Performance-Driven Design Exploration of Biocomposite Facades

Advancing Facade Design through Enhanced Computational Efficiency, Accuracy, and Interpretability: A Novel AI-Driven Facade Design Framework comprising Self-Organising Maps (SOM) and Kolmogorov-Arnold Networks (KAN)

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Introduction

1.1 Introduction

Due to environmental challenges such as climate change, resource depletion, pollution, and biodiversity loss, many industries are strongly encouraged to be more sustainable (Leising et al., 2018). To address these global issues collectively, 196 countries, including the Netherlands, have signed an international climate accord in 2016, the Paris Agreement, to achieve a 100% circular economy by 2050 (Government of the Netherlands, 2023). In addition, the Netherlands' subgoal is to halve its raw material consumption by 2030. The thrust towards a circular economy is a necessary transition, aiming to reduce eco-impact, waste, and pollution, use environmentally friendly materials and extend the lifespan of resources by closing material loops (Ellen MacArthur Foundation, n.d.), as illustrated in Figure 1.1.1.

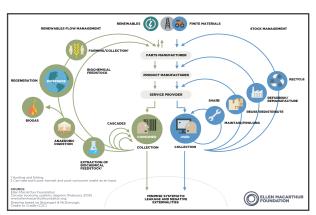


Figure 1.1.1. Circular economy diagram. From "Ellen MacArthur Foundation", by Ellen MacArthur Foundation, 2019 (https://www.ellenmacarthurfoundation.org/circular-economy-diagram).

In this circular framework, the construction sector is key, accounting for approximately 50% of raw material consumption, 42% of energy consumption, and 35% of greenhouse gas emissions in the EU (Gervasio & Dimova, 2018).

Especially housing corporations, which manage around 30% of the residential stock in the Netherlands - or about 2.4 million homes - play a huge role in the sustainability transition, despite their financial limitations. To reach the national circular objectives, they need to upgrade 100,000 dwellings annually towards an energy and CO2-neutral portfolio by 2050, with an average energy label B or higher (Dantuma & Van Sante, 2018).

Facade renovations, which traditionally focus on insulation and infiltration enhancements, are key in this effort as they significantly affect the portfolio's sustainability. Not only because of their impact on energy performance but also due to their exposure to severe climatic conditions which negatively affect the lifespan of its materials (Overend et al., 2021). Using sustainable alternatives could positively impact the environment, by minimising waste and pollution at production and at the end of their lifecycle.

In the EU, construction and demolition waste is the largest sector at 37% of total waste with 839 million tonnes of waste in 2018. Even though recycling rates are high with an average of 74%, over 70% of it is downcycled (European Circular Economy Stakeholder Platform, 2021). Waste wood accounts for approximately 60 million tonnes annually, with around 49% going to energy-to-waste (ETW) plants and around 51% to products like chipboard (Business Waste, 2024), thus massively underutilised, especially as wood is considered to be a valuable bio-based and renewable resource.

In an interview with Hester ten Zijthoff, project manager of Ymere, one of the biggest housing corporations in the Netherlands, challenges in utilising waste wood to its fullest potential were highlighted. Particularly issues of chemical contamination as a result of paints and impregnating agents, metal presence, and varying shapes make high-quality reuse labor-intensive and complex. These issues significantly hinder mass production, leading to prohibitive costs. Additionally, the lack of high-quality reuse examples and an insufficient budget for innovation obstruct its implementation in housing corporations' renovation strategies, despite its potential as a valuable bio-based waste stream resource (Dantuma & Van Sante, 2018).

Wood dust, a byproduct of wood processing, although, offers huge potential for high-value facade applications, as discovered during an internship with "Circular Wood 4 The Neighbourhood," which focuses on reusing waste wood utilising robotic fabrication techniques for furniture projects. Traditionally, wood dust of housing corporations ends up in ETW plants, yet its small uni-

form nature offers vast possibilities for mass production and offers huge amount of design freedom. When wood dust fibers are mixed with a natural matrix, they can transform into a biocomposite with excellent insulating properties (Bahar et al., 2023; Abdallah et al., 2022; Lertwattanaruk & Suntijitto, 2015), which can be of significant value for housing corporations' facade renovations.

