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Computational Optimization of Phase Change Material Integration Using Machine Learning for Enhanced Building Heating Efficiency in Cold Climates

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Abstract

Phase Change Materials (PCMs) represent a transformative approach to improve the energy efficiency and thermal comfort of buildings during winter heating periods. While PCMs offer substantial latent heat storage capacity, their optimal integration and operation pose complex multidimensional challenges involving material properties, placement strategies, and dynamic control responses to weather and occupancy. This study presents an advanced computational framework that combines detailed building thermal simulation, machine learning surrogate modelling, evolutionary optimization, and predictive control techniques. We generate a diverse dataset encompassing multiple climatic conditions and PCM configurations via Energy Plus simulations. Subsequently, we train and validate data-driven machine learning models, including Random Forests and Gradient Boosting Machines, to accurately predict building heating load and indoor thermal comfort metrics. These surrogate models facilitate multi-objective genetic algorithm optimization, identifying PCM property and placement parameters that maximize energy savings and thermal stability. Moreover, reinforcement learning–inspired predictive controls adapt PCM charging and discharging schedules in real time based on forecasted environmental inputs and occupancy patterns. Experimental results demonstrate that the proposed approach achieves up to 40% energy savings and reduces thermal fluctuations by 70%, surpassing traditional design and control methods. This interdisciplinary research advances sustainable building technologies by integrating computational intelligence with material science for intelligent thermal energy management.

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1. Introduction

Heating energy consumption in buildings represents a significant portion of global energy use and related carbon emissions, particularly in cold climate regions with extended winter seasons. Innovative thermal management strategies are imperative to enhance building energy efficiency while ensuring occupant comfort. Phase Change Materials (PCMs) have gained attention as latent heat storage elements capable of absorbing, storing, and releasing substantial amounts of thermal energy during phase transitions, typically between solid and liquid states. This dynamic heat storage reduces the peak heating demand and smoothens indoor temperature variations, thereby offering the potential to significantly decrease energy use in heating applications.

Traditionally, PCM integration strategies in buildings have involved embedding these materials within walls, floors, or roofs to leverage their buffering capacity passively. The effective deployment of PCMs depends critically on selecting suitable melting temperatures, thicknesses,

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thermal properties, and deployment locations relative to climatic conditions and building usage patterns. However, manual configuration and experimentation are impractical given the multidimensionality and complexity of factors influencing PCM performance.

Computational methods offer pathways to explore large design spaces efficiently, predict performance under variable climate and operational conditions, and optimize system behaviour. Simulation environments such as Energy Plus enable detailed building thermal modelling including PCM effects, yet their extensive computational demands limit rapid iteration and optimization efforts. Machine learning (ML) techniques can model nonlinear complex relationships using simulation data and provide fast surrogate models to accelerate design space search and control.

This paper introduces a comprehensive computational framework that integrates thermal simulation, machine learning-based surrogate modelling, evolutionary multi-objective optimization, and data-driven predictive control to design and operate PCM-enhanced buildings for optimal winter heating efficiency. Our contributions include:

- Developing accurate ML surrogate models predicting heating loads and thermal stability metrics from PCM and environmental inputs.
- Implementing a genetic algorithm framework leveraging surrogate predictions to optimize PCM melting temperature, thickness, and location variables.
- Designing ML-driven predictive control that dynamically schedules PCM thermal charging and discharging in response to weather forecasts and occupancy patterns.
- Conducting extensive experiments across multiple cold climate scenarios, quantifying energy savings, thermal comfort improvements, and computational efficiency gains.

2. Literature Review

2.1 Phase Change Materials in Building Thermal Management

Phase Change Materials (PCMs) are widely studied for their ability to store and release latent heat, aiding in reducing peak heating loads and moderating indoor temperature swings [Alvarez et al., 2019; Sharma et al., 2020]. Recent advances in microencapsulation techniques and nano-enhancements have improved PCM thermal conductivity and durability [Wu et al., 2021; Singh et al., 2022]. Various implementation strategies include incorporation within wallboard materials, floors, roofs, and glazing systems, each with unique trade-offs [Zhao et al., 2018; Kumar and Singh, 2019]. Experimental and simulation studies demonstrate potential energy savings from 15% to over 40% depending on climate and integration details [Liu et al., 2020; Bavarian and Zanchini, 2020].

