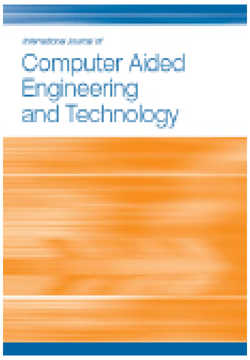
Inderscience Publishers
Linking academia, business and industry through research



International Journal of Computer Aided Engineering and Technology

ISSN online: 1757-2665 - ISSN print: 1757-2657
https://www.inderscience.com/ijcaet

Comparing open-source optimisation algorithms for functionally graded material design: a thermoelastic case study

Ryoichi Chiba

DOI: 10.1504/IJCAET.2024.10063825

Article History:

Received:	02 September 2023
Last revised:	22 January 2024
Accepted:	07 March 2024
Published online:	22 May 2024

Comparing open-source optimisation algorithms for functionally graded material design: a thermoelastic case study

Ryoichi Chiba

Department of Mechanical Engineering,
Sanyo-Onoda City University,
Sanyo-Onoda, 756-0884, Japan
Email: chiba@rs.socu.ac.jp

Abstract: In this study, we apply black-box optimisation (BBO) techniques using an open-source BBO framework, Optuna, to optimise the material composition of functionally graded materials (FGMs), specifically targeting residual thermal stress reduction in a uniformly cooled multi-layered FGM plate. We focus on three algorithms with an aim to compare their performance: the tree-structured Parzen estimator (TPE), the covariance matrix adaptation evolutionary strategy (CMA-ES), and the non-dominated sorting genetic algorithm II (NSGA-II). Our findings indicate that CMA-ES excels in optimisation quality, outperforming TPE and NSGA-II, despite TPE's rapid convergence. We also observe that accounting for interactions among design variables may not always be beneficial and can hinder the optimisation process. This study not only showcases the effectiveness of BBO in material science but also guides material designers in selecting suitable optimisation techniques for complex engineering challenges.

Keywords: optimal design; functionally graded material; FGM; thermal stress; thermoelasticity; black-box optimisation; BBO.

Reference to this paper should be made as follows: Chiba, R. (2024) 'Comparing open-source optimisation algorithms for functionally graded material design: a thermoelastic case study', *Int. J. Computer Aided Engineering and Technology*, Vol. 19, No. 1, pp.1–12.

Biographical notes: Ryoichi Chiba has devoted his career in theoretical research on thermoelasticity in composite materials, with a focus on applying probabilistic methods for engineering issues and developing new reliability designs for advanced materials. His research extends to heat and mass transfer, including experimental and numerical studies on heat transfer with phase change, conducted in partnership with an air-conditioning company. His collaborative efforts have involved multiple Japanese universities, such as Iwate University, Ishinomaki Senshu University and Yamagata University. Since 2008, his focus has shifted towards plastic working, aiming at creating high value-added materials via methods like rolling, extrusion, and drawing. In 2016, he began an atomistic study on grain boundary stability in metals, in collaboration with Thai researchers. His recent efforts are directed towards enhancing sheet metal formability using friction stir processing technology.

1 Introduction

Functionally graded materials (FGMs) are designed with advanced characteristics to serve specific purposes, including reducing thermal stress, enhancing resistance to wear and corrosion, and improving biocompatibility in medical implants (Saleh et al., 2020). These materials, characterised by a gradual change in composition and/or structure, represent a significant advancement in material science and engineering. Arising from the need to mitigate issues of material incompatibility and thermal stress concentration in composite materials, FGMs have been increasingly used since their development in the late 20th century.

The design of FGMs is crucial in applications where materials undergo significant thermal cycles or are subjected to high thermal gradients. Thermoelastic properties of materials govern their response to temperature changes, influencing how they expand, contract, and experience internal stresses. This is particularly pertinent in applications like aerospace and power generation, where materials are regularly exposed to extreme and fluctuating temperatures. To maximise the effectiveness of such heat resisting FGMs, it is essential to tailor the distribution of their material composition to the specific conditions of their intended use. However, finding the optimal material composition profiles of FGMs is challenging due to the intricate relationships between the profile control parameters and the resultant functionality. This optimisation challenge is well-suited for black-box optimisation (BBO) (Alarie et al., 2021), a method used when the objective function is overly complex or not expressible in a closed mathematical form.

