

# Automation & Robotics at Beamlines:

## Lessons from the Field

Automated Sample Handling for Remote Access in Operando  
Catalysis Experiments at Scattering Beamline P65 @ PETRA III



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# JOURNEY: From Concept to Operation

## My Contribution to ROCK-IT

Developing an automated sample changer as a key ROCK-IT use case, with end-to-end responsibility across the entire automation pipeline.

01

### Hardware Integration

Mechanical systems and sensor deployment

02

### Robot Control & Calibration

Precision motion planning and positioning

03

### ROS 2 Architecture

Action-based software framework

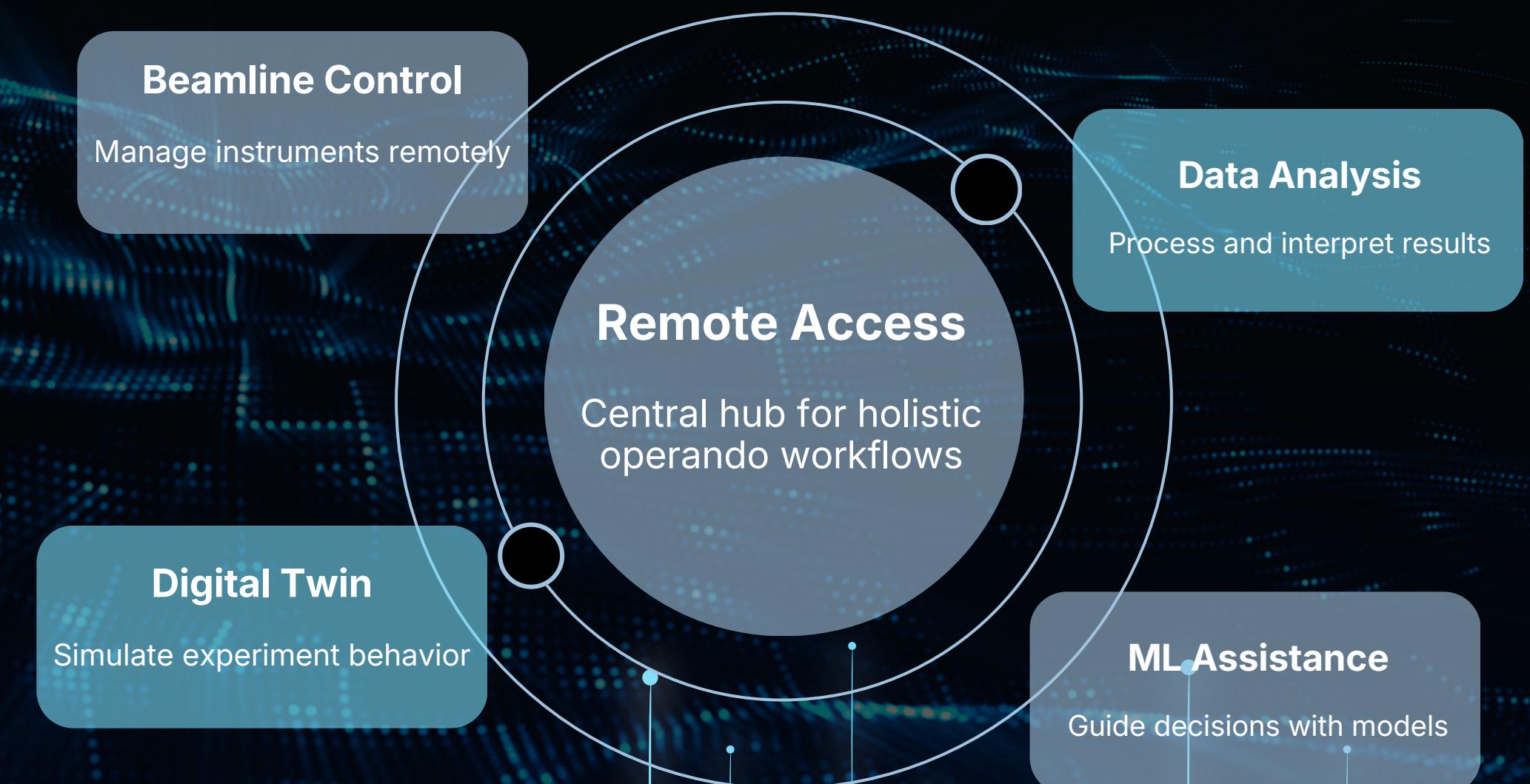
04

### Beamline Commissioning

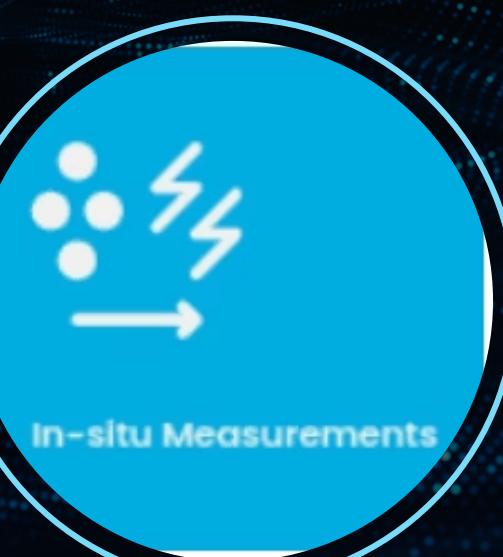
Real-world testing and deployment

# WHAT'S ROCK-IT ?

ROCK-IT (Remote, Operando-Controlled, Knowledge-driven, and IT-based) is a Helmholtz-funded initiative that automates complex operando catalysis experiments, enabling scientists worldwide to conduct research with unprecedented accessibility and scalability.



# Challenges in Operando Catalysis



In-situ Measurements

Complex  
Experimental Design

High-throughput & complex  
environment



Gases Handling

Precise control of  
reaction conditions

Hazardous Gas  
Handling



Sample Positioning

Operando Catalysis  
Experiment

Real-Time Data  
Processing

Beam stability &  
alignment

# Our Aim

## Motivation

Holistic Workflow for Complex Operando Experiments



Common look & feel across institutes for seamless operation

GUI-based experiment control and real-time analysis

Modular components with unified interfaces

Complete data lifecycle from acquisition to archiving

Robust cyber security protecting data and infrastructure

# Why Beamline Automation Is Special ?

## Core Distinctions

### Mixed Environments

Precision mechanics, human interaction, and radiation constraints coexist.

### Low-Volume, High-Variance

Samples are often unique, requiring adaptable handling and analysis protocols.

### Frequent Reconfiguration

Experiments change often, demanding rapid system adjustments.

### Tight Spatial Constraints

Limited space around the beamline necessitates compact and efficient designs.

