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Graph Theoretical Modeling of DNA as a Vehicle for a Course-Based Undergraduate Research Experience

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ABSTRACT: This paper outlines a mathematics course centered around the interdisciplinary topic of modeling self-assembling DNA which was used as a venue for a mathematics course-based undergraduate research experience (CURE). The structure and logistics of designing and teaching such a course in addition to suggestions and student feedback from the course are also included.

Keywords: Undergraduate Research, Graph Theory, Modeling, Course-Based Undergraduate Research Experience

Introduction

The benefits of undergraduate research experiences have been well studied and documented [2, 3, 5, 8, 12, 20, 24, 25, 27]. Engaging in the rich experiences of research are particularly beneficial for underrepresented STEM populations [3, 8, 12]. Course-Based Undergraduate Research Experiences, (CUREs) are a great way to engage whole classes in research experiences in contrast to more selective research internships [1, 2]. While there have been a variety of examples of CUREs implemented in science and engineering labs and classes, there has not been as much written about mathematics-based CUREs [6, 7, 17, 25, 31, 32].

This paper presents the details of a mathematics-based CURE. A CURE is defined in [1] as a course-based undergraduate research experience which involves students in the use of scientific practices, discovery, collaboration, and iteration, and allows students to contribute to broadly relevant work. The structure and logistics of designing and teaching such a course are shared in addition to suggestions and student feedback from the course. Although the class size was only eight, the author believes that this structure could be scaled up to a larger class size perhaps with the use of teaching/research assistants.

1 About the Course

This course was designed to introduce students to a mathematics research topic and provide structure for the students to work together in research cohorts to participate in discovery-based research. Although the course was two credit hours, this structure could easily work for a one credit hour or three credit hour course as well. Students took this course as a special topics mathematics course which could count towards the elective of the mathematics major or minor. Students in this course had a variety of majors including mathematics, computer science, engineering, and biology. Most of the students in the class either were not getting even a mathematics minor, or did not need this course for their major or minor. The main motivation for students to take the class was that they were interested in doing mathematical research and this was a way to “compensate” them for their efforts as an alternative to a stipend. Interest in this course also came through our university’s summer undergraduate research experience. Some of the students applied for the summer research program and the instructor contacted students who were not chosen for the summer program and offered them this opportunity to participate in research.

The theme of this research was “Graph Theoretical Modeling of Self-assembling DNA Nanostructures.” The unique properties of double-stranded DNA molecules make DNA a valuable structural material with which to form self-assembling nanostructures and the field of DNA nanotechnology is largely based on this premise [29]. By modeling nanostructures with discrete graphs, efficient DNA self-assembly turns into a mathematical puzzle which allows construction methods and concepts from undergraduate level graph theory to become useful in the study of self-assembling DNA complexes [11]. To work on this research, students chose families of graphs to use as the base of these nanostructures and then worked to determine optimal design strategies under various given laboratory constraints. One of the benefits of this research topic is that it requires minimal mathematical background and as a result the majority of the students in the class were not mathematics majors.

During the first few weeks, the instructor introduced students to the research topic, appropriate background preliminary mathematics, and some of the known results and techniques used to solve open problems in the field. Specifically the instructor introduced the mathematical model and notation used in this research for DNA self-assembly. Because of the varying backgrounds of the students, the instructor designed short modules to introduce some basic linear algebra, programming, and graph theory. If students were not in need of these introductions or refreshers, then they were free to play with some of the initial warm-up problems for the research. During the first four weeks, students read sections of preliminary research and during our weekly class meetings the instructor went over some of the details of the proofs, techniques, and results. Each week, the instructor assigned some “toy problems” or previously known results as weekly homework for students to discover and prove for themselves. At this time, the students were put into initial research pods or cohorts of four students. These cohorts were initially based on student availability and schedule. Students were required to meet at least once with their cohort to collaborate on the weekly assignments. The cohorts then presented their results during part of the following class period.

After students had learned some of the initial techniques used to solve problems in this field, the instructor had the cohorts work on more complex families of graphs which previous student researchers had explored. These problems were chosen in part because they were slightly more complex to solve

than the initial problems they had seen, but simple enough so that students could make a lot of progress within one week's time. These results were not outlined in any of the papers the students had and thus this gave them a chance to practice using the techniques they had learned to solve these new problems.

For the final third of the class, the instructor broke up the research cohorts students into groups of two or three and each cohort chose their own research problem to solve. In this case, students picked out several families of graphs (usually related graph families like book graphs and stacked book graphs) which had never been explored before. During the next few weeks the students worked on their research and class time was spent as a time to report their current findings and get feedback from the instructor and other students. The instructor would move around the groups providing support and advice when appropriate. The general process for the students was to find optimal designs for their families of graphs in the two least restrictive laboratory conditions and then *prove* that these designs were optimal. As students worked, they updated their results in a research report written in L^AT_EX. The last two weeks of the class were spent wrapping up their current progress, finalizing their written reports, and creating a poster presentation which they would use to present at the Joint Mathematics Meetings and an internal university-wide poster session. After the class was completed, we had a pizza party during which each cohort presented their posters to the class. Later these students presented their research at several local, regional, and national mathematics conferences.