Our study explores the use of BBO techniques, particularly focusing on algorithms available in an open-source BBO framework, Optuna (Akiba et al., 2019), for optimising material composition in FGMs exposed to an extreme temperature change. Optuna has garnered significant academic attention due to its robust framework and the range of algorithms it offers for both single- and multi-objective optimisation. Optuna introduces a novel approach to optimisation in our study, characterised by three key features:

1. Define-by-run context, which allows for dynamic construction of the optimisation search space.
2. Efficient sampling, employing both relational and independent sampling for comprehensive parameter exploration.
3. Ease of setup, facilitating its application across various tasks, enhancing accessibility to advanced optimisation techniques.

The underlying motivation of our study is to demonstrate the broader applicability of Optuna in the intricate domain of material science, particularly for the material composition optimisation of FGMs, beyond its conventional use in hyperparameter tuning for machine learning (Hanifi et al., 2022). Key advantages of Optuna, such as its ease of setup and cost-free access, present a significant opportunity for material designers, offering a viable alternative to the traditionally used costly software or custom-coded optimisation programmes corresponding to each algorithm (Nayak and Armani, 2022).

While our study primarily focuses on the application of Optuna in FGM optimisation, it is worth acknowledging recent advancements in related areas of neural network-based system control and optimisation, as explored in Chaturvedi et al. (2023), Kumar et al. (2017, 2018), Kumar and Srivastava (2020) and Kumar (2023a, 2023b). These works contribute valuable insights into the broader field of computational optimisation and control dynamics. Although they employ different methodologies and focus areas – such as the use of various neural network models for system identification and control – the underlying principles of advanced computational techniques and optimisation strategies present a contextual backdrop to our research. This highlights the multifaceted nature of optimisation challenges across different scientific domains, providing a broader perspective to our exploration of Optuna's capabilities in material design.

On an optimisation problem aimed at minimising the residual thermal stress of a uniformly cooled multi-layered FGM plate (Cho and Ha, 2002), we assess the performances of three key algorithms Optuna offers: the tree-structured Parzen estimator (TPE), the covariance matrix adaptation evolutionary strategy (CMA-ES) and the non-dominated sorting genetic algorithm II (NSGA-II). Each algorithm brings a unique approach to the optimisation problem, and their efficacy in FGM design represents a novel area of exploration. The primary goal of our study is to evaluate and compare the effectiveness of these BBO algorithms in optimising the material composition of FGMs for reduced thermal stress. Through this concise yet thorough analysis, our study aims to provide a clearer understanding of the strengths and limitations of these algorithms in material design applications. Our findings not only contribute to the theoretical understanding of BBO in FGM design but also offer practical insights for material designers in selecting appropriate optimisation techniques.

This paper is structured as follows: Section 2 presents our approach to the material composition design for FGMs, detailing the thermal stress analysis and outlining the optimisation problem to be solved. Section 3 offers an overview of the three BBO algorithms used: TPE, CMA-ES and NSGA-II. In Section 4, we present the results of our optimisation efforts, comparing the performance of the three algorithms in the context of our themoelastic case study. We discuss the implications of these results, both in terms of algorithm efficiency and material design outcomes. Section 5 concludes the paper, summarising key findings.

2 Material composition design workflow

2.1 Thermal stress analysis

Our study focuses on the material composition design of a uniformly cooled Ni-Al_2O_3 FG plate, following the benchmark model proposed by Cho and Ha (2002) and Cho and Shin (2004). As illustrated in Figure 1, the design involves a traction-free 12-layered FG plate with infinite length and width, where the variation in material composition is solely along the thickness direction or z-axis. The plate's total thickness is denoted by h. The first layer, consisting of pure Ni, and the 12th layer, pure Al_2O_3, each have a dimensionless thickness of $a_1 / h = (a_{12} - a_{11}) / h = 0.1$. The intermediate ten layers, sandwiched between these two layers, all have a uniform thickness of 0.08 in dimensionless units. This plate structure is subjected to a uniform temperature drop, from an initial temperature T_0 to a lower temperature T_1.