### Scientific Operators

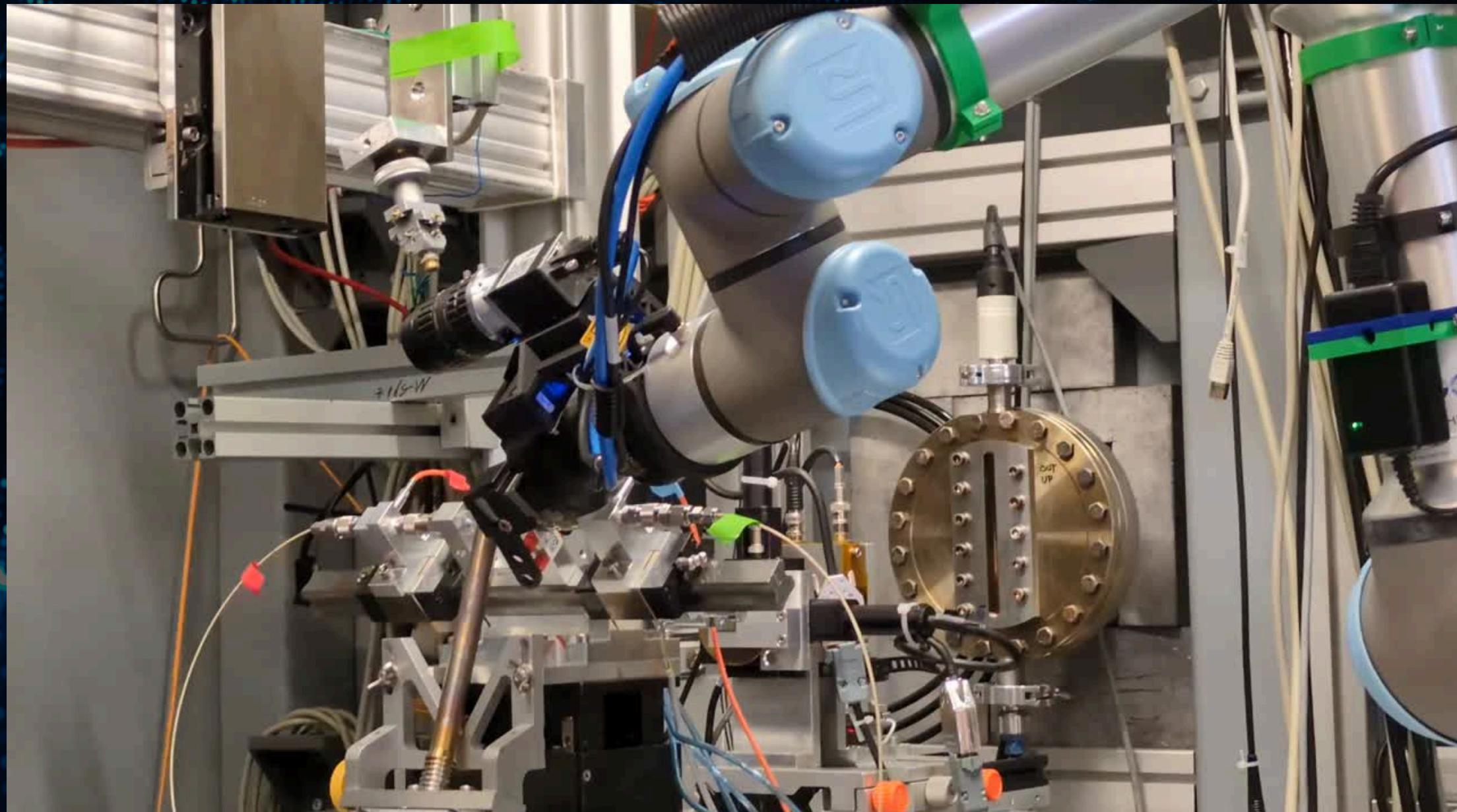
Users are scientists, not industrial operators, requiring intuitive interfaces and flexibility.

# Automated Sample Handling System

## Overview

### Hardware Components:

- UR10e Robotic Arm with RobotIQ 2F-85 gripper for versatile sample handling.
- Basler Camera for accurate QR-code scanning and precise sample localization.
- Pneumatic Clamping Station providing gas connections and controlled heating for operando conditions.
- 6-Slot Sample Magazine enabling parallelized and high-throughput experiments.

