Scalable Multi-Agent Framework for Optimizing the Lab and Warehouse
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Abstract

The field of autonomous physical science – where machine learning guides and learns from experiments in a closed-loop – is rapidly growing in importance. Autonomous systems allow scientists to fail smarter, learn faster, and spend less resources in their studies. The field promises improved performance for various facilities such as labs, research and development pipelines, and warehouses. As autonomous systems grow in number, capability, and complexity, a new challenge arises – how will these systems work together across large facilities? We explore one solution to this question – a multi-agent framework. We demonstrate a framework with 1) a simulated facility with realistic resource limits such as equipment use limits, 2) machine learning agents with diverse learning capabilities and goals, control over lab instruments, and the ability to run research campaigns, and 3) a network over which these agents can share knowledge and work together to achieve individual or collective goals. The framework is dubbed the MULTI-agent Autonomous Facilities - a Scalable framework aka MULTI-TASK. MULTI-TASK allows facility-wide simulations including agent-instrument and agent-agent interactions. Framework modularity allows real-world autonomous spaces to come on-line in phases, with simulated instruments gradually replaced by real-world instruments. Here we demonstrate the framework with a real-world materials science challenge of materials exploration and optimization in a simulated materials lab. We hope the framework opens new areas of research in agent-based facility control scenarios such as agent-to-agent markets and economies, management and decision-making structures, communication and data-sharing structures, and optimization strategies for agents and facilities including those based on game theory.

Introduction

Common challenges link the many fields of science and engineering. As science and engineering researchers seek ever-better materials and devices for next-generation technologies, they exhaust those that are easier-to-make and they are driven to explore materials and devices with greater complexity. Consequently, with each new parameter introduced into their studies, the number of potential experiments (e.g., materials or devices to study) grows exponentially, i.e., the search space grows exponentially. An ever-growing search space is not the only challenge. The relationship between user controlled experimental parameters and the desired material or device properties can also be complex. This vast, complex search space makes traditional one-by-one, expert-driven Edisonian research impractical. Advances in experiment automation (Green et al. 2017; Curtarolo et al. 2013) provide an increasing factor of speed up, but automation alone cannot keep up with an exponentially growing search space. These challenges exist beyond science and engineering. For example, a warehouse operator may seek to improve warehouse performance by optimizing numerous parameters associated with warehouse layout and operation.

Autonomous systems (Stach et al. 2021) offer a solution. For these systems, a machine learning pipeline is placed in control of automated equipment to control experiment design, execution, and analysis, with the system learning and evolving with each new datum in an evolving environment. A machine learning function is used as a surrogate for the unknown relationship between experiment inputs and outputs, mapping the complex and vast search space. Data collected from experiments are preprocessed and then used to improve the surrogate function’s predictive power. Experiment design and selection is guided by active learning (Settles 2010) – the machine learning field of optimal experiment design. Subsequent experiments are selected to provide maximal knowledge to the users.

With such machine learning pipelines, order-of-magnitude improvements in research efficiencies are possible (Stach et al. 2021). Even greater efficiencies are possible by incorporating prior knowledge of the research challenge - such as prior theory and exogenous experimental and simulation data - into the pipeline (Baker et al. 2019). These efficiency gains are exemplified by recent demonstrations of autonomous physical science including successes in optimizing mechanical structure (Gongora et al. 2020), material processing (Nikolaev et al. 2016), device operation protocol (Attia et al. 2020), and mixture rates of liquid-synthesized materials (MacLeod et al. 2020; Burger et al. 2020; Langner et al. 2020). There have also been a few examples of solid-state material exploration and discovery. These studies include mapping the composition-phase and composition-temperature-phase (Ament et al. 2021; Kusne et al. 2020; McDannald et al. 2022) relationships as well as the first autonomous discovery of a best-in-class material (Kusne et al. 2020).

As autonomous systems grow in number, capability, and complexity, a new challenge arises – how will these systems
work together? For example, autonomous control can be extended throughout labs, research and development facilities, and warehouses to achieve many orders-of-magnitude improvements in efficiencies. The benefits may be significant. For example, greater facility efficiencies may be gained by addressing multiple correlated challenges in concert, with each challenge benefiting from knowledge gained for the others. Such autonomous systems would free technical experts to focus on posing questions and gaining insight from results. As the scale of these systems grows, so too does the scope of the questions that can be addressed.