After the cooling process, in-plane thermal stresses remain within the FG plate. The residual thermal stresses can be calculated through an analytical solution derived by Sugano (1987) for a traction-free plate, where the inhomogeneity and temperature variations are exclusively along the thickness direction, as follows:

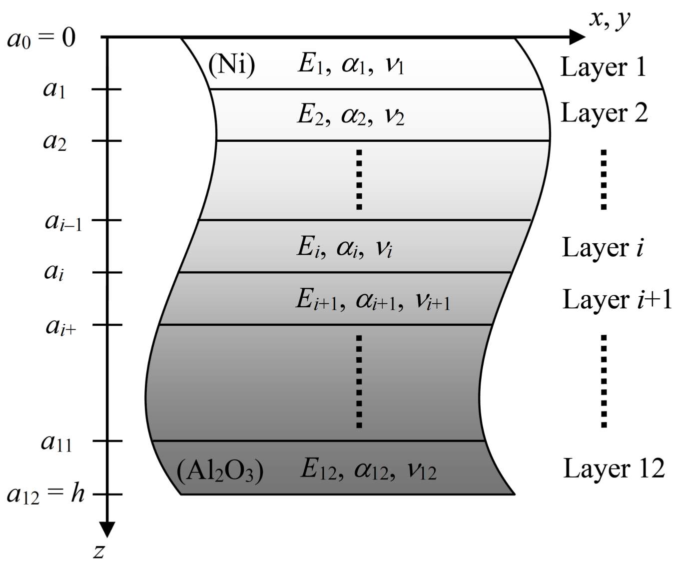
$$\sigma_{xx} = \sigma_{yy} = \frac{E(z)}{1-v(z)}\left[-\alpha(z)\Delta T(z) + \frac{(I_2 z - I_3)\Phi_1 + (I_2 - I_1 z)\Phi_2}{I_2^2 - I_1 I_3}\right], \tag{1}$$

where

$$I_j = \int_0^h \frac{z^{j-1}E(z)}{1-v(z)}dz,\ j = 1, 2, 3, \tag{2}$$

$$\Phi_j = \int_0^h \frac{z^{j-1}E(z)\alpha(z)\Delta T(z)}{1-v(z)}dz,\ j = 1, 2. \tag{3}$$

Figure 1 Analytical model of functionally graded infinite plate and coordinate system



In the above equations, E, α and υ represent the Young's modulus, thermal expansion coefficient and Poisson's ratio, respectively, and ΔT denotes the temperature difference between the temperature T and the initial temperature T_0.

Table 1 Material properties of nickel and alumina

Material properties	*Ni*	*Al_2O_3*
Young's modulus [GPa]	199.5	393
Poisson's ratio [–]	0.3	0.25
Thermal expansion coefficient [$\times 10^{-6}$/K]	15.4	7.4

Source: Cho and Ha (2002)

Table 1 presents thermoelastic material data for Ni and Al_2O_3 (Cho and Ha, 2002). To estimate the effective material properties of the FG plate, the modified rule of mixture method is utilised, which is detailed in Cho and Ha (2001).

2.2 Optimisation problem

The primary goal of our optimisation is to determine the optimal volume fraction of Al_2O_3 in each of the intermediate ten layers of the FG plate. The ceramic (Al_2O_3) volume fractions in these layers are represented as a vector, $\mathbf{V} = [V_2, V_3, \ldots, V_{11}]$. The objective function $f(\mathbf{V})$ to be minimised is defined as the maximum absolute value of non-dimensionalised σ_{xx}, which is evaluated across the entire thickness of the plate. The optimisation problem is thus formulated as:

$$
\begin{aligned}
&\textit{Design variable} && \mathbf{V}, \\
&\textit{Minimise} && f(\mathbf{V}) = \max_{z \in [0,h]} \left| \frac{\sigma_{xx}(z)}{E_{\mathrm{m}} \alpha_{\mathrm{m}} (T_1 - T_0)} \right|, \\
&\textit{Subject to} && 0 \le V_i \le 1,\ i = 2, 3, \ldots, 11, \\
& && V_i \le V_{i+1},\ i = 2, 3, \ldots, 10,
\end{aligned}
\tag{4}
$$

where E_m and α_m are the Young's modulus and thermal expansion coefficient of metal (Ni), respectively.

3 Optimisation algorithms

Out of the optimisation algorithms available in Optuna, three diverse algorithms – TPE, CMA-ES and NSGA-II – are evaluated. These algorithms can be classified under the sequential model-based optimisation approach (TPE) and evolutionary algorithms (CMA-ES and NSGA-II). Each algorithm is described briefly in the following subsections.

Our optimisation calculations are terminated after 10,000 trials, with each trial representing an evaluation of the objective function. These calculations are conducted on a desktop computer with a Core i5-10400 CPU and 8 GB RAM in a Python-based environment. Default settings are applied for each algorithm unless otherwise mentioned. For in-depth information, consult the official Optuna documentation (Optuna_Contributors, 2023).