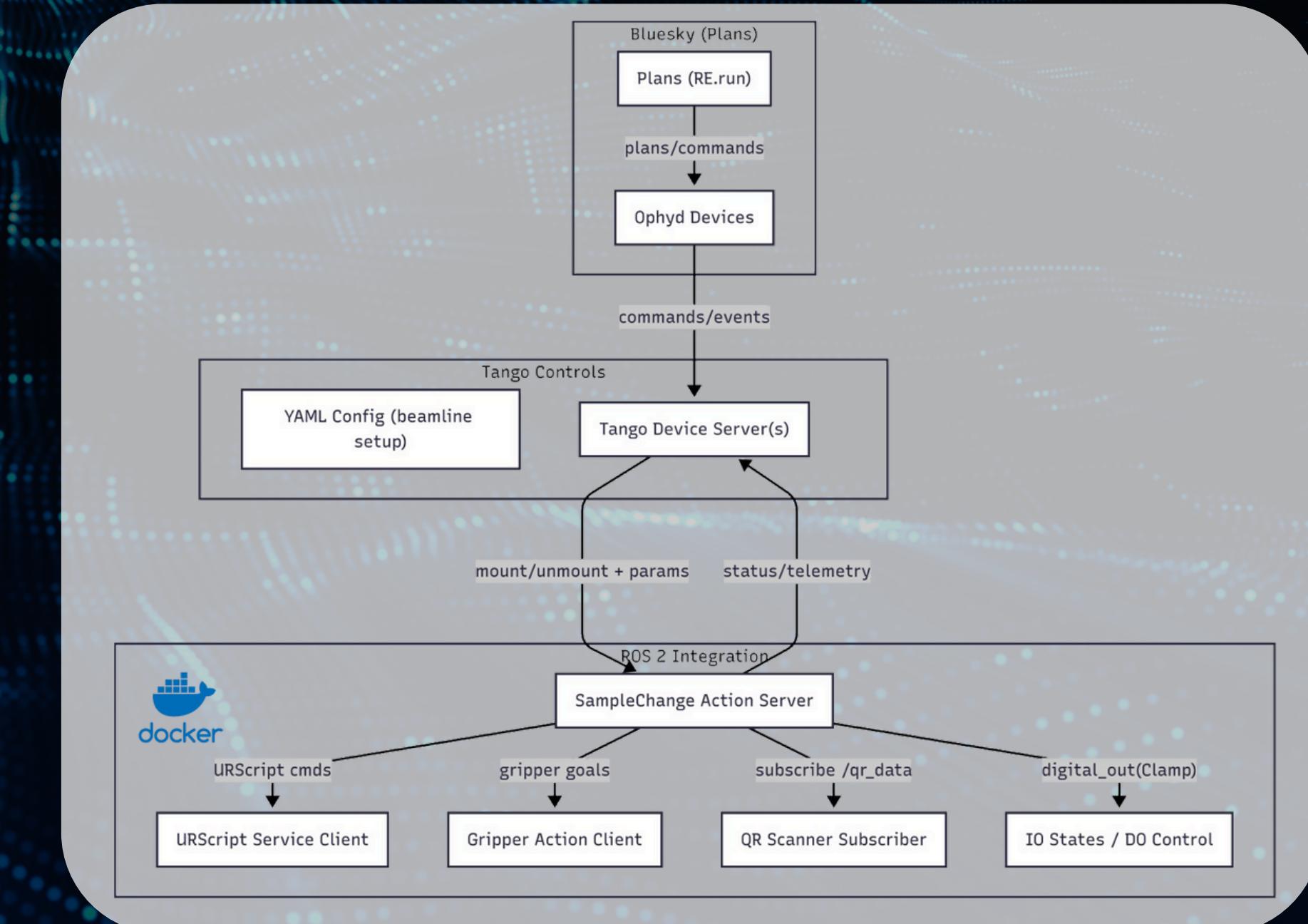


# Automated Sample Handling System

## Overview

### Software & Control Architecture

- Bluesky: High-level experiment orchestration and comprehensive data management.
- Tango Control System: Coordinated control of instruments including the robot, environmental parameters, and detectors.
- ROS 2: Integrated pipeline for robotic motion planning, perception, and feedback control, ensuring reproducibility and user-friendly automation.



# How ROS 2 Served Our System ?

ROS 2 (Robot Operating System 2) proved to be a foundational choice for our beamline automation, offering critical capabilities that addressed the unique demands of our complex scientific environment. It's more than just a framework; it's an ecosystem designed for robust, distributed robotics.

## Why ROS 2 Worked ?



### Hardware Abstraction

Seamless integration of diverse hardware components like robot arms, grippers, and vision systems.



### Action-based Workflows

Manages complex, long-running tasks such as automated sample changes with dedicated action servers.



### Clear Separation of Concerns

Promotes modular code, making development, testing, and maintenance more efficient.



### Modularity & Scalability

Native support for expanding the system and adapting to future autonomous beamline requirements.



