The best way to perform building simulations?

One-at-a-time optimization vs. Monte Carlo sampling

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Abstract

What is the best approach to perform building simulations as means to support decision-making and optimize building performance? Traditionally, the search for a compliant design is carried out in a manual one-at-a-time (OAT) approach where one design parameter is optimized before attention is shifted to the next one. In contrast, the Monte Carlo method makes it possible to combine many design parameters simultaneously and consider numerous input combinations. This paper presents a comparison of design approaches and their ability to optimize the performance of an office room with respect to energy demand and indoor climate. The test case is an office space with eight discretized inputs resulting in 93,750 possible designs. Bootstrapping is used to vary the baseline and fixing order for two systematic OAT approaches and to assess an increasing number of Monte Carlo samples. Summarily, OAT optimization depends heavily on the baseline and reveals only few, local optima close to this baseline, which are potentially far from the best solutions. On average, sampling 32 random simulations unveils better solutions and is less likely to suggest poor solutions. An increased sample of 1024 simulations reveals diverse solutions and favourable input ranges, while enabling sensitivity analysis, metamodeling, and flexible constraints.

1 Introduction

Building design is becoming ever more challenging. It is a complex process involving multiple decision-makers, which have to meet ever-stricter building requirements at a limited budget. Building performance simulation (BPS) software is often used to aid decision-making in the search of a design, where a comfortable and healthy indoor climate is obtained at the lowest environmental impact and cost. In this search, the design team may vary a large set of design parameters such as window-wall-ratio, glazing properties, ventilation rates and insulation levels. When combined, these parameters constitute a vast multi-dimensional "design space" which must be explored to find potential solutions that meet the requirements and ambitions of all stakeholders. However, there is no common, unambiguous way to explore the many opportunities and practice differ between countries, companies and practitioners [1][2]. The adopted approach also depends on the applied software's ability to do parameter variations and optimization which varies considerably between applications [3][4][5]. In this paper, we identify and compare common approaches to do parameter variations as means to explore the design space and optimize building performance.

When exploring design space, the design team often rely on experience and rules-of-thumb to select important parameters, which are varied in series of one-at-a-time (OAT) variations. The latter means that only one parameter is varied between successive simulations in order to assess the consequences of the given input change or to optimize that particular input. It is a laborious task to perform a parameter study manually and the modeller must be methodical to avoid inducing errors. Time limits may cause the modeller to vary only a few, important parameters. Unfortunately, modellers' ability to identify and rank important variables has been shown *not* to coincide with the quantitative ranking based on sensitivity analysis [6]. Consequently, if the parameter study does not involve the most important inputs, it will reduce the potential of finding optimal designs. To remedy this, more parameters can be included when the simulations are automated, which is possible with many simulation programs.[1] Similarly, rapid OAT variations can be made by changing sliders in visual programming applications such as Grasshopper and Dynamo (Figure 1 right) [7][8]. However, such OAT parameter studies reveal only local optima in certain regions of the design space whereas "global" methods are required to cover the multidimensional design space and find globally optimal designs [9].

[1] E.g. Sefaira's "response curves" (Figure 1 left), OpenStudio's "Parametric Analysis Tool", IESVE's "Parametric Tool", and BSim's "BSimBatch".

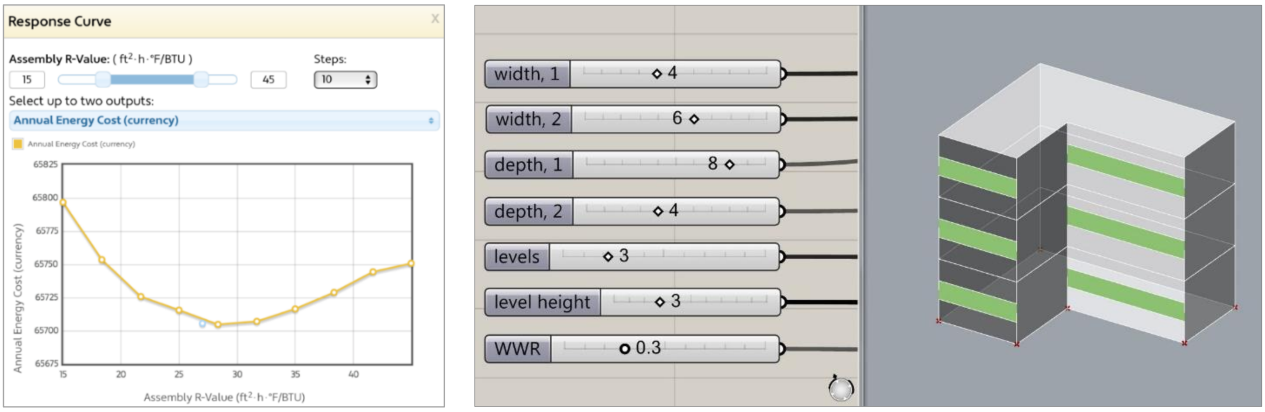

Figure 1 Examples of applications that facilitate one-at-a-time design space exploration. Left: Response curve from 10 OAT variations with Sefaira [10]. Right: Sliders in Grasshopper enables OAT parametric design.

Popular “global” methods to explore a multidimensional design space include Monte Carlo methods, factorial experiments, multivariate optimization, and metamodeling [11][4][12][13][14][15].[2] Their common feature is to vary multiple inputs simultaneously thus taking into account parameter interactions and enabling coverage of the combined design space. Suppose that all design parameters are discretized. In that case, all possible outcomes, and potential solutions, can be obtained using a full factorial experiment as depicted on Figure 4 (top left). However, the number of possible input combinations increases exponentially with the number of varied inputs, which renders full factorial design impractical when addressing many parameters. For instance, 10 parameters, each discretized into five options, would require more than a million simulations (5^{10}). To address this computational challenge, optimization algorithms can be applied to search for optimal input configurations with a reduced set of simulations. The use of optimization is increasing in the field building simulation and a large variety of applications and plugins makes this possible [2][16][17][18][16].

Another approach is to use the Monte Carlo method to select hundreds or thousands of (quasi)-random input combinations to cover the design space evenly. For these simulations, design criteria can be applied to find a subset of high-performing solutions [19][11]. The extent and shape of the design space and the possible solutions can be assessed by uncertainty analysis [20][21]. A related set of statistical methods is sensitivity analysis, which reveals parameter importance and interaction effects [22][23]. This helps decision-makers to focus on the most important design parameters and their interactions while insignificant parameters can be ignored. Finally, Monte Carlo simulations can be used to construct metamodels from which millions of additional input combinations can be evaluated in an instant [24]. The metamodels also enable rapid optimization or instant feedback on specific designs. A growing number of BPS programs now facilitate Monte Carlo simulations, e.g. OpenStudio (~2014) [25], DesignBuilder v. 6 (2019), IDA ICE 4.8 (beta, ~2019), and BSim (2019).

The above trends in the software industry make it easier for practitioners to perform both one-at-a-time parameter studies and global (“all-at-a-time”) design space exploration. Despite the added software features, most practitioners still perform manual parameter studies or automated OAT variations. In this paper, we aim to compare the different approaches to identify best practice for design space exploration. Specifically, we compare two OAT methods, denoted Radial and Winding Stairs, with the Monte Carlo approach for which we consider both random and quasi-random sampling and different sample sizes (number of simulations). In earlier work, we argued that Monte Carlo simulations, combined with sensitivity analysis, metamodeling and interactive visualization, could support decision-making in building design. Here, we seek numerical proof of the allegedly superior Monte Carlo methods as compared to common OAT parameter studies. The use of optimization algorithms is not considered for the following reasons. Optimization have already been addressed thoroughly in literature and, more importantly, the Monte Carlo approach enables uncertainty analysis, sensitivity analysis, and metamodeling. By adding

[2] Metamodels may also be referred to as surrogate models, response surface models, or emulators.

constraints to the sample of Monte Carlo simulations, the design team can easily identify optimal solutions – and non-optimal designs, which too contain valuable information.

1.1 Terminology: Definition of important terms

Before moving on, we describe frequently used terms, which are essential for the understanding of the presented work.

- *Baseline*
  The baseline, or reference model, is the initial design configuration, which has been set up in a building simulation software and quality assured. For one-at-a-time parameter variations, this baseline forms the starting point from which the modeller makes design variations. Due to the large uncertainties in early design, there is no unique, explicit baseline and the modeller has to choose a baseline with specific starting values – also for the design parameters, which are to be varied in the following parameter variations. Similarly, the Monte Carlo approach also requires a fully defined simulation model, which typically contains hundreds or thousands model inputs. In contrast to OAT, there is no need to define specific initial values for the design parameters. These are instead described by probability distributions. [3] Hence, the Monte Carlo method do not rely on the choice of a single, initial baseline, but it does require a complete model for which input values related to the design parameters can be any of those described by their probability distributions.