Biocomposites are gaining momentum as sustainable alternatives to synthetic composites, while insufficient processing methods and high fabrication costs previously limited their development (Zwawi, 2021). Biocomposites, also known as Natural Fiber Composites (NFC), consist of biopolymer-based matrices intermixed with lignocellulosic fibers (Jawaid & Khalil, 2011) - like wood dust - and are the main focus for research and development due to their renewable, biodegradable, and non-toxic nature (Jayamani et al., 2015). Alternatively, synthetic composites, so-called Fiber-Reinforced Plastics (FRP), consist of synthetic matrices intermixed with inorganic fibers (Jawaid & Khalil, 2011). Despite their significant mechanical properties over NFC, there are several drawbacks associated with synthetic composites; they cause pollution, emit toxic byproducts, require enormous amounts of energy for production, have poor recyclability of merely 25%, and negatively impact the depletion of finite petroleum (Zwawi, 2021).

Biocomposites hold the potential to eradicate the dependency on synthetic matrices and fibers, but their inferior mechanical properties and poor UV/water resistance lead to early degradation, affecting their long-term durability and possible applications (Zwawi, 2021). Consequently, the scientific community has been paying considerable attention to developing various methods to alter the properties of biocomposites to attain properties similar to those of synthetic composites (Jayamani et al., 2015).

Particularly biocomposite facade panels hold the potential not only to address insulation and aesthetic shortcomings, as the majority of the building stock is visually outdated, but also to improve the acoustic performance, thermal performance by offering shading, wind conditions, biodiversity, psychological well-being, and mitigate the urban heat island effect.

This circular approach of utilising waste wood dust fibers to create insulating biocomposite facade panels could offer housing corporations an environmentally-friendly - and potentially financially-friendly - solution for upgrading their residential stock to meet their environmental objectives, while simultaneously pushing the construction sector towards a sustainable future.

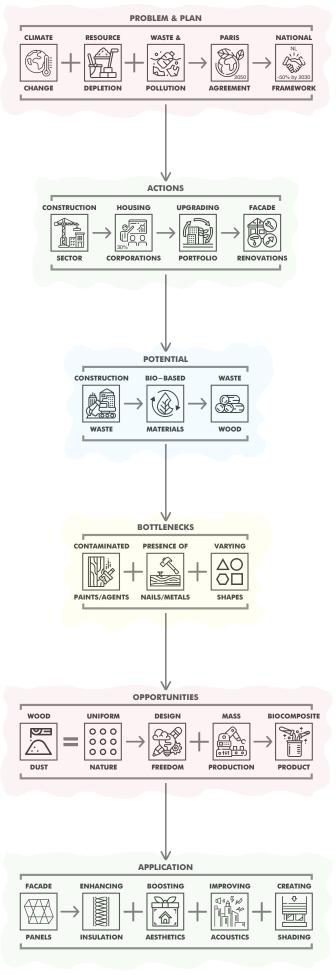


Figure 1.1.2. Introduction scheme. Icons retrieved from Flaticon.com

Current literature is widely spread: from examining the influence of wood dust content on the biocomposites' mechanical properties, UV/water resistance, and acoustic performance, to the effect of various fiber and matrix modification treatments and different fabrication methods. Many of these projects repeat similar experiments with minor changes in material composition or treatment content, and share the same objective of enhancing the biocomposites' properties. None of them have yet considered the bigger picture and combined all the individual pieces of research, making it hard to obtain insight into the potential properties of wood dust grafted biocomposite facade panels, especially because many of these interventions have nonlinear and conflicting impact on its performance.

For this reason, this thesis aims to provide insight into the potential properties of wood dust crafted biocomposite facade panels by developing an interactive design tool that guides its user toward optimal performance based on various material properties and design options.

In a broader perspective, this research on wood dust crafted biocomposite facade panels is rather part of preliminary research than the main focus of this thesis, which instead focuses on improving the design process of building facades in general. Within this thesis, biocomposites serve as a relevant and sustainable case study material, where any facade material could have been chosen.

