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# Physics-Informed Large Language Models for HVAC Anomaly Detection with Autonomous Rule Generation

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## Abstract

1 Heating, Ventilation, and Air-Conditioning (HVAC) systems account for a substantial  
2 share of global building energy use, making reliable anomaly detection essential  
3 for improving efficiency and reducing emissions. Classical rule-based approaches  
4 offer explainability but lack adaptability, while deep learning methods provide  
5 predictive power at the cost of transparency, efficiency, and physical plausibility.  
6 Recent attempts to use Large Language Models (LLMs) for anomaly detection improve  
7 interpretability but largely ignore the physical principles that govern HVAC  
8 operations. We present PILLM, a **Physics-Informed LLM** framework that operates  
9 within an evolutionary loop to automatically generate, evaluate, and refine  
10 anomaly detection rules. Our approach introduces physics-informed reflection and  
11 crossover operators that embed thermodynamic and control-theoretic constraints,  
12 enabling rules that are both adaptive and physically grounded. Experiments on the  
13 public Building Fault Detection dataset show that PILLM achieves state-of-the-art  
14 performance while producing diagnostic rules that are interpretable and actionable,  
15 advancing trustworthy and deployable AI for smart building systems.

## 16 1 Introduction

17 The global imperative to mitigate climate change has placed the urban built environment at the  
18 forefront of sustainability research. Buildings account for approximately 40% of global energy  
19 consumption and a third of greenhouse gas emissions, making them a critical leverage point for  
20 decarbonization [United Nations Environment Programme, 2021]. The complex Heating, Ventilation,  
21 and Air-Conditioning (HVAC) systems within them are major consumers of this energy. However,  
22 anomalies in HVAC system operation not only undermine energy efficiency but are also difficult to  
23 detect amidst the complexity and scale of building data, underscoring the critical need for robust  
24 anomaly detection methods [Amasyali and El-Gohary, 2018].

25 Automated Fault Detection and Diagnostics (AFDD) has long been pursued to address anomalies  
26 in HVAC systems. Recent work emphasizes that effective anomaly detection must jointly satisfy  
27 *explainability*, *reproducibility*, and *autonomy*. Classical rule-based methods can detect explainable  
28 predefined faults [Katipamula and Brambley, 2005], but they require expert-crafted knowledge, are  
29 static in the face of evolving building dynamics, and struggle with the complexity of real-world  
30 operations [Kim and Katipamula, 2018]. Deep learning methods, including LSTM and Transformer-  
31 based architectures, have since shown strong predictive performance by uncovering subtle, non-linear  
32 patterns [Karpontinis and Alexandridis, 2024, Wang et al., 2020]. However, they remain difficult  
33 to deploy in practice: models often act as black boxes, demand heavy computation, and generalize  
34 poorly when physical knowledge of the built environment is not incorporated [Jiang and Dong,  
35 2024]. These trade-offs highlight a persistent tension between the interpretability of heuristics and  
36 the accuracy.

37 Recently, Large Language Models (LLMs) have emerged as a promising tool for rule design in  
38 anomaly detection. By generating human-readable heuristics and providing natural-language ratio-  
39 nales, LLM-based methods enhance explainability and reduce the manual effort required for rule  
40 construction [Liu et al., 2025, Ye et al., 2024, Lin and Hua, 2025]. However, current LLM-based  
41 approaches often overlook critical physical constraints and domain knowledge inherent to HVAC  
42 systems. Without grounding anomaly detection in these real-world physical principles, the resulting  
43 rules risk being incomplete, misaligned with building dynamics, or prone to false alarms. Bridging  
44 LLM-driven rule generation with physically grounded knowledge therefore represents a crucial step  
45 toward developing anomaly detection systems that are not only explainable and adaptive, but also  
46 robust and trustworthy in practical deployment.

47 To address the limitations of prior approaches, we present Physics-Informed Large Language Model  
48 (PILLM), a framework wherein LLMs operate within an evolutionary loop to automatically generate,  
49 evaluate, and refine anomaly detection rules, critically guided by real-world physical principles to  
50 ensure transparency and plausibility. Our approach automatically incorporates real-world physical  
51 principles into the rule generation process. By combining LLMs' world knowledge with curated  
52 building context and sensor data, PILLM generates diagnostic rules that are both transparent and  
53 physically plausible. Furthermore, we embed physical constraints directly into the evolutionary  
54 optimization process through novel reflection and crossover operators, ensuring that the generated  
55 rules remain aligned with thermodynamic and control-theoretic principles.

