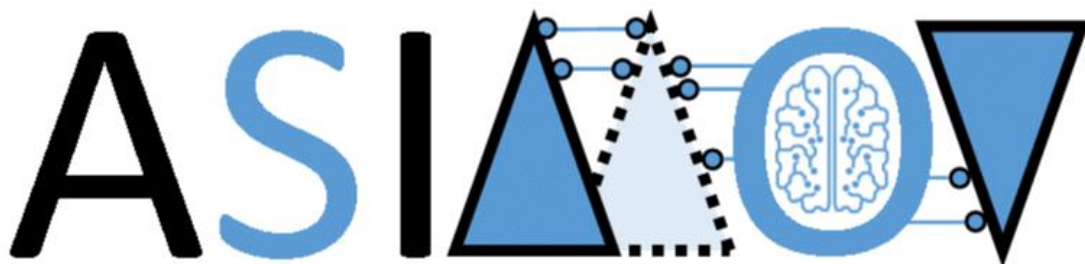


Specifications and Commonality Analysis

[WP1; T1.1; Deliverable: IR1.1]

Confidential



AI training using Simulated Instruments for Machine Optimization and Verification

PROPRIETARY RIGHTS STATEMENT

THIS DOCUMENT CONTAINS INFORMATION, WHICH IS PROPRIETARY TO THE ASIMOV CONSORTIUM. NEITHER THIS DOCUMENT NOR THE INFORMATION CONTAINED HEREIN SHALL BE USED, DUPLICATED OR COMMUNICATED BY ANY MEANS TO ANY THIRD PARTY, IN WHOLE OR IN PARTS, EXCEPT WITH THE PRIOR WRITTEN CONSENT OF THE ASIMOV CONSORTIUM THIS RESTRICTION LEGEND SHALL NOT BE ALTERED OR OBLITERATED ON OR FROM THIS DOCUMENT. THIS PROJECT HAS RECEIVED FUNDING FROM THE ITEA4 JOINT UNDERTAKING UNDER GRANT AGREEMENT NO 20216. THIS JOINT UNDERTAKING RECEIVES SUPPORT FROM THE EUROPEAN UNION'S EUREKA AI RESEARCH AND INNOVATION PROGRAMME AND FINLAND (DECISION PENDING), GERMANY, THE NETHERLANDS.

Version	Status	Date	Page
M30	internal	2022.11.29	1/43

Document Information

Project	ASIMOV
Grant Agreement No.	20216 ASIMOV - ITEA
Deliverable No.	IR1.1
Deliverable No. in WP	WP1; T1.1
Deliverable Title	Specifications and Commonality Analysis
Dissemination Level	internal
Document Version	M30
Date	2023.11.29
Contact	Hans Vanrompay
Organization	Thermo Fisher Scientific
E-Mail	hans.vanrompay@thermofisher.com



The ASIMOV-project was submitted in the Eureka Cluster AI Call 2021
<https://eureka-clusters-ai.eu/>

Version	Status	Date	Page
M30	internal	2022.11.29	2/43

Task Team (Contributors to this deliverable)

Name	Partner	E-Mail
Hans Vanrompay	TFS	Hans.Vanrompay@thermofisher.com
Niklas Braun	AVL	Niklas.Braun@avl.com

Formal Reviewers

Version	Date	Reviewer
M6	2021.12.09	Jacco Wesselius (ESI (TNO)); Remco Schoenmakers (TFS)
M18	2022.12.05	Pieter Goosen (ESI, TNO); Roy van Zuijlen (TU/e)
M30	2023.12.05	Lukas Schmidt (NorCom), J.W. Bikker (CQM)

Change History

Version	Date	Reason for Change
M6	2021.11.26	Initial submission with EM and UUV use case
M18	2022.11.29	M18 update
M30	2023.11.29	M30 update

Version	Status	Date	Page
M30	internal	2022.11.29	3/43

Abstract

In this document, the specifications, commonalities, and fundamental differences between industrial use cases were gathered, analysed, and reported. Electron Microscopy (EM) and Unmanned Utility Vehicles (UUV) are the two target industrial use cases, which comprise sub use cases, are detailed down and described. These target use cases are entitled as (1) automated correction of defocus and astigmatism in the condenser system of a Transmission Electron Microscope, (2) automatic test case generation and sensor optimization from Unmanned Utility Vehicles domain. This document also provides domain analysis and contextual information about these targeted use cases. Additionally, assumptions, constraints, limitations, and dependencies associated with all these use cases are described with enough details.

Version	Status	Date	Page
M30	internal	2022.11.29	4/43

Contents

Specifications and Commonality Analysis [WP1; T1.1; Deliverable: IR1.1]	1
1. Introduction	8
2. Target Use Case: Transmission Electron Microscopy	9
2.1 <i>Overview of Target Use Case</i>	9
2.1.1 Domain Analysis	9
2.1.2 Transmission Electron Microscope (TEM)	9
2.1.3 System Decomposition	10
2.1.4 The Ronchigram	12
2.1.5 Goal	13
2.1.6 Scope	14
2.1.7 Context	14
2.1.8 Assumptions	16
2.1.9 Constraints	16
2.1.10 Dependencies	17
2.1.11 Requirements	17
3. Target Use Case(s): Unmanned Utility Vehicles	25
3.1 <i>Overview of Target Use Case</i>	25
3.1.1 Purpose	25
3.1.2 Scope	26
3.2 <i>Sub Use Case 1 - Automatic Test Case Generation</i>	26
3.2.1 Introduction	26
3.2.2 Context	26
3.2.3 Assumptions	29
3.2.4 Constraints	29
3.2.5 Dependencies	29
3.2.6 Requirements	29
3.3 <i>Sub Use Case 2 - Sensor Optimization</i>	33
3.3.1 Introduction	33
3.3.2 Context	34
3.3.3 Assumptions	35
3.3.4 Constraints	35
3.3.5 Dependencies	35
3.3.6 Requirements	35
4. Analysis of Commonalities and Differences Between Use Cases	36
4.1 <i>System</i>	36
4.1.1 Commonalities	36
4.1.2 Differences	37
4.2 <i>Optimization</i>	37
4.2.1 Commonalities	37
4.2.2 Differences	38
4.3 <i>Envisioned solution</i>	38
4.3.1 Commonalities	38

Version	Status	Date	Page
M30	internal	2022.11.29	5/43

4.3.2	Differences	38
4.4	<i>Digital Twin (DT) modeling</i>	39
4.4.1	Commonalities	39
4.4.2	Differences	39
4.5	<i>Artificial Intelligence (AI) learning</i>	40
4.5.1	Commonalities	40
4.5.2	Differences	40
5.	Terms, Abbreviations and Definitions	42
6.	Bibliography	43

Version	Status	Date	Page
M30	internal	2022.11.29	6/43

Table of Figures

Figure 1: Structure of Transmission Electron Microscope	10
Figure 2: Schematic View of Electron Microscope Components	11
Figure 3: Illustration of Ronchigram features as a function of different aberrations. OF stands for over focus, UF for Under focus. [1].....	13
Figure 4 - Overview of Components Targeted for Sub Use Case 1.....	15
Figure 5: Illustration of the envisioned experimental set-up.....	16
Figure 6 - Electron Microscope Components Included in the Digital Twin.....	18
Figure 7 - Overview of Digital Twin Parameters.....	19
Figure 8 - Unmanned Utility Vehicle on a University Campus [2]	25
Figure 9 - Process Overview Sub Use Case 1.....	27
Figure 10 - Overview Data Management and Processing	28
Figure 11 - Process Overview Sub Use Case 2.....	34

Table of Tables

Table 1 - Details of EM_SUC1_FR_DT_001 Requirement.....	17
Table 2 – Details of EM_SUC1_FR_DT_002 Requirement	19
Table 3 - Details of EM_SUC1_FR_DT_003 Requirement.....	20
Table 4 - Details of EM_SUC1_FR_DT_004 Requirement.....	20
Table 5 - Details of EM_SUC1_FR_DT_005 Requirement.....	20
Table 6 - Details of EM_SUC1_FR_AI_001 Requirement	21
Table 7 - Details of EM_SUC1_FR_SL_001 Requirement	21
Table 8 - Details of EM_SUC1_FR_SL_001 Requirement	21
Table 9 - Details of EM_SUC1_FR_SL_003 Requirement	22
Table 10 - Details of EM_SUC1_FR_SL_004 Requirement	22
Table 11 - Details of EM_SUC1_FR_DA_001 Requirement.....	22
Table 12 - Details of EM_SUC1_NF_CO_001 Requirement	23
Table 13 - Details of EM_SUC1_NF_EX_001 Requirement.....	23
Table 14 - Details of EM_SUC1_NF_PE_001 Requirement.....	23
Table 15 - Details of EM_SUC1_NF_UE_001 Requirement.....	24
Table 16 - Details of UUV_SUC1_FR_DT_001 Requirement.....	29
Table 17 – Details of UUV_SUC1_FR_DT_002 Requirement.....	30
Table 18 – Details of UUV_SUC1_FR_DT_003 Requirement.....	30
Table 19 – Details of UUV_SUC1_FR_DT_004 Requirement.....	30
Table 20 - Details of UUV_SUC1_FR_OA_001 Requirement	31
Table 21 - Details of UUV_SUC1_FR_OA_002 Requirement	31
Table 22 - Details of UUV_SUC1_FR_OA_003 Requirement	31
Table 23 - Details of UUV_SUC1_NF_DA_001 Requirement	32
Table 24 - Details of UUV_SUC1_NF_DA_002 Requirement	32
Table 25 - Details of UUV_SUC1_NF_DA_003 Requirement	32
Table 26 - Details of UUV_SUC1_NF_DA_004 Requirement	32
Table 27 - Details of UUV_SUC1_NF_DA_005 Requirement	33
Table 28 - Details of UUV_SUC1_NF_PE_001 Requirement.....	33
Table 29 - Terms, Abbreviations and Definitions	42

Version	Status	Date	Page
M30	internal	2022.11.29	7/43

1. Introduction

This document provides a detailed analysis of the specifications, commonalities, and fundamental differences between the targeted industrial use-cases; Scanning Transmission Electron Microscopy (STEM) and Unmanned Utility Vehicles (UUV). These use-cases are each composed out of several industrial use-cases, which are detailed below.

The targeted industrial use-cases are:

1. Transmission Electron Microscopy
 - a. Automated correction of aberrations in the electron microscope
2. Unmanned Utility Vehicles
 - a. Automatic test case generation

Further domain analysis on the individual industrial use-cases is provided in the next sections. In addition, information on the requirements, assumptions, constraints, limitations, and dependencies associated with all these industrial use-cases is provided. Based on the derived information of the different industrial applications, the commonalities and fundamental differences are derived.

