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Toward Ontological Alignment: Coordinating Student Ideas with the Representational System of a Computational Modeling Unit for Science Learning

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ABSTRACT


Computational modeling tools present unique opportunities and challenges for student learning. Each tool has a representational system that impacts the kinds of explorations students engage in. Inquiry aligned with a tool's representational system can support more productive engagement toward target learning goals. However, little research has examined how teachers can make visible the ways students' ideas about a phenomenon can be expressed and explored within a tool's representational system. In this paper, we elaborate on the construct of *ontological alignment*—that is, identifying and leveraging points of resonance between students' existing ideas and the representational system of a tool. Using interaction analysis, we identify alignment practices adopted by a science teacher and her students in a computational agent-based modeling unit. Specifically, we describe three practices: (1) Elevating student ideas relevant to the tool's representational system; (2) Exploring and testing links between students' conceptual and computational models; and (3) Drawing on evidence resonant with the tool's representational system to differentiate between theories. Finally, we discuss the pedagogical value of ontological alignment as a way to leverage students' ideas in alignment with a tool's representational system and suggest the presented practices as exemplary ways to support students' computational modeling for science learning.

Introduction

There has been increasing momentum around integrating science and computing in K-12 education (e.g., Sengupta et al., 2013; Weintrop et al., 2016). Computational model building has been found to be one way to integrate computing and science learning. Much of this work has focused on the design of tools and technologies (e.g., Aslan et al., 2020; Bollen & van Joolingen, 2013; Horn et al., 2014; Hutchins, Biswas, et al., 2020), the use of computational modeling for specific learning goals (e.g., Blikstein & Wilensky, 2009; Dickes & Sengupta, 2013; Saba et al., 2020; Wagh & Wilensky, 2018), and students' development of coding and modeling practices (e.g., Farris et al., 2016; Louca & Zacharia, 2008).

As a relatively new representational practice, computational model building offers unique opportunities and challenges that merit more focused research in terms of the teacher's role in supporting students. On the one hand, many aspects of programming computational models can be challenging for students as they try to translate scientific ideas into the ontological structure of

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code (Basu et al., 2016). Teachers need to respond to these challenges with tailored support. Incorporating any new representational tool or practice into a classroom can be a complex task; teachers and students require time and space to negotiate between their goals and the tool's functionality (Wilkerson et al., 2022) before settling on productive engagement practices. On the other hand, students come to the classroom with rich ideas about how the world works (e.g., Rosebery et al., 2010; Smith et al., 1994), and their interpretations of and interactions with computational environments are inherently heterogeneous (e.g., Sengupta et al., 2021). Given this complexity, little work has investigated the role that teachers play in navigating students' multiple ideas to support students in building computational models.

This paper addresses how a teacher and her students coordinated students' ideas with the representational system of a computational agent-based modeling unit for science learning. Much like the work on the establishment of sociomathematical norms in math classrooms (Yackel, Cobb & Wood, 1991), we study how a sixth-grade teacher led her class in building shared practices around computational modeling. We elaborate on the construct of *ontological alignment*, which we define as identifying and leveraging points of resonance between students' existing ideas and the representational system of a tool or unit. We ask: What practices does an experienced science teacher use to ontologically align students' ideas with the representational system of the modeling tool? How are students taking up these practices for scientific sense-making throughout the unit?

Drawing on analysis of whole class discourse from a six-day computational agent-based modeling unit on diffusion, we illustrate three classroom practices that a sixth-grade science teacher and her students engaged in for scientific sense-making. We argue that each of the presented practices supports ontological alignment. In other words, in each practice, the teacher and her students coordinate students' own ideas with the agent-based modeling system of the unit. Finally, we discuss the pedagogical and research value of ontological alignment and the documented practices and suggest them as exemplary ones for supporting students' computational modeling. Our findings contribute to the field's understanding of the role of the teacher in incorporating new representational systems and practices into the science classroom in ways that are responsive to student ideas.

Theoretical background

Our primary goal in this research is to better understand how a teacher can support ontological alignment in a computational modeling unit. To support this goal, we first elaborate on what we mean by *ontological alignment* and then briefly describe the literature around the unit's representational system, agent-based modeling. We also briefly review existing work on how teachers can support computational modeling instruction in classrooms.

Ontological alignment

We are interested in how the representational system of the tool and curricular unit can become explicit for students in ways that leverage their prior ideas about target phenomena. We elaborate on the construct of *ontological alignment*¹ (OA), which we define as coordinating between students' existing ideas with the representational system available in the tool and unit, to illustrate this attention and instructional support (Wagh et al., 2023). While ontological alignment can be supported in many forms, we examine how a teacher and her students engage in classroom discourse that manifests ontological alignment.

By "representational system" of a tool, we mean its epistemic form or its "target structures that drive inquiry" (Collins & Ferguson, 1993, p. 25). A representational system of a tool or a

¹The use of the term "ontology" builds on tradition of its use in the Learning Sciences to characterize the structure and form of knowledge (Chi & Slotta 1993; diSessa 1993) and learning environments (Collins & Ferguson, 1993).

unit highlights the level of perspective on a system that is foregrounded to and manipulable by students. For instance, computational agent-based modeling (ABM) enables students to investigate a system by examining whether and how its constituent entities' properties, behaviors, and interactions result in change at the aggregate level over time (Wilensky & Resnick, 1999). In other words, ABM is a representational system that enables exploring a complex system through the actions and interactions of its component agents.

The representational system of a tool has important implications for learning, as it impacts the kinds of explorations that students can engage in and, subsequently, what learning goals can be supported by it. For instance, in a comparison of the use of algebraic notation and a programming language for physics learning, Sherin (2001) found that each representational system highlighted different kinds of sense-making in physics. While manipulating algebraic formulae highlighted sense-making around balance and equilibrium, programming highlighted student sense-making around underlying processes and causality. Likewise, while ABM enables explorations of phenomena in which the explanatory mechanisms happen at the micro-level (e.g., diffusion), it might be less amenable to explorations of phenomena in which the explanatory mechanism happens at the macro-level (e.g., gravity or electromagnetism).

Representational systems shape student activity and learning in part because they highlight different ontologies. In other words, different representational systems structure disciplinary knowledge in different ways, which can lead to different forms of student sense-making (e.g., Sherin, 2001). This approach to characterizing ontology reorients attention away from ontology as a description of student ideas (e.g., Chi et al., 2012) and toward attention to the structure of representational forms. As a construct, then, ontological alignment focuses on interfacing student ideas with the representational form of a tool.

Just as a tool's representational system shapes learning in important ways, so, too, does students' awareness of that system and ability to work within it. Wilkerson et al.'s (2018) study of fifth-grade students using a stop-motion ABM tool for reasoning about condensation showed that a lack of alignment between students' explorations and the representational system of the tool can make learning more challenging. Students who focused on movements and interactions that aligned with animation and the agent-based representational system of the tool (e.g., particulate representations of water) successfully developed mechanistic, explanatory models representing agent-level behaviors. On the other hand, groups that focused on sequences of events (e.g., transitions between condensation, precipitation, and collection in the water cycle) did not make as much progress using the tool. Perhaps most importantly, student groups benefited from support targeting their modeling strategies—namely, an explicit focus on agent-level behaviors and interactions—instead of the content of their model. Based on this work, Wilkerson et al. proposed that computational model-based instruction requires explicit attention to supporting students in matching their strategies with the representational system of the tool. We aim to respond to this call by documenting ways through which a science teacher and her students highlight the representational system of an ABM tool through whole class discourse.

A teacher can prepare students to productively engage with the representational system of a tool in multiple ways. Existing work suggests that using embodied modeling (e.g., Danish et al., 2011; Dicks et al., 2016; Pierson & Brady, 2020; Rands, 2012), drawings or other physical artifacts (e.g., van Joolingen et al., 2010; Wilkerson, Gravel, et al., 2015) and even a progression to introduce programming with the tool (e.g., Lee et al., 2011) can all help orient students to the tool's representational system. Ontological alignment is a specific form of supporting productive engagement with a tool that considers seriously how a teacher can respond to and build on a variety of such existing resources that students bring to the classroom (e.g., Smith et al., 1994). In the broader science education literature, there is consensus around the importance of responsive teaching as a way to engage with and leverage diverse student ideas in a classroom (Robertson et al., 2015). Building on this work, ontological alignment is a specific kind of responsiveness that

highlights the interfacing between student ideas and the ontology of the tool's representational system.

Computational agent-based modeling for science learning

Computational ABM has been used in many forms: as an environment in which learners run experiments by manipulating parameters (e.g., Yoon et al., 2016), decoding the code to interpret its disciplinary meanings (e.g., Hsiao et al., 2019; Wagh et al., 2022), and programming models by encoding rules (e.g., Louca et al., 2011; Saba et al., 2023; Wagh & Wilensky, 2018; Xiang & Passmore, 2010). Engagement with ABM has been found to support students' mechanistic reasoning (e.g., Blikstein & Wilensky, 2009; Dickes et al., 2016; Fuhrmann et al., 2024; Wilkerson, Gravel, et al., 2015), integrated science and computational learning (e.g., Hutchins, Biswas, et al., 2020; Lee et al., 2011; Sengupta et al., 2013; Wagh et al., 2017), and model-based inquiry (e.g., Wilensky & Reisman, 2006; Xiang & Passmore, 2015).

A considerable amount of research has explored how to lower the barrier to students programming their own agent-based models by using visual block-based programming. A key component of this work involves developing an epistemic structure for designing blocks so students can use them to explore the target domain (e.g., Anderson & Wendel, 2020; Hutchins, Biswas, et al., 2020; Kahn, 2007). One approach identifies the space of target simulations that can enable students to explore the core patterns in a conceptual domain and breaks down those simulations into micro-behaviors that can be combined in different ways to generate patterns (Kahn, 2007; Wilkerson, Wagh, et al., 2015). Alternatively, phenomenological programming structures code blocks that map onto students' intuitive understandings of real-world objects, patterns, and events (Aslan et al., 2020; Sengupta et al., 2018). A third approach maps the mechanism underlying the target phenomena into agents' properties, actions, and interactions (Saba et al., 2023). Each of these approaches instantiates an epistemic structure of the conceptual domain that students can access and build from. However, this structure is typically not made available to students or to the teacher, which we see as a missed opportunity.

Role of teachers in guiding computational modeling in classrooms

Teachers play a key role in facilitating scientific modeling in classrooms and in shaping their students' modeling experiences (Ke & Schwarz, 2016, 2021). However, facilitating scientific modeling in classrooms can be challenging (Danusso et al., 2010; Justi & Gilbert, 2003; van Driel & Verloop, 1999). Teachers have to navigate between modeling as a practice for content learning vs. a practice for generating, exploring, and validating or refuting yet unknown scientific knowledge (Guy-Gaytán et al., 2019). Moreover, teachers may themselves have limited expertise and experience with modeling (Henze et al., 2007; Justi & Gilbert, 2002; Justi & van Driel, 2005; Schwarz, 2009; van Driel & Verloop, 2002; Windschitl et al., 2008), further exacerbating these challenges.

