Active Pathways: Using Active Tangibles and Interactive Tabletops for Collaborative Modeling in Systems Biology

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ABSTRACT

We present *Active Pathways*, an active tangible and tabletop system that aims to support collaborative discovery and learning in biochemical modeling. Our work extends ideas from embodied cognition that suggest that interactive systems that support model building by coupling actions made with the motor system to the dynamic properties of external and internal models can enhance the potential for insight and discoveries. We describe the motivation for our work and the design and development of our system. We also present the results of a user study with pairs of novice modelers, which suggest that our system is not only easy to use and learn but also successful at facilitating an understanding of complex systems and supporting collaboration.

Author Keywords

Tangibles; tabletop; computational science; systems biology; modeling; collaboration.

ACM Classification Keywords

H.5.2 Information Interfaces and Presentation (*e.g.*, HCI): User Interfaces—Input devices and strategies, interaction styles, user-centered design; I.6.7 Simulation and Modeling: Simulation Support Systems—Environments.

INTRODUCTION

Since age old times we have incessantly tried to unveil the inner workings of nature. With the development of computational techniques, we have slowly moved from just offloading basic computations to exploring new avenues of discovery using computers. The complexity of these computational problems demands the use of complex tools, which are used by novice students and researchers as well as

Permission to make digital or hard copies of all or part of this work for personal or classroom use is granted without fee provided that copies are not made or distributed for profit or commercial advantage and that copies bear this notice and the full citation on the first page. Copyrights for components of this work owned by others than ACM must be honored. Abstracting with credit is permitted. To copy otherwise, or republish, to post on servers or to redistribute to lists, requires prior specific permission and/or a fee. Request permissions from Permissions@@@@@m.org. *ISS '16*, November 06-09, 2016, Niagara Falls, ON, Canada @ 2016 ACM. ISBN 978-1-4503-4248-3/16/11...\$15.00 DOI: http://dx.doi.org/10.1145/2992154.2992176 experts. Yet these tools often fail to balance the complexity required to support discovery and the simplicity required to enable learning. Furthermore, few of them provide support for collaboration among students and researchers from various backgrounds. The problem thus, is not merely how to facilitate computation, but how to utilize these tools to enhance our abilities to discover and learn collaboratively.

We propose to harness knowledge from the cognitive sciences to solve the above problem. Theories in embodied cognition underline the importance the physical world and the body play in our cognitive processes [20, 21, 32]. In particular, the common coding theoretical framework can be used to understand this phenomenon [9]. This framework posits that our imagination and perception of movements are linked with our actions (motor system). Building upon this theory, researchers have shown that the act of building computational models, particularly models with dynamic visualizations, can support conceptual understanding and lead to new discoveries [8, 9]. The theory argues that movement acts as a common language between our small-scale internal models (that we form to understand the world) and external models. Hence, manipulating a physical model can help evolve our mental models, leading to comprehension and discovery. One of the most prominent examples of an external model that led to a breakthrough discovery is the DNA model. Watson and Crick created this 3D physical model to help "fit" the experimental data, which helped them solve the mystery of DNA. In parallel, a growing body of research in the field of Tangible and Embodied Interaction (TEI) tries to bridge the gap between the physical and the digital worlds [37, 40] and goes hand in hand with theories of embodied cognition. We believe that bringing together knowledge from embodied cognition with TEI research and design can help us develop tools for supporting learning and discovery in areas of computational scientific practice.

In this paper, we present *Active Pathways*, a tangible system that facilitates collaborative discovery and learning in the modeling of biochemical processes by novice researchers and students. It brings together computational modeling, embodied cognition, and TEI to enable novice students and expert researchers to build and manipulate external models that lend spatial and dynamic properties to abstract scientific problems.

In the following section, we discuss related work. Next, we discuss the cognitive foundations of our work, as well as our overarching research question and design goals. We then describe the design and implementation of the proposed *Active Pathways* system and present results of a user study conducted with novice modelers. We then conclude with a discussion of future work.

RELATED WORK

Researchers have investigated how learning abilities can be enhanced through haptic channels. For instance, Brooks et al. [6] developed Project GROPE to display 6-D force fields of interacting protein molecules augmented with haptic interaction. Their work revealed that the combination of visual and haptic displays improves users' perception and understanding of the force fields. Similarly, Chan and Black [7] conducted a user study to understand how students use cognitive processing to understand structure, purposes, and functional relations among system entities. They taught Newtonian mechanics to a group of students using different methods, including sound, touch, and visuals. Results of the study showed that using haptic channels enhanced students' learning capabilities. None of these projects, however, focus on collaboration or model construction.

