CHEMISTRY ON THE CLOUD: FROM WET LABS TO WEB LABS

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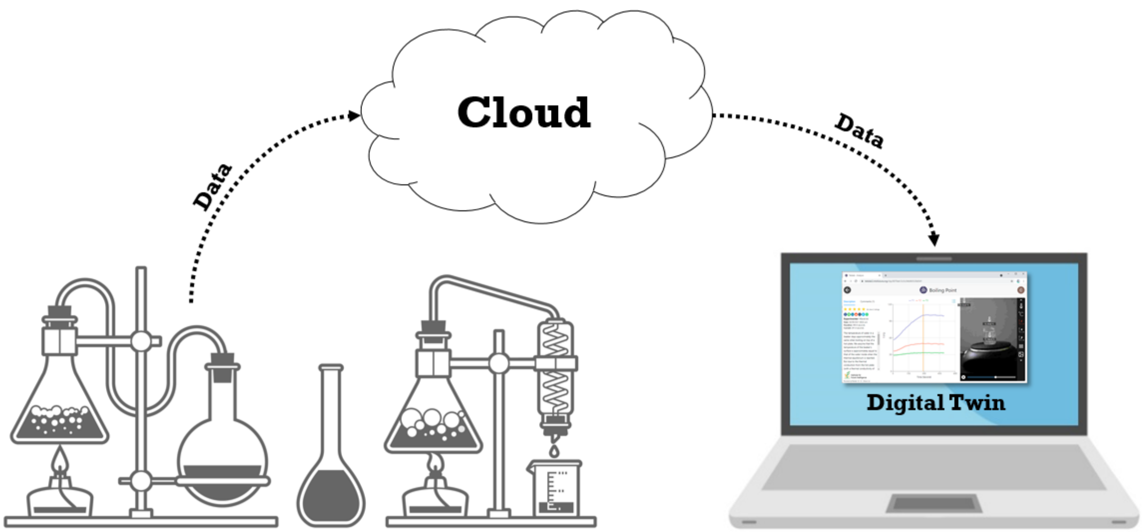
ABSTRACT: Electronic sensors allow people to collect a large quantity of data in chemistry experiments. Using infrared thermography as an example, we show that this kind of data, in conjunction with videos that stream the chemical phenomena under observation from a vantage point, can be used to construct digital twins of experiments to support science education on the cloud in a visual and interactive fashion. Through digital twins, a significant part of laboratory experiences such as observation, analysis, and discussion can be delivered on a large scale. Thus, the technology can potentially broaden participation in experimental chemistry, especially for students and teachers in underserved communities who may lack the expertise, equipment, and supplies needed to conduct certain experiments. With a cloud platform that enables anyone to store, process, and disseminate experimental data via digital twins, our work also serves as an example to illuminate how the movement of open science, which is largely driven by data sharing, may be powered by technology to amplify its impacts on chemistry education.

GRAPHICAL ABSTRACT:



KEYWORDS: High School / Introductory Chemistry, First-Year Undergraduate / General, Laboratory Instruction, Inquiry-Based / Discovery Learning, Internet / Web-Based Learning, Constructivism, Phases / Phase Transitions / Diagrams, Physical Chemistry, Reactions, Thermodynamics

INTRODUCTION

Science experiments often rely on sensors to collect data. Electronic sensors allow people to gather a large quantity of raw data. Traditionally, these data are kept as original records to back some scientific claims. In many cases, the data are used only by the experimenters themselves and may be forgotten or discarded after some time. The purpose of this paper is to uncover the educational potential of these data and present our work on harnessing their value.

Our research was inspired by the technological advancements in the Internet of Things (IoT), particularly with regard to digital twins. In the field of IoT, a digital twin can be loosely defined as a virtual counterpart of a physical object or process[1]. It consists of three essential elements as the bare minimum: 1) a virtual representation of the object or process, 2) a stream of sensor data measuring the change of the object or process's state that the virtual representation maps to, and 3) a mechanism to update the virtual representation with the sensor data[2]. Digital twins play a vital role in Industry 4.0[3]. Likewise, they can also be used to transform science labs.

Theoretically speaking, a chemistry experiment is a process in the material world that can be somehow mirrored on the cloud using the digital twin technology if the experiment is augmented by all the three technical elements mentioned above. But to justify the introduction of this concept to chemistry education, we must first ask: What can students and teachers do with digital twins of experiments that is otherwise unattainable?

This paper starts with attempts to answer the above question, followed by a technical framework for setting up digital twins of chemistry experiments. Based on the framework, we suggest a few educational applications that leverage the affordances of digital twins to support learning and teaching. We then present a reference implementation of the framework that we have developed based on using an infrared thermal camera as a versatile chemical sensor[4-6] and provide concrete examples to demonstrate the educational viability of digital twins. Finally, we conclude this paper by discussing the implications of our work.

