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# Comparative assessment of material homogenisation techniques

Mertol Tüfekci[1,2⋆], İnci Pir[3], and Ekrem Tüfekci[3]

[1] Center for Engineering Research, University of Hertfordshire, Hatfield, AL109AB, UK
[2] School of Physics Engineering and Computer Science, University of Hertfordshire, Hatfield, AL109AB, UK
[3] Faculty of Mechanical Engineering, Istanbul Technical University, Beyoğlu, Turkey

**Abstract:** This study evaluates the accuracy and computational demands of Mean Field Homogenisation (MFH) and Finite Element Method-Based Homogenisation (FEMBH) for composites. FEMBH requires generating a Representative Volume Element (RVE) to capture the essential microstructural characteristics. The focus is on nanoparticle-reinforced composites, considering the distinct mechanical properties of matrix and inclusion phases, as well as the influence of inclusion geometry, such as aspect ratio and reinforcement orientation. A comparative numerical analysis of various homogenisation techniques is conducted, assuming linear and elastic behaviour for both phases. Also, different FEMBH implementations are examined, including voxel and tetrahedral meshes, to assess their precision and computational efficiency. To represent the effect of the RVE size choice on the accuracy of the results, different RVE sizes are evaluated during the homogenisation process. The Mori-Tanaka method, representing MFH, demonstrates good accuracy in predicting macroscopic behaviour, while FEMBH, particularly with detailed meshing, yields precise results. However, FEMBH requires significant computational resources, especially with increasing aspect ratios and volume fractions of reinforcing particles, which demand higher mesh densities for accurate analysis.

**Keywords:** Material homogenisation, Finite element method, Mori-Tanaka method, Nanoparticle reinforcement, Representative volume element, Computational modelling

## 1 Introduction

Material homogenisation techniques are widely used in creating mathematical models that predict the mechanical properties of composite materials. These techniques are particularly valuable for materials with complex microstructures, such as heterogeneous composites and porous materials. By providing a framework to understand and simulate the behaviour of these materials, homogenisation techniques enable researchers to investigate their mechanical responses effectively, ensuring accurate predictions of their performance under various conditions.

Representative Volume Element (RVE) is the smallest three-dimensional element used in materials science and engineering to understand the macro properties of a material and it is small enough to allow the examination of details in its microstructure. It is especially used for composite materials. This way, calculations made with the RVE aim to reflect the general properties of the material in a homogeneous way. While applying this method, the correct boundary conditions should be defined. Periodic boundary conditions (PBC) are a common technique to allow the RVE to represent a larger volume on this microstructure. By using PBC, it is assumed that the material around the RVE has an infinite structure which is especially important in composite materials and materials with repeating microstructures. In microscale analyses, the RVE represents the smallest unit of the material's microscopic structure, with factors such as the type and geometry of the reinforcement material being considered. Especially in polymer matrix composites, RVE models help understand the load-carrying capacity and overall strength of the composite by analysing the inclusion-matrix interactions at the micro level. Such materials are widely used in applications requiring lightness and high strength in the automotive and aerospace industries. Large-scale structures such as wind turbine blades are optimised with RVE-based simulations to increase the strength of such composites Tüfekci (2023) Tüfekci et al. (2021). Similarly, metal matrix composites (MMC) are also used in industrial applications such as turbine blades due to their high-temperature resistance and low-weight properties Rajak et al. (2020) Swetha et al. (2024).

The difference between using RVE in macro- and microscale analyses lies in the level of detail at the respective scale being examined. in macro-scale analyses, RVE is considered assuming that the material is homogeneous and microstructural details are ignored. While the local stress and deformation distributions of the material are examined in detail at the micro-scale, the general behaviour of the material in large-scale engineering applications is considered at the macro-scale approaches. The differences between these two approaches are also reflected in the calculation methods; while high computational power may be required to analyse the detailed microstructure at the micro-scale, a faster and more generalised analysis can be performed at the macro scale.

The determination of the RVE size and its properties is fundamental in capturing the macroscopic behaviour of heterogeneous materials. Various studies have explored different aspects of RVE, from its size determination to the methodologies used for accurate representation in composite materials. The concept of RVE is central to ensuring that the material's microstructural features are appropriately represented, leading to accurate predictions of the material's overall mechanical properties.

Initial efforts focused on establishing the lower bounds of RVE size, particularly for random heterogeneous materials. This foundational work provided an objective tool for determining RVE size by considering the stochastic stability of the material's

⋆ E-mail address: m.tufekci@herts.ac.uk
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properties, which is crucial for materials with varying inclusion distributions Gitman et al. (2006). The importance of stochastic factors in determining the RVE size highlights the complexity of accurately modelling heterogeneous materials.

The advent of advanced imaging techniques, such as X-ray micro-CT, has significantly improved the accuracy of RVE generation. This method enables the creation of realistic RVEs for particulate-filled composites, where the microstructural features, such as filler shapes and distributions, are captured in great detail. The generated RVEs are then used in finite element analysis (FEA) to predict the material's mechanical properties, showcasing the effectiveness of voxel-based and geometry-based approaches Guven and Cinar (2019).

Complementary to these advancements, the development of micromechanics-based nonlocal constitutive equations has provided deeper insights into the estimation of the minimum RVE size necessary for accurate macroscopic predictions. These studies have demonstrated that, for many composite systems, the minimum RVE size is tightly linked to the microstructural features, such as reinforcement particle sizes and distributions Drugan and Willis (1996).

In highly porous materials and composites, numerical homogenisation techniques have been employed to calculate the RVE size. Such approaches have been validated through experimental measurements, achieving results that closely align with theoretical predictions, such as the Hashin-Shtrikman bounds. The integration of 3D printing with these methods has further enabled the production of porous composites with optimised stiffness and mechanical properties Tarantino et al. (2019).

Integrating computer-aided design tools with FEA has led to the development of automated RVE-based design frameworks. These tools allow for the efficient design and analysis of composites with nanofillers, enabling rapid "what-if" scenarios to optimise composite manufacturing processes Pucha and Worthy (2014). Concurrently, mesh generation techniques for RVEs have evolved, particularly in the context of inclusion-reinforced composites. The introduction of periodic mesh generation schemes has enhanced the accuracy and efficiency of computational homogenisation, making it easier to impose periodic boundary conditions on complex microstructures Sohn (2018).

