SimRIX: A Digital Twin for qRIX Motion with a Path Toward Agentic AI Integration

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Background and Motivation

The qRIXS instrument relies on diffractometer and cryo motion to define the geometry between the X-ray beam, sample, and detector. Rotational axes set the scattering angle, while translational axes align the interaction region. This geometric dependence is reflected in Bragg's law: $n\lambda = 2d\sin\theta$

This project develops a TwinCAT-based digital twin to support offline motion testing, validate axis command and readback behavior, and provide a foundation for agentic AI integration.

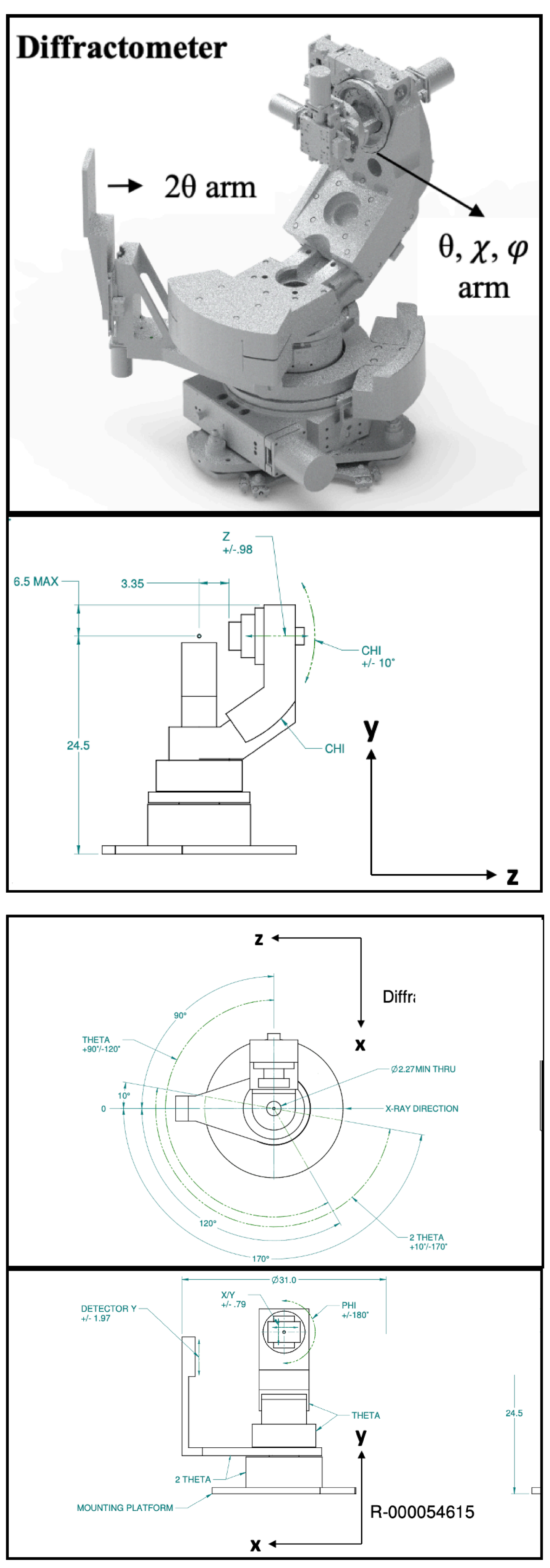

Figure 1. qRIXS diffractometer geometry and approximate dimensions

Simulation Architecture and TwinCAT Implementation

A simulation variant of the qRIX motion project was developed in TwinCAT to simulate the diffractometer and cryogenic motion. Instead of relying on hardware motion, the digital twin:

- preserves the PLC and NC axis structure
- replaces hardware with simulated drive and encoder responses.

