SOCIETY OF PHYSICS STUDENTS

An organization of the American Institute of Physics

SPS Chapter Research Award Proposal

Project Proposal Title	A LEGO Based Low-Cost Autonomous Scientist: Using Machine Learning to Derive the Henderson-Hasselbalch Equation
Name of School	The University of Tennessee - Chattanooga
SPS Chapter Number	7170
Total Amount Requested	**$1998.25**

Abstract

The University of Tennessee-Chattanooga SPS chapter will construct a LEGO-based, low-cost autonomous scientist (LEGOLAS). It will use machine learning techniques to autonomously derive the Henderson-Hasselbalch equation, reducing the tedious experimentation and calculations typically involved in acid-base experiments. It will also be used for demonstrations, recruitment, and outreach.

Proposal Statement

Overview of Proposed Project

The University of Tennessee-Chattanooga chapter of the Society of Physics Students (UTC-SPS) proposes to assemble, calibrate, and operate a LEGO-based, low-cost autonomous scientist (LEGOLAS) that can derive the Henderson-Hasselbalch equation using machine learning techniques. Additional details of the project and LEGOLAS in general are described in the next section.

We have chosen this project as our chapter 2024 research project because:

- After the tremendous success of our previous LEGO project, the LEGO model of the Kibble Watt Balance, which will be featured in the SPS Observer Magazine in the next winter issue, this project will continue our collection of LEGO-based science machines, that really inspires students and kids of all ages. Continuing our work on LEGO science will promote teamwork and growth for our SPS chapter.
- We were inspired to pursue this project after Dr. Aaron Kusne, a coauthor of the LEGOLAS, presented a seminar on machine learning in material science at our department.
- One of our university's top priorities is to promote experiential learning and introduce new technologies, such as machine learning, to all students. This project fits right in.
- The project will allow the UTC-SPS members to learn about areas of physics, material science, and machine learning outside of the scope of standard physics courses.
- At UTC, the first science course most students (including all physics majors) take is chemistry. Chemistry is very important for material science and solid-state physics. Having at least one course in chemistry will allow most, if not all, physics students to be involved in the project and understand the underlying science of the apparatus. Besides physics students, we will be able to recruit chemistry majors and possibly chemical engineers to join our SPS chapter to work on the project.
- The hands-on nature of this project gives us an opportunity to improve our experimental skills.
- The project will require us to work on computer interfacing and machine learning code, which is a very useful skill in today's workplace, but not covered in our physics classes.
- The finalized LEGO-based autonomous scientist will be used for demonstrations, recruiting new physics majors, and outreach events. To our best knowledge, no other group in the Southeast has constructed this apparatus, which will generate interest in our program.
- We will acknowledge that the apparatus is constructed with the help of the SPS Research grant to make students aware of the local SPS chapter and the SPS National.
- The project promotes a duality between rigorous scientific research and fun. We hope this project convinces others that the field of physics/chemistry is fun.

Background for Proposed Project

In the modern world, autonomy has become a necessity to facilitate efficient production of goods, manufacturing of materials, quality assurance, and more. While typical machines found in factories are coded to move an assembly arm or other equipment in a consistent, repetitive manner, for scientific purposes, a more "human" control and reaction is desired. Machine learning, a subfield of artificial intelligence, is one such technique to incorporate autonomous "thinking" and experimentation [1]. Using machine learning, one can design an apparatus to take a set of measurements and interpret the measurements based on an expected model, adjusting the model to better fit the collected data before the next set of measurements [1].

For the apparatus described in this grant as well as other similar machines, Bayesian statistics with Gaussian processes set the underlying framework of machine learning. Specifically, Bayesian optimization is used to compare a model or function to data, optimizing the prior model or function to a posterior version via regression [2]. The models are Gaussian processes that predict data distribution based on initial conditions/inputs [2]. Using these techniques, an apparatus can autonomously mimic the typical steps of researchers by generating a model, collecting data, optimizing the model based on data, and repeating these steps until the model and data agree with statistical significance.