The structure and design of this course clearly aligned within the Course-Based Undergraduate Research Experience spectrum outlined in [1]. All students in the class addressed an interesting research question within the field of nanotechnology which required the use of scientific practices. Students asked questions, proposed hypotheses (in this case conjecturing possible optimal designs for self-assembling DNA), evaluated various methods and techniques they could use to prove or disprove their hypotheses. Students then communicated their findings regularly to each other and the instructor. The course was specifically designed to be very collaborative and required students to work in research cohorts and communicate and present their weekly findings to each other. Students were able to apply previous results and methods to solve new problems and were able to learn from previous misconceptions and misconceptions. Since students chose their own research problems, the research was driven by the students and the instructor's role became that of a mentor or advisor since the outcome of the research problem was unknown to her. At the end of the course, students provided new understanding within the realm of nanotechnology and designs for self-assembling nanostructures. Furthermore, students had to deal with the ambiguity that comes from researching the unknown. One student shared,

“I thought the overall research experience and class was really helpful in understanding how doing research kind of works. For me at least, it was very different in how to approach it since in standard classes, there's always an answer to homework but in research, there was no direct answer we could just search up on the internet or get from [the instructor] since it was all still very new and everything wasn't already all figured out. Making the distinction between the two experiences definitely helped me understand a little of what it's like to do research. Then presenting at JMM was helpful to show what we had learned knowing that there's still a lot to learn about our subject.”

1.1 Time and Effort for Instructor and Student

The time and effort in running this course was similar to the time commitment for other courses. Yet the time which normally would have been spent grading ends up being more of “reviewing” and supporting the research. That being said, a lot of effort, flexibility, and thoughtfulness is required especially for the start of the class. Thinking about scaffolding the initial problems and allowing students to explore the proofs in the initial readings is important and takes some thought. Since students are exploring the research themselves and asking their own problems (in this case, novel problems which had never been solved before), the instructor needs to be able to support and possibly provide additional resources. Structuring the groups or partners also requires some care and thought. Furthermore it is important for the instructor to recognize if the specific research questions asked by the students may not allow them to make meaningful progress within a semester-long course. When this happens, the instructor may want to either suggest a different question or suggest ways to simplify the research question. For example, the instructor could suggest that the students look at specific cases, smaller subsets of the question, or add more requirements/assumptions to the problem to make it easier to explore. The research team could then continue to generalize if they make progress on the adjusted problem. Because of this, it would be

ideal if the instructor of the course had some experience in the research field or had access to someone to vet the student research problems. Like all courses, improvements can be made after an initial run of the course. One thing that I benefited from was having worked on this research before with students during an 8 week university summer undergraduate research experience. Thus I had a better idea about how to scaffold the research and how to choose toy problems and examples which would be the most helpful to the students.

This course also required a lot of time and effort for the students. For many students, especially if this was their first time doing research, this course required them to rethink how they manage time and make progress on a problem. Unlike most of their mathematics courses in which they can refer to their textbook or ask their instructor for immediate feedback, students find that for a CURE like this, they can't easily look up a sample problem which can help with this research. Since the problems they are working on are uncharted territory, the instructor may not be able to provide immediate feedback when asked. As such students are often uncomfortable at first not having the security blanket of problems which have been solved before. Research requires deep thinking and often requires trying a variety of paths which don't work. Students are not always used to this and the instructor should encourage them through this process. Learning what approaches don't work is part of the learning and research process and is still a step in the right direction. Because of this, it may be helpful to make sure students work on sample toy problems which allow them to have some initial success before having them start on a completely unknown problem.

1.2 Structure and Logistics of Course

In this section will provide some details from the course. The course objective for the class was to help each student participate in mathematical research by

- developing his/her ability to solve problems in the field of mathematical research,
- developing his/her ability to read mathematical research articles,
- developing his/her ability to write mathematical proofs and research arguments,
- doing mathematics cooperatively,
- appreciating how abstract ideas and rigorous methods in mathematical analysis can be applied,
- and communicating mathematical ideas clearly.

The course grade was made up of the following categories and most of the assignments were based on completion and effort (usually using a 2 or 3-point scale). Participation was worth 20%, homework was worth 30%, group contribution was worth 10%, presentations were worth 10%, the poster was worth 10%, and the final write-up was worth 20% of the grade. More details regarding these categories are provided below.

Productive Engagement: In order for students to achieve the maximum points for this portion of this portion of their grade, they were required to “actively present, facilitate, and participate in class activities, present problems and proofs from weekly assignments and participate in class discussions.”¹ This was graded based off of completion and effort following a 3-point scale (sufficient participation, partial participation, did not participate).

Homework: Each week, students were given a homework task or research task to work on. This work could be done individually and as part of their assigned research group. This homework was based off of completion and effort following a 3-point scale (sufficient effort/work, partial effort/work, incomplete).

Group Contribution: Students were assigned small groups, called “research cohorts” to work on weekly assignments and tasks. Students were required to meet at least once with their group for at least an hour to work on the weekly research assignment. Their weekly Group Contribution grade included

¹Language for this came through example course materials presented during an IBL workshop ([www.http://www.inquirybasedlearning.org](http://www.inquirybasedlearning.org)).

whether they were able to meet and actively participated as part of the group and was based off of completion following a 2-point scale (met or did not meet).