- *Sampling*
  In a Monte Carlo framework, specific input values for variable design parameters are randomly sampled from their probability distributions. For each new simulation, a set of sampled input values replace the previous values related to the design parameters. There are many sampling strategies such as random sampling, stratified random sampling, Latin Hypercube sampling and quasi-random sampling from space-filling methods such a low-discrepancy sequences (e.g. Sobol and Halton). A final note is that design parameter may affect multiple input values in the model. For example, if we vary the Solar Heat Gain Coefficient for all windows in the models, we consider this a single "design parameter".

- *Fixing order*
  For one-parameter-at-a-time design exploration, the modeller may choose to vary a design parameter, A, and "fixate" it at its optimal value, before shifting his attention to another design parameters, B, which is then optimized and fixated, and so forth. Eventually all design parameters have been optimized, resulting in a final "optimal" design. However, the order of which parameters are optimized and "fixated" may be chosen differently, e.g. optimizing "B", then "A", then "D", and so on. The final design may depend on this so-called "fixing order".

- *Bootstrapping*
  Bootstrapping is a resampling technique, which allows us to estimate the distribution of optimal solutions obtained from different design approaches with varying settings. For example, for a finite set of design combinations (here 93,750), the optimal solution found from 32 randomly sampled Monte Carlo simulations can be poor if unlucky with the random selection, and vice versa. Instead, by resampling 32 simulations (and picking the best one each time) many times, we obtain a distribution of solutions from which we can assess the most likely solutions (median) and extreme solutions (good and poor).

[3] In a design context, "probability" may be misleading since the design team may choose the inputs they desire. However, the term "probability" is commonly used in a Monte Carlo framework where input variations are described by probability density functions (for continuous inputs) and probability mass functions (for discrete inputs).

2 Test case: Generic office room

2.1 Requirements for case study

First, we need to establish the requirements for a test case, which allow us to compare the different design approaches. Firstly, we consider an office space, since it is probably the most common space type in non-residential buildings. In addition to aesthetic and layout concerns, the design of offices must meet requirements for thermal comfort and daylight availability with minimal energy demand and costs. For office rooms located at the facade, a wide range of important and interdependent design parameters can be varied in addition to the internal loads and HVAC strategies. These circumstances render the office a suitable case to test various design approaches.

For the office space, it is possible to simulate all design combinations for a selection of important design parameters by discretizing these parameters and combining them with factorial sampling. Each design combination is assessed with respect to energy demand, daylight availability, and thermal comfort. This all-encompassing set of design combinations enables us to make theoretical comparisons of different design strategies, for which we need to test different baselines, fixing orders, and number of Monte Carlo simulations.

2.2 Context and design parameters

The office space is an ordinary, rectangular room with a single window centred in the South facing facade. It is situated in the heat-dominated, temperate climate of Denmark and there are no obstructions providing shade. System schedules and set points have been defined from Danish building regulations and an industry guideline on indoor climate simulations [27].

Table 1 Discretized design parameters for the generic office room.

Internal load *W/m²*	Room depth *m*	WWR *%*	SHGC -	Overhang °	Shading factor -	Ventilation h^{-1}	Cooling *W/m²*
5	4	40	0.17	0	0.2	2.6	0
11.25	5	52.5	0.21	15	0.6	4	60
17.5	6	65	0.35	30	1	5.4	-
23.75	7	77.5	0.48	45	-	6.8	-
30	8	90	0.57	60	-	8.2	-

The eight variable design parameters and their discretized variabilities are listed in Table 1. The choice of variable inputs is based on a sensitivity analysis in a parallel, ongoing study[4], and their variations are constructed, such that they cover typical designs and layouts for office spaces in Denmark. For example, the room depth ranges from narrow (4 m) to deep (8 m) while the width is fixed at 5 meters. This width allows for two opposing workstations and bookshelves along the interior walls, which is a common interior layout. To elaborate, we provide a short motivation and explanation of the design parameters:

- *Internal load* [5]
  This variation in the total internal load roughly cover the combinations of 1 to 6 persons (1.2 met) with a variable equipment setup, i.e. ranging from a small laptop to a powerful workstation with two monitors [27]. The variable also include a small contribution from efficient LED-lighting.

[4] 14 inputs were ranked with respect to their importance for the three outputs using the TOM method, which is based on estimates of total-orders effects [28]. Based on that ranking, the eight most influential inputs have been kept variable whereas less influential inputs have been fixed, e.g. thermal mass, the façade's U-value, and night cooling.

[5] The internal load is normally a constraint and not a design parameter but the test case and large number of simulations are reused across several studies.

- *Room depth*
  The variable room depth represents both narrow and deep rooms and accommodates 1 to 6 workstations
- *WWR – internal window-to-wall-ratio*
  Measured from the inside, this variation ranges from what is considered minimal and maximal window openings in practice. The small window is centred 0.8 meter above the floor with the top at 2.1 meters. In increasing steps, the windows are first extended sideways, hereafter towards the floor, and finally towards the ceiling.
- *SHGC – Solar Heat Gain Coefficient*
  The glazing type is represented by SGHC but light transmittance and U-value vary simultaneously/correspondingly.
- *Overhang*
  The overhang is defined by the angle from the middle of the window to the tip of the overhang.
- *Shading factor*
  A value of 0.2 represents a nearly opaque screen allowing 20% of the heat to pass, whereas 0,6 represent a semi-transparent screen, and 1 means "no screen". Set points is set such that the screen is active roughly 15% of the yearly working hours in accordance to the "standard" ambition level in Danish guideline [27].
- *Ventilation*
  The variation in ventilation rate approximately span from the minimum rate necessary to meet the requirement for indoor air quality, at the minimum internal load, to a typical maximal rate for which mechanical cooling and draught can be avoided.
- *Cooling*
  The zero-option means no mechanical cooling, whereas the alternative represents "mechanical cooling" with a maximum cooling effect of 60 W/m².

2.3 Extent of design space and solution space

The discretised design parameters are combined, using factorial sampling, into 93,750 possible designs.[6] For each of these, we run a building performance simulation with BSim (version 7.16.8.11) and aggregate the results for energy demand, thermal comfort and daylight. *Energy demand* represents the yearly energy consumption for heating, cooling, ventilation, and lighting, which are combined using primary energy factors of 1 and 2.5 for district heating and electricity, respectively. *Thermal comfort* is assessed by the number of hours above 26°C, which must not exceed 100 hours. The minimum requirement for *daylight availability* is to achieve a daylight factor of 2% in at least 67% of the usable floor area.

The histograms in Figure 2 show the distributions for each of the three performance objectives. The right-skewed distribution for energy demand vary from 15.5 to 161 kWh/m² with a median of 40.0 kWh/m². For thermal comfort, the number of hours with an operative temperature above 26°C range from 0 to 1541 hours. The criterion of 100 hours is met for 81.1% of these outcomes. The results for daylight availability cover the entire range of 0 to 100% of the usable floor area with a daylight factor of 2%. However, only 45,450 simulations (48.5%) meet the criteria of 67%.

[6] Since each parameter in reality could obtain infinitely many values, there are also infinitely many possible solutions, but this large set of combinations is assumed to provide a sufficient representation of the design space.