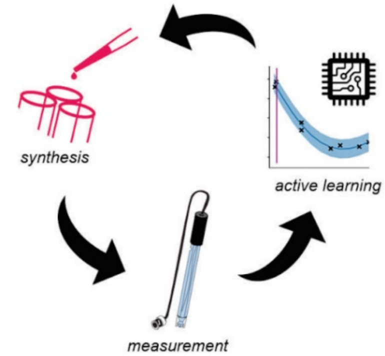

Fig. 1.
Pictorial representation of the automated processes completed by the LEGOLAS apparatus [1].

Fig. 2.
Pictorial representation of Bayesian optimization for machine learning [1].

Machine learning is becoming more and more important in the fields of solid-state physics, chemistry, and material science, especially in developing new materials for optics, electronics, and spintronics. The benefits of machine learning and associated techniques are exemplified in tedious experiments and procedures. As an introduction to machine learning in materials science, one can look at a simple experiment: titration in acid-base chemistry. Typically, these experiments rely on the Henderson-Hasselbalch equation: $pH = pK_a + \log([\text{Conjugate Base}]/[\text{Acid}])$. Generally, a researcher would need to first prepare solutions, titrate the solution of acid with base (or vice versa) based an indicator such as a color change or pH value, record the volume of acid and base used, compare the molar ratios of the acid and base from a chemical equation, and determine a desired quantity such as pH or the acid dissociation constant (K_a). Although these steps are not inherently difficult, they can be laborious. Additionally, these steps only determine a single value based on the Henderson-Hasselbalch equation. With machine learning, these steps could be achieved autonomously, and the underlying equation itself could be derived based on data [1].

Recently, machines have been designed to solve the issue of tedium for material science experiments as shown in [1] and [3]. The LEGOLAS apparatus detailed in [1], which we propose to build, autonomously completes the processes of prepping solutions and mixing ratios of acid and base. Following this, the apparatus takes advantage of machine learning to optimize a model that, after many trials, should take the form of the Henderson-Hasselbalch equation [1]. The comprehensive computer code to control the machine is provided by Saar and is available through a hyperlink in [1]. We believe this project will an excellent introduction to machine learning in material science for our SPS team.

Expected Results

The expected results of this project will be a constructed and functional LEGO-based, low-cost autonomous scientist capable of deriving the Henderson-Hasselbalch equation. We, the UTC-SPS team, expect to gain invaluable experimental experience by assembling and testing this LEGO apparatus. Even though everyone on our team has taken introductory physic and cheimstry courses, we do not have experience with machine learning and only some experience with designing computer controlled experiments. Two years ago, with the hlep of the SPS National grant, we built a LEGO-based model of a Kibble Watt Balance. That was a huge hit among the students and helped us grow our team. We expect that having another LEGO-based project will bring more attention and recognition to the Society of Physics Students chapter at our university and to the physics program as a whole. We believe that the fun nature the apparatus will make it an excellent outreach tool to support physics education at local schools and museums. Additionally, having a serious, funded project will genrate more interest among the students. The material science nature of this project will spark interest not only of physics, but also chemistry and engineering students, allowing us to recruit more members and grow our presence at the University of Tennessee-Chattanooga.

Description of Proposed Research - Methods, Design, and Procedures

The UTC-SPS team will assemble a LEGO-based low-cost automous scientist following the procedures outlined in [1]. The design of our apparatus will be a cartesian gantry with a trolley moving on frame and bridge tracks along the x and y-axes. This design, also used in [1] and [3], gives the trolley freedom of movement to collect and deposit chemical solutions from reservoirs into sample wells via a plunger and syringe that move in the z-axis. The trolley is moved by LEGO motors via gears along gear racks, each of which has a LEGO force sensor to set and calibrate position along the frame and bridge tracks. All of the components are supported by an aluminum frame, and most of them are protected in 3-D printed cases.