Version	Status	Date	Page
M30	internal	2022.11.29	8/43

2. Target Use Case: Transmission Electron Microscopy

2.1 Overview of Target Use Case

In what follows we will first provide the context needed to gain a full understanding of the targeted industrial use case. First, we introduce the field of nanoscience. Next, we highlight the role TEM has played in this field and provide a short summary on the working principles of a TEM. Finally, we introduce the type of images we will use to realize the targeted use-case, and discuss its scope and purpose in detail

2.1.1 Domain Analysis

Nanoscience investigates structures and materials with at least one dimension ranging from 1 to approximately 100 nm. Its focus is on harnessing the distinct properties of nanomaterials, which significantly differ from their bulk counterparts. As materials are scaled down, the surface-to-volume ratio experiences a substantial increase. Consequently, surface atoms play a more significant role, leading to the domination of surfaces in influencing the properties of nanomaterials. This dominance results in unique physical and chemical characteristics not observed in bulk materials, making nanomaterials particularly appealing for diverse applications.

The distinctive features exhibited at the nanoscale have generated heightened interest in nanoscience, driving rapid advancements across various fields, including chemistry, materials science, energy, medicine, electronics, and food. The key to the progress in nanotechnology over the past century lies in research dedicated to understanding the interplay between nanomaterial structure and their physical and chemical properties. This understanding is vital for guiding the synthesis of new nanomaterials with predetermined properties in a systematic and reproducible manner. The specific properties of nanomaterials are intricately linked to their structure, size, and composition. Therefore, a precise structural and chemical characterization is essential to comprehend their unique properties. Transmission electron microscopy (TEM) stands out as an indispensable tool for studying nanomaterials, offering a resolution on the order of 50 pm. However, TEM is constrained to samples thin enough to allow electron passage, requiring technically challenging thinning processes and additional tools.

2.1.2 Transmission Electron Microscope (TEM)

The image formation process in a TEM is very similar to that of an optical light microscope. The main difference is related to the use of electrons as the source of light and the associated replacement of glass lenses by electromagnetic coils. In a TEM, electrons are accelerated towards the specimen using high voltages in order to obtain images with a resolution higher than achievable in optical light microscopes. These electrons are emitted from a thermionic gun or a field emission gun (FEG). Afterwards they pass through a system of condenser lenses, to produce a beam with desired size, intensity and convergence. In TEM mode, a parallel coherent beam is formed, which illuminates the sample uniformly. In STEM mode however, the beam is focused into a fine probe, which is scanned across the specimen.

Once the desired electron beam is formed, it interacts with the specimen, which is placed in a dedicated specimen holder. This holder is located between the two pole pieces of the objective lens. The transmitted electrons are focused by the objective lens into a diffraction pattern in the back focal plane of the objective lens after which they recombine, yielding an enlarged image of the specimen in the objective lens its image plane.

An ideal lens system is expected to image a single point source as a point. Scherzer, however, demonstrated that for round symmetric electromagnetic lenses, spherical and chromatic aberrations are unavoidable. Spherical aberrations cause rays, located far away from the optical axis of the spherical lens, to have a different focal point than rays with the same wavelength, close to the optical axis.

Version	Status	Date	Page
M30	internal	2022.11.29	9/43

Chromatic aberrations are observed when rays with distinct wavelengths, focus differently. All together, these aberrations contribute to blurring of the image.

For both the condenser- and objective lenses, stigmators are present that correct for astigmatism. Astigmatism occurs when the magnetic field in the lens is not symmetrical. Stigmators apply a correcting field to compensate for this asymmetry.

Below the objective lens, a system of intermediate and projector lenses creates a magnified image of either the sample in real space or the corresponding diffraction pattern in reciprocal space. This image can e.g. be visualized using a Charged Coupled Device (CCD) or a direct electron detector. The complete build up of a transmission electron microscope is presented in Figure 1

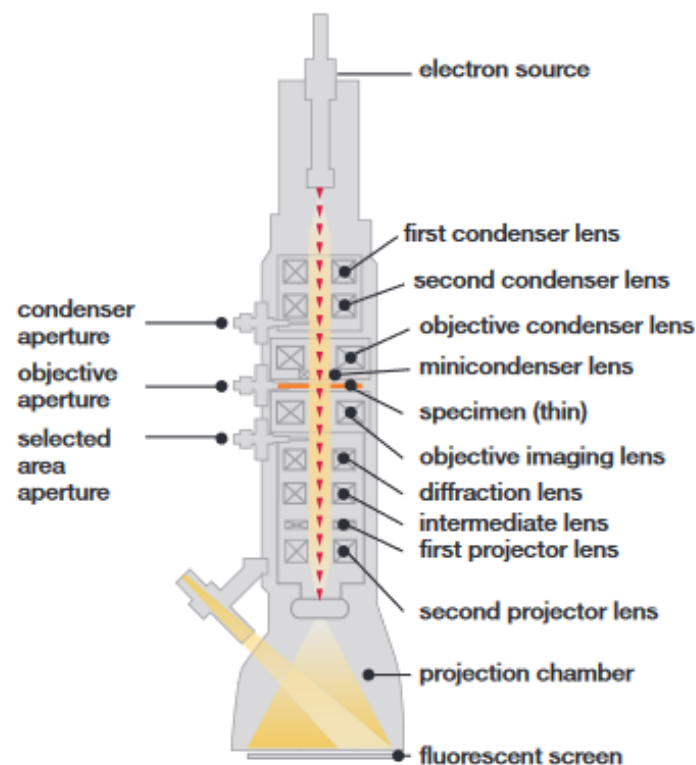


Figure 1: Structure of Transmission Electron Microscope

2.1.3 System Decomposition

Figure 2 shows the high-level view of the transmission electron microscopy. As shown, the transmission electron microscope is composed out of three distinct building blocks: (A) Electron Source, (B) Column, (C) Imaging System. The Electron Source block comprises electron gun, accelerator, monochromator components, and all other parts that are not shown in the figure but available at the real microscope. The Column consists of condenser, objective, projector systems and sample itself. The Imaging System block comprises the components for detectors and cameras.

Version	Status	Date	Page
M30	internal	2022.11.29	10/43

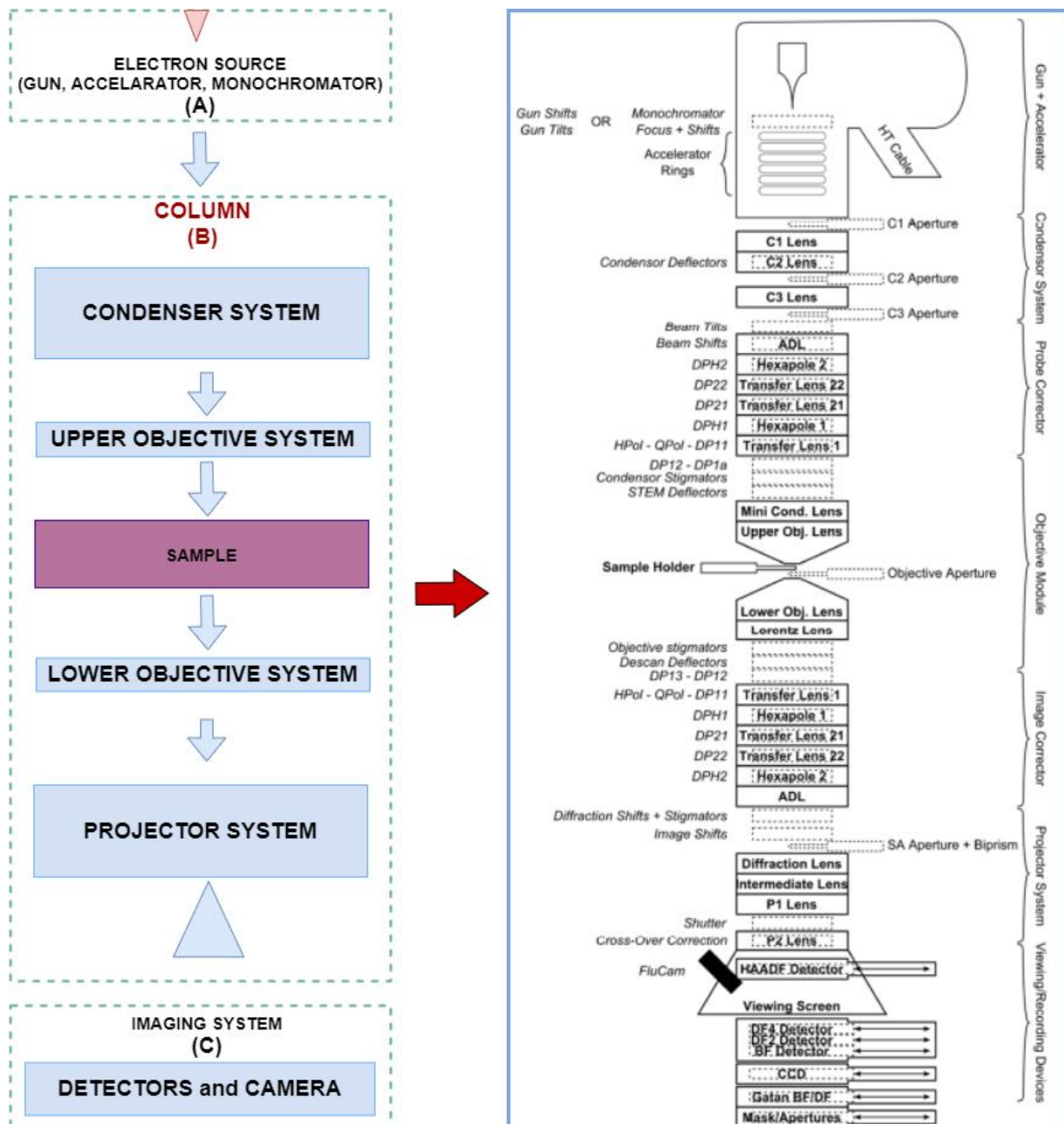


Figure 2: Schematic View of Electron Microscope Components

Version	Status	Date	Page
M30	internal	2022.11.29	11/43

2.1.4 The Ronchigram

In the electron microscope use case, Ronchigram images are the key to finding the right parameters for the microscope's lens system that maximize the spatial resolution. The term Ronchigram is a reference to the "Ronchi test"; a standardized test for shaping aberration-free optical lenses. By placing a diffraction grating within the focus of the optical lens, the imperfections of the lens would be recognizable from the obtained interference pattern.

Constructing Ronchi's grating is not possible in an electron microscope. Due to the high frequency of the accelerated electrons the gratings' spacing would have to be only a few picometers wide for interference to occur. Creating such a grating is therefore extremely challenging. Instead, the atomic arrangement in amorphous materials is used, to provide a nearly random assortment of atomic potentials. This random assortment provides a good approximation of a noisy grating and mimics the Ronchi test by providing interference patterns that reveal aberrations in electromagnetic lenses.

Key features in the Ronchigram which can be exploited to measure the aberrations consist of the Ronchigram's symmetry and magnification (Figure 3). When in focus, the center of the Ronchigram has a high local magnification that represents the aberration-free portion of the electron beam. Further away from the center, thus moving away from the optical axis, aberrations reduce the local magnification. Having as large as possible magnified central region is a first indicator for an optimal defocus. The presence of asymmetric aberrations breaks the rotational symmetry of the Ronchigram. Two-fold astigmatism unidirectionally stretches the region of high magnification, thereby producing distinctive streaks. Axial coma shifts the center of the Ronchigram and higher order aberrations further break the symmetry of the Ronchigram.