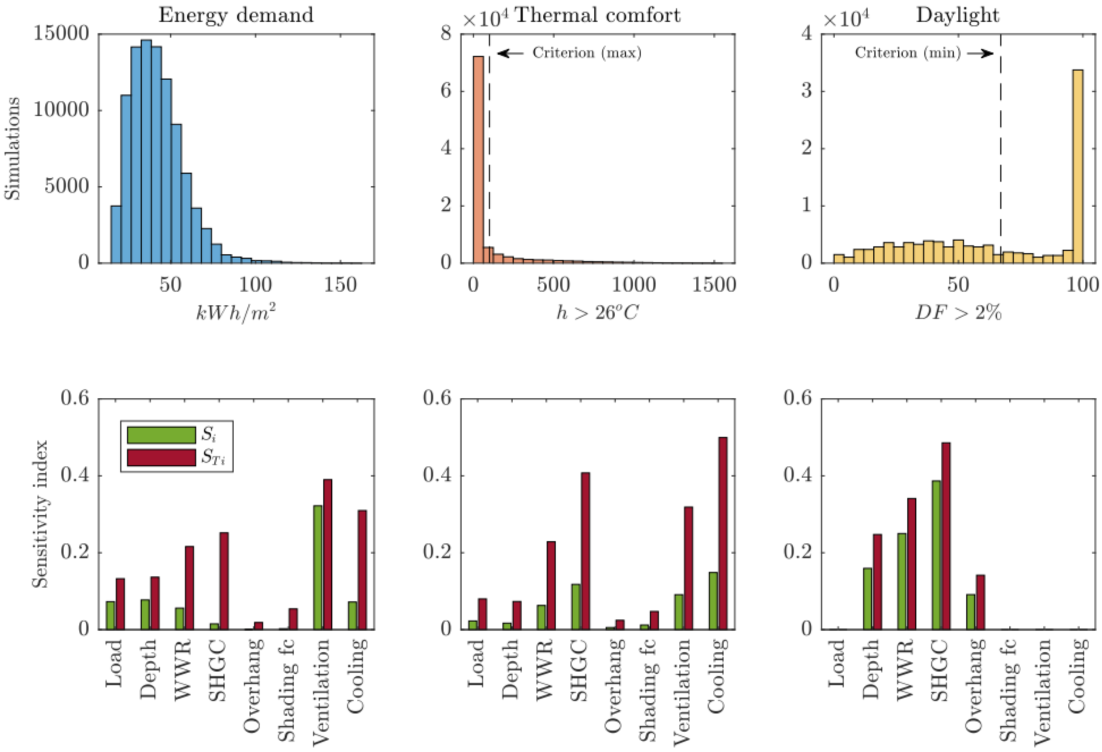

Figure 2 Top) Output distributions obtained by aggregating the results from 93.750 BSim simulations. Bottom) First-order, S_i, and total-order, S_T, sensitivity indices for each of the three outputs.

Figure 3 shows how the individual and combined constraints for indoor climate affects the constrained distribution of energy demand. In combination, the two criteria generate a so-called "solution space" which contains 30,670 simulations corresponding to 32.7% of the total set. Note that the constraints shift the energy distribution to the right and thus remove the designs with lowest energy demand. As a result, the solution with lowest energy demand while meeting the criteria has a value of 21.0 kWh/m². In conclusion, this extreme defines the optimal solution for this test case when ignoring other aspects, such as cost, aesthetics, buildability, etc. Moreover, all solutions are considered equally acceptable in terms of thermal comfort and daylight. That means a design with no hours of overheating is considered equally acceptable as a design with exactly 100 hours above 26°C.

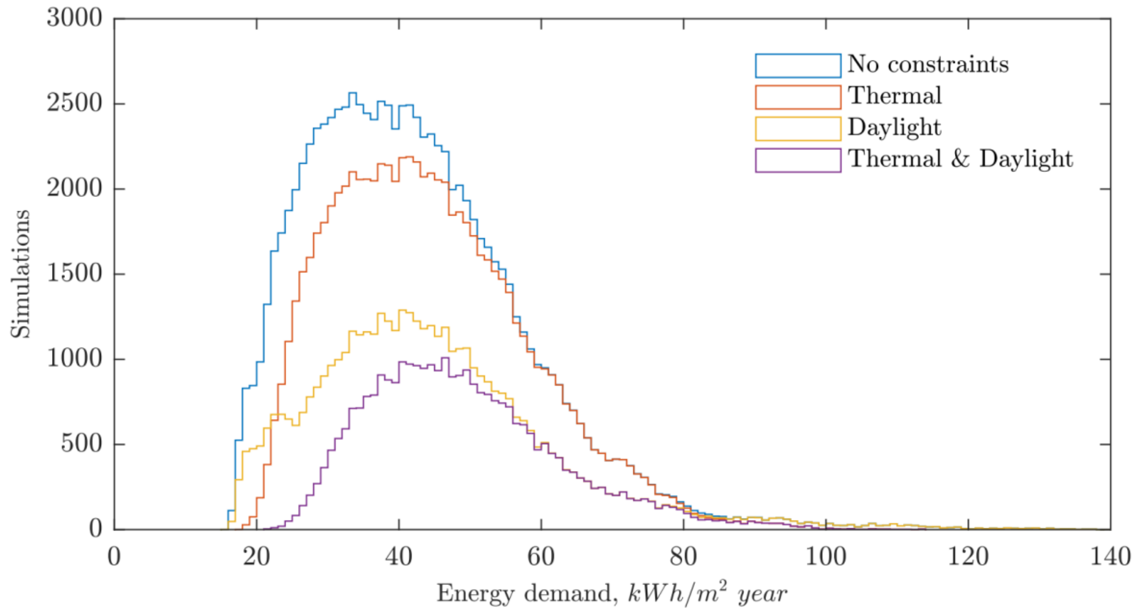

Figure 3 Distribution of the annual energy demand with (and without) constraints for thermal comfort and daylight availability. The bin size is 1 kWh/m².

For each of the three outputs, we have conducted variance-based sensitivity analysis to provide better understanding into the relationships between the design parameters and the performance objectives. The variance-based analysis reveals how much each input contribute to the variance of a given output and to which extent input interactions add to this variance. For this test case, Figure 2 (bottom) displays two sensitivity measures, the first-order index S_i and total-order index S_T, for all inputs for each of the three outputs. The former index, S_i, indicates how much the ith input contribute to the output variance by itself, whereas the total-order index, S_T, denotes how much the ith input and its interactions with other variable inputs contribute to the output variance. S_i is often used to prioritize or rank inputs by importance – and thus requiring the most attention – whereas S_T is used to identify insignificant inputs that could be neglected or fixed without affecting the output notably.

Firstly, we observe that the rankings of both S_i and S_T differ for all three outputs. As an example, only four inputs affect daylight not including ventilation and cooling, which in contrast affect the other outputs greatly. The "solar shading" variable stands out since it has almost no influence on any of the three outputs. This may sound surprising but keep in mind that its activation is limited to only 15% of the in-use hours. Most importantly, we observe large differences between the first-order and total-order effects for all inputs for energy demand and thermal comfort. This indicate a great deal of interaction effects. Thus, the model's response to a change of a given input depends considerably of the values of the other inputs. Ultimately, this suggests that design space optimization is challenging due to the high degree of interactions between the inputs.

3 Methodology

3.1 Design space exploration methods

There is no explicit, well-defined list of methods to explore the multidimensional design space. Though, trends and recurrent approaches can be seen in literature and consultancy practice, and many software applications enable similar features to perform automated building simulations. We have identified the following design space exploration methods (see Figure 4 for visual descriptions):

- *Heuristic approach*
  Perhaps the most common practice is to test different designs based on rules-of-thumb, educated guesses and experience. This approach is highly dependent on the individual modeller

and variations are typically unstructured and performed manually.

- *Radial* [7]
  Starting from a random point (the baseline), each input is varied while keeping the others fixed. Thus, each parameter is varied in turn – each time with respect to the same original baseline. When each input has been varied, the optimal solution may be any of the assessed variations or, alternatively, by combining the best input values obtained for each set of parameter variations. Therefore, this "combined" design point is also assessed and may be the optimal point for linear problems with no or little interaction between inputs (see Figure 4). Some BPS software applications enable this radial approach, e.g. Sefaira's response curves.

- *Winding Stairs* [8]
  Starting from a random baseline, a single, randomly selected, input is varied and eventually fixed at its optimal value, which creates a starting point for the next, randomly selected, input to be varied and optimized. This OAT optimization continues until all of the selected inputs have been addressed and sequentially optimized. The resulting solution will depend on the choice of baseline and the order of which the parameters are addressed, i.e. "fixing order". Windings stairs occur in practice when modellers use "sliders" in e.g. Grasshopper to find a local optimum before changing additional sliders in the same manner.

- *Factorial*
  Factorial sampling is used to consider all possible combinations of a discretized design space. As stated in the introduction, this extensive, global approach is often not applicable in practice due to the exponential growth in possible design combinations making it too time-consuming.

- *Monte Carlo method*
  The Monte Carlo method rely on repeated random sampling from a multidimensional input space. Thus, all inputs are varied randomly between consecutive simulations in this global approach. The Monte Carlo simulations can be continued infinitely, and the "experiment" is therefore stopped when the desired objective is achieved, e.g. providing a sufficient large set for uncertainty analysis or sensitivity analysis or, as in this study, until a desired optimal solution is found.

As mentioned, different sampling strategies exist for Monte Carlo simulations. The simplest version is plain "random" sampling for which each input value is picked at random without considering the other inputs or previously sampled values. Therefore, some samples (i.e. design combinations) may be picked closely together and others far apart – leaving "gaps" and "clusters" in the investigated design space. A more sophisticated strategy is to apply quasi-random sampling using a space-filling technique, where each new "quasi-random" point is picked in the largest gap among the previously selected samples. Such strategies are statistically more efficient and cover the design space more evenly. Though, the quasi-random sampling are apparently not available in the surveyed software applications, which currently facilitate Monte Carlo simulations. In this work, we consider both simple random Monte Carlo simulations (MC) and quasi-random simulations (qMC) to assess the potential of the latter.