### Strong Ecosystem

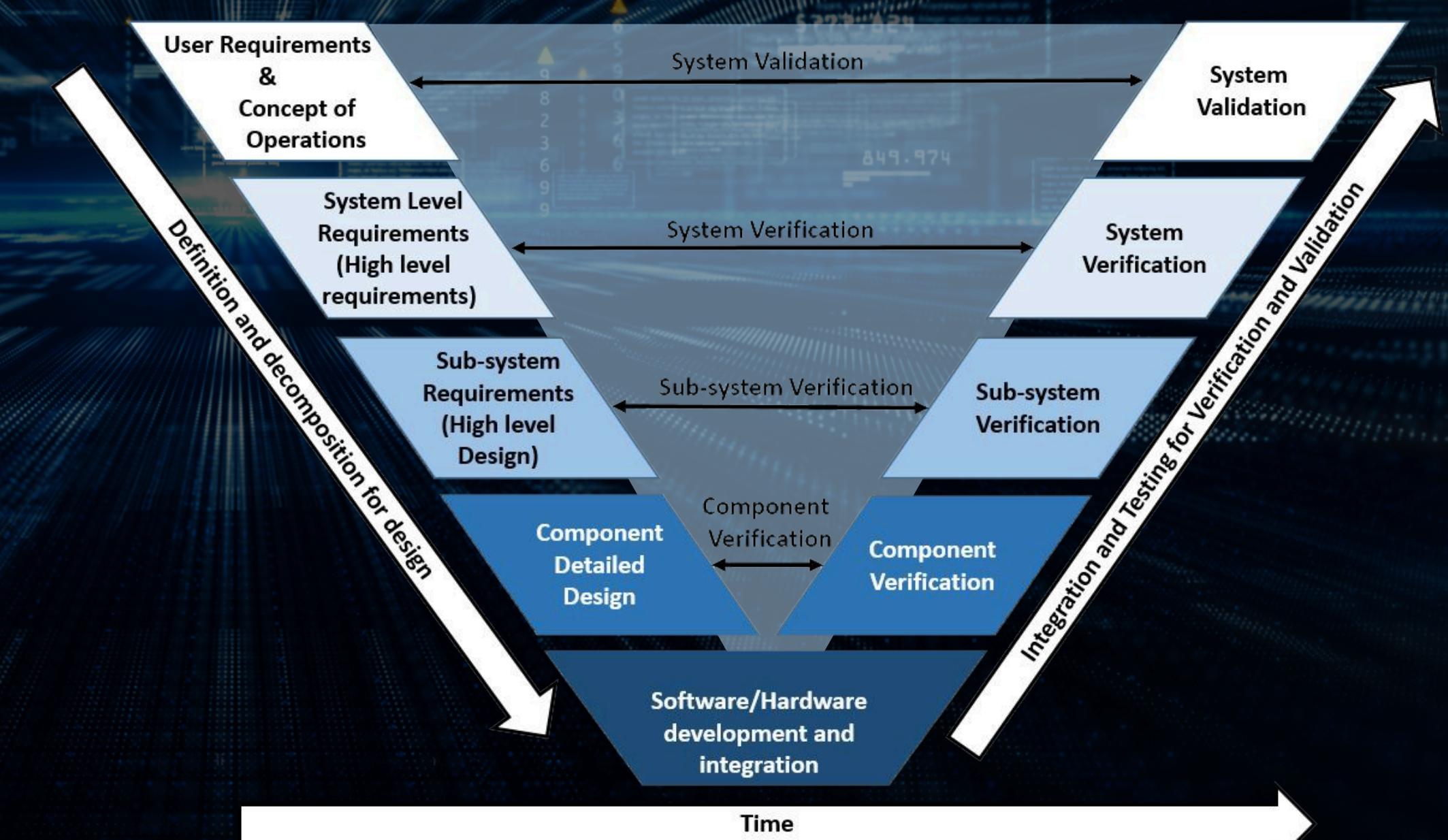
Access to a rich community and powerful tools for robotics development and perception.

