Methods and Tools for Training AI with Digital Twin

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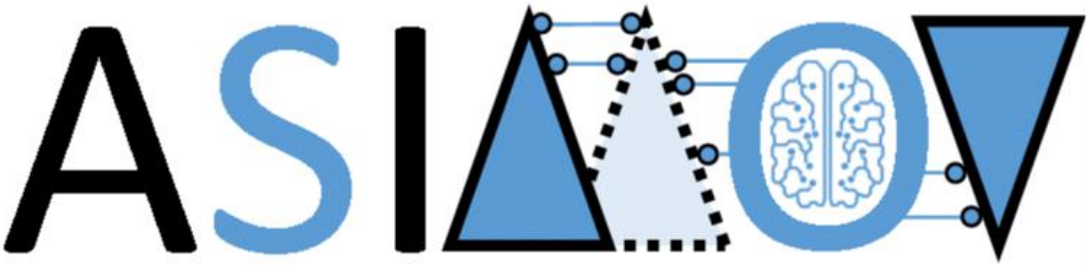

AI training using Simulated Instruments for Machine Optimization and Verification

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Contact	Jilles van Hulst
Organization	TU/e
E-Mail	j.s.v.hulst@tue.nl

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Task Team (Contributors to this deliverable)

Name	Partner	E-Mail
Jilles van Hulst	TU/e	j.s.v.hulst@tue.nl
Roy van Zuijlen	TU/e	r.a.c.zuijlen@tue.nl
Maurice Heemels	TU/e	m.heemels@tue.nl
Duarte Antunes	TU/e	d.antunes@tue.nl
Michael Wild	DLR	michael.wild@dlr.de
Niklas Braun	AVL	niklas.braun@avl.com
Jan Willem Bikker	CQM	janwillem.bikker@cqm.nl
Narges Javaheri	TFS	narges.javaheri@thermofisher.com
Maurits Diephuis	TFS	maurits.diephuis@thermofisher.com
Sebastian Moritz	TrianGraphics	sebastian.moritz@triangraphics.de

Formal Reviewers

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Abstract

One of the main premises of the ASIMOV project is that optimal settings and behavioural policies of cyber-physical systems can be found through Artificial intelligence (AI) techniques that leverage digital twins (DTs). DTs generate artificial data to feed the training of AI data-hungry algorithms, dramatically reducing the needed data from system trials. In this setting, it is crucial to define the interface between the DT/real-system and the AI agent or algorithm. This interface establishes how the DT generates training data for the AI algorithms so that the behaviour and optimization possibilities of the system can be understood by the AI algorithms. The present document defines this interface with generality and shows that it is broad enough to capture the two main use cases, namely the Electron microscope and the Unmanned Utility Vehicle. The proposed interface relies on three main components: pre-processing, post-processing and variations. Pre-processing matches high-level actions/decisions to be taken by the AI agent to proper low-level inputs of the system. Post-processing translates real observations generated by the system and/or simulated observations generated by the DT into suitable information for the AI agent to respond to, e.g., the State and the Reward in Reinforcement Learning (RL). Variations pertain to informative data generation, namely by considering sufficiently rich variations or scenarios to provide a suitable training set. Related literature associated with these three main components of the interface is surveyed. For each of the two main use cases of the project, the Electron Microscope, and the Unmanned Utility Vehicle, the three main components are instantiated, and use-case-specific training features are discussed.

Contents

List of Abbreviations

Abbreviation	Meaning
AI	Artificial Intelligence
ALE	Arcade Learning Environment
CPS	Cyber-physical System
DQN	Deep Q-Learning
DT	Digital Twin
EM	Electron Microscope
FL	Federated Learning
GAN	General Adversarial Network
GPS	Global Positioning System
HMM	Hidden Markov Model
ICA	Independent Component Analysis
KPI	Key Performance Indicator
LDA	Linear Discriminant Analysis
MDP	Markov Decision Process
MSE	Mean Squared Error
NN	Neural Network
ODD	Operational Design Domain
PBRS	Potential-Based Reward Shaping
PCA	Principal Component Analysis
PID	Proportional Integral Derivative
POMDP	Partially Observable Markov Decision Process
PT	Physical Twin
RL	Reinforcement Learning
RLA	Reinforcement Learning Agent
RM	Reward Machine
RS	Real System
SEM	Scanning Electron Microscope
STEM	Scanning Transmission Electron Microscope
TEM	Transmission Electron Microscope
TG	TrianGraphics
UC	Use Case
UUV	Unmanned Utility Vehicle
VAE	Variational Autoencoder

1 Introduction

Cyber-physical systems (CPSs) are increasing in complexity and number, which emphasises the need for more advanced methods to control how they behave. The goal of the ASIMOV-project is to optimise the process of determining optimal settings or behavioural policies for these systems. Due to the complexity of such systems, Artificial Intelligence (AI), especially reinforcement learning (RL), is considered a promising direction for controlling CPSs. In RL, an AI agent learns to perform desired behaviour by interacting with an environment (Sutton & Barto, 2018). By exploring the complete domain of the environment, namely from all-encompassing experiences, an optimal policy can be discovered.

A challenge within RL is the need for a huge amount of experience to eventually discover the optimal policy. It is often impractical to gather the needed amount of experience from the actual system/environment. Consider for example the two CPSs under consideration in the ASIMOV-project: the electron microscope (EM) and the unmanned utility vehicle (UUV). These systems have a highly complex structure with many inputs. Using these systems for collecting the needed experience is unfeasible. Furthermore, training time is very costly on these real systems (RS's). To overcome these two drawbacks, digital twins (DTs) are used in the ASIMOV-project. In fact, synthetic data generated by the DT can replace or complement the actual environment data. Moreover, DTs allow faster than real-time training, in a cost-efficient digital environment.

A crucial aspect in a DT-supported training environment, is the interface between the AI agent and the DT. This interface will be created in this task. In particular, the central question addressed in T2.2 is:

How can a DT create corresponding training data for an AI, so that behaviour and optimisation characteristics of the modelled product can be understood by the AI?

The interface between the AI agent and the DT should be applicable to the RS as well. The structure of the interface between DT/RS and AI agent can be seen in Figure 1. The interface consists of three blocks: pre-processing, post-processing and variations. Pre-processing matches (high-level) actions/decisions to be taken by the AI agent to proper (low-level) inputs of the system. Post-processing translates real observations generated by the RS and/or simulated observations generated by the DT into suitable information for the AI agent to respond to, e.g., the State and the Reward in RL. The block variations pertain to informative data generation. It considers sufficiently rich variations or scenarios to provide a good training set. In particular, the DT-based training setting in ASIMOV allows to introduce more "exceptional/rare" cases in the variation of the training set, to properly prepare the AI agent for these scenarios. This is in contrast with the generation of data based on the RS, in which such rare cases are often not (sufficiently) encountered. Hence, the trained AI agent is typically not trained for choosing proper actions in these cases. This is a potentially strong benefit of DT-based training (certainly for safety-critical applications or when calibrating fragile expensive equipment).

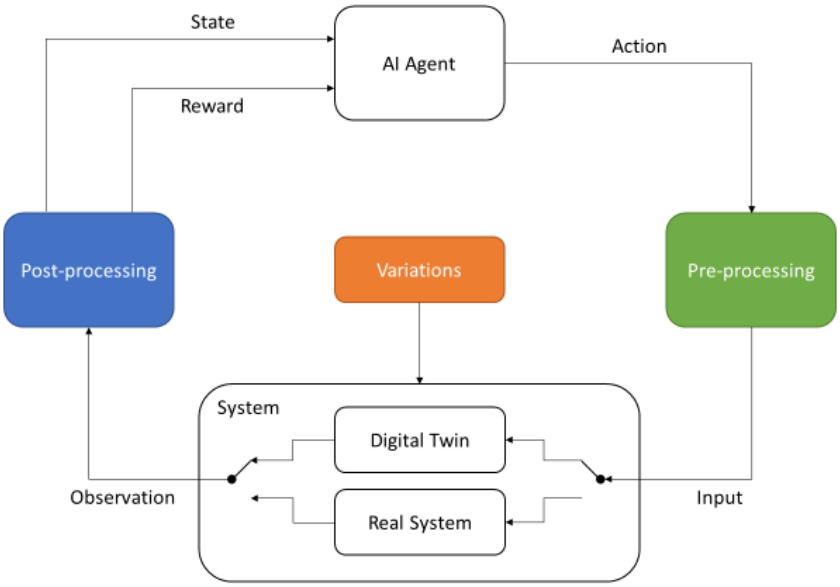

Figure 1 Overview of Task 2.2 contents

In this task these three blocks are elaborated in detail and eventually mapped to the use-cases.

The remainder of the chapter is organized as follows. Chapter 2 presents definitions of terms that will be used throughout the deliverable. Chapter 3 gives the current state of the art of the interface; in particular is provides an overview on the methods corresponding to pre-processing, post-processing and variations that can be found in literature. Chapters 4 and 5 give the view on the interface from the perspective of the EM and UUV use-case, respectively. Chapter 6 discusses the generic solution of the interface by comparing the use-cases of Chapters 4 and 5. In particular, it finds commonalities and differences between the interface of the EM and UUV. In Chapter 7, the conclusions and a summary the most important results and achievements are given.

2 Definitions

This chapter provides an overview of the definitions of terms that will be used throughout the remainder of this document. Since two fields are combined in this chapter (the control and the machine learning fields), there are discrepancies between the terms, see, e.g., (Busoniu, de Bruin, Tolic, Kober, & Palunko, 2018). These discrepancies motivate the present chapter. A total of nine main terms are listed in this chapter: State, Reward, Observation, Action, Input, Internal state, Pre-processing, Post-processing, and Variations. The underlying relation between these terms can be seen in Figure 1. The first five terms are briefly mentioned, since they are discussed in detail in D2.1. Internal state is an important term as will turn out later in the document, related to the Markov property. The last three terms are the main focus of this deliverable. The definitions are as follows:

State	*State* (s) is the signal that is used by the AI agent and forms a representation of the current environment. This choice of *State* is user-determined. The state is obtained or estimated from the *Observation.*
Reward	*Reward* (r) is the signal that represents the goal. The *Reward* is also user-determined from the *Observation*. It is used by the AI agent to update its policy.
Observation	*Observation* (y) is the signal that the system (DT or CPS) outputs from receiving an input. This signal is then *post-processed* to generate the *State* and the *Reward*.
Action	*Action* (a) is the signal that the AI agent generates, based on the *State* and *Reward.*
Input	*Input* (u) is the signal that is entered into the system after *pre-processing* of the *Action.*
Internal state	The *internal state* (x) characterizes the current environment completely. This means that history is implicitly embedded in the internal state. In a Markov Decision Process (Ghavamzadeh, Mannor, Pineau, & Tamar, 2015) , we can give the probability of ending in a new internal state from the current internal state and the current input using a state transition function. The internal state satisfies the Markov Property by definition. The *Observation* is usually a function of the Internal state and often has reduced dimensionality (partial observability).
Pre-processing	In this document and in the ASIMOV project in general, pre-processing refers to the manipulation of the signals that the AI agent produces before they are put into the DT or RS. Note that this definition is different from the definition of pre-processing in most literature on data analysis. There, pre-processing refers to the process of manipulating data before it is used for analysis.
Post-processing	*Post-Processing* refers to the manipulation of the *Observations* produced by the system in order to create the *State* and the *Reward* to be used for the AI agent. Note, this is also different from the definition of post-processing in data analysis literature. In data analysis, post-processing concerns the manipulation of data after the main analysis has been performed. In this document, the 'post' refers to the fact that the signals have been produced by the system.
Variations	The system on which the training of the AI agent is being done is one instance of the digital prototype, which corresponds to one intended purpose. Variation can be used: • To improve the AI agent's robustness by changing the DTs properties slightly and therefore imitating artefacts of the RS (e.g. manufacturing anomalies). This also can account for uncertainty in the internal state (partial observability).

