Interpretable Digital Twins for Autonomous STEM Aberration Correction

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Abstract

Achieving sub-ångström resolution in scanning transmission electron microscopy (STEM) requires precise correction of lens aberrations. Current aberration correction workflows rely on iterative estimation of aberration coefficients from tableau- or Ronchigram-based measurements, followed by manual or semi-automatic adjustment of corrector lens currents [1-2]. Although effective, this process is slow, highly sensitive to operator expertise, and complicated by the nonlinear and strongly coupled nature of aberrations: correcting a single term often perturbs multiple others. Such cross-coupling leads to unstable convergence, repeated trial-and-error tuning, and limited throughput and reproducibility. In this hackathon project, we develop a proof-of-concept framework for machine-learning-assisted aberration correction in STEM (Fig. 1). The framework integrates four key components: (i) a large-language-model-based parsing pipeline that extracts and organizes aberration coefficient trajectories from real human-generated STEM aberration correction logs, (ii) symbolic regression to identify coupled response relationships between corrector settings and aberration evolution (Fig. 2a), (iii) a simplified aberration corrector simulator that embeds nonlinear and cross-coupled response models identified through the symbolic regression (Fig. 2b), and (iv) a reinforcement learning agent that automatically predicts multi-parameter correction steps from measured aberration coefficients or image-based features (Fig. 2c). By learning the nonlinear interactions between corrector adjustments and aberration evolution, the proposed approach aims to accelerate convergence and enhance correction stability compared to conventional iterative tuning. Initial results focusing on low- to mid-order aberrations demonstrate reduced correction steps and decreased reliance on expert intervention, highlighting the potential of machine learning for automated and reproducible STEM alignment.

Methodology:

1. Aberration Correction Trajectory Extraction and Parsing: To ground the learning framework in realistic aberration correction behavior, we begin by extracting aberration correction trajectories from real STEM alignment sessions with human operators on the TEAM 0.5 instrument at the National Center for Electron Microscopy. These trajectories consist of time-ordered aberration coefficient measurements, human-selected correction actions, and convergence trends recorded during manual or semi-automatic tuning. Because such logs are often unstructured or instrument-dependent, we employ a large language model (LLM)-based parsing pipeline to automatically interpret, standardize, and organize the correction history into structured datasets. The parsed output provides aligned sequences of aberration states and corresponding correction steps, enabling downstream data-driven modeling without manual annotation.

2. Symbolic Regression for Coupled Aberration Response Modeling: To characterize nonlinear and cross-coupled relationships between corrector adjustments and aberration evolution, we apply a sparsity-promoting symbolic regression approach based on the Sparse Identification of Nonlinear Dynamics (SINDy) framework to the parsed correction trajectories [3]. This approach identifies analytical expressions that describe how changes applied in the corrector simultaneously affect multiple aberration coefficients. The resulting models provide interpretable representations of aberration coupling and serve as a data-driven approximation of corrector behavior.

3. Aberration Corrector Simulator with Learned Coupling: We construct an aberration corrector simulator that embeds the learned response functions obtained from the symbolic regression, along with a graphic user interface (GUI). Given an initial aberration state and a user action of aberration correction, the simulator predicts the updated aberration coefficients in a single step. Measurement noise and bounded actuation constraints are optionally included to mimic realistic experimental conditions. This simulator serves as a fast and controllable environment for training and evaluating automated correction strategies, while remaining grounded in experimentally observed correction behavior.

4. Reinforcement Learning–Assisted Correction Strategy: Aberration correction is cast as a sequential decision-making problem and solved with a Proximal Policy Optimization reinforcement learning algorithm (PPO) [4]. In each step, the agent observes the current aberration state as a vector of numerical coefficients and outputs a multi-dimensional correction command that is applied simultaneously to all aberrations. The correction dynamics in the simulator include cross-coupling relationships (encoded by a user-specified coupling matrix based on user expertise and real experiment logs) and stochastic disturbances with parameter-dependent scales, so the agent must learn a robust closed-loop policy rather than independent one-at-a-time updates. The reward encourages rapid reduction of the overall aberration magnitude while penalizing unstable trajectories and limiting the number of iterations via early termination when the deviation exceeds a safety bound. Training is performed with many parallel simulator instances and optional observation/reward normalization to stabilize learning, and the learned policy is periodically evaluated and checkpointed to track and preserve the best-performing controller.

