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EXPLORING THE INTEGRATION OF LARGE LANGUAGE MODELS AND THE MODEL CONTEXT PROTOCOL FOR AUTOMATED SIMULATION MODELING: FEASIBILITY CHECKS WITH A MATRIX PRODUCTION SYSTEM

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ABSTRACT

This paper proposes a conceptual framework for automating simulation model generation by integrating Large Language Models (LLMs) with the Model Context Protocol (MCP). The framework standardizes the interaction between generative agents and structured system data by using MCP as a context delivery mechanism for LLMs. This enables the automatic construction of discrete event simulation (DES) models through context-grounded reasoning and standardized data access. To demonstrate its potential, a conceptual sequence diagram illustrates how MCP could exchange model requirements, system data, and generated artifacts between an LLM host, MCP servers, and simulation environments. Proof-of-concept tests using simple DES models, such as an M/M/1 queuing system implemented in SimPy, evaluate the feasibility of generating executable simulation code from MCP-delivered context. Finally, a case study on the Matrix Production System (MPS) highlights the types of structured information that could be formalized via MCP, supporting scalable, context-grounded, LLM-driven simulation modeling workflows.

1 INTRODUCTION

Automating the development of simulation models remains a major challenge in the analysis and implementation of complex production systems. In the manufacturing sector, growing demands for customization, flexibility, and resilience have made traditional discrete event simulation (DES) workflows resource-intensive and highly dependent on domain expertise (Gu et al. 2024). These workflows typically include problem formulation, data structuring, model implementation, verification, and validation (Banks et al. 2010).

Recent advances in Large Language Models (LLMs) have introduced new opportunities for automating knowledge-intensive tasks (Wang and Shao 2025). However, while LLMs can generate plausible outputs, they often lack grounding in real-world context, resulting in inconsistencies or hallucinations, also referred to as unfaithful or arbitrary generations (Farquhar et al. 2024). Model Context Protocol (MCP) has emerged as an open protocol that standardizes how LLM agents access structured data and external tools, enabling more reliable and grounded reasoning, although it remains in its early stages (Anthropic 2024; Hou et al. 2025). Beyond automated modeling, MCP can serve as a foundational layer for broader context-aware AI agent workflows by allowing agents to access, interpret, and act upon structured system data in a consistent manner (Yang et al. 2025).

This paper proposes a framework for integrating MCP and LLMs for automated simulation modeling. The focus is on demonstrating how MCP could be applied in the simulation domain using sequence diagrams and simple proof-of-concept DES experiments before extending the approach to more complex scenarios. To this end, the Matrix Production System (MPS) is introduced as an advanced testbed for evaluation. The MPS, with its inherent complexity including dynamic routing, modular layouts, and diverse resource interactions, provides a representative manufacturing system to assess the scalability and adaptability of the proposed framework.

2 METHODOLOGY

The methodology consisted of three stages. First, the current capabilities and limitations of MCP and LLMs for supporting automated modeling were analyzed. A conceptual sequence diagram was created to capture interactions between LLM hosts, MCP servers, and simulation tools. Second, simple test models, such as an M/M/1 queuing system, were implemented in SimPy to assess whether LLMs could generate executable DES code when provided with structured context, such as system parameters and data schemas, through MCP. These experiments focused on testing feasibility rather than full automation. Third, the framework was conceptually extended to the more complex MPS case. The MPS scenario demonstrates how production system data, such as modular layouts, routing rules, and resource capacities, could be formalized into MCP-compatible schemas to enable automated modeling.

3 RESULTS

Initial experiments using the M/M/1 test model showed that natural language descriptions of system characteristics could be successfully transformed by the LLM into executable DES models in SimPy when structured context was provided. The integration with MCP was conducted using static context definitions delivered to the LLM, as full MCP-to-tool integration was not yet implemented. The extended MPS case further illustrated the structured context requirements for complex manufacturing systems. These results suggest that MCP-compatible data formats could enable scalable automated modeling. While some of the generated models required iterative prompting and minor corrections, the experiments confirmed that using MCP to deliver structured context can support standardized, context-aware simulation model generation.

4 DISCUSSION AND CONCLUSION

This study identifies the architectural requirements and feasibility considerations for using MCP as a foundation for LLM-driven simulation modeling. MCP's modular design, comprising Host, Client, and Server components, has the potential to standardize the delivery of system context, reduce manual modeling effort, and increase reusability once integrated with simulation tools. Future work will focus on developing prototype MCP extensions for simulation environments, validating the approach on larger and more complex models such as the MPS, and incorporating verification and human-in-the-loop workflows. These efforts aim to move toward context-grounded, semi-automated simulation modeling pipelines that are scalable and adaptable to complex production environments.

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