One option for the agent architecture – defining how the agents work together – is autonomous control by a central machine learning agent that collects all data and makes all decisions. This framework has its benefits, including reducing the need for redundancies in data storage and computational resources by centralizing both. Another architecture is one with a central decision-making agent combined with distributed learning-only agents based on federated learning (Yang et al. 2019). Each learning agent collects and analyzes data from its dedicated pool of instruments. Learned model parameters from learning agents are then integrated by the central agent for subsequent centralized decision making. This architecture reduces the network burden of transmitting all data to a central site.

A third architecture of multiple independent agents (Dorri, Kanhere, and Jurdak 2018) working in concert, has its own advantages. These advantages mirror those of having multiple human experts working together to solve large challenges. For instance, agents of differing algorithmic bias (similar to individual human bias due to education and training) can validate each other’s results. Additionally, multi-agent interactions of data sharing, learning, and decision making can be varied to achieve task-based optimal performance. For example, consider the collaboration between two teams of agents working on disparate tasks. Collaboration between the teams may provide research acceleration when the data from one task is informative of the other (e.g., phase maps and material properties (Küse et al. 2020)). However, if data sharing is extraneous, it may serve only to increase the computational cost for data analysis tasks. In the latter case, non-collaborating teams may be preferable. For either coupled or non-coupled research tasks, architecture impacts the need for data sharing and learning. Architecture can also impact decision making. For example, distributed decision making may be preferable when agent teams have disparate goals, compared to centralized decision making for when teams share a common goal. Furthermore, the optimal agent architecture may depend on research objectives and the type and size of the data being analyzed. The multi-agent framework presented herein is flexible enough to allow for different agent architectures including centralized agent, federated learning agents, and multiple independent agents. The framework also facilitates optimizing dynamic architectures that vary in response to time-varying challenges.

The presented framework for multi-agent architectures can also demonstrate clear technical benefits. For example, facilities may have systems from which collected data is large (volume, velocity, etc.), resulting in network bandwidth issues when centralizing data. Distributed agents, with associated data storage and computing, can overcome this challenge by performing local experiment design, data collection and reduction, and data analysis. A local agent operating a diffraction system can convert a gigabit-size diffraction image into a short description of identified phases, share this data while also guiding subsequent diffraction experiments. Also, specialized agents can be paired with instruments that require specialized machine learning tools for data analysis, resource optimization, and decision making. For example, different machine learning tools are needed for autonomous control of a scanning electron microscopy or a current-voltage device characterization instrument.

A multi-agent framework also offers the flexibility of modularity. Framework modularity allows real-world autonomous spaces to come on-line in stages, with simulated instruments gradually replaced by real-world instruments. As facilities change in size and scope, and even grow to contain distributed instruments (e.g., across states or countries), a networked, multi-agent framework can scale to demand, varying the number and type of agents. If two disparate facilities overlap in some instruments, successful agents from one facility can be copied to the other. Additionally, local agents can focus on local challenges and collaborate with agents working on larger scale challenges, such as agents working to optimize both local and shared resources.

There are also potential instrument manufacturer benefits to a multi-agent framework. Many instruments manage internal signals that may be beneficial to users if exposed. However, instrument manufacturers limit access to these inner workings due to intellectual property concerns. Manufacturers can offer customers a specialized agent paired with the purchased instrument. The agent would provide the customer access to information of internal signal trends while maintaining intellectual property protections through data privacy, federated learning, and other techniques. Similar agent-based tools may be used to allow facilities to collaborate through agent-agent interactions without exposing intellectual property.

We demonstrate the multi-agent framework with an example challenge of autonomous materials optimization. Past work into agent-based machine learning for the materials sciences includes three studies. The first study utilizes data processing and learning agents for identifying the composition-phase map from previously performed X-ray diffraction experiments (Gómez et al. 2019). Prior physics knowledge of phase mapping is encoded as a set of constraints, with different sets of learning agents able to apply different sets of constraints. One set of learning agents works together to identify viable phase map descriptions for small regions of the composition space. These results are unified by another set of learning agents to generate multiple
viable solutions. The second study uses agents to identify a stable, optimal material by running density functional theory simulations (H. Montoya et al. 2020). In this study, a set of identical agents are instantiated, each runs a fully independent campaign, and results are combined at the end. The third study describes a framework where again independent agents (called ‘orchestrators’) run independent research campaigns (Rahmanian et al. 2022). For all of these studies, ‘agents’ refer to independent learners, optimizers, or algorithmic units with predefined interactions. To the authors’ knowledge, there have been no investigations of agent-agent interactions on autonomous facilities optimization, where each agent is a potential decision maker.