Version	Status	Date	Page
M30	internal	2022.11.29	12/43

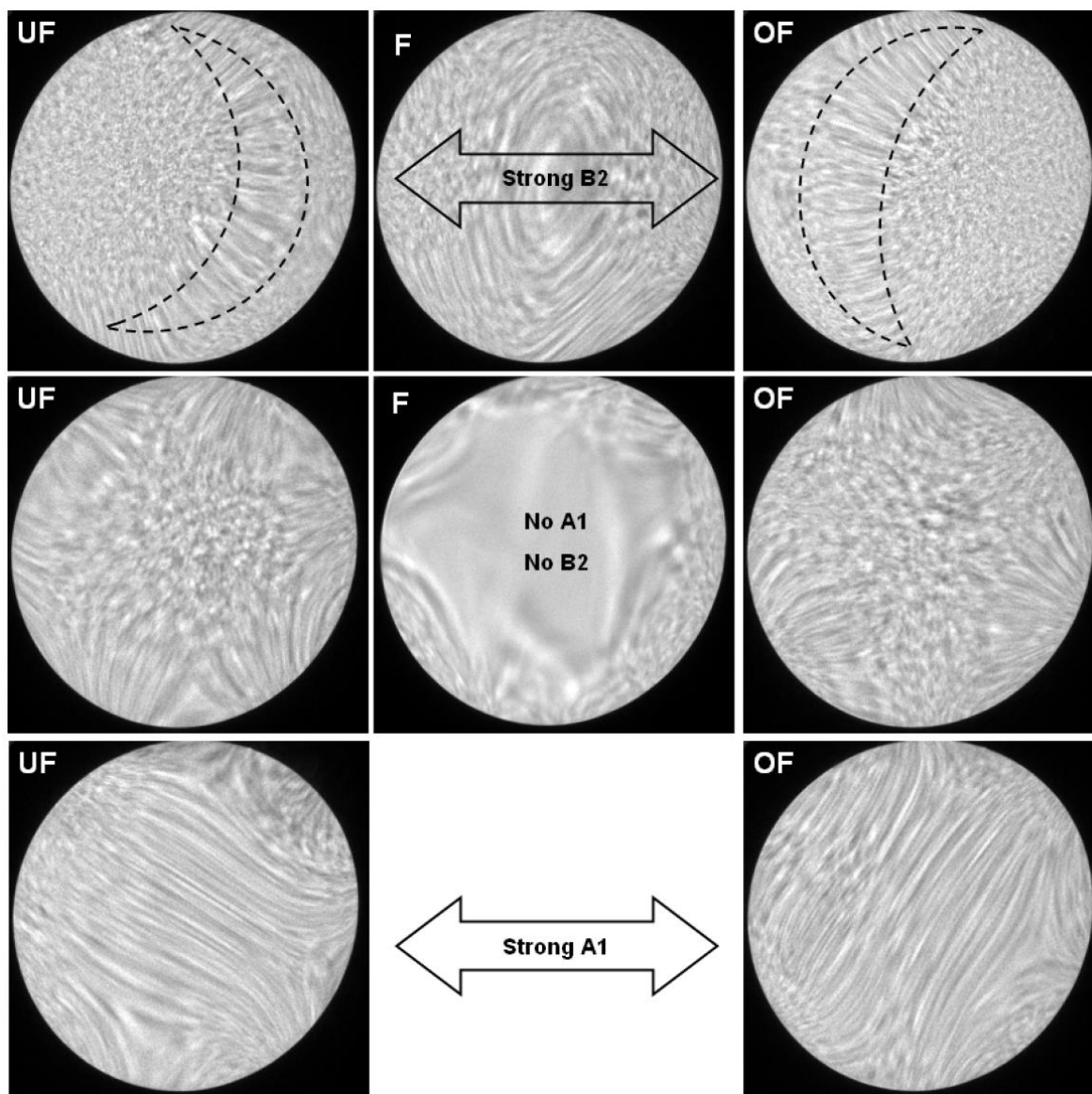


Figure 3: Illustration of Ronchigram features as a function of different aberrations. OF stands for over focus, UF for Under focus. [1]

2.1.5 Goal

Prior to shipping a microscope, it must be calibrated to ensure it can reach the desired resolution. This calibration is an intensive alignment procedure during which various experimental parameters have to be optimized to ensure that the electron beam coincides with the optical axis of the electron microscope (e.g. centering the apertures, gun tilt, gun shift, etc.). In addition, the current through the various electromagnetic lenses and correctors needs to be adjusted such that an electron beam with minimal aberration is formed.

As of today, the microscope operators spent on average 200 working hours on the alignments of the electron microscope before the microscopes can be shipped to customers. Roughly half of that time is correlated to aberration corrections. Therefore, there is a clear need to automate this process, as it will lead to a large cycle time reduction, and ability to produce more microscopes in the same amount of time.

Version	Status	Date	Page
M30	internal	2022.11.29	13/43

2.1.6 Scope

For the new use-case, the objective is to align and calibrate electron microscopes. As of today, microscope operators need to correct aberrations manually and go through time-intensive routines to calibrate the TEMS.

All components that are integral part of the electron microscope column and required for generation of a Ronchigram are within the scope of the target use case. For digital twinning and training an AI model, the condenser system, electron beam interaction and detector are targeted. The electron source system (i.e., comprising the electron gun, accelerator, and monochromator) and imaging system will be ignored within the context of ASIMOV. The electron source system is considered as an ideal point source and is used as an input parameter to the condenser system. Given that we will focus on the Ronchigram image, the output of the column system, and not the final magnified STEM image, simulating the full imaging system is not required.

Within the ASIMOV project we will investigate the use of digital twinning and AI-based optimization for automated microscope calibration. We envision that an AI based solution will allow for a faster, more reliable and automated calibration of the electron microscope.

2.1.7 Context

The main challenges that Thermo Fisher Scientific is facing regarding aberrations correction during electron microscopy calibration are:

- Time-intensive and tedious procedure to minimize aberrations. Especially the correction of higher order aberrations can take multiple hours, thereby wasting valuable experimental time.
- Images with a limited resolution due to the presence of aberrations
- Requiring expert microscope knowledge to minimize the aberrations
- The aberration correction needs to be performed repeatedly.
- Since the systems are uncalibrated and agnostic approach is required with a notion of 'better' to calibrate and align the microscope

An overview of the EM components targeted for sub use case 1 is depicted in Figure 4. As can be seen, the column block is subdivided into two sub blocks:

- (B.1) condenser system (composed out of: condenser lenses, apertures, stigmators and deflectors), upper objective system, and sample
- (B.2) lower objective and projector systems.

For this subcase we aim to pursue an agile way of working. Therefore, we will first focus on modeling B.1 and train an AI model to aberrations. In Figure 4, the components targeted for sub use case 1 are indicated in red. However, the end goal is to model both B.1 and B.2.

Version	Status	Date	Page
M30	internal	2022.11.29	14/43

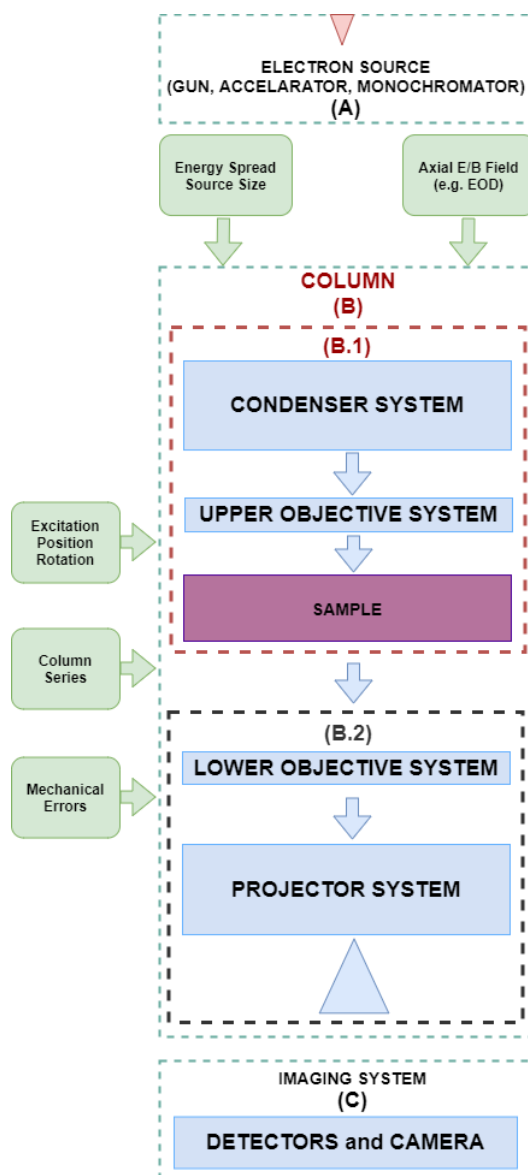


Figure 4 - Overview of Components Targeted for Sub Use Case 1

2.1.7.1 Envisioned experimental set-up

Figure 5, displays the envisioned scenario for the correction of the defocus and astigmatism. The illustrated components are:

- **Digital Twin:** The DT is composed out of models for all components in B.1 including; condenser system, upper objective lens, and electron-sample interaction.
- **AI Agent:** an AI agent is trained on simulated data from the digital twin. Its purpose is to create necessary actions (e.g., values for multifunction and defocus knobs) to tune the microscope to reduce the condenser astigmatism.
- **Electron Microscope:** Enable the AI agent to interact with the electron microscope. Based on experimental images, it will estimate the required actions and apply them autonomously.

Version	Status	Date	Page
M30	internal	2022.11.29	15/43

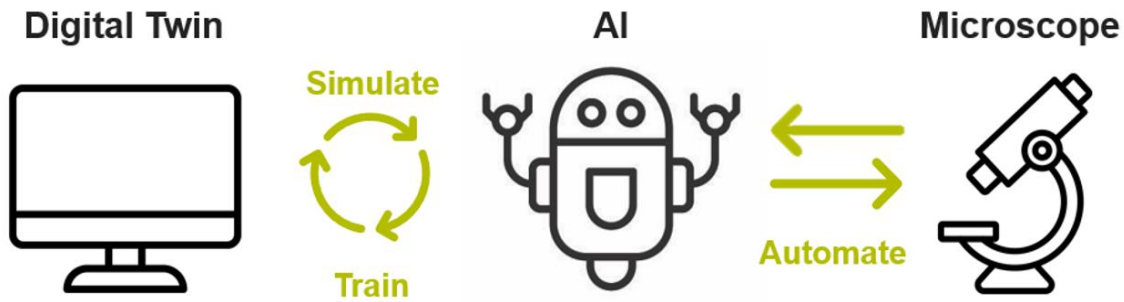


Figure 5: Illustration of the envisioned experimental set-up

2.1.8 Assumptions

The following assumptions are made for the presented use-case:

I) ASIMOV Solution

1. The axial electron beam field is generated by an external application (e.g., Electron Optical Design (EOD) Software output) and provided as an input to the system.
2. The electron source (i.e., electron gun, accelerator, and monochromator) and the imaging system of the electron microscope are excluded.
3. The aberration corrector module is trained offline with the output of digital twin.