3.1 Tree-structured Parzen estimator

TPE (Bergstra et al., 2011) is a sophisticated method used for BBO, particularly useful for high-dimensional and complex problems. It is the default algorithm in Optuna for single-objective optimisation tasks and is frequently used for hyperparameter optimisation in machine learning. Being a Bayesian optimisation technique, TPE skilfully incorporates prior probability to guide its search for the optimal parameters.

In Bayesian optimisation, the goal is to find the minimum (or maximum) value of an unknown objective function by constructing a probabilistic model. TPE models the conditional probability $P(x|y)$ in a unique manner, dividing the observed parameter space into two regions based on a performance threshold y^*, where x represents a design variable (e.g., material composition in a layer) and y the associated objective function (e.g., thermal stress). It employs two density functions: $l(x)$ for observations with performance better than the threshold, and $g(x)$ for those worse than the threshold. This is expressed mathematically as

$$P(x \mid y) = \begin{cases} l(x) & \text{if } y \le y^* \\ g(x) & \text{if } y > y^* \end{cases}. \tag{5}$$

This bifurcation facilitates a more effective search as TPE samples more from regions where the performance is better. The expected improvement (EI) criterion used in TPE is then derived from these densities, guiding the selection of the next set of design variables to evaluate.

In Optuna, the best observed objective function value so far is adopted as y^*. Therefore, the EI has the following simple relation (Bergstra et al., 2011):

$$EI(x) \propto \frac{l(x)}{g(x)}, \tag{6}$$

where Gaussian mixture models are used to form $l(x)$ and $g(x)$ (Optuna_Contributors, 2023). This formula indicates the likelihood ratio of having improved performance at a new point x. By maximising this EI, TPE selects the next design variables, effectively balancing exploration and exploitation.

This approach focuses the search on areas of the design space that appear most promising based on prior computations. While independent sampling is used by default in Optuna, which assumes that the design variables are independent, we also consider joint sampling (i.e., relational sampling) to account for possible interactions among the design variables.

3.2 Covariance matrix adaptation evolutionary strategy

CMA-ES (Hansen and Ostermeier, 2001) is a robust evolutionary algorithm widely used in BBO, particularly suited for non-separable, ill-conditioned and multi-modal continuous domain optimisation problems. CMA-ES has demonstrated superior performance in various benchmark problems (Loshchilov et al., 2013). This algorithm is employed in the Optuna framework primarily for single-objective optimisation tasks.

At its core, CMA-ES operates by generating a population of candidate solutions, initially modelled as a multivariate normal distribution. The algorithm's primary mechanism involves iteratively updating the distribution's mean $\mathbf{m}$ and covariance matrix $\mathbf{C}$ to adapt to the objective function's landscape. The mean $\mathbf{m}$ represents the centre of the distribution, guiding the search towards regions with optimal fitness values.

The adaptation of the covariance matrix $\mathbf{C}$ is a distinctive feature of CMA-ES. It enables the algorithm to learn the shape of the objective function's contours. The update rule for $\mathbf{C}$ is based on the concept of cumulative step-size adaptation. In each iteration, the algorithm selects a subset of the fittest candidate solutions and computes the weighted average of their covariance matrices. This step ensures that the search distribution adapts to the most promising regions of the solution space.

Mathematically, the update of the mean $\mathbf{m}$ and the covariance matrix $\mathbf{C}$ in each generation g can be expressed as

$$\mathbf{m}_{g+1} = \mathbf{m}_g + \omega \sum_{i=1}^{N} w_i \left(\mathbf{x}_i - \mathbf{m}_g \right), \tag{7}$$

$$\mathbf{C}_{g+1} = \left(1 - c_1 - c_\mu\right) \mathbf{C}_g + c_1 \mathbf{p}_c \otimes \mathbf{p}_c^{\mathrm{T}} + c_\mu \sum_{i=1}^{N} w_i \mathbf{y}_i \otimes \mathbf{y}_i^{\mathrm{T}}, \tag{8}$$

where $\mathbf{m}_g$ and $\mathbf{m}_{g+1}$ are the means of the distribution in the current and next generation, respectively, ω is the learning rate, N is the number of candidate solutions, w_i are the weights assigned to each candidate solution based on its fitness, with fitter solutions receiving higher weights, $\mathbf{x}_i$ represents the i^{th} best candidate solution; $\mathbf{C}_g$ and $\mathbf{C}_{g+1}$ are the covariance matrices in the current and next generation, c_1 and c_μ are coefficients for the rank-one and rank-μ updates of the covariance matrix, respectively, $\mathbf{p}_c$ is the evolution path, which accumulates information about the direction of successive steps, and

$$\mathbf{y}_i = \left(\mathbf{x}_i - \mathbf{m}_g \right) / \eta, \tag{9}$$

in which η (> 0) is a step size.