EDUCATIONAL AFFORDANCES OF DIGITAL TWINS

Learning and teaching through experiments are fundamentally important in chemistry education[7]. Just like applications of digital twins in other fields, a chemistry experiment equipped with a digital twin can engender additional learning and teaching opportunities that would be difficult to provide without such a cyber-physical linkage. These educational affordances include, but are not limited to, 1) a digital twin permits an experiment to go online in an interactive form, such that students who are not present can participate in the experiment to some extent through the Internet; 2) a digital twin can live on indefinitely as a data-rich resource on the cloud even after the experiment ends, such that anyone with access can still retrieve the complete details of a past experiment for further analyses; and 3) a digital twin can be easily cloned, edited, and redistributed on the cloud by any authorized user, such that the encapsulated data can be shared, reused, and aggregated to support a community of practice[8] on a given topic.

We are aware and in support of the policy position of the American Chemical Society that states "computer simulations that mimic laboratory procedures have the potential to be a useful supplement to student hands-on activities, but not a substitute for them"[9]. But it needs to be clarified that, although digital twins of experiments rely on virtual representations to provide information to students in a way similar to simulations, they are by definition tied to a current or past experiment. In that sense, it can be argued that digital twins can actually open up new possibilities to increase authentic experimental content in the curriculum, rather than eroding it. Through digital twins, a significant part of laboratory experiences such as observation, analysis, and discussion can be delivered on a large scale. Thus, the technology can potentially broaden participation in experimental chemistry, especially for students and teachers in underresourced communities who may lack the expertise, equipment, and supplies needed to conduct certain experiments.

From Wet Labs to Web Labs: A Technical Framework

Digital twins in real-world applications can be very complex and expensive to construct. In this section, we propose a practical framework for building digital twins for chemistry experiments. As illustrated in Figure 1, this technical framework consists of three parts: the Wet Lab, the Web Lab, and the IoT Layer that couples them. A Web lab in the context of this paper refers to a virtual representation of a wet lab (not to be confused with a pure simulation lab that has never been connected to a real-world counterpart through IoT data links). The reason that we aspire to this term is because we expect a digital twin to provide a highly interactive user interface, so much so that it can mimic some rudimentary laboratory experiences in the corresponding wet lab and even create a sense of telepresence through remote control and immersive technologies.

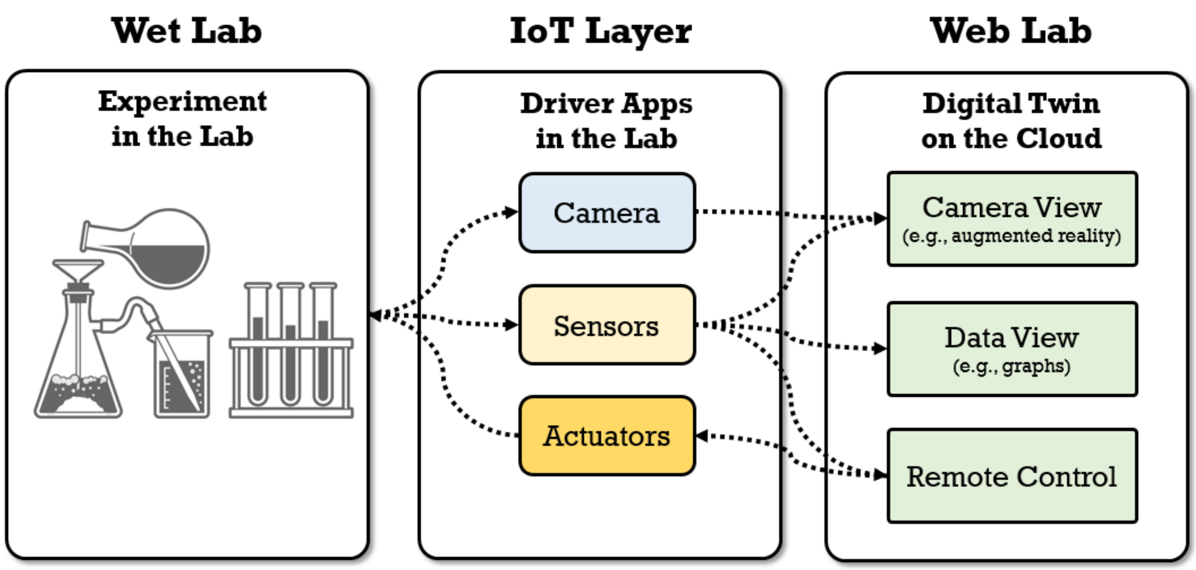


Figure 1. A conceptual framework for building practical digital twins of chemistry experiments. The rationale and details are provided in the following subsections. Note: Technically, a camera is also a sensor, but we single it out as a special case because it can be used to implement augmented reality.