Research using computational model-based learning has shown that there can be diverse teaching approaches to model-based learning (Hmelo-Silver et al., 2015) and that how teachers facilitate instruction is impacted by their own comfort and leanings with computational modeling (Hsiao et al., 2019). When we add the use of coding tools in classrooms with which students create explanatory computer programs, challenges remain. The time required for students to become adept modelers (Xiang & Passmore, 2010) and the need to better integrate modeling with other scientific practices (e.g., Berland & Reiser, 2009; Clark & Sengupta, 2015) can make integrating computational modeling instruction for science learning challenging. Moreover, several aspects of programming computational models—e.g., identifying relevant science content, grappling with programming structures and syntax, and translating scientific ideas into the ontological structure

of code—can be challenging for students (Basu et al., 2016). As a facilitator, the teacher needs to offer tailored support in response to these varied challenges.

Finally, and perhaps most importantly, there is an inherent heterogeneity in the ways in which computational modeling work is taken up by students (Sengupta et al., 2021). Teachers need to experience agency in being responsive to students' multiple ideas and their computational modeling work (e.g., Swanson et al., 2024; Wilkerson, Wagh, et al., 2015). One way in which teachers can manage this heterogeneity is by supporting the establishment of classroom norms that support students and the teacher in using the computational tool as an expressive medium to articulate and refine their ideas (e.g., Sengupta et al., 2021). We examine the classroom practices that emerge as a teacher, and her students address this inherent heterogeneity by leveraging students' ideas and work to align with the agent-based representational system of the unit.

Research questions

This manuscript examines how a 6th-grade science teacher and her students work through a week-long computational agent-based model-building unit to understand how ink spreads through water by diffusion. We are guided by the following research questions:

1. What practices does an experienced science teacher use to ontologically align students' ideas with the representational system of the modeling tool?
2. How are these alignment practices taken up by students throughout the unit?

Methods

MoDa: Integrating agent-based modeling with real-world data

MoDa is a web-based environment that combines creating computational models using domain-specific code blocks with comparison against real-world data (Wagh et al., 2022). MoDa builds on research in the design of domain-specific blocks-based programming (e.g., Wilkerson, Gravel, et al., 2015) and efforts to support learners in comparing computational models with real-world data (Blikstein, 2014; Fuhrmann et al., 2018).

MoDa consists of a modeling area and a real-world data area (Figure 1, areas A and B, respectively). The modeling area includes: a coding area where students can drag and drop domain-specific blocks (e.g., properties, actions, control mechanisms) built on Google's Blockly library to program models of the target phenomenon; a simulation of students' coded models built on the NetLogo engine (Wilensky, 1999) in which students can control different parameters of the simulation (e.g., temperature); and data visualizations that illustrate the modeling results in graphs. By comparing their computer modeling results with video data, quantitative datasets, or other sources featured in the real-world data area, students can refine and validate their models. In this specific unit on the topic of diffusion of ink in hot and cold water, MoDa embeds video data in the form of two video clips within the computational modeling environment itself rather than leaving such integration to supplementary curricular activities. Corresponding to the experiments students conducted in the unit, the two videos available to students in the unit were of ink spread in hot and cold water (Figure 1).

Instructional sequence

Over 6 class periods, students investigated how and why ink spreads differently in hot and cold water (See Table 1). Students first conducted two experimental trials to collect, plot, and compare data on the rate of spread of ink in hot and cold water. Ms. K led a whole-class discussion to

How does ink spread in water?

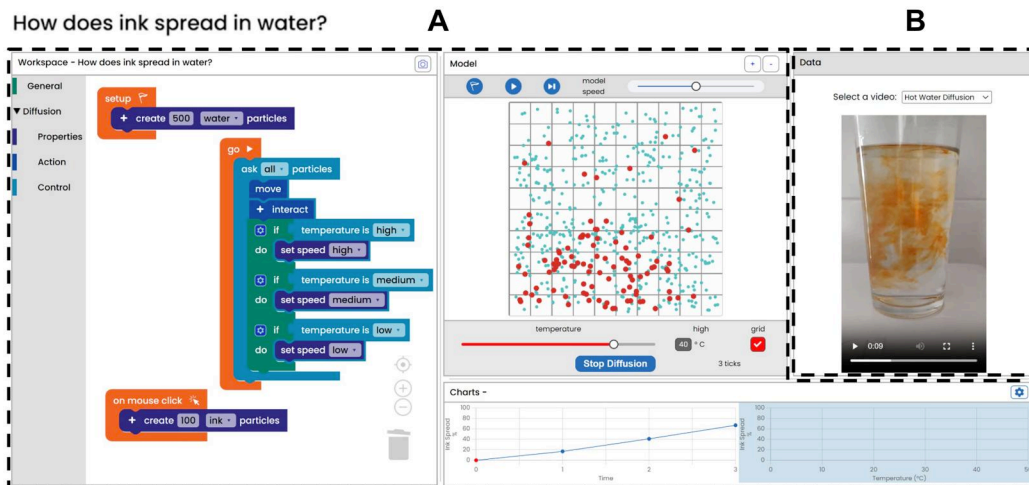


Figure 1. The MoDa interface: The environment consists of a modeling area (A) and a real-world data area (B).

Table 1. Instructional Sequence of the Diffusion Unit.

Days	Description	Activities
Day 1	Students conducting the Ink diffusion experiment Analyzing data and discussing the experiment's results.	Demo Ink diffusion experiment Data discussion
Day 2	Students develop paper models to account for their observations of the data	[No data]
Day 3	Students present their paper models in a gallery walk. Introduction to MoDa & students work on challenges to get introduced to MoDa. Some students design an initial model in MoDa to explain the data	Present paper model MoDa work MoDa feedback
Day 4	Teacher reviews their work and asks some students to present their MoDa models. The teacher hands out a "code cheat-sheet" with student code examples. Working in pairs, students continue to design a model to explain diffusion.	Present MoDa models MoDa work
Day 5	Teacher asks students to make a case for which explanatory model they are supporting. She highlights the video data as a resource with which to align their models. Students have work time to work on their models. In a whole-class discussion, students present their models and compare them with the video data. The teacher brings in new evidence to address one of the explanatory models. Students have additional work time to revise their models. The teacher shows students a 3-minute video describing diffusion.	Review and video comparison work Present models Evaporation experiment MoDa work Video
Day 6	Students have work time to wrap up their models.	[No data]

identify trends in the scatter plot and generate initial explanations for these trends. Students then drew paper models of their explanations and shared their paper models in a gallery walk. Ms. K organized students' drawings into conceptual themes, posting each theme and the corresponding drawings on a large Post-it board in different parts of the room. Students walked around the class to familiarize themselves with the conceptual themes and paper models made by their classmates. Ms. K then asked a few students to present their models to the class.

Next, Ms. K introduced MoDa, the computational modeling environment. Students worked in pairs through four challenges designed to introduce and familiarize them with MoDa's block library. After reviewing their work on these challenges in a whole-class discussion, students

worked in pairs to design a computational model of their explanation of diffusion. On the 5th day, students presented their computational models to the class for feedback. To validate their models, students compared them with video data and external resources to collectively critique their models and reach a shared understanding of how diffusion works. At the end of the class period, they watched a video that presented a canonical explanation for diffusion.

It is important to note that though the unit occurred over a 6-day period, our data corpus only includes 4 days of the unit. We do not have data from the second day—during which students made their paper models—or from the last day—on which they watched a video explaining diffusion and reflected on their experiences. As students did not use MoDa on these two days, these gaps in our data corpus minimally affect our ability to analyze classroom practices of ontological alignment.

Representational system of the unit: agent-based modeling

The representational system of the unit is agent-based modeling. The agent-level perspective on the system was highlighted in the design of the curricular materials available to students. For instance, the prompt to students in the paper modeling activity encouraged them to articulate their ideas about what was happening at the level of the individual entities in this system (See [Figure 2](#)). This practice is grounded in the literature about how agent-level behaviors and interactions can be an accessible entry point into sense-making of phenomena (e.g., Schwarz et al., 2009; Wilensky & Reisman, 2006).

MoDa, as an agent-based modeling tool, also highlighted the perspective of individual agents in the system. In designing the library of blocks for this unit, we attempted to balance between providing adequate blocks to address the target learning goals of the unit while giving students expressive power to be able to design different kinds of models. Blocks in the library were divided into four sections: General, Properties, Action, and Control. The last three sections were specific to diffusion.

The General collection included basic blocks to form conditional statements ([Figure 3](#)). Diffusion-specific Properties blocks enabled students to create ink or water particles and manipulate their properties, including color, speed, position, and heading ([Figure 3](#)). The Action blocks

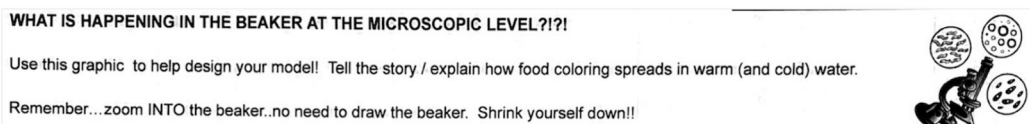


Figure 2. Ms K's worksheet prompt for drawing a paper model of diffusing students to "zoom in" to explain.

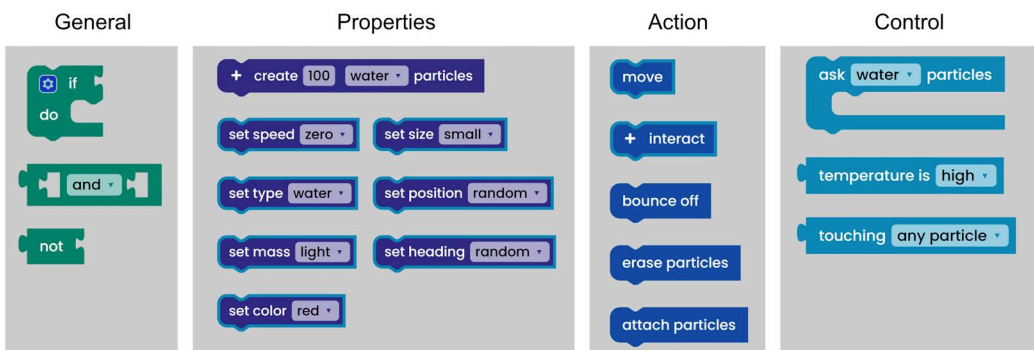


Figure 3. MoDa block library.

included rules for students to encode for ink and water particles, including a “bounce” block that changed the heading of a particle, a “move” block that made a particle move forward by 1 unit in the direction of its current heading, an “attach” block, and an “erase” block. The former two blocks could be used together to represent Brownian motion. The latter two blocks were anticipated based on prior work with middle school students studying diffusion (Fernandez et al., 2021). The Action blocks also included an “interact” block that could be used as a procedure. In other words, it contained code inside it that could be viewed and edited by selecting the “+” symbol. Finally, using the Control blocks (Figure 3), students could encode rules for specific particles (water, ink, or all) and under certain conditions (temperature, touching other agents). By combining blocks from different sections, students could encode different properties and actions for different particles under different conditions (e.g., setting a higher particle speed when temperatures are higher, setting different colors for ink and water particles).

The MoDa blocks were designed to readily map onto the experiment students conducted in the unit. For instance, in addition to “setup” and “go,” the interface also included an “on mouse click” block, which made it possible for students to create ink particles in the simulation with a mouse click, similar to dropping ink into a beaker as they did in class.

Though students had a fairly limited number of blocks in the library, we have found that students devise ingenious ways to represent a multitude of explanations using different combinations of these blocks (For details, see Fuhrmann et al., 2022).

Data collection

The study was conducted in a public school in the Bay Area, California. The school population is 48% White, with 18% of students identifying as two or more races, 16% as Latine, 10% as African American, and 7% as Asian American. Roughly 25% of students come from low-income families, and 6% of students are English language learners.