The LEGO motors and force sensors are monitored and controlled by two Raspberry Pi Build HATs which are ultimately controlled by two Raspberry Pi computers. Additionally, the trolley's vertical position and the pump action of the syringe is controlled by the Raspberry Pi computers, utilizing gear ratios of the LEGO parts. Although some modification will be needed, the code for movement of the trolley and associated equipment is provided in [1], and should issues arise, we will have assistance from Dr. Aaron Kusne from NIST, an advisor of the original LEGOLAS project. We will also attach a USB camera to the trolley to better view the trolley's point of view and motion (the camera can also be used for color-based sensing in future experiments).

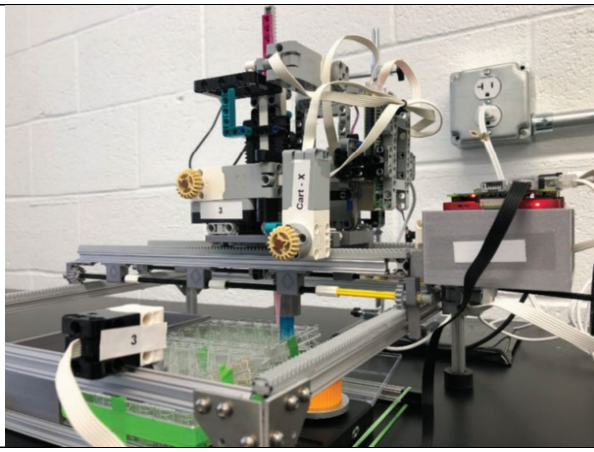

Fig. 3. LEGOLAS apparatus [1].

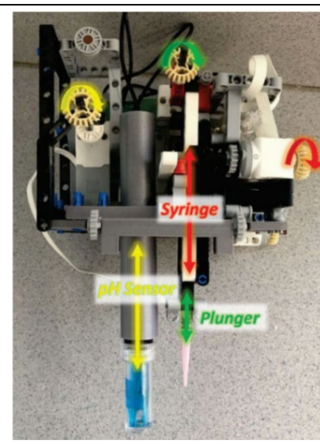

Fig. 4 LEGOLAS trolley and trolley equipment [1].

Under normal operation, the trolley and its equipment will transport solutions from the acid and base reservoirs to sample wells in varying ratios of acid and base. We will use glacial acetic acid and sodium acetate, a weak acid and strong base in water, respectively. These chemicals are relatively safe and suitable for demonstrations to the public. After mixing different concentrations of acid and base, the trolley will dip an Arduino pH sensor into each sample for measurements, cleaning the tip of the sensor in a reservoir of deionized water before each sample. Following data collection, machine learning will be incorporated for the apparatus to autonomously adjust a model to explain the data. Code for machine learning, including Bayesian statistics and Gaussian processes, is provided in [1]. After many iterations of the experiment, the apparatus should derive the Henderson-Hasselbalch equation based on its best model.

After assembling and calibrating the LEGOLAS apparatus, we will begin machine learning operations and test the capability of the apparatus in deriving the Henderson-Hasselbalch equation. This will demonstrate the usefulness of the apparatus in completing tedious experimentation and computational "thinking".

Plan for Carrying Out Proposed Project

All current members of the UTC-SPS (currently fifteen members) will participate in the project, and the project leaders are Matthew Boone (UTC-SPS President) and Evan Humberd (UTC-SPS Vice President). When parts and electronics are obtained, we will divide responsibilities among the members (construction, assembly, coding, calibration, etc.) and hold regular working meetings. We will enlist help from our faculty advisor, Dr. Tatiana Allen, for general questions and from Dr. Ichiro Takeuchi (UMD) and Dr. Aaron Kusne (NIST) for LEGOLAS code and assembly. The Physics Department will provide research space on the second floor of the Grote Hall (Advanced Physics Lab and Physics Study room) and necessary additional resources, such as tools and measurement equipment not covered by this grant.