	• To make the trained AI agent applicable in other intended purposes, in which the CPS behaves substantially differently. Training the AI agent with such variations can be seen as a way to enable a zero-shot approach for calibration of the RS (Degrave, et al., 2022).

3 State of the art

In this section, the state of the art regarding pre-processing, post-processing and variations as defined in Chapter 2 is presented.

3.1 Pre-processing

The goal of pre-processing for interactions with the system is to reduce the complexity of the RL problem. While the *Inputs* (u) might be required to be very complex in order to maximize the obtained *Rewards* (r), it might be possible to obtain almost the same *Rewards* with simple *Actions* (a) using smart pre-processing. Additionally, the pre-processing block can be used to change the *Inputs* (u) in order to increase safety or satisfaction of constraints.

3.1.1 Input Shaping

In this section, different methods for shaping the input are detailed. In general, the dimensionality of the input space for typical CPSs can be very high. For example, consider the problem of generating a trajectory for a pen in order to replicate handwriting. This problem could be formulated as finding a sequence of points that, when connected, produce written text. Finding an appropriate sequence of positions on a 2D plane which together constitute handwritten text presents an extremely complex task. Using what we call input shaping, we can reduce the complexity and learn to solve the problem more quickly. There exist many ways of doing this, such as discretization of the action space into a finite set of positions, parametrizing the inputs into a reduced set of sub-trajectories, learning an encoding of possible moves, and smart interpolating between points or actions. An important concept to consider is whether the shaped input satisfies controllability of the system.

3.1.1.1 Discretization

The first question that arises is why the action space should be discretized in the first place. Firstly, the theoretical analysis behind discrete action space problems is more developed than that of continuous action spaces. However, many CPSs have a continuous input space by design, which results in an infinite set of possible inputs at every timestep (Tang & Agrawal, 2020).

There are multiple ways in which the action space can be discretized. The simplest is to consider a continuous input space and to simply divide the space into many discrete parts. This method causes a problem however, as for a high dimensional input space, the number of discrete actions quickly rises. An alternative approach is to factorize the joint distribution over discrete actions, which achieves the same discretization but reduces the amount combinations which are possible (Tang & Agrawal, 2020). These considerations reveal a trade-off between lowering the dimensionality of the actions and maintaining the accuracy of the inputs, as the methods that result in lower dimensionality also compromise on the possible inputs that can be given.

Another consideration to make when discretizing actions is whether the actions should be relative or absolute. This concept is best illustrated with an example. Consider UC1, the electron microscope. In this use case, the objective is to calibrate the instrument by tuning knob values which improve the resulting image quality. For instance, if the image is under-focused the focus knob should be turned until focus is achieved. The value of the signal that is being sent to the focus lens, which is a voltage, is not necessarily relevant to the calibration solution and might have an offset in between different attempts. Additionally, using relative actions can improve numerical conditions, and can turn static problems into dynamic problems by creating trajectory through the input space. Note that when there are input constraints, the relative actions should be canceled when they would result in violation of the constraint.
The concept of discretization can be generalized into parametrized inputs, which are introduced in the next section.

3.1.1.2 Parametrized inputs

In order to simplify the AI training problem, we can reduce the complexity of the Action space compared to the Input space that is used in the environment through parametrization. In general, a parametrized input looks as follows:

$$u_k = \phi(a_k)$$

where ϕ is the parametrization function. Note that for multi-dimensional actions and inputs, the parametrization becomes a matrix of functions. Note that discretization is a special case of parametrization where we restrict the AI Agent to choose from a finite set of (indexed) actions a_k, after which a corresponding u_k from the input set is fed into the system.

Additionally, the input can be parametrized using basis functions which makes use of aspects of the actions generated by the AI agent. A general basis function parametrization looks as follows:

$$u_k = \sum_{i=0}^{n} \theta_k[i] \cdot \phi_i(a_k),$$

in which $\theta_k[i], \forall\, i \in \{1, \dots, n\}$ are the parameters and $\phi_i, \forall\, i \in \{1, \dots, n\}$ are the basis functions (Yamaguchi, Takamatsu, & Ogasawara, 2009). Examples of basis functions include radial basis functions, derivative approximations, etc. It is important to note that appropriate selection of the basis functions is inherently dependent on the system. Also note that a_k can be discrete or continuous. In Reinforcement learning, the AI Agent selects the values for both the parameters and the actions simultaneously. This can be viewed as making a high-level choice between different actions, and then supplying this choice with parameter values.

Examples of RL with parametrized inputs can be found in literature. For instance, in (Hausknecht & Stone, 2015), Deep RL is applied to a soccer robot. In the paper, the actions that the AI agent can perform operate on a higher level than the soccer robot's input signals. The AI agent can choose between different discrete actions such as moving on the field or shooting the soccer ball, and has to assign continuous parameters such as the movement distance or shooting direction to complete the command. (Masson, Ranchod, & Konidaris, 2016) analyzes RL with an input parametrization similar to (Hausknecht & Stone, 2015). The paper focuses on analyzing the learning problem under this parametrized structure. As an extension, the set of discrete high-level commands can be chosen by the AI agent itself. This method is called encoding/decoding.

3.1.1.3 Encoding/Decoding

Often, the inputs required to be performed by the AI agent in order to achieve the objectives for the system are very complex in nature. However, it is also true that these same complex signals can often be grouped into families with similar characteristics. These groups operate on a higher level and are usually of lower dimension and less complex. This helps the overall AI training problem by reducing the complexity of the action space.

An encoder can use AI techniques in order to learn a mapping from complex input signals to a set of higher-level commands to choose from. For instance, in an EM, a sample manipulation platform can be controlled using commands such as ‘higher focus’ or ‘lower focus’. These commands can then be decoded back into lower-level signals, i.e., trajectories of currents to a motor driving the stage to desired point using low-level feedback controllers

As an example, consider openings in chess. Rather than interpreting every move as an action, an AI agent might instead be able to choose from a catalogue of known valid openings which are sequences of multiple moves. This way, there are fewer options to choose from which enables faster training.

The state of the art regarding action encoding learns these higher-level commands using supervised learning. In (Chandak, Theocharous, Kostas, Jordan, & Thomas, 2019), an “embedding” is inserted as an intermediate step of the RL policy and represents the high-level commands. The high-level policy (state-to-embedding) can be learned by the AI agent simultaneously with the set of high-level commands (embedding-to-input mapping). This can be seen in Figure 2.

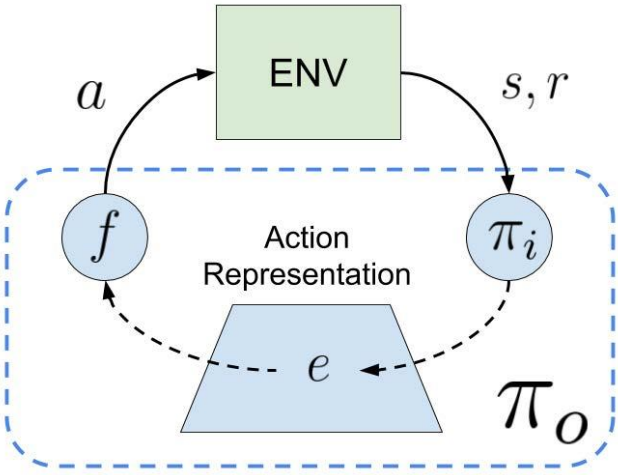

Figure 2 structure of "action representation" in (Chandak, Theocharous, Kostas, Jordan, & Thomas, 2019). The AI agent learns to map states (s) and rewards (r) to inputs (a) by separating into a state-to-embedding mapping and an embedding-to-action mapping. The embeddings are a reduced dimensionality abstraction of the possibly high dimensional input space.

In (Kim, Yamada, Miyoshi, Iwata, & Yamakawa, 2020), the same type of idea is employed except using an autoencoder. This autoencoder learns different high-level (called "latent space") commands based on a set of expert demonstrations. Afterwards, the AI agent learns a policy network that outputs the encoded actions in the latent space rather than the system inputs.

3.1.1.4 Interpolating input signals

Most real-world applications operate in continuous time, while their digital controllers operate in discrete time. This poses the question: what input should the physical system use in between discrete timesteps of the controller? Answers to this question come in the form of interpolation. In control applications, there are many common interpolation strategies such as zero-order-hold (Aström, Hagander, & Sternby, 1984), generalized hold (Chou, Bruell, Jones, & Zhang, 756-761; Bai & Dasgupta, 1990). The theory behind these methods, as well as analysis of benefits and shortcomings, are quite mature (Aström, Hagander, & Sternby, 1984). Special attention should be paid to ensure that the continuous-time system still behaves as desired, for instance with stability or without inter-sample behavior.

3.1.1.5 Reachability

Reachability is a classical concept in the field of control theory, which becomes relevant for RL when pre-processing the system inputs. The reachability of a system is the ability to bring the system from a specific initial state to any other state. By shaping the input, we might lose reachability of the system, potentially making it impossible to reach high-rewarding states. This is illustrated in a simple example. Consider the following nonlinear state-space which describes a dynamic system, which we want to control to $x_k = 0$:

$$x_{k+1} = x_k^2 + u_k.$$

If we discretize the action space as follows: $u_k \in \{-1,1\}$, then, for certain initial values of x_k, e.g., $x_k = 10$, it is impossible to control $x_{k+1}$to the origin given the allowable inputs. The idea of explicitly considering reachability for problems with input limitations can be found in recent literature on RL. Specifically, safe operation through recursive constraint satisfaction can be ensured by using reachability analysis (Yu, Ma, Li, & Chen, 2022). Alternatively, reachability in combination with Lyapunov analysis to ensure stable operation within the constrained space (Huh & Yang, 2020).

3.1.2 Constraint Handling

Systems have physical limitations while operating that should be taken into account in the control architecture. These limitations may contain constraints on the feasible input space, or constraints on internal states/observations. Constraints on the inputs are for example valves that have physical

constraints on their positions, or voltages that only have a limited domain. Constraints on internal states or observations can either be physical constraints that certain positions cannot be reached, or safety constraints to ensure safe operation of the system. The process of dealing with all these constraints is called constraint handling. This section elaborates on the current state of the art on constraint handling.

There are different approaches to deal with input and output constraints. (Glattfelder & Schaufelberger, 2003) gave an extensive overview of different techniques that can be applied on controllers, mainly focused on classical controllers. Controllers are designed to deal with input constraints, output constraints, or a combination of both. The controllers in the overview are viewed from three perspectives; structure, transient response, and stability. This overview is useful when guarantees about stability have to be given. Since the overview is mainly focused on classical controllers, the proposed methods do not take optimality into account.