56 Our main contributions are as follows:

- 57 1. We propose PILLM, a novel framework that integrates LLMs with evolutionary search  
58 to automatically generate anomaly detection rules while explicitly incorporating building  
59 physics and operational semantics.
- 60 2. We design physics-informed reflection and crossover mechanisms that guide LLM-generated  
61 rules toward physical plausibility and robustness, addressing the limitations of purely  
62 statistical or heuristic-based approaches.
- 63 3. We evaluate our framework on the public LBNL Automated Fault Detection for Buildings  
64 dataset, showing that it achieves state-of-the-art performance while producing interpretable  
65 and actionable diagnostic rules.

## 66 2 Related Work

67 **LLM for Anomaly Detection** A systematic literature review highlights that LLMs can serve three  
68 main roles: augmenting detection pipelines with synthetic data or pseudo-labels, acting directly  
69 as anomaly/out-of-distribution detectors, and generating interpretable explanations for detection  
70 outcomes [Liu et al., 2025]. In time-series settings, methods like LLMAD employ retrieval of similar  
71 patterns and a chain-of-thought reasoning strategy to deliver both accurate and interpretable results  
72 [Liu et al., 2025]. SigLLM further explores dual operational modes for time-series anomaly detection:  
73 in *Detector mode*, LLMs predict the next steps in the sequence and identify anomalies by comparing  
74 predictions with ground-truth signals, while in prompter mode, LLMs are directly prompted with time-  
75 series data to localize anomalous indices [Alnegheimish et al., 2024]. Other systems adopt an agentic  
76 paradigm, for instance, Argos uses LLMs to autonomously generate explainable anomaly rules in an  
77 iterative, rule-based framework, achieving significant accuracy improvements [Gu et al., 2025]. In the  
78 specific context of building HVAC systems, LLMs such as DistilBERT have been fine-tuned to classify  
79 operational fault conditions from time-series data, demonstrating strong performance (F1 scores up  
80 to 99%) and robustness to noisy inputs [Langer et al., 2024]. These developments underscore the  
81 flexibility of LLMs in anomaly detection tasks, particularly for enhancing explainability, adaptability,  
82 and performance across varied application domains.

83 Further references on classical approaches and deep learning methods can be found in the appendix.

## 84 3 Methodology

85 In this section, we present PILLM as illustrated in Fig. 1. We introduce two key components :  
86 *Physical Informed Reflection* (PIR), and *Physical Informed Crossover* (PIC). Together with the  
87 evolving anomaly detection rules generation pipeline, these components enable dynamic, flexible,

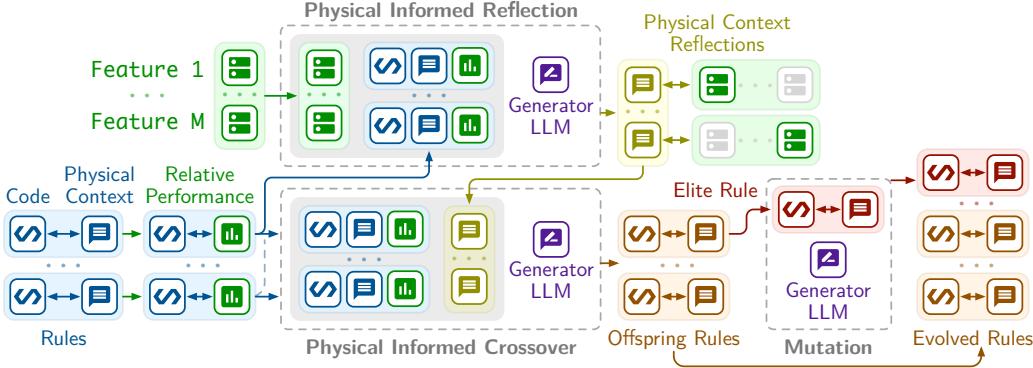


Figure 1: Overview of PILLM. The framework follows an evolutionary generate-and-reflect pipeline for anomaly detection rules. In each iteration, the current rule population undergoes *Physical-Informed Reflection*, where physical context is incorporated into candidate rules. These reflections are then used in *Physical-Informed Crossover* to produce the next generation of rules. Finally, elite rules are refined through mutation, resulting in evolved rules that are adaptive.