In this work, we provide a scalable multi-agent framework capable of addressing these challenges. The framework is dubbed the MULTI-agent auTonomous fAcilities - a Scalable frameworkK aka MULTITASK. The contributions are:

- A visual language for describing multi-agent, facility-control frameworks.
- A unifying environment for an autonomous research lab, and a basis for similar facilities. The environment allows for real-world modules to come on-line unit by unit (replacing simulations and digital twins).
- Autonomous agents (here demonstrated as Bayesian learning agent) capable of running individual and joint research campaigns through sharing data and making multi-agent-based decisions.
- Demonstration of a network environment for autonomous agents to collaborate.
- A comparison of different facility architectures for materials discovery challenges.
- A coregionalization algorithm for learning the composition-structure-property relationship of solid-state materials.

In the next section Framework Description, we describe the working parts of the framework, present example code for instantiating an autonomous facility, and demonstrate a visual language for communicating different instantiations. In Demonstration, we describe a materials optimization challenge and framework results. For more information about implementation, see the Methods section. We conclude with the Discussion section. First, we provide a brief description of materials optimization and discovery.

**Background: Materials Discovery**

The discovery of novel solid-state materials is key to the success of numerous next-generation technologies such as quantum computing, carbon capture, and low-cost medical imaging. These materials must possess advanced properties selected for their technology applications. To find these advanced materials, researchers utilize a fundamental relationship between how a material is made and its resulting structure and properties - the synthesis-structure-property relationship (Graef and McHenry 2012). For example, a material’s properties are dependent on its elemental composition (e.g., iron, copper, etc.) and its phase—a description of the atomic organization within the material.

A useful tool in the search for advanced materials is the ‘composition-phase map’ which maps unique elemental compositions (and potentially other properties such as the temperature at which the material was synthesized) to its phase (Graef and McHenry 2012). These maps are segmented into regions separated by boundaries, known as phase regions and phase boundaries, respectively. Optimal materials of certain properties tend to occur within specific phase regions (e.g., magnetism and superconductivity) or along phase boundaries (e.g., caloric-cooling materials). The phase of a material is determined through characterization techniques including X-ray diffraction, Raman spectroscopy, and transmission electron microscopy. With these measurements, materials researchers identify phase regions and boundaries of a composition-phase map and use this map to guide their search for advanced materials.

**Framework Description**

There are a list of ‘objects’ (for background on object-oriented programming, see: (Lutz 2013)) that can be instantiated, consisting of: agents, resources such as instruments, individual samples (i.e., items) used for the machine learning campaigns, and repositories for either physical samples or data. Physical instruments include those used for sample synthesis, processing, and measurement. Instruments also include computational tools used to generate sample simulation data (not used in the demonstration). Physical and computational instruments are represented as shared resources that produce or consume countable objects. For example, a synthesis instrument produces physical samples and devices while a computational instrument produces data for simulated samples and devices.

To instantiate an agent, synthesis instrument, measurement instrument, or other object just requires calling the class, i.e., agent(), instr_synthesis(), instr_measure(). In Python, list comprehension can be used to instantiate a list of these objects with a call such as: agents = [agent(index, *properties) for index, properties in agent_descriptions]. These objects can be combined into facility units with multiple agents, shared instruments, and shared sample and data repositories.

**Agents**

Agents consist of four basic properties. Internal representation (IR): An internal representation of the world. This includes a perception of the materials search space, the tools and samples available, past collected data, and the other
agents. 

**Goals**: Each agent has a set of goals with an associated set of active learning acquisition functions, which quantify the utility of future experiments. Agents can work together in a group by combining their acquisition functions (i.e., goals), to identify the next set of experiments that benefit the group as a whole. **Machine learning (ML)**: They have machine learning capabilities for data analysis, prediction, and decision making (i.e., active learning). Each agent can have its own unique ML capabilities. In principle these capabilities can be any sort of algorithm for data analysis and prediction, be that deep learning models, Bayesian inference models, physics-based analytical models, etc. In the present work, agents employ Bayesian models as they are particularly well suited for active learning. When sharing data between agents, agents employ a coregionalization learning algorithm to exploit shared trends across the data sources (See Methods Section). **Communication**: Agents use functions for requesting, sending, and receiving data to share knowledge between individual agents, groups of agents, or with the full agent community through a central data repository. The four basic capabilities of IR, ML, goals, and communication are demonstrated through agent-agent collaboration for accelerated research campaigns.