A popular method that can deal with input and output constraints, as well as optimality is model-predictive control (MPC), see e.g. (Camacho & Alba, 2013; Kouvaritakis & Cannon, 2016; Grüne & Pannek, 2017) In MPC a model is used for prediction of future outputs. Based on a given cost function and constraints, an optimal sequence of control inputs is calculated. Only the first control input is applied, and afterwards the procedure is repeated again. Recent advances in MPC are focusing on combining data-driven techniques with MPC (Hewing, Wabersich, Menner, & Zeilinger, 2020; Berberich, Köhler, Müller, & Allgöwer, Data-driven model predictive control with stability and robustness guarantees, 2020; Berberich, Köhler, Müller, & Allgöwer, Data-driven model predictive control: closed-loop guarantees and experimental results, 2021).

In RL, constraint handling is covered in the field of safe RL. A survey on this topic can be found in (Garcia & Fernández, 2015). In safe RL the goal is still to maximize the expected rewards (similar to ordinary RL) but also to respect safety constraints on either states or actions. (Garcia & Fernández, 2015) considered two types of safe RL:

- Optimization criterion, where a safety factor is included in the reward calculation.
- Exploration process, where the goal is to only select safe actions.

Both types have their benefits and disadvantages. Depending on the type of problem, one type may be preferred over the other.

One of the recent advances within safe RL is the use of a predictive safety filter (PSF), see Figure 3 (Wabersich & Zeilinger, 2021). The idea behind the PSF is that the RL controller still has all the freedom to give actions, while the PSF verifies whether the actions are allowed with respect to the pre-determined constraints. (Wabersich & Zeilinger, 2021) uses MPC techniques within the PSF, to ensure a safe system.

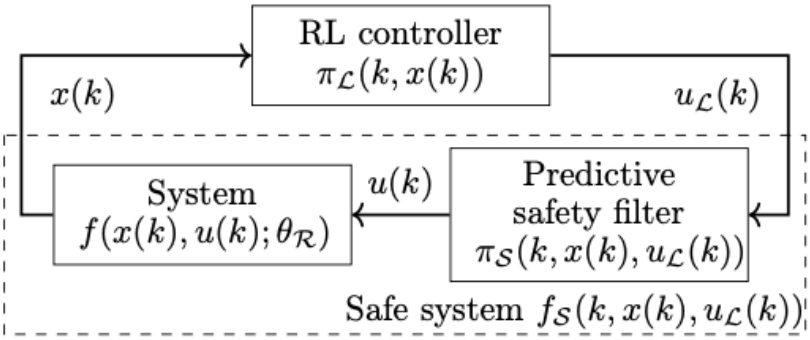

Figure 3 Structure of a system with an RL controller attached, which uses a predictive safety filter to ensure safe operation. Figure adopted from (Wabersich & Zeilinger, 2021).

3.1.3 Tuning controller parameters

To further simplify the RL problem, one can make use of an existing standard feedback controller design with some freedom in the form of tunable parameters. Then, the parameters of this controller can be tuned using the AI agent, possibly dynamically. Notions like stability and robustness can be enforced due to the known character of the controller. In (Qin, Zhang, Shi, & Liu, 2018), RL is used to dynamically tune three parameters of a proportional-integral-derivative (PID) controller. A PID controller is a widely used feedback controller because of its effectiveness and simplicity. The user only needs to tune three parameters in the form of the proportional (P), integral (I), and derivative (D) gains. By allowing the AI agent to tune these parameters, the controller can become adaptive to changes in the system. Furthermore, the properties of the feedback system can be analysed using mature theoretical tools available to PID feedback structures. The structure of this concept is shown in Figure 4.

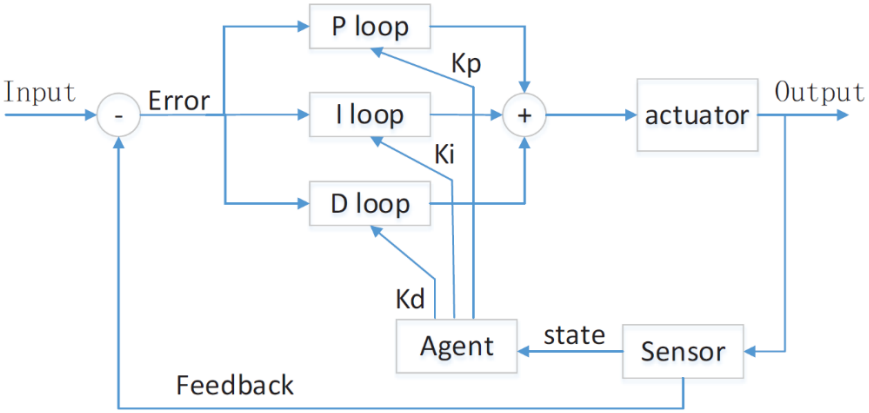

Figure 4 structure of RL-tuned PID controller.

3.2 Post-Processing

The system (either a RS or its DT) and the AI agent are connected to each other by the post-processing step. Post-processing converts the information available from the system in such a way that it can be used by the AI agent. The post-processing can be divided into several categories:

1. Information preparation
2. State shaping
3. Reward function formulation

In Figure 5, a general structure of the post-processing is visualized, containing the above mentioned three categories. Within the post-processing, first all the available data is prepared in the **information preparation** part. Information preparation includes collecting all the available data and then making it a suitable, cleaned up, dataset for the next steps, without affecting the dimensionality. For preparation one could think of restoring corrupt data or normalization. The second part of post-processing is **state-shaping**. State shaping can either add dimensions to the state or reduce it. Adding dimensions is useful when there is not enough information available in one observation, which can be done by adding history of previous states to the current state, or make use of observers. State reduction can be used when the dimension of the observation is very high (e.g., an image), while the usable information in it can be captured in a low-dimensional vector. The purpose of state reduction is to decrease the load on the AI agent by reducing the dimensionality of the state information. The last category is the **reward function formulation**. The goal of that part is to formulate a reward function which the AI agent should maximize. The reward may depend on the observations, the estimated states or the control inputs.

Information preparation and state reduction are two well-known concepts in Big Data Analytics (see e.g., (García, Ramírez-Gallego, Luengo, Benítez, & Herrera, 2016)). Adding information by using observers is a concept from Control Theory to restore the Markov property, which is important in the learning process of an AI agent (Sutton & Barto, 2018). The remainder of this section is structured as follows: Firstly, an overview of methods of information preparation is given. Secondly, state shaping is explained and concepts are given that can help restoring the Markov property or reduce the load on the AI agent. Furthermore, the formal definition of the Markov property, Markov Decision Process (MDP) and Partially Observable Markov Decision Process (POMDP) are given. At the end the reward function is elaborated in more detail.

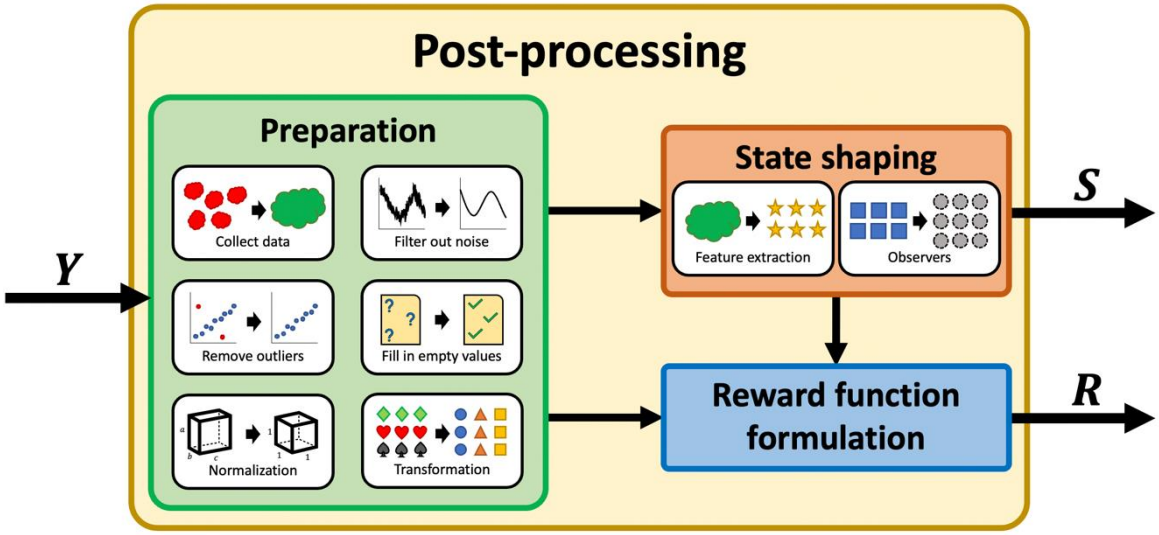

Figure 5 Overview of post-processing process.

3.2.1 Information preparation

The first step within post-processing is information preparation, where all available data is collected and made suitable for the subsequent steps. In the literature there are several authors who wrote methods on this topic, see e.g., (García, Ramírez-Gallego, Luengo, Benítez, & Herrera, 2016; Saleem, Asif, Ali, Awan, & Alghamdi, 2014; Famili, Shen, Weber, & Simoudis, 1997). Among all the methods mentioned, there are six main methods covered in almost every overview:

1. **Integration:** gather all available data and merge it. This should be done carefully to prevent, for example, duplicates.
2. **Noise handling:** measurements that contain irrelevant high frequent noise should be treated to suppress that noise.
3. **Cleaning:** removing and correcting bad data. Data which does not make sense, should be removed from the dataset. An example of cleaning is the removing of outliers.
4. **Missing data imputation:** within control systems this includes the handling of different sample times of sensors. The AI agent operates at a particular frequency, so the state information should be available at the same frequency. More information regarding missing data imputation can be found in (Luengo, 2012).
5. **Normalization:** can be used to scale the data.
6. **Transformation:** convert the data such that it becomes easier for processing in the subsequent steps. Transformation includes changing the units of the data or the rounding of numbers.

These six methods are visualized in Figure 5.

No major recent advantages in information preparation have been made, since the mentioned methods are highly dependent on the specific use case and the expertise of the researcher (Mansingh, Osei-Bryson, Rao, & McNaughton, 2016). General methods are given in (García, Ramírez-Gallego, Luengo, Benítez, & Herrera, 2016; Saleem, Asif, Ali, Awan, & Alghamdi, 2014; Mansingh, Osei-Bryson, Rao, & McNaughton, 2016), however, it is not possible to determine beforehand which methods should be used.

3.2.2 State shaping

A crucial part within RL is the state. The state contains all the information available to the AI agent at a particular time. The state can either be directly the output of either the RS or DT (solely with some preparation steps), or the result of some intermediate state-shaping steps. Depending on the type of process, different approaches have to be taken in the state-shaping part of the post-processing. An important process property that relates to this is the Markov property. The first part of this section is therefore dedicated to the Markov property with its various types.

When the type of process is known, the next steps within state shaping can be taken. This includes restoring the Markov property if that is required, extracting features from the output of the process, and/or building observers to estimate hidden information. These steps are elaborated in the remainder of this section from the second part onwards.