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[7] The term "radial" is borrowed from [30] even though the authors use "radial design" to describe iterated OAT variations.

[8] In this analogy, the descend of a flight of winding stairs represents the optimization (minimum) of a given input, until we make a quarter-turn a descend the next flight, i.e. optimize the next input (in a new direction). Inspired from [31].

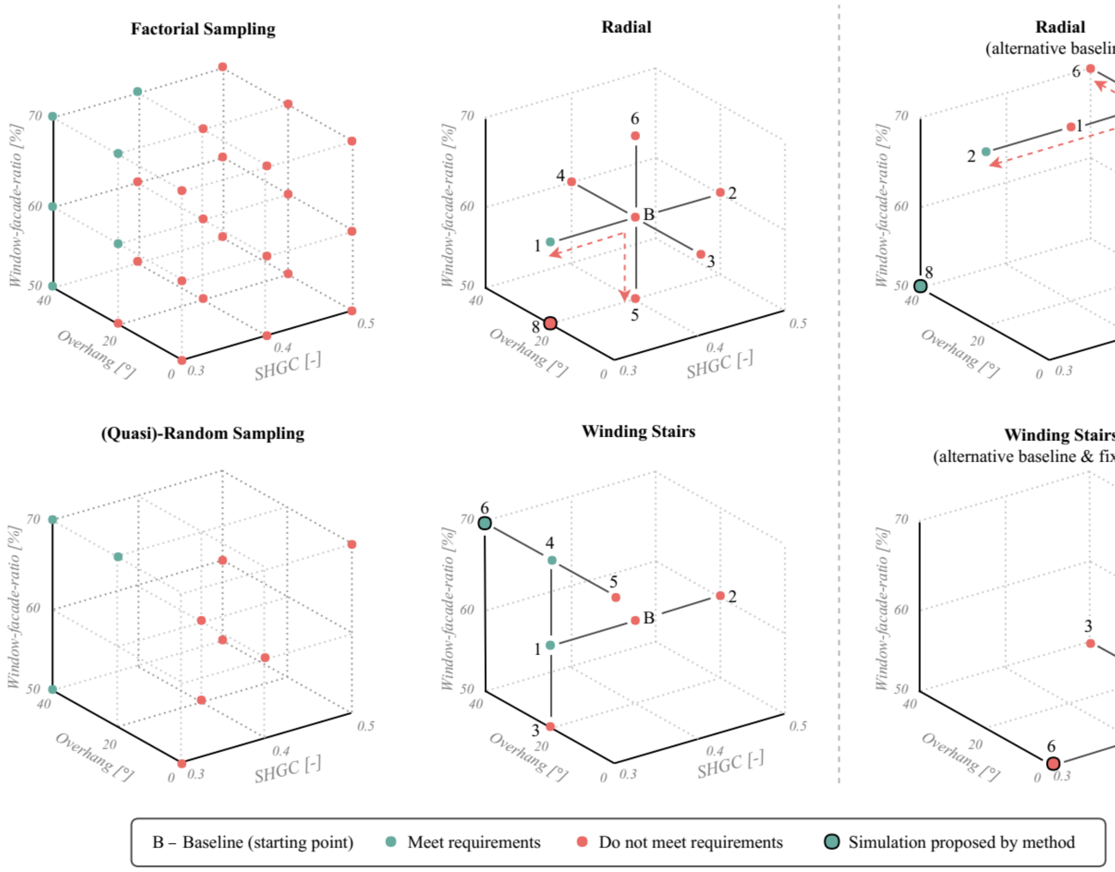


Figure 4 Conceptual visualizations of approaches to explore of a (discretized) 3-dimensional design space. The local methods are shown with an alternative baseline and fixing order.

3.2 Theoretical comparison of OAT and MC approaches

A design team must meet both qualitative and quantitative requirements, but in this study, we provide a *numerical* comparison of "optimal" solutions obtained from different design strategies. The term "optimal" is somewhat controversial, since different stakeholders may emphasize different aspects of building performance. In multi-objective optimization, Pareto fronts are often used to present a range of solutions including the trade-offs between two opposing objectives. However, such visual presentations are not viable here, where we wish to compare optima under all kind of settings. However, Cost and Energy demand are popular objectives to optimize while constraining other performance objectives, e.g. by minimum or maximum values [16]. Since construction costs are difficult to assess during conceptual design, we aim to compare office designs with the minimal energy demand while meeting constraints for daylight availability and thermal comfort.

Each design method will produce different optimized solutions depending on method-specific settings, such as baseline and fixing order. We therefore apply bootstrapping to vary these settings, which lead to distributions of optimal solutions for each design approach [26]. Finally, these distributions are compared using statistics and illustrated with boxplots showing both common and extreme values. These statistics indicate which approach is most likely to reveal the best solution and how robust each approach is.

For Radial design, the optimal solution depends on the choice of baseline (initial set of input values). For Winding Stairs, the proposed solution also depend on the fixing order. If, for at specific baseline, none of the OAT variations complies with the constraints for thermal comfort and daylight, we cannot carry out this particular design optimization in an unambiguous and systematic manner. We have therefore chosen to give these methods an advantage by selecting the baseline from the set of 30,650 simulations that do meet the constraints. Thus, all 30,650 compliant baselines are tested for the Radial approach. For Winding Stairs, a randomly selected, compliant baseline is combined with one of the 40,320 possible fixing orders (factorial of 8). Testing all combinations is unfeasible. Instead, bootstrapping is applied to test 100,000 random combinations of baselines and fixing orders.

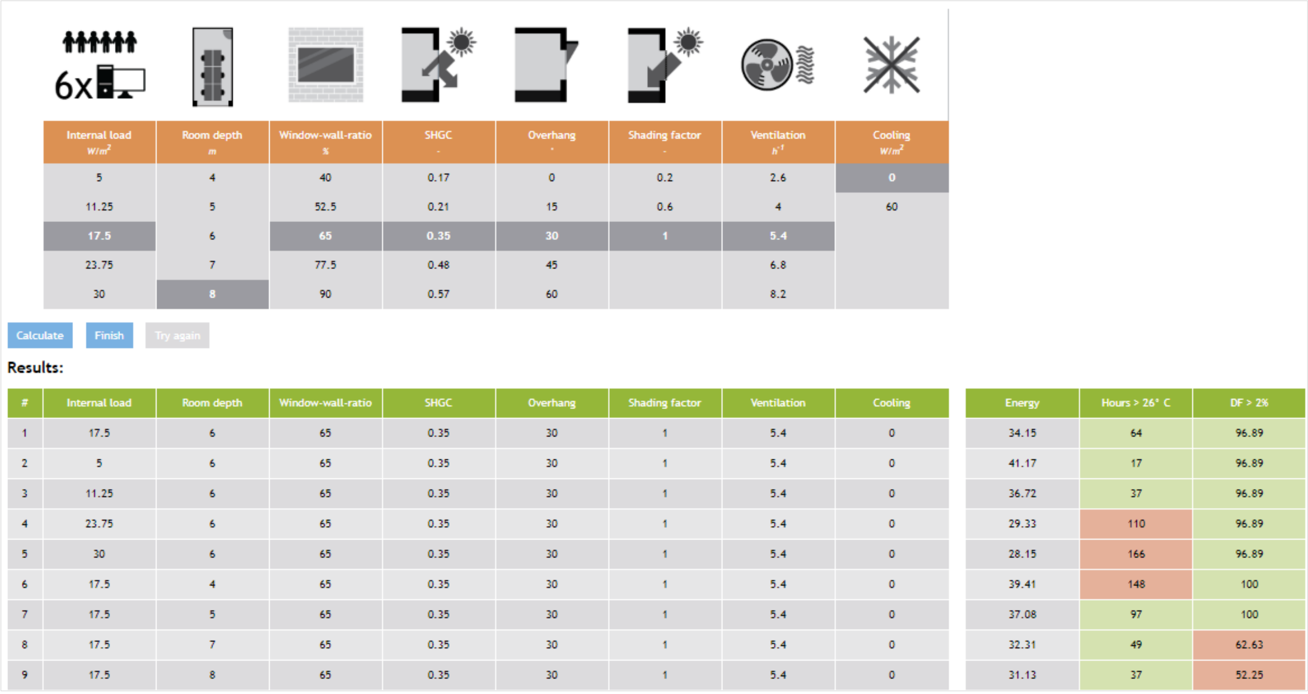
Bootstrapping is also used to test the Monte Carlo methods under different settings. Thus, for a given sample size, sampling is repeated 100,000 times. The number of quasi-random samples are considered in exponentially increasing sizes, i.e. 32, 62, … , 1024. Knowing that quasi-random sampling is more efficient than random sampling, we consider only the sample sizes of 32 and 1024 when applying random sampling. This upper limit of sample size originate from earlier work, which indicates that highly accurate metamodels can be constructed from 1024, or less, building simulations [24]. The variation in sample size makes it possible to assess how many simulations, on average, is needed to outperform the OAT approaches. Sobol low-discrepancy sequences are used to select the quasi-random samples.[9] For each sample size, we select 100,000 different Sobol sequences by varying the starting point of the Sobol sequence. This completes the setup for all but the heuristic design approach, which requires a more practical setup.