There have been several attempts to provide users with flexible Graphical User Interface (GUI) based tools for the visualization of biological pathways. For example, a Webbased system called VisANT [16] provides a framework for visualizing and analyzing different types of networks of biological interactions and associations. Another system called Cytoscape [31] supports the visualization and integration of molecular interaction networks and biological pathways. Neither system allows model construction, but manipulation of the data through using various filters. They also do not facilitate learning or collaborative exploration.

Many projects have also focused on tangible interfaces to support scientific practices. Mackay et al. [19], for example, developed augmented laboratory notebooks, termed *a*-books, for linking paper, physical artifacts such as lab specimens, and online data. While both novices and experts can benefit from a-books, it does not allow complex model construction. It also does not support collaboration directly, but allows users to share notes with each other. In a different project, Schkolne et al. [29] used a number of tangible input devices along with a stereoscopic display for DNA molecule design. The system, however, is designed for experts, and therefore does not facilitate learning. It is also unclear if the system enables collaboration among the users or allows model construction. Augmented Chemistry [13, 14] is an augmented reality based tool that employs tangibles to help teach organic chemistry. It combines the strengths of graphical and tangible user interfaces to provide an involved learning experience to students by helping them construct and visualize molecules in 3D. However, the system does not support a collaborative environment.

Many researchers have designed scientific support systems based on interactive tabletops. For example, the eLabBench [35] is a digital tabletop-based laboratory bench that supports molecular biologists in both capturing experimental work and working with standard tools such as spreadsheets using a combination of stylus, mouse and keyboard, and tangibles. This system supports learning and collaboration among the users, but does not support modeling. It does, however, allow users to apply various statistical tests on a dataset. Other examples include the G-nome Surfer [30], a multi-touch tabletop system for collaborative exploration of genomic databases; SynFlo [39], a tangible tabletop for introducing synthetic biology concepts to non-experts, and Eugenie [15], a tangible tabletop interface for helping synthetic biologists to explore of large datasets through the construction of complex queries. A more recent tabletop and active tangiblebased system called Sparse Tangibles [1] supports crossplatform collaborative gene network exploration using a Web interface. It enables query construction and filtering the data both on- and off-the-table using the active tangibles. None of these techniques provide the support for model construction.

Technique	Interaction Modalities	Learning	Collaboration	Modeling
Project GROPE ^[6]	Visual and haptic displays	Yes	Unclear	No
Direct-manipulation animations ^[7]	Interactive animations with auditory, visual, haptic feedback	Yes	No	No
VisANT ^[16]	Conventional desktop interactions on a Web browser	No	No	Partially
Cytoscape ^[31]	Conventional desktop interactions	No	No	Partially
Augmented Chemistry ^[13, 14]	Desktop and tangible interactions, and augmented reality	Yes	No	Yes
<i>a</i> -book ^[19]	Augmented notebooks as active tangibles and stylus	Yes	Partially	No
Immersive interface for DNA ^[29]	Various tangible 3D input devices	No	Unclear	Unclear
eLabBench ^[35]	Stylus, mouse/keyboard, tangibles, and physical buttons	Yes	Yes	Partially
The G-nome Surfer ^[30]	Multi-touch tabletop	Yes	Yes	No
Systems Dynamics ^[27]	Tabletop and tangibles, and external display	Unclear	Yes	Unclear
SynFlo ^[39]	Tabletop and active tangibles	Yes	Unclear	No
Eugenie ^[15]	Tabletop and active tangibles	Yes	Yes	No
Sparse Tangibles ^[1]	Tabletop and active tangibles	Yes	Yes	No
Kinesthetic Pathways ^[38]	Tabletop and active tangibles	Yes	Yes	No
Active Pathways	Tabletop and active tangibles	Yes	Yes	Yes

Table 1. An overview of the most relevant data visualization and manipulation projects.

Systems Dynamics [27] is a tangible-tabletop system for studying complex feedback systems in fields such as business and social sciences. It allows users to change various parameters of computer models to simulate the outcome. However, it is unclear how the system can aid the process of learning.

