Digital Twins For Urban Mitigation: Modelling City-Wide Carbon Neutrality Scenarios Via High-Performance Computing (HPC)

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Abstract: This paper presents a comprehensive framework for the context of integrating urban digital twins with the high-performance computing (HPC) to model, analyse, as well as accelerate pathways to city-wide carbon neutrality. Urban abstract simulations consist of digital twins of cities integrating heterogenous streams of data, physical models, and machine learning surrogates to simulate the behaviour and conditions of cities both spatially and temporally. HPC provides computational envelope capable of executing detailed building energy modelling, transport systems modelling, renewable generation modelling and coupled atmosphere-urban microclimate modelling both at city scale and at a temporal scale suitable to do sound policy analysis. The modular digital twin system comprises a system of interaction between building energy simulation and urban mobility models and distributed energy resource (DER) models and an urban carbon scoring engine. Its structure experiences HPC in order to compute a great number of scenarios in order to measure uncertainty and apply multi-objective analysis with the aim of minimizing emissions, costs and resilience. To explain the approach, a case study of synthetic city is conducted, and sensitivity experiments of electrification, deep retrofit, distributed photovoltaics, storage, and demand response portfolios is carried. Results quantify trade-offs between decarbonization rate, cost of energy, and stressors resilience and show that HPC-based digital twin's communities can be used to discover near-Pareto-optimal trade-offs in the presence of epistemic and aleatory uncertainty. The last point is on the implementation problems, data handlings and research plans to operationalize the city digital twins as a decision support system to simplify into carbon neutral city.

Keywords: *Digital twin; Urban decarbonization; Carbon neutrality; High-performance computing; City digital twin; Urban energy systems.*

How to cite this article: Patil NM, Maram B. Digital Twins For Urban Mitigation: Modelling City-Wide Carbon Neutrality Scenarios Via High-Performance Computing (HPC). Int J Drug Deliv Technol. 2026;16(6s): 833-844; DOI: 10.25258/ijddt.16.6s.110

1. Introduction

Cities are responsible for the majority of global greenhouse gas emissions and play a vital role in achieving carbon neutrality targets. The measures related to buildings, transport, energy supply, land use, and consumption that would lead to the realization of carbon-neutral cities were implemented through interventions synchronized over time, taking into account technical feasibility, social acceptability, and economic limitations. Decision-makers therefore require methods that can integrate large volumes of heterogeneous data, simulate complex physical and human systems, and estimate a range of alternative interventions under uncertainty. (Turner *et al.*, 2023). To satisfy this demand, a new technology, urban digital twins (UDTs), is introduced in order to create the high-fidelity and data-driven virtual replication of an urban system that, in its turn, can be used to simulate, analyse, and explore the possible scenario. Recent reviews indicate that urban digital twin (UDT) research and practice have expanded rapidly over a short period. The scope of applications has become highly diverse, highlighting the need to establish standardized approaches for achieving sustainability goals.

Nonetheless, the actual application of the idea of the existence of digital twins, which can be reputable to have some ability to run the planning of carbon neutrality at the city level, implies a huge burden to the computation. In full-city scales and detailed building energy modelling of large building portfolios, coupled transport and emissions modelling, and spatiotemporally resolved simulation of renewable generation and interaction between atmospheric conditions and urban environments require large numbers of compute hours and large memory and I/O throughputs when solved (Hodorog *et al.*, 2023). This can be closed by high-performance computing (HPC) systems that are enhanced with latest parallelization methods, surrogate modelling and workflow coordination that are necessary in order to facilitate large scenario ensembles and uncertainty quantification (UQ) that are essential in supporting good policy analysis. Recent developments in the application of HPC in the urban environmental modelling have their positive results of the application of parallel model to massively reduce wall-clock time in performing a city-scale run.

It is the generalization into current practice and in concept of carbon neutrality that provides both realistic, practical architecture which provides pathway estimation by combining urban digital twins with high performance computers. The aspects can be specified of the digital twin, HPC designs to scale, scenario generation and ensemble management and methods to multi-criteria evaluation (Ye *et al.*, 2023). Then, the findings are presented of a synthetic case study that is aimed to resemble to the medium-sized European and Asian cities. The case study demonstrates the use of an HPC-enabled digital twin to find answers to thousands of intervention portfolios within a short time and quantify uncertainties and trade-off between emissions, cost, and resilience.

2. Literature review

According to Ali (2025), the concept of the digital twins is mainly positioned as a transformative enabler for the climate resilience within the smart cities, with a very much strong emphasis on the sustainability-driven within the urban governance. The author adds that digital twins do not stop at preset urban models as they use real-time information, predictive analytics and simulation solutions to support positive climate adaptation and mitigation plans. The article highlights how digital twins have an opportunity to model climate risks such as floods, heatwave, and energy shortages and plan scenarios, on which policy-makers can decide. Ali highlights the role of interoperable data platforms, IoT and geospatial intelligence integration in resilient urban ecosystem development. Other institutional and technical challenges that limit large-scale adoption, including data fragmentation and governance challenges are also discussed in the paper. Broadly, when grounding digital twins to the framework of the sustainable city development, the paper provides a sustainability-oriented point of view where the smart city development is oriented to the long-term goals of climate resilience and carbon neutrality rather than operational efficiency in the short-term perspective only.