Further advancements include the development of embedded solid element models within RVEs, which facilitate the prediction of effective elastic constants in discontinuous fibre-reinforced composites. These models simplify the meshing process while maintaining high accuracy, offering an alternative to traditional finite element methods Liu et al. (2016). Additionally, the Extended Multiscale Finite Element Method has emerged as a powerful tool for multiscale analysis, particularly in heterogeneous materials, by bridging the microscopic and macroscopic properties without relying on assumptions of scale separation Liu et al. (2021).

The study of size effects in discontinuous fibre composites has also contributed to understanding the critical RVE size required for accurate property predictions. These investigations have revealed that the critical RVE size is often several times larger than the fibre length, depending on the material's tensile and shear stiffness characteristics Qian et al. (2012). Moreover, the analysis of particle-reinforced composites has shown that microstructural geometry plays a significant role in determining the necessary RVE size for accurate homogenisation Gentieu et al. (2019).

In parallel, the development of Python codes for calculating effective RVE properties under periodic boundary conditions has provided researchers with accessible tools for multiscale optimisation. Such codes facilitate the computation of mechanical properties for composites with periodic structures, allowing for a wide range of material and geometric design experiments Ye and Wang (2017). The boundary element method has also been adapted for homogenising particulate composites, providing a highly efficient approach for analysing large RVEs Okada et al. (2004).

The incorporation of fibre-matrix interphases within RVEs, especially in 2D and 3D microstructures, has been facilitated by the development of specific plugins for commercial software like ABAQUS$^{TM}$. These tools streamline the early stages of analysis by automating geometry generation, thus saving significant time and effort Riaño and Joliff (2019). Exploring the existence and size determination of RVEs across different material response stages, including both elastic and softening behaviours, has further refined the understanding of the RVE concept Gitman et al. (2007).

Advanced algorithms for generating random spatial distributions of fibres and spherical fillers have proven effective in predicting the elastic, damping, and plastic properties of composites. These algorithms enable the creation of RVEs that accurately reflect the microstructural randomness observed in real composite materials, offering improved predictions of macroscopic behaviour Pathan et al. (2017). Voxel-based FEA has also been employed to assess the elastic properties of cementitious materials, demonstrating the robustness of this approach in handling heterogeneous microstructures Shahzamanian et al. (2014).

Mesh generation for complex 3D woven composites remains a challenging task, but recent methodologies have made significant strides in creating conforming meshes at the numerous interfaces within these materials. Such advancements are critical for accurately capturing the mesoscopic behaviour of woven composites Ha et al. (2016). In addition, new techniques for imposing PBC in explicit finite element solvers have been introduced, enhancing the efficiency and reliability of multiscale computational homogenisation Sádaba et al. (2019).

The study of composites reinforced by spatially random distributions of discontinuous fibres has revealed that these materials behave homogeneously at the macroscopic scale despite their microstructural complexity. This finding underscores the importance of accurately generating and analysing RVEs to predict the effective properties of such composites Tian et al. (2015). Efficient methods for generating RVEs with diverse fibre volume fractions have also been developed, enabling researchers to explore the impact of microstructural variations on the elastic properties and anisotropic behaviour of composites Park et al. (2019).

Finally, hybrid approaches that combine the Mori-Tanaka model with finite element methods have been shown to model composites with various reinforcement shapes and orientations effectively. These hybrid methods provide a good balance between computational efficiency and accuracy, particularly for materials with misaligned inclusions Ogierman (2019). The continuum mechanics approach has also been applied to evaluate the effective properties of carbon nanotube-based composites, demonstrating the significant load-carrying capacity of carbon nanotubes within a matrix Chen and Liu (2004).

This study specifically focuses on composites reinforced with nanoparticles, emphasising understanding how the geometry of inclusions—such as their aspect ratio and orientation—affects the mechanical properties of the composite materials. By comparing different Finite Element Method-Based Homogenisation (FEMBH) techniques, including those using tetrahedral and voxel meshes, this research assesses both the accuracy and computational demands of these methods. While the Mean Field Homogenisation (MFH) method, particularly the Mori-Tanaka approach, is well-regarded for making reliable macroscopic predictions, it is less detailed than FEMBH, which, although more computationally intensive, offers precise insights at the microscale level. A key aspect of this study is the generation of RVE that encapsulate the essential microstructural features required for accurate analysis, including the distribution of material properties and the application of periodic boundary conditions. The novelty of this work lies in its comprehensive comparison of various FEMBH implementations, with a particular focus on the influence of mesh types and the geometrical aspects of nanoparticle inclusions on the homogenised properties of composites. This research provides critical insights into the trade-offs between computational efficiency and accuracy in the application of these techniques, offering valuable guidance for future studies and practical applications in material design and analysis.

## 2 Modelling Framework and Computational Approach

### 2.1 Material Properties and Characteristics

This study examines the mechanical behaviour of nanoparticle-reinforced composites using two mathematical homogenisation techniques: Mori-Tanaka Homogenisation MFH and FEMBH. Both approaches treat the matrix and inclusion phases as linear, elastic, and isotropic materials. The matrix material is epoxy resin with an elasticity modulus of 2400 MPa, while the inclusion material is fumed silica, with an elasticity modulus of 70 GPa, details about the material properties are given in Table1 Tüfekci et al. (2023). These material properties were selected to reflect common industrial composites and to enable a comparative analysis across different modelling approaches.

Tab. 1: Material properties of Epoxy and Fumed Silica

| Material | Elasticity Modulus [MPa] | Poisson's Ratio |
|---|---|---|
| Epoxy | 2400 | 0.3 |
| Fumed Silica | 70000 | 0.2 |

### 2.2 Geometric Modelling of Inclusions

To analyse the impact of inclusion geometry on the composite's mechanical properties, three aspect ratios of the inclusions are modelled: 1, 3, and 5. These aspect ratios represent different shapes of the inclusions, varying from spherical (aspect ratio 1) to more elongated forms (aspect ratios 3 and 5). Additionally, the mass fraction of the inclusions within the composite is varied at three levels: 0.5%, 1%, and 1.5%. The variation in the mass fraction is intended to assess how the concentration of inclusions influences the overall mechanical behaviour of the composite.