1.2 Problem analysis

Aligning with today's world, where everything is more data-driven than ever before, designers increasingly rely on quantifiable metrics for decision making, especially in the early design stage (Turrin et al., 2020). However, given the immense architectural impact of building facades, qualitative metrics will always remain of great importance. As an alternative to the traditional design framework where designers make decisions based on their knowledge and experience, optimisation frameworks employ genetic algorithms to search for optimal solutions in vast design spaces. Exploring design alternatives based on both geometry and performance is often challenging. While manual exploration of the design space is impractical due to the huge number of design alternatives, optimisation frameworks overlook a huge part of the qualitative aspects that are crucial in facade design. However, performance-driven design exploration frameworks are posing a solution, by leveraging machine learning techniques, giving designers the ability to navigate the entire design space according to geometry typology and performance (Danhaive & Mueller, 2021; Turrin et al., 2020).

Current literature related to the design process of building facades, generally focuses on multi-objective optimisation (Brown et al., 2016; Vazquez & Walker, 2021), potentially missing out on valuable design alternatives with high qualitative value. In some cases (Minaei & Aksamija, 2020; Choo & Janssen, 2015), surrogate models are employed to optimise the computational process of multi-objective optimisation frameworks, by substituting slow performance simulations with fast approximation models. Nevertheless, these frameworks still revolve around optimisation, and have the same limitations of overlooking crucial qualitative aspects. In very rare cases, when performance-driven design exploration frameworks are used in facade design, several critical parts are missing, making them significantly less effective.

As an example, Bertagna et al. (2021) employed a Self-Organising Map (SOM) in the design process of a load-bearing concrete diagrid facade, as illustrated in Figure 1.2.1, clustering 12,758 design variants onto a two-dimensional network of nodes, according to their geometric characteristics.

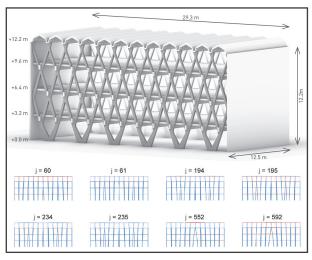


Figure 1.2.1. Diagrid facade. Adapted from "Holistic Design Explorations of Building Envelopes Supported by Machine Learning", by Bertagna et al., 2021 [17].

After assessing each design alternative' structural and thermal performance, the self-organising map allows for exploration, considering qualitative and quantitative metrics. However, the absence of a surrogate model not only makes the design framework computationally intensive, but also limits its ability to adapt to more complex design problems.

Additionally, non-geometry related design variables are often excluded from the design process due to limitations of the self-organising map, which clusters based solely on geometry features. This limits design optimisation, as non-geometry related design variables, such as facade panel perforations, hold the ability to influence quantitative performance as well, such as affecting the Sound Pressure Level (SPL) in front of the facade.

Furthermore, the complex relationship between geometry - driven by design variables - and performance lacks interpretability, for both optimisation frameworks and performance-driven design exploration frameworks. This is particularly true for complex design problems with high-dimensional design spaces and multiple performance criteria, as their relationship is often highly non-linear and conflicting. While both multi-objective optimisation' genetic algorithms and surrogate models are able to effectively showcase which combinations of design variables result in well-performing geometries across various performance criteria, they are, without employing sensitivity analysis tools, unable to inform the designer about how each individual design variable affects the performance.

An enhanced interpretability between geometry and performance would have a significant beneficial impact on the design process by offering the designer the ability to reconsider their initially selected design variables, as some of them might not have as big of an impact on the performance as expected and might predominantly affect the geometry, therefore able to be freely tweaked within their original domain. Selecting relevant design variables, affecting both geometry and performance, is crucial as most design problems require high-dimensional design spaces and Self-Organising Maps (SOM) face the curse of dimensionality where the number of design variables have to be limited to prevent sparsity and to ensure it is able to reflect the design space correctly, potentially selecting design variables that predominantly affect geometry, and neglecting those that are highly-relevant, thus significantly affecting the design process' efficiency.

As an example, Turrin et al. (2020) employed a performance-driven design exploration framework comprising a Self-Organising Map (SOM) and a Multi-Layer Perceptron (MLP), in the design process of a long-span roof structure of an indoor arena. Partly due to the curse of dimensionality, as it is asserted that a nine-dimensional design space can be effectively reflected by a two-dimensional SOM, only 4/30 design variables were considered without even knowing their effect on performance.

By solely focusing on design variables that are truly significant, designers can mitigate noise introduced by non-relevant design variables. This not only makes the design process more efficient, but also creates design vectors with stronger underlying patterns, enhancing the surrogate model's performance approximation capabilities. This is particularly beneficial for design problems with high-dimensional design spaces, as their high complexity generally make them more prone to overfitting and a lot harder to generalise.