**Instruments**

Instruments can perform certain operations with associated capacity and delays. An example set of instruments for materials or device research would consist of sample synthesis, processing, property simulation, and characterization instruments. For instance, a synthesis instrument can be defined so that it makes 2 material samples at a time, with a synthesis time of 10 minutes. Agents place requests to instruments to perform desired operations (e.g., a synthesis instrument to make a sample, a measurement instrument to measure a sample) and these requests are put into operation queues for the instrument. In performing their operations, instruments can draw on or create limited, consumable resources. For example, a sample synthesis instrument may consume 1 silicon wafer to produce one material sample.

**Repositories**

Two types of repositories exist – ones that store physical samples and ones that store data. Each type has a dedicated management system for agent interaction. **Sample repository**: Once a sample is synthesized, it is transferred to a sample repository to await a request to the repository management system for the sample to be processed or measured. When the sample is unused, it is returned to the sample repository. The sample-repository relationship is analogous to that of a book and library. The management system allows agents to identify which samples are in the repository and which are being lent out. **Data repositories**: These serve as central data storage facilities, where agents can share collected data including measurement data as well as data analysis, prediction, and decision-making acquisition function data. Management provides agent read and write access to databases.

**Visualizing the Network**

A diagrammatic language can facilitate network description and comparisons through displaying the lab network in-
structure. Here we use shaped icons to indicate the physical and computing instruments (rectangle), repositories (hexagon), agents (oval), and humans (cut-off oval). Different forms of agent-agent and agent-instrument interactions can be indicated through the graph connections. Here data sharing is shown with a graph edge (connection between objects, i.e., nodes). The additional icon ▷ indicates that this data sharing path also permits sharing data on acquisition function which impacts decision making. The direction of the icon indicates the hierarchy of decision making with { Leader ▷ Follower}. If both directions are shown, both agents share their acquisition functions and impact the other’s decision making. Edges marked with ■ indicate physical sample sharing between objects. An example is shown in Figure 1.

Figure 2. The two materials optimization challenges. The materials data challenge is drawn from the perovskite oxide material system as characterized by [23] for piezoelectric response and structure. Data for samples near the Bi1-xSmxFeO3 edge of this composition space is shown. a1) The functional property challenge is to identify the maximum value of the piezoelectric coefficient d_{33} (pm/V) (maximum indicated with red dot) and the associated composition. This parameter is strongly dependent on the phase diagram as indicated by the maximum located near the second phase boundary. The maximum occurs with a single peak which extends the entire shown composition range. a2) A more complex synthetic example where the target functional property peaks near the second phase boundary and is characterized by a narrow peak. b) Raman spectra for samples in the phase regions (1-3) are shown.

Figure 3. Diagrams for portions of facility units, each uses the plate notation with M multiples. a) The physical lab portion of the facility unit consists of a sample repository and the following instruments: sample synthesis, Raman-based structure measurement, and d_{33} functional property measurement. One sample repository is used for the M repeated objects. b) The software portion of the facility unit, containing two independent agents, agent1:PM focused on composition-structure relationship (i.e., phase map) and agent2:FP focused on the composition-property relationship. c) an alternative software portion where agents share sample data through the data repository. All agents share the same data repository. d) an alternative software portion where agents share sample data and acquisition functions. All agents share the same data repository.
Demonstration

The material synthesis-structure-property relationship (‘synthesis’ here includes composition) is fundamental to materials science and presents an excellent opportunity to demonstrate the multi-agent approach. Functional properties are intrinsically linked to phase – i.e., elemental composition and lattice structure. Through shared trends, knowledge of one can provide knowledge of the other, as demonstrated by recent autonomous materials discovery informed by the composition-structure-property relationship (Kusne et al. 2020).

For this work, individual agents either investigate the composition-structure relationship or the composition-property relationship. The former agents utilize an acquisition function that investigate subsequent samples that maximize knowledge of the composition-structure relationship. These agents are labeled ‘PM’ for phase map. The latter agents work to maximize knowledge of the property extrema and are labeled ‘FP’ for functional property. In collaboration, the agents combine data of composition, structure, and property to learn the composition-structure-property relationship and thus improve analysis and prediction of their individual target objectives. By combining their acquisition functions, agents can balance their goals with that of the community, selecting subsequent investigations that benefit overall community knowledge.