### 2.3 Mori-Tanaka Homogenisation

The Mori-Tanaka MFH Method is based on the calculation of the elastic properties of the matrix and inclusion phases. First, the elastic moduli and volume fractions of the matrix and inclusion materials that are made up of the composite material are determined. Then, a single inclusion is assumed to be homogeneously distributed in an infinite matrix, and the stress and strain conditions around this particle are calculated. By modelling this local effect with the Eshelby tensor, inclusion-matrix interactions are calculated. The Mori-Tanaka approach determines the effective elasticity modulus of the composite material at the macro scale, considering the average effect of these local effects on the entire material. The mechanical properties of the composite material can be estimated using this method.

The Mori-Tanaka method is applied to predict the effective mechanical properties of the composites. This method relies on the inclusion-matrix interaction to estimate the overall behaviour of the composite material. The MFH technique is used as a benchmark for comparison with the more detailed finite element-based simulations. In this method, the inclusions are assumed to be embedded within the matrix, and their interaction is modelled to derive the macroscopic properties of the composite. This approach is commonly employed for its efficiency in providing quick estimates of composite properties without the need for complex numerical simulations.

### 2.4 Finite Element Method-Based Homogenisation

FEMBH is an important method for understanding the macro-scale behaviour of heterogeneous materials. In this method, a specific displacement is assigned to the RVE representing the composite material. This process involves analysing the deformations and stress distributions in the internal structure of the material. This displacement is the starting point for understanding the macro-level behaviour of the material. The displacements in the volume element are used to determine the stresses in the internal structure of the material. The stress distributions play a critical role in the calculation of the effective elasticity modulus of the composite material because these distributions are directly related to the mechanical properties and behaviours of the matrix and conclusion phases, which affect the elastic properties and deformation response of the material. Thus, the stress data obtained from the determined displacements contribute to the calculation of the macroscopic properties of the composite material and to a better understanding of the overall mechanical behaviour of the material. This approach provides an effective basis for the analysis and design of more complex material systems in engineering applications.

For the FEMBH approach, an RVE is constructed to simulate the microstructural characteristics of the composite, given in Figure 1. The RVE is designed to include the essential features of the microstructure, ensuring that it represents the material's overall behaviour under loading conditions. Periodic boundary conditions are applied to the RVE to replicate the repetitive nature of the microstructure across the material. Two types of mesh configurations are used in the FEMBH simulations: tetrahedral and voxel meshes. These configurations are chosen to investigate the impact of mesh type on the accuracy and computational requirements of the homogenisation process. The tetrahedral mesh, with its flexibility in conforming to complex geometries, and the voxel mesh, with its straightforward grid-based structure, provide a basis for comparing different numerical discretisation strategies.

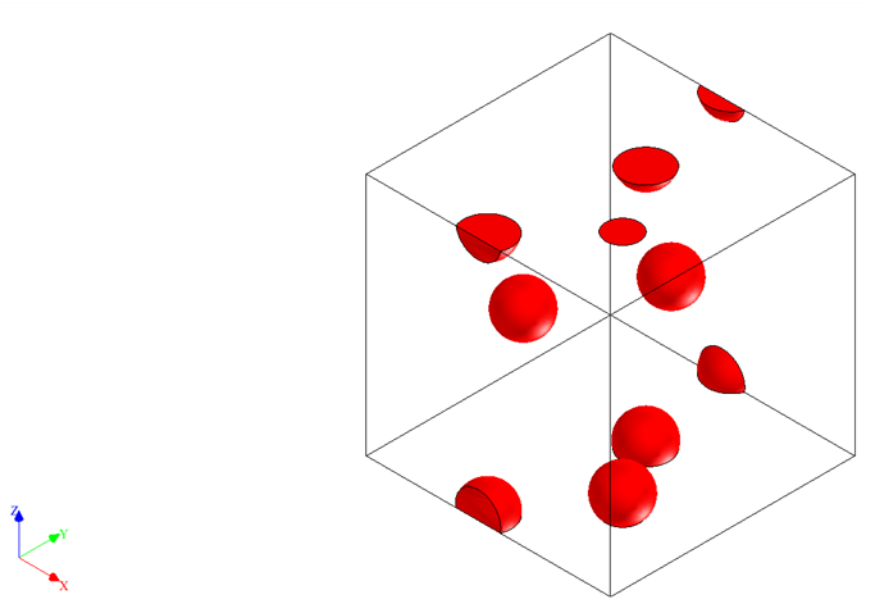
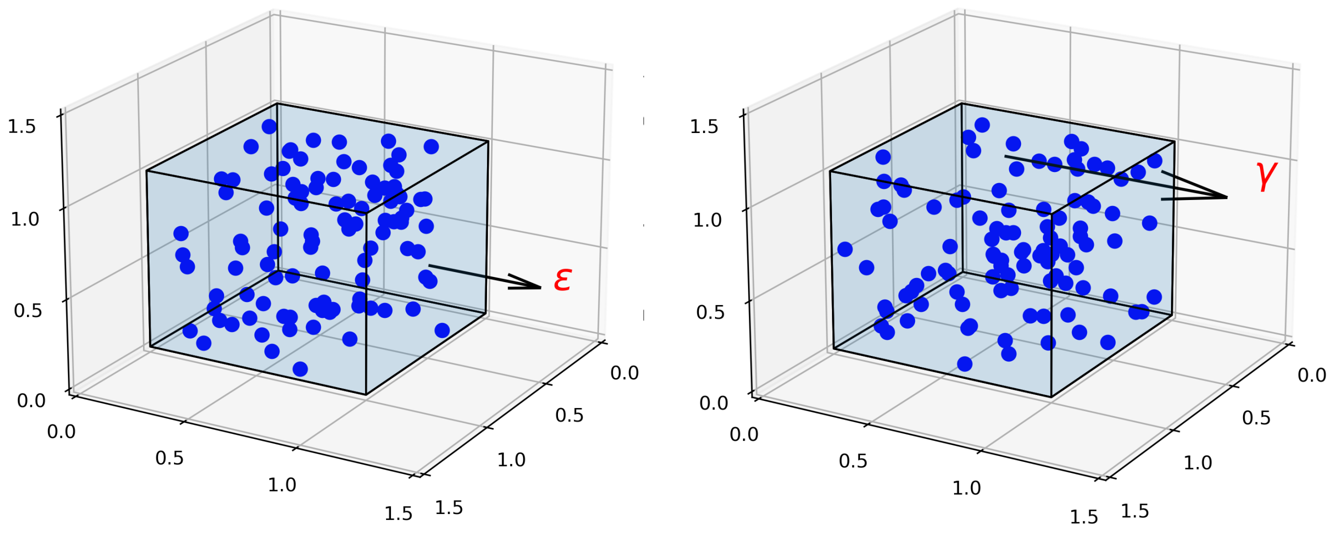