Sensing Wet Labs

A digital twin requires using one or more sensors to collect data on an ongoing basis from a physical thing that can be subsequently processed and mapped onto the corresponding virtual representation. In this way, anyone looking at the digital twin can immediately get an idea about what is happening out there in the real world. The technology fits science labs very well, because sensors are already used to measure physical or chemical changes over time or space in many experiments. Even in science education, sensors have also been widely used as inquiry tools[10]. Most sensors can now be connected to a computer or a smartphone for data storage and visualization (the resulting apps are sometimes dubbed “probeware”[11]). If the manufacturer of a sensor also provides an application programming interface (API) for a third party to extract the raw data, an app can be developed to capture and transmit the data to a cloud database for use in a digital twin. As it stands, augmenting sensors with digital twins seems a logical next step of innovations for science labs if we can find a practical way to build the matching virtual representations.

Building Web Labs

If a chemistry experiment can be conducted on a lab bench, we can simply create a virtual representation of it by using a camera to capture the scene from a vantage point, streaming the images to the cloud, and displaying the livestream in a window within the client's Web browser. Unlike other types of digital twins that rely on a computer model to represent the evolving state of an object or process in the real world, using a video stream as a virtual representation has the following advantages: 1) *Cost-effectiveness*: there is little to no cost for producing it as no computer modeling is required; 2) *Realism*: the video contains many real-world details of an experiment, including noises and errors that are inevitable in a lab; and 3) *Generality*: the method can be applied to many types of experiments and used by anyone with a smartphone and a broadband connection for shooting and streaming videos. Moreover, using a video stream to represent an experiment does not mean that it cannot be enhanced with computationally generated elements. For example, computer vision can be used to recognize certain objects in the scene or even estimate their real-world sizes to automatically generate a geometric model. Similar to augmented reality (AR), we can also use the video stream as a backdrop and add virtual tools on top of it to support intuitive user interactions with the experiment, such as selecting a virtual sensor to view the data supplied by its real counterpart. Other representations such as graphs can be added to visualize the temporal evolution or spatial distribution of incoming sensor data and even the results of analysis based on mining these data (data visualization and analytics are often touted as a value proposition of digital twins that supplements their physical counterparts).

Coupling Wet Labs and Web Labs

Part of the appeal of digital twins comes from their novelty in organizing, processing, and presenting various types of sensor data gathered from the real world, sometimes known as the homogenization of data. Without a digital twin as the unifying model, these heterogeneous data would be isolated from one another. In our framework for digital twins, data from an experiment can still be collected, managed, and transmitted separately by multiple driver apps deployed in the wet lab to connect and control individual sensors and actuators. But even though they may run on a variety of devices such as a computer, a smartphone, or a Raspberry Pi in the lab, these driver apps can all livestream the timestamped sensor data through the Internet to the digital twin. The digital twin then synthesizes the data and uses the results to update its virtual representation, resulting in the synchronization of state with the experiment in the real world (in terms of the state variables being monitored by the sensors, of course). Thus, anyone who accesses the digital twin automatically gets a copy of the latest data and comes to the same page of the experiment. This synchronization is the reason why an experiment can be shared with others in real time through its digital twin.

Educational Applications of Digital Twins

In typical experiments, students propose testable hypotheses, plan investigations, perform hands-on procedures, observe phenomena, collect data, analyze results, and write lab reports. Digital twins of experiments support a substantial part of this scientific process in a virtual learning environment, such as observation and analysis that are fundamental science practices. The persistence of an experiment in the form of its digital twin also gives rise to additional learning and teaching possibilities. In the following subsections, we outline a few educational applications.

Digital Twins in Synchronous and Asynchronous Experiments

As in the case of online instruction[12], digital twins can afford both synchronous and asynchronous modes of learning and teaching. In the synchronous mode, students interact with the digital twin of an ongoing experiment conducted by the teacher (or a lab assistant). They are in the same virtual workspace, though not necessarily at the same physical location, at the same time. Their learning paces are typically orchestrated by the teacher as the experiment unfolds. In the asynchronous mode, students access the digital twin of a previous experiment in different times and spaces and carry out observation and analysis at their own paces. Such a previous experiment can be conducted by the teacher or anyone else in the past. Although asynchronous experiments may be less dramatic than synchronous ones, they are generally more flexible to adopt.