Ms. K taught two class periods. Both class periods used the same artifacts and revealed similar patterns in the kind of whole-class discussions that took place. Of these two class periods, we selected the class in which a greater number of students spoke and presented their ideas for analysis. Given the nature of the analysis, selecting a focal class period enabled us to do an in-depth investigation of our research questions. Out of 29 students in the focal class, 18 students consented to participate in this study. To answer the research questions above, we analyzed observational field notes taken by a researcher who was present in the classroom. These notes included rough transcriptions for whole class discussions and brief notes about students’ work. We also collected video data of whole-class discussions that took place over all four days. Our data corpus also included teacher artifacts (e.g., Ms. K’s slides, a MoDa sample code handout, a reflection worksheet) as well as student artifacts (e.g., the paper and computational models, their worksheet responses). Finally, we conducted an hour-long interview with Ms. K at the end of the implementation to document her reflections on how the unit supported student learning in her two class sections.

It is important to note that though the driving phenomenon of the unit was why ink spreads more quickly in hot than cold water, the class focused on how and why ink spreads in water. Students fundamentally disagreed about the behavior of the ink and water particles, so, in the spirit of responding to students’ interests, Ms. K took that up as the central line of inquiry.

This was Ms K’s second year teaching this unit and her third year in the project. She was very comfortable with MoDa and the available blocks in this unit. Two researchers were present in class throughout the unit. However, the teacher taught the unit independently. Moments when the teacher relied on the researcher for support have been marked as such. To the best of our knowledge, students did not have prior experience with MoDa or other agent-based modeling environments.

Data analysis

Our analysis focused on our two research questions: What practices does an experienced science teacher use to ontologically align students' ideas with the representational system of the modeling tool? How are these alignment practices taken up by students throughout the unit?

To identify Ms. K's practices, we used observation notes to identify videos of whole-class discussions in which she introduced, reviewed, or contextualized the computational modeling activity (roughly 4.5 hours of video were identified). Consistent with interaction analysis methods (Jordan & Henderson, 1995), members of the research team reviewed the videos independently and collaboratively to identify the teacher's high-level pedagogical practices framing her students' computational modeling work. Through this initial work, our focus of analysis expanded to include how students took up the practices modeled by Ms. K in class.

Through discussion and comparison, four preliminary themes were identified (See [Appendix C](#) for a detailed account of the analytical process, supplementary material). Each of these themes was related to how the teacher supported students in adopting the agent-based representational system in the unit by leveraging their own ideas and models. This common thread led us to define the construct of "ontological alignment" as moves that reflect explicit attention to identifying resonances between students' ideas and the representational system—in this case, agent-based modeling—of the tool and unit being used. Through iterative bottom-up coding of transcripts of video data of whole-class discussions, we identified a total of *ten moves*. These moves were categorized into *three classroom practices* based on their role in supporting students' thinking and work. The moves may have been introduced by either the teacher or students, and they may have been subsequently taken up by either the teacher or other students in the classroom.

The final codebook, as presented in [Table 2](#), underwent several rounds of revision through collaborative discussion with the research team. For instance, because the "Label" code and the "Categorize" code co-occurred frequently and were challenging to distinguish between in some instances, "Label" was deemed to be a specific subcase of "Categorize." An initial code for "surfacing student ideas" was removed, as it was found to occur almost constantly and, thus, lost meaning. Additionally, as analysis proceeded, the decision was made to focus only on moves that specifically fostered ontological alignment. Thus, the codebook also does not include certain, recognizable valuable pedagogical moves that Ms. K engaged in (e.g., such as revoicing student ideas).

Videos of whole-class discussions were transcribed, and the resulting transcripts were coded at the level of each turn of talk for the teacher and students, with each turn eligible for as many codes applied (See [Appendix C](#) for details about the exception to this norm, supplementary material). Three researchers collaboratively coded a small portion of the whole class discussions from each instructional day to reach a consensus about how the codes should be applied. The remaining bulk of the whole-class discussion transcripts were then independently coded by the three researchers. Discrepancies were identified and, with a few exceptions, resolved collaboratively through discussion. In the remaining cases where all three researchers did not agree (8 disagreements out of 296 utterances coded), the code agreed upon by two researchers was assigned.

We then constructed heat maps of the coded data by counting the frequency of each code within 5-minute increments² of the four days of available classroom data. We annotated these cells with the particular classroom activity occurring at that time. Time periods for which we do not have whole-class data recordings (e.g., pair work time) were removed. We then calculated the frequency of each move as performed by the teacher and the students within each cell. For this calculation, the practices "Categorize" and "Label" were combined, as were the practices "Compare & Contrast" and "Crossover;" each practice in these two sets was closely related and

²While we display frequencies for 5-minute intervals, codes were applied at the level of turns of talk, of which there were often many per minute.

Table 2. Codebook of classroom practices and associated moves.

Move	Description	Example(s)
Classroom Practice #1: Elevate Student Ideas Elicit Causal Explanation (Teacher only)	Relevant to the Representational System of the Tool Prompt a causal explanation of diffusion	Teacher: "Now let's talk about why. Why do you think the data looks this way? [...] [Pointing to different data points on a scatter plot of the class data] Why is the cold here? Why is the warm-up here? And why is the cold spreading less than the warm?" Student: "Basically he was just saying that the molecules or whatever capture, I think, the coloring and move around faster, spreading it faster." Teacher: "Yes, we got five theories, and you'll notice that I've color coded them" Student: "Because some are kind of similar theories, so you like, explanation #1 and explanation #4. They're kind of similar, so you made them the same color." Teacher: "So this is the bounce-off model" Student: "Oh, that's kind of the water and ink particles/ are mixing but not attaching." Teacher: "Ok, so that was one difference. Anything else that was different?" Student: "Kind of the same as that one [pointing to one of the posters in the room], but also consuming it a little bit." Teacher: "And you're doing 5 and 4?" Student: "[we] are a mix of 1 ('infect') and 3 ('bounce') [...] they are like infecting and also they are bouncing ..."
Provide Causal Explanation (Student only)	Offer a causal explanation of diffusion	
Categorize	Allude to clusters, groups, camps, or buckets of explanations (including difficulty categorizing)	
Label	Assign a name (e.g., "bounce," "attach," "infect") to ideas expressed in code, simulation, or explanations. Does not include observations (e.g., "The particles are bouncing off.") or naming the categories (e.g., "Are you going to make the attach theory?")	
Connect or Contrast	Compare or contrast ideas	
Crossover	Acknowledge elements of a theory across different explanations	
Classroom Practice #2: Explore & Test Links between Students' Conceptual & Computational Models Link Conceptual & Computational	Explain how a conceptual idea is represented in the code or simulation	Teacher: "[observing the simulation] Yellow is the ink that just infected something." Student: [describing their code] "So we made it so that the particles would bounce off of each other, but we also made it so that when an ink particle and a water particle, it changes the color, but it also changes the [water] to an ink particle." Teacher: "[Just watch their model. Pick an ink or a water particle and see what happens." Student: "What the heck, they're attaching!" Teacher: "Differentiate between Theories Teacher: "The experiment had, how many times did we drop in ink? [...] So, on your mouse click, you're gonna click twice." Student: "And then, also, pause it [the simulation] when the video pauses." Teacher: "how could we test the idea that the water has been infected? What would happen, how could you test this?" Student: "We could look at it in a microscope."
Strategies for Observing Simulation	Direct attention to particular ways of watching the simulation	
Observing Simulation	Voicing observations of the simulation	
Classroom Practice #3: Draw on Evidence Resonant with the Representational System of the Tool to Differentiate between Theories Matching	Matching the simulated model and real-world data or video data	
Supporting / Refuting Evidence	Gathering evidence to support or refute a theory	

often temporally linked, lending little value to continuing their separation. Finally, we color-coded the cells by frequency value, from light gray (a value of 1) to black (a value of 10+).

We primarily present Findings at the level of classroom practice (not moves) so as to emphasize the collection of moves through which the teacher supported her students' developing ontological alignment. In addition to constructing the classroom practices heatmap (Figure 13), we also used the codes to identify excerpts from the class discussions to illustrate, in a qualitative way, how each practice played out in the classroom, as presented in the Findings below. All student names are pseudonyms.

Findings

Guided by our research questions, analysis of video data led us to identify three classroom practices through which an experienced science teacher facilitated classroom discourse to support ontological alignment:

1. Elevating student ideas relevant to the representational system of the tool;
2. Exploring and testing links between students' conceptual and computational models; and
3. Drawing on evidence resonant with the representational system of the tool to differentiate between models.

We see each practice as supporting ontological alignment between students' ideas and the representational system in MoDa, the computational tool, and the curriculum in use.

Classroom practice 1: Elevating student ideas relevant to the representational system of the tool

This first classroom practice consisted of moves through which Ms. K elicited student ideas about particle-level behaviors and interactions, categorized and labeled these ideas, and connected them with each other. Students took up this practice as they repeatedly labeled their own and others' ideas and connected and contrasted them with one another. In what follows, we describe the origins of this practice in Ms. K's teaching and show how the class took it up over the rest of the unit.

Illustration 1.1: Eliciting student ideas about particle interactions

After students conducted the ink diffusion experiment and generated a class-level scatter plot of their data on Day 1, Ms. K prompted students to describe any patterns or trends they observed in the data representation. In sharing their observations of the scatter plot, the class established a consensus that the ink spread more quickly in hot than cold water. Ms. K then asked her students to explain these results:

1	Ms. K: Now let's talk about <i>why</i> . ³ <i>Why</i> do you think the data looks this way? <i>Why</i> ? Turn
2	and talk to your partner first. I want everybody to talk. <i>Why</i> is the cold here? (<i>gestures to</i>
3	<i>the middle/bottom of the scatter plot</i>) <i>Why</i> is the warm-up here? (<i>gestures to the top of</i>
4	<i>the scatter plot</i>) And <i>why</i> is the cold spreading less than the warm? Turn and talk to your
5	partner (<i>Makes a note on the chart; Student pairs talk to each other for 50 seconds</i>)

Ms. K emphasized that her students needed to generate a causal explanation for their observations (lines 1–5). As students in the class began to share their ideas, Ms. K captured some of the ideas on the class scatter plot (Figure 4). Though some students provided descriptions of the phenomenon rather than causal explanations, the ideas that Ms. K chose to document addressed

³Italics indicate Ms. K's verbal emphasis.

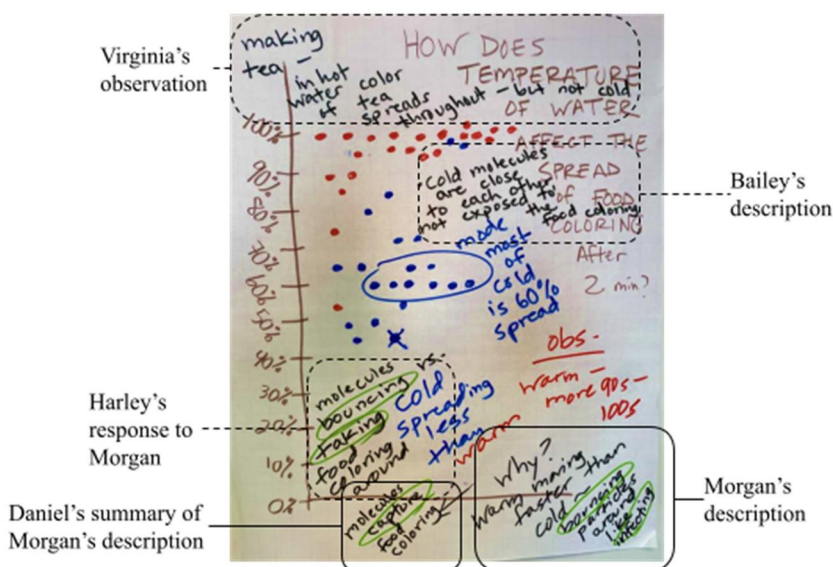


Figure 4. The collective scatter plot, annotated (black text) with student explanations. Annotations in dashed regions occurred after the discussion excerpted above.

particle-level behaviors and interactions. For instance, as seen in Figure 4, some of the ideas she jotted down were “bouncing,” “capture,” “infecting,” “molecules taking the ink around,” and a sense of density that “cold molecules are close to each other.” As she wrote them down, she told students that these were “great descriptive words” and acknowledged that it could be “really hard to describe a phenomenon.” These initial ideas seeded the conceptual categories that served as the foundation for the subsequent paper modeling activity and the rest of the unit.