3.2.2.1 Markov Property

The goal of the ASIMOV project is to optimize the process of determining optimal control settings for complex high-tech systems by use of Artificial Intelligent (AI) technologies. In WP3, where the AI-agent is developed, RL is selected as a promising direction to achieve the goal of the ASIMOV project. The performance that the AI agent can achieve depends on the information (the state) that the complex high-tech system (the process) gives to the AI agent. A property that can be assigned to a process is the so-called Markov property. When a process is said to have the *Markov property*, it means that the new state X_{t+1} only depends on the current state X_t, and not on the states before.

In total there are four different Markov types, which are given in Table 1. These four types can be distinguished based on observability and whether actions are involved or not. If the complete internal state of the process is available at each time instance, it is said to be fully observable. In a lot of processes, only a part of the internal state is available at each time instance since not every relevant property can be measured/observed at each time step. Therefore, these processes are said to be partially observable. If there are no actions involved in the process, the process is autonomous and acts independently of the AI agent/user. On the other hand, the process is controlled if the AI agent/user can interact with the process. In the remainder of this section, these four types are elaborated in more detail.

Table 1 Overview of Markov types.

	Fully Observable	**Partially Observable**
Autonomous	Markov Chain	Hidden Markov Model
Controlled	Markov Decision Process	Partially Observable Markov Decision Process

The first type is a *Markov Chain*, which is autonomous and fully observable. Formally, the Markov Chain can be written down as:

$$P(X_{t+1} \parallel X_t, \ \dots, X_0) = P(X_{t+1} \parallel X_t)$$

The equation states that the transition from current state X_t to new state X_{t+1} is independent of the previous states.

The second type is a *Markov Decision Process* (MDP), which is controlled and fully observable. If a process is an MDP, the new state X_{t+1} only depends on current state X_t and current action U_t. MDP is an extension of the Markov chain and satisfies

$$P(X_{t+1} \parallel X_t, U_t, \ \dots, X_0, U_0) = P(X_{t+1} \parallel X_t, U_t)$$

Since actions U are involved, this Markov type is noted as a decision process rather than a chain.

The third type is a *Partially Observable Markov Decision Process* (POMDP), which is controlled and partially observable. In a POMDP, observations (Y) are typically not the same as (do not represent the same information as) the internal state (X). The observations represent only a part of the information collected in the internal state. The underlying process however, with internal state X, does satisfy the properties of an MDP. Processes which are considered from the perspective of the observations do not necessarily satisfy the Markov property as an MDP:

$$P(Y_{t+1} \parallel Y_t, U_t, \ \dots, Y_0, U_0) \neq P(Y_{t+1} \parallel Y_t, U_t)$$

Since only limited information of the process internal state is considered, adding previous states could change the transition probabilities for the next state.

The fourth type is a *Hidden Markov Model* (HMM), which is autonomous and partially observable. The difference between the HMM and POMDP is that HMM is autonomous (as the Markov Chain). Similar to POMDP, HMM does have observations which give only partial information rather than full state information. The HMM can formally be written down as:

$$P(Y_{t+1} \parallel Y_t, \ \ldots, Y_0) \neq P(Y_{t+1} \parallel Y_t)$$

In the remainder of this report, we will say that the state is Markov if state X satisfies the conditions of an MDP.

3.2.2.2 Restoring Markov property

In many processes that have to be controlled, the output only partially represents the internal state. In these cases, the process is a POMDP (assuming that the internal state does satisfy the properties of an MDP). Therefore, using the output of a process directly as state, results in the state not being Markov. In RL however, all algorithms in (Sutton & Barto, 2018) assume that the state available to the AI agent is Markov, and satisfies the MDP properties. This assumption emphasises the need for restoring the Markov property to make the state for the AI agent Markov again.

Two solutions are briefly discussed in order to restore the Markov property: (i) add a history of the process to the state; and (ii) use (state) observers. These two solutions can be understood from the following traditional and simple example. Suppose that we want to make decisions for the pedal of an autonomous car (brake or accelerate) based on positioning data (e.g. obtained from GPS). Using only the current position measurement to this effect is clearly not enough as it neglects velocity. In fact, braking or accelerating decisions will be very different if the car is still (zero velocity) or moving at high speed, while having the exact same position. One solution is to keep track of the history of positions. Another solution is to estimate the velocity based on previous position measurements. Both of these related solutions allow for informative pedal decisions to be taken.

Adding history is one way to transform a POMDP to an MDP in certain simple cases. However, measurements are often noisy. In such a case, the larger the history window, the better the noise in the measurements can be mitigated. For such problems (which encompass most cases of interest) the complete process history should be stored. However, this is often infeasible.

It is well-known (see (Bertsekas, 2012)) that the state probability distribution given the measurement history is a sufficient statistic for decision making. This means that all the information contained in the process history can be summarized in the state probability distribution given the previous measurements.

An ideal state observer is then one that provides this state probability distribution given the measurements. This is known as the Bayes' filter. A special case, under strong assumptions such as Gaussianity and linearity, is the Kalman filter

In general, this ideal Bayes filter is hard to synthesize and run due to the curse of dimensionality and therefore other forms of observers are used. Such observers aim at simply recovering the internal state (and not the full state probability distribution) from previous measurements. Typically, an observer estimates the hidden internal states using the available observations in a recurrent manner. Such an observer turns a POMDP into an MDP when the state is replaced by the state estimation. This is not an optimal procedure as the information in the state probability distribution is lost, but an often used one in practice. Since the literature on observers is extensive, the complete next section is dedicated to them.

3.2.2.3 Observers

Knowledge of a system's internal state (X) is useful for the purposes of controlling the system to exhibit desired behaviour. In many cases, the full internal state is not directly measured, as detailed in Section 3.2.2.1. However, indirect effects of the internal state can be visible through observations. A *state observer* or *state estimator* can estimate the internal state (X) from measurements of these observations (Y) along with the past system inputs (U).

As seen from the example, observers typically require knowledge of the underlying prescribing equations. In this case, the relationship between position and velocity.

The simplest version of an observer is a Luenberger Observer (Luenberger, 1964). Consider a general linear dynamical system in state space formulation:

$$\dot{x} = Ax + Bu + v,$$
$$y = Cx + w\,,$$

where $x \in R^n$ are the internal states, $y \in R^o$ are the output measurements or observations, $u \in R^m$ are the system inputs, $v \in R^n$ are disturbances acting on the system, $w \in R^o$ is measurement noise, and $A \in R^{n\times n}$, $B \in R^{n\times m}$ and $C \in R^{o\times n}$ describe the behaviour of the system. Now, if $o < n$, then at least one of the internal states is hidden (note that this condition is not sufficient or necessary). In order to estimate this state, we use the observer described by:

$$\dot{\hat{x}} = A\hat{x} + Bu + L(y - \hat{y}),$$
$$\hat{y} = C\hat{x},$$

where $\hat{x} \in R^n$ is our state estimate, $\hat{y} \in R^o$ is our output estimate and $L \in R^{n\times o}$ is the observer gain. We update our estimate based on the difference between our output estimate and the real measured outputs. Under certain conditions, the state estimate x will eventually converge to the real internal state x.

We can design the observer gain L using an optimization problem which minimizes the least squares estimation error, in which case the observer becomes a Kalman filter ((Bertsekas, 2012), Appendix E).

A Bayes' filter generalizes the concept of a Kalman filter to application for general POMDPs, see Section 3.2.2.1. Similarly, the Bayes' filter uses recursive state estimate updates based on measured outputs and inputs. The core idea behind these updates lies in Bayesian statistics, namely Bayes' rule:

$$P(X \parallel Y) = \frac{P(Y \parallel X)P(X)}{P(Y)},$$

in which we update our belief of the internal state X based on the new observations Y.
There exist observers for nonlinear dynamical systems which also use a model of the system and observations to update estimated beliefs, such as the extended Kalman filter or high-gain observers (Khalil, 2015).

Additionally, observers can be used for simultaneous state and parameter (system property) estimation, in which the internal state of the model is appended with a state for the parameter to be estimated. This concept might be of special interest to ASIMOV Task 2.1, in which the relevant parameters of the DT are identified.

In ASIMOV, the idea of observers can be used to restore the Markov property for POMDPs. Additionally, Use Case 1 can potentially be reformulated as an estimation problem, in which estimation of the internal state of the electron microscope can result in easy calibration. Observer-like logic is key in estimation problems which underlines its relevance.

3.2.2.4 Feature extraction

Depending on the application, the output of the system in the form of the observations can take on different forms and different dimensionality. Simple examples of the output are discrete with few possible values, or a single continuous number. A bit more complex is a vector of continuous values. However, in real applications, the output could be a curve (e.g., quantity-over-time) or even an image, such as in the EM use case. The curve is typically described by a set of points; an image consists of gray values for each pixel. Here we give some examples and ideas on how to extract features of the complex shape that are still sufficiently informative as a Markov state. Here, domain knowledge and problem experience plays a large role in the choice.

Principal Component Analysis (PCA) is a well-known and established technique in multivariate statistics. In machine learning, it is considered as belonging to the class of unsupervised learning. The starting point is a dataset with many variables that is summarized using only a few scores belonging to the first, second, third, … principal components. As an example, if a dataset consists of people with many variables describing their height, length of arms, legs, belly size, etc., the first component might pick up on the general size of the person. Mathematically, the first component is a linear function of the original variables. In PCA, the first component is the linear combination with the most variance in the dataset. The second component also finds the most variance, but is "orthogonal" to the first; here it might be a score on the axis along fat vs thin. This way, the original possibly large number of output variables is approximated by a summary using a short vector of scores, all using linear expressions.

There are other variants of this theme using linear expressions; Factor analysis from statistics addresses similar problems to PCA, but is more model-based. Linear Discriminant Analysis (LDA) can be applied if there are known groups in the data; it finds components that are most suitable for separating the groups, i.e., a multivariate dataset where each datapoint belongs to a pre-specified group. For more details on Factor analysis and LDA, see (StataCorp, 2007).

Standard examples often use tens or hundreds of variables as a starting point. Curves and images may be treated as a long vector of values and could be analyzed using the same tools. However, note that positional information is lost here. A somewhat dated example is recognition of faces (Turk, Pentland, Belhumeur, & Hespanha, 1991).

There are more elaborate variants of the discussed techniques as well, described in section 14.5 of (Hastie, Tibshirani, & Friedman, 2009). There, non-linear variants of PCA are discussed, called Kernel Principal Components. Section 14.6 discusses non-negative matrix factorization which is a variant for non-negative scores and strictly positive data, such as grey values in an image. Section 14.7 explains Independent Component Analysis (ICA). ICA tries to find scores in the data such that the projection scatterplots of the scores are as different as possible from multivariate normal as possible. In practice, this can give better results than PCA if some time series is the result of mixing "independent components".

Autoencoders are another technique to handle complex inputs, see (Efron & Hastie, 2021), section 18.3. Here, a complex input is fed into a neural network with several layers. The target output is taken to be a copy of the input. The middle layer has relatively few nodes. As the neural net tries to translate input to (identical) output, the information has to pass through the middle layer. The model therefore has to "code" the information using only the information corresponding to the few nodes in the middle layer. Such a model is considered in the UUV use case, not for defining a state but to generate a reward. The idea is to learn an autoencoder based on a dataset of previous simulation runs. Then, a new simulation run is passed as input to the trained network. The goal is to assess whether this new point is "surprising" in light of the earlier simulations. If the new point is more difficult to predict, i.e., the autoencoder's error is large, then this new point contains new information and therefore gives a higher reward.