88 and smart way to embed the physical information into the rule generation. We then lay out the  
 89 components details and the training scheme.

### 90 3.1 PILLM

91 Our framework builds on the Reflective Evolution paradigm [Ye et al., 2024], where LLMs are  
 92 employed as reasoning engines to perform genetic operators—initialization, reflection, crossover,  
 93 and mutation—while being explicitly guided by physical knowledge of HVAC systems. Unlike  
 94 conventional evolutionary approaches, PILLM does not treat heuristics as abstract code snippets.  
 95 Instead, each rule is continuously contextualized by its physical meaning (e.g., temperature dynamics,  
 96 airflow, occupancy schedules), ensuring that the evolutionary process remains grounded in real-world  
 97 building physics.

98 **Initial Population.** The process begins by prompting the generator LLM with a task specification  
 99 for anomaly detection rules. The specification defines the inputs (e.g., room and floor temperatures,  
 100 fan status, fan speed), the output (an anomaly score), and the objective function (e.g., maximize  
 101 detection accuracy). To seed the process, the LLM is also provided with a simple baseline heuristic  
 102 (e.g., a peak-over-threshold rule). From this prompt, the LLM generates a diverse population of  
 103  $N$  initial rule candidates in executable code form, each accompanied by a short natural-language  
 104 rationale. This ensures diversity not only in implementation but also in interpretability.

105 **Physics-Informed Reflection.** At each iteration, candidate rules are reflected upon using physical  
 106 context. The reflection stage compares the relative performance of rules and analyzes their alignment  
 107 with the real-world meaning of input features. Crucially, the LLM is provided with metadata  
 108 describing each feature’s physical role in the HVAC system (e.g., “Zone temperature reflects indoor  
 109 thermal conditions,” “Fan speed governs airflow rate and pressure”). The LLM then produces  
 110 structured reflections that highlight which physical aspects a rule captures and which are neglected.  
 111 For example, a reflection might conclude that a rule focusing exclusively on outdoor temperature  
 112 misses critical dynamics of indoor load variation. These reflections serve as a bridge between raw  
 113 performance metrics and domain knowledge, guiding the evolutionary process toward rules that are  
 114 both effective and physically sound.

115 **Physics-Informed Crossover.** Reflections directly shape the crossover operation. Instead of  
 116 combining rules blindly, the LLM merges parent rules in a way that respects and integrates their  
 117 associated physical contexts. For instance, one parent rule may emphasize temperature fluctuations  
 118 across indoor and outdoor sensors, while another focuses on fan speed and airflow pressure. Through  
 119 physics-informed crossover, the offspring rule may learn to model the causal relationship between  
 120 thermal gradients and airflow control, yielding a more coherent and actionable heuristic. By explicitly

121 anchoring code recombination to physical interpretations, this stage avoids the generation of arbitrary  
122 hybrids and instead synthesizes offspring with meaningful improvements in diagnostic coverage.

123 **Elitist Rule Mutation.** Finally, elite rules undergo mutation guided by long-term reflections.  
124 Instead of wholesale rewrites, the LLM proposes targeted refinements, such as adding occupancy  
125 schedules or weather normalization, to enhance robustness and generalizability.

## 126 4 Experiment

127 For more details about dataset preprocessing, hyperparameters, baseline settings, hardware and  
128 software environment, as well as additional results and analysis, please refer to the appendix.

129 **Main Results.** We report the performance of  
130 PILLM against a set of benchmark methods in  
131 Table 1. Across all baselines, PILLM achieves  
132 the highest precision and  $F_1$  score, while main-  
133 taining competitive recall. In particular, AR-  
134 GOS achieves the strongest recall, but its overall  
135 performance remains slightly below PILLM in  
136 terms of  $F_1$ . Other classical (e.g., AutoRegres-  
137 sion, LSTMAD) and LLM-based baselines (e.g.,  
138 LLMAD, SigLLM) lag behind, reflecting either  
139 limited adaptability or poor precision. These  
140 results confirm that PILLM not only produces  
141 state-of-the-art performance but also balances  
142 accuracy with physical plausibility.