According to Agostinelli (2024), the microgrids optimization and management of the built environment are one of the main successes of intelligent digital twins. The author cogitates about the concept of digital twins resulting in the ability to locate distributed energy resources (photovoltaics, storage system, and controllable loads) in real time, to conduct predictive control, and optimize them in an adaptive manner. The authors observe that physics-based energy models should be combined with the implementation of artificial intelligence to enhance the reliability, efficiency and resiliency of the microgrids. Agostinelli stresses that digital twins can act in the condition of uncertainty, process operational scenarios, detect anomalies and decide directly on decentralized energy management. Of particular importance to the ongoing research is the decarbonization of cities because the study demonstrates how the local energy infrastructure can be optimized to reduce emissions without disrupting the supply grid. Difficulties in the scalability, interoperability, and cybersecurity capabilities also are the area of concern, which can be included in the future study, the author suggests the reasonable standardization of the architectures, and their implementation with the city-scale digital twins.

Myers (2023) further makes it clear that digital twins can be considered as the pillars of developing successful smart cities since they enable systemic understanding of complex city communications. The author does not depict digital twins as technical simulations but rather forms the idea of digital twins as the types of socio-technical infrastructures relating data, model and processes of stakeholders to each other. The article also underscores the notion that to achieve successful smart cities, the concept of digital twins is some of the essentials as they will moderate between technological innovation and the humanistic approach to urban planning, government, and economic development. Myers describes their application in field of mobility, energy, healthcare, as well as in the sphere of the public services and the possibilities of digital twins to contribute to the evidence-based policymaking and resilience of cities in the long term. The paper also increases the topicality of semantic interoperability, common data standards, and participatory governance to also scale digital twin efforts. Providing the idea of digital twins as a manifestation of urban transformation rather than optimization per se, the chapter does provide the theoretical background which may be of invaluable interest to the studies of sustainability and carbon neutrality.

According to Hui (2025), both experimental and computational approaches have resulted in the phases of urban canyons wind and thermal environment development through the use of data-driven simulation and numerical modelling. As the authors note, the microclimatic processes which define urban heat islands, ventilation, and comfort of individuals can be discovered only with the help of high-resolution digital models. The review highlights the growing relevance of machine-based learning and data-driven strategies to supplement traditional computational fluid dynamics models to increase accuracy and create models of reduced computational cost. Hui emphasizes that such models can be applied not only to climate sensitive cities but also to the low-carbon city planning in particular, due to the high-density nature of the city. Some of the weaknesses present in the research include data availability, the model generalizability, and computational scalability. Overall, the article provides a high scientific foundation of urban microclimate digital twins introduction in the context of the greater city-level sustainability and decarbonization models.

According to Singh (2025), technologies of digital twins can be mentioned among efficient instruments to organize urban planning and management of resources in the healthcare segment of society. The authors argue that by developing healthcare-oriented digital twins, the real-time and predictive analytics can be integrated to plan the infrastructure, and services and an emergency response system. The paper recognizes the opportunity to streamline the use of resources, patient flow, and hospital energy consumption with the assistance of digital twins through the use of the study to enhance resilience of the system during the pandemic times. One more trend described by Singh is a combination of IoT, city analytics, and digital twins as the basis of smarter and more sustainable healthcare systems in the smart cities as shown in Figure 1. Other ethical and governance issues, including privacy of data and equity in relation to access to digital health infrastructure are also discussed within the work. This paper broadens the range of application of the concept of digital twins since the study links the concept of urban sustainability to human well-being and the population health outcome.

According to Hakiri (2023), digital twins play a more critical role in shaping the future of the communication networks and emerging internet of things based industrial world. The article involves a comprehensive review that talks about the digital twin architecture, enabling technologies, and application sector within the networking, manufacturing, and smart infrastructure. The author emphasizes the importance of digital twins in simplification of networks, predicting maintenance, and real-time control in highly complex and decentralized environments. The joint implementation of AI, edge computing, and cloud is also suggested by Hakiri as the fundamental requirements of size in the deployment of a digital twin. The issues which have been highlighted in the survey as the hurdling factors to extensive implementation comprise of standardization, interoperability, latency and security. This contribution is particularly beneficial to the study of digital twins in the city context as it provides conceptual background of what a network and data infrastructure should be concerning supporting digital twins in a large city.