## An Honest Note

Debugging distributed systems is hard and requires stringent discipline in defining and maintaining interfaces between components.

# The V-Model for Mechatronics Systems

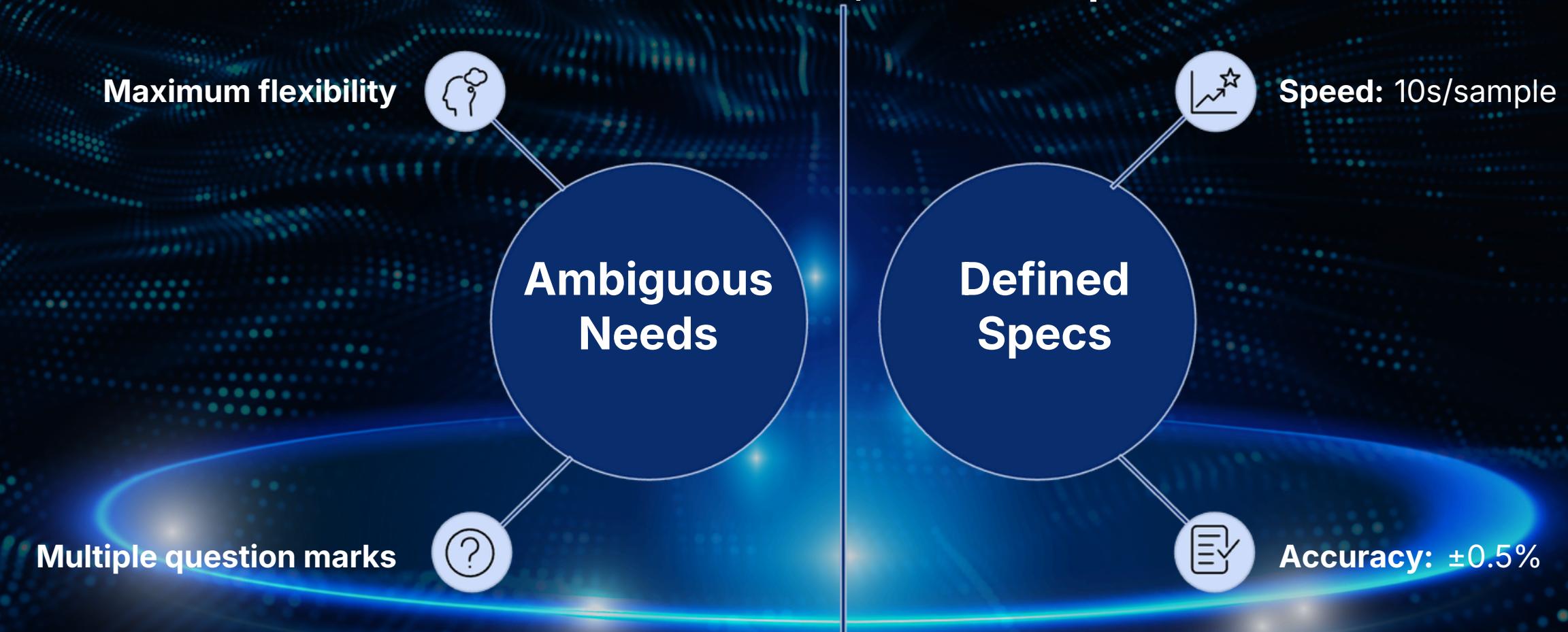
Let's delve into the V-Model, a structured development process that integrates specification, design, integration, and validation phases. This framework is particularly powerful for complex mechatronic systems, ensuring quality and traceability throughout the project lifecycle.



# Phase 1: Requirements

## The "Why" Trap

The initial phase of any project, especially in scientific automation, is fraught with the challenge of translating broad scientific desires into actionable, technical specifications.