Arias et al. [1] developed a research platform that explores a socio-technical environment to bring together people from different backgrounds to frame and solve complex problems. They employ tabletop computing and tangibles to combine action and reflection spaces, and to create "boundary objects" that help people communicate and build a common ground. The research, spanning over two decades, explains how such an environment can support design, creativity and learning. While their explorations are more geared towards open ended problems where human opinions are the parameters, we employ these methods in mathematical "what-if" situations.

Kinesthetic Pathways [38] is a tangible tabletop system for visualizing biochemical reaction networks. It was developed as a result of a two-year ethnographic study conducted in two systems biology research labs. The studied labs build Ordinary Differential Equation (ODE) models that represent how the concentrations of different metabolites change over time for a particular pathway. Without any visualization tools specific to their practice, they have to work with bare chemical and ODE equations. Most of them resort to drawing sketches on paper to augment their mental model of the pathway. Kinesthetic Pathways provided a tabletop visualization of a built-in chemical network to facilitate exploration of parameters to fit model data using a limited set of passive tangibles (*e.g.*, [22]). It did not support model construction.



Figure 1. Users collaboratively building a biochemical pathway model using the *Active Pathways* system.

MOTIVATION

Motivated by the idea that building computational models can support conceptual understanding as discussed above [8, 9], our research aims to extend the tabletop visualization work of Kinesthetic Pathways in order to support collaborative model construction for graduate students and novice researchers [38]. The ethnographic research conducted in systems biology labs outlined the practices and problems of novice graduate students from various backgrounds, including engineering, mathematics, and biology, as they build biochemical pathways to understand different natural phenomena [38]. Often these students also take modeling courses, many of which have adopted problem-based learning approaches that are grounded in real research problems. This type of classroom setting provides an interesting context for our research as students not only try to gain new knowledge, but also try to apply it to solve real problems. Additionally, these classes bring together students from varying backgrounds with differing levels of biomedical engineering or modeling expertise to work on complex scientific problems.

For modeling, the students receive experimental data, often in tables or spreadsheets, which can be used to develop the pathway and validate the model. The modeling phase is divided into three main phases, namely *building*, *fitting* and *perturbation*. These models usually deal with metabolic processes and are often sketched on paper as a network, *i.e.*, nodes connected by arrows, where the nodes represent molecules and the arrows represent the reactions between them. Ordinary Differential Equations (ODEs) are derived from the pathway to describe the change of concentration of metabolites over time and coded in a numerical computation language such as MATLAB. The parameters (*i.e.*, kinetic order and rate constant) are then iteratively estimated and simulations are run to check the "fit" of the model with the experimental data [9, 38].

It is evident from the description above that the elements of the modeling process are scattered across different representations, *i.e.*, numerical, graphical, computational, etc., and it is up to the student to bring all of these together and create a coherent mental model. Moreover, with students of varying backgrounds coming together to solve these problems, there is a need for a platform to share and gain knowledge. Our research operates within this problem domain, and seeks to apply TEI approaches to facilitate collaboration, learning, and discovery in systems biology by novice students and researchers. The following questions encompass our broad research goals.

- What functionality is required for supporting collaborative modeling of biochemical pathway in terms of model construction, data fitting/testing, validation, and collaborative tasks?
- What combinations of control and representation effectively capture and support the modeling process and allow researchers to work together in building, navigating, and testing the model?
- Can the designed system facilitate peer-level collaboration in and understanding of the modeling task for novice researchers from different backgrounds?

DESIGN OBJECTIVES

Transforming abstract data into physical form is challenging. In an investigation, Shaer et al. [30] listed several challenges of computational scientific practices and pointed towards possible TEI interventions with respect to understanding complex problems, visualizing biological data, enabling large collaboration, and supporting diverse audiences. During the design process, we looked into each of these in greater detail, in an attempt to introduce new interaction techniques that employ active tokens and interactive tabletops in a robust system for building and simulating biochemical models and fitting them to experimental datasets.