3.3 Heuristic approach and student challenge

Assessment of the heuristics approach requires a group of test persons with knowledge of building physics and building performance simulations. This study has involved two consecutive classes with a total of 22 students enrolled at a master's program in Indoor Environmental and Energy Engineering. The students are given a description of the case study and its context, and then asked to use domain knowledge, educated guesses and experience to minimize energy demand while meeting the indoor climate constraints. For this experiment, we provide a specific baseline from the solution space since we are interested to see how skilful the participants are at optimizing the design rather than how "lucky" they have been at choosing a starting point. The baseline is defined by the middle option for most design parameters, which is believed to reflect a realistic scenario with initial guesses "in-the-middle" after which the inputs are varied to higher and lower values. Exceptions for this baseline are the parameters solar shading and mechanical cooling, which in a Danish context are often biased towards "no external shading" and "no cooling". Finally, the baseline is chosen such that it meets the indoor climate criteria in order to compare the heuristic approach with Radial and Winding Stairs that also benefit from a compliant starting point.

For this experiment, we created a small web application enabling rapid, error-free parameter variations for the office room. Figure 5 shows a screenshot of the web application, which has access to the aggregated inputs and outputs from the 93,750 BSim simulations – however these are not visible to the student. The top part displays a table with the eight design parameters and the available, discrete values. Small visualizations illustrate the chosen input value. The user selects a combination of input values (highlighted in dark grey) and press the "Calculate" button after which the chosen input values and the resulting outputs values are inserted into a new row in the "Results" table. Conditional formatting of cell colour is used to highlight whether the indoor climate objectives meet the requirement (green) or not (red). With this setup, each student were asked to find an optimal solution with a maximum of 28 iterations, which corresponds to the number of evaluations needed to perform a Winding Stairs optimization. Such limit is considered realistic based on common practice[10]. Upon completion of the parameter study, all variations including the optimal one were submitted to the lecturer (first author).

[9] Sobol sequences has been chosen over alternative methods, as Halton Sequences or Latin Hypercube Sampling, due to expectedly improved efficiency [32][33].
[10] Based on common practice at MOE, which is one of the largest engineering consultancies in Denmark. From collaborations and employee experiences with other companies, such practice is believed to be representative for large companies in Denmark.



Internal load W/m²	Room depth m	Window-wall-ratio %	SHGC -	Overhang °	Shading factor -	Ventilation h⁻¹	Cooling W/m²
5	4	40	0.17	0	0.2	2.6	0
11.25	5	52.5	0.21	15	0.6	4	60
17.5	6	65	0.35	30	1	5.4	
23.75	7	77.5	0.48	45		6.8	
30	8	90	0.57	60		8.2	

Calculate Finish Try again

Results:

#	Internal load	Room depth	Window-wall-ratio	SHGC	Overhang	Shading factor	Ventilation	Cooling	Energy	Hours > 26° C	DF > 2%
1	17.5	6	65	0.35	30	1	5.4	0	34.15	64	96.89
2	5	6	65	0.35	30	1	5.4	0	41.17	17	96.89
3	11.25	6	65	0.35	30	1	5.4	0	36.72	37	96.89
4	23.75	6	65	0.35	30	1	5.4	0	29.33	110	96.89
5	30	6	65	0.35	30	1	5.4	0	28.15	166	96.89
6	17.5	4	65	0.35	30	1	5.4	0	39.41	148	100
7	17.5	5	65	0.35	30	1	5.4	0	37.08	97	100
8	17.5	7	65	0.35	30	1	5.4	0	32.31	49	62.63
9	17.5	8	65	0.35	30	1	5.4	0	31.13	37	52.25

Figure 5 Screenshot of our web page used by the students to test the heuristic approach (Daylight Factor abbreviated DF).

3.3.1 Students trying out Winding Stairs

Leading up to above experiment, the students are asked to try the Winding Stairs approach. This exercise is meant to give them better understanding of the Winding Stairs approach and to give them hands-on experience with a systematic, manual optimization study. Interestingly, this exercise has revealed some surprising learnings and therefore the results are included in section

4 Results

4.1 Theoretical comparison of design approaches

As described in the methodology section, we vary the baseline and fixing order for the OAT approaches and resample the Monte Carlo based simulations, which allows us to make a statistical comparison of their ability to identify low-energy solutions. The boxes in Figure 6 show the median along with the 25th and 75th percentiles for the distributions of energy-optimized solutions. Extreme outliers are omitted by setting the whisker length equal to the interquartile range (Matlab default) which corresponds to 2.7 standard deviations for normally distributed data (i.e. 99.3% of the data). [11] A quick glance of the boxplots reveals that the Monte Carlo based methods results in smaller variance and a lower median. Thus, they are more robust and, on average, provide better solutions. To elaborate, 29 and 28 parameter variations are needed for the Radial and windings stairs optimization, respectively, but the design team is more likely to find a better design from 32 random simulations and has less risk of ending up with a poor-performing design. Increasing the number of Monte Carlo samples gradually improves both performance and robustness. With 256 quasi-random samples, the upper limit is less than the average solutions obtained from the OAT approaches. When comparing simple random sampling with the supposedly more efficiently quasi-random sampling, we observe slight improvement for the size of 32 samples. At higher samples sized, here 1024, the improvement apparently becomes insignificant.

[11] For Monte Carlo, 32 simulations can be sampled infinitely times, and at some point the 32 worst simulations will be sampled. Thus, extreme outliers become a result of the number of bootstraps and are of no interest in this study.

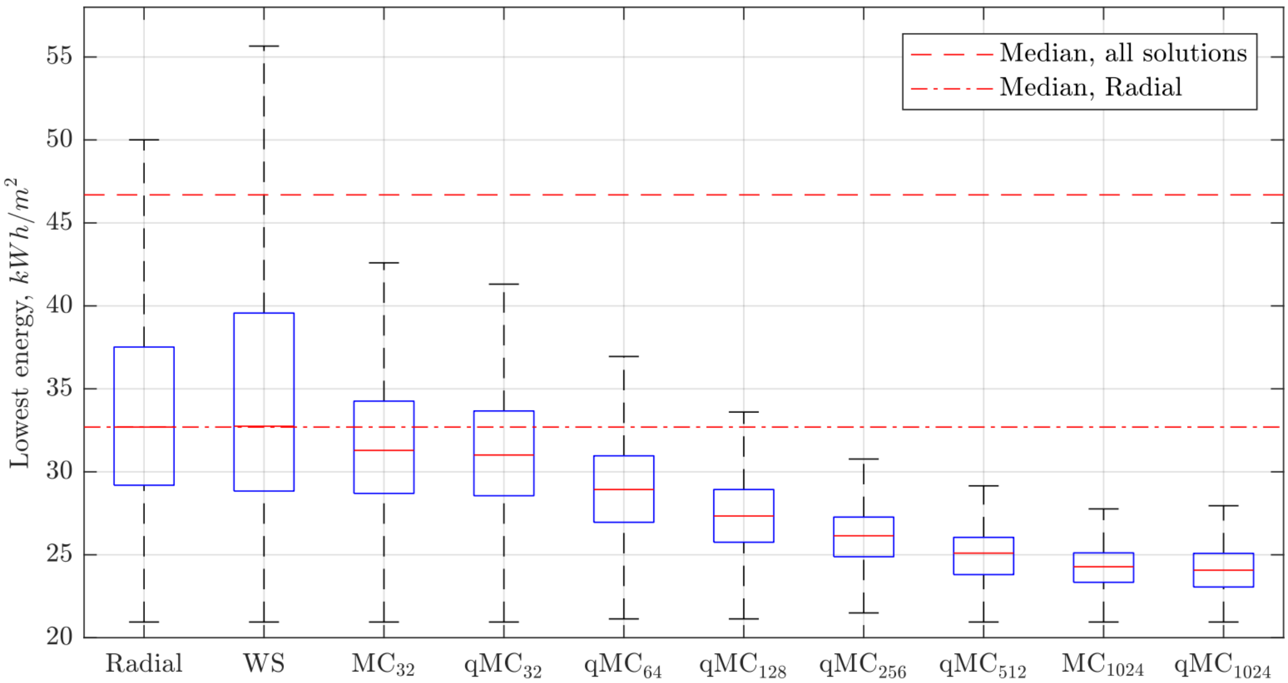


Figure 6 Box plots showing the lowest energy demand found when varying method-specific settings. qMC denotes quasi-random Monte Carlo sampling using Sobol low-discrepancy sequences whereas MC refer to random sampling. The subscript denotes the number of samples.