In the EM use case, the output consists of an image on which the organization has much fundamental knowledge from physics and years of experience. Here, a spatial Fourier transform of the image gives a new image but with easier to recognize patterns. From here, it is also easier to apply *filters* to block certain frequency bands (e.g., block higher frequencies if the information is in the low frequencies). This example uses 2D images; a similar 1-dimensional variant is the domain of time series, signal processing, which finds many applications in audio signals.

Curves as output of some process may be parameterized or summarized by making use of the understanding of the problem. Here we think of an output y=f(t) for sampled points, typically equidistant. Examples of the predictor t could be time, angle designating a point on a round object, or location. A simple approach could be to work with simple summaries of f(t), such as mean, standard deviation, or percentile-based such as median, IQR, the 95-percentile. Also, these could be made of horizontal intervals. More elaborate summaries could be the (t, y) coordinate of where the curve is steepest.

Alternatively, understanding of the problem could propose a parametric description of f(t), such as y=f(t)a+b*exp(-c*t) with parameters a,b,c. . One observation gives many points on the curve (y, f(t)+error) which can be fit using e.g., least squares. The resulting parameter vector (a,b,c) is then the state summary. Other common fits are polynomials, straight lines, and the Fourier transform for time series mentioned above.

3.2.3 Reward function formulation

Part of the post-processing is the reward function formulation, where a reward signal is created based on the systems' outputs. The reward signal should express the performance on a predetermined task in a single value, $R \in \mathbb{R}^1$. The AI agent then maximizes the total cumulative rewards, such that the performance of the AI agent is as good as possible in the long term. The reward function is not the place where the trajectory to the goal should be shaped in terms of a-priori knowledge. The reward function should include the overall objective and not reward intermediate steps deemed reasonable by the user. By doing so, we let the AI agent figure out the way to the objective itself with as much freedom as possible. In general, the reward function contains not how you want to achieve an objective, but only what you want to achieve (Sutton & Barto, 2018). In the remainder of this section several publications regarding reward function formulation are highlighted and discussed.

In (Eschmann, 2021), an overview with the history, links to behaviour sciences and evolution, and surveys on reward function design is given. A distinction is made between sparse and dense reward functions:

- **Sparse reward functions**: Rewards are only given to the AI agent when the final objective is achieved.
- **Dense reward functions**: Informative intermediate rewards are given to the AI agent while approaching the final objective, although the final objective has not been achieved yet.

Preference is given to dense reward functions to guide the AI agent to the final objective. Sparse rewards may be infeasible in terms of training time, since it could take a long time before rewards are found at all. If sparse reward functions are used, the training time can be decreased when curiosity-based exploration methods are used. Other popular methods to improve exploration when only sparse rewards are available are reward shaping and intrinsic motivation. The first theoretical publication on reward shaping is (Ng, Harada, & Russell, 1999), where potential-based reward shaping (PBRS) is formalized. In PBRS a term is added to the original (sparse) reward function to already achieve rewards in the vicinity of the sparse rewards. The disadvantage of PBRS is that a-priori knowledge is included in the reward function, something undesirable according to (Sutton & Barto, 2018). At intrinsic motivation rewards are given when new states are explored. This method encourages the exploration of new states in order to speed up the search for sparse rewards. The foundation for intrinsic motivation in RL is laid in (Singh, Lewis, Barto, & Sorg, 2010).

(De Moor, Gijsbrechts, & Boute, 2022) applied PBRS in combination with deep-RL in inventory management. The goal of using PBRS was to improve learning behavior by using an existing policy. The same shaped reward function as in (Ng, Harada, & Russell, 1999) has been used:

$$R' = R + F$$

where F is the shaped reward term and R' is the new reward function. In (De Moor, Gijsbrechts, & Boute, 2022), F is a feedback term from the existing policy. By using reward shaping, an important condition is **policy invariance**. Policy invariance means that reward shaping should not change the original desired goal. Interesting publications related to PBRS are (Wiewiora, Cottrell, & Elkan, 2003) and (Harutyunyan, Devlin, Vrancx, & Nowé, 2015), where different types of shaped reward functions are discussed.

A completely new direction in reward function formulation is reward machines (RMs). The background of RMs comes from the question whether the reward function formulation should be a black-box for the AI agent or not (Icarte R. T., Klassen, Valenzano, & McIlraith, 2018). As mentioned before, the reward is expressed as a single value in $\mathbb{R}^1$. If the AI agent could have access to the structure of the reward function, it could help to create subproblems to increase the learning rate. RMs consist of pre-determined high-level states of the environment. The language used in RMs is Linear Temporal Logic (Icarte R. T., Klassen, Valenzano, & McIlraith, 2018). An example of an RM is given in Figure 6. The goal is to collect a cup of coffee (c), and reach the office (o), while avoiding obstacles ($*$). The corresponding reward machine can be seen on the right. It consists of four high-level states: u_0 no coffee, not on an object; u_1 Coffee, not on an object; u_2 on an object; u_3 in office with coffee. This level of abstraction can be useful for the AI agent during training. In (Icarte R. T., Klassen, Valenzano, & McIlraith, 2018) also the algorithm Q-Learning for RMs is provided which explicitly uses the structure of the RM. (Camacho, Icarte, Klassen, Valenzano, & McIlraith, 2019) gave a formal language to the RMs, and extended RMs with shaped rewards. Follow up work and extensions are provided in (Icarte R. T., Klassen, Valenzano, & McIlraith, 2022).

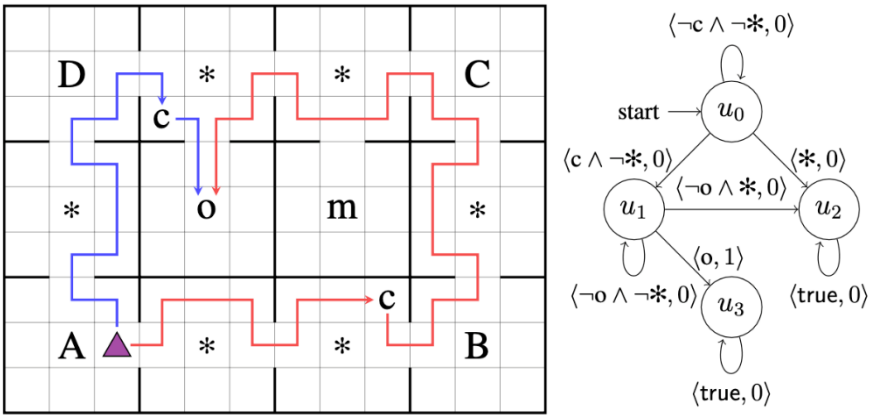

Figure 6 Example of a reward machine (adopted from (Icarte R. T., Klassen, Valenzano, & McIlraith, 2018)*).*

3.3 Variations

It is of great importance to generate data with the DT, that is relevant for the AI agent's training process. As the AI agent will be paired with a RS in the operational phase, it is therefore not only important for the training data to be accurate, but also to represent imperfections in the behavior of the RS and differences in the configuration of multiple systems.

When producing and operating CPSs, there will always be machine-to-machine differences due to, for instance, manufacturing inconsistencies or wear over time. Therefore, even if a perfect model of one instance of a machine is available, an AI agent trained on this model is not guaranteed to have good performance on other instances of that machine. Engineers at NASA state that in DTs "manufacturing anomalies that may affect the vehicle are also explicitly considered, evaluated and monitored" (Glaessgen & Stargel, 2012). Furthermore, it is often impossible to have a perfect model of an RS. This can lead to the AI agent relying on features that are only present in the simulation and not in the RS. Hence, there is almost always a model mismatch. Training an AI agent on a model which does not fully match the RS has detrimental effects on the AI agent's performance on the RS. For these reasons, we seek to train the AI agent in a varying environment that switches between multiple machine instances, multiple models or even multiple domains. Good performance on the varying environment is then much more likely to result in good performance on the RS.

A lot of research on ensuring AI agents perform well in multiple domains is done on arcade games. This concept is called generalization. Arcade games are useful to this end because they are well known, require similar strategies (in other words small variations of high-dimensional control tasks) to win, and

offer widely available frameworks (e.g., Arcade Learning Environment (ALE)) and benchmarks. A method to evaluate the generalization of a policy is to “inject extra stochasticity to the environments during the evaluation process” (Zhang, Vinyals, Munos, & Bengio, 2018). This and other techniques can be used as a regulizer to prevent overfitting or as an evaluation to detect overfitting. Generalization of the AI agent to perform well in other environments can be seen as the AI agents being invariant to changes in the observation space (Farebrother, Machado, & Bowling, 2018). The authors in (Cobbe, Klimov, Hesse, Kim, & Schulman, 1282-1289) address the issue of an AI agent overfitting to a specific environment (which is the DT in the case of ASIMOV) and find, that “deeper convolutional architectures improve generalization, as do methods traditionally found in supervised learning, including L2 regularization, dropout, data augmentation and batch normalization.” More general-purpose features are learned, which can be adapted to similar problems via fine-tuning. On a similar note, the authors in (Farebrother, Machado, & Bowling, 2018) show that Deep Q-Networks (DQN) overspecialize to the training environment. They offer the solution to reuse learned representations to improve the generalization capabilities of DQN. Further, the approach to fine-tune the weights of a learned neural network is discussed, where the authors found that “reusing a regularized representation in deep RL might allow [them] to learn more general features which can be more successfully fine-tuned.” In our use cases, the trained policy can ideally also be applied, or at least be the training basis for the application, on slightly different physical systems, to cover the product family aspects.

Independent of which of the above-mentioned problems, variation needs to be applied at some point during the training process. In (Moos, et al., 2022), possible ways of handling this variation are discussed. Depending on how the variation is included, the authors distinguish between different types of robustness that can be achieved.

A system is **Transition Robust** when it can cope well with every - even with the least likely - state transition.

It is **Disturbance Robust** when it can cope with a system that is influenced by parameter changes or modeling errors not in control of the AI agent.

Action Robust describes a system that can be controlled, even though the AI agents' actions are manipulated by an adversary.

Lastly, an **Observation robust** system is characterized by the fact that the system is robust against adversarial attacks that try to generate observation data, that is indistinguishable from real data, but influences the RL agents’ output to a great extent.

We can further distinguish which type of parameters are changed during variation. For a common understanding of the different parameter types, the nomenclature used in the ASIMOV T2.1 document shall be used. In this scheme, u is introduced as the input into the system, which is controlled by the AI agent. Typically, these inputs can be set independently and are the means for optimizing the system in ASIMOV.

Disturbances d are another input type that influences the system. Disturbances can be seen as external signals acting on the system, that cannot be controlled by the AI agent. There are however ways to include them in the simulation.

The system parameters c are not inputs, but rather a set of parameters that define the behavior of the system itself. They are, besides the internal model structure, the main influence on how a system translates its inputs to outputs.

The output of each system is described as y .

3.3.1 Three Kinds of Variations

Variation can be introduced in different ways in the DT. Depending on where the variation is introduced and which parameters are varied, we distinguish between different variation types in ASIMOV, that are explained below. For a wider view on the consequences for the use cases, the Use Case Mapping sections provide further details.

3.3.1.1 Disturbance Variation

The disturbance variation targets the disturbances d . . As they are varied, small changes of the system can be introduced for improved robustness of the AI agent. It forces the AI agent to cope with varying responses of the CPS.