It is important to note that digital twins are not limited to supporting remote labs. As a matter of fact, many demo experiments that chemistry teachers routinely perform in the classroom to entice students may be transformed into synchronous or asynchronous experiments enhanced by digital twins. Even in the case where all the students are present, they are typically not offered hands-on opportunities in a demo experiment. But they can interact with its digital twin on their own computers. In this way, they may become more involved in the experiment than passively watching it from a distance. Furthermore, they are automatically given a copy of the digital twin of the experiment for their own analyses and records after it ends, making it more useful than just a demo.

Digital Twins as Intellectual Properties of Students

When an experiment ends, its digital twin does not necessarily vanish (unlike the physical counterpart). Since a digital twin is stored on the cloud, it can always be revisited by anyone with an access right at any time. Hence, a digital twin of an experiment can become an intellectual property that can be "shown, discussed, examined, probed, and admired"—as advocated by Papert in his constructionism theory[13]. This attribute of digital twins may be leveraged to motivate science learning through challenging students to design their own experiments to prove or disprove a hypothesis. Experiment design is an indispensable part of science investigation that has been underexplored in science education. This may be partly due to the fact that, unlike engineering design and computer programming that generate demonstrable products personally relevant to students, experiment design tends to generate only abstract science knowledge for the sake of generalizability. Through a quest that converges at the abstract knowledge, experimental details and personal relevance fade away, leaving no well-defined artifact as a "take-home" end product for students to own and share. Digital twins of experiments may offer presentable and personalizable products that record students' very own processes of scientific discovery and preserves important details that matter to them. By enabling and engaging students to produce digital twins of experiments as their own intellectual properties that can be shown to others, science learning can also take advantage of the psychological and cognitive effects of constructionism.

Digital Twins for Learning in Open Science Environments

Open science is a movement to make scientific research and its dissemination accessible to all citizens. The same spirit of open science that is responsible for accelerating research[14], such as sharing, critique, and collaboration, can promote the learning of science among students as well. In open science, open data plays a key role. With a cloud platform that empowers anyone to easily store, process, and disseminate experimental data via digital twins, open science can take root in schools. As digital twins live on the cloud, we can catalog them as open resources for sharing among learners interested in certain topics. For example, digital twins generated by a class of students can be used to create interactive displays in a virtual gallery walk in which students review and discuss one another's experiments using analysis tools, online chats, or comment areas. The openness even makes it possible for students to collect a set of digital twins and perform meta-analyses based on aggregating and stratifying data distilled from them. This meta-analytical capability on the cloud creates collaborative learning opportunities when used in conjunction with a divide-and-conquer strategy that enlists a group of students to crowdsource a problem space by each focusing on a smaller subspace tractable within their respective time budgets. In this way, students have chances to explore science both independently and collectively.

A Reference Implementation: Telelab

To realize the ideas described in the above sections, we have developed an open-source reference implementation, branded as Telelab, and pilot-tested it in online settings with a few high schools in the United States during the COVID-19 pandemic. Currently, the main sensor that we have used with Telelab is a low-cost thermal camera, FLIR ONE, which can be connected to a smartphone and reprogrammed. We started with thermal cameras because of their unique power for visualizing chemistry[4-6]. As chemists often rely on visually striking color changes shown by pH, redox, and other indicators to detect or track reactions, thermal imaging, which uses false color heat maps on a display screen instead of chemical compounds, can similarly be used as a "green" indicator of chemical processes. What is even more compelling with this virtual indicator is its versatility, originated from the universality of thermal energy change in every chemical process (anything that leaves a trace of heat leaves a trace of itself under a thermal camera[4]).

In the following subsections, we present five examples to demonstrate how digital twins of experiments may be used to support chemistry education. Note that, with these digital twins, students who do not have an actual thermal camera can still benefit from its power.

Experiment 1: Condensation Warming

This is a simple experiment that the first author has reported in 2011[4], but it can now be shared through a digital twin. As we know, due to the effect of evaporative cooling, an open petri dish filled with water settles at a lower temperature than the room temperature. If we place a piece of paper on top of the dish (Figure 2), the evaporated water molecules will condense onto the underside of the paper, resulting in the rising of temperature by up to 2°C, depending on the relative humidity of the air. This effect is nanoscopic as the lowering rate of water surface in an open dish due to evaporation is estimated to be less than 20 nanometers per second[15]. But the condensation of such a microscopic amount of water suffices to warm up the macroscopic paper to a remarkable degree (to be more accurate, the warming effect is also contributed by the formation of hydrogen bonds when the water molecules first encounter the cellulose molecules of the paper).