Additionally, allowing designers to understand the complex non-linear relationships between design variables and performance criteria early on in the design process, based on just a small representative dataset of design vectors and their simulated performance values, would allow for an optimised stratified sampling logic for training the surrogate models. This not only reduces the amount of training data required, reducing the computational demands, especially for higher-complex design problems with detailed simulations, but also improves the surrogate model's generalisation capabilities by focusing on the most relevant design vectors.

Furthermore, it would empower designers with actionable insights to explore the design space faster and more effectively, allowing them to adjust design variables more strategically towards finding optimal solutions from a qualitative and quantitative perspective, facilitating more informed decision making in the early design stage, potentially leading to better architectural and sustainable solutions.

Currently, there are 3 main types of performance-driven design exploration frameworks which are used in the AEC sector, as illustrated in Figure 1.2.2. They all commence similarly by employing a parametric model, controlled by geometry-related design variables, creating a vast design space with numerous design alternatives, and all have some sort of performance assessment, often utilising surrogate models to optimise the computational process. Apart from their similarities, each design framework has its distinct characteristics and qualities, and choosing between them fully depends on the specific nature of the design problem.

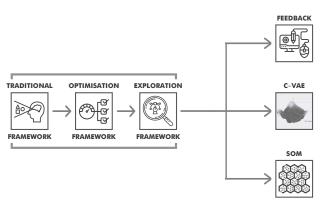


Figure 1.2.2. Design frameworks scheme. Icons retrieved from Flaticon.com

The first performance-driven design exploration framework that is utilised in the AEC sector is the real-time feedback framework. This design framework allows the designer to tweak design variables freely with real-time changing performance approximations guiding the design exploration process towards high performance. Despite empowering the human designer with control over the design process and AI assisting - rather than taking over

control completely, enhancing the design framework's reliability and making it easier to adapt to from a traditional design framework - it has two significant limitations: a huge number of design alternatives will not be explored and it is difficult for the designer to understand how to adjust the design variables to achieve higher performance, making the design framework more suitable for relatively simple and low-dimensional design problems.

The second performance-driven design exploration framework that is utilised in the AEC sector is called the performance conditioned variational autoencoder framework (c-VAE). This design framework, particularly employed for structural design problems (Danhaive & Mueller, 2021; Balmer et al., 2024), is able to compress high-dimensional data into low-dimensional representations, thereby creating distributions within a so-called latent space. Once created, it is able to project back out of this latent space into high-dimensional data again. In simple terms, the c-VAE projects design alternatives, paired with their approximated performance, from a huge design space onto a threedimensional surface and focuses on the ones that perform well, based on an adjustable predefined threshold, enabling the designer to explore the design space. Despite offering excellent guidance towards high quantitative performance, the design framework lacks overview of the design space from a qualitative perspective, making it highly performance-oriented. Although this would be perfectly fine for most structural design problems, it is less suitable for most facade design problems due to their superior architectural impact.

The third performance-driven design exploration framework that is utilised in the AEC sector is the Self-Organising Map (SOM) framework. By clustering design alternatives onto a two-dimensional network of nodes, according to their geometric characteristics, the designer is able to navigate the entire design space according to geometry typology and approximated performance. While offering an excellent overview of the design space from a qualitative perspective, their design exploration process, consisting of between-cluster and insidecluster exploration, lacks balanced human-AI interaction. Particularly, inside-cluster exploration, involving the exploration of hundreds of similar design alternatives, is overly AI-dominant and lacks interactivity with the human designer, making the design framework less effective and intuitive.

Consequently, the problem statement of this thesis is: "The implementation of performancedriven design exploration frameworks in facade design is in a very early stage, and significant enhancements must be made to make them more effective."

1.3 Objective

In light of these challenges, this thesis proposes a novel performance-driven design exploration framework, inspired by the SOM framework, employed in the design process of a biocomposite facade. Instead of Multi-Layer Perceptrons (MLP), today's foundational deep learning models for approximating non-linear functions, this thesis hitches on recent groundbreaking research by Liu et al. (2024), from Massachusetts Institute of Technology, introducing Kolmogorov-Arnold Networks (KAN) as a highly-promising surrogate model alternative.