This adaptive mechanism allows CMA-ES to efficiently explore complex, multimodal optimisation landscapes. It is particularly adept at adjusting its search strategy based on the problem's intrinsic properties, a feature that proves invaluable for challenges like optimising the material composition of FGMs, where the objective function may be complex and poorly understood.

3.3 Non-dominated sorting genetic algorithm II

NSGA-II (Deb et al., 2002), an evolutionary algorithm, serves as Optuna's default algorithm for multi-objective optimisation tasks. In contrast to TPE and CMA-ES, which primarily target single-objective optimisation, NSGA-II is specifically designed to tackle situations where multiple conflicting objectives must be balanced, a common scenario in complex engineering problems.

NSGA-II applies a population-based search approach, employing the principles of natural selection to iteratively evolve a population of candidate solutions. The algorithm utilises concepts such as dominance, crowding distance, and elitism to ensure diversity in the solution set whilst converging towards the Pareto-optimal front. The algorithmic process is described as follows:

1 *Initialisation:* NSGA-II starts with a randomly generated initial population of potential solutions.

2 *Non-dominated sorting:* The population is sorted based on non-domination levels. Here, let $f_i(\mathbf{x})$ be the value of the i^{th} objective function for solution $\mathbf{x}$. It can be said that solution $\mathbf{x}$ dominates $\mathbf{y}$ if

$$\forall i,\ f_i(\mathbf{x}) \le f_i(\mathbf{y}) \text{ and } \exists j,\ f_j(\mathbf{x}) < f_j(\mathbf{y}). \tag{10}$$

Solutions are classified into fronts based on domination. The first front (front 1) is completely non-dominated, the second front is dominated only by those in front 1, and so on.

3 *Crowding distance:* Within each front, solutions are assigned a crowding distance, which measures the proximity of neighbouring solutions. The crowding distance ensures diversity in the solution set. For each solution, the crowding distance is calculated as the sum of normalised distances between the adjacent solutions in each objective.

4 *Selection, crossover, and mutation:* A binary tournament selection based on non-domination rank and crowding distance is used to select parent solutions. Crossover and mutation operators are then applied to create a new population.

5 *Elitism:* Elitism is implemented by combining the parent and offspring populations and selecting the best solutions for the next generation.

6 *Termination:* The algorithm iterates until a termination criterion is met, typically a set number of generations.

Optuna's default crossover operator, the uniform crossover, can sometimes reduce the efficiency of GAs for real-valued representation, as indicated in Picek and Golub (2010). To address this, we have implemented the blend crossover alpha (BLX-α) and the unimodal normally distributed crossover (UNDX) as alternative crossover operators. Furthermore, given NSGA-II's specialisation for multi-objective tasks, we address its less optimal performance in single-objective scenarios by transforming these into bi-objective problems, a technique detailed in Watanabe and Sakakibara (2005). This transformation leverages NSGA-II's strengths by introducing an auxiliary objective, thereby enhancing the algorithm's applicability and effectiveness. The details of this transformation are provided in the Appendix.

4 Numerical results and discussion

Optimisation results obtained with different algorithms are summarised in Table 2. Within the table, the column 'number of trials to reach optimal result first' indicates how many trials are required for the first attainment of the minima of the objective function $f(\mathbf{V})$. Figure 2 illustrates the progression of the optimisation process. The horizontal axis represents the trial number, whilst the vertical axis depicts the cumulative minimum objective values up to that trial.

Table 2 Summary of optimisation results achieved with different algorithms

Algorithm	*Number of trials to reach optimal result first*	*Optimisation result*
TPE with independent sampling	4,212	0.0848
TPE with joint sampling	1,968	0.0901
CMA-ES	6,946	0.0724
NSGA-II* with BLX-α	9,862	0.0725
NSGA-II* with UNDX	9,424	0.0725

Note: *multi-objectivisation is applied.

From Table 2, the superior performance of CMA-ES in optimisation is evident. Additionally, the evolutionary algorithms consistently yield favourable results. A notable observation from Figure 2 is the rapid convergence of the TPE algorithms to the minima, a characteristic of Bayesian optimisation methods like TPE. The TPE methods utilise prior information to make more informed sampling decisions, leading to quicker convergence. On the other hand, the evolutionary algorithms, although slower initially, eventually achieve more desirable outcomes.