Illustration 1.2: Categorizing and labeling student ideas about particle interactions

After class on Day 2, Ms. K collected all the students’ paper models of ink spread, took them home with her, and categorized them into five groups (Figure 5), which she shared with the class to start Day 3 of the unit. She created a whiteboard for each category, labeled each group with a title taken from students’ explanations for the ink spread differently in hot and cold water, and attached student paper models that she saw as corresponding to it (Figure 5). Where applicable, she included the names of the corresponding blocks that the students would encounter in MoDa (e.g., “attach” and “bounce”). For models she was unclear about, she invited students to assign their paper model to a category (Figure 5, bottom right).

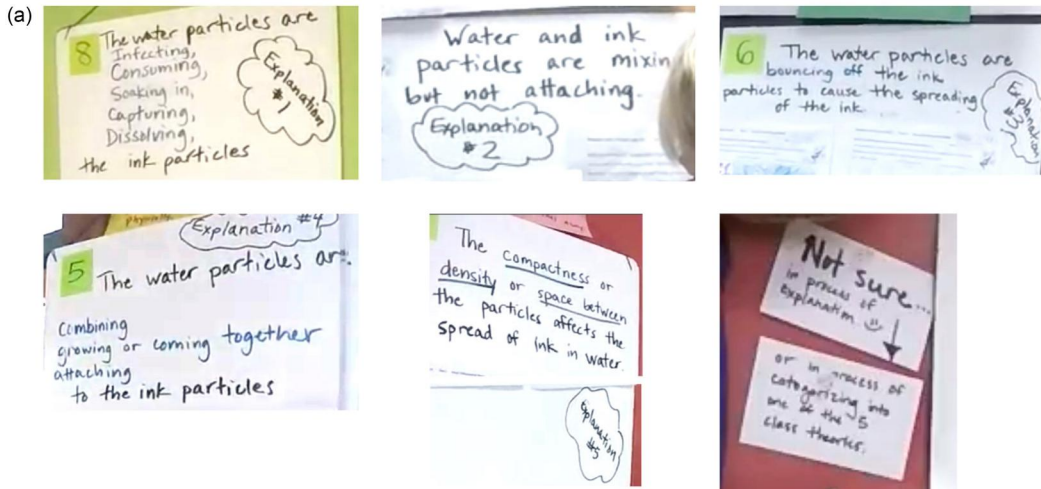
Ms. K instructed students to do a gallery walk to review their classmates’ drawings (Figure 5a), spending roughly 5 minutes for each category. These five “explanations” or conceptual models served as reference points for students’ work throughout the rest of the unit. Ms. K repeatedly organized and brought up these five conceptual models to orient students to their modeling work (Figure 5b).

Following the gallery walk, Ms. K asked a few students to explain particular models about which the class had expressed curiosity during the previous lesson. As Bailey’s presentation illustrates below (Figure 6), Ms. K continued to categorize and label explanations during these presentations.

- 1 Bailey: So when we first put in the drops (pointing to image on the left in Figure 6), I saw
- 2 they were really staying together near the top, so that is the ink. And, of course, there is
- 3 water everywhere [...] And because the water was just poured, it’s all cold still. And then,
- 4 for this one (pointing to the middle image in Figure 6), again there’s water everywhere
- 5 because there’s water everywhere, and the ink is starting to spread out a little bit more. [...]

(continued)

- 6 Ms. K: So in your model, you're showing that the ink and the water are not attaching or
 7 combining, they are separate. (*Bailey nods*) And I put you in this category, "the water and
 8 the ink particles are mixing but they are not attaching." And did you have an explanation
 9 for what is causing the food coloring to spread?
 10 Bailey: Like, the movement of the water. Like, because the temperature, I noticed that with the hot, it was moving a
 lot more versus the cold.
 11 Ms. K: So the heat was causing the movement of the particles to spread it around (*Bailey nods*).



(b)

Explanation #1	Explanation #2	Explanation #3	Explanation #4	Explanation #5
The water particles are infecting, consuming, soaking in, capturing, dissolving the ink particles. (Similar to 4)	The water and ink particles are mixing but not attaching. (Similar to 3)	The water particles are bouncing off the ink particles to cause the spreading of the ink. (Similar to 2)	The water particles are combining, growing or coming together and attaching. (Similar to 1)	The compactness or density or the space between the particles affects the spread of ink water.

We observe the water and ink particles INTERACTING, but still not exactly sure how...

We also have observed that heat seems to cause the spreading of the ink faster.

Question...is the heat expanding or changing the size of the particles or just moving them around? Is the heat separating? Detaching? Pushing the particles?

Figure 5. (a) Five clusters of paper models for the gallery walk, with a "Not sure" (bottom right) area for uncategorized models. (b) The five conceptual models organized into a table on Ms. K's class slide.

Bailey begins her account by primarily describing the phenomenon without a causal mechanism to explain it (lines 1–5). In response, Ms. K repeated the idea that the particles would stay separate (lines 7–8: "they are separate" and "mixing but they are not attaching") and articulated this as her rationale for categorizing Bailey's model under the "mixing but not attaching" theory (lines 7–8). Importantly, this label also highlighted the level of analysis students would encounter in MoDa: *an agent-based level that emphasizes particle-level behaviors and interactions*.

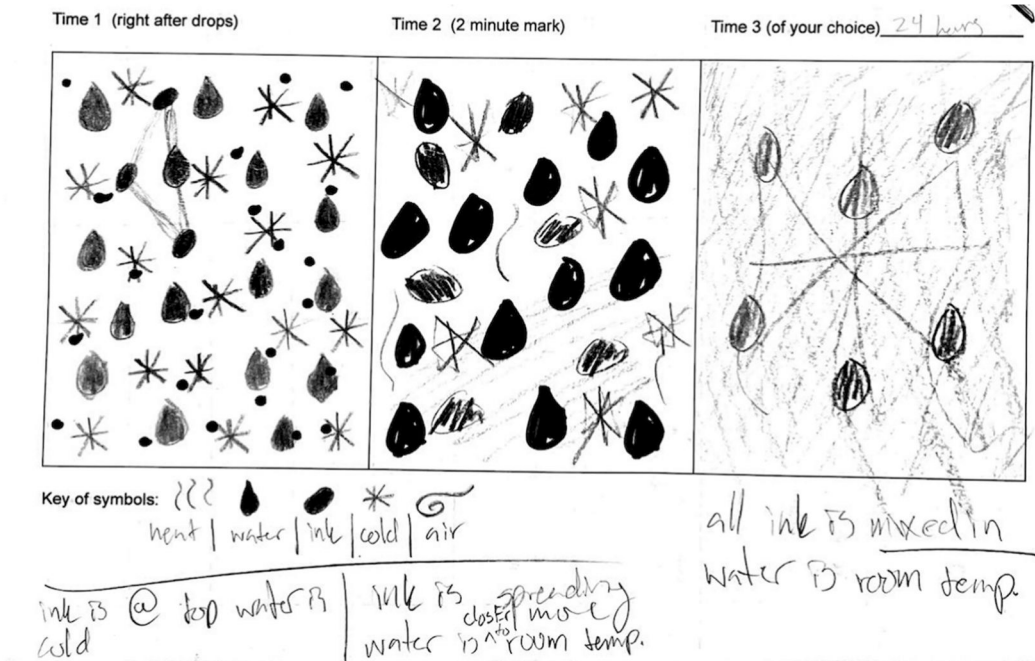


Figure 6. Bailey's paper model.

By underscoring that the ink and water will not combine, Ms. K labeled Bailey's model at a level of interaction that flagged for students what they would see in their upcoming model simulations (e.g., particles would not attach or combine). However, Bailey's initial explanation was not readily programmable; she did not identify particles or a causal behavior that they would follow. Ms. K's follow-up question about what *caused* the ink to spread gave Bailey an opportunity to propose a causal, programmable explanation. Ms. K even paraphrased Bailey's response to introduce agent-level behavior ("the heat was causing the movement of the particles"). We interpret these moves as working to ensure students understood that diffusion's key explanatory mechanisms were at the agent level so that students were prepared to use MoDa to express, explore, and refine their ideas.

Illustration 1.3: Connecting student ideas with each other

The next student's model presentation demonstrates how the practices of labeling and categorizing theories laid the foundation for yet another pedagogical practice: connecting ideas to one another.

1	Molly: the reason that I think the dye was moving around, and why I think it was moving
2	around faster in the warm water, is because particles in the warm water, they're moving
3	faster because they need to, like, move to create the energy that heats up the water, and I
4	thought that it was like kind of swirling the dye around and bringing it to other places. Kind
5	of the same as that one (<i>points to a poster in the room</i>) but also consuming it a little bit (<i>points to another poster</i>).
6	Ms. K: Yes, that's the other thing. Even though these are in buckets, you probably noticed
7	there is some crossover, it's not. As we're trying to explain this phenomenon, it might be a
8	little bit of one and a little bit of another, or it might just be one.

Molly's idea was that because warm water particles move faster (than cold water), it causes the dye to spread more quickly in hot water (lines 1–5). This explanation accounted for the behaviors and interactions between particles in the phenomenon. Molly then labeled her idea as related to two other theories in the class (lines 4–5). In response, Ms. K reinforced this

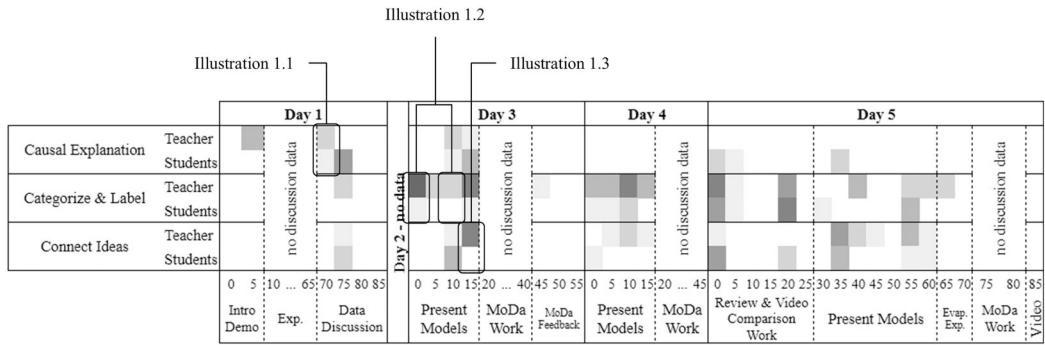


Figure 7. Ms. K and students offer causal explanations, categorize and label, and connect ideas over time. Shading indicates move frequency (light gray: 1, black: 10+). Code frequencies for each 5-minute interval were obtained by counting codes that were applied at the level of turns of talk.

connection by clarifying that even though the theories “are in buckets,” they are related to each other and that some explanations might belong to more than one category (lines 6–8, “crossover”). This marked the origin of “crossover models” in the class. MoDa’s programming environment supports the creation of models that include elements of multiple theories; thus, by validating the comparison and even mixing of conceptual theories, Ms. K again flagged for students the kinds of work they could do in the computational modeling platform they would use.