TwinCAT v3.1.4026.17

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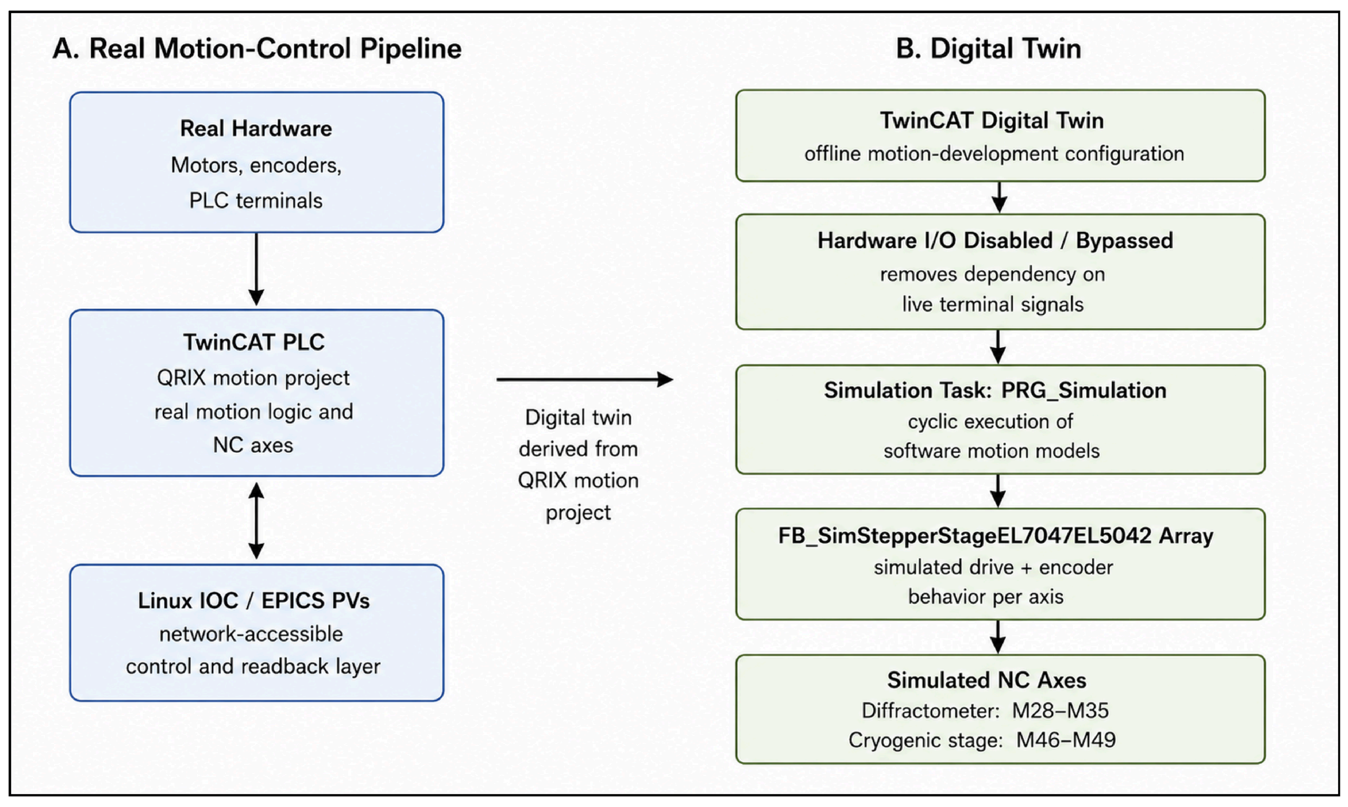

Figure 2. Workflow for the SimRIX digital twin. The left side shows the real PLC-based motion pipeline, while the right side shows the digital twin.

Number	Axes	S..	Link to I/O	Link to PLC
1 (Id 46)	M46 - CRYO X	☐		Main.M46.Axis (qrix_motion Inst
2 (Id 47)	M47 - CRYO Y	☐		Main.M47.Axis (qrix_motion Inst
3 (Id 48)	M48 - CRYO Z	☐		Main.M48.Axis (qrix_motion Inst
4 (Id 49)	M49 - CRYO ROT	☐		Main.M49.Axis (qrix_motion Inst

Number	Axes	S..	Link to I/O	Link to PLC
1 (Id 29)	M29 - Diff Y	☐		Main.M29.Axis (qrix_motion Inst
2 (Id 30)	M30 - Diff Z	☐		Main.M30.Axis (qrix_motion Inst
3 (Id 31)	M31 - Diff 2Theta Y	☐		Main.M31.Axis (qrix_motion Inst
4 (Id 32)	M32 - Diff Phi	☐		Main.M32.Axis (qrix_motion Inst
5 (Id 33)	M33 - Diff Chi	☐		Main.M33.Axis (qrix_motion Inst
6 (Id 35)	M35 - Diff 2Theta	☐		Main.M35.Axis (qrix_motion Inst
7 (Id 34)	M34 - Diff Theta	☐		Main.M34.Axis (qrix_motion Inst
8 (Id 28)	M28 - Diff X	☐		Main.M28.Axis (qrix_motion Inst