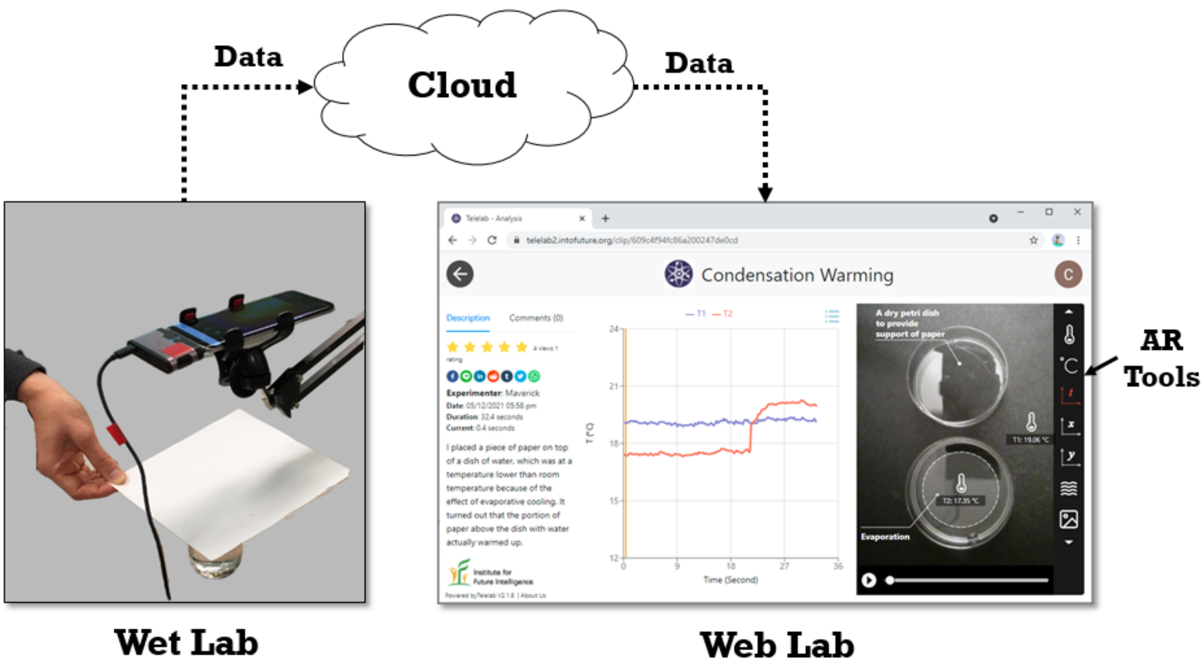


Figure 2. This illustration shows how a digital twin for an experiment works in Telelab. A smartphone with a FLIR ONE thermal camera is used to stream video and sensor data to the cloud. The data is then distributed to a client's browser for constructing a Web lab interface through which the client can observe and analyze the phenomenon using a set of augmented reality tools.

URL: https://telelab2.intofuture.org/clip/607a26431750b00022aef788

As seen in Figure 2, the digital twin of this experiment displays a camera view with augmented features such as text annotations and analytical tools, as well as a graph that shows the temperature changes over time at different locations measured by two virtual thermometers placed in the view. The virtual thermometers can be moved by users freely, just like what they might do with real temperature sensors in a physical lab. Users can also add more thermometers as necessary. The graphs and readings for the virtual thermometers will automatically update as they change, using the sensor data stored in a cloud database. As the digital twin always keeps track of past data, a slider is provided for revisiting any past moment and a button for playing the whole session back just like a video.

Experiment 2: Breaking a Dynamic Equilibrium

Following the experiment described above, the warming effect disappears after the paper stays atop the dish for some time (10-30 seconds). This is because after condensed water molecules form a layer of liquid on the underside of the paper, evaporation from that layer starts to take place. When the rate of evaporation equals that of condensation on the surface of that layer, a dynamic equilibrium is established, resulting in no net gain of thermal energy. Hence, the paper once again reaches a thermal balance with the environment. If we now nudge the paper sideways, the thermal image exhibits a three-color pattern (Figure 3), indicating that the dynamic equilibrium is broken in a subtle way. The upper crescent zone, which has a layer of condensed water newly exposed to the air with no water vapor, cools down as evaporation dominates in it. The lower crescent zone, which has a dry surface newly exposed to water evaporated from the dish, warms up as condensation dominates in it. The average temperature in the football-shaped zone between the two crescents remains approximately the same as before because the dynamic equilibrium in that zone is hardly disturbed by the move of the paper.