The cases in Illustrations 1.1, 1.2, and 1.3 characterize Ms. K’s and her students’ work of eliciting/offering causal explanations, categorizing and labeling those explanations, and connecting them to one another in ways that align with the agent-based representational system in MoDa. [Figure 7](#) illustrates that those few cases were not isolated events but rather representative of practices that continued throughout the lesson sequence. From here onwards, throughout the unit, these five conceptual models served as reference points for the explanatory ideas students brought to the unit. Ms. K and her students repeatedly compared and contrasted the ideas with one another and connected them when meaningful ([Figure 7](#)).

Summary of ontological alignment in classroom practice #1

To summarize, the first classroom practice involved Ms. K eliciting and elevating student ideas about particle-level behaviors and interactions, which she and the students then categorized, labeled, and connected with each other. Consistent with the agent-based representational system of MoDa, this practice served to highlight ideas around particle-level activities and interactions. For instance, when Ms. K documented students’ initial explanations ([Illustration 1.1](#)), she elevated those involving particle behaviors and interactions as “really great descriptive words.” This documentation seeded the five conceptual models that Ms. K subsequently presented to the class ([Figure 5](#)), and that became a touchstone for how the class categorized and labeled their ideas for the remainder of the unit ([Figure 7](#)). Each of the theory categories highlighted particle-level behaviors and interactions that could be represented and observed in MoDa (e.g., “attaching” or “not attaching” would be visually obvious in a simulation). Finally, the class began comparing these explanation categories to one another and recognizing that they were not mutually exclusive. Linking theories in this way led to the idea of “crossover” models. By highlighting how theories could include elements from multiple explanations, Ms. K encouraged students to consider ideas and models that aligned with the representational structure offered by MoDa.

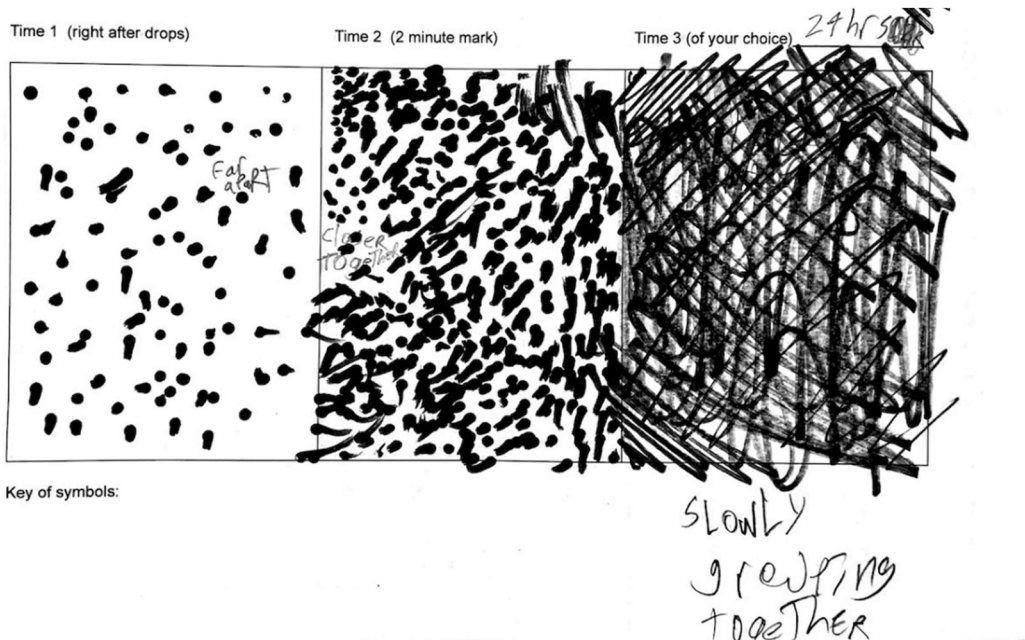


Figure 8. Parker's paper model.

Classroom practice 2: Exploring and testing links between students' conceptual and computational models

The second classroom practice involved exploring and testing links between students' conceptual ideas about diffusion and their computational modeling work, both in the model code and resulting simulations. Below, we present three illustrations to show how this practice was initiated by Ms. K and subsequently taken up by her students.

Illustration 2.1: Preparing students to translate their conceptual ideas into a computational form

The following episode occurred a few minutes after Illustration 1.3 above as students continued to present their paper models on Day 3 of the unit. Ms. K invited one of two students who developed conceptually similar models to explain his idea to the class (Figure 8).

1	Ms. K: Alright. Parker or Jamal, you both had a similar idea. Would one of you be willing to present yours from this board, this idea that the water particles are combining or growing or coming together with the ink particles. Would one of you be willing to explain yours?
2	
3	
4	Parker: In this one, the ink was far apart. In a little bit more time, it was closer together.
5	Ms. K: Did the ink particles increase or break apart? How did there get to be more ink particles?
6	Parker: It slowly increased because the ink particles were splitting apart.
7	Ms. K: So that'll be super interesting to think about when you make this computer model, like how can you take an ink particle and split it apart?
8	

Comparing two paper models developed by two different students, Ms. K pointed out the conceptual similarity between them (lines 1–3). She invited Parker to explain his model to the class. Parker described that the ink was initially further apart (Figure 8, left panel), and then after some time, it was closer together (Figure 8, middle and right panels) (line 4). Ms. K asked him to explain how the total number of ink particles in the model increased (line 5), and Parker's explanation involved the ink particles "splitting apart" (line 6). Aware that there was no block in

MoDa to directly represent this idea, Ms. K asked him to consider how this explanation could be computationally represented. In other words, Ms. K flagged for this student a potential challenge that he would encounter when translating his conceptual model into the computational medium.

Ms. K enacted a similar move during Bailey’s model presentation (excerpted in Illustration 1.2). Bailey’s initial explanation was descriptive rather than causal (“the drops [...] were really staying together near the top [...] And then later, [...] the ink is starting to spread out a little bit more,” lines 1–5). As she did not identify particles or a behavior that they followed, her explanation was not readily programmable. Ms. K followed up by asking for “an explanation for what is causing the food coloring to spread” (lines 8–9). Bailey’s pro-offered response (“I noticed that with the hot, it was moving a lot more versus the cold,” line 10) was still not readily programmable. Accordingly, Ms. K rephrased Bailey’s reply to introduce agent-level behavior (“the heat was causing the movement of the particles,” line 11), making her explanation more conducive to modeling. In this way, Ms. K helped prepare both Parker and Bailey to express/translate their conceptual ideas into a computational form. The class then spent the rest of the day exploring MoDa through four coding challenges and beginning to code their own theories of diffusion.

Illustration 2.2: Highlighting MoDa models as computational representations of students’ conceptual models

Complementing her practices in Illustration 2.1 that prepared students for coding, Ms. K also guided the class in reflecting on how their computer code, once written, represented the conceptual ideas they had been discussing. At the beginning of class the next day (Day 4), Ms. K reviewed the four coding challenges. When reviewing challenge #2, she highlighted the role of the “interact” code block as a container for students’ different conceptual models:

1	Ms. K: And then over here, Challenge 2. Somebody just summarize, what was Challenge 2? Rachel?
2	Rachel: To make the water particles move and interact with each other instead of just moving around.
3	Ms. K: Ok, so instead of just moving around, we want them to actually interact. And this is
4	where we go into, are they infecting each other? Are they growing together? Are they
5	combining? Are they bouncing off each other?

In this segment, Ms. K explicitly linked code blocks to student theories of diffusion, building off one student’s explanation of the “interact” block to emphasize that this is where students could represent any of the five different conceptual models being considered by the class (lines 3–5).

Ms. K devised other ways to help students link their conceptual models and the computational models they developed in MoDa. Using students’ code from their first day of programming, she created what she called a “code cheat-sheet”⁴ of example code for each of the five conceptual models about particle-level interactions (excerpt in [Figure 9](#)). With this “code cheat sheet,” students could see how other students were representing the different theories about particle interactions in code. In addition, Ms. K asked students to save their models by the name of the theory that they were representing (“I want you to rename whatever is, if you are doing explanation 1, explanation 2, you don’t have to type ‘explanation,’ just do ‘ex,’ that’s fine. 3, 4, 5.”). This naming convention gave students yet another opportunity to establish and remind themselves of the connection between their conceptual theory and their MoDa code.

Ms. K’s framing of the expressive power of MoDa—both in discussing the “interact” block and in creating the code cheat sheet—supported students in seeing MoDa and its block library as computational tools to represent their ideas. Indeed, many students found unanticipated ways to

⁴The “cheat-sheet” part of the term “code cheat-sheet” could be seen as problematic even though the resource was created using students’ own models. We retain it to represent the teacher’s work and language with integrity.

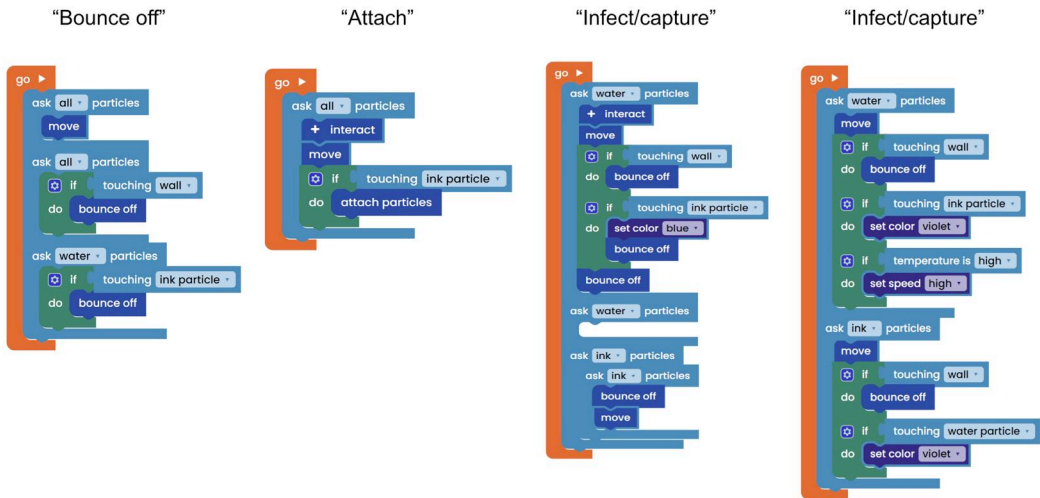


Figure 9. Selected student code from the share-out worksheet: Sample models developed by students for Bounce, Attach, and Infect/Capture Theories.

represent their conceptual models within MoDa. For instance, to begin Day 5 of the unit, Ms. K invited students to share how they computationally represented each of the five different conceptual models. Bailey shared that she had found a way to represent the “infect” theory (Explanation #1):

1	Bailey: I don't think that, our explanation is not really attaching. What we are doing is more
2	like infecting the ink and the water, so the water is capturing the ink, so making the ink...
3	so in our model, the ink goes around and touches the water particle, and it mixes the ink...
4	become more ink... so it's like more like what... this is just what we saw... because
5	Ms. K: So, is a better word, we can call it more like the “infect” model? Do we have an infect in the program?
6	Student: Ya... Yes, I think we do, maybe no, we don't.
7	Student: No no, I don't think so.
8	Student: We have attached or bounce off.
9	Bailey: But you can make it so when particles touch each other, it turns into a different
10	color. Which is like infecting... Whatever the ink particle is touching, it makes a new color.
11	Ms. K: Oh, it makes a new color, ok, so it is like infect. Cool.