The materials data challenge is drawn from the perovskite oxide material system as characterized by (Kan et al. 2012) for piezoelectric response and structure. Data for samples near the Bi$_{1-x}$Sm$_x$Fe$_3$O$_9$ edge of this composition space are shown in Figure 2. For this system, composition, lattice structure, and piezoelectric properties are strongly linked. Figure 2(a1) shows the relationship between composition and the piezoelectric coefficient $d_{33}$ ($\text{pm/V}$) which has its maximum near the second phase region boundary. This is an easy maximization challenge as the extrema is characterized by a peak profile that stretches the full composition domain. Experiments performed on either side can use simple gradient ascent to find the maximum. A synthetic and more difficult challenge is presented in Figure 2(a2). Here the maximum is characterized by a highly local peak profile in the third phase region and the first two phase regions are described by their own broad peak profiles and local maxima. Additionally, for samples near the Bi(Fe$_{1-y}$Sm$_y$)O$_3$

Figure 4. Materials optimization performance for different agent architectures in materials optimization for a) one run of challenge 1 and, a2) challenge 2. Performance is shown using % minimum regret. b1 and b2 show the 95 % confidence interval for the performance mean over ten runs for each challenge. Example of combining acquisition functions: c1) Before combination, using Gaussian Process Upper Confidence Bounds, c2) acquisition functions for other 3 agents (PM$_0$, PM$_1$, FP$_0$), c3) combined acquisition function. d) Example predictions for Challenge 2 after 10 iterations: d1) and d2) for independent functional property predictions for two different agents, d3) coregionalization without acquisition sharing, d4) coregionalization with acquisition sharing.
composition binary, structure is measured using Raman spectra, with example spectra shown for phase region (1) through (3) in Figure 2b.

An agent requests a composition to investigate, the sample is synthesized if needed, and the agent then requests for the sample to be characterized for either d3 or Raman spectra based on their agent type (PM or FP). Synthesis and characterization have associated delays. Agents, instruments, and data repositories are instantiated with facility units composed of the simulated physical portion diagramed in Figure 3a and a selection of the software portion given by either: Fig 3b) fully independent agents, Fig 3c) agents that share sample data, or Fig 3d) agents that share sample data and where the PM agent shares acquisition function results with the FP agent. The ‘M’ in the top right corner of each of these ‘plates’ indicates that these objects are reproduced M times, as in the plate notation of probabilistic graphical models (Koller and Friedman 2009). All objects associated with the physical lab share the same sample repository and all objects for the software portion of the lab share the same data repository. For the demonstration, M=2.

Diagrams of agent performance for each of the 3 facility types is shown in Figure 4a1 and 4a2 for the two challenges. For the simpler challenge, the pair of independent composition-property agents (red line) identify the best material in 8 experiment design, execution, and analysis iterations. The more advanced agents show a dramatic improvement at lower iterations, with the agents sharing only data and learning coming close to the best material in 7 iterations and the agents sharing decision making coming close to the best material in only 4 iterations. For the significantly more complex Challenge 2, knowledge of the phase boundary locations provides a significant boost to both types of data sharing agents bringing them close to the optimal material within 6 iterations while one of the non-sharing agents got stuck in a local optimum. Figure 4b1 and 2 show the 95% confidence intervals for the performance mean for each architecture and for each challenge over ten runs. Shared information provides a significant performance boost for both challenges and shared decision making provides a moderate performance boost for challenge 2. Figure 4c provides an example of acquisition function combination. Figure 4d provides FP agent’s predictions for the functional properties after 10 iterations. In this case, one of the non-sharing agents (F4d2) is able to identify the optimal material despite operating under the incorrect assumption that the functional property has a uniform behavior (covariance length scale) across the entire composition space.

Discussion

This preliminary work demonstrates the different performance achievable using diverse agent architectures. For these simple challenges, joint learning and decision making performed better than only joint learning, which itself performed better than independent agents. The presented framework can be extended for diverse research possibilities. For example, one can investigate: the impact of agent heterogeneity in learning and decision-making capabilities; the relationship between agent-facility architecture and challenge type and difficulty; as well as agent-agent interactions. This latter possibility includes investigating agents with internal representations of other agents (e.g., expected beliefs and actions), adversarial agents capable of introducing poisoned data or models to throw off their competitors, and collaborative agents working together to improve the certainty of their individual results (i.e., cooperative validation).