Presentations: Most weeks, one student from each research cohort was asked to present the weekly results from the group. This presentation grade was based off of completion and so each group was expected to rotate presenters.

Poster: Each group designed a poster summarizing their research and results. Research cohorts will present this poster as a final summary of their semester-long progress. The rubrics used for the poster and presentation are provided in Appendices A and B.

Write-Up: Each research cohort was required to write a L^AT_EX report of their work over the semester. A template and some examples of this write-up were provided. (This write-up was also able to serve as a first draft for their senior seminar project if they were a math major.) A sample rubric used for the paper is included in Appendix C.

1.2.1 Course Schedule and Timeline

Table 1 provides a general 16-week schedule which was used for this course. A more detailed course schedule can be found in Appendix D. This could be adapted for a variety of research topics.

Week(s):	Task
1	Introduction to research topic and notation: Students will read introductory material and be introduced to the general research topic and notation used in the class.
2-5	Introduction to Methodology: Students will be introduced to the methodology and theory used in the research and verify known results themselves in order to practice using the methods for the research.
6-8	Research Exploration: Students will work on toy research problems whose results are known to the instructor, but not known to the students.
9	Choose Research Question: Research Cohort groups will choose their own research topic within the general research they have been exploring. The instructor will make sure each cohort has different graphs to work on.
10-15	Research: Students will explore their research questions, present their weekly progress and questions in class, and begin writing up their results.
16	Presentation and Write-Up : Group presentations of final results and progress. The final Write-up and Poster for each group are due.

Table 1: General Course Timeline

1.3 Research Aims and Goals

Motivated by the rapid advancements in nanotechnology and the discovery of new laboratory techniques using the Watson-Crick complementary properties of DNA strands, the study of self-assembling DNA complexes and self-assembly in general, can be assisted by graph theoretical techniques [26,30]. Synthetic DNA molecules have been designed that self assemble into given nanostructures [4, 13–16, 22, 23, 28, 33–38, 41, 42]. Furthermore, there is great promise in the ability to create and engineer synthetic DNA nanostructures which in turn supports new applications in nanoelectronics, biosensors, biomolecular computing, drug delivery systems, and directed organic synthesis, all of which can lead to more effective diagnosis and treatment of illness [18, 19, 21, 39, 40]. Since modeling this self-assembling process requires

designing the component molecular building blocks, which can often be modeled through surface meshes, lattice subsets, and other graph-like structures, construction methods developed with concepts from undergraduate graph theory have resulted in increased efficiency [9]. Thus this research topic opens up problems within the scope of graph theory and provided the general motivation for the research conducted in this class.

The introduction of a graphical methods for exploring the combinatorial properties of self-assembly of DNA molecules was first introduced in the early 2000s [29]. Based upon this use of graph-theoretical design strategies, one can model the self-assembly of DNA by equating DNA molecules to the vertices of a graph and cohesive-ends (bond-ends) as an alphabet placed on the edges of the graph. Thus, given a DNA complex, we can then model this complex using a graph. The research goal is to determine the optimal placement of an alphabet on the edges. Design strategies for realizing a target graph are considered under three different levels of laboratory restrictions, which depend on whether or not smaller or non-isomorphic structures are acceptable byproducts of the process. In order to optimize the construction of a target graph, we usually first find upper bounds on the number of letters needed to construct the complex and then refine these results until we can prove that no smaller alphabet can be used. While the general fundamental research questions were consistent for all research cohorts (that is optimizing the number of tiles/bond-edge types used in the construction of complexes), the cohorts picked specific families of graphs to explore. All of the main research problems tackled by the students were novel in nature and had not been previously proven. Figure 1 provides an example of one group's poster.

In addition to gaining research experience and creating a summary poster and report, students were able interact in a comfortable and collaborative research environment in which students and instructors worked together to discover new knowledge. Students were able to improve their presentation and communication skills along with learning firsthand the need for persistence, patience, and resilience in research. Furthermore the experience of presenting the research at regional and national conferences helped students and gave them an identity as a researcher. Reading research papers was also a challenging experience. Several students commented on the difficulty of reading through an intensive research paper and verifying the known results. Finally, it also helped motivate several participants to pursue graduate studies in their field. Two of the participants went on to go to graduate school in a math-related field. Two others are considering attending graduate school when they graduate or after they spend some time in the workforce.

1.4 Student Feedback

The feedback on the course was overwhelmingly positive. Several students continued to work on their projects throughout the following semesters and some of their results were submitted to an undergraduate research journal. Below are some of the comments from students in the course.

- Working on this research project showed me what the higher levels of academia would be like. I was challenged by having to create and evaluate new techniques based on what I had learned in previous courses. This experience ultimately led me to pursuing a graduate degree in mathematics.
- When I joined the Modeling DNA Self-Assembly course I was still at the beginning of my math career. I had never worked on math outside of the classroom scope and had no idea what a proof looked like or how to write a mathematical paper. This course helped prepare me for higher level math courses, as well as gave me the opportunity to experience presenting at math conferences, such as JMM. Thanks to this experience, I was accepted into an REU the following summer that I felt better prepared for since I had already gotten a feel for the mathematical research process.
- The structure was done nicely. We learned about the subject and then we were set loose to do our individual work. Still being required to put so many hours in per week and also being able to get help anytime in class is what kept productivity up.
- Graph Theoretical Design Strategies For Modeling Self-Assembling DNA was one of my most interesting courses that I wish could have invested more time in because I enjoyed the feeling of exploration figuring something out that nobody else really had. All of my undergraduates course were learning how things are already understood and demonstrating that I understood it too, so it was very different to be introduced to a topic and then set free to see what I could map out in the uncharted territory along with everyone else in the research group. On top of that, presenting

our research was very important. Not only did I love going to the 2019 JMM for the sake of travel, I once heard a line about how something isn't truly discovered in science until it has been shared with others. Writing the research paper, making the poster, and presenting was the full experience of doing research. I want to stress that the group aspect was also very important because research is ultimately collaborative.