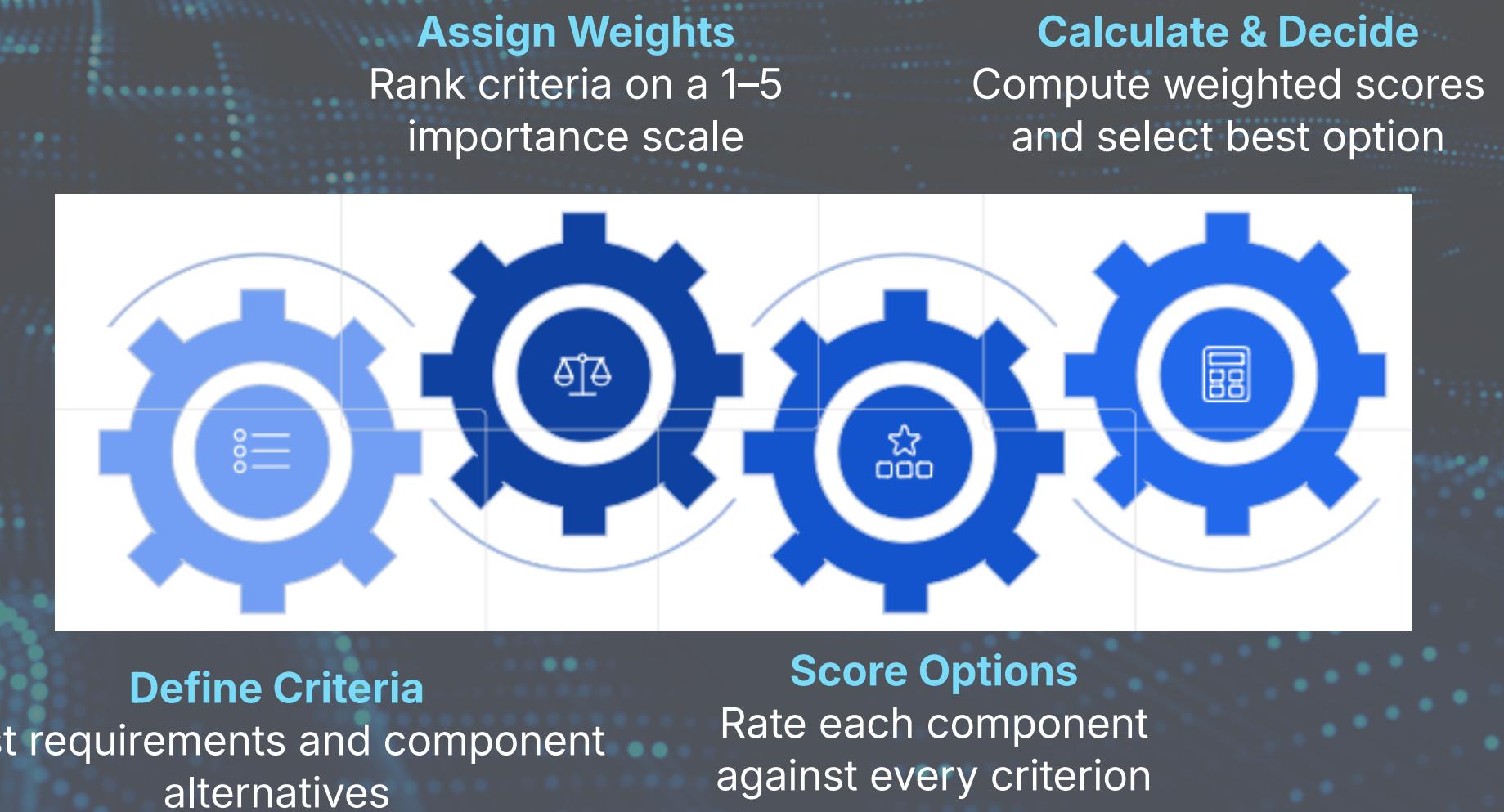
**The Lesson:** A signed requirement document is your best friend. It formalizes needs and prevents scope creep.

## Phase 2: Design

# Navigating the Component Maze with Structured Decision-Making

From Subjective Choice to Objective System Design

To move beyond arbitrary selections, we adopt a systematic 4-step framework based on Multi-Attribute Decision Making (MADM) [2]. This ensures that every component choice is thoroughly evaluated against our defined requirements, reducing risk and optimizing performance.