Fig. 1: A constructed RVE.

### 2.5 Numerical Implementation and Simulation Setup

The numerical simulations are conducted by applying uniaxial strain to the RVE models, enabling the computation of effective mechanical properties such as the elasticity modulus, shear modulus, and Poisson's ratio and the simulation steps are picturised in Figure 2. The simulations are executed on a Dell 7820 Tower equipped with an Intel(R) Xeon(R) Gold 6230R CPU and 262144 MB of RAM, which provided the necessary computational resources to handle the detailed FEMBH models. The choice of this high-performance computing setup is dictated by the need to manage the large computational load associated with FEMBH, mainly when using fine mesh resolutions and when simulating composites with high aspect ratio inclusions. The simulations are carefully designed to ensure that the results from the different mesh types and homogenisation methods could be directly compared, allowing for a comprehensive assessment of the strengths and limitations of each approach.




(a) An RVE under uniaxial loading with PBC. (b) An RVE under shear loading with PBC.

Fig. 2: RVEs under uniaxial and shear loding undergoing homogenisation through stress averaging.

## 3 Test Cases for Performance Assessment

In this study, the impact of nanoparticle inclusions on the mechanical properties of composites is investigated, focusing on several important variables. The parameters varied in our simulations, including the aspect ratio of the inclusions, mass fraction of inclusions, and RVE size. The study compares results from the Mori-Tanaka MFH method and the FEMBH using two types of meshes: tetrahedral and voxel. Aspect ratio, mass fraction and RVE Size factors are investigated within the scope of this study. For the aspect ratio of the inclusion case, three distinct inclusion shapes, represented by aspect ratios of 1 (spherical), 3, and 5, are modelled. For the mass fraction of the inclusion case, the mass fractions of nanoparticle inclusions in the composite are varied at three levels: 0.5%, 1%, and 1.5%. For RVE sizes three different RVE sizes, which are 1.5, 3, and 5 times the inclusion diameter, to assess how the choice of RVE size influences the accuracy of the homogenisation techniques are considered. For each set of parameters that are investigated using FEMBH, the procedure is repeated three times to also account for the repeatability. Test cases utilising the FEMBH approach with tetrahedral and voxel meshes and the Fast Fourier Transform (FFT) method are summarised in Figure 3 and test cases evaluated with the MFH method are given in Table 2.