- Honestly it's just very exciting to explore something not many have looked at before. To do research means my perspective will help cultivate some new idea out of the newly searched concept, even if it's wrong, knowing you're contributing even in a small way makes the experience very motivating and exciting.


2 Tips for running such a course

Below I provide some general tips for running a course like this.


- Ellis Monaghan and Pangborn's *An Example of Practical Organization for Undergraduate Research Experiences* was a very helpful resource for designing the structure and timeline for this class [10].
- The design of this course could be used for a senior research class, but allowing students to have this type of research opportunity earlier in their career, as mentioned in [1], is very valuable. The benefit of having upper classmen in the class is added maturity and possible prerequisite knowledge. One possible design for this course could be to have a CURE like this with a different research topic each year and then have them work on the write-up in a follow-up course. The first semester could be a CURE with an informal write-up with a seminar/writing course the following semester in which the student writes a formal research paper.
- This structure for a course could be used for a variety of research areas, but would be most successful if conducted using a research topic the instructor is very familiar with. Another option could be to have a faculty consultant who could provide additional feedback when necessary.
- Allow for the flexibility of changing research groups. Some group dynamics may not be amenable for all participants so having a plan to allow for changing groups or a chance for students to provide feedback on which group they want to be a part of would be helpful.
- Since students will be choosing their own research questions, the instructor's role may be to give advice on whether the research question can be completed in the time allowed for the course.
- Additionally, since students are working on different research questions, the progress made by the different cohorts may vary. It is important for the instructor to recognize this and encourage all groups and celebrate any progress made. For example, in this class, I had one group who picked a much more challenging family of graphs and so they only worked in the most relaxed of the laboratory conditions.
- Since the research will be done during the semester, the progress expectations need to be adjusted when compared with a summer research internship.
- If you want students to work in groups and present, I suggest making it a requirement for the course and part of the grade.
- Just like when you are mentoring a summer research project, it is helpful to provide practice problems and exercises for students to work on as they learn the background and current known results.
- Students may be able to participate in your research without taking all the prerequisite courses. It may be helpful to think of the bare minimum knowledge required in order for a student to engage in research and create mini-modules for them to go through in order to prepare them for the research project.

3 Conclusion


Overall designing and teaching this course was a great experience. It was incredibly rewarding to watch the participants grow in their mathematical abilities and reasoning. It was also great to watch students form a comfortable research environment. As someone who enjoys working with students on research, this type of course allowed me to engage more students in the research process. It also provided me a good non-monetary “compensation” for the students since they were able to earn course credit for their efforts. Having the students present their results at various mathematics conferences following this course was a great way to finish and celebrate their results.




Modeling Crossed Prism and Petersen Graph Families in Self-Assembling DNA Using Graph Theory and Linear Algebra




Background
In this research, we are exploring the graph theoretical formalism of nanotube construction and related design strategy problems.



We will order to the n -mered molecules as tiles, and to a collection of tiles as a pot



A pot realizes a graph G if the tiles in said pot constructs the same structure as G .



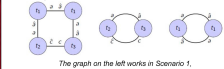
Lata generally prefer complete complexes, where every bond edge is matched with a complement. The complex on the left is complete, the complex on the right is incomplete.

Fundamental Questions
The fundamental questions for this research include:
Given a target graph, G .

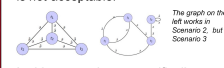
- What is the minimum number of tile types needed to realize the graph?
- What is the minimum number of bond types needed?
- What is the combinatorial structure of the molecules in a minimum set which realizes the target graph?

In answering these questions, we consider three different laboratory constraints.

- Scenario 1:** The incidental construction of graphs smaller than the target graph is acceptable.
- Scenario 2:** The incidental construction of a graph smaller than the target graph is *not* acceptable, but a graph of the same size that is not isomorphic to the target graph is acceptable.
- Scenario 3:** The incidental construction of any graph other than the target graph and its isomorphisms is *not* acceptable.



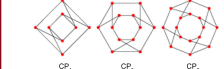
The graph on the left works in Scenario 1, but not Scenario 2.



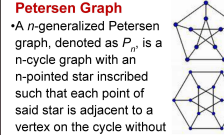
The graph on the left works in Scenario 2, but not Scenario 3.

In this research, we specifically focused on cross-prism and Petersen graphs in **Scenario 1 and 2**, using the construction matrix methodology and computational methods for generating pots acceptable for **Scenarios 1 and 2**.