Project Timeline (2024)

January: Order parts and electronics, begin 3-D printing parts as necessary, schedule work parties for SPS members.
February-May: Assemble and calibrate the LEGOLAS apparatus.
5/31/2024: Submit the Interim Report.
August: Test the LEGOLAS apparatus and make final adjustments. Present the LEGOLAS demostration during the UTC student organizations promotion week to promote the UTC-SPS.
September-November: Finallize the project and present it at the South Eastern Section of the American Physical Society 2024 Meeting. The LEGOLAS apparatus will also be used for demonstration purposes by SPS memebrs for recruitment (Departamental and University events) and outreach events at local schools.
12/31/2024: Submit the Final Report

Budget Justification

To construct the LEGO-based low-cost autonomous scientist apparatus we request the following equipment:

LEGO parts: according to the list specified in [1], 298 parts total, from the LEGO web site and other sources. Includes LEGO bricks as well as LEGO sensors and motors.	$336.95
Non-LEGO construction components: aluminum extrusions, end caps, corner cubes, L-brackets, nuts, and bolts from MakerBeam.	$98.20
Computer and associated components: 2 Raspberry Pi 4GB 64-bit, 2 Raspberry Pi Build HATs to control LEGO motors/sensors, Raspberry Pi Buildhat Chargers, 2 Plug adapters for Build HAT chargers (US-Aus), Arduino pH sensors, Arduino Uno microcontroller, ELP USB camera for viewing trolley motion and color-based sensing.	$508.95
Cables and adapters: USB 2.0 A Male to B Male, Jumper wire cables to connect components, WeDo Extension Cables for LEGO sensor/motor, 25-ft ethernet cable to connect Raspberry Pi to Wi-Fi and establish wireless control, USB Anker micro-SD card reader for Raspberry Pi memory reading/editing, 5-ft HDMI to micro-USB cable to connect Raspberry Pi to monitor.	$44.41
Monitor equipment: 24-in Sceptre monitor to connect to Raspberry Pi, 24-in ASUS portable monitor to connect to Raspberry Pi and be used for demonstrations/conferences display; USB keyboard, USB mouse.	$472.94
Other equipment and chemicals: mg-accurate digital scale to weigh chemicals, Chem Lab stand and rings to hold cables/components, 1mL syringes, 20-gauge dispensing tips, 24 well cell to hold various ratios of solutions, plastic funnel, 100 mL graduated cylinder, 100 mL storage bottles to hold solutions, 500 mL wash bottle, plastic weighing dishes, Nitrile disposable gloves for handling chemicals, safety goggles for visiting guests and students who may not already have safety goggles, glacial acetic acid sodium acetate anhydrous, potassium chloride (pH electrode storage solution)	311.63
Subtotal (Equipment and Parts) = $1773.08	
Shipping and handling (estimated at 12% of the parts)	$212.77
3-D printed parts: according to files provided by [1], includes bases, supports, and other assembly pieces (based on $30.24/kg for PLA filament)	$12.40
LEGOLAS software/code: provided by Logan Saar (author of [1]) on GitHub	Free
Total	**1998.25**

Bibliography

1. Saar, L., Liang, H., Wang, A. *et al.* The LEGOLAS Kit: A low-cost robot science kit for education with symbolic regression for hypothesis discovery and validation. *MRS Bulletin* **47**, 881–885 (2022). https://doi.org/10.1557/s43577-022-00430-2
2. Garrido-Merchán, E.C., Hernández-Lobato, D. Dealing with categorical and integer-valued variables in Bayesian optimization with gaussian processes" Neurocomputing **380**, 20-35 (2020)
3. Gerber, L.C., Calasanz-Kaiser, A., Hyman, L. *et al*. Liquid-handling Lego robots and experiments for STEM education and research. PLOSBiology (2017) https://doi.org/10.1371/journal.pbio.2001413