II) Pre-conditions for the Correction Procedure

1. The electron beam is nearly coherent, meaning that a small energy spread (e.g., 0.1eV) and a small angular distribution is assumed.
2. The electron beam is already aligned along the optical axis; gun and aperture alignments have already been completed.
3. A sample with amorphous areas (e.g., amorphous carbon) is inserted.
4. The electron microscope is operating in STEM mode.

III) Assumptions for the Correction Procedure

1. There is no need to tilt the sample.
2. The specimen is at eucentric height.
3. The electron beam is axially well aligned

2.1.9 Constraints

The following constraints are relevant to the presented use case:

- While calibrating a microscope, there exists no 'linear' relationship yet between the 'buttons' you use to control the microscope and the measured aberrations. Therefore, an agnostic approach is required which has a notion of 'better'
- On a real microscope, lower objective system (if applicable) or projector systems might still add some aberrations. Their influence should be considered for digital twinning.
-

Version	Status	Date	Page
M30	internal	2022.11.29	16/43

Dependencies

The following are the dependencies that are relevant to this use case:

- The B.1 part of the digital twin has to be completed before the AI can be obtained.
- The Digital twin is potentially dependent on third-party applications for simulating the electron beam generation.
- Each hardware component in the B.1 depends on the output of the previous component.
- Internal programming interfaces to the electron microscope are needed to translate the output of the AI agent to changes in excitation values for the lenses of the electron microscope and vice versa.

2.1.10 Requirements

2.1.10.1 Functional Requirements

2.1.10.1.0 Digital Twin

Table 1 - Details of EM_SUC1_FR_DT_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_DT_001
Type	Digital Twin Components
Priority	High
Purpose	The digital twin must model all components that contribute to the Ronchigram image formation including aberrations. These components are: (1) condenser system + upper objective system and (2) electron-sample interaction in the electron microscope chamber and (3) the detector. Electron source system, lower objective system and the projector system are out of scope for the model design as part of sub use case 1. Therefore, the digital twin should include the following components: • Condensor system • Upper part of objective lens • Electron-sample interaction • The used camera for the experimental acquisition
Rationale	These are the required components in a generic TEM system
Mandatory	Yes
Dependency	N/A

Version	Status	Date	Page
M30	internal	2022.11.29	17/43

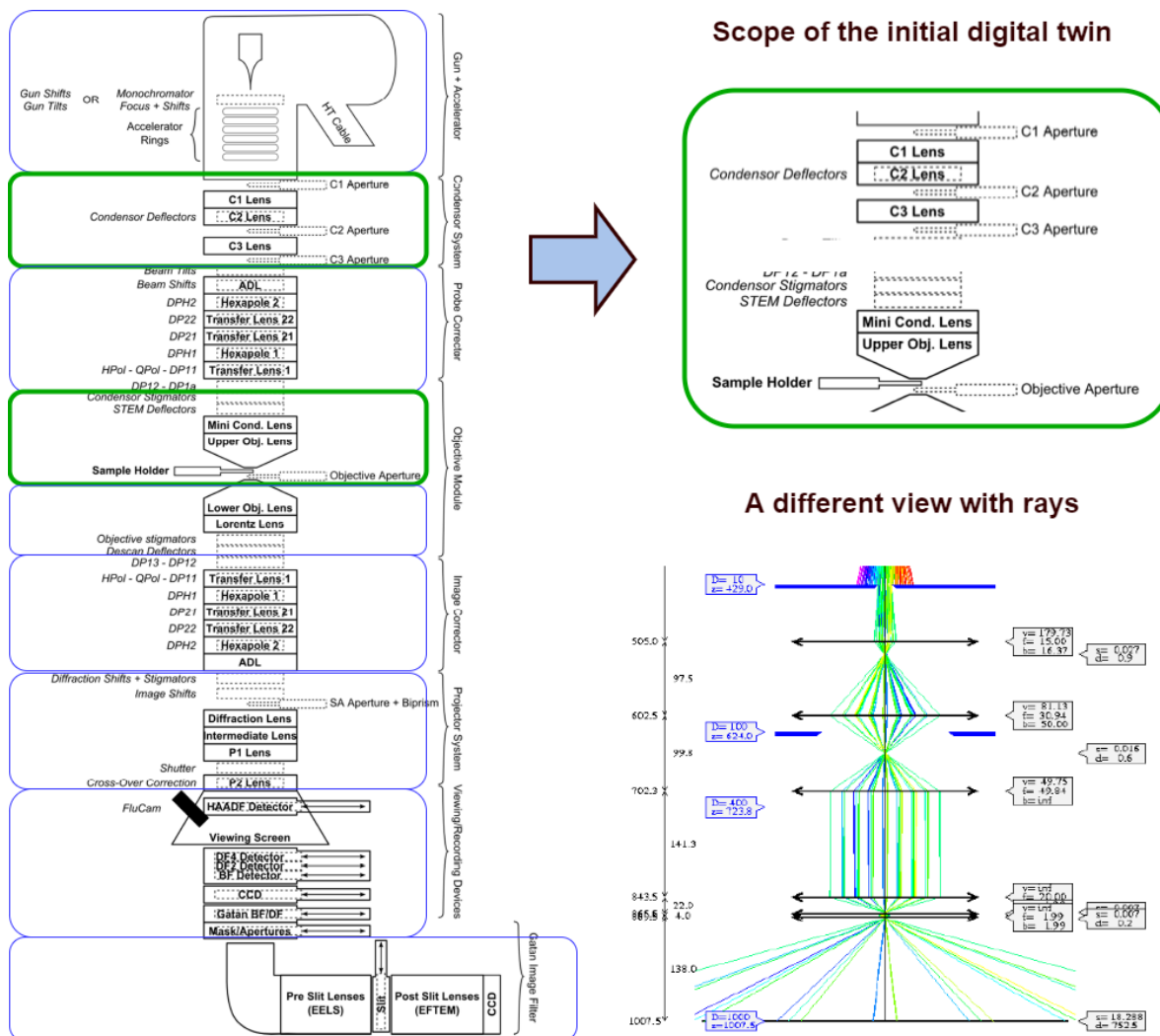


Figure 6 - Electron Microscope Components Included in the Digital Twin

Version	Status	Date	Page
M30	internal	2022.11.29	18/43

Table 2 – Details of EM_SUC1_FR_DT_002 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_DT_002
Type	Digital Twin Input Parameters
Priority	High
Purpose	The digital twin should have tunable input parameters which are similar to the tunable settings of the physical electron microscope, In this way, the digital twin can mimic microscope operation when for instance correcting aberrations. Figure 6 shows the overview of different types of parameters in the digital twin model. The following are some of the input parameters for the digital twin of condenser system: • Source energy • Source spot size • Aperture diameter • Lens current • Sample thickness
Rationale	Digital twin needs to mimic the behavior of a physical microscope
Mandatory	Yes
Dependency	N/A

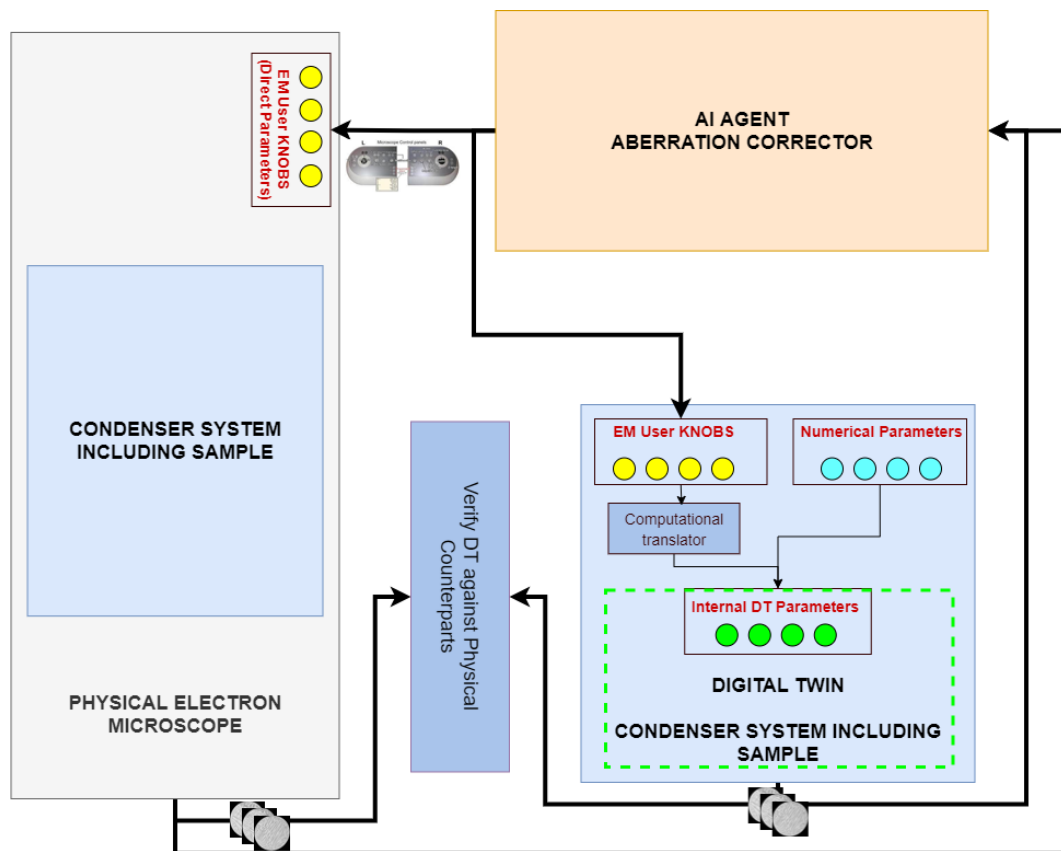


Figure 7 - Overview of Digital Twin Parameters

Version	Status	Date	Page
M30	internal	2022.11.29	19/43

Table 3 - Details of EM_SUC1_FR_DT_003 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_DT_003
Type	Digital Twin Subcomponent Interactions
Priority	High
Purpose	The digital twin must model all components that contribute to the Ronchigram image formation and the condenser astigmatism. Several components are composed out of different sub components. These need to interact with each other accordingly. The condenser component contains for instance: • Condenser lenses (C1, C2, C3) • Condenser apertures (C1, C2, C3) • Condenser stigmators • STEM deflectors • Probe corrector (only if needed in the next steps) • Mini condenser Lens
Rationale	Components in the column are connected to each other by nature
Mandatory	Yes
Dependency	N/A

Table 4 - Details of EM_SUC1_FR_DT_004 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_DT_004
Type	Electron-sample Interaction Output
Priority	High
Purpose	Sample Simulation refers to the simulating electron-sample interaction. The sample itself is placed on a TEM grid within a sample holder, which is inserted between the pole pieces of the objective lens. The digital twin of electron-sample interaction system should generate realistic exit waves.
Rationale	Ronchigram/Probe images are necessary to capture aberrations
Mandatory	Yes
Dependency	N/A