Similar to the existing Eugenie [15] and SyFlo [39] systems, we employ active tangibles in combination with an interactive tabletop, however we focus more on the building, as well as the visualization and exploration of dynamic models to support conceptual understanding. To achieve this, we extended the Kinesthetic Pathways project to provide a complete system for both model construction and fitting tasks that is based on the use of multiple active tangibles, programmable physical objects with integrated display, sensing, or actuation technologies, that can be used both off and on an interactive tabletop display surface. Kinesthetic Pathways focused on visualizing a dynamic system on an interactive tabletop with manipulation of parameters using passive tangible controls. In contrast, our aim was to provide users with a comprehensive system that would let users build, edit, manipulate, and simulate their model, as well as test its performance against imported real-world experimental results. The use of active tangibles is central to this goal, as they can serve not only as controls for manipulating visualized data, but can also physically become components of the dynamic system that have changing properties over time, such as molecules and reactions.

Our research team is interdisciplinary, and includes six human-computer interaction researchers, two biomedical engineers, and one cognitive scientist. The human-computer interaction researchers worked closely with the biomedical engineers, who provided domain expertise in systems biology in order to inform the design of the system's features and functionality. The cognitive scientist provided theoretical and empirical knowledge in embodied cognition to inform the design of tangible interactions and visualizations that could facilitate model construction and the development of shared conceptual models by novice and expert users. To fully utilize the interdisciplinary nature of our research team, we adopted an iterative design process where all design decisions were evaluated and analyzed by the team members, and interactions were redesigned until every member found them satisfactory. This process was particularly beneficial, as the experienced biomedical engineers on our team are can also be identified as potential users of the system. Primarily, we attempted to achieve the following goals while designing and testing/pre-evaluating the system.

- *Easy to learn and use:* As our system targets both novice and experienced biologists, and collaboration among them, our primary goal was to make input and interactions with the system intuitive and easy to learn.
- *Facilitates understanding of complex systems:* Through an external model that resonates with the complex analogical problem, we attempted to support the development of a mental model and a way to explore the problem space [23]. We also tried to strengthen the understanding of relationships among the different components by enabling users to see the effect on the system of changing any of its parts.

- *Facilitates discovery and problem solving:* Attempts were also made to assist the process of discovery by exploiting the connection between mental and physical models through tangible interactions. While changing the external model helps novices discover new states, visualizations help shape their imagination and nudge their internal models into new states [9]. This also supports problem solving by allowing users to gauge the accuracy of the solution and a gradual evolution of their internal models.
- *Facilitates collaboration:* With multiple tangibles as inputs and a tabletop system that can accommodate several people, we attempted to create a common space for users to work together. With the shared external model that can be perceived by several people at once, we potentially enable the creation of shared mental models that can help users work together in real time and reach a consensus.
- *The learning and discovery process is enjoyable:* Enjoyment is created not only through involvement of different senses (visual, touch), but also through satisfaction gained from a better understanding of the task at hand.

ACTIVE PATHWAYS

We designed and developed *Active Pathways*, an active tangible and tabletop application for collaborative modeling of biochemical reaction networks. The system seeks to help novice students and researchers in the processes of discovery and learning through building external models. It also explores the use of active tangibles as a means to provide flexible physical attributes to digital data.

Tangible Interactions

The interaction flow is defined around the two major tasks involved in modeling biochemical pathways. First, building the model, and second, fitting the model to experimental data by adjusting parameters. Multiple active tangibles, *i.e.*, Sifteo Cubes [33], are used both on and off the tabletop for both model construction and fitting tasks. Unlike tangible widgets [28], the cubes contain a hierarchy of menu options. We categorize the menu into two initial high-level options: "Model" for creating and editing components and "Data" for uploading experimental data, each having multiple options to choose from, illustrated in Figure 2 (a). Grouping the building and fitting functions creates an agile environment wherein users can quickly build, modify, and test their pathways iteratively without having to switch context. One can switch between the options inside each of these categories by tilting the cube. A selection is made by a single tap on the cube's screen. Shaking the cube takes one back to the parent category. A good analogy to understand the navigation is a tree structure. For the purpose of this prototype we use three Sifteo cubes. Among these, two can be used to build and fit, while one is reserved to play and stop the simulation.

The "Model" Category

This includes the options to create and modify molecules, enzymes, and reactions. Each of these components is a menu in itself and holds an array of related actions that can be performed on the respective components.



Figure 2. (a) The top-level menus on the active tangibles. (b) Model creation with active tangibles. Here, the user first selects the "Concentration" option from the menu on the tangible, places it on a molecule on the table, and then uses it like a dial to adjust the concentration parameter. S/he can also create a reaction by touching two molecules together and tilting to set the direction. (c) Data visualization in *Active Pathways*. The directional graph visualization represents the pathway, while the radial chart and scatterplot visualizations are for comparing model and experimental data.