Cross-Prism Graph
A n -cross prism graph for a positive even n , denoted as CP_n , is a graph obtained by taking two disjoint cycle graphs, C_n , and adding edges (v_i, v_{2i+1}) and (v_{i+1}, v_{2i}) for $k = 1, 3, \dots, (n-1)$. Examples of cross-prism graphs are shown below.



Petersen Graph
•A n -generalized Petersen graph, denoted as P_n , is a n -cycle graph with an n -pointed star inscribed such that each point of said star is adjacent to a vertex on the cycle without crossing edges



Construction Matrix
The construction matrix can be used to determine if a pot has the minimum number of tiles needed to create a graph with n -vertices. The matrix's solution is the proportion of each tile in the graph. This is used in **Scenario 2**.

$$\begin{bmatrix} 2 & 0 & -2 & 0 & 0 \\ 1 & 0 & 0 & -3 & 0 \\ 0 & 3 & -1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{bmatrix} \text{ rref} \rightarrow \begin{bmatrix} 1 & 0 & 0 & 0 & 3/8 \\ 0 & 1 & 0 & 0 & 3/8 \\ 0 & 0 & 1 & 0 & 3/8 \\ 0 & 0 & 0 & 1 & 1/8 \end{bmatrix}$$

Above is an example of the method applied to a pot that constructs a K_5 graph

Results
Scenario 1
K-Regular Graphs, Odd Vertices

- $B_1(CP_n) = 1$
- $T_1(CP_n) = 2$
- $B_1(P_n) = 1$
- $T_1(P_n) = 2$

$P = \{a^2\bar{a}, \bar{a}^2a\}$

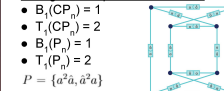
Scenario 2
Cross-Prism Graph

- $B_2(CP_n) = n/4$
- $T_2(CP_n) = n/4 + 1$

Ex. Hexagonal Graph $n = 12$

- $B_2(CP_6) = 3$
- $T_2(CP_6) = 4$

$P = \{a^2\bar{a}, \bar{a}^2b, \bar{a}bc, \bar{a}c^2\}$



Scenario 2
Petersen Family Graph
Five-Point Graph

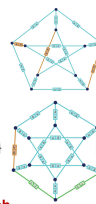
- $B_2(P_5) = 2$
- $T_2(CP_5) = 3$

$P = \{a^3, \bar{a}^2b, \bar{a}^2\bar{b}\}$

Six-Point Graph

- $B_2(P_6) = 3$
- $T_2(CP_6) = 4$

$P = \{a^2\bar{a}, \bar{a}^2b, \bar{a}bc, \bar{a}c^2\}$



Future Research.

- The following pots could potentially realize a graph of size 10 based on results from construction matrices: $\{\{a^2, b\}, \{a, b^2\}, \{a, b^3\}\}, \{\{a^2, b\}, \{a^2, b\}, \{a, b^2\}\}$
- An upper bound for tiles and bond types was found for cross-prism and Petersen graphs, as mentioned in the results section, but a lower bound is yet to be found for Scenario 2
- Graphs larger than size 16 for cross-prism graphs and size 12 for Petersen graphs have yet to be tiled

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Figure 1: Sample end of semester poster

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References

- [1] Lisa Corwin Auchincloss, Sandra L Laursen, Janet L Branchaw, Kevin Eagan, Mark Graham, David I Hanauer, Gwendolyn Lawrie, Colleen M McLinn, Nancy Pelaez, Susan Rowland, et al. Assessment of course-based undergraduate research experiences: a meeting report, 2014.
- [2] Gita Bangera and Sara E Brownell. Course-based undergraduate research experiences can make scientific research more inclusive. *CBELife Sciences Education*, 13(4):602–606, 2014.
- [3] Amy EL Barlow and Merna Villarejo. Making a difference for minorities: Evaluation of an educational enrichment program. *Journal of research in science teaching*, 41(9):861–881, 2004.
- [4] Junghuei Chen and Nadrian C Seeman. Synthesis from dna of a molecule with the connectivity of a cube. *Nature*, 350(6319):631, 1991.
- [5] Lisa A Corwin, Mark J Graham, and Erin L Dolan. Modeling course-based undergraduate research experiences: an agenda for future research and evaluation. *CBELife Sciences Education*, 14(1):es1, 2015.
- [6] Erin L Dolan. Course-based undergraduate research experiences: Current knowledge and future directions. *Paper commissioned for the Committee on Strengthening Research Experiences for Undergraduate STEM Students Board on Science Education, Division of Behavioral and Social Sciences and Education Board on Life Sciences, Division of Earth and Life Studies*, 2016.
- [7] Erin L Dolan. Undergraduate research as curriculum. *Biochemistry and Molecular Biology Education*, 45(4):293–298, 2017.
- [8] M Kevin Eagan Jr, Sylvia Hurtado, Mitchell J Chang, Gina A Garcia, Felisha A Herrera, and Juan C Garibay. Making a difference in science education: the impact of undergraduate research programs. *American educational research journal*, 50(4):683–713, 2013.
- [9] J Ellis-Monaghan and G Pangborn. Using dna self-assembly design strategies to motivate graph theory concepts. *Mathematical Modelling of Natural Phenomena*, 6(6):96–107, 2011.
- [10] Joanna Ellis-Monaghan and Greta Pangborn. An example of practical organization for undergraduate research experiences. *PRIMUS*, 23(9):805–814, 2013.
- [11] Joanna Ellis-Monaghan, Greta Pangborn, Laura Beaudin, David Miller, Nick Bruno, and Akie Hashimoto. Minimal tile and bond-edge types for self-assembling dna graphs. In *Discrete and Topological Models in Molecular Biology*, pages 241–270. Springer, 2014.
- [12] Sandra R Gregerman, Jennifer S Lerner, William Von Hippel, John Jonides, and Biren A Nagda. Undergraduate student-faculty research partnerships affect student retention. *The Review of Higher Education*, 22(1):55–72, 1998.
- [13] Yu He, Tao Ye, Min Su, Chuan Zhang, Alexander E Ribbe, Wen Jiang, and Chengde Mao. Hierarchical self-assembly of dna into symmetric supramolecular polyhedra. *Nature*, 452(7184):198, 2008.
- [14] Ryosuke Inuma, Yonggang Ke, Ralf Jungmann, Thomas Schlichthaerle, Johannes B Woehrstein, and Peng Yin. Polyhedra self-assembled from dna tripods and characterized with 3d dna-paint. *science*, page 1250944, 2014.
- [15] Nataša Jonoska, Phiset Sa-Ardyen, and Nadrian C Seeman. Computation by self-assembly of dna graphs. *Genetic Programming and Evolvable Machines*, 4(2):123–137, 2003.
- [16] Neville R Kallenbach, Rong-Ine Ma, and Nadrian C Seeman. An immobile nucleic acid junction constructed from oligonucleotides. *Nature*, 305(5937):829, 1983.
- [17] Daniel S Kissel. Integrating faculty research into the undergraduate chemistry curriculum: A cure using porous composite materials for water remediation. In *Environmental Research Literacy: Classroom, Laboratory, and Beyond*, pages 79–104. ACS Publications, 2020.

