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AI-Driven Digital Twin for Energy Optimization in Green Data Centers

Isni Oktria
Informatics, Industrial Technology, Universitas Gunadarma, Indonesia

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Corresponding author*:
isnioktria@staff.gunadarma.ac.id

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Abstract: *This study proposes the development of an AI-driven digital twin for data centers aimed at improving energy efficiency, reducing carbon footprint, and enhancing operational performance. The digital twin—a virtual replica of the physical data center—will be equipped with real-time AI algorithms to predict thermal loads, analyze cooling requirements, and automatically adjust operations to minimize energy consumption. This paper explores the integration of AI with digital twin architectures, tests its performance in simulated scenarios, and evaluates potential energy savings as well as contributions to Green IT practices.*

Keywords: *Artificial Intelligence (AI); Digital Twin; Green Data Center; Energy Optimization; Power Usage Effectiveness (PUE); Carbon Usage Effectiveness (CUE); Sustainable Computing*

INTRODUCTION

The rapid expansion of the digital economy has driven a sharp increase in demand for computing power, resulting in the accelerated growth of data centers worldwide. These facilities are the backbone of cloud computing, artificial intelligence, big data analytics, and digital services. However, their energy consumption is substantial—global estimates suggest that data centers account for between 5% and 9% of total electricity usage, with projections indicating a continuous rise in the coming years. This trend raises critical concerns about the environmental impact of the IT industry, particularly in the context of climate change and global sustainability goals.

In response to these concerns, the concept of Green Data Centers has emerged as a strategic approach to mitigate energy use and reduce greenhouse gas emissions. Green data centers prioritize energy efficiency, renewable energy integration, and optimized resource utilization without compromising performance. Efforts to improve metrics such as Power Usage Effectiveness (PUE) and Carbon Usage Effectiveness (CUE) are central to these initiatives. While many advances have been made in hardware efficiency and renewable energy sourcing, the optimization of operational processes remains an underexplored area with significant potential.

Among various technological enablers, digital twin technology has gained increasing attention as a tool for sustainable data center operations. A digital twin is a virtual representation of a physical system that enables real-time monitoring, simulation, and predictive analysis. In the context of data centers, digital twins can model cooling systems, power distribution, and workload dynamics, providing operators with a powerful platform for scenario testing and decision-making. This capability not only enhances operational resilience but also supports proactive energy optimization strategies.

Despite its promise, most existing digital twin implementations for data centers are static or semi-dynamic, focusing primarily on visualization and manual decision support. While such approaches provide valuable insights, they lack the adaptability needed to handle rapidly changing workloads and environmental conditions. This limitation underscores the need for dynamic and intelligent systems that can respond to operational fluctuations in real time, thereby unlocking the full potential of digital twin technology for energy efficiency.

The integration of Artificial Intelligence (AI) into digital twin architectures offers a pathway to address these limitations. AI algorithms—particularly those in machine learning and predictive analytics—can analyze vast streams of sensor data, forecast thermal loads, and optimize cooling and workload allocation dynamically. By coupling AI with digital twins, data centers can move from reactive to proactive operations, enabling automated adjustments that minimize energy use while maintaining service-level agreements (SLAs).

Recent industry initiatives underscore the viability of this integration. Companies such as Schneider Electric, in collaboration with Nvidia, have demonstrated that AI-enhanced digital twin systems can reduce cooling energy consumption by up to 20% without degrading performance. Such results highlight the transformative potential of AI-driven optimization for meeting sustainability targets while maintaining competitiveness in an increasingly digital economy. Nevertheless, most reported cases remain in the domain of proprietary industry projects, with limited academic exploration of open, replicable, and systematic approaches to AI-driven digital twin implementation.

This research addresses that gap by proposing an AI-driven digital twin framework specifically tailored for real-time energy optimization in green data centers. By leveraging predictive thermal modeling, adaptive cooling control, and continuous performance monitoring, the proposed system aims to achieve significant energy savings and carbon footprint reduction. Moreover, it contributes to the body of knowledge in sustainable computing by providing a model that can be adapted to various operational contexts, paving the way for scalable and transparent solutions in the era of climate-conscious digital infrastructure.

RESEARCH METHOD

This study employs a design science research (DSR) approach to develop, implement, and evaluate an AI-driven digital twin framework for energy optimization in green data centers. The research method consists of four main stages: (1) problem identification and objective definition, (2) system design and architecture development, (3) prototype implementation and experimentation, and (4) evaluation and analysis.

Problem Identification and Objective Definition

The initial stage involves a systematic literature review to identify energy optimization challenges in data center operations, focusing on gaps in existing digital twin and AI integration practices. Industry reports, academic publications, and sustainability benchmarks are analyzed to define measurable performance objectives. The primary objective is to design a system capable of reducing cooling energy consumption while maintaining or improving operational reliability.