Figure 3. Diffractometer axes M28–M35 and cryo axes M46–M49 were selected for the simulation variant. The "Link to I/O" field is cleared, indicating that the axes are no longer connected to live hardware terminals, while the "Link to PLC" field remains active, preserving the normal PLC/NC motion structure.

```
{attribute 'TcLinkTo' := '
      [1].SimEL7047.DrvI := TINC^NC-Task 1 SAF^Axes^M28 - Diff X^Drive^Inputs^In;
      [1].SimEL7047.DrvO := TINC^NC-Task 1 SAF^Axes^M28 - Diff X^Drive^Outputs^Out;
      [1].SimEL5042.EncI := TINC^NC-Task 1 SAF^Axes^M28 - Diff X^Enc^Inputs^In;
      [1].SimEL5042.EncO := TINC^NC-Task 1 SAF^Axes^M28 - Diff X^Enc^Outputs^Out;
```

Figure 4. Example TcLinkTo mapping that connects one simulation block to the NC drive and encoder interfaces

```
{IF defined (Simulation)}
FOR i := 1 TO 12 BY 1 DO
    fbSimStepperStage[i]();
END_FOR
{END_IF}
```

Figure 5. Simulation loop that cyclically updates all simulated axis blocks when the Simulation is enabled.

A TwinCAT simulation task executed an array **FB_SimSteppetStageEL7047EL5042** blocks, each linked to a diffractometer or cryo axis to reproduce simulated drive or encoder behavior.