Table 5 - Details of EM_SUC1_FR_DT_005 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_DT_005
Type	EM mode for Target DT
Priority	High
Purpose	The digital twinning should model the components that are relevant to the condenser system aberrations and target STEM mode
Rationale	Aberration correction is more crucial for STEM mode than TEM mode
Mandatory	Yes
Dependency	N/A

Version	Status	Date	Page
M30	internal	2022.11.29	20/43

2.1.10.1.1 Artificial Intelligence

Table 6 - Details of EM_SUC1_FR_AI_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_AI_001
Type	AI Input Parameter
Priority	High
Purpose	AI model should use the output of the digital twin for training and verification.
Rationale	This allows offline training of aberration corrector module without interaction with real instrument
Mandatory	Yes
Dependency	N/A

2.1.10.1.2 System Level

Table 7 - Details of EM_SUC1_FR_SL_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_SL_001
Type	Target Configuration
Priority	High
Purpose	The system should have the following setup configurations: • Operate in STEM mode • Sample type is amorphous carbon or crystalline nanomaterials on an amorphous support
Rationale	Ronchigram/Probe images can be acquired when placing the STEM probe on an amorphous region within the sample
Mandatory	Yes
Dependency	N/A

Table 8 - Details of EM_SUC1_FR_SL_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_SL_002
Type	Target Aberration Type
Priority	High
Purpose	The system should reduce the lower order aberrations.
Rationale	Start with simplest aberration
Mandatory	Yes
Dependency	N/A

Version	Status	Date	Page
M30	internal	2022.11.29	21/43

Table 9 - Details of EM_SUC1_FR_SL_003 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_SL_003
Type	System Flexibility
Priority	Medium
Purpose	The system should be flexible and generic enough to adapt the other aberrations such as Axial Coma (B2), Three-fold Astigmatism (A2), etc.
Rationale	This allows the system to be independent from aberration type
Mandatory	Yes
Dependency	N/A

Table 10 - Details of EM_SUC1_FR_SL_004 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_SL_004
Type	Target Tuning Actions
Priority	High
Purpose	The system should be able to generate appropriate tuning actions to correct Astigmatism (A1) and Defocus (C1) As can be seen in the Figure 7, the EM operator can physically control the level of Astigmatism by tuning the stigmator X and Y knobs. Through an existing python interface to the microscope, the stigmator values can also be tuned from command line. The RL agent should be able to interact with the python interface.
Rationale	These are the knobs used by the microscope operator
Mandatory	Yes
Dependency	N/A

2.1.10.1.3 Data

Table 11 - Details of EM_SUC1_FR_DA_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_FR_DA_001
Type	Output Format
Priority	Medium
Purpose	The system should be able to generate and process tif/png/jpg formatted Ronchigram images of 256x256/512x512/1024x1024 and mp4 formatted Ronchigram videos
Rationale	Generated images have certain dimensions and format
Mandatory	Yes
Dependency	N/A

Version	Status	Date	Page
M30	internal	2022.11.29	22/43

2.1.10.2 Non-Functional Requirements

2.1.10.2.0 Compatibility

Table 12 - Details of EM_SUC1_NF_CO_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_NF_CO_001
Type	Integration with External Application(s)
Priority	Medium
Purpose	The system should be compatible with the output of the Electron Optical Design (EOD) application or a similar one.
Rationale	Since the Digital Twin will not comprise the electron source part, third party application(s) generate the required input data for condenser system
Mandatory	No
Dependency	N/A

2.1.10.2.1 Extensibility

Table 13 - Details of EM_SUC1_NF_EX_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_NF_EX_001
Type	Modular Architecture
Priority	High
Purpose	The system architecture should allow adding or removing extensions to the digital twin.
Rationale	Correction of each aberration requires a change in excitation of different lenses and/or stigmators
Mandatory	No
Dependency	N/A

2.1.10.2.2 Performance

Table 14 - Details of EM_SUC1_NF_PE_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_NF_PE_001
Type	Performance of Automated Correction
Priority	Low
Purpose	The system should be able to optimize the electron microscope, faster than a typical microscope operator, yet obtain the same robustness
Rationale	An automated system is expected to function better or close to manual scenario
Mandatory	No
Dependency	N/A

2.1.10.2.3 User Experience

Table 15 - Details of EM_SUC1_NF_UE_001 Requirement

REQUIREMENT	DESCRIPTION
ID	EM_SUC1_NF_UE_001
Type	User Interface
Priority	Low
Purpose	The user should be able to monitor the progress of the correction and should be notified in case of a failure that might require manual intervention.
Rationale	The system could freeze at a certain step during the correction
Mandatory	No
Dependency	N/A

3. Target Use Case(s): Unmanned Utility Vehicles

3.1 Overview of Target Use Case

3.1.1 Purpose

Unmanned Utility Vehicles offer a great possibility to deliver goods and lead to a sustainable alternative in public transportation while improving safety. In order to deploy a system of UUVs, which could support critical supply chains during lockdown, multiple different UUVs need to be developed and calibrated. Calibration reaches from UUV individual parameters for control units of the drive train up to parameters for communication between the UUVs or a teleoperator, which can act as Incident Management. Considering the large variety of possible UUVs, each designed with a specific purpose in mind, individual manual calibration becomes unfeasible when deploying a fleet of vehicles. To improve scalability of mass fleet deployment, as well as leading to a significant reduction in application cost during development, digital twins and AI-based system optimization can be used as an enabler for smart mobility solutions.



Figure 8 - Unmanned Utility Vehicle on a University Campus [2]

Digital Twins and AI-based system optimization for UUVs offers a tool to significantly lower the need for testing on proving grounds and public streets and therefore lead to a reduction in cost. ASIMOV not only provides large companies the possibility to scale in production, but also serves as a tool for development of alternative vehicle concepts in a more research orientated organisation.

Digital Twinning and AI-Parameter optimization is also not limited to vehicle parameters but can also be applied to the testing itself. The testing process as such can benefit in two ways from the ASIMOV idea. A well calibrated test bed leads not only to more accurate data but also to a wider accessible range of possible tests, including highly dynamic ones, which offer insight into vehicles driving characteristics in safety relevant scenarios. Additionally, optimizing the parameters of the relevant test scenarios leads to a more effective way of gathering meaningful measurement data and therefore reduces the required testing time in the lab and on the road.

Version	Status	Date	Page
M30	internal	2022.11.29	25/43

3.1.2 Scope

The Unmanned Utility Vehicle Use case will be focusing on improving the testing itself by automatically creating a test plan that is best suited to test the vehicle while focusing on a specific component.

As access to such a vehicle is rather limited, the use case will rely on virtual validation of the developed toolchain and methods. The autonomous driving (AD) stack itself will not be part of the optimization.

3.2 Sub Use Case 1 - Automatic Test Case Generation

3.2.1 Introduction

This sub use case focuses on automatically creating a set of test case scenarios to test a specific vehicle component for development of complex UUVs. The created test case scenarios shall maximize information about the component under test with as little testing required as possible. As a starting point we therefore focus on a vehicle that offers a "Track & Follow"-Function. This function is mainly based around three basic functionalities. An Active Cruise Control (ACC) offers the functionality to adapt the speed of the unmanned utility vehicle based on the distance to and the velocity of the vehicle in front. A Lane Keep Assist System (LKA) takes over the lateral control of the vehicle in such a way that it follows the vehicle in front. Finally, an Autonomous Emergency Braking (AEB) system serves as a safety net to ensure that the UUV is aware of its surroundings and can avoid accidents caused by traffic or pedestrians that get in between the platoon of following vehicles. Each of these automation functions needs information about the vehicle and its behavior to be used successfully. While functions like ACC and LKA require models that reflect the real vehicles behavior in non-critical situations, the AEB system relies on more complex models that take more detailed dynamic physical effects into account.

Using the ASIMOV approach, reinforcement learning is used to iteratively suggest new variations of a scenario template to find the most critical combination of parameters based on analyzing a variety of criticalities. A Digital Twin of vehicle and environment is therefore used to enable such an automated parameter identification process.

3.2.2 Context

Creating such an automated scenario suggestion requires several components that interchange and process data.

Figure 9 shows an overview of the whole process. It can be divided into two separate tasks and the environment for data processing. As a first step, the environment model has to be set up manually. This is done with a specific environmental domain in mind. In our case, this will be a university campus.

Version	Status	Date	Page
M30	internal	2022.11.29	26/43

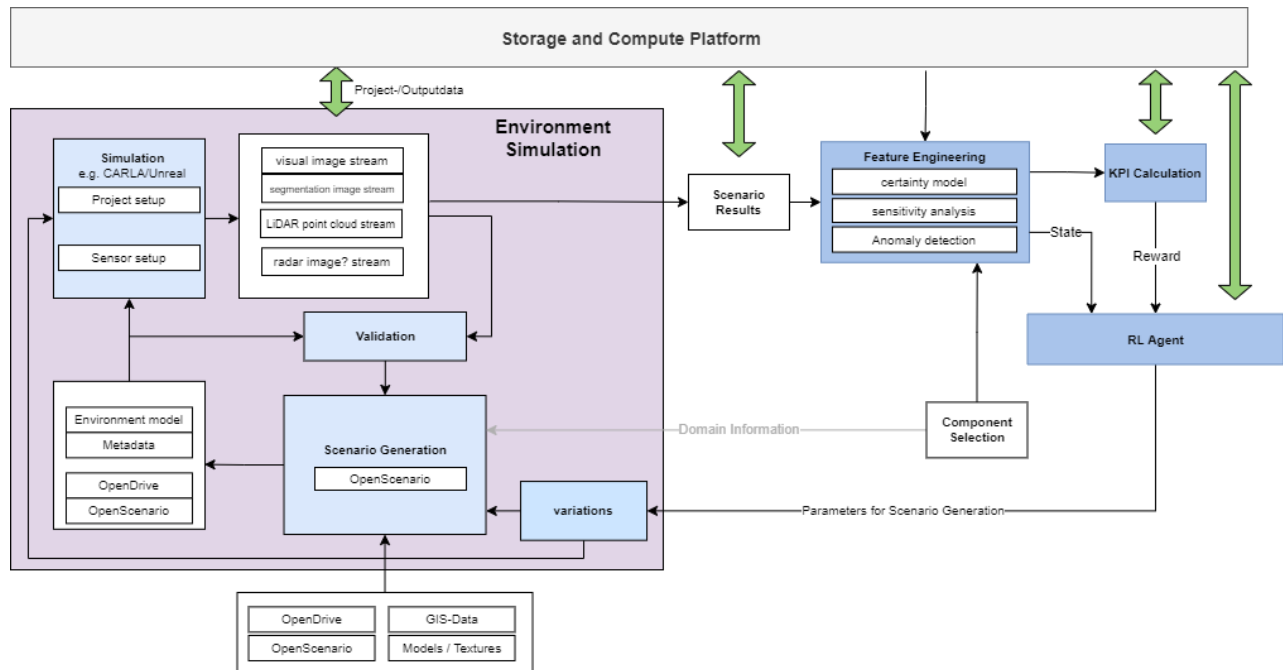


Figure 9 - Process Overview Sub Use Case 1

To create the campus environment, input data is required. For this process it can be measurement data of the road network (ASAM OpenDRIVE [3]) and GIS data for the environment. Both data sets can be manually adapted or extended depending on the requirements. This is a one-time process. During the operational phase of the automatic Scenario Generation, some parameters for the static environment and the dynamic traffic maneuvers (ASAM OpenSCENARIO [4]) will be varied by the reinforcement learning agent.