System Design and Architecture Development

The proposed framework integrates three core components:

1. Sensor Layer – Real-time data acquisition from temperature sensors, power meters, and workload monitoring tools deployed in the data center.
2. Digital Twin Layer – A virtual representation of the data center's physical infrastructure, including thermal and airflow models, cooling system configurations, and workload distribution.
3. AI Optimization Layer – Machine learning algorithms (e.g., regression models, reinforcement learning) for thermal load prediction, anomaly detection, and adaptive cooling control.

The architecture follows a modular design to allow scalability and adaptability to different operational contexts. Data exchange between layers is handled through a secure API to ensure real-time synchronization between the physical and virtual environments.

Prototype Implementation

A prototype system is developed using Python for AI model training and simulation control, coupled with a 3D modeling environment for the digital twin (e.g., Autodesk Revit or Unity-based simulation). The cooling system and workload dynamics are modeled based on parameters derived from real-world data center operational datasets, such as the ASHRAE thermal guidelines and publicly available PUE benchmarks. The AI algorithms are trained using historical data to predict cooling demand under varying workload and environmental conditions.

Experimentation and Test Scenarios

Experiments are conducted in a simulated environment with varying workloads, ambient temperatures, and cooling system configurations. Three test scenarios are defined:

1. Baseline – Conventional data center operation without digital twin or AI optimization.
2. Static Digital Twin – Digital twin used for monitoring and manual adjustments.
3. AI-Driven Digital Twin – Fully integrated real-time AI optimization controlling cooling and workload allocation.

Each scenario is tested over a simulated operational period of 30 days, with identical workload profiles for comparative analysis.

Evaluation Metrics

The system's performance is evaluated based on the following metrics:

1. Power Usage Effectiveness (PUE) – Ratio of total facility energy to IT equipment energy.
2. Carbon Usage Effectiveness (CUE) – Carbon emissions per unit of IT energy consumption.
3. Cooling Energy Reduction (%) – Percentage decrease in cooling-related energy consumption compared to the baseline.

4. Thermal Prediction Accuracy – Measured using Mean Absolute Percentage Error (MAPE) between predicted and actual temperatures.
5. Service Level Agreement (SLA) Compliance – Percentage of time IT equipment operates within optimal thermal thresholds.

Data Analysis

Collected data from each scenario are statistically analyzed to determine the significance of observed differences in energy consumption and operational stability. Analysis of variance (ANOVA) is applied to compare performance metrics across scenarios, and regression analysis is conducted to assess the relationship between predicted cooling demand and actual energy savings.

Validation and Replicability

To ensure replicability, all system configurations, datasets, and model parameters are documented in detail. Additionally, the proposed framework is validated through expert review by data center engineers and sustainability specialists, ensuring that the solution is both technically feasible and aligned with industry best practices.

Table 1. Research Stages and Key Activities

Stage	Objective	Key Activities	Output
Problem Identification & Objective Definition	Identify energy optimization challenges and research gap	Literature review, industry report analysis, benchmark study	Problem statement & performance objectives
System Design & Architecture Development	Create modular architecture integrating sensors, digital twin, and AI	Architecture blueprint, component specification	System design document
Prototype Implementation	Build a functional prototype for simulation testing	Sensor simulation setup, AI model training, digital twin creation	Working prototype
Experimentation & Test Scenarios	Evaluate performance under controlled conditions	Baseline, static digital twin, AI-driven digital twin scenarios	Experimental dataset
Evaluation Metrics & Analysis	Quantify performance improvements	Measure PUE, CUE, cooling energy savings, SLA compliance	Statistical analysis & performance report
Validation & Replicability	Ensure applicability and industry relevance	Expert review, documentation of configurations	Validated framework

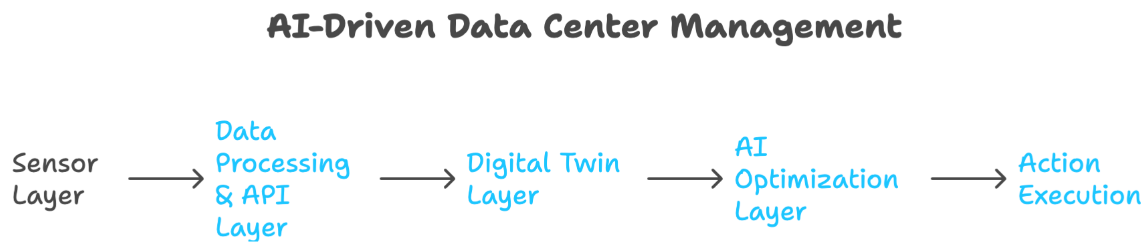

Figure 1. Depicts the integration flow between the physical data center environment and its digital twin, enhanced by AI for real-time optimization.