For example, consider that two users, Sara and Rahul, want to create the pathway GLC \rightarrow G6P with enzyme Hexokinase acting on it. Towards that, Sara takes a cube, navigates to the desired molecule (GLC), places the cube on the table, and then taps. This creates the molecule GLC on the table that is now "bound" to that cube, *i.e.*, 'GLC' can now be controlled using that cube. She moves the cube to place the molecule at a desired position on the interactive table. She sets the initial concentration of the molecule by navigating and selecting "Concentration" and then rotating the cube like a VCR dial, *i.e.*, clockwise to increase and anti-clockwise to reduce, till it reflects the value she wants. See Figure 2 (b).

Rahul follows a similar process to create G6P. He then "unbinds" the cube from the molecule by shaking it so that he can create the Hexokinase enzyme. He later realizes that he forgot to initialize the concentration of G6P, so he puts the cube back on the molecule G6P and taps on "Molecule". This enables him to make the necessary changes. Sara and Rahul now bring together the two cubes bound to the molecules to create a reaction between them. See Figure 2 (b). The direction is set by the action of "pouring" the cube bound to the reactant (GLC) onto the one bound to the product (G6P). The rate constant of the reaction is set by binding a cube to it and then rotating the cube. Since the Hexokinase enzymes acts on the GLC \rightarrow G6P reaction, the enzyme is connected to the reaction by touching a cube bound to the enzyme with a cube bound to the reaction.

A scatter plot can be viewed for each molecule by tapping on the option "Graph" inside the molecule category. Once the pathway is set up, Sara and Rahul can run the simulation by hitting play and see how their model fits the experimental data in real time. The process can be repeated until a good fit is obtained.

The "Data" Category

We users with the ability to input the experimental data using a .CSV or .XLS file via a Web form. Once the file is uploaded, a Data cube can be used to transfer data points from the file onto the model on the table. Users can choose the files associated with the model and go inside the menu to look for the Root Mean Square (RMS) error related to each of them.

Visualizations

The visualizations of our system were inspired by the design and evaluation of Kinesthetic Pathways [38]. While different modelers have different ways of representing pathways, we borrow the directional graph, which is evidently a common representation used by most [38]. This depicts molecules and enzymes as nodes with reactions as arrows connecting them, illustrated in Figure 2 (a). We use fill color to differentiate between molecules and enzymes. We incorporate animations like "breathing" of molecules to make the pathway feel more organic. The name and concentration of the molecule are placed within the circle, whereas the rate constants are situated above a reaction arrow.

Keeping in mind the importance of graphs to validate the accuracy of the results, we use scatter plots and radial charts as graphical aids to realize a fit, illustrated in Figure 2 (c). It has also been shown that different people like to organize the same pathway in different ways to suit their mental models. With the aim of providing a comprehensive representation and the flexibility of arranging their own models, we provide the freedom to move around the different components on the interactive table.

Hardware Implementation

Active Pathways is a tangible tabletop system built around three main components: Sifteo Cubes as active tangibles, a Diffused Surface Illumination (DSI) interactive table, and the CCV and ReacTIVision computer vision framework. Figure 3 illustrates the setup.



Figure 3. The Active Pathways system setup.

We selected Sifteo Cubes to prototype the active tangibles in our system, as each cube has a small Liquid-Crystal Display (LCD) and built-in sensors that detect shake, touch, tilt, and adjacency with other cubes. They communicate wirelessly with a base that is connected to a computer via USB. They can thus communicate bi-directionally with the computer in the interactive table and can be easily programmed to listen to and create events that are communicated via WebSockets. In our system, ReacTIVision fiducial markers [17] are affixed to the base of the cubes, allowing them to be manipulated both on and off the tabletop. The size of the Sifteo Cubes also factored into our decision to use them in our system: they are small enough to not take up significant screen real-estate and occlude visualizations on the table, but big enough to be held comfortably in hand.

We use a DSI table constructed with four PS3 Eye Cameras viewing the four quadrants of the table from underneath. The PS3 Eye Camera is a webcam that can record an image of 640×480 at 60 Hz or 320×240 at 120 Hz. We use a short-throw projector to rear-project an image on the table's 43.3×30.9 -inch active surface. The pictures from different cameras are stitched together by the Community Core Vision (CCV) engine [25] to form a single image. It tracks both the position and orientation of the small ReacTIVision fiducial markers attached to the cubes as they are moved around the tabletop.