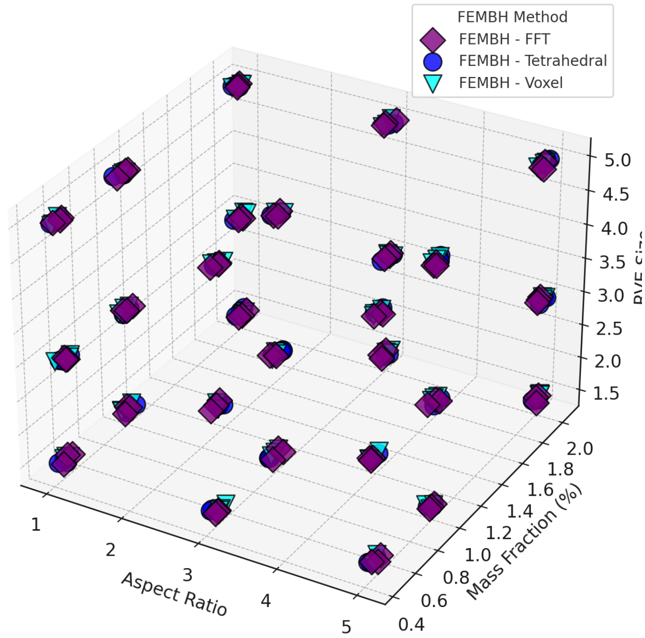



Fig. 3: 3D Scatter Plot of FEMBH configurations by applied method

Tab. 2: Test cases evaluated with MFH method

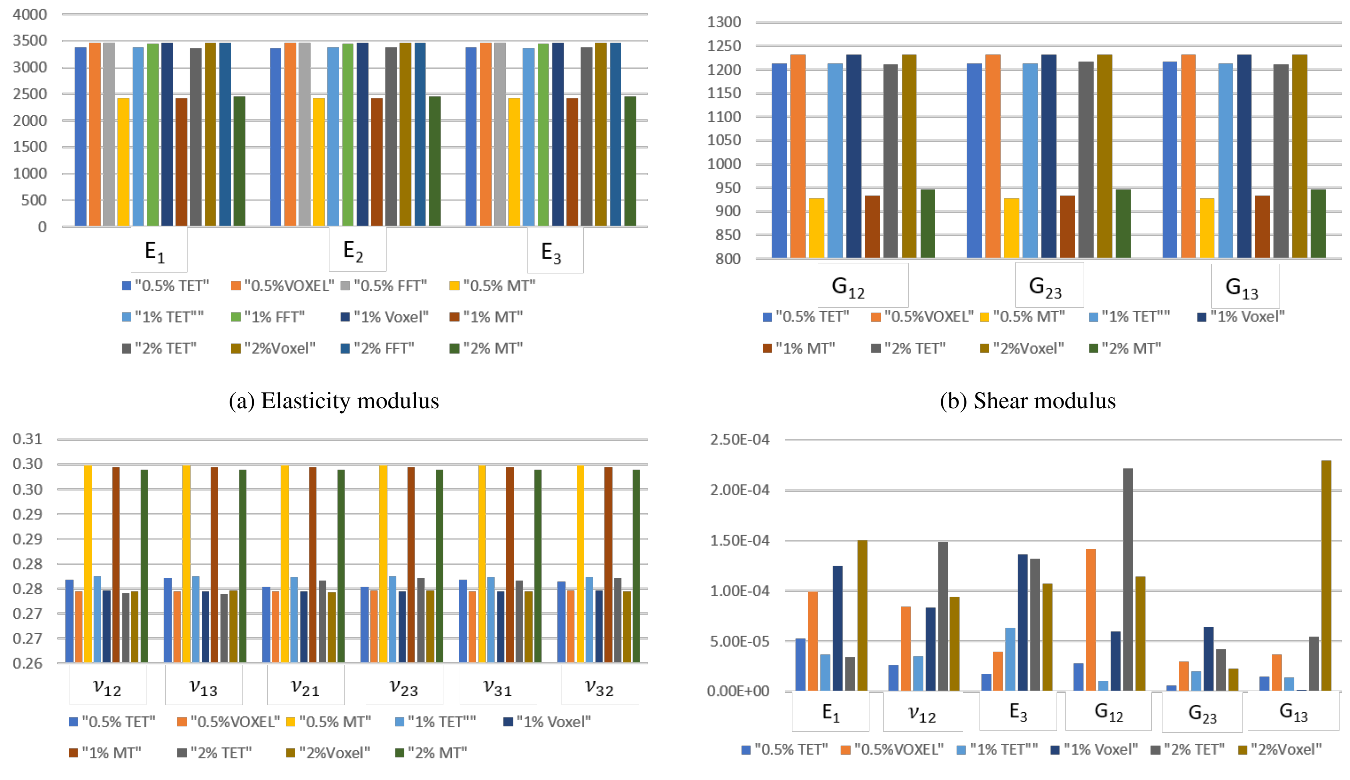
| Aspect Ratio | Mass Fraction (%) | Homogenisation Method |
|---|---|---|
| 1 | 0.5 | MFH |
| 1 | 1 | MFH |
| 1 | 2 | MFH |
| 3 | 0.5 | MFH |
| 3 | 1 | MFH |
| 3 | 2 | MFH |
| 5 | 0.5 | MFH |
| 5 | 1 | MFH |
| 5 | 2 | MFH |

The aim of the investigation is to explore the relationships between these parameters and their effects on the predicted mechanical properties, such as elasticity modulus, shear modulus, and Poisson's ratio. The numerical methods applied include the Mori-Tanaka method for macroscopic property predictions and FEMBH for detailed microscale analysis. By comparing these methods under various configurations, the study demonstrates the trade-offs between accuracy and computational efficiency.

## 4 Results and Discussion

As discussed in the previous section, MFH and FEMBH methods with tetrahedral and voxel meshes are employed to evaluate the effective elasticity modulus, shear modulus, and Poisson ratio values of silica-reinforced composites with different reinforcement aspect ratios and mass fractions with various RVE sizes. Results are presented in this section with bar graphs.
In Figure 4, the mechanical properties of the spherical model (aspect ratio 1) with an RVE size of 1.5 (which is 1.5 times the inclusion diameter), as well as changing mass fractions, are presented. From that figure, it can be seen that there is a significant and

notable discrepancy between the results obtained from the MFH and FEMBH approaches. This can be attributed to the selection of the RVE sizes. With FEMBH, RVE size can be arranged; however, the RVE approach is not followed in MFH. Additionally, an increase in elasticity modulus and shear modulus values can be observed with increasing mass fraction of inclusions.



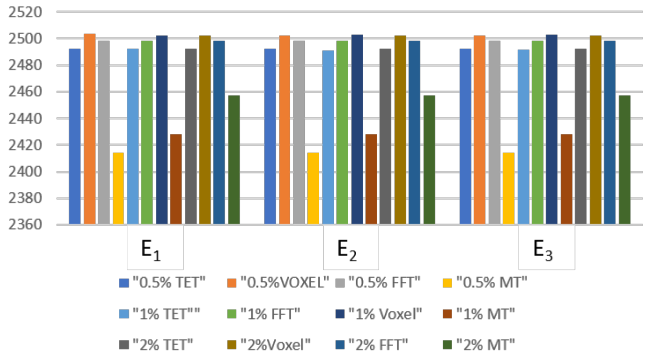

(a) Elasticity modulus (b) Shear modulus

(c) Poisson's ratio (d) Mismatch

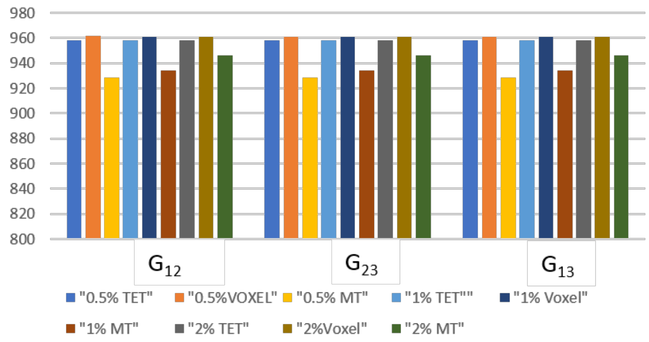
Fig. 4: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 1, RVE = 1.5).

Similar properties are evaluated for the same spherical inclusion for the RVE 3 case; results are given in Figure 5. From that figure, it can be seen that the difference between the MFH and FEMBH results decreases compared to the previous case, yet there is still a difference. This can be attributed to the expanding the RVE size. Further, similar to the previous results, elasticity modulus and shear modulus values increase with increasing mass fractions of inclusions. When the effect of mesh types in results is obtained, voxel meshes always represent the highest elasticity and shear modulus values. Then, the FFT approach follows them with elasticity modulus results. Yet, the FFT approach is insufficient to calculate the shear properties of the composite materials. While the FEMBH results with different mesh types are compared, it can be stated that there is a difference in the results, which is to be expected and is within an acceptable range. The difference is not significant, indicating that the results are accurate.