5. Proof-of-Concept Evaluation: As a proof of concept, the framework is evaluated on low- to mid-order aberrations (up to third-order coefficients) under diverse initial conditions. Note that, due to the limited availability of mid- and high-order aberration logs, only low-order coupling relationships identified through symbolic regression are incorporated into the simulator here. High-order corrections are rare on a day-by-day basis during real-world operation, but can be further accumulated over long-term usage. Performance is assessed by comparing convergence speed, stability, and the number of correction steps against conventional iterative correction schemes. These results demonstrate the feasibility of combining symbolic-regression-based modeling with reinforcement learning to achieve faster and more stable aberration correction with reduced reliance on expert manual intervention.

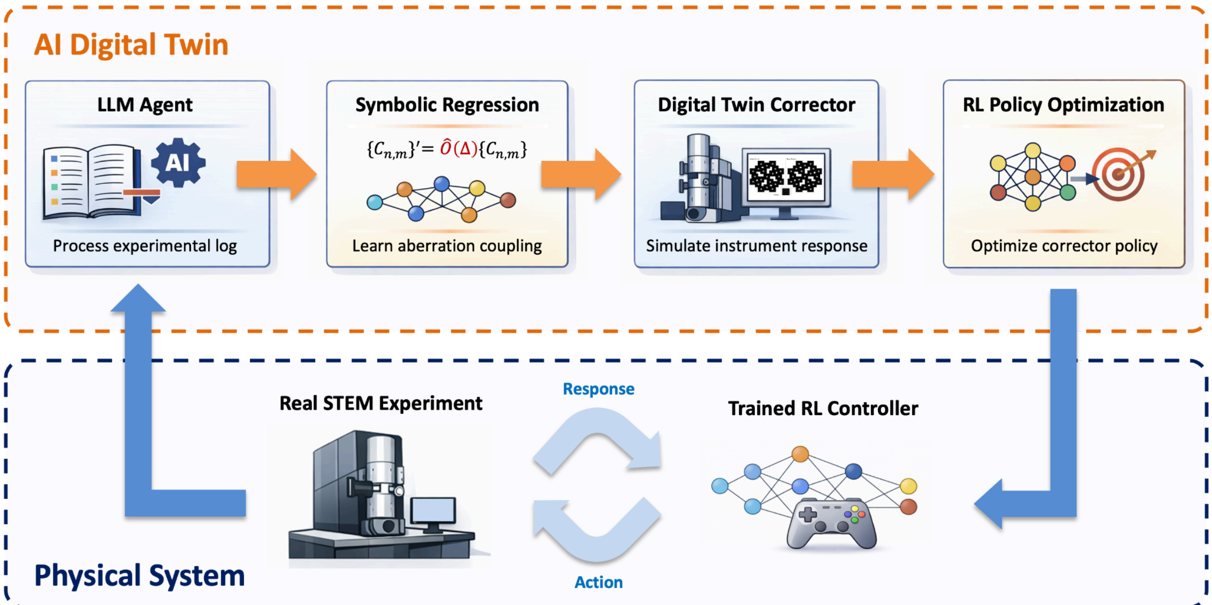

Figure 1: AI-based digital twin framework for STEM aberration correction, integrating LLM-based experimental log parsing, symbolic regression-derived coupling models, a simplified corrector simulator, and reinforcement learning-based optimization, operating in a closed loop with the physical microscope through bidirectional action–response exchange.