- [18] Anton Kuzyk, Robert Schreiber, Zhiyuan Fan, Günther Pardatscher, Eva-Maria Roller, Alexander Högele, Friedrich C Simmel, Alexander O Govorov, and Tim Liedl. Dna-based self-assembly of chiral plasmonic nanostructures with tailored optical response. *Nature*, 483(7389):311, 2012.
- [19] Thom H LaBean and Hanying Li. Constructing novel materials with dna. *Nano today*, 2(2):26–35, 2007.
- [20] Sandra Laursen, Anne-Barrie Hunter, Elaine Seymour, Heather Thiry, and Ginger Melton. *Undergraduate research in the sciences: Engaging students in real science*. John Wiley & Sons, 2010.
- [21] Jiang Li, Chunhai Fan, Hao Pei, Jiye Shi, and Qing Huang. Smart drug delivery nanocarriers with self-assembled dna nanostructures. *Advanced materials*, 25(32):4386–4396, 2013.
- [22] Di Liu, Gang Chen, Usman Akhter, Timothy M Cronin, and Yossi Weizmann. Creating complex molecular topologies by configuring dna four-way junctions. *Nature chemistry*, 8(10):907, 2016.
- [23] Di Liu, Yaming Shao, Gang Chen, Yuk-Ching Tse-Dinh, Joseph A Piccirilli, and Yossi Weizmann. Synthesizing topological structures containing rna. *Nature communications*, 8:14936, 2017.
- [24] David Lopatto. Undergraduate research experiences support science career decisions and active learning. *CBELife Sciences Education*, 6(4):297–306, 2007.
- [25] Catherine M Mader, Christopher W Beck, Wendy H Grillo, Gail P Hollowell, Bettye S Hennington, Nancy L Staub, Veronique A Delesalle, Denise Lello, Robert B Merritt, Gerald D Griffin, et al. Multi-institutional, multidisciplinary study of the impact of course-based research experiences. *Journal of microbiology & biology education*, 18(2), 2017.
- [26] John A Pelesko. *Self assembly: the science of things that put themselves together*. Chapman and Hall/CRC, 2007.
- [27] Susan H Russell, Mary P Hancock, and James McCullough. Benefits of undergraduate research experiences. *Science*, 316(5824):548–549, 2007.
- [28] Phiset Sa-Ardyen, Nataša Jonoska, and Nadrian C Seeman. Self-assembling dna graphs. In *International Workshop on DNA-Based Computers*, pages 1–9. Springer, 2002.
- [29] Nadrian C Seeman. An overview of structural dna nanotechnology. *Molecular biotechnology*, 37(3):246, 2007.
- [30] Nadrian C Seeman. *Structural DNA nanotechnology*. Cambridge University Press, 2016.
- [31] Casey Shapiro, Jordan Moberg-Parker, Shannon Toma, Carlos Ayon, Hilary Zimmerman, Elizabeth A Roth-Johnson, Stephen P Hancock, Marc Levis-Fitzgerald, and Erin R Sanders. Comparing the impact of course-based and apprentice-based research experiences in a life science laboratory curriculum. *Journal of microbiology & biology education*, 16(2):186, 2015.
- [32] Rachelle M Spell, Judith A Guinan, Kristen R Miller, and Christopher W Beck. Redefining authentic research experiences in introductory biology laboratories and barriers to their implementation. *CBELife Sciences Education*, 13(1):102–110, 2014.
- [33] Wei Sun, Etienne Boulais, Yera Hakobyan, Wei Li Wang, Amy Guan, Mark Bathe, and Peng Yin. Casting inorganic structures with dna molds. *Science*, page 1258361, 2014.
- [34] Hui Wang, Russell J Di Gate, and Nadrian C Seeman. An rna topoisomerase. *Proceedings of the National Academy of Sciences*, 93(18):9477–9482, 1996.
- [35] Yinli Wang, John E Mueller, Börries Kemper, and Nadrian C Seeman. Assembly and characterization of five-arm and six-arm dna branched junctions. *Biochemistry*, 30(23):5667–5674, 1991.
- [36] Erik Winfree. *Algorithmic self-assembly of DNA*. PhD thesis, California Institute of Technology, 1998.