Different from MLPs static activation functions on neurons and learnable weights on edges, KANs have static sum operations on their neurons and learnable 1D parametrised B-spline univariate activation functions on their edges between their neurons, allowing them to fully understand how each individual input variable affects the surrogate model's predicted output (Liu et al., 2024). Where SOM-MLP-based design frameworks are highly inefficient at providing insights into the relationship between geometry and performance, due to their complex architectures based on weights, and the addition of sensitivity analysis tools result in overengineered frameworks with poor usability, SOM-KAN-based design frameworks hold the ability to overcome these hurdles as an all-in-one solution.

Additionally, making the surrogate model's decision-making process transparent, unlike sensitivity analysis tools which are only able to offer output-level insights, fosters trust between human designers and AI, crucial for AI to be smoothly integrated into current design practices, especially as many designers remain hesitant to shift from traditional workflows to AI-driven workflows due to concerns about AI's reliability coupled with their partial loss of control over the design process.

Furthermore, Liu et al. (2024), Yang et al. (2024), Bozorgasl & Chen (2024), and Samadi et al. (2024) claim that KANs are capable of outperforming MLPs from an accuracy, convergence, neural scaling efficiency, and a catastrophic forgetting perspective as well, achieving this with much smaller model architectures. This not only reduces computational demands significantly, particularly due to its faster convergence, minimising the amount of training data required to yield acceptable prediction accuracies - assuming sufficient representativeness of the dataset - as well as for optimising the surrogate model's stratified sampling logic, but also make them more adaptable to higher-complex design problems and a lot easier to work with.

In addition to providing interpretability between geometry and performance through the integration of Kolmogorov-Arnold Networks (KAN) into

a SOM-based design framework, this thesis proposes a novel design exploration process, consisting of an orientation and fine-tuning phase, not only aiming to balance human-AI interaction more efficiently, making design exploration more interactive, thereby more effective and intuitive, but also to include less-geometry related design variables, enhancing its optimisation capabilities.

Consequently, the objective of this thesis is to develop a novel performance-driven design exploration framework integrating Self-Organising Maps (SOM) and Kolmogorov-Arnold Networks (KAN), that advances the facade design process by enhancing computational efficiency, performance approximation accuracy, interpretability, reliability, and usability, to facilitate more efficient decisionmaking in the early design stage.

1.4 Research questions

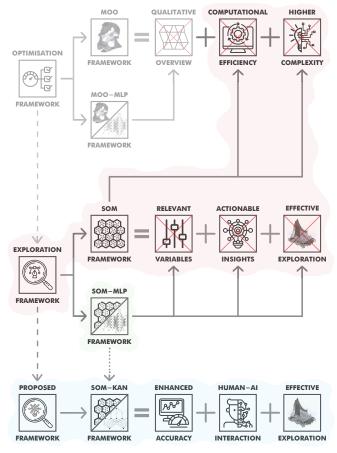
Hence, the main research question of this thesis is: "How can a performance-driven design exploration framework, integrating Self-Organising Maps (SOM) and Kolmogorov-Arnold Networks (KAN), advance the facade design process by enhancing computational efficiency, performance approximation accuracy, interpretability, reliability, and usability, to facilitate more efficient decision-making in the early design stage?". Following this, the sub-questions are:

- 1. "How can a parametric model using Rhino 3D and Grasshopper create a vast design space of biocomposite facade design alternatives, controlled by geometry-related design variables?"
- 2. "How can a Self-Organising Map cluster these biocomposite facade design alternatives onto a two-dimensional network of nodes, according to their geometric characteristics?"
- 3. "How can a Kolmogorov-Arnold Network predict the performance of these biocomposite facade design alternatives, while providing interpretability between geometry and performance?"
- 4. "How can interpretability between geometry and performance enhance the design exploration process during the fine-tuning phase, guiding the designer interactively towards optimal performance?"

1.5 Relevance

The main relevance of this thesis lies in its ability to not only advance the facade design process by integrating Kolmogorov-Arnold Networks (KAN) as a surrogate model within a Self-Organising Map (SOM) based design framework, which is currently the most advanced performance-driven design ex-

ploration framework in facade design, overcoming limitations associated with its computational efficiency and adaptability to higher-complex design problems, but also to offer a design framework that can be extended to advance design practices across the entire AEC sector by offering more accurate performance approximations and more informative interactions between human designers and AI, ultimately making the design process more effective, intuitive, reliable, and less computationally intensive.