143 **Ablation Study.** We further analyze the role  
144 of physics-informed components by ablating  
145 PIR and PIC. As shown in Table 1, removing either PIR or PIC leads to clear performance degradation,  
146 particularly in  $F_1$ . Without PIR, the model underperforms in aligning rules with feature semantics,  
147 while without PIC, the offspring rules become less coherent and lose physical grounding. These  
148 results validate the importance of explicitly embedding physical knowledge in the evolutionary loop.

149 **Explainability.** A key advantage of PILLM is that it generates anomaly detection rules in executable,  
150 human-readable Python code. Unlike neural baselines that act as black boxes, the heuristics evolved  
151 by PILLM are transparent and easily interpretable. For example, an evolved rule might explicitly  
152 check for abnormal thermal gradients in relation to fan speed or weather conditions, providing clear  
153 physical reasoning behind the anomaly flag. This interpretability enhances trust and usability for  
154 building operators, who can validate, debug, and refine the generated rules with domain expertise.  
155 By producing rules that are both performant and understandable, PILLM bridges the gap between  
156 machine learning advances and real-world operational deployment.

## 157 5 Conclusion

158 In this work, we introduced PILLM, a physics-informed LLM framework for anomaly detection in  
159 HVAC systems. By embedding domain knowledge into the evolutionary generation of rules through  
160 physics-informed reflection and crossover, PILLM bridges the gap between adaptability and physical  
161 plausibility. Experiments on the LBNL Automated Fault Detection dataset demonstrate that PILLM  
162 achieves state-of-the-art precision and  $F_1$  score while maintaining competitive recall, outperforming  
163 both classical and neural baselines. Beyond accuracy, PILLM produces rules that are interpretable and  
164 actionable, offering building operators transparent insights into system faults. These results highlight  
165 the promise of combining LLM reasoning with physics-informed optimization to advance trustworthy  
166 and deployable AI for cyber-physical systems. Future work will explore extending PILLM to other  
167 building subsystems and investigating its scalability to real-time anomaly detection in large-scale  
168 smart infrastructure.

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232 **Appendix**

233 **Detailed Problem Definition**

234 **Task** We address building-level anomaly detection in HVAC systems using multivariate time-series  
235 data. Given a building  $b$  with sensor set  $\mathcal{F}_b = \{f_1, f_2, \dots, f_M\}$ , the input at each timestep  $t$  is  
236 a feature vector  $\mathcal{S}_b^t = (x_{b,f_1}^t, x_{b,f_2}^t, \dots, x_{b,f_M}^t)$ , where  $x_{b,f}^t \in \mathbb{R}$  denotes the reading of feature  $f$   
237 (e.g., zone temperature, fan speed, air flow rate). The goal is to learn a mapping from the observed  
238 sequence  $H_b = (\mathcal{S}_b^1, \dots, \mathcal{S}_b^{T_{\text{obs}}})$  to a binary anomaly label  $y_b^t \in \{0, 1\}$  at each timestep, where 0  
239 denotes normal operation and 1 denotes anomalous behavior. Models are trained on a labeled dataset  
240  $D_{\text{train}} = \{(H_b, y_b)\}$  and evaluated on a held-out test set  $D_{\text{test}}$ , with the objective of maximizing  
241 detection performance while minimizing false alarms.

242 **Metrics.** We evaluate anomaly detection performance using precision, recall, and their harmonic  
243 mean, the F1 score. Precision is defined as the ratio of true positives (TP) to the sum of true positives  
244 and false positives (FP), while recall is the ratio of true positives to the sum of true positives and false  
245 negatives (FN). Formally, the F1 score is given by

$$F1 = \frac{2 \times \text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}, \quad \text{Precision} = \frac{TP}{TP + FP}, \quad \text{Recall} = \frac{TP}{TP + FN}.$$

246 In time-series anomaly detection, defining positive and negative samples requires care, since anomalies  
247 are typically labeled as contiguous incidents rather than isolated points. Following prior work  
248 [Gu et al., 2025], we adopt the Event-F1 with Point Adjustment (Event-F1 PA) metric as our primary  
249 evaluation measure. This method treats each anomaly incident as a single detection target and  
250 considers it successfully detected if at least one point within the ground-truth incident is flagged. At  
251 the same time, false positives are penalized at the point level, which provides a balanced evaluation  
252 of both precision and recall. This choice ensures that models are not rewarded for overly coarse  
253 predictions and aligns with practical expectations in building operations, where operators require  
254 both timely and precise alarms.