Software Implementation

Active Pathways is built on top of Web technologies, i.e., Node.js [24], JavaScript, and HTML 5, for easy portability to other potential platforms, such as tablets and smartphones. For tabletop interactions, we use the CCV computer vision engine, which recognizes the ReacTIVision fiducial markers and touch events on the DSI table. CCV communicates the events occurring on the table using the TUIO protocol. We use the TUIO.js JavaScript library [36] to detect touch and tangible interactions on a Web browser. We use the Sifteo SDK to communicate with the Sifteo Cubes and Socket.IO [34] as the pipeline between the table and the Sifteos. As users interact with the cubes, events are created that are broadcast via Socket.IO. We use the D3.js JavaScript library [4] to create and manage our visualizations and animations. Formation of ODEs is an integral part of modeling and these are created behind the scenes as the model is built. We use the Numeric.js JavaScript library [26] to solve these equations as the simulation is run while performing fitting tasks.

A USER STUDY

We conducted an empirical study to gauge the usability and usefulness of *Active Pathways* for collaborative modeling and fitting tasks.

Apparatus

The user studies were conducted in a lab on a Windows 7 machine. The interactive table was $124 \times 90 \times 94$ centimeters in dimension, with an active surface of 110×78.5 centimeters resolution of 1280×800 pixels. The application does not have any touch capabilities hence the touch sensitivity was turned off to ensure proper behavior. The indoor lights were turned off while using the DSI table for proper detection of the fiducial markers. All sessions were video-recorded with due permissions from the participants for the purpose of analysis.

Participants

Since almost all existing work on supporting systems biology modeling on an interactive tabletop has focused on expert users while our system is targeted primarily at novice researchers, we recruited novice modelers for our study. Fourteen paid participants from the university community participated in the study. Twelve of them were from the age group 18-24 and the remaining two were from 25-39. Ten of them were male and four of them were female. They all had prior experience with modeling through coursework, *i.e.*, about four months on average, but had never used an interactive table before. Since we aim to support collaborative modeling, the study was conducted in pairs. Each participant was given a \$10.00 Starbucks gift card for participating in the study.

Procedure

The user study started with a semi-structured interview to understand the background of the participants and their familiarity with modeling practices. Since this is a novel approach towards modeling and not many people are familiar with a tabletop system, the interview was followed by a brief demo of the functionalities of the system. Participants were then given some time to get familiar with the system, at the end of which they were asked to fill in a perceived usefulness and ease of use questionnaire, *i.e.*, pre-task questionnaire. It used a 7-point Likert scale and was based on a combination of the System Usability Scale (SUS) [5], the Technology Acceptance Model (TAM) [10], and our own questions regarding specific features of the system. Participants were instructed to rate the evaluated system in comparison with the system they use most frequently for modeling tasks.

We then gave them a small modeling task, in which they were asked to first build the Glycolysis pathways and then to perform a fitting task based on the experimental data already fed into the system. Glycolysis is the metabolic pathway that converts glucose into pyruvate. This particular pathway is commonly used to teach the process of modeling to novices. Although, in practice experimental data is obtained through research, we used synthetic data for simplicity. We manually selected initial concentration values for each molecule, *i.e.*, higher values for reactant and lower values for products, and rate constants for each reaction. The simulation then produced the value for each molecule per unit of time for a total of 10 units.

Participants were given 20 minutes to complete the task. This was decided in consultation with several expert modelers, who responded that it would take them less than 20 minutes to complete the presented task with conventional tools. Upon completion of the task, they were asked to revisit the usefulness and ease of use questions, *i.e.*, post-task questionnaire. We ended each session with a short subjective debrief interview to gather additional feedback.

RESULTS

We converted user response on seven-point Likert scales to three-point scales using linear transformation to calculate ratios (%). All ratings below four were mapped to one, all fours to twos, and all ratings above four were mapped to three. We also converted some responses to binomial data. That is, everything above four was rated as "accept" and below four as "reject" or vice versa, depending on the phrasing of the question. Ratings of four were disregarded. Such a mapping is common practice in statistics [11].