Bailey and her partner labeled their model as representing the “infect” theory (lines 1–4). Aware that there is no “infect” block in MoDa, Ms. K asked the class if MoDa included such a block. There was no clear agreement among students on whether such a block was included in the library (lines 6–8). Even though an “infect” block did not actually exist, Bailey’s response made clear that she and her partner had found a way to represent the “infect” theory using the available code blocks. They programmed their model such that when a particle touched another particle, its color would change (lines 9–10), which they saw as conceptually representing the “infect” theory (lines 9–10, “which is like infecting”). Hiding her surprise, Ms. K acknowledged that this way of using the code blocks does computationally represent this conceptual idea (line 11). Here, we see evidence that these students took up the practice of using the computational modeling environment to represent their conceptual ideas, even in the absence of a clear way to do so.⁵

⁵Though her explanation does not (yet) align with canonical science, we also note the remarkable progress in the extent to which Bailey thought about and worked with ideas about particle interactions; in two days working with MoDa, she advanced from a purely descriptive account of diffusion (Illustration 1.2) to a fully agent-based account that she and her partner expressed through innovative coding.

Illustration 2.3: Observing simulations to evaluate theory

Besides linking students' conceptual models with their computational models through code, Ms. K also supported students in learning how to observe their resulting simulations to look for their represented theories. On Day 4, after reviewing the four coding challenges, Ms. K selected a model from each of the five conceptual categories coded by the students to share with the class. She projected MoDa—including the code, simulation, and video areas—to the whole class as she played each model's simulation, creating space for students to familiarize themselves with the different theories and their simulated outcomes, even ones they had not coded themselves.

The episode below begins as Ms. K projected Molly and her partner's model:

1	Ms. K: Pick an ink or a water particle and see what happens.
2	Molly: [] we used the code from making the ink particles and the water particles bounce
3	off each other to make it so that all the particles bounce off the wall just to make it easier.
4	So we haven't brought back more code to make it so that they bounce off each other. So they're not bouncing off each other yet.
5	Ms. K: So they're not bouncing off each other. Do people see it bouncing off the walls?
6	Few students: Yes

In this episode, Ms K directed students to watch an ink or water particle (line 1). One of the model authors, Molly, described their model code to clarify that they were still revising their model—particles in their model did not yet bounce off each other; they only bounced off the walls (lines 2–4). In response, Ms. K directed students' attention to the area where the encoded behavior was expected to occur (line 5) so students could see what the encoded rule of bouncing off the wall looked like in the simulation (line 6).

Ms. K spent the majority of class time on Day 5 repeating this practice of projecting students' models to draw attention to encoded behaviors and collectively observing how they played out in the model. As illustrated by their response in this vignette, students began to adopt Ms. K's suggested observation strategies.

1	Ms. K: [Labeling this pair's model using cues from the name they have used to save the model, "Second attach"] So they're doing kind of an interact and they're attaching, they're
2	doing the attaching theory. Ok, so watch what happens to the particles here. [7 sec pause]
3	What do you notice? What's happening to the particles?
4	Student: What the heck? They're all attaching.
5	Jordan: (unclear) and some of the other ones bounce off, it's kind of weird. Can't make them stay/stick (?)
6	Maddie: Yeah, they attach for ...
7	Ms. K: ^ a short period of time and then they bounce.
8	Maddie: Yeah and then they attach with others and then they
9	Student: Oh, that's kind of the "water and ink particles are mixing but not attaching" [Explanation #2].
10	

Using the name students had saved the model by, "Second attach," Ms. K presented this model as representing the "attach" theory and asked students to attend to the particle interactions (lines 1–4). One student noticed, much to their apparent surprise, that the particles attach to each other (line 5), while another student added that some other particles seem to bounce off one another (line 6). These responses indicate that students picked up the strategies (e.g., "pick a particle" in the previous episode) that Ms. K suggested for observing the simulations at a particle level (line 6, "bounce," lines 7 & 9, "attach," line 10, "not attach") and also began to make observations about aggregate trends (line 10, "mixing"). This exercise of collectively observing models gave students the opportunity to develop strategies to attend to the behavior of particles in the simulation and resulting aggregate trends and to label the models based on their observations. For instance, in the episode above, a student categorized this model under Explanation #2 (line 10, "that's kind

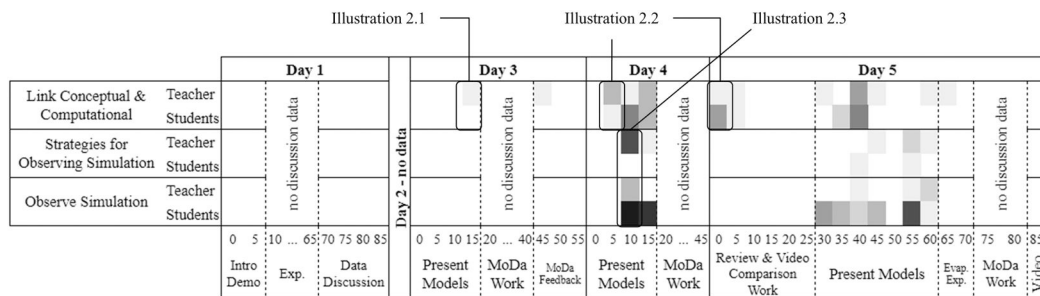


Figure 10. Ms. K and students link conceptual and computational ideas and observe the simulation over time. Shading indicates move frequency (light gray: 1, black: 10+).

of the water and ink particles are mixing but not attaching”), which is different from how the model authors had labeled it.

Figure 10 demonstrates how the cases presented in Illustrations 2.1, 2.2, and 2.3 represent broader classroom trends around linking conceptual and computational ideas and proposing/enacting strategies for observing the model simulation. We note that students’ observation work, especially on Day 5, continued even as Ms. K’s pro-offered strategies for such observations decreased.

Summary of ontological alignment for classroom practice #2

This second classroom practice involved exploring and testing links between the conceptual ideas that arose from students’ paper modeling work and their computational modeling in the remainder of the unit. Even before introducing the class to MoDa, Ms. K flagged for students certain challenges they might encounter when working to translate their conceptual ideas (e.g., Parker’s “growing” and Bailey’s “the hot, it was moving a lot more”) into MoDa; at those moments, Ms. K pushed her students to express their ideas in terms of particle-level behaviors that could be encoded in MoDa (Illustration 2.1). This move served to realign students’ ideas with the MoDa blocks library. Then, once students started expressing their ideas in MoDa, Ms. K helped students structurally map their nascent models back to the five familiar conceptual categories (Illustration 2.2). The “code cheat sheet,” which included model code developed by students in the class, provided concrete examples to help students identify the various theories within MoDa code, even theories they did not program themselves. By asking students to name their models with the theory number, Ms. K presented another opportunity for students to reevaluate and label their computational artifacts using their own conceptual ideas. One student, Bailey, took this translational practice to heart, finding a way to represent her “infect” theory in a way that even Ms. K didn’t anticipate and, in the process, illustrated how she was beginning to think about diffusion in terms of the representational tools available in MoDa. Finally, as the class began watching simulations of different student models, Ms. K’s prompts to attend to specific aspects of the model (“watch what happens at the wall” or “pick a particle”) drew students’ attention to how each encoded theory played out in simulated behavior. This practice added yet another way for students to explore and test how their conceptual ideas about particle-level behaviors and interactions were embodied in their computational models.

Classroom practice 3: Drawing on evidence resonant with the representational system of the tool to differentiate between theories

This practice involved Ms. K leveraging evidence that was tied to claims about particle-level behaviors and interactions to help students discriminate between their modeled theories. Here,

our intention was to facilitate connections across instructional materials including the computational tool as well as external resources. Thus, we observe Ms. K leveraging evidence both within and across the platform and external resources. We share two illustrations of this practice: 1. comparing the model and video data and 2. strategically selecting evidence to refute an argument. By pointing out areas of agreement and disagreement to converge to a normative explanation for how ink spreads in hot and cold water, this practice emphasized the accountability of scientific theory to evidence.

Illustration 3.1: Matching the computational model and video data

On Day 4, Ms. K asked students to “compare your [their] code to the video experiment and see what does work with your model and what does not work.” After students worked in pairs for about 20 minutes, Ms. K brought the class together to present their models. In the vignette below, she projected Marina and Jordan’s model that the students had labeled as representing the infect theory⁶ and asked them, “How is your model different than the video”?

1	Marina or Jordan ⁷ : Well, it keeps going, it doesn’t stop after a certain amount of time.
2	Because, you know, all videos end, but
3	Ms. K: Oh you’re right, your model keeps when the video stops. Good point. What else?
4	Marina or Jordan: They are not the same color.
5	Ms. K: Yeah, one is orange. Pasha is going to change his ink to orange just to connect it.
6	Anything else that you noticed about the diffusion on the right (<i>points to the video</i>) versus
7	the diffusion on the left (<i>points to the simulation</i>)? Anybody else, too, can add in. Molly?
8	Molly: The diffusion on the right, I kind of noticed that it didn’t soak very well. That might
9	just be because the video wasn’t as long.

Watching the model simulation of the “infect” theory side by side with the video led students to notice differences between the two (e.g., duration, lines 1–3; color, line 4; saturation, lines 8–9), only some of which were relevant to the phenomenon. Students attempted to account for these differences in terms of the set-up (e.g., a different ink color; the video stops, whereas the model continues indefinitely). Their statement about the length of the video was indicative of their recognition of the emergent nature of diffusion, namely that it took time to unfold. This emphasis on matching simulated and experimental conditions was common throughout Days 4 and 5 of the unit (Figure 11).

However, students did not yet attribute differences between the modeled “infect” theory and the video data to the underlying theory itself. In this instance, simply observing the simulation and video side by side did not give students enough evidence at the level of particle interactions to reliably refute the “infect” theory, which had become the most popular theory in the class. In the teacher interview following this lesson, Ms. K explicitly discussed this tension:

10	Ms. K: ... when you run the computer model with infect, it looks like it works. It’s more
11	convincing because, like diffusion, your water goes from clear to blue with the naked
12	eye. And in the infect model, the water particles go from gray or clear to blue at the particle level, so that matches the real world.

Ms. K recognized that the MoDa video data by itself would not invalidate the “infect” theory based on a visual comparison (lines 10–12). In her interview, she then discussed how this tension

⁶Following Ms K’s prompt of saving their model by a name that labeled the theory they were representing, this pair had saved their model as “final explanation 1 pt. 2”. Explanation 1 came to be referred to as the “infect theory” in this class.

⁷Given the similarity of their voices and the camera focus on Ms K, we cannot distinguish precisely which student spoke each line.