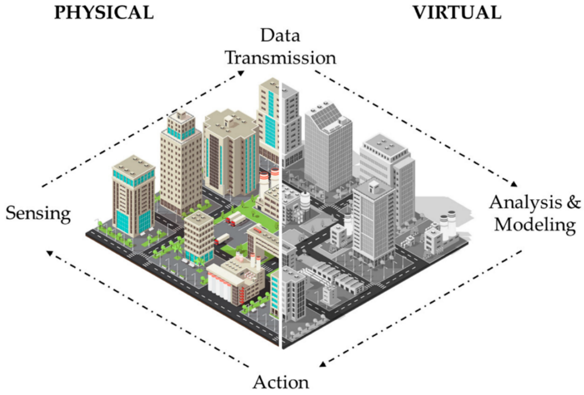


Figure 1: HPC-driven simulation workflow applied to an urban environment, highlighting parallel processing of large-scale urban models, scenario ensembles, and real-time analytics — directly relevant to city-wide carbon neutrality modelling.
(Source: Iossa *et al.,* 2025)

According to Wedi (2023), the current administration of digital twin technologies should be democratized to maximize their values to society overall and within an organization. The author provides a management platform, which can be implemented to transmit, share, and reapply digital twin assets and between industries and stakeholders. The dissertation emphasizes the fact that the currently existing digital twin markets are proprietary and marketable so as to inhibit cooperation and innovation. According to Ubomah (2024), it may minimise entry and participation barriers imposed by open platforms and standard asset management structures, particularly in suppliers who are smaller municipalities or organisations. The other reasons, as addressed in the study, are governance, intellectual property and trust as the necessary aspects in the digital twins sharing settings. The contribution that this work makes is the management and policy-based understanding of which technological development cannot be sufficient without participatory and open digital twin ecosystems.

3. Methodology

This section presents with the digital twin architecture, the HPC scaling strategy, scenario generation approach, and the evaluation of the metrics which are used in the experiments.

3.1 Digital twin architecture

The proposed urban digital twin shown in Figure 2 is modular in design and is composed of four primary layers: data ingestion and semantic integration, physics-based simulation engines, surrogate modelling and uncertainty quantification modules, and decision-support analytics with visualization.

Data of heterogeneous nature (building footprints and typologies, asset registers, IoT sensor streams (energy meters and traffic detectors), historical demand profiles, weather and solar irradiance, and socio-demographic data) is received by the ingestion layer, which reconciles it (Meschini et al., 2025). The data are overlaid onto semantic ontology that will help in defining the relationship among the urban objects such as buildings, roads, busses and substations therefore enabling the exchange of similar and read up information in different simulation models.

The simulation layer contains building (detailed EnergyPlus or other physics engines), urban mobility (agent-based or macroscopic traffic models), distributed energy resources (PV, storage, EV charging models), and microclimate (reduced-order urban canopy models) domain models (Iraola *et al.*, 2025). Models are constructed with shared interfaces to ease coupling (as a run and staged execution) like the construction of load outputs (feed) DER scheduling models.

The surrogate and uncertainty quantification (UQ) layer provides computationally efficient emulators and enables probabilistic assessment of uncertainty. Surrogate models, such as Gaussian process regressors and neural network–based approximations, are trained to replicate the response of computationally expensive simulations, allowing rapid exploration of the scenario space. Uncertainty quantification is performed using ensemble sampling methods, including Latin hypercube sampling and Monte Carlo techniques, along with Bayesian calibration using observed data to estimate confidence intervals for projected emissions.

The analytics and visualization layer also aids in multi-objective evaluation, exploration of scenarios in an interactive environment, and automatic reporting (Ali *et al.*, 2025). It possesses a city carbon accounting engine that aggregates the emissions based on the sector, spatially maps the emissions and determines such variables as per-capita emissions, marginal cost curve of abatement and resiliency.

A workflow manager coordinates the coordination of graphical distance and computational distance which can divide simulative tasks to dissimulation clusters of local HPC capabilities, the cloud HPC solutions or node-based systems equipped with GPUs as defined by processing requirement.

3.2 HPC scaling strategy

The HPC strategy addresses the three scaling axes: horizontal ensemble scaling, vertical model scaling (higher spatial/temporal resolution), as well as the hybrid parallelism for individual models. Horizontal scaling Scenario members can still be run in parallel on nodes, this can be done without difficulty when handling embarrassingly parallel ensembles. Vertical model scaling core principles are decomposition, domain parallelism (MPI) of models, which require a fine grid resolution; spatial elements represented by urban microclimate and CFD components are distributed to a scheme of spatial partitioning (Canfora *et al.*, 2025). Hybrid parallelism involves the application of MPI at the node-to-node boundary, and thread-level parallelism (also known as OpenMP or GPU kernels) within the nodes on those components of the solution that are compute-intensive such as radiative transfer and power flow solvers. The elasticity of providing resources in the form of efficient checkpointing is used to alleviate the bottlenecks and the efficient utilization of parallel file systems to optimize the I/O.