# Phase 2: Design Simulate or Stumble

Roadblock: TCP & Gripper Reality vs CAD

## Key Challenges:

- Custom fingers ≠ simple offset
- Tilted fingers introduce orientation-dependent error
- Teaching precise grasp poses manually is exhausting and unreliable

How to Pass It:  
Aggressive use of CAD & kinematics simulation



Fig: Sample changer @ MySpot beamline

# RODBLOCK 2

# Teaching Poses in Constrained Spaces

Precision in robotic manipulation isn't just about the robot's capabilities; it's heavily influenced by the environment and the methods used for teaching. Our second major hurdle emerged when attempting to program precise poses within the physically restrictive beamline environment.

## The "Feel" of Free-Drive

Relying on constant human force during free-drive mode is fatiguing and inherently imprecise, making it difficult to maintain stability for accurate pose teaching.

## Human Precision Limits

Even highly skilled operators struggle with the sub-millimeter accuracy required. Small angular errors at the robot's base translate into significant deviations at the gripper's fingertip.

## Amplified Angular Errors

Due to the robot's kinematics, a tiny angular misalignment (e.g., 0.1 degree) can cause the gripper to miss its target by several millimeters or even centimeters over the length of the arm.

## Solution Strategies for Robust Pose Teaching

01

Teach Approach & Retreat

02

Separate Precision Needs

03

Utilize Mechanical Truth

**The Lesson:** If a pose is consistently hard to teach, it's often a **design problem** in the setup or tooling, not a user problem. Rethink the interface between robot and environment.

# RODBLOCK 3

# Software-Hardware Contract Violations

Robotics systems fail at interfaces, not in components.

## Stale Poses

Poses recorded once were reused after hardware components were subtly changed, leading to misalignments and collision risks.

## QR Data Assumptions

Assumptions that QR code data would always arrive perfectly formed and in time led to errors when environmental factors interfered.

## Small Gripper Tweaks Break Workflows

Even minor changes in gripper finger geometry or material can alter grasp mechanics, requiring entire pick-and-place routines to be re-taught and re-verified, disrupting established automated workflows.

**The Lesson:** Robust system design requires explicit interface contracts and thorough validation at every integration point. Anticipate and handle discrepancies between the expected and actual states of hardware and software.

# Integration Is Not Linear



The V-model often depicts a smooth, sequential flow from requirements to validation. However, in complex robotic systems, integration is rarely a linear process. Changes in one phase can cascade, invalidating work done in others, forcing continuous adaptation.

## The Ripple Effect of Change

### Mechanical Changes Invalidate Software

A slight modification to a physical component, like a sample holder, can render existing software trajectories and CAD models obsolete, demanding costly re-programming and re-validation.

### Calibration Affects Motion Planning

Recalibrating a robot's TCP or adjusting sensor offsets can subtly shift its kinematic model, leading to motion planning errors and potential collisions if not carefully re-integrated.



**The Lesson:** Integration must be a continuous, ongoing process, not a final phase. Embrace iterative development and build in mechanisms for rapid adaptation to changes across all system layers.

# Outlook & Future Improvements

## Parametric Positioning

Transition from manual "teaching" of robot poses to defining them parametrically in code or through precisely engineered physical fixtures. This drastically reduces human error and boosts repeatability.

## Enhanced Calibration

Develop automated and adaptive calibration workflows for TCPs, robot base frames, and sensor offsets. Implement continuous monitoring to detect and correct any deviations in real-time, maintaining high precision.

## Increased Autonomy & Resilience

Integrate advanced decision-making capabilities and sophisticated fault detection/recovery mechanisms. This allows the system to self-correct and handle unexpected events, minimizing downtime and human intervention.

# Acknowledgements



[rock-it-project.de](http://rock-it-project.de)

The ROCK-IT team at the 4th ROCK-IT project meeting at HZDR, October 2024.

# Q&A Session



Thank You for  
Attention