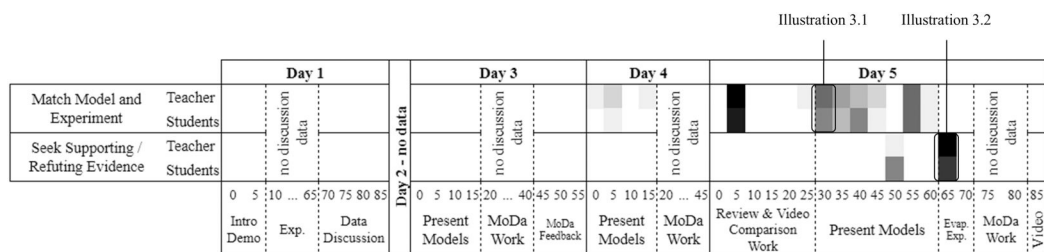


Figure 11. Ms. K and students match the model and video data to seek supporting/refuting evidence over time. Shading indicates move frequency (light gray: 1, black: 10+).

led her to identify an external source of data (the evaporation experiment) to challenge the popular “infect” theory.

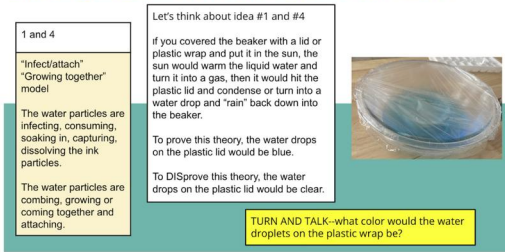
Illustration 3.2: Strategically selecting evidence about particle-level interactions

By Day 5, students’ commitments remained divided between the infect and bounce-off theories, with the “infect” theory remaining the most popular. In close collaboration with the in-class researcher, who is the third author of this paper, Ms. K modified the unit design to introduce a new data source: an experiment that would help refute the underlying claim about particle interactions in the “infect” theory.

After the model presentations shared above, Ms. K asked the class how they could test their idea that “the water has been fully infected with blue ink.” Students came up with several different ideas: “evaporating,” “look[ing] at it in a microscope,” and using “a really, really fine strainer.” Ms. K then projected a slide showing an evaporation experiment in which a dish of water mixed with blue dye was covered with plastic “Saran” wrap (Figure 12, left). She asked students to discuss with their partners what color the water particles on the plastic wrap would be when the covered dish was placed in the sun.

1	Ms. K: Ok, let’s go with the evaporation [1] (<i>Projects a slide with blue ink and water in a beaker with plastic wrap</i>). And, here we go, so if we put Saran wrap on top of the blue ink
2	and water mixed here (<i>pointing to the bowl in Figure 12</i>), if we put that in the sun, what do you think is gonna
3	happen?
4	Student: Precipitation
5	Ms. K: What is gonna happen to the Saran wrap, turn and talk to your partner. (<i>Students</i>
6	<i>discuss</i>) Alright, so what should happen if we put this in the sun, what is gonna happen?
7	Student: Water would go.
8	Ms. K: Where would the water go?
9	Student: To the top (<i>other students talking</i>)
10	Ms. K: Ok, it would go to the Saran wrap. What color would it be?
11	St: Blue
12	Ms. K: Hey, it should be blue if the infection theory is correct. If the water is not blue on the
13	top of the Saran wrap, what does that mean?
14	Student: That the infection theory ...
15	Ms. K: (<i>points to a student</i>) That the infection theory is not correct. (<i>Projects slide showing</i>
16	<i>an image of clear water on the plastic wrap; Figure 12, right</i>). What color is the water?
17	Students: Not blue.
18	Ms. K: It is not blue, it’s clear. So does the ink infect or get captured by the water?
19	Students: No
20	Ms. K: No. (<i>X appears on the theories 1 and 4 on the slide; Figure 12, right</i>) So, is this
21	infecting theory correct?
22	Students: No.
23	Ms. K: So, what are we left with? [<i>multiple student voices</i>] So we are left out with this explanation about the water
	and the ink particles are mixing, but not attaching, and the water particles are bouncing off the ink particles, or
	there is something going on with density. And what do I want you to do? I want you to go back to your
	models and see if you can turn out the infection and turn in the particles, go back and fix your models.

Explaining Diffusion....Let's recap.....Explanation #1 and #4



1 and 4

"Infect/attach" "Growing together" model

The water particles are infecting, consuming, soaking in, capturing, dissolving the ink particles.

The water particles are coming, growing or coming together and attaching.

Let's think about idea #1 and #4

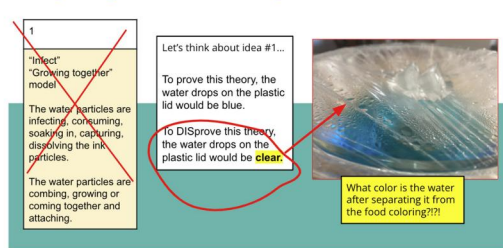
If you covered the beaker with a lid or plastic wrap and put it in the sun, the sun would warm the liquid water and turn it into a gas, then it would hit the plastic lid and condense or turn into a water drop and "rain" back down into the beaker.

To prove this theory, the water drops on the plastic lid would be blue.

To DISprove this theory, the water drops on the plastic lid would be clear.

TURN AND TALK--what color would the water droplets on the plastic wrap be?

Explaining Diffusion....Let's recap.....IDEA #2



1

~~"Infect" "Growing together" model~~

~~The water particles are infecting, consuming, soaking in, capturing, dissolving the ink particles.~~

~~The water particles are coming, growing or coming together and attaching.~~

Let's think about idea #1...

To prove this theory, the water drops on the plastic lid would be blue.

To DISprove this theory, the water drops on the plastic lid would be **clear**.

What color is the water after separating it from the food coloring?!!

Figure 12. Ms. K's slides of the "Saran wrap" evaporation experiment set-up (left) and results (right).

Table 3. Sample student responses to the reflection worksheet.

Marina	"At first I thought that the correct theory was Explanation #1 [the infect theory] but what changed my mind was when we evaporated the water and food coloring and the water was clear. At first, we modeled the infecting theory, but we changed it to the bounce theory."
Morgan	"... Now I understand that the ink mixed in with the water but it did not infect or attach, they just bounced. I learned this when we saw the evaporation experiment."
Marcy	"... After that, I thought that it was more like ex #1 [the infect theory] because I thought that it was dissolving the ink into the water particles. Now I think it's ex #2 [the mixing theory] because of the water evaporating and it being proven that it's not ex #1 or #4 [the infect theory]."
Molly	"... What changed my mind was that if you evaporated the water, the droplets were clear."

In this whole-class discussion, Ms. K built on students' ideas and strategically brought in new evidence to invalidate a theory that could not be disproved within MoDa itself. Here again, Ms. K was operating from an understanding of the strengths and limitations of the kind of computational agent-based modeling possible within MoDa and finding ways to support students where it fell short. This was a powerful moment for many students, as evidenced in their reflection worksheets. Of the 18 consented student responses from the class, seven students explicitly alluded to the evaporation experiment as changing their minds. A sample of five student responses (Table 3) illustrates how this evidence shifted their thinking.

Because the "infect" theory was one of the most popular theories in class, the evaporation experiment played a powerful role in shifting many students' thinking. As seen in student responses, evidence from the evaporation experiment convinced them that the ink particles were not infecting water particles. This specific evidence successfully led students to reconsider their ideas because it directly addressed their theory about the nature of interactions between ink and water particles.

Summary of ontological alignment for classroom practice #3

Classroom practice three involved matching or selecting empirical data to compare with computational simulations to support or refute modeled theories. As students compared their simulations to the empirical video data, it was evident that they were starting to make sense of the emergent nature of the phenomenon (e.g., their requests for a longer video to see diffusion run to completion). When matching video data to their simulations, students attended to some dimensions (e.g., duration, speed) that were relevant to the target phenomenon but also to other dimensions (e.g., color, pathway) that were not. It could be that commitment to a sense of esthetic alignment with the video data somewhat interfered with establishing stronger ontological alignment. As evidenced by her interview, Ms. K recognized this shortcoming of the available video data and worked with the third author, a researcher in the classroom, to identify a data source that would more effectively challenge the "infect" theory's claims about particle-level

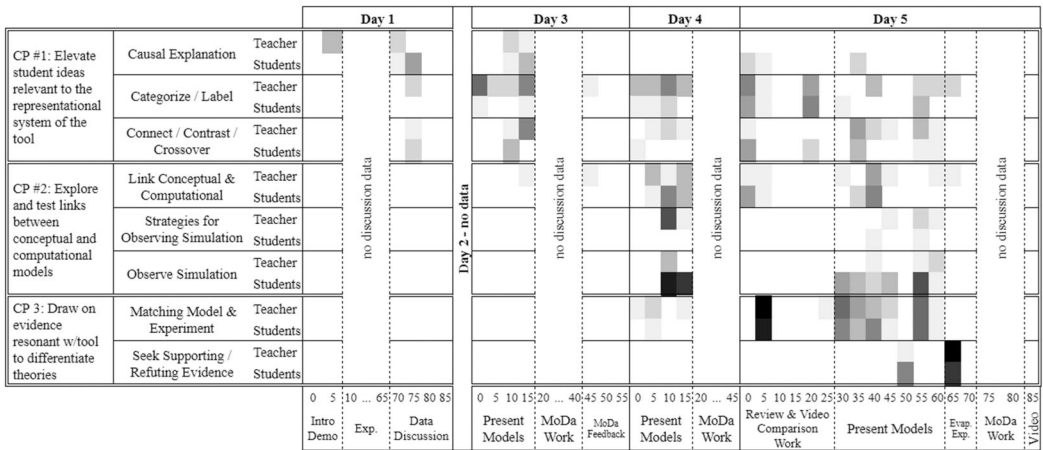


Figure 13. Time series over the unit. Shading indicates move frequency (light gray: 1, black: 10+).

interactions. This external data source played a powerful role in unsettling students' commitments to the "infect" theory as the explanation for how ink spreads in water. In these two illustrations, Ms. K revealed ontological alignment in her awareness of the specific kinds of evidence that would serve to validate or invalidate students' claims about particle-level interactions in the model.

Relationships between practices over time

The illustrations above characterize how Ms. K initiated the three classroom practices and how students took them up. Figure 13 shows when each classroom practice and corresponding move first appeared and how it was appropriated by the class over the unit. In what follows, we highlight some of the key relationships between the classroom practices and how those relationships developed over the course of the unit.

Over the four days of our data corpus, we see a shift in the epicenter of classroom practice. On Days 1 and 3, the teacher and class primarily engaged in CP#1 as they generated explanations for the phenomenon and categorized and drew distinctions between them. Once the class began working with MoDa on Day 4, the focal practice shifted to CP #2 as the class explored and tested links between their existing conceptual theories and the newly generated computational models. Finally, on Day 5, Ms. K and the class focused their attention on CP#3 as they matched the video data with their models and identified external evidence to support or refute their theories.

Even as the focal classroom practice changed over time, it did not replace previously established ones. For example, as Ms. K led the class in connecting conceptual ideas and computational representations (CP#2) on Day 4, the class continued to categorize and label models and connect them to one another (CP#1). Similarly, while they focused on using evidence to distinguish between theories (CP#3) on Day 5, the class continued to express ideas about particle interactions (CP#1) and link conceptual ideas and computational representations (CP#2), often without overt prompting from the teacher (see lower teacher frequency in those practices, Figure 13). We interpret these consistent co-occurrences as indicative of the ways the three classroom practices—and related moves—support and build upon one another; linking scientific ideas to code or identifying them within a simulation (CP#2) typically involves labeling those concepts (CP#1), often using the phrases selected by Ms. K to emphasize causal relationships (also CP#1). Matching a model to video data (CP#3) involved identifying certain concepts within that model (CP#2) and comparing the video data to how those concepts play out in the simulation (also CP#2).