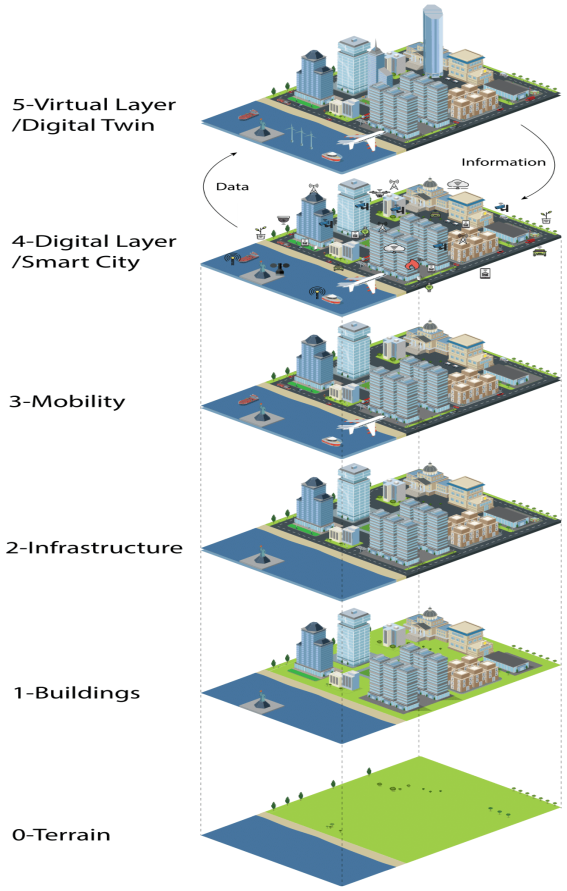


Figure 2: A layered urban digital twin system integrating multi-source data (IoT, sensors, geospatial), analytics, and simulation engine (Source: Mohammed *et al.,* 2025)

The file based and lightweight exchange of the coarse data and the utilization of tightly coupled messaging among the components of the system is two different communication strategies. Nevertheless, the initial message is ambiguous and logically different. Direct messaging between components can lead to model dependency in tightly coupled systems due to the existence of components that are most likely in direct contact with each other, particularly when latency requirements are high enough to reach product specifications.

Surrogate models are used to alleviate the effect of computational complexity through reduced full-fidelity simulations. In the first stage of exploration, computationally costly kernels are substituted by learned approximations, thus enhancing their efficiency but without an unacceptable accuracy.

3.3 Scenario generation and ensemble design

Those are policy levers (retrofit rates, rate of electrification, renewable build-out), technology options (heat pumps, EV penetration, battery rates), behavioural option (occupancy patterns, mobility mode share), and climatic variability. The ensemble design assumes factorial stratified sampling on probabilistic sampling to parameters that are uncertain (Taşyaran *et al.*, 2022). Each scenario exercise produces demand, supply, emission, costs, and time series of the resilience indicators during the 30 years of demand with one hour of time resolution.

Sensitivity analysis employs global variance-based techniques, such as Sobol indices, to decompose the input–output variance and quantify the contribution of each input parameter to the overall model uncertainty.

Multi-objective optimization is performed using high-performance computing (HPC) ensemble-based evolutionary algorithms. These methods are used to analyze trade-offs among multiple objectives, including cumulative emission reduction, net present value (NPV) of investment, and resilience measures.

3.4 Case study setup

To demonstrate the technique, we model the configuration of a fictitious city of about 300,000 inhabitants, inventory of residential, commercial and industrial buildings, a hodgepodge transport network and a medium carrying distribution net (Wedi *et al.*, 2023). The parameters of archetype building are trained on open datasets and refined on synthetic traces of meters. Time series of weather uses past reanalysis data, which is re-sampled to hourly time interval. Interviewee portfolio includes deep retrofit (insulation, glazing, HVAC replacement), electrification of heating and transport, rooftop PV installation, community storage and flexible demand.

3.5 Evaluation metrics

The main indicators are cumulative CO2e emissions (30-year horizon), peak demand reduction, levelized cost of avoided emissions, net present cost to the city and resilience indicators (hours of critical load served during grid stress situations). It is said that the uncertainty is 90 percent credible intervals of the outcome of the ensemble.

3.6 Data Source Clarification and Synthetic City Justification

In the current study, no single real-world city dataset has been mainly directly employed due to limitations related to the data accessibility, privacy constraints, as well as interoperability challenges across the heterogeneous urban systems. This has instead been constructed with a model of a synthetic city in order to provide a real but controlled experimental landscape. The synthetic city is a statistically calibrated model urban system, which is grounded on publicly accessible benchmark data and archetypical buildings along with the general urban distribution of infrastructure observed in the existing literature (Taşyaran *et* *al*.,2022). An artificial city is a structured method in urban systems modelling and is particularly applied to the methodology research stage; when a multiplicity of variables is being investigated without being confined to incomplete or biased actual world information. The synthetic dataset used in this study is constructed based on representative distributions of building typologies, energy consumption patterns, transport demand profiles, and renewable energy supply characteristics (Turner et al., 2023). These distributions are derived from publicly available benchmark datasets and established urban system modelling practices to ensure realism and statistical validity.