2.2 Computational Modelling and Simulation Tools

Energy Plus and TRNSYS remain the predominant simulation platforms for PCM performance assessment [Liu and Gou, 2020; He and Langensiepen, 2018]. Finite element and computational fluid dynamics (CFD) models extend insight into transient PCM behaviour [Gupta et al., 2019;

Tang et al., 2021]. However, their high computational cost restricts large parametric studies [Nguyen et al., 2020]. Reduced-order thermal models offer a faster alternative though often with reduced accuracy [Patil et al., 2021].

2.3 Machine Learning for Building Energy Applications

Machine learning has been increasingly applied to model and predict building thermal dynamics and energy consumption with high accuracy and low computational latency [Wang et al., 2020; Zhang et al., 2019]. Techniques such as Support Vector Regression, Random Forests, and deep neural networks capture nonlinear relationships between environmental variables and performance metrics [Chen et al., 2021; Li et al., 2022]. Hybrid physics-based and data-driven approaches provide robustness across varying scenarios [Mukherjee and Debnath, 2021].

2.4 Optimization Techniques in PCM Design

Mult objective optimization, particularly genetic algorithms and particle swarm optimization, have been applied to PCM design problems, balancing energy, cost, and occupant comfort [Jiang et al., 2019; Dhas et al., 2020]. Surrogate-assisted optimization reduces computational overhead by replacing full simulations with data-driven models [Banerjee and Biswas, 2021; Xu et al., 2020]. Recent studies integrate uncertainty quantification to address variability in climatic and occupancy conditions [Vega et al., 2022].

2.5 Data-Driven Control Strategies

Advanced control mechanisms employing reinforcement learning and predictive analytics maximize PCM benefits by actively adjusting thermal storage states [Singh et al., 2020; Patel et al., 2021]. These approaches improve system responsiveness and adaptivity beyond passive PCM operation, yielding additional energy savings and enhanced comfort [Choi and Kim, 2019].

2.6 Summary of Literature Gaps

While numerous studies address PCM properties, integration, and passive benefits, comprehensive data-driven optimization and intelligent control frameworks remain under-explored. Bridging physics-based models, surrogate ML predictors, and adaptive control represents a promising research frontier essential for practical PCM-enabled building solutions.

3. Methodology

3.1 Overview of Computational Framework

This research proposes a comprehensive computational approach integrating detailed physical simulations, machine learning (ML) models, multi-objective evolutionary optimization, and intelligent control strategies to optimize PCM integration in building envelopes for enhanced winter heating performance. The framework comprises four major modules:

1. **Data Generation:** Using Energy Plus simulations to generate high-fidelity data reflecting building performance across varied PCM properties and climate conditions.

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2. **Machine Learning Modelling:** Training and validating surrogate ML models to predict key performance indicators (KPIs) such as heating load and thermal comfort metrics, reducing reliance on computationally expensive simulations.
3. **Optimization Module:** Employing a genetic algorithm (GA) that utilizes the ML surrogate models to efficiently explore the design space and identify Pareto-optimal PCM configurations balancing energy savings and comfort.
4. **Predictive Control System:** Designing an ML-enabled real-time control strategy that dynamically manages the PCM charging and discharging schedule based on environmental forecasts and occupancy patterns.

3.2 Data Generation via Energy Plus Simulations

Energy Plus (Version 9.6) serves as the core simulation engine to model the heat transfer and energy balance of buildings equipped with PCM-enhanced components. The simulations are configured as follows:

- **Building Prototype:** A typical residential building with insulated walls, windows, floor, and roof, modelled according to ASHRAE standards.
- **PCM Variations:** Parameters varied include PCM melting temperature (18°C to 28°C), PCM layer thickness (10 mm to 50 mm), and placement location (wall, floor, roof).
- **Climate Profiles:** Weather data representing cold climates, specifically subarctic (e.g., Fairbanks, Alaska) and continental (e.g., Minneapolis, USA), with hourly temperature, solar radiation, and humidity inputs.
- **Simulation Outputs:** Hourly heating energy demands, indoor temperature profiles, and thermal comfort indices (PMV, PPD) over heating season.

An initial design of experiments (DOE) approach using Latin Hypercube Sampling generates ~500 diverse simulation scenarios covering the parametric space to construct a robust dataset.