Disturbance Variation can vary after each action of the AI agent.

In the STEM use case, such disturbance variation could include effects that cannot be influenced by the configuration or control of the microscope. This could be room temperature, camera noise, electron source noise, vibrations, etc.

In the UUV use case, such effects could be noise in camera or Radar images, as well as gusts of wind in the virtual environment.

3.3.1.2 System Configuration Variation

Digital Models used in traditional simulations represent a typical instance of the physical counterpart. Due to manufacturing inaccuracies, wear and slightly different operating configurations, multiple systems of the same type can behave differently. These effects are captured by system parameters c , which generates different CPS instances when varied. Ideally, the AI agent should be able to perform well for all common CPS instances, be it new or worn-out, for instance. Furthermore, this can help to overcome the inadequacies of the simulation due to insufficient parameter choices. In other words, we want to avoid that the model overfits one some specific parameters choices, that do not reflect the actual behavior that shall be learned.

This type of variation can also include a switch to a different model of the same system, as proposed in (Khairy & Balaprakash, 2022), which could be first-principles-based or purely data-driven. If the RL loop switches between these models in between episodes, the optimal policy is one that performs well for both models. Hence, bias to one type of modeling error is reduced.

As it is unnatural for a system to change its behavior in terms of system configuration during an optimization process, this variation can only be applied in-between episodes.

System Configuration Variation can also be realized in two different ways, both of which are compatible with the concept explained in Figure 5. One way is to create arbitrary system parameter combinations to build a virtual fleet of fictional systems without a link to RSs. The other way is to create a real fleet of multiple RSs, linked to their DTs. The diversity in the fleet and the resulting differences in the system configuration parameters of their DTs defines the system configuration variation.

Examples of the System Configuration Variation in the STEM use case could be the high-tension voltage, the magnification, targeted resolution, sample type, sample thickness, aperture dimension, position, etc.

The UUV use case offers such possibilities in the form of varying the properties of Vehicle, Sensor and Driving Function.

3.3.1.3 Domain Variation

This is the type of variation which typically results in the largest differences in the environment. It is represented by a major change in the interaction of the system with the AI agent. This can include different outputs y and actions u .

The idea is to switch to a completely different system which is required to perform the same type of task. This way, the optimal policy of the AI agent is more generalized in the sense that it can solve the whole task type, rather than only the specific system. This idea is employed in the RL benchmark AlphaZero.

AlphaZero by Google DeepMind (Silver, et al., 2017) is able to play multiple different games (chess, go, shogi) at an extremely high level using a single AI agent. It is able to do so by exploiting commonalities in high-performing playing strategies in these games. To understand this, consider the games it is able to play. The games are all examples of combinatorial games, where both players have perfect information and make moves in sequence. These games can typically be represented as decision trees, in which the different choices that players can make are different branching paths of the tree. The difficulty in solving such games typically stems from the fact that these trees can grow very large, resulting in many possible ways a game can play out, too many to compare explicitly.

AlphaZero makes use of a neural network to perform tree searches more efficiently, drastically reducing the time to evaluate the tree. The key lies in the fact that certain tree branches should be given more attention than others. This is also how human players approach these games. Rather than evaluating and comparing every possible option, often only a few promising candidate moves are considered. For example, in chess, if one of the move choices leads to a forced checkmate by the opponent, the entire branch following this move choice can be disregarded. This idea generalizes to alpha-beta pruning (Knuth & Moore, 1975), in which any move that can lead to a worse position than the current best candidate is disregarded. Using neural networks, AlphaZero is able to learn an advanced tree-search algorithm with many tricks similar to alpha-beta pruning, making the search even faster. But because tree-search generalizes, AlphaZero is able to perform well for not just chess, but any combinatorial game.

AlphaZero learns the tree-search algorithm through self-play on increasingly complex games. By starting with a simple combinatorial game, the solution to the game can be found by the AI agent in relatively little time. By switching to a new game which is more complicated, the lessons from the simple game can still apply so long as both are combinatorial games. This concept is called c*urriculum learning* (Soviany, Ionescu, Rota, & Sebe, 2022). Since the structure of the inputs and the outputs of the system may change with the variation of the domain, a wider view of the consequences is necessary. It also typically introduces manual intervention and happens after successful complete training of the AI agent for one type of system.

Examples in the STEM use case could be the application of the AI agent on a new type of microscope with other controls, or estimating aberrations from a different type of output image, e.g., a STEM image rather than a diffraction pattern.

In the UUV use case, the change of Operational Design Domain (ODD) would be an example for such a variation.

3.3.2 How to introduce variations

There are several techniques to introduce variations. In this section, a selection of these techniques is summarized.

3.3.2.1 Random

The first, and easiest approach is to have variations at random. To be able to select variations at random with a uniform distribution, bounds on the variation domain should be provided. If the random values are selected by means of a normal distribution, the mean and standard deviation should be provided. Normal distributions can be very useful when the parameter is approximately known with uncertainties if these uncertainties are normally distributed. If the parameter can have a value within a large domain and shows a uniform distribution on that domain, random values with a uniform distribution are useful. The advantage of random variations is that no bias is introduced. The disadvantage, however, is that this method is extremely time-consuming, as covering every possible combination of variations often results in a huge variation space. Furthermore, there is no preference for specific variations. That results in “common” variations having the same probability as “uncommon” variations.

3.3.2.2 3.3.2.2 Space-Filling

The second approach, that deals with the disadvantage of the variations at random that there is no equal distribution, is to use a space-filling Latin-hypercube design, see e.g. (Gramacy, 2020). In (Eriksson, Johansson, Kettaneh-Wold, Wikström, & Wold, 2000), more techniques are given when experiments have to be chosen from fixed ranges. All the aforementioned techniques still have no preference for specific variations; all these techniques are determining the variations beforehand, without any interaction with the system.

3.3.2.3 Neural Networks

A technique that introduces variations that became of great interest in the last couple of years within the field of neural network, is the variational auto-encoder (Doersch, 2016). As a consequence of a low-dimensional hidden layer in the neural network, which forces the reproduction of the input to be summarized in a low-dimensional projection. The idea is to remove the encoder part, and only sample from the low-dimensional layer, to produce a high-dimensional layer. The advantage is that a lot of feasible variations can be created, based on real data. Also, anomaly detection can be executed to find rare cases, see e.g., (An & Cho, 2015). Furthermore, techniques such as Generative Adversarial Networks (GANs) may be of interest to introduce variations (Creswell, et al., 2018). GAN's also aim to create "fake" situations that are useful to train a network.

3.3.2.4 Curriculum Learning

Within curriculum learning, variations are introduced by task generation. In task generation, sub-targets are determined that the AI agent should solve. Ideally, these tasks have an increased difficulty. The tasks are created manually. Automated task-generation is still an open-research question (Narvekar, et al., 2020).

3.3.3 How to convert DT performance to RS performance?

The goal when training an AI agent with a DT should be that the learned policy can be applied to the RS directly. In accordance with (Degrave, et al., 2022), this can be seen as a zero-shot approach. If the performance of the policy is not satisfactory, the AI agent can be fine-tuned on the DT of the RS. Here, DT is to be understood as an instance of the DT Prototype, that is linked to one physical twin (PT) and therefore contains all details about it (Glaessgen & Stargel, 2012). In (Nichol, Pfau, Hesse, Klimov, & Schulman, 2018) the authors mention a trend in RL to "train on the test set". They introduce a meta-learning dataset, consisting of many similar tasks sampled from a single task distribution, to construct a suitable benchmark. This dataset can be used to evaluate few-shot RL algorithms.

By not having realistic variations of the digital environment, it is unlikely for the AI agent to perform well on the RS. Like detailed above, three kinds of variations were considered when training the AI agent.

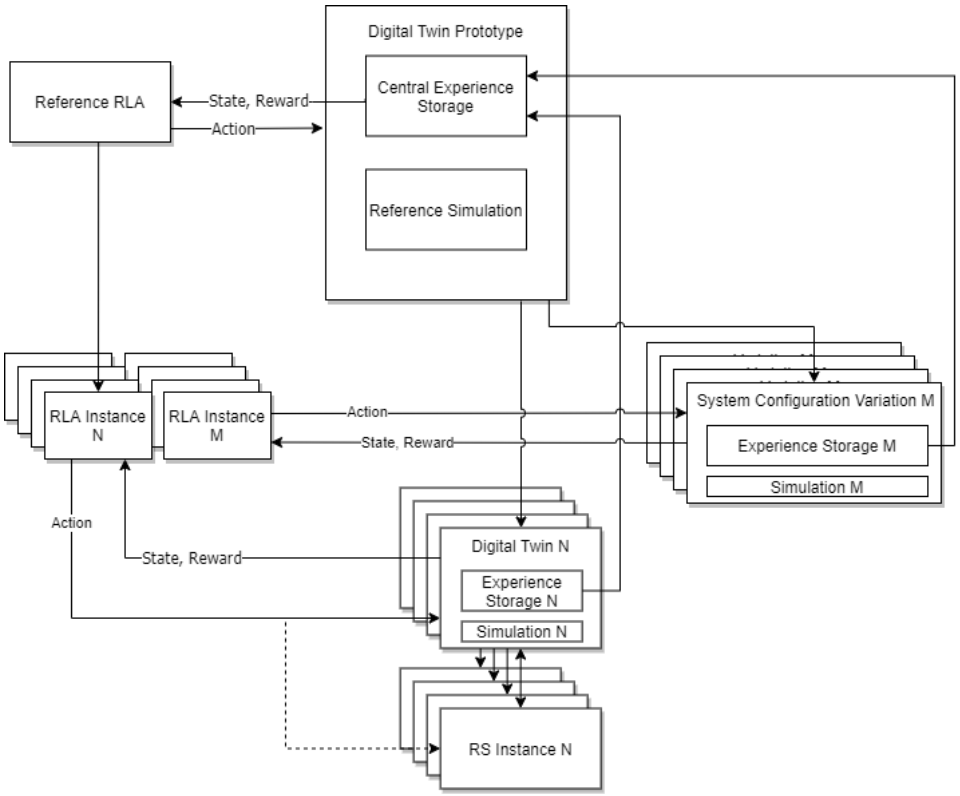

Figure 7 This Figure introduces an interpretation, in which System Configuration Variations are seen as instances of a DT Prototype (further details about the differences to the DTs in the text). The boxes indicate the different entities and the arrows indicate either dataflow, an instantiation from a generic entity, or (in the case of a double arrow) a twinning process. The dotted arrow indicates that the action can in principle be applied to the RS instance directly, but this is not the preferred option, at least not during training. The two stacks of RL Agent (RLA) instances are in theory the same, but hint at the difference between the DTs and the System Configuration Variations.

In the architecture described in Figure 7, a reference RL Agent is trained on a centralized experience storage that was fed by all the instances of the DT Prototype. Those have in turn been used to train the instances of the RL Agents. This option requires the experiences to be stored locally, which might not always be desired.