 $\textbf{Figure 1.5.1.} \ \textbf{Relevance overview scheme.} \ \textbf{Icons retrieved from Flaticon.com}$

In a broader perspective, this thesis contributes to the research community by demonstrating the potential of Kolmogorov-Arnold Networks as a promising surrogate model alternative to traditional Multi-Layer Perceptrons, by systematically comparing KANs with identical MLPs, as well as those with four, eight, and sixteen times as many nodes, across varying levels of performance approximation complexity, evaluating R²-scores at intervals of 300 samples up to 6,750 samples, offering insights into KAN's efficiency in approximating non-linear functions as training data and performance approximation complexity increases, relative to MLPs.

Additionally, this thesis advances the body of knowledge on biocomposites, through the development of an interactive design tool, providing insight into the potential properties and applications of those crafted from wood dust and polylactic acid.

1.6 Methodology

In phase I, a parametric model using Rhino 3D and GH will be employed to create a vast design space of biocomposite facade design alternatives, controlled by 9 out of 19 optional geometry related design variables, creating a nine-dimensional design space. Aiming to consider 27,000 design alternatives, each variable will be assigned an own range and interval.

In phase II, a SOM will be trained using all possible combinations of normalised geometry-related vectors of 3 out of 9 design variables, identified as the most influential on geometry, clustering 125 design variants onto a two-dimensional 15x15 hexagonal node network, according to their geometric characteristics. After optimising the SOM's clustering performance through a hyperparameter tuning process, the 125 node design vectors, together with 6,625 vectors sampled during stratification to ensure proper generalisation - representing 25% of the entire dataset - will be used to conduct performance simulations for material use (GH), solar heat gains (Ladybug), and sound pressure level (PachyDerm), creating representative labeled datasets for training three KANs, one for each metric.

In phase III, the KAN models will be trained to approximate the performance of all design alternatives with maximum accuracy. After optimising their prediction accuracy through a hyperparameter tuning process, they will be systematically compared with various MLP models to evaluate their prediction accuracy as training data and comlexity increases. Following this, the KAN models will be used to create plots showing the percentual impact of each design variable on performance predictions, enabling designers to identify and focus on relevant design variables that affect both, while also empowering them with actionable insights to adjust design variables strategically toward optimal performance. These plots will be validated through sensitivity analysis results and personal assessment.

In phase IV, two design exploration phases will be employed: an orientation phase allowing designers to navigate the SOM according to geometry typology and approximated performance, facilitating fast design orientation based on variables with high influence on geometry, and a fine-tuning phase focusing on smaller geometric changes within a selected best-performing design from the orientation phase, allowing designers to adjust design variables strategically based on real-time performance feedback and actionable insights provided by the KAN models. To validate the design exploration framework's effectiveness, it will be employed in practise and compared with traditional SOM-based between cluster and inside cluster design exploration phases with feedback obtained through a questionnaire.

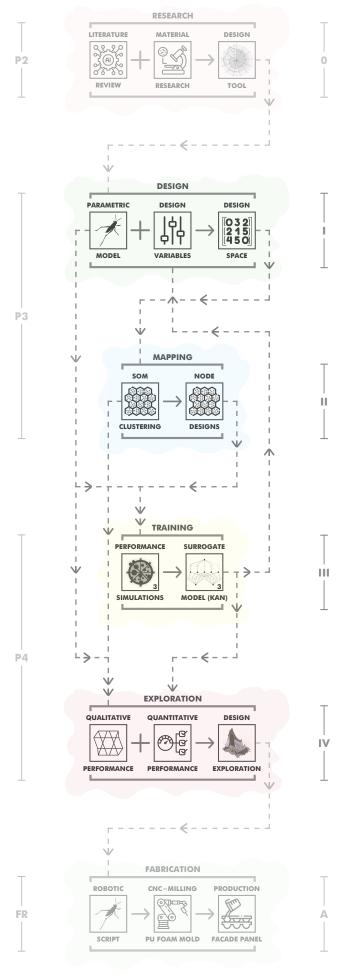


Figure 1.6.1. Methodology scheme. Icons retrieved from Flaticon.com