Let us take a closer look at the two OAT methods. Their medians are almost identical so, on average, the will provide equally good solutions. Though, the Radial design approach is more robust since Winding Stairs is more likely to suggest poor-performing solutions with higher energy demand. From the upper limits, we see that both OAT methods will sometimes propose optimized solutions that are worse than the median for the entire set of simulations meeting the indoor climate criteria (dashed line). This indicates that the OAT methods will propose "worse-than-average" solutions if the baseline is poorly, or unluckily, selected. In such cases, they cannot "escape" a poor starting point and instead they find a local minimum and fail to identify a high-performing design. Figure 7 shows the results of variance-based sensitivity analysis, which reveals how the energy demand for the proposed solutions from Windings Stairs depends on the choices of baseline and fixing order. From the first orders effects, we learn that the choice of baseline has the largest impact on the proposed solution but the fixing order do also contribute to the variation of solutions. Interaction effects account for roughly one third of the lowest energy variation, which means that the fixing order and baseline are mutually dependent and that the optimal fixing order depends largely on the chosen baseline. Thus, the design team cannot know, in general, in which order to assess and optimize the design parameters.

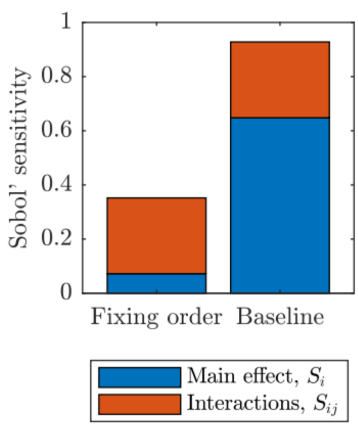


Figure 7 Variance-based sensitivity analysis for energy demand when varying baseline and fixing order for Winding Stairs.

4.2 Heuristic design and students' challenge

Now we turn our attention to the heuristic approach represented by 22 graduate students. As described in 3.3, the students have been offered a specific, compliant baseline, which is also applied for the Radial and Winding Stairs optimization in this comparison. We remind that the baseline consists of the "midpoint" options for the first six parameters and has no cooling nor shading. It is worth to notice that this baseline has an Energy Demand of 34.2 kWh/m² which is considerably lower than the solutions' median of 46.7 kWh/m². The distribution of optimized designs found by the students and the systematic approaches are illustrated on Figure 8. First and foremost, the students perform better than both OAT approaches with solutions in the range of 21.5 and 32.1 kWh/m² (outliers are included to present this range). Note that the Radial approach has a unique solution for this baseline since it does not depend on fixing order. In contrast, Winding Stairs has 40,320 possible fixing orders but, interestingly, only 15 unique solutions, or local minima, are found. The Monte Carlo based approach do not benefit from a favourable baseline and somewhere between 256 and 512 quasi-randomly sampled simulations are needed to obtain the same median as the students.

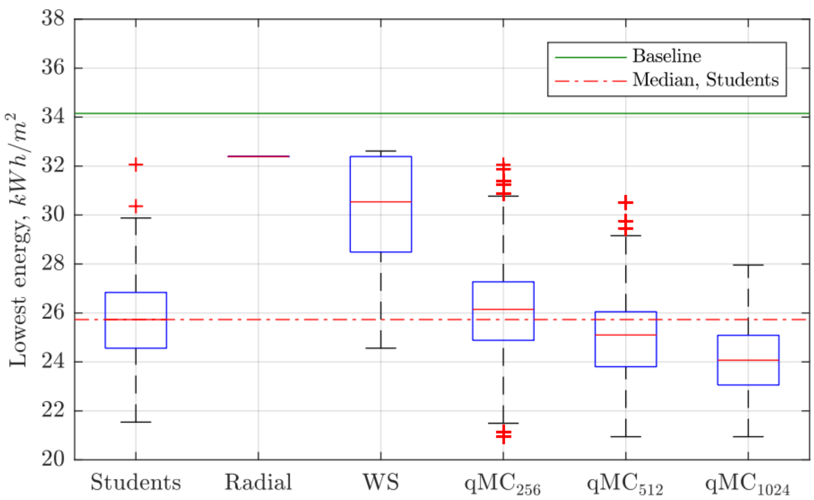


Figure 8 Variations of solutions' energy demand found for the specific "in-the-middle" baseline used in the student case study.

Figure 9 provides an alternative depiction of the above experiment. The small subplots represent the entire solution space, whereas the leftmost plot shows only a small section of the cumulative distribution containing the 8% most energy-efficient designs. It illustrate how narrow the solution space becomes when searching for the energy-optimal designs. Moreover, we observe how the doubling of Monte Carlo samples gradually improves the probability of finding the optimal solution in the distribution's tail.

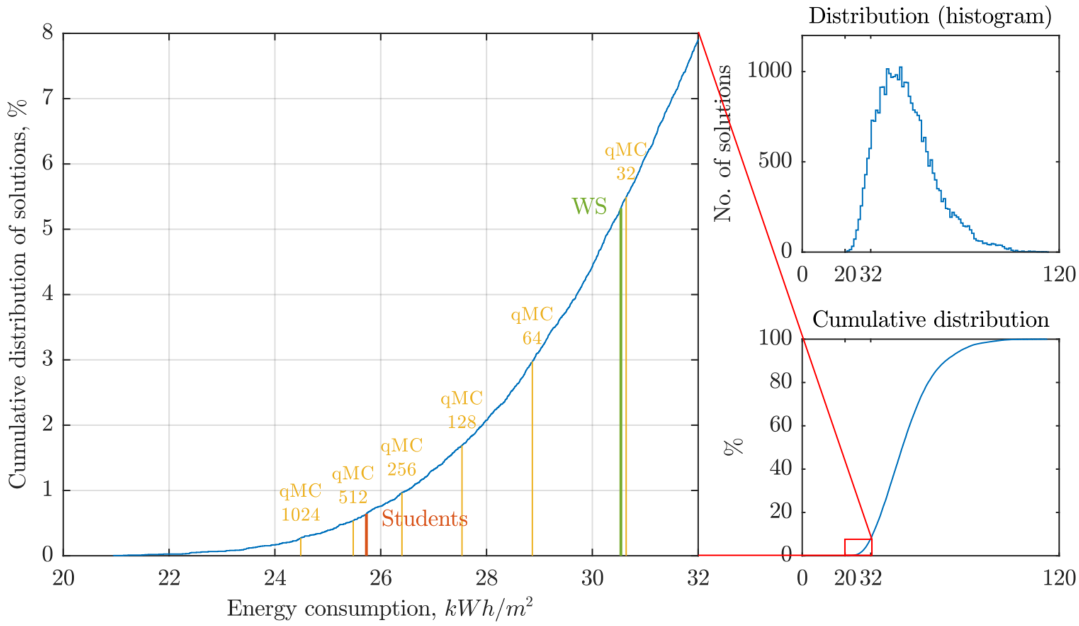


Figure 9 Topright) Distribution of energy demand for all simulations meeting the indoor climate constraints (bin size 1 kWh/m²). Bottomright) Corresponding cumulative distribution. Left) Left-most section of the cumulative distribution along with the medians of the best solutions identified from different design approaches.