- [37] Erik Winfree, Furong Liu, Lisa A Wenzler, and Nadrian C Seeman. Design and self-assembly of two-dimensional dna crystals. *Nature*, 394(6693):539, 1998.
- [38] Gang Wu, Natasha Jonoska, and Nadrian C Seeman. Construction of a dna nano-object directly demonstrates computation. *Biosystems*, 98(2):80–84, 2009.
- [39] Zeyu Xiao, Changwei Ji, Jinjun Shi, Eric M Pridgen, Jillian Frieder, Jun Wu, and Omid C Farokhzad. Dna self-assembly of targeted near-infrared-responsive gold nanoparticles for cancer thermo-chemotherapy. *Angewandte Chemie International Edition*, 51(47):11853–11857, 2012.
- [40] Hao Yan, Sung Ha Park, Gleb Finkelstein, John H Reif, and Thomas H LaBean. Dna-templated self-assembly of protein arrays and highly conductive nanowires. *science*, 301(5641):1882–1884, 2003.
- [41] Yuwen Zhang and Nadrian C Seeman. Construction of a dna-truncated octahedron. *Journal of the American Chemical Society*, 116(5):1661–1669, 1994.
- [42] Jianping Zheng, Jens J Birktoft, Yi Chen, Tong Wang, Ruojie Sha, Pamela E Constantinou, Stephan L Ginell, Chengde Mao, and Nadrian C Seeman. From molecular to macroscopic via the rational design of a self-assembled 3d dna crystal. *Nature*, 461(7260):74, 2009.

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A Poster Rubric

Category	4	3	2	1
Organization	Student presents information in logical, interesting sequence which audience can follow. Student has a clean and clear presentation!	Student presents information in logical sequence which audience can follow. Most of the presentation is clear and clean.	Audience has difficulty following presentation because student jumps around or the presentation is a bit disorganized.	Audience cannot understand presentation because there is no sequence of information or because presentation is very disorganized.
Graphics	Student's graphics explain and reinforce screen text and presentation with references.	Student's graphics relate to text and presentation.	Student occasionally uses graphics that rarely support text and presentation.	Student uses superfluous graphics or no graphics.
Quality of Information	Information clearly relates to the main topic. It includes several supporting details and/or examples.	Information clearly relates to the main topic. At least 1-2 supporting details and/or examples are provided.	Information clearly relates to the main topic. No details and/or examples are given.	Student is unable to accurately answer questions posed by classmates about the topic.
Sources/References	All sources (information and graphics) are accurately documented in the desired format.	All sources (information and graphics) are accurately documented, but a few are not in the desired format.	All sources (information and graphics) are accurately documented, but many are not in the desired format.	Some sources are not accurately documented.
Mechanics	Presentation has no misspellings or grammatical errors.	Presentation has no more than 2 misspellings and or grammatical errors.	Presentation has 3 misspellings and or grammatical errors.	Student's presentation has 4 or more spelling errors and/or grammatical errors
Mathematics Presentation	The mathematics in the paper are presented in a correct, logical, and easy to follow manner.	The mathematics in the paper are correctly presented, but is at times difficult to follow or does not always flow in a logical manner.	The mathematics in the paper are correctly presented, but is sometimes difficult to follow or does not always flow in a logical manner.	The mathematics in the paper are at times incorrect and often is presented in a way that is difficult to follow.

B Presentation Rubric

Category	4	3	2	1
Speaking	Speaks clearly and distinctly all (100-95%) the time, and mispronounces no words.	Speaks clearly and distinctly all (100-95%) the time, but mispronounces one word.	Speaks clearly and distinctly most (94-85%) of the time. Mispronounces no more than one word.	Often mumbles or can not be understood OR mispronounces more than one word.
Enthusiasm	Facial expressions and body language generate a strong interest and enthusiasm about the topic in others.	Facial expressions and body language sometimes generate a strong interest and enthusiasm about the topic in others.	Facial expressions and body language are used to try to generate enthusiasm, but seem somewhat faked.	Very little use of facial expressions or body language. Did not generate much interest in topic being presented.
Vocabulary	Uses vocabulary appropriate for the audience. Extends audience vocabulary by defining words that might be new to most of the audience.	Uses vocabulary appropriate for the audience. Includes 1-2 words that might be new to most of the audience, but does not define them.	Uses vocabulary appropriate for the audience. Does not include any vocabulary that might be new to the audience.	Uses several (5 or more) words or phrases that are not understood by the audience.
Preparedness	Student is completely prepared and has obviously rehearsed.	Student seems pretty prepared but might have needed a couple more rehearsals.	The student is somewhat prepared, but it is clear that rehearsal was lacking.	Student does not seem at all prepared to present.
Content	Shows a full understanding of the topic.	Shows a good understanding of the topic.	Shows a good understanding of parts of the topic.	Does not seem to understand the topic very well.
Comprehension	Student is able to accurately answer almost all questions posed by classmates about the topic.	Student is able to accurately answer most questions posed by classmates about the topic.	Student is able to accurately answer a few questions posed by classmates about the topic.	One or more topics were not addressed or there were not enough topics for the paper.
Listens to Other Presentations	Listens intently. Does not make distracting noises or movements.	Listens intently but has one distracting noise or movement	Sometimes does not appear to be listening but is not distracting.	Sometimes does not appear to be listening and has distracting noises or movements.
Time-Limit	Presentation is within 2 minutes of time limit.	Presentation is 3 minutes long or short.	Presentation is 4 minutes short or long	Presentation is over 5 minutes short or long