The 3D environment model, as well as the corresponding description of the road network (ASAM OpenDRIVE) and description of the scenario (ASAM OpenSCENARIO) are then generated from this data. The environment model is converted into a format that is best supported by the simulation environment to be used. Geometry, texture, Physically Based Rendering (PBR) material description and segmentation information have also to be taken over. At present, the open-source simulation package CARLA [5], which is based on the Unreal Engine [6], could be a good option, since it fulfils all current requirements. Native Unreal will also be looked into.

In the simulation environment, the project must initially be set up in terms of lighting, performance, and determinism. Likewise, CARLA offers multiple sensor models, whose position and parameters must be initially adjusted. Sensors for the visual image, LiDAR point clouds and radar images have to be modeled.

OpenDRIVE and OpenSCENARIO data can be used to simulate scenarios on the environment model, which are recorded as data streams via the sensors set up. The measurement data can then be processed by the feature engineering to quantify the information value of the already gathered data. From this, a KPI value with the information density of the data set, obtained by the latest scenario is calculated as a reward. This reward and the state, formed by information about the tested component and the operational areas, where there is still high uncertainty in the data, is fed to the reinforcement learning agent. The reinforcement learning agent aims for the highest long-term reward and therefore modifies future scenarios in such a way that their simulation obtains the most amount of new data possible. That maximizes the information obtained over the course of the entire test plan.

The automatic scenario generation relies on feedback about the criticality of the driven scenario. Therefore, an essential part of this process is the Feature Engineering, that quantifies the quality of data in different driving situations. Based on this information, the reinforcement learning agent tries to find parameters for scenario generation that would deliver valuable data in operational areas, where the RL agent expects critical scenarios or has a high uncertainty in the behavior of the vehicle.

Version	Status	Date	Page
M30	internal	2022.11.29	27/43

The parameters that are being tuned by the reinforcement learning agent can be divided into a static and a dynamic part. The dynamic parameters control the routes the ego vehicle drives on, as well as where and when other traffic participants, such as cars, pedestrians, cyclists, etc. interact with the ego vehicle. Static parameters will setup the scene and define the road sampling, tree density, etc.

Using different vehicles and components to adapt the test plan for, would be part of the training process for the reinforcement learning agent to make it more robust.

When applying this technique to real components in Hardware-in-the-Loop (HiL) tests or a vehicle on a testbed (ViL), the corresponding components from the simulation have to be replaced by their physical counterparts. The scenario generation and therefore the stimulation of the components of interest will not change compared to a fully simulated setup. That way, the reinforcement learning agent can apply its experience to the real system.

3.2.2.1 Data Management & Processing

To enable repeated learning and counter-testing of scenarios later, data and project information are managed in an experiment and experience data store. This process runs automatically without manual intervention.

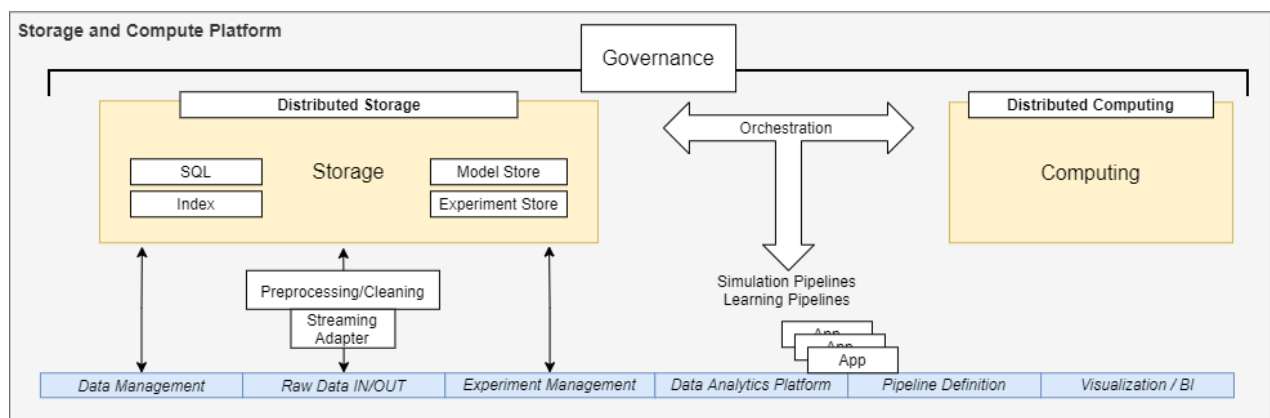


Figure 10 - Overview Data Management and Processing

In the data processing environment, there are 6 main interfaces for computing, storing and displaying results.

To store and access data in the form of files and folders on a distributed filesystem there will be a Data Management Platform which can also be used to browse, search data and to make additional annotations.

In addition, a streaming adapter will be developed and evaluated for raw data input and output of sensor data. This solution would accept a stream of data in a previously decided format with support to “replay” it. This would allow to save simulated sensor data while it is generated and to use it as an input source that is close to the conditions of a real environment.

To keep track of the experiments that were made, an experiment management system is used to systematically store all experiment related information which allows to compare and analyze the results on the Analytics Platform.

On the Data Analytics Platform the gathered information can be exploited by providing an environment to analyze data efficiently in a distributed environment. All computational tasks can be defined as apps or pipelines that are able to scale to multiple compute nodes.

Version	Status	Date	Page
M30	internal	2022.11.29	28/43

A visualization platform allows to easily visualize key information of the simulations and the progress. Depending on the integration of the streaming adapter this could also allow to visualize the simulation in near-real time.

3.2.3 Assumptions

The creation of driving scenarios and sceneries based on a set of parameters needs to be possible and the restrictions of the vehicle or component under test must be known as input parameters. Furthermore, it is assumed that there is a way to quantify the uncertainty of a model in different driving situations.

3.2.4 Constraints

Due to costs and availability, the test bed can only be used for a limited time span. The lack of permanent availability of a physical UUV itself leads to further restrictions regarding the usage of real-world measurement data.

The scenario generation is constraint to non-destructive scenarios. The limitations of test system and system under test must be respected at every time.

3.2.5 Dependencies

Creating the digital representation of a campus environment and the vehicle with its sensors lay the foundation and can be done in parallel. During implementation of the environment model, interfaces for scenario and static environment variations need to be developed. As information about the current density of the data in different operational areas serves as input for the RL agent, the feature engineering function needs to be developed next. The reinforcement learning agent has to be developed closely with the feature engineering function, as their interplay in combination with the KPI calculation is crucial.

3.2.6 Requirements

3.2.6.1 Functional Requirements

3.2.6.1.0 Digital Twin

Digital Twins need to be modelled, to enable the Reinforcement learning agent to gain experience. Instead of creating one large DT, that represents the whole vehicle, separate DTs for individual parts of the vehicle are being used. This approach offers greater compatibility for HiL and ViL testbeds, where individual components exist as real physical components.

Table 16 - Details of UUV_SUC1_FR_DT_001 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_DT_001
Type	DT of the Driving Function
Priority	High
Purpose	The driving function needs to be represented as if it was in the real system.
Rationale	Vehicle will be controlled via this function block
Mandatory	Yes
Dependency	N/A

Version	Status	Date	Page
M30	internal	2022.11.29	29/43

Table 17 – Details of UUV_SUC1_FR_DT_002 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_DT_002
Type	DT of the Vehicle dynamics
Priority	High
Purpose	Reflect the vehicle dynamics as a DT
Rationale	The vehicles behavior will deliver measurement data that is used to optimize the scenario generation. In the training stage, many different configurations of vehicles will be tested, to achieve robust AI functionality in the operational phase. An interface must be provided, to change vehicle configurations easily.
Mandatory	Yes
Dependency	N/A

Table 18 – Details of UUV_SUC1_FR_DT_003 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_DT_003
Type	DT of the Sensors
Priority	High
Purpose	At least LiDAR and camera sensor models need to be modelled, as they serve the perception of the vehicle.
Rationale	The sensors behavior will deliver measurement data that is used to optimize the scenario generation and is key for the driving function to be able to run.
Mandatory	Yes
Dependency	N/A

Table 19 – Details of UUV_SUC1_FR_DT_004 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_DT_004
Type	DT of the Environmental model
Priority	High
Purpose	Provide a digital campus environment that the vehicle can drive in. The campus environment defines our operational design domain and is the basis for any sensor in- and output.
Rationale	The digital campus environment will serve as a proving ground for the optimized scenario generation.
Mandatory	Yes
Dependency	N/A

3.2.6.1.1 Optimization-AI

Table 20 - Details of UUV_SUC1_FR_OA_001 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_OA_001
Type	KPI
Priority	High
Purpose	Implement a useful metric to measure the amount of new information in measurement data.
Rationale	The KPIs will serve the Reinforcement Learning Agent as reward. Good KPIs will lead to more effective parameter optimization. The AI aims for maximizing the amount of new information contained in every test run.
Mandatory	Yes
Dependency	N/A

Table 21 - Details of UUV_SUC1_FR_OA_002 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_OA_002
Type	Reinforcement Learning Agent
Priority	High
Purpose	Implement the Reinforcement Learning agent itself.
Rationale	The Reinforcement Learning agent will deliver optimized parameter sets for the scenario generation, based on the current state of information.
Mandatory	Yes
Dependency	N/A

Table 22 - Details of UUV_SUC1_FR_OA_003 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_FR_OA_003
Type	Experiment Storage and Analyzer
Priority	High
Purpose	Create an experiment storage, which collects all gathered data and an experiment analyzer that improves future actions of the AI
Rationale	Data Storage for improving AI performance with knowledge acquisition
Mandatory	No
Dependency	N/A

3.2.6.2 Non-Functional Requirements

3.2.6.2.0 Data

Table 23 - Details of UUV_SUC1_NF_DA_001 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_NF_DA_001
Type	Vehicle State
Priority	High
Purpose	Vehicle State, generated by the vehicle model, need to be accessible by the environmental model
Rationale	Vehicle interacts with the virtual environment and therefore has to be accessible
Mandatory	Yes
Dependency	N/A

Table 24 - Details of UUV_SUC1_NF_DA_002 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_NF_DA_002
Type	Environmental data
Priority	High
Purpose	Input data for sensor model
Rationale	Sensor Model needs to have access to the environmental model in order to deliver sensor information to the driving function
Mandatory	Yes
Dependency	N/A

Table 25 - Details of UUV_SUC1_NF_DA_003 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_NF_DA_003
Type	Sensor data
Priority	High
Purpose	Sensor data for driving function
Rationale	Sensor model needs to forward its information to the driving function for action planning
Mandatory	Yes
Dependency	N/A

Table 26 - Details of UUV_SUC1_NF_DA_004 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_NF_DA_004
Type	Driving instructions
Priority	High
Purpose	Controlling the vehicle
Rationale	Driving instructions from the Driving function block need to be forwarded to the vehicle model.
Mandatory	Yes
Dependency	N/A

Version	Status	Date	Page
M30	internal	2022.11.29	32/43

Table 27 - Details of UUV_SUC1_NF_DA_005 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_NF_DA_005
Type	Actions / States / Rewards
Priority	High
Purpose	Linkage between the DT and the RL Agent
Rationale	The Optimization AI needs feedback in order to optimize its actions
Mandatory	Yes
Dependency	N/A

3.2.6.2.1 Performance

Table 28 - Details of UUV_SUC1_NF_PE_001 Requirement

REQUIREMENT	DESCRIPTION
ID	UUV_SUC1_NF_PE_001
Type	Overall simulation time
Priority	High
Purpose	The automated scenario generation has to lead to a reduction of overall simulation time, while delivering more relevant information compared to current methods.
Rationale	If the automated scenario generation is slower than the conventional method, the ASIMOV optimization is unsuitable
Mandatory	Yes
Dependency	N/A

3.2.6.2.2 Availability

The ASIMOV approach would only be used for efficient data gathering in a development phase of the vehicle. The availability has to be high, as test bed use is expensive.