Therefore, the dataset does not correspond to any specific geographic city but is instead generated using a parameterized and scalable urban prototype. This approach enables the systematic exploration of decarbonization pathways while ensuring that the findings remain generalizable across different urban contexts. The results in the present study are through a systematic sequence of computation formed in a high-rate computing (HPC) facility (Ugbomah *et al*.,2024). The workflow will consist of the sequence of process of data introduction, scenario generation, and simulation performance, as well as post-processing. In the first step, probabilistic techniques (e.g. Monte Carlo) assist in sampling the input parameters (e.g. retrofit, electrification, renewable deployment and behavioural variables). The parameters set sampled selects a given scenario in the ensemble. In both instances, coupled simulation models are implemented, and they consist of building energy models, transport demand models, distributed energy resource models, and carbon counting modules. These scenarios are run at HPC nodes simultaneously in parallel fashion which allows exploration of large scale scenarios to be realized. Both simulations have results in the form of time-series energy demand output, emissions, and system costs and measures of the resilience (Ye *et al*.,2023). The summation and evaluation of the products will be done to determine the ensemble statistics, sensitivity indices along with the optimization results. Thus, they are not determined by some deterministic computation, but rather, on ensemble basis simulation experiments, which makes them resistant to uncertainty.

3.7 Computational Workflow and Result Generation Process

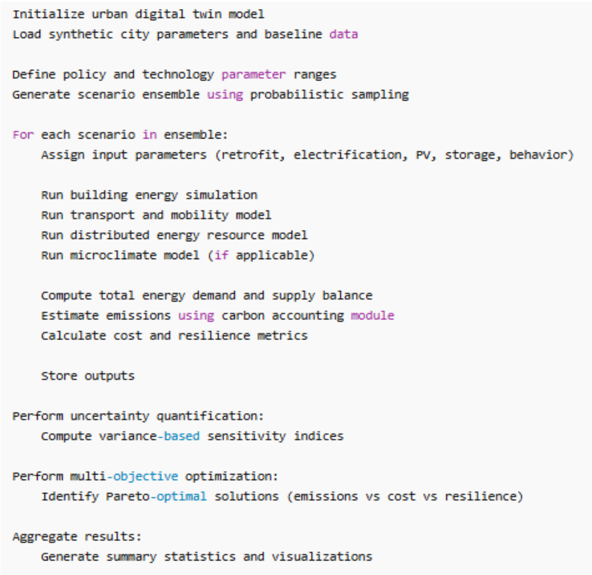
The results obtained in this research are designed using a systematic computational workflow and implemented using supercomputers with a high-performance computing (HPC) platform. The workflow is divided into a number of steps that follow each other, such as data preparation, scenario generation, simulation execution, and post-processing (Vazquez-Novoa et al., 2025). The first stage is to sample the key input variables, i.e. retrofit rates, electrification levels, deployment of renewable energy and behavioural parameters, by applying probabilistic methods, such as Monte Carlo simulation and stratified sampling. The set of parameters sampled is a set of parameters in each scenario in the ensemble.

In both scenarios, coupled simulation models are run, which are building energy models, transport demand models, distributed energy resource models, and carbon counting modules. These simulations are scaled to multiple HPC nodes which can be used to effectively search through many scenarios with an acceptable time constraint. The simulation outputs will be time-series data on the energy demand, emissions, the cost of the systems, and resilience measures across the specified planning horizon (Veigas et al., 2025).

After the execution of the simulation, the results are summarized and analysed to calculate the below statistics: ensemble, sensitivity indices, and optimization. This ensemble technique makes the results not to rely on a deterministic single simulation but rather on statistically sound estimates of the results of the many realizations of the scenarios. The findings thus give a valid foundation on the measurement of uncertainty, intervention effect, and evidence-based urban decarbonization planning.

3.8 Algorithmic Framework (Pseudo-code Representation)

To improve methodological transparency, the computational process followed in this study can be summarized through the following high-level pseudo-code (Wedi *et al*.,2023) as in Figure 3:



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Initialize urban digital twin model
Load synthetic city parameters and baseline data

Define policy and technology parameter ranges
Generate scenario ensemble using probabilistic sampling

For each scenario in ensemble:
    Assign input parameters (retrofit, electrification, PV, storage, behavior)

    Run building energy simulation
    Run transport and mobility model
    Run distributed energy resource model
    Run microclimate model (if applicable)

    Compute total energy demand and supply balance
    Estimate emissions using carbon accounting module
    Calculate cost and resilience metrics

    Store outputs

Perform uncertainty quantification:
    Compute variance-based sensitivity indices

Perform multi-objective optimization:
    Identify Pareto-optimal solutions (emissions vs cost vs resilience)