Furthermore, just as multi-agent frameworks have been used to study markets (Tesfatsion 2006) and political systems (Gao et al. 2022), this framework provides an opportunity to model the interactions of physical scientists. The framework can be used to evaluate the impact of varying scientist capabilities and behaviors, their facilities, and their scientific challenges. This model can then be used to investigate how scientist-scientist interactions, resource and instrument limitations, and others scientific factors impact learning, decision making, and discovery.

Methods

Agents: Independent Learning

Independent phase mapping is performed by first clustering the materials $s_i$ with collected Raman data using Spectral Clustering with a cosine measure applied to the Raman data (here intensities measured at different Raman shift values form individual vectors. The cosine measure is applied between vectors to define dissimilarity). The result is an approximate phase region labels $y$ for each sample. Extrapolation of phase region knowledge is then performed using Bayesian inference. Two change points values $c$ are sampled uniformly over the composition domain. These change points are then used to define a categorical distribution $M_{c}$ for the structure measured materials $s_i$ with the boundary between categories defined by the change points, using one-hot encoding. The sum log likelihood $L^c$ of the observed phase region labels, given the categorical distribution is then computed. Bayesian inference is used to identify the most likely change points values $c$, given the observed data. This Bayesian inference operation is performed using the Pyro* (Bingham et al. 2019) package and allows for probabilistic structure labels as inputs.

The posterior over categorical probability $c_{post}$ will tend to have greater uncertainty at the change points.

Independent functional property regression is performed using the Matern52 kernel over the composition domain.
with the standard Gaussian process regression function using the GPFlow package (Matthews et al. 2017) for materials $x_j$ with measured functional properties $y_j$.

**Agents: Collaborative Learning**

A custom Bayesian inference-based coregionalization function is used to combine the tasks of phase mapping and materials property regression. First samples with Raman are clustered as with the independent phase mapping. The cluster labels define potential phase regions. Within a Bayesian inference model, change points are sampled and converted to a categorical distribution to compute the likelihood of the observations given the distribution, as in the independent phase mapping. The previous model is extended by using each defined categorical region (bounded by either a change point or the edge of the search space) to compute a Gaussian process (GP) likelihood for the observed functional property values within that region, using the same method as the independent functional property regression. The combination of likelihoods from functional property regression and phase mapping is used to identify the most likely change points and regression models within each region.

**Agents: Independent Decision Making**

PM agents, which are focused on learning the composition-structure relationship, select subsequent compositions based on risk minimization (Zhu, Lafferty, and Ghahramani 2003) using the Bayesian inference sampled change point values to compute the probability of each material sample belonging to each phase region. FP agents, which are focused on learning composition-property relationship use Gaussian Process Upper Confidence Bounds given by $\arg\max_{\alpha} \left\{ \mu + \sigma \sqrt{\ln(Dn^2\pi^2)/3\lambda} \right\}$ (Shahriari et al. 2016). Here, $\mu$ and $\sigma$ are the GP mean and standard deviation, respectively; $n$ is the current iteration number; at each iteration a grid of $D$ compositions is selected to search over; $\lambda$ is a predefined constant, here set to 0.1.

**Agents: Collaborative Decision Making**

For this demonstration, each FP agent $i$ takes the collection of all other agents’ normalized acquisition functions and computes the mean acquisition function $\alpha_{\text{m}}$. The agent’s normalized acquisition function $\alpha_i$ is combined with $\alpha_{\text{m}}$ using the equation: $\alpha_i' = 0.75\alpha_i + 0.25\alpha_{\text{m}}$. By combining acquisition functions focused on function property optimization with identification of changepoints, the combined functional property acquisition function will have greater utility near the phase boundaries. Points in the range of the expected change points can be more heavily weighed through a direct function similar to that of (Kusne et al. 2020).

**Data Repositories**

Each data repository is designed as an object with a Pandas DataFrame-based database and operational functions for common tasks such as adding and updating entries.

**Simulation Environment and Resources**

The simulation environment and resources are built using the Simpy library (Matloff 2008). Measurement times and synthesis times are set to 1 time unit.

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