

Agentic Workflow for AFM Digital Twin with Theory-Experiment Integration

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Abstract

Foundation models and agentic workflows offer transformative potential for accelerating materials science research by bridging the gap between theoretical simulations and experimental observations. In this work, we present an integrated system that combines ferroelectric domain simulations (FerroSim) with real Atomic Force Microscopy (AFM) experimental data analysis through the Model Context Protocol (MCP). Traditional AFM workflows often require manual switching between simulation tools, data analysis software, and experimental control interfaces, leading to inefficiencies and difficulties in theory-experiment comparison. Here, we introduce FerroSim-AFM MCP Server, an automated workflow that integrates ferroelectric domain theory simulations with multi-format AFM experimental data processing, enabling AI-driven comparative analysis and decision-making.

Our system builds upon the DTMicroscope Digital Twin framework [1] and leverages Claude's foundation model capabilities through MCP to provide a unified interface for: (1) running physics-based FerroSim simulations with configurable electric fields, defects, and material properties; (2) loading and analyzing real AFM data from multiple experimental formats (Igor .ibw, HDF5/USID, NumPy, MATLAB, text files); (3) automated theory-experiment matching with quantitative metrics (correlation, MSE, RMSE); and (4) natural language-driven workflow orchestration enabling domain scientists to interact with complex experimental and simulation tools conversationally.

The workflow demonstrates enhanced reproducibility in ferroelectric materials characterization, reduces manual effort in data format conversion and analysis, and facilitates rapid iteration between theoretical predictions and experimental validation. By exposing both simulation and experimental capabilities through a standardized MCP interface, this approach enables foundation models to reason about physical systems, suggest parameter adjustments, and guide experimental design based on theory-experiment discrepancies.

Methodology

The system architecture consists of three primary components orchestrated through MCP

1. FerroSim Theory Engine: Implements phase-field simulations of ferroelectric domain evolution using the FerroSim library [1]. The engine supports initialization of domain structures, application of external electric fields, introduction of defects (charged, elastic, electrostatic), and time-evolution of polarization dynamics. Simulation outputs

include polarization field maps, domain statistics, and energy landscapes.

2. AFM Digital Twin: A unified data loader and analyzer supporting multiple experimental AFM data formats commonly used in ferroelectric characterization. The module automatically detects file formats and extracts Piezoresponse Force Microscopy (PFM) amplitude and phase channels. Key capabilities include:

- Multi-format data loading with automatic channel detection
- Domain structure analysis (up/down domain quantification, wall density metrics)
- Piezoresponse signal extraction and processing
- DTMicroscope-compatible API for integration with existing tools
- Line-by-line scanning emulation for progressive data analysis

3. Theory-Experiment Matching Layer: Implements automated comparison between simulation outputs and experimental AFM data using multiple quantitative metrics. The matching algorithm accounts for scale differences, performs spatial alignment when needed, and computes correlation coefficients, mean squared error, and root mean squared error to assess theory-experiment agreement.

The workflow is exposed through 15 MCP tools that enable foundation models to:

- Initialize and configure ferroelectric simulations with specific material parameters
- Load experimental AFM scans from laboratory instruments
- Analyze domain structures in both simulated and experimental data
- Compare theoretical predictions with experimental observations
- Visualize results with automated plot generation
- Iterate parameters based on theory-experiment discrepancies

Each tool provides structured JSON responses with metadata, enabling the AI agent to reason about results and suggest next steps. The system maintains state across multiple scans and simulations, allowing for comparative studies and parameter space exploration.

Integration with Claude Desktop through MCP enables natural language interaction with the entire workflow. Domain scientists can request complex multi-step analyses (e.g., "Load the experimental scan, run a simulation with similar parameters, and compare the domain wall densities") without writing code or manually switching between tools. The foundation model interprets requests, orchestrates appropriate tool calls, analyzes results, and provides scientific insights based on theory-experiment comparisons.

References

- [1] DTMicroscope Digital Twin Framework, <https://github.com/pycroscopy/DTMicroscope>
- [2] FerroSim: Phase-field simulations of ferroelectric domains,
<https://github.com/ramav87/FerroSim>

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