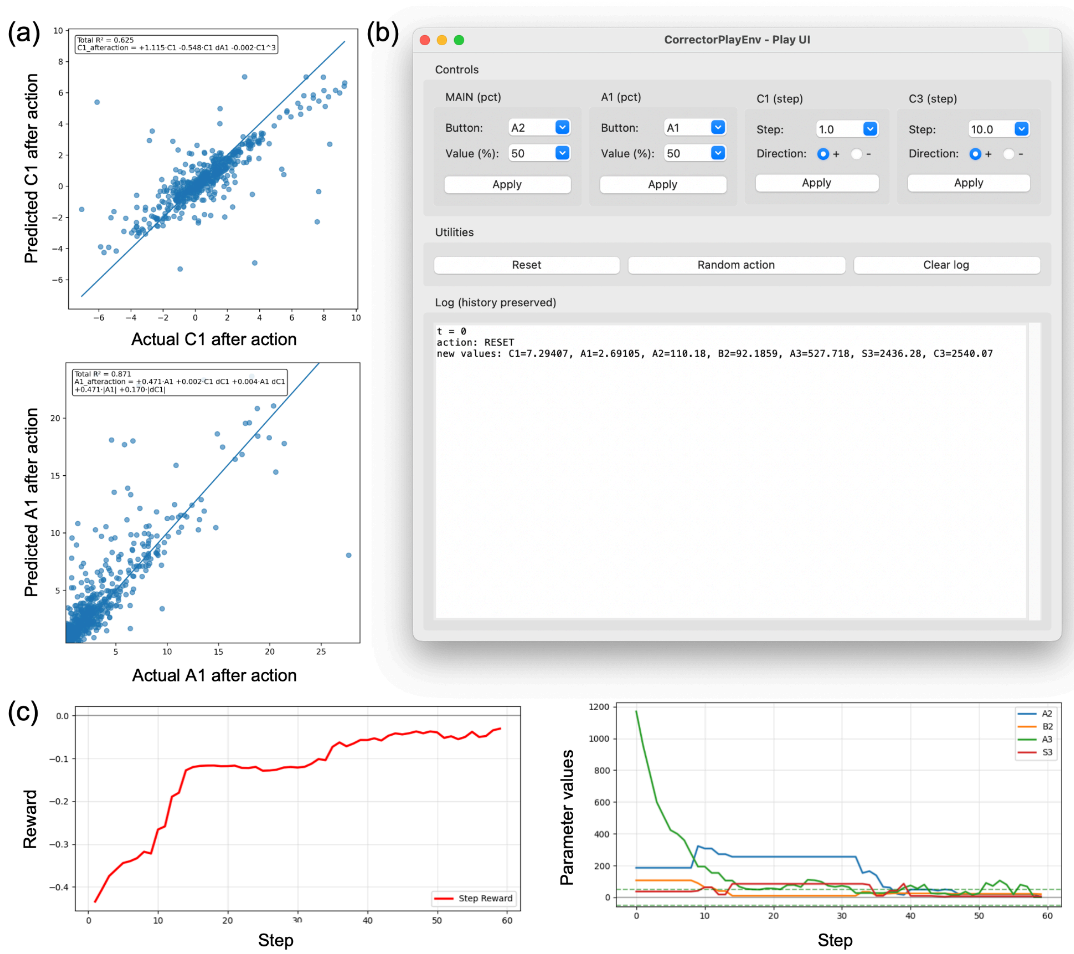

Figure 2: Components and performance of the AI-based digital twin for STEM aberration correction. (a) Symbolic regression results showing predicted versus measured aberration values after corrective actions, illustrating response function coupling with two aberration modes (e.g., A1–C1). The high correlation demonstrates that the symbolic model captures dominant response relationships of the corrector. (b) Graphical user interface of the aberration corrector simulator, designed to emulate the experimental corrector control software, including percentage-based and step-based corrections, logging, and reset/random actions for closed-loop interaction. (c) Reinforcement learning–based optimization results, showing progressive improvement of the reward function (left) and concurrent reduction of multiple aberration coefficients over iterations (right), indicating stable convergence toward an optimized aberration state.

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