3.2.6.2.3 Compatibility

The automated scenario generation has to be adaptable to different vehicle components and vehicle specifications. Finding lumped parameters for a one-track model of a vehicle must be possible just like finding physical parameters for a sensor model.

3.2.6.2.4 Resource Usage

On vehicle resource usage shall be reduced to a minimum.

3.3 Sub Use Case 2 - Sensor Optimization

As the creation of a suitable DT of the vehicle and its optimization is a big topic on its own, Sensor optimization can be seen as a separate subtopic, which is described below.

3.3.1 Introduction

In contrast to sub use case 1, where the analysis of measurement data and model uncertainties is used to create an automatic test scenario generation, sub use case 2 uses the scenario generation for optimizing the configuration of vehicle sensors themselves. The Positioning, Orientation, Field of View and other internal Parameters of a LiDAR Sensor will be optimized exemplarily so that objects are detected reliable and fast across different situations.

Version	Status	Date	Page
M30	internal	2022.11.29	33/43

3.3.2 Context

Positioning and configuration of vehicle sensors have a large impact on the perception quality and therefore must be optimized for different vehicles. This sub use case will use the approach from sub use case 1 to adapt and test these parameters.

As in sub use case 1, the initial step is to generate a suitable family of scenarios to test the sensors perception. Ideally, the scenarios that were found useful in sub use case 1, are also useful for optimizing the sensors parameters for best perception.

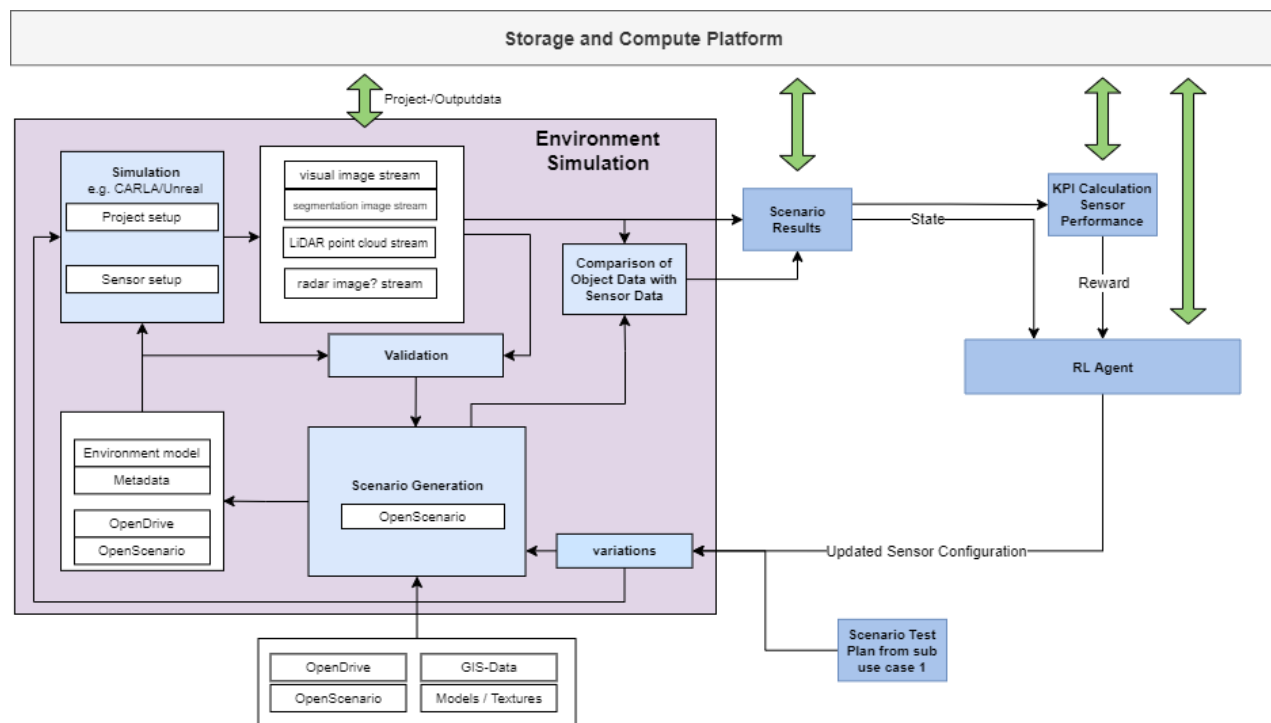


Figure 11 - Process Overview Sub Use Case 2

In contrast to finding the best test plan in sub use case 1, the reinforcement learning agent in sub use case 2 focuses on finding the best parameters for the sensor setup, using the earlier developed test plans. Therefore, the environment simulation will still function in the same way, but instead of changing the parameters of the scenario generation, the reinforcement learning agent will change the parameters of the sensors. The whole process can be seen in Figure 11.

Based on these inputs and the tailored test plan from sub use case 1, measurement data from the sensor can be acquired. These data streams will be used as training data for the AI algorithm. By using a segmentation image stream directly from the environment as a ground truth source, it can be checked if objects or situations are correctly recognized by the sensor. In order to recognize in time during the process whether the generated data streams are suitable for evaluation, a validation process has to be integrated. It checks the output data of the generation process for plausibility and consistency, as well as the data streams from the simulation itself.

Information about the objects recognized by the sensor and those that were initially generated in the scenario, serves the reinforcement learning as input to further tune the sensor parameters.

Version	Status	Date	Page
M30	internal	2022.11.29	34/43

3.3.3 Assumptions

See sub use case 1.

3.3.4 Constraints

See sub use case 1.

Besides the constraints from sub use case 1, the positioning of sensors itself is constraint due to the vehicle's dimensions and possible mounting points. The optimization process must respect these limitations.

3.3.5 Dependencies

To optimize the position and configuration of a sensor, an adequate sensor model, as well as information about how its parameters were obtained, are required. Sub use case 1 offers the possibility to satisfy these dependencies.

As backup, a traditional test plan can be used in place of the optimized test plan from sub use case 1 as well.

3.3.6 Requirements

3.3.6.1 Functional Requirements

See sub use case 1.

3.3.6.2 Non-Functional Requirements

3.3.6.2.0 Performance

See sub use case 1.

3.3.6.2.1 Availability

See sub use case 1.

3.3.6.2.2 Compatibility

See sub use case 1.

3.3.6.2.3 Resource Usage

See sub use case 1.

Version	Status	Date	Page
M30	internal	2022.11.29	35/43

4. Analysis of Commonalities and Differences Between Use Cases

In this section we analyze the use cases, described in the previous sections, to identify commonalities and fundamental differences that may be relevant for technology development in the work packages. The commonalities indicate opportunities for reuse and collaboration across the use cases. The differences, on the other hand, indicate required variation points in the overall ASIMOV methodologies and technologies.

In the following subsections we describe our observations classified around 5 main themes:

1. System
2. Optimization
3. Envisioned solution
4. Digital Twin (DT) modeling
5. Artificial Intelligence (AI) learning

In general, observations for earlier themes (like system) also apply to later themes (like DT modeling).

We use the following abbreviations to refer to the use cases and sub use cases:

- STEM: Scanning Transmission Electron Microscopy
- UUV: Unmanned Utility Vehicle
 - UUV.1: Automatic Test Case Generation
 - UUV.2: Sensor Optimization

General impression based on the more detailed observations below:

- STEM looks more like UUV.2 than like UUV.1
- UUV.2 uses the results of UUV.1, but there is a workaround if necessary
- 2D Image processing is a technological common denominator

4.1 System

In this subsection we focus on the characteristics of the system to be optimized.

4.1.1 Commonalities

- Product family of similar (but different) systems:
 - STEM: product families of microscopes
 - UUV.2: product families of vehicles
- Control parameters are dependent:
 - STEM: different control parameters of the lenses influence the same image
 - UUV.2: different control parameters of the sensor influence the same image
- Control parameter values:
 - STEM: limited (but large) number of microscope settings
 - UUV.1: unlimited functional scenarios, limited number of concrete scenarios
 - UUV.2: limited number of sensor positions
- Limited number of parameters to change;
 - RL is specifically only allowed to change a certain number of knobs in a controlled manner.
- Sensitivity to an uncontrollable physical environment:
 - STEM: high(e.g., we will attempt to align uncalibrated microscopes and are very dependent of its unknown starting conditions)
 - UUV.1: low (e.g., measurement and stimulation inaccuracies)

Version	Status	Date	Page
M30	internal	2022.11.29	36/43

4.1.2 Differences

- Pre-existing API to control the system:
 - STEM: Python API available for controlling the electron microscope
 - UUV: No API for dynamically changing the 3D environment established.
- Control parameters have boundary conditions for safety:
 - STEM: potential damage to the microscope and the sample
 - UUV.1: no potential damage to the vehicle and the environment

General Conclusion: Broadly speaking, there is a significant intersection between the two usage scenarios. In both cases, our efforts are directed towards creating artificial intelligence and digital twin technologies capable of maneuvering through extensive and unfamiliar application domains. Nevertheless, these AI/DT solutions operate within constraints, having only a finite set of 'control knobs' available for optimization. They therefore share the same aspects in terms of system safety and AI interface. While in the STEM use case, an already existing API can be used to control the system, such an equivalent had to be developed for the environment variation in the UUV use case.

4.2 Optimization

In this subsection we focus on system optimization.