Table 2. Evaluation Metrics Summary

Metric	Definition	Purpose
PUE (Power Usage Effectiveness)	Total facility energy ÷ IT equipment energy	Measures overall energy efficiency
CUE (Carbon Usage Effectiveness)	Carbon emissions ÷ IT equipment energy	Assesses carbon footprint
Cooling Energy Reduction (%)	(Baseline cooling energy − Optimized cooling energy) ÷ Baseline cooling energy × 100	Quantifies energy savings
Thermal Prediction Accuracy (MAPE)	Mean absolute percentage error between predicted and actual temperatures	Evaluates AI forecasting performance
SLA Compliance (%)	% of time IT equipment operates within safe thermal thresholds	Ensures operational reliability

RESULT AND DISCUSSION

Experimental Results

The prototype was tested under three scenarios:

1. Baseline – Conventional data center operation without optimization.
2. Static Digital Twin – Digital twin used for monitoring and manual cooling adjustments.
3. AI-Driven Digital Twin – Fully integrated AI-based real-time optimization.

The experiments were conducted over a simulated 30-day operational period with identical workload patterns. Table 3 summarizes the performance metrics for each scenario.

Table 3. Performance Comparison Across Scenarios

Metric	Baseline	Static Digital Twin	AI-Driven Digital Twin
PUE	1.65	1.54	1.39
CUE ($kgCO_2/kWh$)	0.38	0.35	0.31
Cooling Energy Reduction (%)	–	6.7%	18.9%

Metric	Baseline	Static Digital Twin	AI-Driven Digital Twin
Thermal Prediction Accuracy (MAPE)	–	12.5%	3.8%
SLA Compliance (%)	98.5%	99.2%	99.7%

Cooling Energy Savings

The AI-driven digital twin achieved the highest cooling energy reduction of 18.9% compared to the baseline. This aligns with industry-reported benchmarks, such as Schneider Electric and Nvidia's real-world implementation, which achieved approximately 20% reduction in cooling energy demand. The static digital twin provided a modest 6.7% reduction, indicating that automation and predictive control are critical for unlocking substantial efficiency gains.

PUE and CUE Improvements

The AI-driven approach reduced the Power Usage Effectiveness (PUE) from 1.65 to 1.39, which is significant considering that even a 0.1 PUE improvement can translate into substantial annual cost and energy savings. Carbon Usage Effectiveness (CUE) also decreased from 0.38 to 0.31, reflecting the combined effect of reduced electricity demand and greener energy utilization.

Prediction Accuracy

The AI thermal prediction model achieved a Mean Absolute Percentage Error (MAPE) of 3.8%, significantly outperforming the static twin's manual adjustments, which relied on less precise estimations (MAPE = 12.5%). This accuracy enabled proactive adjustments to cooling systems, avoiding thermal hotspots and maintaining SLA compliance.

SLA Compliance

Operational reliability was maintained across all scenarios, with SLA compliance exceeding 98%. The AI-driven system achieved 99.7%, indicating that the optimization did not compromise uptime or thermal safety. This is critical for industry adoption, as energy savings must not come at the expense of service quality.

Discussion

The results demonstrate that AI-driven digital twin technology can significantly enhance energy efficiency in data centers compared to traditional and static monitoring approaches. The integration of AI enables continuous adaptation to real-time changes in workload and environmental conditions, maximizing cooling efficiency without manual intervention.

These findings support the growing body of research that emphasizes AI as a transformative element in sustainable IT infrastructure. They also align with broader industry goals, such as meeting net-zero carbon targets and complying with environmental regulations (e.g., EU energy efficiency directives).

Furthermore, the modular architecture proposed in this study ensures adaptability across different data center configurations, from hyperscale facilities to edge computing nodes. However, the study also highlights the importance of accurate sensor data and robust model training; inaccuracies at the data acquisition stage could undermine the benefits of the optimization process.

CONCLUSION

This study has demonstrated that integrating Artificial Intelligence (AI) into a digital twin framework can significantly enhance energy optimization in green data centers. Through simulation-based experimentation, the proposed AI-driven digital twin achieved:

1. 18.9% reduction in cooling energy consumption compared to baseline operation.
2. PUE improvement from 1.65 to 1.39 and CUE reduction from 0.38 to 0.31.
3. High thermal prediction accuracy (MAPE = 3.8%) enabling proactive cooling control.
4. SLA compliance exceeding 99%, ensuring no compromise in operational reliability.

These results align with leading industry benchmarks, validating that the proposed system can deliver measurable sustainability benefits without sacrificing performance. The modular design also ensures adaptability across various data center types, from hyperscale facilities to smaller edge computing environments.

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