4.3 Optimal input values

So far, emphasis has been on optimal values for the output *energy demand* obtained by the various design approaches. We now focus on inputs and investigate whether the different methods are able to indicate specific input values, or ranges of input values, which are most likely to produce energy-efficient solutions. For this investigation, we compare the distributions of input values that lead to energy efficient solutions using the following approaches:

- Heuristic approach conducted by students
- Winding Stairs performed by students starting with the "in-the-middle" baseline
- Winding Stairs using all 40,320 theoretical fixing orders starting with the "in-the-middle" baseline
- A single set of Monte Carlo simulations using 1024 random samples
- Factorial sampling of all combinations which lead to the benchmark of "optimal" input values

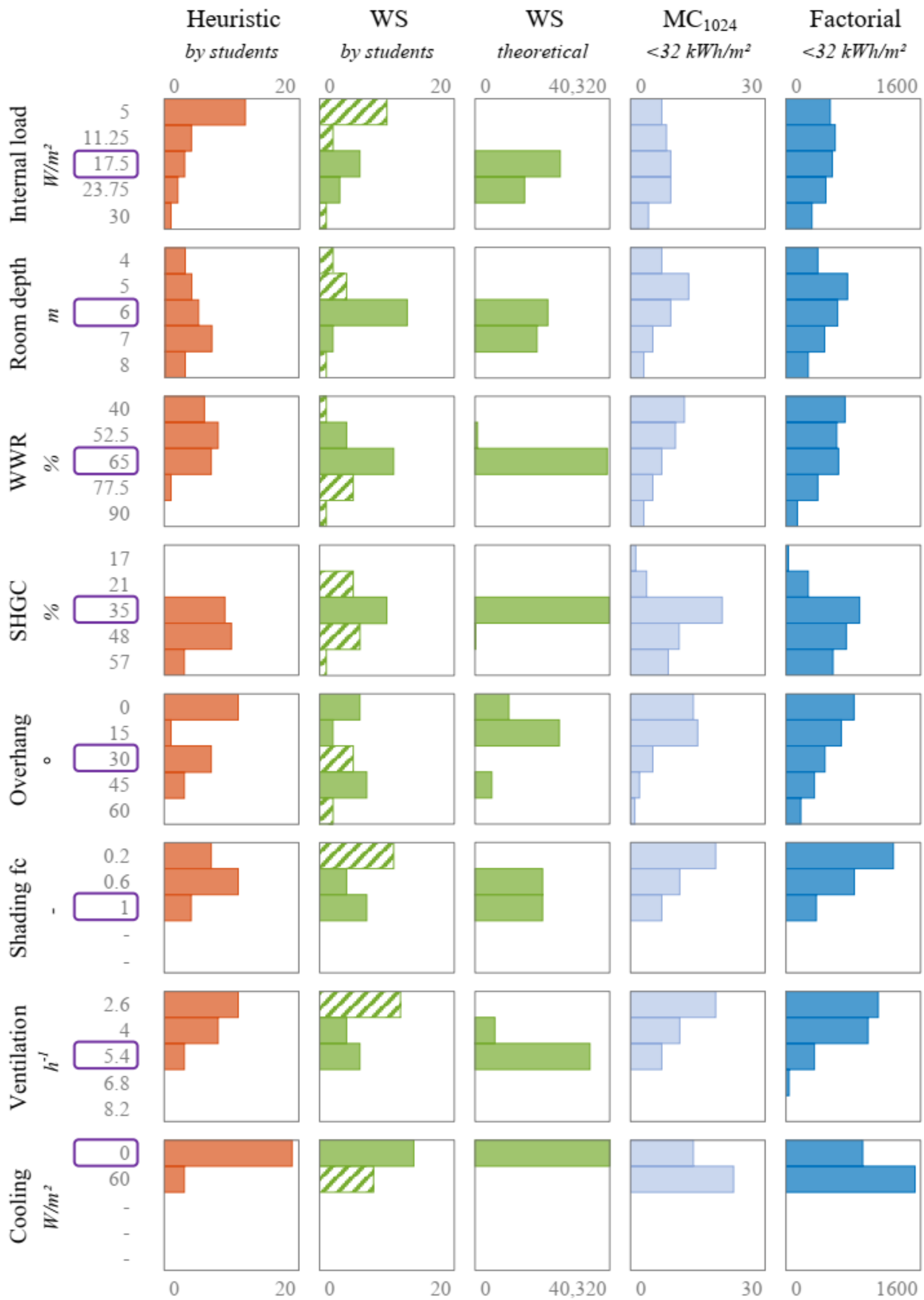


Figure 10 Input distributions for the solutions obtained by the students (heristic and Winding Staris), theoretical Windings Stairs with a fixed baseline, Monte Carlo with 1024 random samples, and factorial sampling. Baseline values are highlighted with purple boxes.

For the comparison, we first need to establish a benchmark as to what "optimal" or "favourable" input values are. In other words, we seek the input values that are most likely to produce solutions with low energy demand. We therefore define a "high-performing" solution space by selecting solutions with an energy demand less than 32 kWh/m² year, since these are all better than the median solutions for Radial and Windings Stairs (see Figure 6). This set of high-performing solutions comprise of 2448 simulations, which is 5.4% of all simulations meeting the indoor climate criteria. The histogram related to the factorial approach on Figure 10 shows the input distributions that lead to these high-performing solutions. These input distributions cover almost the entire range for each design input. Exceptions are a few options for WWR (90%), SHGC (17%), and ventilation (6.8 and 8.2 h^{-1}) for which there are no or few solutions. These results indicate that a high-performing set of solutions can be reached with thousands of diverse combinations of input values. The peaks show the most prevalent input values leading to energy-efficient solutions. Thus, it is favourable to fix a variable input within such peaks if the design team hopes to maintain the most design freedom when addressing the remaining inputs. However, the presence of bins with fewer simulations shows that it also possible to find high-performance solutions for such values.

Turning our attention to the students, we compare their input choices with the benchmark distribution acknowledging that the number of participants is limited. For the heuristic approach, the students manage to avoid the aforementioned unfavourable input options for WWR, SHGC, and Ventilation. Apart from that, there is seemingly no or little correlation, i.e. their choice of inputs do not align with the favourable distributions of the high-performing set of solutions. Examples of contradictory trends are the prevalence of an internal load of 5 W/m² and the option of "no mechanical cooling". This could be an unintentional consequence of the order, for which the inputs are presented on the webpage. It may also be due to student bias, e.g. that mechanical cooling is preferably avoided.

As mentioned, Winding Stairs results in only 15 different solutions for this particular baseline despite the numerous fixing orders. The most remarkable result is that for all design parameters, except one (SHGC), the most frequent input value is the same as the baseline. Apparently, the Winding Stairs approach rarely "escapes" the baseline, which underlines the importance of guessing a fortunate baseline. The obtained solutions only reveal a tiny part of the possible solutions and do not reflect the diversity of solutions nor which input values are favourable. Neither does it yield very good results as shown in Figure 8. Another important outcome is deduced from the input distributions for Winding Stairs as performed by the students. Their solutions include the selection of several input values (coloured with diagonal strips) that should not be possible with this baseline. It turns out that 19 of 22 students failed to follow the systematic approach strictly. For example, they did not continue with best, or a compliant, option when addressing a new parameter or they made "an illegal jump" in the input space. These mistakes may be due to the limited timeframe but time is also limited when performing building simulations in consultancy. When making 28 consecutive parameter variations manually, errors are likely to occur.

Finally, we consider the Monte Carlo based approach using a single set of 1024 randomly selected simulations. When the same criteria of 32 kWh/m² is applied, a set of 37 simulations remain – also meeting the indoor climate constraints. The input distributions for these Monte Carlo solutions are almost identical to those from factorial sampling. Monte Carlo therefore reveals similar trends and ranges of favourable input values as the benchmark, for which all design combinations have been simulated. As seen on Figure 9, Monte Carlo approach will seldom find the single "optimal" solution but trends to be used for design guidance are as informative as when considering all of the design space.

5 Discussion

In the above comparison, we aimed to provide an objective comparison of design approaches based on quantitative measures and statistics. Here, we discuss the design methods from a more subjective perspective and comment on other aspects of the design approaches and the office test case.

In the theoretical study of the Radial and Winding Stairs approach, their performance is based on all compliant baselines. However, an experienced modeller is expected to identify and begin with a decent performing baseline and avoid extreme starting points, e.g. high airflow and mechanical cooling for a room with a modest internal load and small windows. In our comparison, we compensate for this by using only compliant baselines that meet the indoor climate criteria. Moreover, when considering all compliant baselines and fixing orders, the comparison is not biased towards specific input configuration, which modellers could be prone to use. In practice, a potential bias, due to experience or preferences, could hinder the modeller from finding extreme solutions – both good and bad. Finally, from experience with Danish practice, we believe that it is uncommon to perform systematic, manual optimization of as much as eight design parameters. If less parameters are considered, the optimized solution lie closer to the baseline and the performance of the OAT approaches will be worse.