Constructing the policy of the Reference AI agent can be seen as an application of federated learning (FL), which “is an approach to machine learning, in which the training data is not managed centrally.” (Ludwig & Baracaldo, 2022) While the biggest motivation to apply federated learning might be in applications in which data privacy and data ownership are paramount, there are also more practical reasons. Especially with big datasets in settings where the bandwidth is not great, it can be very practical not having to send the data to a central storage. In FL the parties performing the local training are called *clients*, and the instance that orchestrates the training is called *aggregator*. In our case the Generic AI agent can serve as aggregator and the instances are the clients. Each client is trained on an environment (which is the instantiated and twinned DT), which contains all the manufacturing anomalies of the RS (Glaessgen & Stargel, 2012). The aggregator receives the trained models from the clients and performs *model fusion.* In the case artificial neural nets, this could be realized in averaging the weights. This merged model will then be deployed either to all the existing instances, where the next iteration of this process can start, or to a completely new instance, where it serves as the starting point for the local instance. If the performance is not satisfactory, the fine tuning with the instantiated DT happens. Since the instance of the DT shall be connected to, and twinned with the RS, this translates into a good performance on the RS. Note, that there may be multiple aggregators, each commanding a party of clients. This is relevant for our domain variations, where the structure of the models may vary significantly.

4 Mapping UC1 (STEM)

The first ASIMOV use case (UC1) concerns transmission electron microscopy. To achieve state-of-the-art resolution, Transmission Electron Microscopes (TEM) require a tuning procedure, often by an expert user. Such a procedure is crucial to bringing TEM to its lowest aberration state. Aberrations cause deviations in electron trajectories, or, equivalently, in the electron wavefront, thus deteriorating the imaging resolution. Our aim in the ASIMOV project is to automate the aberration correction process using a new method which takes advantage of an AI agent, trained on the data simulated by a DT of a TEM.

To estimate and correct aberrations different output images can be used. Here we use so-called Ronchigram images, of an amorphous sample in Scanning Transmission Electron Microscope (STEM) mode. We initially aim at controlling 1st order aberrations, namely, 2-fold astigmatism, and defocus and assume that all higher-order aberrations are controlled to be near-zero by methods already available in the TEM software. A Ronchigram is a convergent-beam electron diffraction pattern (CBED) that carries information both about the properties of the specimen and the properties of an electron beam, such as aberrations. Depending on the amount and type of aberrations present in the electron beam, different patterns emerge in the Ronchigram image. For instance, if 2-fold astigmatism is present, the Ronchigram of an amorphous sample shows stretched patterns in the presence of defocus (see Figure 8).

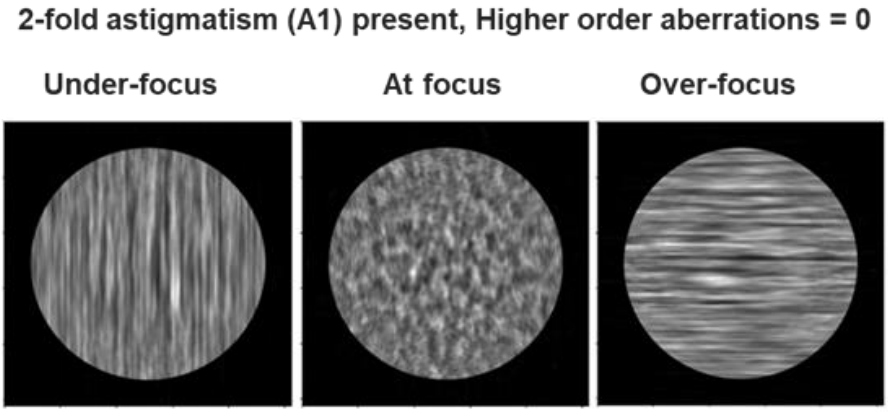

Figure 8 Response of Ronchigram image to 1st order aberrations, defocus and 2-fold Astigmatism: In presence of 2-fold astigmatism, Ronchigram pattern rotates by 90 degrees while changing focus settings.

For the objective of ASIMOV, the AI agent should learn how to move the state of the TEM system, via control knobs for defocus and astigmatism, towards a state with zero aberrations (zero defocus and 2-fold astigmatism in this case). Table 2 shows how the concepts explained in this document map to the TEM use case (UC1). The remainder of this section is dedicated to pre-processing, post-processing, and variation methods used in the UC1.

Table 2 Mapping of concepts used in this document to the TEM use case (UC1).

Concept	Definition in UC1
Observation	Ronchigram images
State	Aberration values accessible via Ronchigram images
Internal state	Full state of the electron microscopy system, including, but not limited to, aberrations of the electron beam (due to imperfections in optical components, such as lenses), electron beam energy, the detection device and the specimen. The system is only partially observable.
Reward	A function representing the lower or zero aberration values.
Action	The signal that the AI agent generates from which the aberration controller values (input) is inferred.
Input	The value of the controller knobs for defocus and 2-fold astigmatism

4.1 Pre-processing

The AI agent used in UC1 defines the actions in the form of the step size and the direction for a change in the aberration values, namely, the defocus, and the 2-fold astigmatism in 2 directions (real and imaginary part of the astigmatism). On a TEM system the change in aberration is, in practice, achieved via a lower-level control which is the change in the current of the magnetic lens coils. Therefore, the action set by the AI agent needs to be translated to the lower-level control parameters. However, assuming a linear relation between the lens current and the aberration values, the relative changes set by the AI agent can be directly used for controller knobs of a TEM. The accuracy of this assumption will be further investigated in future experiments.

Additionally, the TEM controller knobs impose limitations on the range of input values, to ensure the operator remains in the reasonable working regime of the TEM. Therefore, constraint handling is also relevant for UC1. Currently, the AI agent is aware of the boundaries of the possible actions via the environment. The environment is limited to aberration values that are within the boundaries of allowed values for the controller knobs.

4.2 Post-processing

4.2.1 Information preparation

Currently, we apply the following transformations to prepare the images for the RL algorithm:

1. Cropping the image, so that it only includes the diffraction pattern within the disk (the so-called bright field disk)
2. Normalizing the image
3. Applying a window function (e.g., Kaiser window)
4. Applying the 2d Fourier transform

The above steps result in an image that shows the presence of aberrations in a more obvious way, at least to the human eyes. Although, one can start with the Ronchigram image itself as the input to the RL algorithm, from experience we have noticed that using these post processing steps makes the AI training more efficient.

In the post-processed image in the case of zero aberration, the Ronchigram image corresponds to a small circle. As defocus increases, the disk radius increases, and with large 2-fold astigmatism an ellipse-like shape appears. Figure 9 shows two examples of Ronchigram images and their transformed form after the 4 steps described above.

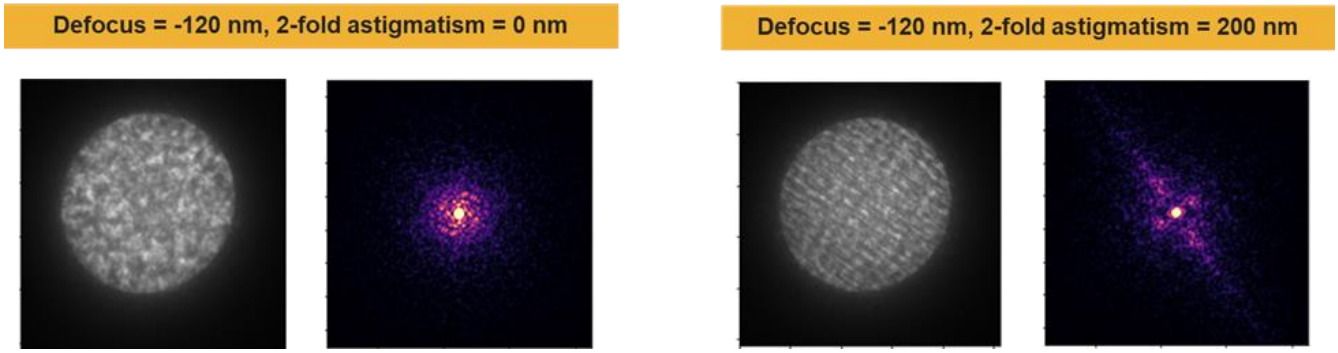

Figure 9 A Ronchigram image and its transformed form for two cases with different aberrations. Left: Only defocus is present, right: Both defocus and 2-fold astigmatism are present.

4.2.2 Reward function formulation

In UC1, the reward should represent the level of aberration, which should be as small as possible, ideally zero. Aberrations, i.e., the deviation of the electron wavefront from an ideal spherical shape, are caused by imperfections in an optical system. Theoretically, knowing the exact geometry and location of the optical elements in an electron microscope, one can calculate the deviations in the electron wavefront, to which an aberration function is fitted and the aberration coefficient values are calculated. However, the

exact geometry and locations are usually unavailable and also not in the scope of the current DT. In electron microscopy it is more common to estimate the values of the aberration coefficients from the effects it has on the captured image. This is also the method that we use here. The image we use for estimating the aberration level is Ronchigram image of an amorphous specimen and from there we further define a reward function.

Using the domain knowledge, a reward function, representing the level of aberration, was carefully formulated. This was done, firstly, by feature reduction on the post-processed image (the Fourier transform image) and, secondly, by defining reward as a function of the reduced features. The process is as follows. The prepared (post-processed) image is smoothed with a Gaussian kernel. Subsequently, the shape appearing in the smoothed image is quantified. This is done by interpreting the spectra as an unknown realization of a 2-dimensional bivariate Gaussian distribution. We then determine the eigenvalues of its covariance matrix. For an ellipse this gives 2 non-equal values. A scaled ratio of these numbers was used as the reward function in the proof-of-concept case. In this proof of concept, the reward is now a direct function of the state, next to being near convex and an example of a so-called shaping reward. Finally, it is not sparse, which can make learning more efficient.

Additionally, a new method for defining a state & reward is being developed. The goal is to achieve a reward that is more general in terms of extendibility to other types of aberrations and needs less human involvement in defining the reward function. In this method, the state is ascertained using a neural network (currently a resnet18 encoder) which uses the entire prepared image, rather than the image with reduced features, as the input. The AI agent, in short, needs to take a decision based on an image alone, outputting new knob values every turn. The reward can be sparse, simply zero everywhere except for the goal state, or inverse shaping based on the distance the knob settings are from an ideal value.

4.2.3 State shaping

In general, the full internal state of the physical TEM system is unknown. The aberration level of the system is inferred via the observation, the Ronchigram image in our case. The full internal state of the system is only partially observable. This is also the case for the DT of the system. Although several parts of the physical system are abstracted by simple models in the DT, there are some parameters of the system which are hard to estimate using only one image.

A few cases for which the internal state cannot be inferred from one observation (one Ronchigram image) are as follows. One Ronchigram does not necessarily provide sufficient information to infer both first order aberration coefficients, namely, the 2-fold astigmatism and the defocus values. For instance, a large astigmatism and no defocus can result in an almost identical image as a large defocus and no astigmatism. Another case is when the accurate parameters describing the performance of the camera are not available and they cannot be estimated from one Ronchigram. In this case a pre-estimation process is most likely required. Another example is if a magnetic lens in an electron microscope shows significant hysteresis effect. This means that using the coils' current value as a control parameter will result in different magnetic fields and thus different beam quality, depending on whether the preceding change in current was in decreasing or increasing direction. The hysteresis effect is not currently covered in the DT, and due to its complexity, it should be investigated whether this effect is significant enough to merit a further modelling step.

To restore the Markov property for the system one approach is to use the system's history, i.e., use a sequence of images over time, or use a different parameter estimation process before running the DT simulations. This can provide the Markov property, which is important for the AI agent. This means that an AI agent bases its decision solely on the state that the system is currently in.