Figure 2 Minimum objective values obtained up to each trial in Optuna (see online version for colours)

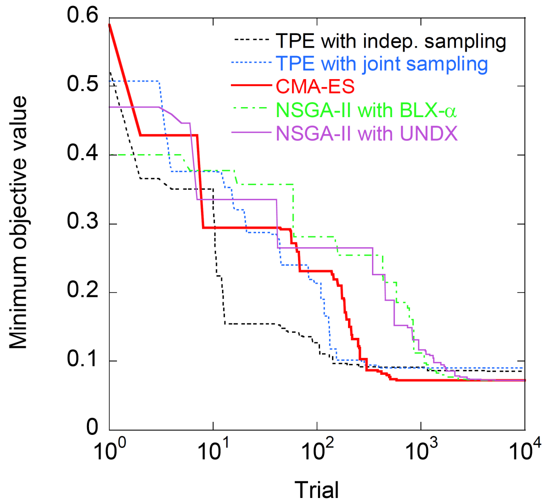
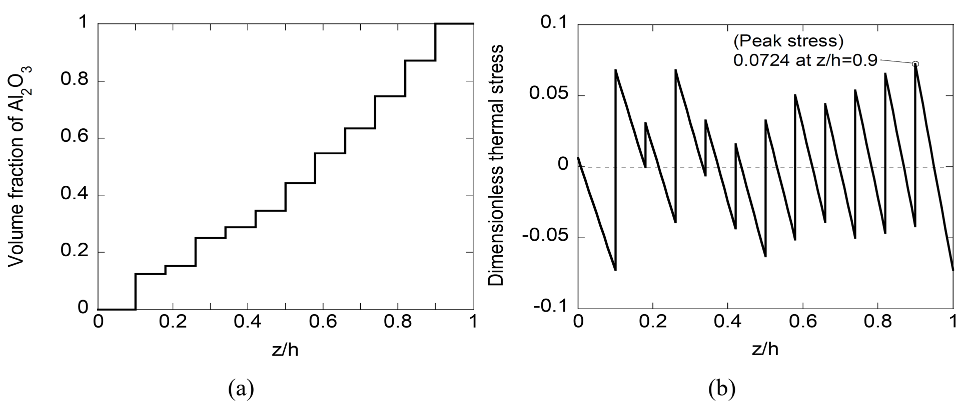


Figure 3 Optimisation results derived from the CMA-ES algorithm, (a) distribution of alumina volume fraction throughout the plate's thickness (b) profile of the residual thermal stress



A comparative analysis between the TPE sampling methods reveals that TPE with joint sampling is more efficient in achieving the initial optimal result, as seen in Table 2. However, its optimisation quality is slightly compromised. When comparing the two variants of the NSGA-II algorithms, negligible differences are observed in their convergence rates and the final optimisation outcomes. The UNDX crossover operator, which can consider interactions among design variables (Ono et al., 1999), shows only a marginal advantage over BLX-α. These suggest that in this specific optimisation problem, such interactions may not be crucial, and factoring them in might sometimes hamper the results.

Figures 3(a) and 3(b) present the optimised volume fraction distribution and its associated residual thermal stress profile, respectively, both derived using the CMA-ES algorithm. An upward concave trend is discernible in the volume fraction changes within the intermediate ten layers, as shown in Figure 3(a). The stepwise nature of these volume fractions causes Figure 3(b)'s stress profile to have pronounced jumps at layer interfaces. The maximum absolute value of residual thermal stress occurs at a dimensionless coordinate value of 0.9 in the pure alumina layer.

5 Conclusions

This study utilised Optuna, an open-source BBO framework, to optimise the material composition of FGMs, with a focus on reducing residual thermal stress in a uniformly cooled multi-layered FGM plate. Our investigation centred on comparing the performance of three algorithms: TPE, CMA-ES and NSGA-II. The key findings are as follows:

1. The CMA-ES algorithm demonstrated the highest optimisation quality, outperforming both TPE and NSGA-II, making it particularly suitable for the challenge of this optimisation task.
2. While TPE algorithms converged quickly, their optimisation quality was surpassed by the evolutionary algorithms, indicating a trade-off between speed and thoroughness.
3. Our study suggests that explicitly considering interactions among design variables may not always be advantageous in optimisation. In certain cases, it could potentially impede the optimisation process.