4.2.1 Commonalities

- Classical techniques for system optimization are/become infeasible:
 - STEM: optics is well-understood, but does not deal with un-happy flow
 - UUV: number of optimization parameters is too large
- Optimize the control parameters of a CPS:
 - STEM: find parameters to minimize lens aberrations
 - UUV.1: find parameters to generate critical scenarios
 - UUV.2: find parameters to optimize sensor configuration
- Optimize a fleet of systems instead of a single system:
 - STEM: train an AI capable of optimizing various microscopes
 - UUV: train the AI to come up with meaningful test scenarios for various vehicles.
- Need for virtualization:
 - STEM: expensive microscope time is hard to come by.
 - UUV: driving many critical scenarios is impractical, costly and potentially dangerous on public roads
- Optimize non-deterministic systems:
 - UUV Variety and complexity of vehicles is high, which leads to slightly different results every time.
 - STEM: There are unknown parameters such as sample thickness/structure which can change the obtained data from day to day.
- Frequency of applying system optimization:
 - STEM: Each time when calibrating an electron microscope to a certain high tension
 - UUV: iteratively during the development of a vehicle's ADAS/AD system for a specific domain of operation
- Required quality of the resulting optimization:
 - STEM: Predefined quantitative benchmarks need to be reached to ensure final resolution
 - UUV: leverage Vehicle-in-the-Loop capabilities to full extent by providing more representative detail compared to conventional scenario-based testing

Version	Status	Date	Page
M30	internal	2022.11.29	37/43

4.2.2 Differences

- Feasibility of manual optimization:
 - STEM: feasible, but requires scarce expertise (extensive training)
 - UUV: infeasible for a fleet of various UUVs
- Required performance of the optimization process:
 - STEM: not dramatically slower than a human operator (low priority)
 - UUV: reduction of the overall simulation and testbed time (high priority)
- Concreteness of the optimization:
 - STEM: control values with a visible effect on microscope images
 - UUV.1: set of test scenarios with a quantitative notion of criticality
 - UUV.2: control values with a visible effect on sensor images and perception accuracy

General remark: Both use cases focus on optimizing a calibration process, which is essential before deployment. However, the application spaces are vast and filled with unknowns, posing challenges for classical techniques. Consequently, we explore AI-based solutions. Due to expensive and scarce machines, data generation using digital twin (DT) technology becomes crucial. While STEM already benefits from human operators for optimization, the UUV use case seeks to expand optimization parameters through DT/AI approaches.

4.3 Envisioned solution

In this subsection we focus on the envisioned high-level structure of the optimization procedure.

4.3.1 Commonalities

- Use of DTs (see the dedicated subsection for a deeper analysis)
- Use of AI (see the dedicated subsection for a deeper analysis)
- Required performance of the optimization subprocesses:
 - STEM: efficient computation times (scalability)
 - UUV: efficient computation times (scalability)
- Use of Flask for managing microservices
- DT-trained AI is used to optimize the physical system
- Online learning with modular docker set-up

4.3.2 Differences

- Training situations:
 - STEM: virtual STEM + virtual environment and physical STEM + physical environment
 - UUV: virtual vehicle + virtual environment and physical vehicle + virtual environment
- Hybrid solutions:
 - STEM: aside from AI based solutions we also explore DT based optimisations solutions and even hybrid solutions where we combine the best of both worlds.

General remark: Both use cases will use the same solution architecture. The difference lies in the use of a physical system during deployment. While in the STEM use case, the AI is directly optimizing a physical device, in the UUV use case, the AI optimizes a virtual environment, with which a physical device

Version	Status	Date	Page
M30	internal	2022.11.29	38/43

interacts. This makes interaction with a physical STEM during training much more important than in the UUV use case. As a result, more direct feedback is available for the STEM use case.

4.4 Digital Twin (DT) modeling

In this subsection we focus on modeling the system as a Digital Twin (DT).

4.4.1 Commonalities

- The type of environment (which cannot be controlled) that needs to be modelled:
 - STEM: the starting conditions of the to be aligned/calibrated microscopes
 - UUV: the unmanned vehicle, other vehicles and pedestrians as well as the majority of the 3D environment
- The DT is expected to be imperfect (deviating from the physical system):
 - STEM: properties of the sample, contamination, slight mechanical misalignments
 - UUV: dynamics of the vehicle and its sensor models
- The DT is expected to have limited fidelity (less than the physical system):
 - STEM: omitting quantum effects
 - UUV: limited details and resolution of the environment, limited set of physical effects in the sensor models
- Common types of technologies:
 - STEM: 2D image processing (Ronchigram)
 - UUV: 2D image processing (camera)
- Reuse requirements:
 - STEM: compositional collection of DTs for interdependent system components
 - UUV: compositional collection of DTs for sensors and vehicles from multiple suppliers

4.4.2 Differences

- Different types of technologies:
 - STEM: electron optics, microscopy, micro mechanics, thermodynamics
 - UUV: mechanics, 3D images (Lidar)
- Modelling challenge:
 - STEM: detailed physics (hysteresis, drift, contamination)
 - UUV: dynamic environment based on a limited number of parameters
- Ease of comparing DT with physical system:
 - STEM: relatively easy (comparing experimental Ronchigram/Probe images)
 - UUV: hard (comparing realism of 3D environment with reality)
- Already available DTs:
 - STEM: some models and tools are available for electron microscopes
 - UUV: mature models for vehicles with drivers, but not for unmanned vehicles

General Remark: When developing a Digital Twin (DT), a critical consideration is determining the necessary level of detail for simulating realistic data. The ultimate metric for data quality lies in the AI's ability to train on simulated data and generalize to experimental data. However, striking a balance between detailed simulations (which can become slow and unwieldy) and the AI's capacity to generalize is crucial.

Version	Status	Date	Page
M30	internal	2022.11.29	39/43

Additionally, imperfections are inherent in DTs across both use cases. While some existing models vary in maturity, a commonality emerges in their composition from multiple sub-DTs. By composing the DT in a modular approach one obtains more control over the simulation and can more easily adapt the DT based on the AI needs.

4.5 Artificial Intelligence (AI) learning

In this subsection we focus on learning the optimization procedure using Artificial Intelligence (AI).

4.5.1 Commonalities

- Use of Reinforcement Learning
- Training a single AI model to deal with multiple scenarios:
 - STEM: different kinds of aberrations/ microscope conditions
 - UUV.1: different scenarios from a scenario class (e.g., a driving situation)
- Actions by the AI must be restricted by boundary conditions for safety reasons
- Huge state space of the virtual or physical system that needs to be explored by the AI
- Need to acquire training data sets, including sampling of dependent parameter spaces:
 - STEM: acquire Ronchigram images with set aberrations
 - UUV.2: derive object list from sensor images
- Test environment:

In both cases the test environment consists of a Cyber-Physical System CPS:

 - STEM: The AI is evaluated both on simulated data from the DT as on the PS under operation conditions
 - UUV: The AI is evaluated mostly on DT and most likely on a scale model of vehicle and testbed.
- Components:
 - Both systems consist of a highly-interdependent chain of components for which an AI is trained on a virtual environment, applied and evaluated on a PS
- Number of AI models for the sub use cases:
 - STEM: Preference to restricted models which can operate in a smaller state space.
 - UUV: 2 different AI models corresponding to the 2 sub use cases

4.5.2 Differences

- Optimal parameters and quality KPIs:
 - STEM: optimal conditions known upfront in the DT;
 - UUV: not known upfront in a DT
- Type of AI; The STEM use-case also explores to usage of supervised learning
- Usage of AI:
 - STEM: to control the electron microscope directly
 - UUV: to directly control scenario generation
- Online vs offline learning
 - STEM; Offline learning
 - UUV; Online learning

Version	Status	Date	Page
M30	internal	2022.11.29	40/43

General remark: The methods for handling the complex CPS are very similar between the use cases and include purpose-built AI models for different applications, training on variations of scenarios for better generalization and applicability on a real system, as well as constrained AI, that is affected in its control output by the same limits a human operator would have. The main differences lie in the upfront knowledge of how an ideally tuned system would look like, as well as the fact, that in the STEM use case, the AI directly controls the Electron microscope, while in the UUV use case, the scenario generation is purely digital and indirectly effects the UUV.

Version	Status	Date	Page
M30	internal	2022.11.29	41/43

5. Terms, Abbreviations and Definitions

Table 29 - Terms, Abbreviations and Definitions

ABBREVIATION	EXPLANATION
A-Cor	Automated Correction of Astigmatism in the Condenser System
AAP	Advanced Analytics Platform
ACC	Active Cruise Control
AD	Autonomous Driving
AEB	Autonomous Emergency Braking
AI	Artificial Intelligence
CBED	Convergent Beam Electron Diffraction Pattern
CCD	Charge-Coupled Device
CPS	Cyber-Physical System
DT	Digital Twin
EELS	Electron Energy Loss Spectra
EM	Electron Microscopy
EOD	Electron Optical Design
GIS	Geographic Information System
HiL	Hardware-in-the-Loop
KPI	Key Performance Indicator
LKA	Lane Keep Assist
OEM	Original Equipment Manufacturer
PBR	Physically Based Rendering
PS	Physical System
SEM	Scanning Electron Microscopy
STEM	Scanning Transmission Electron Microscopy
TEM	Transmission Electron Microscopy
UUV	Unmanned Utility Vehicle
ViL	Vehicle-in-the-Loop

6. Bibliography

- [1] FEI, "FEI Application Instructions: How to tune STEM probe on Cs-corrected Titan."
- [2] "Unmanned Utility Vehicle on a University Campus," [Online]. Available: <https://www.continental.com/de/presse/pressemitteilungen/2019-12-12-hmi-cube-204622>. [Accessed 25 11 2021].
- [3] "ASAM OpenDRIVE," [Online]. Available: <https://www.asam.net/standards/detail/opendrive/>. [Accessed 25 11 2021].
- [4] "ASAM OpenSCENARIO," [Online]. Available: <https://www.asam.net/standards/detail/openscenario/>. [Accessed 25 11 2021].
- [5] "CARLA," [Online]. Available: <https://carla.org/>. [Accessed 25 11 2021].
- [6] "Unreal Engine," [Online]. Available: <https://www.unrealengine.com/en-US/>. [Accessed 25 11 2021].
- [7] ASIMOV-consortium, *ASIMOV - Full Project Proposal*, 2020.
- [8] "Transmission (TEM) vs. Scanning (SEM) Electron Microscopes: What's the Difference?," [Online]. Available: <https://www.thermofisher.com/blog/microscopy/tem-vs-sem-whats-the-difference/>. [Accessed 25 11 2021].
- [9] "Exploring Uncharted Realms with Electron Microscopy Brochure," [Online]. Available: <https://assets.thermofisher.com/TFS-Assets/MSD/Handbooks/Exploring-uncharted-realms-with-electron-microscopy.pdf>. [Accessed 25 11 2021].
- [10] "Tuning the Cs probe corrector S-CORR User's Guide," [Online]. Available: <https://assets.thermofisher.com/TFS-Assets/MSD/manuals/nanoport-tuing-cs-probe-s-corr-user-guide.pdf>. [Accessed 25 11 2021].
- [11] L. A.R., "The Electron Ronchigram. In: Pennycook S., Nellist P. (eds) Scanning Transmission Electron Microscopy," New York, NY, Springer, 2011.

Version	Status	Date	Page
M30	internal	2022.11.29	43/43