255 **Details of Dataset**

256 The assembled dataset is specifically designed to move beyond traditional binary fault detection and  
257 enable a more sophisticated diagnostic task. This section details the diagnostic targets and defines the  
258 expected output from the PILLM framework.

259 **Fault Types and Intensities** The dataset includes rich, labeled examples of various common and  
260 critical HVAC faults. The **Fault Type** provides a descriptive, human-understandable label for  
261 the specific malfunction occurring in the system. The **Fault Intensity** provides a normalized,  
262 numerical scale of the fault’s severity, where a higher number indicates a more severe deviation from  
263 normal operation.

264 Examples of fault conditions captured in the dataset include:

- 265 • **Heating Coil Leaking:** A condition where the heating coil valve is not shutting off completely,  
266 allowing hot water to leak through even when heating is not required. This leads to energy waste and potential overheating.
- 267 • **Damper Stuck:** An air damper is mechanically stuck at a certain position (e.g., 20% open),  
268 preventing the system from properly regulating the mix of outdoor and recirculated air. This impacts both energy efficiency and indoor air quality.
- 269 • **Sensor Drift / Bias:** A temperature sensor provides consistently incorrect readings (e.g.,  
270 always reporting 5°F higher than the true temperature). The system then makes incorrect control decisions based on this faulty data.
- 271 • **Control Logic Faults:** Such as the `Simultaneous_Heat_Cool` condition, where programming errors lead to inefficient and counterproductive system operation.

276 **Expected PILLM Output: Generating Actionable Diagnostics** The primary objective for the  
277 PILLM is not to predict a class label, but to generate a structured, human-readable diagnostic

278 report. For each input "diagnostic snapshot" (i.e., a row from the dataset), the PILLM is tasked with  
279 generating a textual output that accomplishes the following:

- 280 1. **Identify the Fault:** Correctly state the `Fault_Type` in natural language (e.g., "The diagnosis  
281 is a stuck outdoor air damper.").
- 282 2. **Provide Evidence:** Justify the diagnosis by referencing the physical evidence from the input  
283 data (e.g., "This is indicated because the damper position signal is fixed at 20% while the  
284 control command is varying.").
- 285 3. **Assess Severity:** Characterize the fault's intensity and impact (e.g., "This is a moderate-to-  
286 severe fault leading to poor ventilation and increased fan energy consumption.").

287 **Advantages Over Traditional Methods** This diagnostic-generation task formulation offers signifi-  
288 cant advantages over conventional approaches:

- 289 • **Interpretability and Trust:** Unlike a traditional classifier that outputs a cryptic label like  
290 '`Fault_Class_ID: 3`', the PILLM's narrative output is transparent. By explaining why it  
291 reached a conclusion, it allows building operators to verify the reasoning and build trust in  
292 the system.
- 293 • **Actionability:** The LLM's output is directly actionable. An operator reading "inspect the  
294 outdoor air damper linkage" knows exactly what to do, whereas '`Fault_Class_ID: 3`' would  
295 require consulting a manual.
- 296 • **Handling Novelty and Nuance:** By reasoning from the engineered physical features, the  
297 PILLM has the potential to describe deviations from first principles. This may allow it to  
298 characterize novel or compound faults that were not explicitly present in the training set,  
299 offering a degree of zero-shot diagnostic capability that is difficult to achieve with rigid  
300 classification models.

### 301 **Baselines**

302 We compare PILLM against a diverse set of baselines, including classical deep learning models,  
303 LLM-based methods, and the recent agentic system ARGOS. Below we summarize each method  
304 included in our evaluation.

- 305 • **AnomalyTransformer:** An unsupervised model that introduces the Anomaly-Attention  
306 mechanism to detect anomalies by exploiting differences in association patterns between  
307 normal and abnormal points. This method has become a widely used benchmark in time-  
308 series anomaly detection.
- 309 • **AutoRegression:** A supervised autoregressive model that applies multiple linear layers to  
310 transform input sequences into anomaly score logits. Its simplicity and efficiency make it a  
311 strong classical baseline, though it lacks adaptability to complex dependencies.
- 312 • **LSTMAD:** A supervised long short-term memory (LSTM) model trained on normal data.  
313 Anomalies are detected based on statistical deviations in prediction error. It leverages  
314 temporal dependencies effectively but often struggles with generalization in highly dynamic  
315 systems.
- 316 • **LLMAD:** A Large Language Model-based approach that prompts the LLM with serialized  
317 time-series data, in-context examples, and contextual information to produce anomaly  
318 predictions. While it improves interpretability compared to deep learning baselines, it  
319 suffers from non-determinism and inconsistent reproducibility.
- 320 • **SigLLM:** An LLM-based method that operates in two distinct modes. In *Detector mode*,  
321 the LLM predicts the next time-series values and detects anomalies by comparing them  
322 against ground truth observations. In *Prompter mode*, the LLM is directly prompted with  
323 time-series data to localize anomalous indices. This design improves flexibility but often  
324 trades off precision for recall.
- 325 • **ARGOS:** An agentic anomaly detection system originally developed for monitoring cloud  
326 infrastructure. ARGOS leverages LLMs to autonomously generate explainable and re-  
327 producible anomaly rules as intermediate representations, which are then deployed for