These insights underscore the effectiveness of BBO techniques in FGM design and highlight the practical implications of choosing suitable optimisation algorithms for specific engineering applications.

References

Akiba, T., Sano, S., Yanase, T., Ohta, T. and Koyama, M. (2019) 'Optuna: a next-generation hyperparameter optimization framework', in *The 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, Anchorage, USA, pp.2623–2631.

Alarie, S., Audet, C., Gheribi, A.E., Kokkolaras, M. and Le Digabel, S. (2021) 'Two decades of blackbox optimization applications', *EURO Journal on Computational Optimization*, Vol. 9, p.100011, DOI: 10.1016/j.ejco.2021.100011.

Bergstra, J., Bardenet, R., Bengio, Y. and Kégl, B. (2011) 'Algorithms for hyper-parameter optimization', in *The 24th International Conference on Neural Information Processing Systems*, Curran Associates Inc., NY, USA, pp.2546–2554.

Chaturvedi, S., Kumar, N. and Kumar, R. (2023) 'A PSO-optimized novel PID neural network model for temperature control of jacketed CSTR: design, simulation, and a comparative study', *Soft Computing*, DOI: 10.1007/s00500-023-09138-0.

Cho, J.R. and Ha, D.Y. (2001) 'Averaging and finite-element discretization approaches in the numerical analysis of functionally graded materials', *Materials Science and Engineering: A*, Vol. 302, No. 2, pp.187–196, DOI: 10.1016/S0921-5093(00)01835-9.

Cho, J.R. and Ha, D.Y. (2002) 'Volume fraction optimization for minimizing thermal stress in Ni-Al_2O_3 functionally graded materials', *Materials Science and Engineering: A*, Vol. 334, No. 1, pp.147–155, DOI: 10.1016/S0921-5093(01)01791-9.

Cho, J.R. and Shin, S.W. (2004) 'Material composition optimization for heat-resisting FGMs by artificial neural network', *Composites Part A: Applied Science and Manufacturing*, Vol. 35, No. 5, pp.585–594, DOI: 10.1016/j.compositesa.2003.12.003.

Deb, K., Pratap, A., Agarwal, S. and Meyarivan, T. (2002) 'A fast and elitist multiobjective genetic algorithm: NSGA-II', *IEEE Transactions on Evolutionary Computation*, Vol. 6, No. 2, pp.182–197, DOI: 10.1109/4235.996017.

Hanifi, S., Lotfian, S., Zare-Behtash, H. and Cammarano, A. (2022) 'Offshore wind power forecasting – a new hyperparameter optimisation algorithm for deep learning models', *Energies*, Vol. 15, No. 19, p.6919, DOI: 10.3390/en15196919.

Hansen, N. and Ostermeier, A. (2001) 'Completely derandomized self-adaptation in evolution strategies', *Evolutionary Computation*, Vol. 9, No. 2, pp.159–195, DOI: 10.1162/106365601750190398.

Kumar, R. (2023a) 'Double internal loop higher-order recurrent neural network-based adaptive control of the nonlinear dynamical system', *Soft Computing*, Vol. 27, No. 22, pp.17313–17331, DOI: 10.1007/s00500-023-08061-8.

Kumar, R. (2023b) 'Memory recurrent Elman neural network-based identification of time-delayed nonlinear dynamical system', *IEEE Transactions on Systems, Man, and Cybernetics: Systems*, Vol. 53, No. 2, pp.753–762, DOI: 10.1109/TSMC.2022.3186610.

Kumar, R. and Srivastava, S. (2020) 'Externally recurrent neural network based identification of dynamic systems using Lyapunov stability analysis', *ISA Transactions*, Vol. 98, pp.292–308, DOI: 10.1016/j.isatra.2019.08.032.

Kumar, R., Srivastava, S. and Gupta, J.R.P. (2017) 'Modeling and adaptive control of nonlinear dynamical systems using radial basis function network', *Soft Computing*, Vol. 21, No. 15, pp.4447–4463, DOI: 10.1007/s00500-016-2447-9.

Kumar, R., Srivastava, S., Gupta, J.R.P. and Mohindru, A. (2018) 'Self-recurrent wavelet neural network-based identification and adaptive predictive control of nonlinear dynamical systems', *International Journal of Adaptive Control and Signal Processing*, Vol. 32, No. 9, pp.1326–1358, DOI: 10.1002/acs.2916.