Across the unit, there is also a shift in who performs each practice. While Ms. K initiates many of the practices, students take them up and come to enact them somewhat independently. For example, whereas on Day 1, Ms. K prompted students for causal explanations (CP#1), students offered such explanations organically, without prompting, when making sense of diffusion on Day 5. Likewise, once Ms. K initiated CP#2 on Day 4, the class repeatedly linked their conceptual ideas with the computational models as they observed their peer's simulations on Days 4 and 5.

Notably, the four days of classroom activity represented in the visualization are, nominally, the same: from the perspective of the instructional sequence, all were periods of “presenting models,” that is, whole-class discussion around student-generated artifacts, be they paper or computational models. However, the practices that Ms. K modeled and the class took up clearly evolved over time. We interpret this shift as likely influenced by 1) the change in the media used for modeling (from paper to computational models) and 2) the instructional sequence itself, which shifted focus from representing student ideas with computational models to comparing those models with real-world data to converge on a canonical explanation for diffusion.

Discussion

In this manuscript, we examined (RQ1) the practices an experienced science teacher used to ontologically align students' ideas with the representational system of the modeling tool and (RQ2) how students took up these practices through the unit. Based on analysis of whole-class video data, we presented three practices adopted by both the teacher and students:

1. Elevate student ideas relevant to the representational system of the tool.
2. Explore and test links between students' conceptual and computational models.
3. Draw on evidence resonant with the tool's representational system to differentiate between theories.

For each practice, we identified associated moves that the teacher and students enacted as they engaged in a computational agent-based modeling unit about diffusion. Each practice and its associated moves manifested ontological alignment—that is, identifying points of resonance between students' existing ideas and the representational system of the tool. Moreover, the three practices together linked students' conceptual models, their computational models, and real-world evidence to explain the target phenomenon (Figure 14).

The first classroom practice elicited and underscored student ideas about particle-level behaviors and interactions in alignment with MoDa's and the unit's representational system. For example, Ms. K organized students' initial explanations of data trends into five conceptual models (Illustration 1.1) that became touchstones for reference and comparison throughout the unit. Ms. K and, later, students used these conceptual models to label students' work (Illustration 1.2), laminating each conceptual model and later linking it to computational representations. Categorizing and labeling models also enabled students to compare and contrast their ideas with each other, a practice initiated by a student (Illustration 1.3). Collectively, these moves leveraged students' existing ideas and made them available for the class to reuse and link to the computational abstractions they would create later. In doing so, this classroom practice privileged students' ideas that aligned with the representational system of the unit and made them available for use as an entry point into the computational tool (e.g., Sengupta et al., 2018).

The second classroom practice provided opportunities for students to explore and test links between their conceptual and computational models. For instance, as students presented their paper models, Ms. K flagged interactions and mechanisms they could expect to see (or not) when programming their models in MoDa (e.g., Illustration 2.1). This move foreshadowed connections

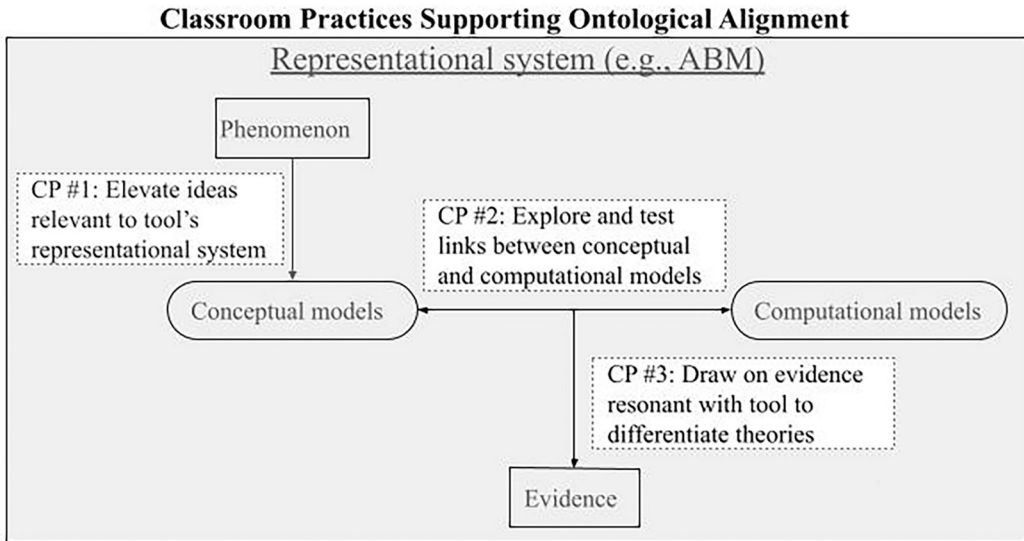


Figure 14. Roles of classroom practices (CP) in scientific sense-making with a computational modeling unit. Rectangles are resources, ovals are student artifacts, and dashes are classroom practices.

between students' conceptual models and the computational models they would soon build. Conversely, Ms. K also made space for students to link their developing computational models back to their conceptual models. For example, positioning MoDa's "interact" block as one in which students could program behaviors to represent their conceptual models (e.g., "infect" or "bounce off") helped students identify the code block as one in which they could encode these multiple explanations. Moreover, sorting students' early computational models into categories on the "code cheat sheet" established how students' conceptual models could be computationally represented. Such bi-directional linking of conceptual and computational models enabled students to use the representational system of MoDa to represent and test out their own ideas about how diffusion works. Indeed, one student even invented a way to express a conceptual model in a way that neither Ms. K nor the model and curriculum designers had anticipated (e.g., Bailey's model in Illustration 2.2), where this innovation went on to become the most popular model in class. Finally, Ms. K offered students strategies to identify their conceptual models within the simulation in ways that highlighted the level of analysis available in the tool (e.g., Illustration 2.3). This move supported students in verifying how a conceptual model, represented in code, played out in the simulation. Together, these three moves solidified links between students' own ideas, their conceptual models, and the computational models they were building and refining. Prior work has noted that mapping code to content in this way can be challenging for students (Basu et al., 2016). By using the representational system of the tool as a foundation for this mapping, Ms. K made these connections more accessible to students.

The first and second practices maintained conceptual space for students to consider a range of explanations to account for their observations of the experiment and video data. On the other hand, the third practice drew students' attention to evidence resonant with the tool's representational system to differentiate between the various theories they proposed. For instance, when MoDa's video data failed to provide evidence refuting the claim that particles were infecting each other, Ms. K devised a thought experiment to speak directly to this claim (Illustration 3.1) and asked her students about the kinds of evidence that would support or refute this claim (Illustration 3.2). While prior work has identified discrepancies between models and data as productive for sense-making more generally (e.g., Blikstein et al., 2016), this classroom practice highlights the value of using evidence responsive to students' claims.

Finally, the heat map analysis illustrated how Ms. K's moves shaped whole-class discourse beyond her or a student's initial introduction of them. Students continued to enact each classroom practice even after Ms. K stopped prompting or modeling it overtly (Figures 7, 10, and 11). Though the focus of activity migrated across the practices as the unit progressed, the earlier practices remained (Figure 13). We interpret these two trends together as suggesting a somewhat sustained ontological alignment between the tool's representational system and students' scientific sense-making.

Responding to calls for thinking carefully about how to support students by making the representational system of tools visible (e.g., Su et al., 2023; Wilkerson et al., 2018), we describe how a teacher can provide this support. Our work positions ontological alignment as an important construct in supporting discourse around the use of innovative computational modeling tools for sense-making. In the work described here, classroom practices around ontological alignment were not a set of sporadic, one-off practices used to introduce a new tool in the classroom. Instead, this expert teacher repeatedly aligned and realigned students' conceptual and computational models and drew on real-world evidence resonant with the representational system of the tool to validate or refute those models. Similar to how Sengupta et al. (2021) traced a teacher's use of classroom norms to manage the heterogeneity involved in the scientific and computational enterprise of modeling, we investigated how a teacher was responsive to the heterogeneity of student ideas in the context of the tool's representational system. Moreover, the recurrence of these moves resonates with existing literature on establishing sustained practices for science learning (e.g., Pierson & Clark, 2019).

Our findings focused on students' sense-making about the particle interactions that gave rise to an emergent phenomenon, because that is where the work around establishing ontological alignment happened in this class. Our analysis didn't focus as much on how students' attention to these particle-level interactions supported their sense-making of emergent patterns at the aggregate level, though this trend has been well-documented in the literature (e.g., Samon & Levy, 2017; Sengupta and Wilensky, 2009; Wilensky & Reisman, 2006).

Finally, we acknowledge that the tool and the phenomenon are inextricably related to each other. For instance, the unit and model blocks we presented were built on previous work that established the fit between the phenomenon and the representational systems of agent-based modeling (Fuhrmann et al., 2022). Because the tool was provided to the teacher, our analysis and findings emphasized how she supported discourse that was ontologically aligned with the tool. However, we do not see the selection of the representational system of a tool as independent of the phenomenon. Instead, it depends on a careful consideration of which representational system best highlights the phenomenon's mechanistic explanation and supports the key science learning goals.

Implications of ontological alignment

We argue that ontological alignment and the specific practices presented here have implications beyond their use in the learning environment described in this paper. For instance, they can be applicable to other representational systems such as systems modeling (e.g., Sage Modeler) or data modeling (e.g., CODAP). While the substance of student investigations would differ, the work of finding points of resonance between students' ideas and the tool's representational system would still be important.

Our work also highlights the importance of attuning teachers to the representational system of the tool, its corresponding learning objectives, mapping and fit with the phenomenon, and how they play out in both tool and curriculum design. Doing so can better prepare teachers to support their students and make the representational system of the tool visible for more productive engagement with modeling. Ontological alignment also raises the call for designers to consider

why a particular tool and representational system are a good fit for a phenomenon of study. Finally, our work provides recommendations for ways in which teachers can respond to student ideas in the classroom. In particular, teachers could attend not only to students' utterances but also to their constructed physical and computational artifacts as a way to cultivate scientific sense-making aligned with the representational system of the tool.

Limitations and future work

We acknowledge the limitations of this work, especially in regard to investigating student uptake of the moves through which the focal teacher supported ontological alignment. While whole-class discussion data illustrated how tightly coupled exchanges between the teacher and her students shifted over time, they omitted significant swaths of class time when students were working alone or in pairs to refine their models. An analysis of pair discourse during modeling work (vs. solely during whole-class discussion and presentation time) could provide a clearer picture of the ways students adopted and adapted the focal moves to reason about the phenomenon of interest in terms of the tool's representational system.

Finally, we suspect that the three classroom practices presented above do not capture all the ways in which teachers support ontological alignment in class. Our hope is that naming ontological alignment as a construct can support further research around investigating ways to be responsive to the heterogeneity of student ideas in the context of the representational systems in science. While this study focused on ontological alignment for a particular computational modeling platform, the construct may be useful for similar investigations of other epistemic tools (e.g., data tables, particular modes of gesture, and concept mapping tools; Stroupe et al., 2019). We can also imagine ontological alignment providing a methodological lens for characterizing classroom discourse around epistemic tools in science. Going forward, we hope ontological alignment can help illuminate the work that teachers are doing at the intersection of student ideas and particular epistemic tools and offer new approaches to teacher learning that emphasize the resonances between students' ideas and the tools and practices of science.

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