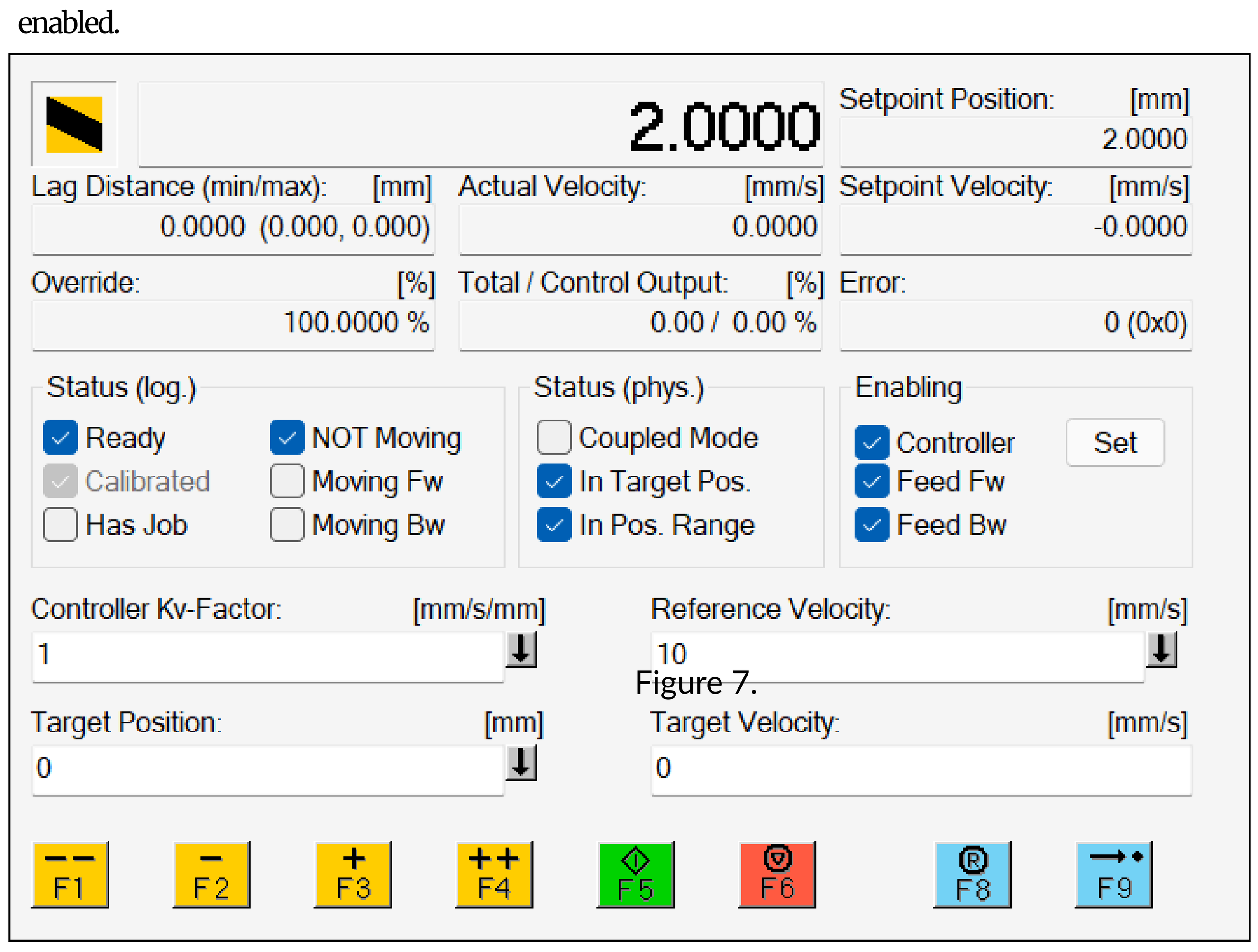

Figure 6. Example TwinCAT online state for a simulated diffractometer axis (M28), showing that the axis reaches ready and in-target conditions in the offline simulation environment.

Figure 7. TwinCAT PLC hardware used in the sRIX environment.