3.3 Machine Learning Model Development

To overcome the computational bottleneck of repeated high-fidelity simulations during optimization, ML surrogate models are developed. The process entails:

- **Feature Engineering:** Inputs include PCM melting temperature, thickness, placement, outdoor temperature, solar irradiance, occupancy schedule, and time-of-day indicators.
- **Model Selection:** Three model families are evaluated—Random Forest Regression (RFR), Gradient Boosted Trees (GBT), and Feedforward Neural Networks (FNN).
- **Training and Validation:** The dataset is split into training (70%), validation (15%), and test (15%) subsets. Hyperparameter tuning employs grid search and cross-validation.
- **Performance Metrics:** Predictive accuracy is measured via root mean squared error (RMSE), mean absolute error (MAE), and coefficient of determination (R^2).

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The best-performing models are used as surrogates to predict heating load and thermal comfort metrics for new design points rapidly (~milliseconds per prediction).

3.4 Surrogate-Assisted Multi-Objective Genetic Algorithm Optimization

A non-dominated sorting genetic algorithm II (NSGA-II) framework drives the multi-objective optimization of PCM design parameters aiming to:

- **Objectives:**
    - Minimize annual heating energy consumption.
    - Minimize indoor temperature fluctuations during occupied periods (improving thermal comfort).
    - Minimize computational cost proxies related to PCM quantity and installation complexity.
- **Decision Variables:**
    - PCM melting temperature (continuous, 18-28°C).
    - PCM layer thickness (continuous, 10-50 mm).
    - PCM location (categorical: wall, floor, roof).
- **Constraints:** Compliance with building codes, feasibility of PCM layer thickness, and practical installation considerations.

Each candidate solution is evaluated using the ML surrogate models. The population is evolved over 100 generations with crossover, mutation, and elitism to approximate the Pareto front.

3.5 ML-Enabled Predictive Control Strategy

To further enhance energy savings and comfort, a data-driven control strategy manages the PCM thermal state dynamically:

- **Input Data:** Weather forecasts (temperature, solar radiation), occupancy schedules, and current indoor conditions.
- **Predictive Model:** A recurrent neural network (RNN) predicts short-term occupancy and temperature trends.
- **Control Algorithm:** An optimization-based controller, guided by reinforcement learning principles, determines optimal charging (heat storage) and discharging (heat release) times for PCM layers.
- **Actuation:** Communicates with building management systems to operate HVAC and thermal actuators, coordinating with PCM response characteristics.

This adaptive control aims to maximize PCM efficacy by pre-conditioning thermal storage before anticipated cold periods and utilizing stored heat efficiently.

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4. Experimental Setup and Results

4.1 Dataset and Simulation Environment

The computational experiments utilized the Energy Plus simulation platform integrated with custom Python scripts for automation. The residential building prototype comprised:

- Floor area: 150 m²
- Insulation: per ASHRAE 90.1 standards
- Windows: double glazed, U-value 1.2 W/m²K
- HVAC system: standard furnace with a coefficient of performance (COP) of 0.9

Two climate zones formed the basis of climate scenarios:

- Fairbanks, Alaska (subarctic, ~6700 heating degree days)
- Minneapolis, USA (cold continental, ~4400 heating degree days)

The heating season was defined from October 1 to April 30, with hourly meteorological inputs sourced from Typical Meteorological Year (TMY3) data.

The PCM properties were varied across:

- Melting temperature: 18°C – 28°C
- Thickness: 10 mm – 50 mm
- Locations: wall, floor, roof

A dataset of 500 parametrized simulations was generated to train the ML models.

4.2 Performance Metrics

The effectiveness of PCM integration was evaluated using:

- **Annual heating demand (kWh/year):** total energy required to maintain occupant comfort.
- **Temperature standard deviation (°C):** fluctuations in temperature during occupied hours, indicating comfort stability.
- **Predicted Mean Vote (PMV):** average thermal sensation index.
- **Predicted Percentage Dissatisfied (PPD):** percentage of occupants likely to feel uncomfortable.

Computational efficiency of ML surrogate models was measured by prediction latency and scalability.

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4.3 Machine Learning Model Performance

Multiple ML models were trained and their results compared:

Model	RMSE (kWh)	MAE (kWh)	R²	Prediction Time (ms)
Random Forest	230	180	0.94	2
Gradient Boosting	210	165	0.96	4
Neural Network	250	195	0.92	3

The Gradient Boosting model exhibited the best balance between accuracy and speed and was selected for surrogate predictions during optimization.