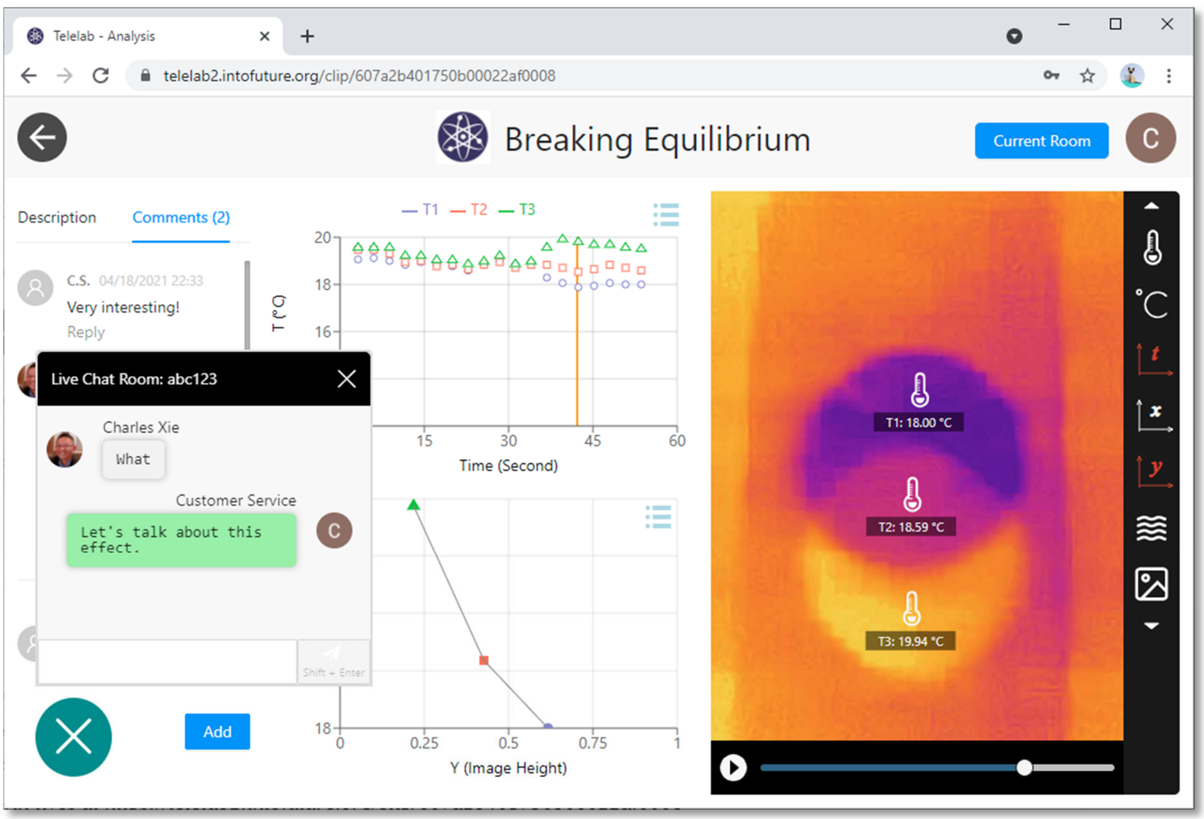


Figure 3. To facilitate student discussions, Telelab provides a comment area for each digital twin. If the "room" (a virtual space where students go to participate in an experiment) is still open, they can also interact with one another through a chat channel.

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As also shown in Figure 3, Telelab provides tools to support social interactions among students around each digital twin so that they can discuss about the experiment. For example, they can propose a different interpretation of the result or a new idea for further experimentation.

Experiment 3: Ice Melting and Latent Heat

In this experiment, a petri dish filled with ice is taken out from a freezer to melt. If students add a virtual thermometer to the center of the dish, they observe that the temperature stays relatively unchanged (close to 0°C with some minor fluctuations) for a long while before it can rise. In this way, they discover the latent heat.