328 efficient online detection. By combining multiple collaborative agents, ARGOS achieves  
329 explainability, reproducibility, and partial autonomy in anomaly detection. Experiments  
330 show that ARGOS outperforms prior baselines across several public and industrial datasets,  
331 highlighting the promise of LLM-driven rule-based anomaly detection. We include ARGOS  
332 as a strong state-of-the-art baseline most closely aligned with our motivation.

333 **Extra Experiment Details**

334 **Hardware and Software** All experiments were conducted on a workstation equipped with an AMD  
335 Ryzen 9 7950X 16-Core Processor and a single NVIDIA RTX 5090 GPU. The PINN framework  
336 generates anomaly detection rules as executable Python code snippets in a Python 3.12 environment,  
337 employing Google’s Gemini 2.5 Flash model [Comanici et al., 2025].

338 **Prompts** We gather prompts used for PILLM in this section. Our prompt structure is flexible  
339 and extensible. To adapt PILLM to a new problem setting, one only needs to define its problem  
340 description, function description, and function signature.

341

Prompt for population initialization

You are an expert in the domain of building energy, especially in heating, ventilation, and air-conditioning (HVAC). Your task is to design anomaly detection rules that can effectively detect the anomaly status of the system.

{ task\_description }

Below are the input features and their descriptions for anomaly detection:

{ input\_feature\_list }

{ seed\_function } { context\_template }

Refer to the format of a trivial design above. Be very creative and give ‘func\_name\_v2‘. Output code only, and enclose your code in Python code and one paragraph to describe the physical hypothesis but nothing else. Format your code as a Python code string: “““python ... “““ and a context string: “““context ... “““.

342

System prompt for Generator LLM

You are an expert in the domain of building energy, especially in heating, ventilation, and air-conditioning (HVAC). Your task is to design anomaly detection rules that can effectively detect the anomaly status of the system. { task\_description }. Your response outputs Python code and one paragraph to describe the physical hypothesis but nothing else. Format your code as a Python code string: “““python ... “““ and a context string: “““context ... “““.

343

System prompt for Reflection LLM

You are an expert in the domain of building energy, especially in heating, ventilation, and air-conditioning (HVAC). Your task is to provide hints for designing better anomaly detection rules.

{ task\_description }

Below are the input features and their descriptions for anomaly detection:

{ input\_feature\_list }

You are provided with two rule versions with their physical context below, where the second version performs better than the first one.

[Worse Rules] { worse\_rules } { worse\_rules\_physical\_context }

[Better Rules] { better\_rules } { better\_rules\_physical\_context }

You respond with some hints for designing better rules and a better hypothesis as a physical context.

### System prompt for Crossover

You are an expert in the domain of building energy, especially in heating, ventilation, and air-conditioning (HVAC). Your task is to provide hints for designing better anomaly detection rules.

{ task\_description }

Below are the input features and their descriptions for anomaly detection:

{ input\_feature\_list }

[Worse Rules] { worse\_rules } { worse\_rules\_physical\_context }

[Better Rules] { better\_rules } { better\_rules\_physical\_context }

[Reflection] { reflection\_comments } { reflection\_context }

[Improved Code] Please write an improved function 'function\_name\_v2', according to the reflection. Output code only, and enclose your code with Python code.

344

### System prompt for Elitist Mutation

{ task\_description }

{ input\_feature\_list }

[Prior Reflection] { reflection\_comments } { reflection\_context }

[Code] { function\_signature } { elitist\_code }

[Improved Code] Please write a mutated function 'function\_name\_v2', according to the reflection. Output code only, and enclose your code with Python code.