Aggregate results:
    Generate summary statistics and visualizations
```

Figure 3: Pseudo-code Representation

4. Results and Analysis

This section presents and interprets the results obtained from various high-performance computing (HPC)–enabled urban digital twin simulations. It is interested in the performance of the ensemble, the correctness of decarbonization of baseline calibration, quantified effect of decarbonization interventions, propagation of uncertainty in diverse circumstances, performance of multi-objective optimization, and computational efficiency (Geenen *et al.*, 2024). The discussion proves the application of scenario exploration, large scale and uncertainty exposure optimization in order to provide a practical information about the city-wide planning of carbon neutrality.

4.1 Ensemble outcomes and baseline calibration

A total of 2,400 members of a scenario were simulated on a mixed CPU/GPU computing cluster using the HPC based simulation system. All scenarios consisted of various assumptions of building retrofitting rate, electrification introduction rate, renewable energy introduction rate, and behavioural adoption parameters selection and climate conditions in the future. The ensemble based algorithm allowed the digital twin to search an extensive solution space rather than limited set of deterministic paths.

The calibration of the baselines was carried out with the comparison of the simulated electricity and thermal demand traces with synthetic smart-meter traces of residential, commercial and mixed-use buildings. The results are represented in Table 1 and Figure 4 below. The accuracy of the calibration was measured using the measurement of the mean absolute percentage error (MAPE) as well as the peak deviation measure of the demand (Tan *et al.*, 2024). The MAPE values of aggregated daily energy demand were less than 8 always and the errors of peak hourly demand could not be more than 12 with all building archetypes. The size of these error margins falls within reasonable ranges already documented in the literature on urban energy models, which implies that the digital twin can effectively reproduce a wide range of demand variations at the urban scale.

In the absence of additional mitigation policies, and under current trends, cumulative operational emissions over a 30-year horizon are projected to be moderately higher. The main causes of this growth were population growth, urbanization, end use partially electrified over time, without a decarbonate supply of electricity. The current bottom case therefore served as the comparison of all the mitigation cases on their absolute and relative reduction of emissions.

Table 1. Baseline calibration accuracy and emissions indicators

Indicator	Value
Mean absolute percentage error (daily demand)	7.6%
Peak demand error	11.4%
Annual baseline electricity demand (TWh)	2.35
Annual baseline heat demand (TWh)	1.92
Cumulative CO_2e emissions over 30 years (Mt)	48.7

The pattern of emissions at the ground level illustrates how vulnerable the cities are during the process of electrification which do not coincide with the supply-side decarbonization which emphasize the reasons why the cities must be designed as the entire system.

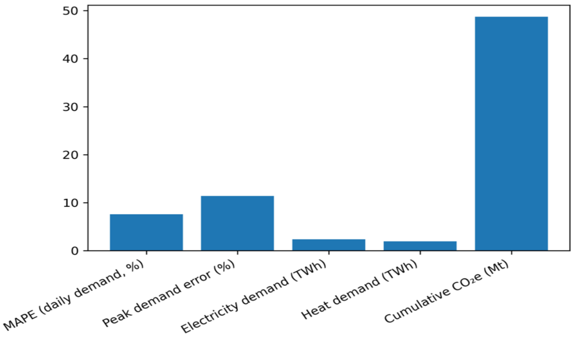

Figure 4: Baseline calibration accuracy and emissions indicators

4.2 Intervention impacts

It is shown in the simulations of the ensembles that there are great variations upon the outcomes of the emissions depending on the combinations and sequences of the intervention. The mitigation effect on individuals of reinvestments of deep building with high-efficiency heat pump had the strongest effect on reduction in sectors. The average reduction in the total construction industry emission was an estimated 45 percent below the base over the 30 years period (Veigas *et al.*, 2025). This was because of the lower final energy requirement together with the higher conversion efficiency which augmented the profits of future electrification.

As the battery storage has been installed in community-scale and flexibility of the building, the deployment of rooftop photovoltaic systems led to the further reduction of the system-wide emissions. Interventions reduced imports of the grid electricity in the peak periods, reduced the amount of curtailment of the renewable generation and demand shifted to the low marginal emission periods. PV-plus-storage strategies (when used with retrofit strategies) offered a cumulative emission reduction of 8-12 per cent incremental to retrofit-only strategies.

Transport electrification significantly reduced the carbon dioxide emission levels at the tail pipes particularly with passenger transport at the urban levels. However, the net system effects of transport electrification are highly time-dependent, and assessing them depends critically on the pace of grid decarbonization. (Nechesov *et al.*, 2025). The cases in which the progress in electric vehicles increased more rapidly than that of renewable electricity were partially offsetting the advantages of the decrease in the number of emissions due to a higher rate of increase in upstream atmosphere emissions by electricity generation based on fossil. Having said that, it has high net reductions which were attained via co-controlled rollout of renewables and electrification.

The combination of grid decarbonization with building retrofit and distributed energy resource deployment was proposed to be the most effective one to solve the issue of grid decarbonization in multiple dimensions of mitigation (Hlal *et al.*, 2025). One approach to this, in which deep retrofits were done over the initial 10 years and thereafter faster electrification applied, as part of ambitious renewable procurement, the synthetic city model would have the operational emissions of the synthetic city approaching net-zero by around 2045.

Table 2. Cumulative emissions outcomes under selected intervention scenarios (30-year horizon)

Scenario	**Cumulative CO_2e emissions (Mt)**	**Reduction vs. baseline (%)**
Baseline (no intervention)	48.7	0
Deep retrofit + heat pumps	26.8	44.9
Retrofit + PV + storage	22.9	53.0