Popular Modeling Tools

Results revealed that most participants use MATLAB for data visualization and modeling tasks. The remaining use various tools, including SolidWorks, AutoCAD, Microsoft Excel, and Simulink. See Figure 4. Interestingly, about 57% participants responded that they often use paper or whiteboard along with these tools. In regard to usability of the tools, half of them responded that they often find these difficult to use, especially when working with large datasets. It is also takes extra time to discover and learn a previously unknown feature due to the systems' unintuitive user interface. Therefore, most participants (80%) felt that more user friendly and responsive systems can improve their modeling performance. Regarding collaboration, most participants (80%) responded that they often collaborate with their peers.



Figure 4. The most used data visualization and modeling tools.

Usability

When asked about the perceived learnability and ease of use of the system in the pre-task questionnaire, most participants (93%) responded that they think that the system will be easy to learn and use. Their responses did not deviate much after using the system. In the post-task questionnaire, most participants responded that the system either met or exceeded their expectations, both in terms of learnability (80%) and ease of use (71%). The remaining 20% and 29% participants found the system more difficult to learn and use, respectively, than they initially expected. See Figure 5.



Figure 5. User responses regarding learnability and ease of use, respectively.

Functionality

In the pre-task questionnaire, most participants (about 90%) responded that they found the various functions are well integrated in the system and data visualization on the tabletop is beneficial. Similar to usability, their responses regarding functionality did not deviate much after using the system. In the post-task questionnaire, most participants responded that the system either met or exceeded their expectations in terms of various function integrations (57%) and data visualization (71%). Nevertheless, about 43% and 29% participants did not find the functions as well integrated and the visualizations as useful, respectively, as they initially expected. See Figure 6.



Figure 6. User responses regarding function integration and data visualization, respectively.

Usefulness

In the pre-task questionnaire, all participants (100%) felt that the system will make them better understand the model, the molecules, the reactions, and the relationships between them. They all believed that this will make fitting process easier, as a result make them more confident performing fitting tasks (93%) and enhance their effectiveness on the job (71%). Likewise, in the post-task questionnaire, 86% responded that the system either met or exceeded their expectations in terms of its effectiveness on their performance. However, the remaining 14% were not as convinced. See Figure 7.



Figure 7. User responses regarding the easiness of the fitting process.

Collaboration

The complete session lasted for about one hour, including demonstration, interviews, questionnaires, and breaks. Each modeling session lasted for about 20 minutes (on average 19 minutes, SD = 3.6). Four out of seven groups (57%) were able to complete the model and run at least one simulation, while the remaining three groups (43%) failed to complete the task. This is not surprising, considering that we recruited novice modelers to perform a task that is usually performed by experts. In the pre-task questionnaire, most participants (80%) replied that the system will most probably make collaboration easier. Their responses did not deviate much after using the system. In the post-task questionnaire, about 80% of them stuck with their initial responses, when the remaining 21% found it less collaboration-friendly then they anticipated. See Figure 8.



Figure 8. User responses regarding collaboration.

To better understand how well the examined system supports collaboration, we studied the video recordings of the sessions to observe if participants worked exclusively or collaboratively, and if both participants were handling the active tangibles and performing actions or if only one participant was actively performing tasks when the other was either providing directions or passively watching. We then classified the groups based on Shaer et al.'s [30] classification of roles taken by pairs of users working together on a task: Independent, Driver-Passenger, Driver-Navigator, and Turn-Taker.

Based on our observations, all of our groups can be classified as Turn-Takers. That is, both participants in all groups were equally involved in the task, actively participated, and accepted suggestions from their partner. Even in cases where one participant was more knowledgeable, the other was still actively involved with the system, making suggestions and trying actions to move through the tasks. In all groups, each participant assumed ownership of one tangible throughout the duration of the experiment.

User Experience

In the pre-task questionnaire, most participants (over 90%) responded that they will enjoy using the system and can see themselves using it for modeling tasks in the future. However, after using the system about 36% did not find the system as enjoyable as they initially expected. About 21% also changed their minds about using it in the future. See Figure 8.

DISCUSSION

Active Pathways aims to help students and researchers in the processes of systems biology learning and discovery by building external models using active tangible and tabletop interaction. The results of the study provide an opportunity to revisit our design goals.



Figure 9. User responses regarding whether the system was enjoyable (above) and whether they see themselves using it in the future (below).