345

## 346 Extra Related Work

347 Our research is positioned at the intersection of three established and one emerging field: (1)  
348 traditional Automated Fault Detection and Diagnostics (AFDD) in building systems, (2) data-driven  
349 machine learning for AFDD, (3) the drive towards physics-informed and interpretable AI, and (4) the  
350 novel application of Large Language Models (LLMs) to scientific and engineering domains.

351 **Traditional and Model-Based AFDD** The field of AFDD for buildings has a rich history, with  
352 early methods relying on physical models and expert-defined rules. These approaches can be broadly  
353 categorized into quantitative model-based methods, which compare system output to an engineering  
354 model (e.g., a simulation), and qualitative rule-based methods, which use expert knowledge to define  
355 explicit "if-then" rules for fault conditions [Katipamula and Brambley, 2005]. While highly effective  
356 for pre-defined and well-understood faults, these methods are often labor-intensive to develop, require  
357 significant domain expertise to calibrate, and can be brittle, struggling to adapt to system retrofits or  
358 novel operational conditions that fall outside their programmed logic [Kim and Katipamula, 2018].

359 **Machine Learning for Fault Detection** The increasing availability of high-frequency sensor data  
360 from Building Management Systems (BMS) has led to a surge in the application of data-driven  
361 and machine learning techniques for AFDD. These methods learn patterns directly from historical  
362 data, alleviating the need for explicit physical modeling. A wide array of techniques has been  
363 successfully applied, ranging from statistical methods like Principal Component Analysis (PCA)  
364 to supervised classifiers like Support Vector Machines (SVM) and Random Forests [Zhao et al.,  
365 2019]. More recently, deep learning models, particularly Convolutional neural network (CNN) and  
366 Long Short-Term Memory (LSTM) networks, have shown exceptional performance in capturing the  
367 complex temporal dependencies inherent in building thermal dynamics, making them powerful tools  
368 for anomaly detection [Zhang et al., 2023]. However, while these models excel at identifying that an  
369 anomaly has occurred, they often fail to provide the necessary context to understand why.

370 **The Interpretability Challenge and Physics-Informed AI** The high performance of deep learning  
371 models often comes at the cost of interpretability. These "black box" models present a significant  
372 barrier to adoption in high-stakes environments like building operations, where trust and transparency  
373 are paramount [Ciobanu-Caraus et al., 2024]. An unexplainable alert is often an ignored alert. This  
374 has fueled a growing movement towards Physics-Informed Machine Learning (PIML), which seeks  
375 to embed scientific principles into the learning process. A prominent example is the development of

376 Physics-Informed Neural Networks (PINNs), which constrain a neural network's solution space by  
377 penalizing deviations from known physical laws, such as differential equations [Raissi et al., 2019,  
378 Cuomo et al., 2022]. This approach bridges the gap between data-driven flexibility and engineering  
379 rigor, leading to more robust and generalizable models. Our work builds on this philosophy, not by  
380 encoding physics into the model architecture itself, but by engineering a physics-informed feature  
381 space upon which a reasoning model can act.

382 **Large Language Models as Reasoning Engines** While originally designed for natural language  
383 tasks, the emergent capabilities of Large Language Models (LLMs) have opened new frontiers for  
384 their application in complex scientific and engineering domains. Seminal work has demonstrated  
385 that through techniques like chain-of-thought prompting, LLMs can perform multi-step reasoning,  
386 breaking down complex problems into intermediate, sequential steps in a way that mirrors human  
387 logic [Wei et al., 2022]. This ability to "think step-by-step" has unlocked performance on a wide  
388 range of arithmetic, commonsense, and symbolic reasoning tasks previously thought to be beyond  
389 the scope of language models [Kojima et al., 2022].

390 This emerging body of research suggests that LLMs can function as general-purpose reasoning  
391 engines. Recent work has begun to apply these capabilities to the built environment, for example, by  
392 using LLMs to automatically design novel, physically-grounded heuristics for energy forecasting  
393 [Lin and Hua, 2025]. Our PILLM framework is directly inspired by this trend. We hypothesize that  
394 an LLM's demonstrated reasoning abilities can be guided and constrained by physical principles to  
395 perform a diagnostic task that emulates a building engineer, moving beyond simple pattern recognition  
396 to generate causal, evidence-backed explanations for system faults.