Loshchilov, I., Schoenauer, M. and Sèbag, M. (2013) 'Bi-population CMA-ES algorithms with surrogate models and line searches', in *The 15th Annual Conference Companion on Genetic and Evolutionary Computation*, Amsterdam, Netherlands, pp.1177–1184.

Ma, X., Huang, Z., Li, X., Qi, Y., Wang, L. and Zhu, Z. (2023) 'Multiobjectivization of single-objective optimization in evolutionary computation: a survey', *IEEE Transactions on Cybernetics*, Vol. 53, No. 6, pp.3702–3715, DOI: 10.1109/TCYB.2021.3120788.

Nayak, P. and Armani, A. (2022) 'Optimal design of functionally graded parts', *Metals*, Vol. 12, No. 8, p.1335, DOI: 10.3390/met12081335.

Ono, I., Satoh, H. and Kobayashi, S. (1999) 'A real-coded genetic algorithm for function optimization using the unimodal normal distribution crossover', *Journal of the Japanese Society for Artificial Intelligence*, Vol. 14, No. 6, pp.1146–1155, DOI: 10.11517/jjsai.14.6_1146.

Optuna_Contributors (2023) *Optuna: A Hyperparameter Optimization Framework* [online] https://optuna.readthedocs.io/en/stable/ (accessed 2 September 2023).

Picek, S. and Golub, M. (2010) 'Comparison of a crossover operator in binary-coded genetic algorithms', *WSEAS Transactions on Computers*, Vol. 9, No. 9, pp.1064–1073.

Saleh, B., Jiang, J., Fathi, R., Al-hababi, T., Xu, Q., Wang, L., Song, D. and Ma, A. (2020) '30 years of functionally graded materials: an overview of manufacturing methods, applications and future challenges', *Composites Part B: Engineering*, Vol. 201, p.108376, DOI: 10.1016/j.compositesb.2020.108376.

Segura, C., Coello, C.A.C., Miranda, G. and León, C. (2016) 'Using multi-objective evolutionary algorithms for single-objective constrained and unconstrained optimization', *Annals of Operations Research*, Vol. 240, No. 1, pp.217–250, DOI: 10.1007/s10479-015-2017-z.

Sugano, Y. (1987) 'An expression for transient thermal stress in a nonhomogeneous plate with temperature variation through thickness', *Ingenieur-Archiv*, Vol. 57, No. 2, pp.147–156, DOI: 10.1007/BF00541388.

Watanabe, S. and Sakakibara, K. (2005) 'Multi-objective approaches in a single-objective optimization environment', in *2005 IEEE Congress on Evolutionary Computation*, IEEE, Edinburgh, UK, Vol. 2, pp.1714–1721.

Appendix

In the field of optimisation, the consensus traditionally leans towards using specific algorithms tailored for the kind of problem at hand – either single or multi-objective. However, recent studies suggest a nuanced approach. Contrary to traditional practices, certain researchers advocate for the utility of multi-objective evolutionary algorithms even in single-objective optimisation tasks (Ma et al., 2023; Segura et al., 2016). Their premise is rooted in the adaptability and potential performance enhancements these algorithms can offer.

In this study, when applying the NSGA-II to the present single-objective task [i.e., equation (4)], we adopt a multi-objectivisation approach as proposed by Watanabe and Sakakibara (2005). This approach necessitates the introduction of an auxiliary objective function, commonly termed as 'helper-objective'. Their method ingeniously uses a slightly modified version of the original objective function as the helper-objective. This modification is achieved by introducing noise to the design variables as follows:

Original objective (to be minimised):

$$F_1(\mathbf{V}) = f(\mathbf{V}), \tag{A1}$$

Helper-objective (to be minimised):

$$F_2(\mathbf{V}) = F_1\left(\mathbf{V} + D \cdot Gauss\,(0,1)\right), \tag{A2}$$

where D is the parameter for adjusting the magnitude of the noise. Based on the findings of Watanabe and Sakakibara (2005), we use $D = 0.05$ for our computations. Note that the value of $\mathbf{V} + D \cdot Gauss\ (0, 1)$ is clipped to the interval between the upper and lower bounds of $\mathbf{V}$.

While this introduction of noise might appear minor, it can significantly influence the optimisation process. The method proposed by Watanabe and Sakakibara is particularly effective in multi-modal optimisation problems with interactive design variables. In these scenarios, introducing such a helper-objective as equation (A2) can considerably enhance the performance of the NSGA-II algorithm.