Graphical User Interface

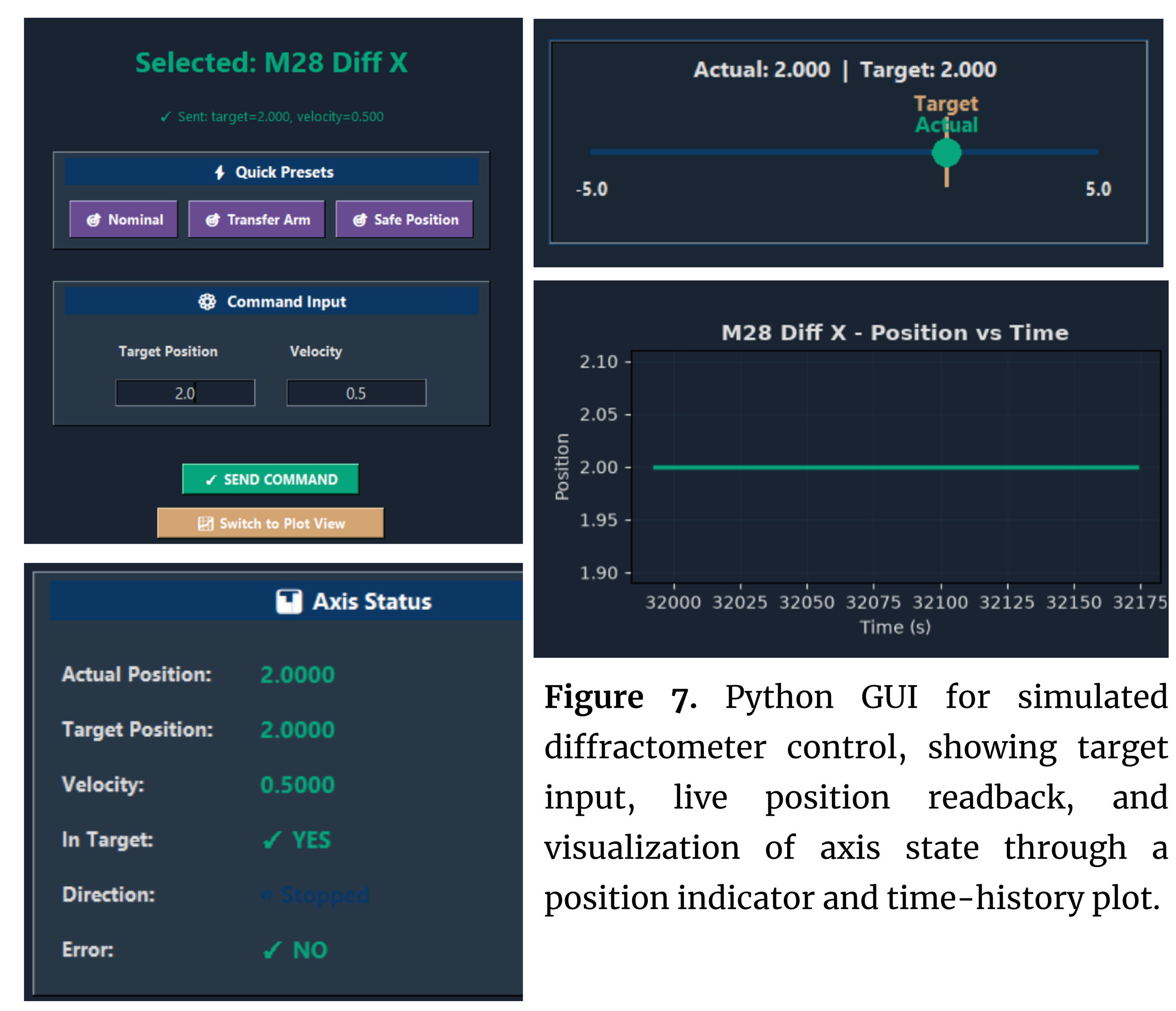

Figure 7. Python GUI for simulated diffractometer control, showing target input, live position readback, and visualization of axis state through a position indicator and time-history plot.

Copilot Agent Assisted Simulation

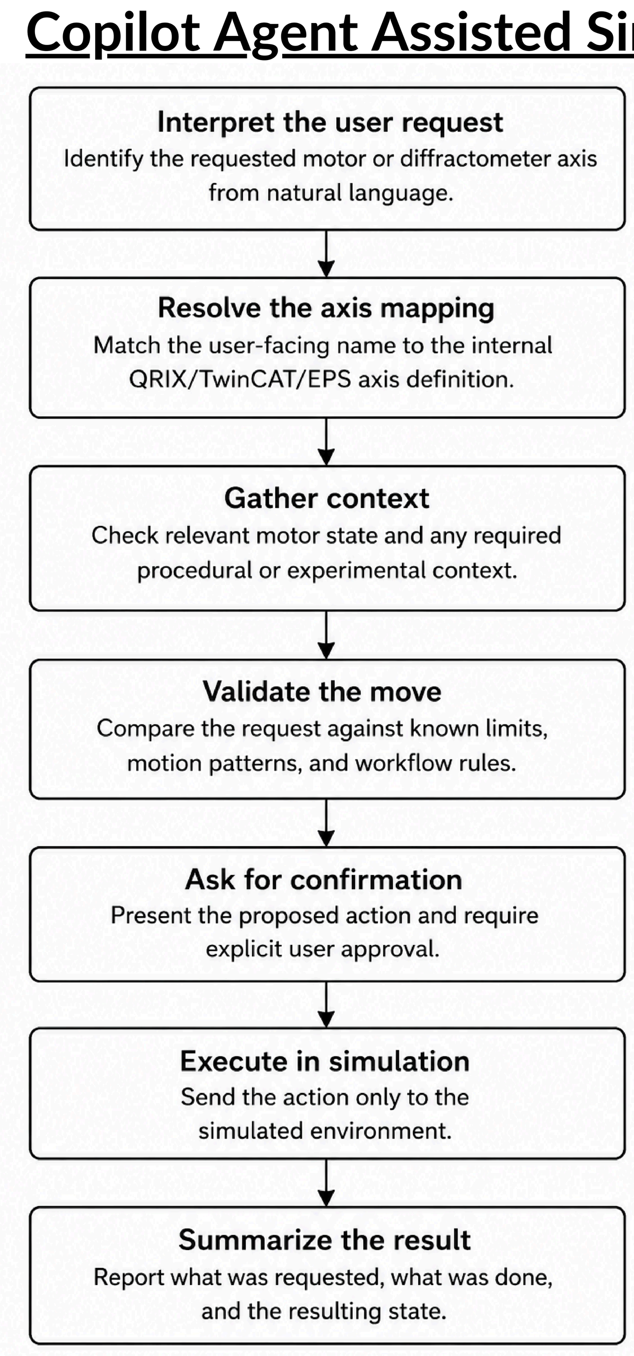

Figure 9. Copilot agent-assisted simulation workflow

Figure 10. OpenCode enviroment

```
~/sim-diffractometer/
├── SKILL.md
└── references/
    ├── axis-map.md
    ├── eps-limits.md
    ├── motion-patterns.md
    └── fault-reference.md
```

Figure 11. The copilot agent uses a skill-based design in which a central SKILL.md file defines how the agent should respond to diffractometer. The reference files include axis mappings, motion patterns, safety limits, and elog workflow context. This gives the agent content to reference when reasoning about motor movement.

Future Work

- Connect the agent to simRIXS to test end-to-end diffractometer interaction in simulation.
- Expand this skill-based framework to other parts of the qRIX

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