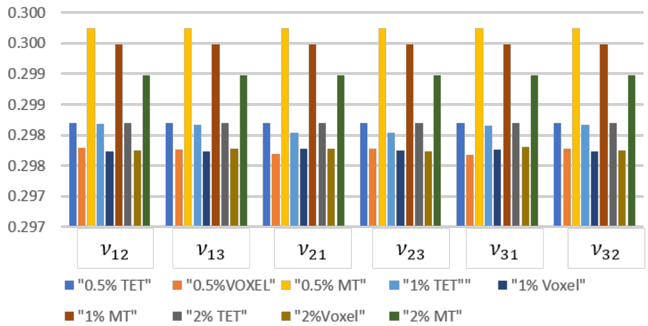
As mentioned in the previous section, different RVE sizes are considered within this study. Figure 6 represents the results of RVE 5 for the spherical inclusion case. These results clearly show that the difference between the MFH and FEMBH results is slightly close. With increasing inclusion, mass fraction, elasticity, and shear modulus values are getting higher, as expected. Moreover, the Poisson's ratio values are also getting closer when comparing the results with other RVE (1.5 and 3) cases. In calculated values, the highest one belongs to the voxel meshes; similar to previous results, differences get lower with larger RVE geometry sizes. Moreover, when the mismatch values are examined, mismatch values get lower in general. This can be attributed to the increased RVE size facilitating uniform and random distribution of nanoparticles and getting better quality meshes and results.



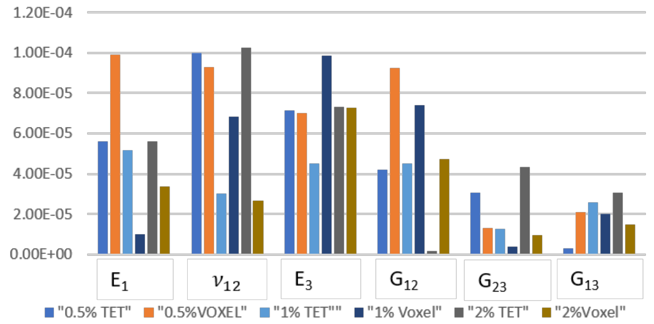

(a) Elasticity modulus




(b) Shear modulus

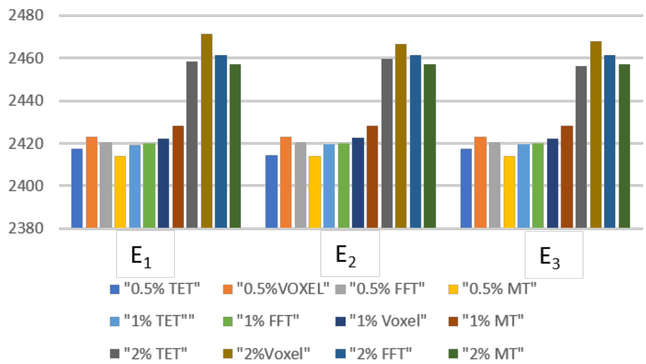



(c) Poisson's ratio

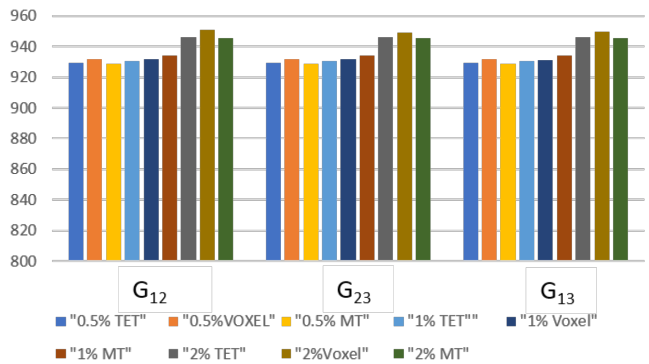



(d) Mismatch

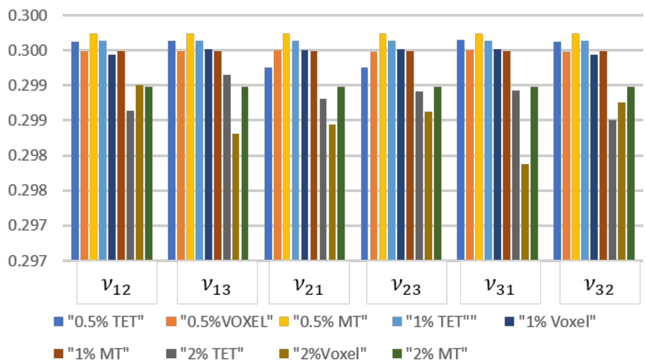
Fig. 5: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 1, RVE = 3).