4.4 Optimization Results

The NSGA-II algorithm was run with a population size of 100 over 100 generations, amounting to approximately 10,000 evaluations accelerated by the surrogate model.

Key insights from the Pareto front:

- **Optimal melting temperature:** 20°C to 25°C for wall integration, 22°C to 28°C for floor.
- **Thickness trade-off:** higher thickness (>40 mm) increased storage but at diminishing returns due to cost and installation complexity.
- **Location preference:** floor integration yielded highest energy savings (up to 40%), followed by walls and roofs.
- **Energy savings:** averaged 35% reduction compared to baseline on all optimized solutions.
- **Thermal stability:** temperature standard deviation decreased by over 65%, indicating improved comfort.

Selected Pareto solutions demonstrated excellent compromises between the multiple objectives, enabling flexibility for stakeholders.

4.5 Predictive Control Evaluation

Employing the ML-based predictive controller, simulations showed:

- Reduction in peak heating demand up to 12%
- Further decrease in indoor temperature fluctuations by 7%

- Adaptive charging ahead of cold spells enhanced PCM effectiveness

Control strategies dynamically modified thermal energy storage, capitalizing on pre-heating opportunities during solar gain periods.

4.6 Computational Efficiency

The surrogate-assisted optimization reduced computational time dramatically:

- Original simulation time per scenario: ~10–15 minutes
- Surrogate model prediction time per scenario: <5 ms
- Overall optimization runtime reduced from months to hours

This efficiency positions the framework for real-time application and iterative design processes.

5. Discussion

5.1 Advantages of the Proposed Approach

This study demonstrates that integrating machine learning within a computational optimization framework substantially enhances the design and operation of PCM-based thermal management in buildings. Key advantages include:

- **Accelerated Optimization:** Surrogate models trained on simulation data enable rapid evaluation of candidate designs, reducing computational costs from hours to milliseconds per evaluation.
- **Improved Multi objective Trade-offs:** The use of a genetic algorithm with accurate surrogate models allows simultaneous optimization of energy consumption, thermal comfort, and economic factors, providing a Pareto front for informed decision-making tailored to stakeholder priorities.
- **Adaptive and Intelligent Control:** The incorporation of predictive ML-based control strategies dynamically improves system responsiveness to environmental variability and occupant needs, outperforming passive PCM management.
- **Scalability and Generalization:** The framework accommodates varying climatic conditions and building types, showing promise for scalable deployment in diverse geographic regions.

5.2 Limitations and Challenges

- **Model Generalization:** While surrogate models demonstrated excellent accuracy within the training domain, extrapolation beyond sampled input ranges may reduce reliability. Periodic retraining with new data is essential for robustness.

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- **Data Acquisition Burden:** Generating comprehensive simulation datasets or real-world measurements requires significant computational or experimental effort.

- **Control System Complexity:** Implementing ML-driven control in existing building management systems demands integration of sensors, forecasting modules, and communication infrastructure.

- **Uncertainty Modelling:** Future work must incorporate uncertainties in weather predictions, occupancy behaviour, and material degradation to ensure resilient system performance.

5.3 Future Research Directions

- **Hybrid Physics-ML Models:** Combining mechanistic and data-driven models may enhance interpretation and improve confidence in unexplored scenarios.

- **Real-time Adaptive Learning:** Online learning algorithms can continuously update surrogate and control models based on live sensor data.

- **Multi-modal Energy Systems:** Integration with solar PV, battery storage, and other renewable systems warrants exploration.

- **Human-Centric Models:** Incorporating occupant feedback and adaptive comfort models would increase practical relevance.

6. Conclusion

This paper presents a novel computational framework leveraging machine learning to optimize Phase Change Material integration in building envelopes for enhanced heating efficiency in cold climates. By constructing accurate surrogate models from detailed simulations, we enable efficient Multi objective optimization across PCM design parameters. Coupling these designs with intelligent ML-based control strategies further advances thermal management efficacy, achieving up to 40% energy savings and superior occupant comfort.

The approach represents a significant stride toward data-driven sustainable building design, combining thermal physics, optimization algorithms, and artificial intelligence to deliver adaptable, high-performance solutions. Future enhancements incorporating uncertainty quantification, continuous learning, and multi-energy integration will expand applicability and impact.

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