C Paper Rubric

Category	4	3	2	1
Organization	Information is very organized with well-constructed paragraphs, subheadings, and labels.	Information is organized with well-constructed paragraphs.	Information is organized, but paragraphs are not well-constructed.	The information appears to be disorganized.
Amount of Information	All topics are addressed and all questions answered with sufficient details.	All topics are addressed and most questions answered with sufficient details.	All topics are addressed, and most questions answered, but lacks sufficient details.	One or more topics were not addressed or there were not enough topics for the paper.
Quality of Information	Information clearly relates to the main topic. It includes several supporting details and/or examples.	Information clearly relates to the main topic. At least 1-2 supporting details and/or examples are provided.	Information clearly relates to the main topic. No details and/or examples are given.	Information has little or nothing to do with the main topic.
Sources	All sources (information and graphics) are accurately documented in the desired format.	All sources (information and graphics) are accurately documented, but a few are not in the desired format.	All sources (information and graphics) are accurately documented, but many are not in the desired format.	Some sources are not accurately documented.
Number of Sources	There are 5 quality sources referenced.	There are 4 quality sources referenced.	There are 3 quality sources referenced.	There are 0-2 quality sources referenced.
Mechanics	No grammatical, spelling or punctuation errors.	Almost no grammatical, spelling or punctuation errors.	A few grammatical spelling, or punctuation errors.	Many grammatical, spelling, or punctuation errors.
Mathematics Presentation	The mathematics in the paper are presented in a correct, logical, and easy to follow manner.	The mathematics in the paper are correctly presented, but is at times difficult to follow or does not always flow in a logical manner.	The mathematics in the paper are correctly presented, but is sometimes difficult to follow or does not always flow in a logical manner.	The mathematics in the paper are at times incorrect and often is presented in a way that is difficult to follow.
Mathematics	There is significant and sophisticated, college-level Mathematics present in this paper.	There is significant but not sophisticated, college-level Mathematics present in this paper.	There is college-level Mathematics present in this paper, but not a significant amount.	There is neither significant nor sophisticated, college-level Mathematics present in this paper.
Research	The exploration in the topic goes beyond what is already known. Student exceeds expectations in the project.	The exploration stays within the known realm of their topic, but is thoroughly examined. Student meets the expectations for his/her project.	The exploration stays within the known realm of their topic and is not thoroughly examined. Student is progressing with his/her project, but needs more work.	The exploration stays within the known realm of their topic, but only the surface is examined. Student is not there yet with his/her project.
Quality of writing	Writing is sophisticated and at the college level. The length of the paper is appropriate and there is good flow to the paper.	Writing is sophisticated and at the college level, but sometimes does not flow well. The length of the paper is appropriate.	Writing is often not at the college level and lacks sophistication or the paper is not at the appropriate length.	Writing is not at the college level and does not meet the required length.

D Detailed Course Timeline

Week:	Task
1	Introduction to research topic and notation: Students will read <i>Using DNA self-assembly design strategies to motivate graph theory concepts</i> pages 96-101 for next class.
2	Scenario 1 Techniques: Students will begin reading <i>Minimal tile and bond-edge types for self-assembling DNA graphs</i> pages 239-245, and Scenario 1 section (page 247-249) for next class.
3	Scenario 2 Techniques and Construction Matrix: Students will continue reading <i>Minimal tile and bond-edge types for self-assembling DNA graphs</i> pages 245-247 and Scenario 2 section pages 250-253 for next class.
4	Scenario 2 Techniques Continued: Students should have finished reading <i>Minimal tile and bond-edge types for self-assembling DNA graphs</i> pages 254-256, 260-264 for next class.
5	Scenario 3 Techniques: Students should have finished <i>Minimal tile and bond-edge types for self-assembling DNA graphs</i> .
6-8	Toy Research Problems: Students will work to create optimal pots on toy research problems whose results are known to the instructor.
9	Choose Research Question: Research Cohort groups will pick and rank 3 graphs which have not been research to start exploring.
10-15	Research: Students will explore their research questions, present their weekly progress and questions in class, and begin writing up their results.
16	Presentation and Write-Up : Group presentations of final results and progress. The final Write-up and Poster are due.

Table 2: Detailed Course Timeline