Several participants mentioned that seeing and feeling the model helped their understanding. One group liked how binding makes it feel like one is holding the molecule and another mentioned how physically putting things together helped them "see" better, which is hard to do in MATLAB. Moreover, they found the approach better than paper, as one can easily modify the pathway.

Roughly half the groups were able to complete the task and we received mixed feedback with respect to how well the system supports problem solving. This appears to be due to a combination of reasons. First, as all our participants were new to modeling tasks, it is not surprising that they would require more time for the tasks than expert modelers. Instead, the fact that about the half the groups (57.14%) were able to compete the tasks without having any prior knowledge of the system or the tasks assigned to them highlights the system's usability and how both experts and novices can be productive with it. Second, the accuracy of detection and the limited interactions using active tangibles affected participants' experiences with the system. Since the tabletop interactions in the system currently are entirely based on the positioning and movement of active tangibles on the tabletop (i.e., no support for multi-touch), their detection needs to be accurate and smooth. It can get frustrating for a user if a molecule is constructed at an unexpected position. In the post-study interviews, some also complained about the absence of realtime feedback on parameter changes. There were also some disagreements among the participants regarding how many active tangibles are required to perform the tasks. Some complained that there were not enough active tangibles for the given tasks, while some suggested that not many tangibles are required. A male participant, 25-39 years, commented, "...everything can be accomplished with one cube (active tangible)". Nevertheless, we aim to improve these limitations in future revisions.

From the perspective of collaboration, it is evident from the study that in all the groups both participants worked together not just while planning the next steps but also while performing the tasks. Relevantly, a female participant, 18-24 years, commented, "*(the) tasks were easily divisible between partners*." We speculate that having multiple tangibles to hold, as opposed to simply a large shared display, encouraged joint action and turn-taking, hence increasing focus on the task, opening up a space for discussion, and fostering collaboration among participants. However, we acknowledge the fact that all our participants took courses together may have contributed to this behavior, thus further investigation is necessary to fully understand collaboration behaviors with the system.

While most participants agreed that working on the system would be enjoyable, post task some of them felt it was not as enjoyable as they had initially expected. As active tangibles were a novel form of interaction to all users, several of them did not feel comfortable with the interactions based around the tangibles alone (*i.e.*, without multi-touch), or would have liked more active tangibles. This feedback can be easily incorporated into future iterations of the system. It is worth noting that the system needs to strike the right balance between using tangibles as a novel interaction to most users [18], and providing interactions that they are familiar and comfortable with. For example, swiping the screen to scroll through the options has become so ingrained in us that it was hard for some of our participants to get accustomed to tilting a cube to change the menu. Future design iterations could employ new kinds of active tangibles that address some of these issues.

Lastly, our goal of facilitating discovery is difficult to assess at this stage of the research. Boden [1] describes how individuals generate knowledge that is either new to them as individuals ("P-Creative"), or new to humanity as a whole ("H-Creative"). Assessing how well the system facilitates discovery will require deploying the system in actual learning or research settings to evaluate its impact on individual and/or broader creativity.

The foundation for our work lies in the ideas advanced by embodied cognition, which suggest that interactive systems that couple actions made with the motor system to the movement properties of internal models can enhance the potential for insight and discoveries. While much TEI research focuses on improving ease-of-use and collaboration in a given task, there remain unexplored avenues when it comes to understanding how we can design scientific support systems that can better leverage the connection between our motor, perceptual and cognitive processes. We hope *Active Pathways* can help further the research in this direction and possibly be extended to computational modeling in areas beyond systems biology.

CONCLUSION

Based on ideas from embodied cognition, we designed and developed *Active Pathways*: an active tangible and tabletop system that aims to support collaborative discovery and learning in biochemical modeling. We evaluated the system in a user study with pairs of novice modelers. Results of the study suggest that the system is easy to use and learn and can facilitate an understanding of complex systems and collaboration.

FUTURE WORK

Our future plans include refining the tangible and tabletop interactions based on the feedback collected in the study, including more tangibles and exploring the combination of tangibles and multi-touch on the tabletop. Additionally, we are beginning to explore additional tangible devices to better support the fitting task by providing simultaneous control over multiple parameters. Ultimately, we aim to incorporate additional features to provide a more comprehensive tool to support modeling practices in the systems biology classroom or research lab. On the empirical side, we plan to deploy the system in an undergraduate modeling class to understand how it may aid novice modelers in the process of collaborative learning and discovery of complex systems.

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