Transport electrification only	34.5	29.2
Integrated portfolio (sequenced)	6.3	87.1

These results given in Table 2 and depicted in Figure 5 confirm the hypothesis that the accomplishment of carbon neutrality through single intervention is insufficient and should strive to adopt systemic strategies in an attempt to fill the gap between interventions.

4.3 Uncertainty quantification

The measures of global sensitivity used on the whole ensemble in terms of variance were used to implement the analysis of the uncertainty quantification (Vázquez-Novoa *et al.*, 2025). The results indicate that uncertainty in future grid carbon intensity is the largest contributor of future grid carbon energy outcomes to cumulative emission outcomes which is an indication that shows that future grid carbon intensity has approximately 42% of variance. Behavioural adoption parameters applied to obtain variance not only included electric vehicle charging schedule but also building occupancy schedule about 27% contribution.

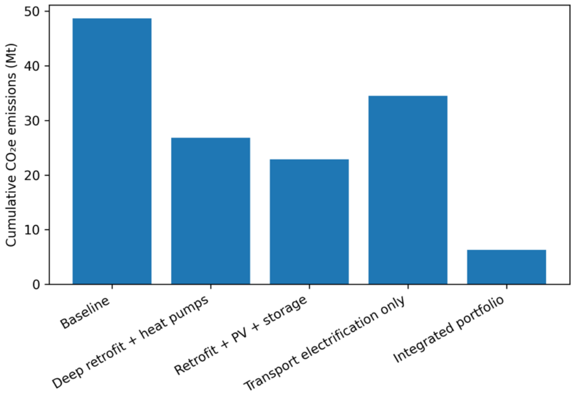

Figure 5: Cumulative emissions outcomes under selected intervention scenarios

The remaining variance was attributed to the trends in cost of the technology particularly on the batteries and heat pumps as well as uncertainty of the retrofit rates which had been attained. All these findings lead to the fact that technology spending matters, but the policy and infrastructure decisions that characterize decarbonization of electricity supply are more significant to final emissions.

It is pointed out in the uncertainty analysis that demand-side intervention must be accompanied by supply-side decarbonization. Uncertainty discrepancy was high when compared to situations which only decreased the demand and not the strength of grid emissions, which had a probability of performing poorly when they happened during the pessimistic grid futures.

4.4 Multi-objective optimization and Pareto frontiers

The trade-offs between cumulative reduction of the emissions, and net present cost of interventions were studied by use of evolutionary optimization based on multi-objectives. The derived Pareto frontiers indicate that there exists a non-linear relationship between expense and reduction of emissions (Bakhouya *et al.*, 2025). The moderate investments of deep retrofit and selective photovoltaic installation gained large starting illness at a relatively low marginal cost, and commanded the best portion of the Pareto frontier.

On the other hand, less renewable growth accompanied by more aggressive short-term electrification shifted solutions to a higher and less efficient mode of eliminating the emission. These strategies increased the level of electricity intensity during periods when the grid remained carbon-intensive hence decreased the abatement returns relative to unit of investment and lock-in effects.

The uncertainty maximization produced good portfolios which would perform reasonably on both the pessimistic and optimistic grid decarbonization paths. Such portfolios were also aimed at demand flexibility, local renewal generation along with gradual electrification. They reduced the ultimate limit by a considerable margin on cumulative emissions in the long-term having paid somewhat more in the short-term capital expenditure and were therefore improving the performance at risk in the long-term.

4.5 Computational performance

The success of such analysis of this number of ensembles relied on the presence of HPC infrastructure. It was estimated to require approximately 18 weeks of computing time to execute the full 2,400 fluctuations of the entire ensemble on a single high-performance workstation even with the standard non-parallelization. In comparison, in a mixed CPU- GPU cluster of 256 nodes, time to execute took around 10 hours overall.

Hybrid MPI/OpenMP parallelism enabled parallelism to embrace scenario executions in an effective manner across nodes and the surrogate model analysis as well as computationally toxic kernels were quickened through the employment of the NCLC (Canfora *et al.*, 2025). Little idle time was experienced and data bottlenecks were reduced by employing parallel input-output strategies and intelligent scheduling of tasks. There was also the reduction of full-fidelity simulations to assist the pre-screening by about 60 due to substitution of surrogate models which boosted further throughput.

These gains in performance indicate that HPC is not a luxury, but a pre-condition to operationalising urban digital twins that can be employed to inform the policy-related, as well as the uncertainty-sensitive, decarbonization analysis.

5. Discussion

The discoveries demonstrate that the combination of HPC and urban digital twins can allow city planners to achieve new opportunities. To begin with, since UQ can now handle ensemble of large scenarios, the decision makers have gained the chance of not limiting their actions to one deterministic path any more, and now they have the chance to examine robust strategies when they encounter profound uncertainty (Taşyaran *et al.*, 2022). This is illustrated by the prevalence of grid carbon intensity of outcome variation demonstrating that decarbonization in cities cannot be regarded independent of regional and national power system directions, it has to be co-ordinated in the scales.

Second, sequencing matters. According to the findings of the experiment, the first retrofits with deep constructions require a lower energy demand in totality and further electrification are less energy-demanding and more efficient. This finding aligns with the available knowledge on energy systems according to which the importance of demand abatement is a requirement towards low-carbon electrification scenarios. The digital twin offers a concise examination and analysis of progression by regions and with time, and training on portfolios, which can be both short period decrease of emission and long term impartiality.