So far, we have paid little attention on how the setup of Monte Carlo based simulations differs from traditional, manually configured, simulations. The Monte Carlo method requires a slightly different way of thinking and careful consideration when dealing with correlated or interdependent inputs. For example, the glazing properties SHGC, light transmittance (LT), and U-value are mutually interdependent. If the variability of SHGC is described by a probability density function, its relationship with LT and U-value may be described from correlation matrices. Alternatively, the modeller may define a number of distinct windows from which to sample in the Monte Carlo experiment. Another distinction from common practice relates to the comparison of designs with entirely different systems with diverse properties, e.g. mechanical cooling system and natural ventilation. One way to handle this unambiguity is to perform sequential Monte Carlo runs and combine the simulation data afterwards. However, with manually configured simulations, it is also challenging to set up and compare such systems. As mentioned in the introduction, there seems to be a tendency of software vendors integrating Monte Carlo based methods into their building simulation software. This makes Monte Carlo based simulations more accessible and easier to use. The inconvenience of increased computing time can be reduced by parallel or cloud computing, which may reduce computation time significantly. For this study, computing 1000 BSim simulations took between 5-8 hours using a combination of Excel and inefficient Windows automation software. In ongoing development, the software developer has parallelized the simulations and removed redundant display of graphics, which has led to a vast decrease in computing time, such that 1000 simulations can be run in a few minutes.

The results of this study obviously reflects the chosen test case, i.e. the early design of an office space with large variabilities and many interdependent design parameters. What about rooms or buildings with fewer, less interdependent inputs having smaller uncertainties? In such cases, the advantage of applying Monte Carlo instead of OAT approaches is probably less significant. Due to the better coverage of the design space, the Monte Carlo approach is still expected provide more and better solutions while offering additional information from sensitivity analysis. If, during early design, the design team only considers a few design parameters with limited variability, they are likely to miss the most promising designs. With a mediocre early design solution, it may become expensive and time-consuming to ensure compliance during later design stages, in which changes almost inevitably occur. Another aspect of the applied test case is the limited selection of only three performance objectives (outputs). If more objectives and constraints are introduced, it will further reduce the solution space making it harder to find compliant solutions. Moreover, we applied static constrains, but in practice constraints and ambitious may change during the design process, e.g. when trying to achieve specific points in environmental assessment schemas, such as LEED or DGNB. These circumstances augments the use of a Monte Carlo approach, which allow for a design space exploration that is much more thorough and, in addition, constraints can be adjusted after the simulations have been completed.

Access to numerous Monte Carlo simulations facilitate new ways to analyse and communicate the simulation data. The interactive parallel coordinate plot as illustrated on Figure 11 offers an effective way to visualize and explore multidimensional data. In real-time, a multi-actor design team can apply constraints to inputs and outputs and immediately observe the consequences and find solutions that meets everyone's wishes. Combined with histograms and sensitivity analysis, such interactive plots help reveal favourable inputs ranges dependent on the flexible constraints [28]. In this manner, the search for potential solutions is influenced by multiple stakeholders with different opinions, and not governed by the modellers own design optimization strategy and constraints.

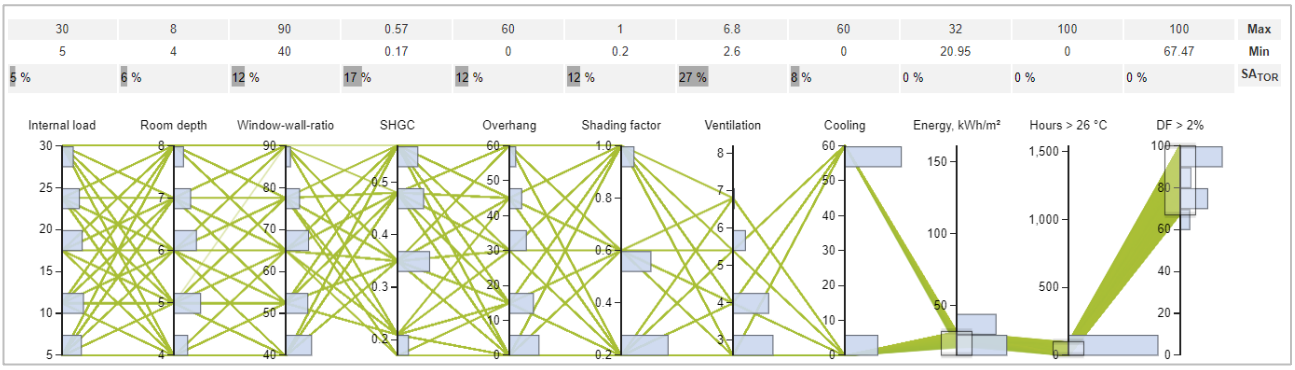


Figure 11 Screenshot of an interactive parallel coordinate plot combined with histograms showing the parameters' distributions [29]. Based on criteria-dependent sensitivity analysis, SA_{TOR}, the bar plots above the coordinates indicate how much the parameters have been affected by the applied criteria [28].

6 Conclusion

In this research, we compare different approaches to explore a multidimensional design space using building simulations as means to find high-performing solutions. The design space is represented by an office room for which eight important design parameters have been discretized to allow for exhaustive factorial sampling, which results in 93,750 possible input configurations. The simulation software, BSim, is used to perform whole-year simulations, from which we aggregate the results for energy demand, thermal comfort, and daylight availability. This complete set of simulations facilitates a statistical comparison of two common OAT optimization strategies, Radial and Winding Stairs, and a Monte Carlo based approach. For our test case with eight discrete inputs, Radial and Winding Stairs optimization require 29 and 28 systematic variations, respectively, whereas the Monte Carlo approach is assessed with an exponentially increasing number of samples. A complementary study based on 22 students was conducted to assess a manual, heuristic approach where the design optimization is based on domain-knowledge and experience. The main findings of this research include:

(1) On average, 32 randomly selected simulations will contain a solution (~31 kWh/m²) that is more energy-efficient than those from Radial and Winding Stairs (both ~32 kWh/m²). The upper-limits of the distributions are 50 and 56 kWh/m² for Radial and Winding Stairs whereas the extreme for 32 random samples is 43 kWh/m² indicating Monte Carlo as the most robust approach – even with low samples.

(2) For Winding Stairs, variance-based sensitivity analysis shows that the optimal solution depends mostly on the baseline. More importantly, the combination of baseline and fixing order has significant influence on the proposed solutions (S_{ij} is 0.28), which means there is no global best order in which to address and optimize design parameters. In addition, the proposed solution lies close to the baseline as shown for the "in-the-middle" baseline, which resulted in only 15 local optima.

(3) Increasing the number of samples gradually improved the performance of the Monte Carlo approach, which reveal more and better solutions. Even with extremely unfortunate sampling of 1024 simulations, it will reveal solutions with lower energy demand than the 25%-quartiles obtained from Radial and Winding Stairs optimization.

(4) Only the Monte Carlo approach can reveal favourable input values or ranges, which are most likely to lead to high-performing designs. The distributions shapes are very similar when comparing the inputs producing the best solutions (<32 kWh/m²) obtained from 1024 random samples and all 93,750 simulations.

(5) When applying the Monte Carlo method with few simulations, quasi-random sampling will typically reveal slightly better solutions compared to random sampling due to a better coverage of the design space. However, with larger sample sizes, the difference becomes insignificant.

(6) In the experimental study, the students have been provided with a compliant, "in-the-middle" baseline which is slightly better than average. With this starting point, the students perform significantly better than both OAT approaches and between 256 and 512 quasi-random simulations are necessary to obtain better solutions.

(7) In a training exercise, 19 of 22 students made mistakes when asked to carry out a set of Winding Stairs parameter variations. This illustrate how difficult it is to be systematic and avoid error in manual parameter studies.

This study of an office space involves eight interdependent design parameters with large variabilities. In general, the design variabilities are often smaller and correspondingly less is the energy-savings potential. However, the building physics remains the same with many inputs, outputs, and complex interdependencies, which advocates the use of the multidimensional, global Monte Carlo approach. Monte Carlo makes it easier to address many design parameters, whereas heuristic OAT approaches seldom encompasses as many as eight design parameters. More often, only a few design parameters is considered and the design space investigation is less structured and thorough. Thus, the potential of using Monte Carlo is expected to be even more significant than shown in this study.

In addition to revealing more energy-efficient designs, we have argued that a large set of Monte Carlo simulations provide more flexibility to vary constraints and inputs, which supports decision-making during design meetings with multiple stakeholder having different preferences. In addition, the Monte Carlo approach facilitate global sensitivity analysis and the construction of metamodels, which enable additional optimization and rapid feedback. However, heuristic OAT approaches are still the dominating approach in common practice and, despite recent developments, the integration of Monte Carlo methods are still immature in most building simulation software. This study shows that a Monte Carlo based approach has great potential to help designers create better designs with low energy and high performance. To realize this potential, software developers must make Monte Carlo methods more accessible and easy-to-use for practitioners.

In conclusion, Monte Carlo simulations cover the design space thoroughly and therefore reveals a variety of high-performing solutions whereas OAT optimization lead to only one of the local optima close to the arbitrarily chosen starting point.

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