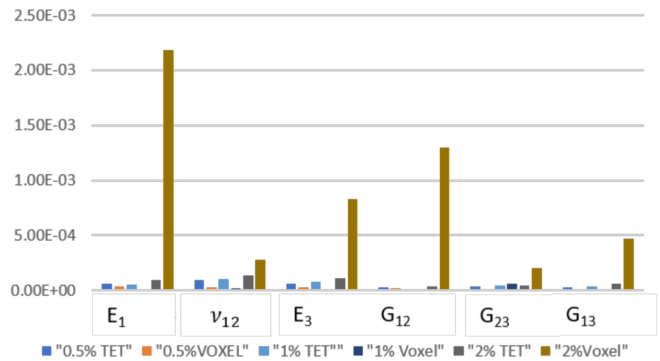

(a) Elasticity modulus




(b) Shear modulus



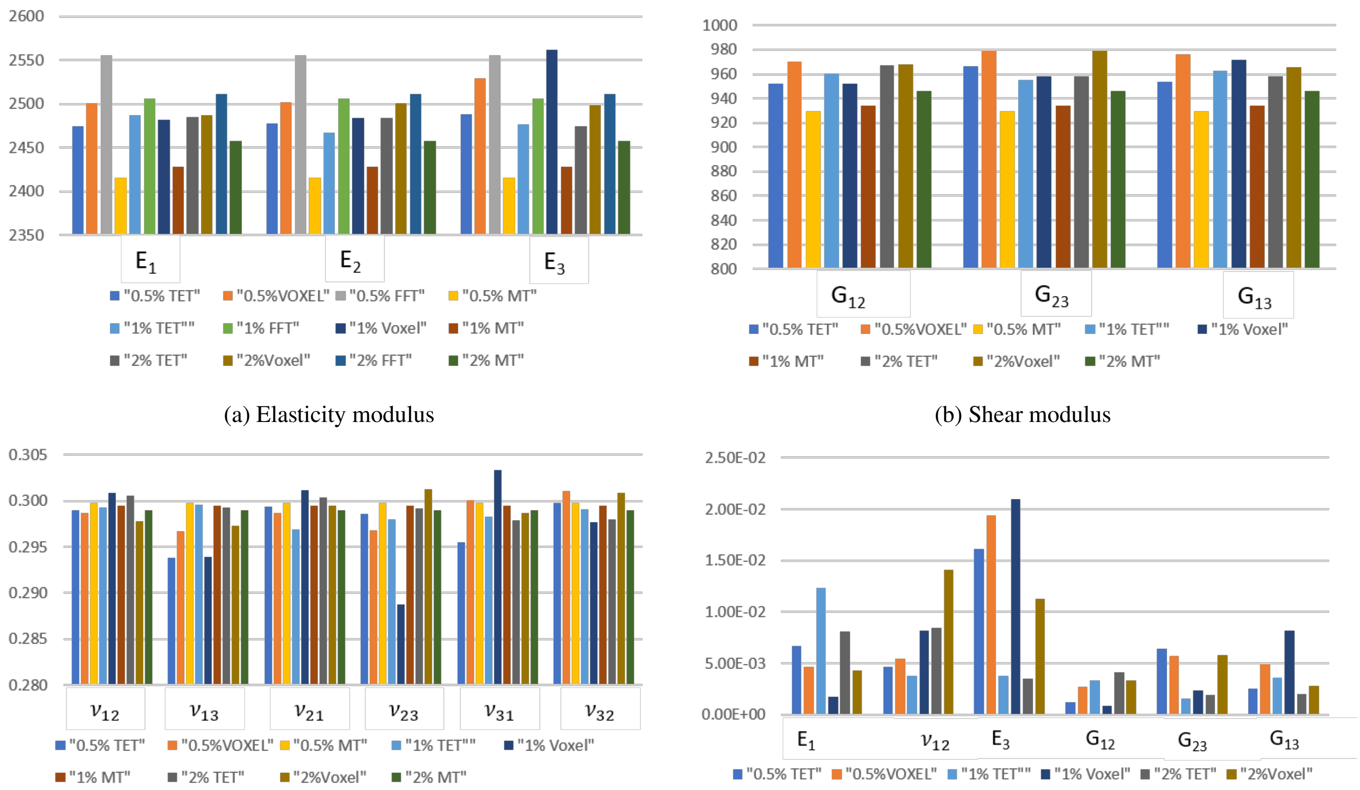

(c) Poisson's ratio




(d) Mismatch

Fig. 6: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 1, RVE = 5).

The influence of aspect ratio is further examined for inclusions with an aspect ratio of 3. Figures 7, 8, and 9 present the mechanical property predictions for aspect ratio 3 across different RVE sizes. When the results are considered, the effect of RVE size on calculated mechanical properties displays a similar role to that of spherical inclusion cases. The difference between the computed values decreases with increasing RVE sizes. Additionally, when the inclusion's mass fraction increases, the composite material's elasticity modulus and shear modulus properties are advanced.




(a) Elasticity modulus

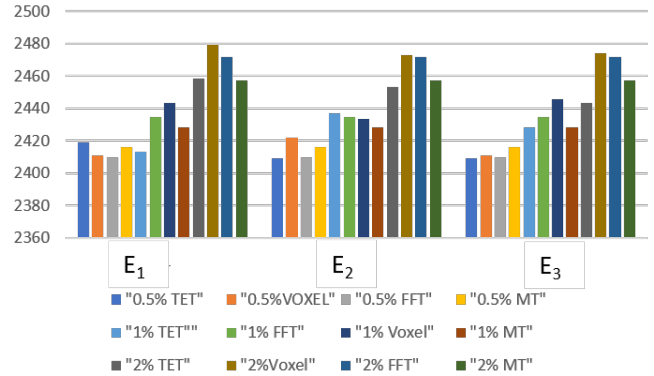
(b) Shear modulus

(c) Poisson's ratio

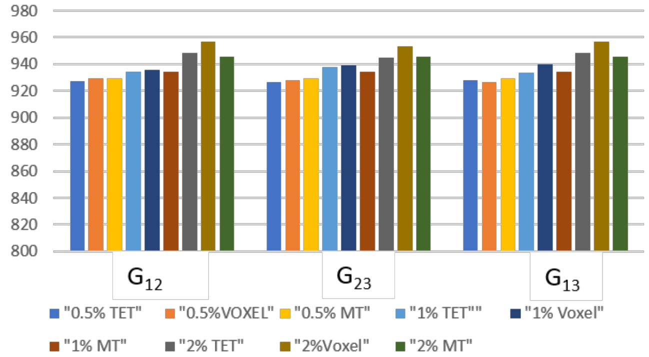
(d) Mismatch

Fig. 7: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 3, RVE = 1.5).

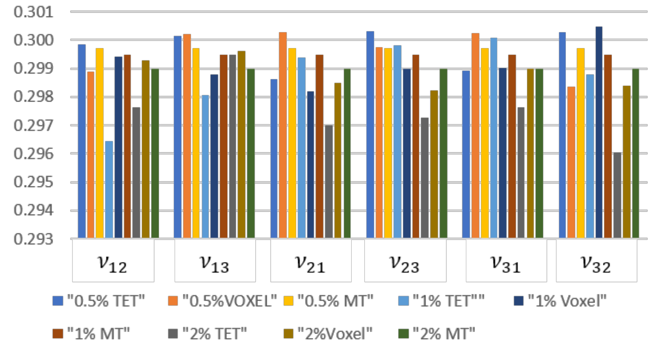
When the aspect ratio increases for the same RVE sizes are considered, results show more consistency. This can be attributed to the increasing RVE sizes with increasing aspect ratios. While RVE sizes are arranged, a multiplication process is conducted with the maximum size of the inclusion, which is the multiplication of aspect ratio and diameter. So, with increasing aspect ratio, RVE sizes also increase, and accuracy could be gathered.



