Cellular Automata - A Discrete Universe. World Scientific (2001). https://doi.org/10.1142/4702
4. Lachiany, M., Louzoun, Y.: Effects of distribution of infection rate on epidemic models. Physical Review E. **94**(2) (2016)
5. National Research Council: A Framework for K-12 Science Education - Practices, Crosscutting Concepts, and Core Ideas. The National Academies Press (2012)
6. Shiflet, A.B., Shiflet, G.W.: Introduction to Computational Science - Modeling and Simulation for the Sciences. Princeton University Press, 2^{nd} edn. (2014)
7. Stauffer, D., Aharony, A.: Introduction to Percolation Theory. CRC Press (1994)
8. Winter, V., Hickman, H., Winter, I.: A Bricklayer-Tech Report. World Scientific and Engineering Academy and Society (WSEAS) Transactions on Computers pp. 92–107 (2021)
9. Winter, V., Love, B., Corritore, C.: The Bricklayer Ecosystem - Art, Math, and Code. Electronic Proceedings in Theoretical Computer Science (EPTCS) (2016)

ICCS Camera Ready Version 2022
To cite this paper please use the final published version:
DOI: 10.1007/978-3-031-08760-8_55