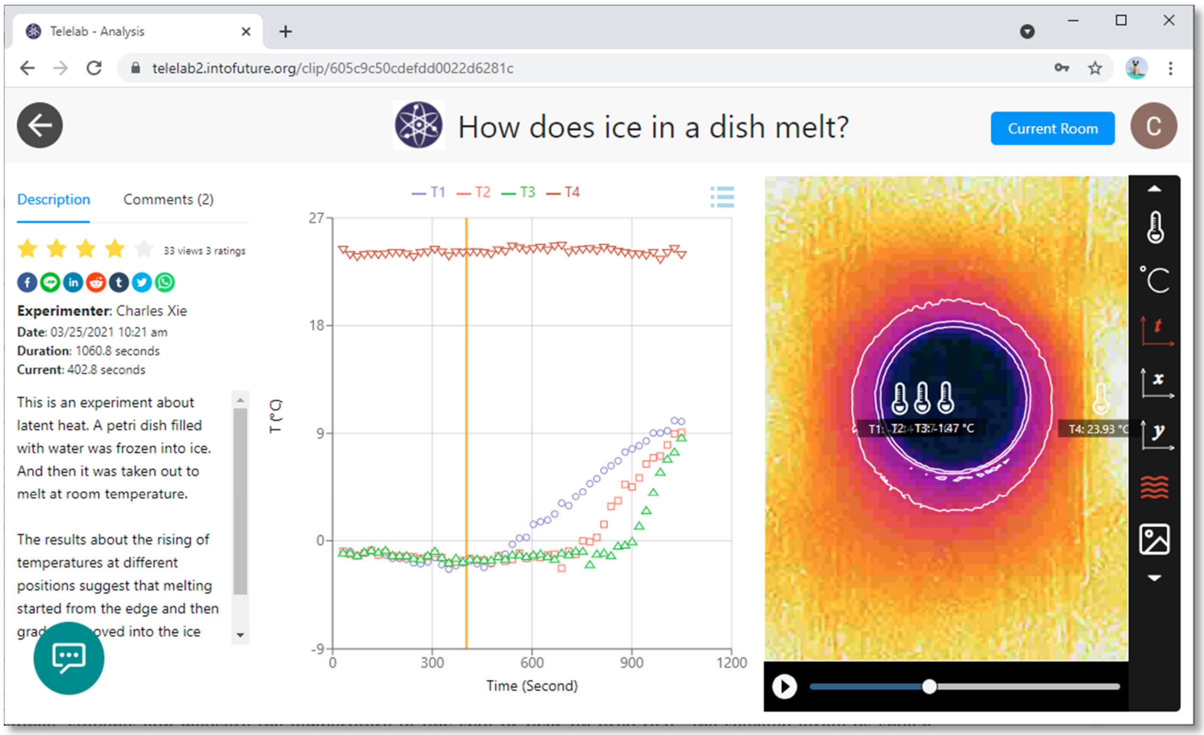

Figure 4. The large dataset stored in a digital twin provides a considerable room for exploration. Students can measure the temperature at any spot or over an area and retrieve the entire historical records for analysis.

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In Telelab, the driver app based on the FLIR ONE thermal camera transmits 96,000 temperature values per second to the cloud. At such a rate, the digital twin of the experiment shown in Figure 4 accumulates over 100 million data points in just 18 minutes. With the ability to collect and visualize such "big data," Telelab can provide opportunities for students to make their own scientific discoveries from digital twins. For example, students can place additional thermometers, as shown in Figure 4, to monitor the rising of temperatures at different positions. The results suggest that the melting of ice in a dish starts from the edge and then gradually moves into the center.

Experiment 4: An Anomalous Temperature Gradient

As the first author discovered in 2011[4], there exists an anomalous temperature gradient in a cup of salt solution that persists until all the water evaporates. This phenomenon is counter-intuitive because the bottom of the cup is slightly warmer than the top, which is against the conventional wisdom that cooler water sinks and warmer water rises due to thermal convection. In the experiment shown in Figure 5, we used two cups of salt solution with different concentrations, contrasted by a cup of pure water in the middle. The anomalous temperature gradient existed in both solutions.