4.2.4 Offline vs. online RL

Note that in the current setting the DT generates an image dataset with sampling over the control parameters and small variations over the rest of parameters, accompanied by a metadata file describing the parameter values for each image. The AI agent then starts the learning and interacts with this already prepared dataset, rather than with the DT itself. This is known as offline RL. This has been convenient for proof-of-concept. However, this approach has limitations. For instance, the AI agent is limited by the

sampling resolution in the dataset. Moreover, it will become increasingly difficult to generate an offline dataset once the number of control parameters increases. Therefore, the preferred method for the future is for the AI agent to directly interact with the DT.

4.3 Variations

In addition to parameters controlled by the AI agent there are other parameters in the DT that are varied to provide a more realistic scenario for training the RL algorithm. Below is a list of variations considered in the system according to three types described in Section 3.3.

Disturbance Variation: Effects that cannot be influenced by the configuration or control of the microscope. For example, when controlling first order aberrations (defocus and 2-fold astigmatism) it is possible that higher order aberrations still have small, nonzero, values. Therefore, small random values of higher order aberrations are added to produce variations in the DT outputs. Moreover, sources of noise, such as camera noise, are added to the DT to create variations.

System Configuration Variation: Another source of variations can be the parameters, which are unknown in the physical measurements. For instance, when the thickness of the sample is unknown, the DT can produce outputs with several thickness values so that the AI agent can learn to become robust to it.

Domain Variation: An example of domain variations is in the STEM use case where the AI agent could be applied on a different microscope type with different inputs or outputs, e.g., a STEM image rather than a diffraction pattern (Ronchigram). However, this type of variation so far has not been used in the RL training.

5 Mapping UC2 (UUV)

The following chapter will explain how the concepts of the previous chapters can be mapped to the Unmanned Utility Vehicle (UUV) use case.

5.1 Pre-processing

In the pre-processing step, the actions provided by the AI agent need to be transformed into a file that describes the environment variations. For that, it is currently planned to use a JSON file as data structure. In this JSON file, information about the density of trees in certain areas, as well as the positioning of vehicles on the roadside, will be stored. To eliminate false combinations (like vehicles overlapping each other) a correction needs to be incorporated in this block as well, while keeping in mind that error correction might lead to the AI agent not being able to learn correctly. After this, the Variation JSON file is used to create the varied Unreal Environment, which can then be loaded together with the respective OpenDRIVE and OpenSCENARIO files, to run an instance of the simulation. Figure 10 shows the pre-processing pipeline from the JSON file to the Unreal engine. The JSON file is passed to a variant process that evaluates the variation information contained in the JSON file and creates a Triangraphics (TG) project file. The TG project file contains all the variants specified in the JSON file. Since the TG project file cannot be processed directly by Unreal, the next process generates data that can be imported by Unreal. After the import, the data is then available for simulation.

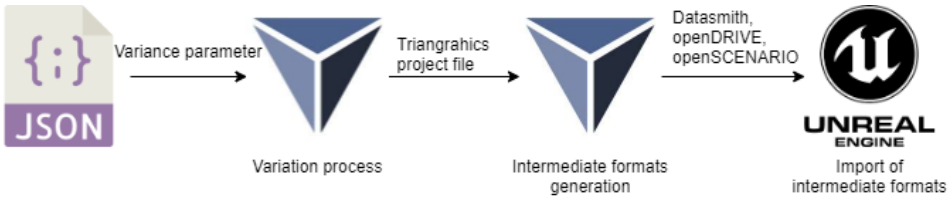

Figure 10 Pre-processing pipeline

5.2 Post-processing

Post-processing takes all the measurement data collected during the simulation runs and calculates relevant states and rewards out of that. In the UUV.1 use case, this will contain two aspects, representing the goals of the optimization process. On one hand, an anomaly detection, based on an autoencoder neural network, will be used to measure the information gain of every simulated scenario. On the other hand, criticality metrics will be used.

An Autoencoder is a neural network, which has the same number of neurons in the input and output layer. Its main purpose is to reconstruct the input data in the output layer, with as little error as possible. The easiest way to do this would be to learn the identity function, meaning that every input is passed through the network without any modifications to it. To suppress this behavior, the hidden layers in-between input and output layer, have less neurons. This ensures compression of the input data and therefore an automatic extraction of relevant features of the input vector. This also means that the autoencoder can cope with data of similar type better than when confronted with completely new data. This makes it applicable for use as anomaly detection, by measuring how good the autoencoder can reconstruct the data, it is confronted with.

The Anomaly Detection will be using the entire set of measurement data, gathered during one simulation run, and will calculate the reconstruction error of every signal by providing it as input to the autoencoder network. The overall reconstruction error will be used to measure the anomaly value and therefore the information density of the dataset. A high reconstruction error represents a high information value. This will be part of the reward function. After calculating the information value, the neural network will be retrained, also incorporating the just seen dataset as additional training data. That way, when confronted with similar data, a low reconstruction error and therefore low information value will be determined by the anomaly detection. The individual contributions of every signal to the overall anomaly score will represent part of the state.

The criticality metrics will be scenario specific and will be evaluated for every simulated scenario as well. It is planned to use an ensemble of different key performance indicators (KPIs) to measure the criticality

of scenarios based on different aspects. The selection process for the KPIs can be found in (Westhofen, et al., 2022).

In Figure 11, the entire post-processing workflow for reward calculation can be seen.

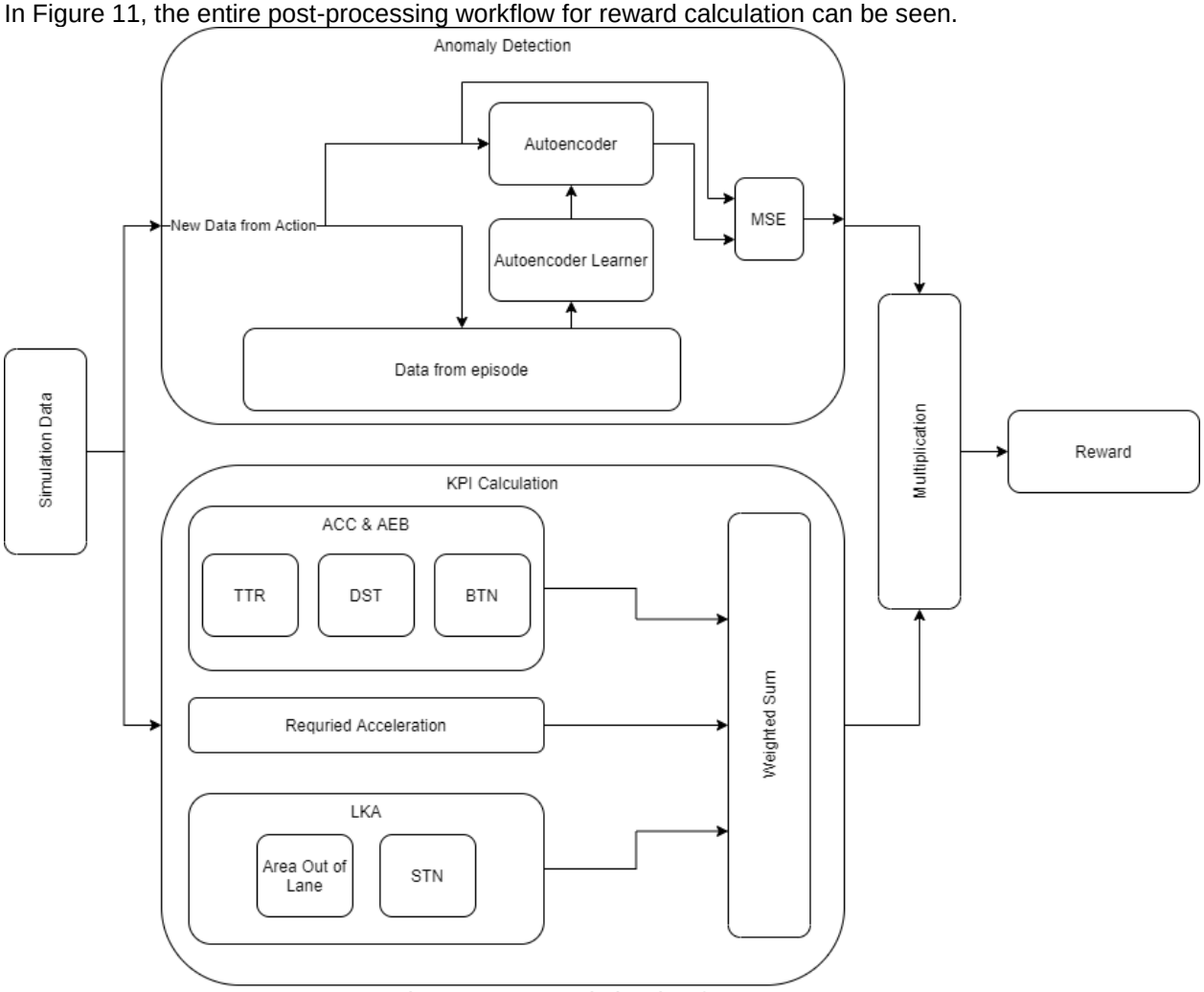

Figure 11 Reward shaping for UC2.

5.3 Variations

Variations are needed to make the AI agent more robust during training. Slight variations in the vehicle's response to actions lead to the AI agent proposing more general actions, which avoids overfitting to the DT. This allows for an easier transfer of the learned actions to the RS, which slightly differs from the DT. For the variation to work as intended and to yield an advantage, it has to be ensured that the actual physical twin lies in-between the boundaries of the variation. The variation can therefore include experts' knowledge about typical parameter ranges of certain vehicle types.

Variation will happen in between different episodes of learning as part of resetting the environment from the AI agent's perspective. During an episode, i.e., a sequence of actions that include requests for test cases, the vehicle will not be varied, as it has to be ensured, that each varied vehicle offers a consistent response across its test sequence.

Variation itself can happen either by randomly changing certain parameters of the vehicle inside some limiting boundaries, or by systematically changing parameters to ensure an evenly covered space of vehicle properties.

6 Generic solution

Based on the described methods in the state of the art in chapter 3, combined with the use case mapping to these methods in chapter 4 and 5, a generic solution can be formulated that fits within the ASIMOV context. In the next version of this report, this generic solution is being formulated.

7 Conclusions

This document puts forward the proposed interface between the DT and the AI agent to be used in the ASIMOV project. The proposed interface relies on three main ingredients: pre-processing, post-processing and variations. In the context of pre-processing, existing solutions include input shaping through discretization or, more generally, input parameterization, encoding and decoding, and input interpolation. Pre-processing solutions must ensure constraint handling. Post-processing can be divided into the following categories: information preparation, state shaping, and reward function formulation. Information preparation encompasses integration, noise handling, cleaning, missing data imputation, normalization and transformation. State shaping techniques include restoring the Markov property, extracting features from the output of the process, and building observers to estimate hidden information. Solutions for formulating reward functions include reward shaping and reward machines. Variations can be introduced in different places in the model, including disturbance variations, system configuration variations and domain variations, and can be introduced randomly, via space-filling, or via neural networks. For each of the two main use cases of the project, the Electron microscope and the Unmanned Utility Vehicle pre-processing, post-processing and variations were instantiated, and use-case-specific training features were discussed.

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