Third, HPC makes the barrier of performing detailed scenario analysis simpler, which has new governing and operation implications. All towns cannot be linked to national supercomputing centres, and cloud HPC is also quite costly, and can be forbidden in the cities lacking enough resources (Wedi *et al.*, 2023). The technologies used to accomplish access democratization are regional shared HPC consortia, tiered fidelity model: model components are used as surrogates to enable local office communication with fast approximation models, and full fidelity runs are done by connecting with remote HPC systems, and open workflow by allowing the reuse of model components.

Uniting physics-based models with high-fidelity and machine learning surrogates proved methodologically effective, particularly when the computational cost of high-fidelity models was prohibitive. This integration resulted in the development of hybrid modelling approaches. Surrogates accelerated the rate of exploration while maintaining fidelity to key measures through calibration with observed data. However, the reliability of surrogate models must be continuously evaluated, especially when interventions introduce regime shifts in the system that were not represented in the training data.

The privacy of the data, ownership and trust are essential in the regards of the governance. The data of the fine-grained human behaviour is combined in digital twins, and it is concerning in terms of the surveillance and equity (Geenen *et al.*, 2024). There must be open systems of governance, data sharing contracts with articulation and model processes with participation, which would facilitate attainment of legitimacy of model processes and their adoption in policy settings. The recommendation of digital twin cities offered by the world economic forum gives an outline to institutional design but more applied research and pilot projects are required in implementation of governance at local levels.

Finally, integration with procurement, financing and regulatory tools will subject the effectiveness of city twins that provides carbon neutrality basing on pragmatics. The outputs must be modelled in such a manner that this can be translated to programs that must be implemented and programs that must be put in place as investments and schemes that would keep a check between planning and implementation.

6. Implementation challenges and operational considerations

The technical, institutional, and social issues also are connected with the process of operating the proposed architecture. Technical concerns include the ability of data to be interoperable across scales, model validation of systems, scalable workflow reproducibility and accessibility of HPC (Tan *et al.*, 2024). These institutional problems consist of the integration across departments, sustainable investment plans and academic capacity to decipher model findings. The social problems addressed by the modelled interventions should be equity rather than to put aside the well-intended policies, and to ensure the confidence of the masses.

They can be alleviated by a number of prudent measures. Reuse and interoperability is improved through the usage of open standards and semantic ontologies. The cohort development involving the local stakeholders is local knowledge inclusive and adopted. The value can be established by implementing a gradual process which gives priority cases at the beginning (e.g. building retrofit targeting or EV charging network planning) and which can be then used to justify further investment. Privacy-enhancing aggregated indicators visible on public dashboards facilitates visibility and stakeholder interaction.

7. Policy implications

The analysis implies three policy implications. To begin with, the cities need to emphasize the demand-side policies particularly deep retrofit as initial interventions to ensure that the additional electrification gains maximum (Viegas *et al.*, 2025). Second the decarbonization planning of cities must be linked to the plans to decarbonize the regional grid whereby the emissions during the electrification process do not experience undesired tradeoffs. Third, strategic enables such as modelling and computational resources are highly returned with minimal returns and could be arrived at by the finding of cost-effective and resilient portfolios and the reduction of the threat of maladaptation.

To make these possible, the policy-makers would need to consider shared HPC to regional networks of cities, promote data sharing with apparent privacy safeguards, and invest in pilot digital twins that can swap modelling with purchasing conduits and fund vehicles such as green bonds.

8. Conclusions

This paper mainly presents a properly integrated framework that couples urban digital twins with high-performance computing (HPC) to model city-wide carbon neutrality scenarios. These elements of a modular architecture and scaling of an HPC infrastructure and surrogate-enhanced ensemble design allow quantified uncertainties in thousands of intervention portfolios to be estimated. As the synthetic case study shows, coordinated portfolios, especially those that focus on demand reduction, which is then followed by electrification in line with grid decarbonization, provide the most successful route to deep cuts in emissions. Moreover, HPC lowers time-to-insight by months and down to hours, which allows interactive policy analysis at decision-making scales. The study is limited in a number of ways. It uses a synthetic city model as opposed to an actual working model entirely based on a real world implementation and not all interactions in the system like the dynamics of the distribution network are simplified. Future studies are needed in cross-city pilot applications, better data integration, better behavioural adoption socio-technical models, and creation of viable implementation routes with proper financing mechanisms. A high level of potential can be achieved in the implementation of city digital twins to attain carbon neutrality. This however needs long term investment in data infrastructure, computer ability, institutional capacity and participatory governance systems. HPC-enabled digital twins can be useful decision-support systems when properly combined and help in achieving multi-sectoral decarbonization transitions in urban settings.

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