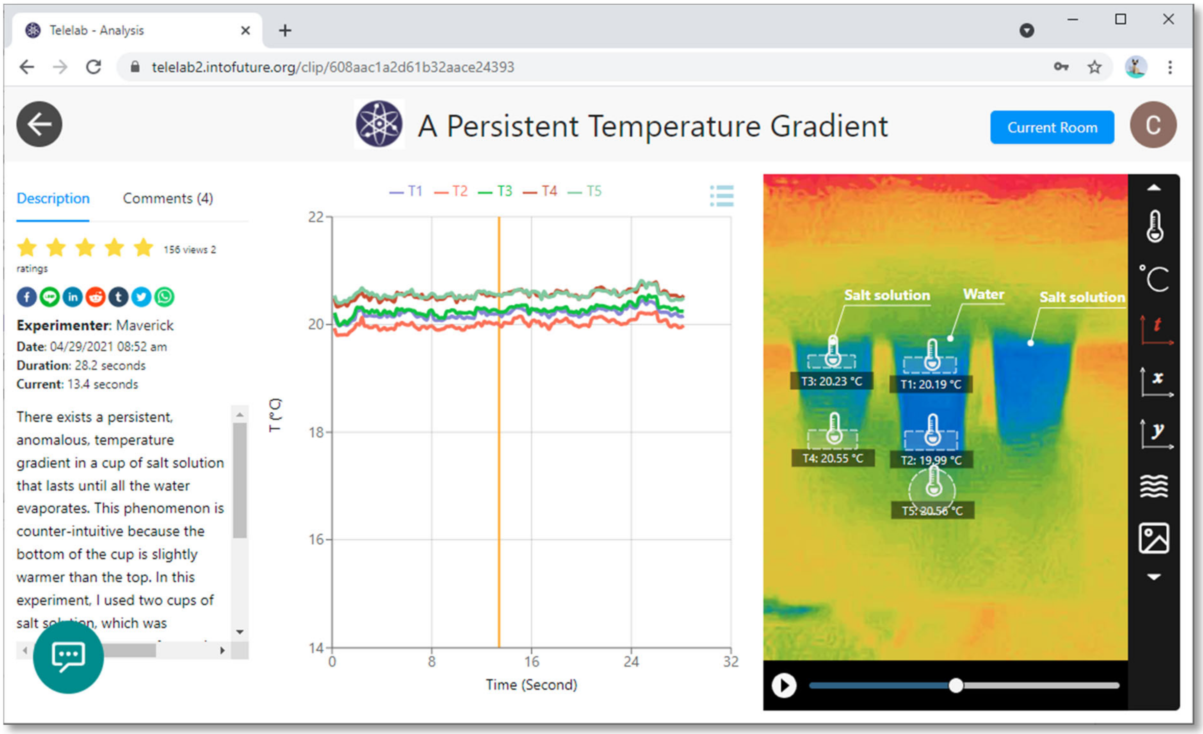

Figure 5. The plastic cups on the left and right each contain a salt solution, whereas the one in the middle contains pure water. The salt concentration in the left cup is higher than that in the right cup.

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This phenomenon is difficult to explain and there are competing theories[4]. Through Telelab, we can now provide open data to the public and invite everyone, including readers of this paper, to analyze it through a digital twin (Figure 5). To facilitate such an open science challenge, Telelab allows users to copy and edit a digital twin, perform a different analysis, write a brief report, and then share the new version on the cloud. These capacities of Telelab enhance the nature of science that permits an experiment to have multiple interpretations until they are disproven. So game on!

Experiment 5: Effect of Concentration on Reaction Rate

This experiment investigates the relationship between the concentration of a reactant and the rate of the reaction. It uses the reaction between baking soda and vinegar with four different concentrations: 0% (pure water), 5%, 10%, and 15%. The cooling in the case of pure water is due to the endothermic dissolving of baking soda in water. Figure 6 shows that, compared with the effect of the endothermic reactions under the other three conditions, dissolving absorbs much less heat.

Figure 6 also demonstrates the ability of Telelab to trim the historical data stored in a digital twin (as indicated by the break symbols in the line plot and the play slider). Such a data cleaning tool allows users to remove unwanted data in a way similar to editing a video clip.

Figure 6. Baking soda are added to four petri dishes with different concentrations of vinegar. Their temperature drops are used as indicators of the reaction rates.

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Discussions and Conclusions

As an example of practical applications, digital twins delivered through Telelab have provided intuitive user interfaces for remotely accessing science labs during the COVID-19 pandemic, resulting in improved student engagement and learning in online environments[16-18]. In a teacher's own words, "In real labs, I ask students to do free exploration before giving specific instructions on where to observe and what to analyze. Then we share, as a whole class, what we find. With Telelab, I can do the same thing. They can add thermometers anywhere and share what they find. Some focus on purple colors (cold) and some focus on red colors (hot). From their choices of places, they start to ask questions of why it happens as it shows."

Unlike videos that contain only pixels, massive sensor data stored in digital twins of past experiments allow for in-depth data analyses. This makes digital twins better alternatives to videos for teachers to demonstrate science phenomena without having to redo the experiments, which is helpful when teachers have only limited instructional time to cover a topic in their lesson plans. Furthermore, digital twins can also be used directly by students to explore science through experiments conducted by others when they do not have the facilities needed to do the experiments themselves or fail in achieving the desirable results within the given time frame.

Last but not least, just like the industrial and medical applications of digital twins in condition monitoring[19-20], a digital twin is automatically generated on the cloud for each experiment conducted by students using our technology. These digital twins of student experiments can then be used by researchers or teachers as holistic artifacts to gauge or predict students' laboratory performance post lab (diagnostic) or in real time (prognostic). Automatic assessment of such artifacts and their digital traces based on machine learning can even make personalized formative feedback feasible in complex laboratory environments[21].

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