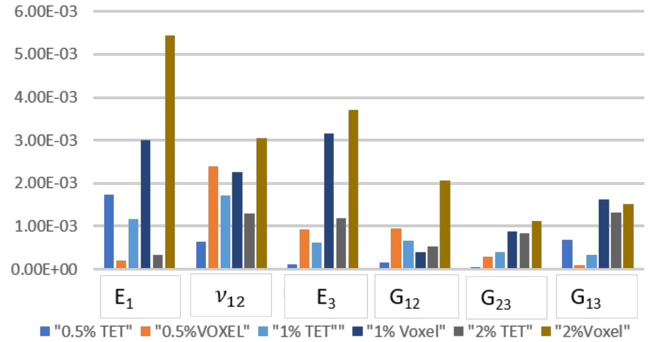

(a) Elasticity modulus




(b) Shear modulus

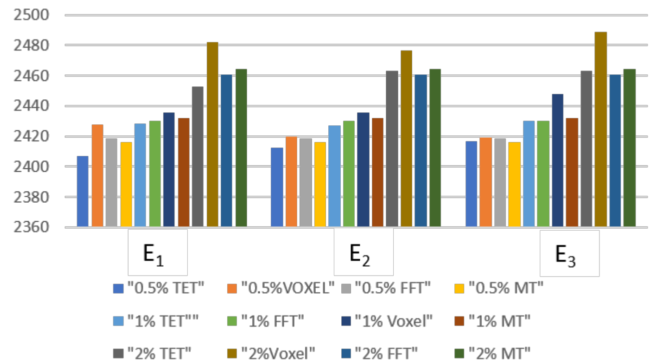



(c) Poisson's ratio

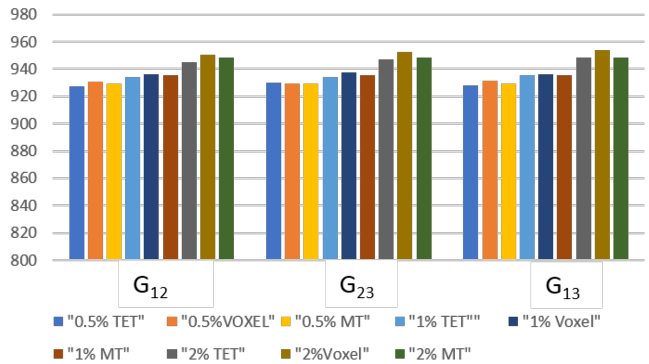



(d) Mismatch

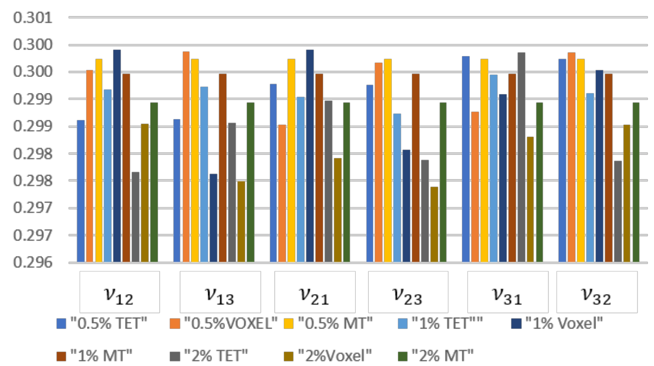
Fig. 8: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 3, RVE = 3).



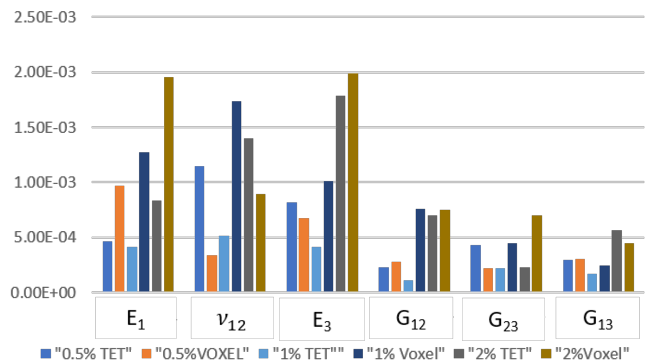

(a) Elasticity modulus




(b) Shear modulus



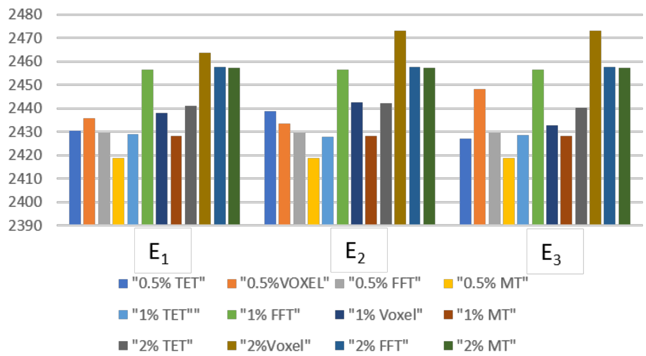

(c) Poisson's ratio



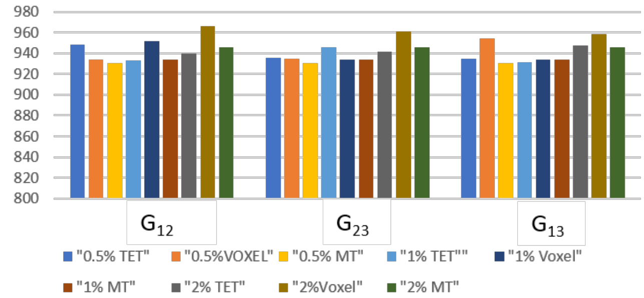

(d) Mismatch

Fig. 9: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 3, RVE = 5).

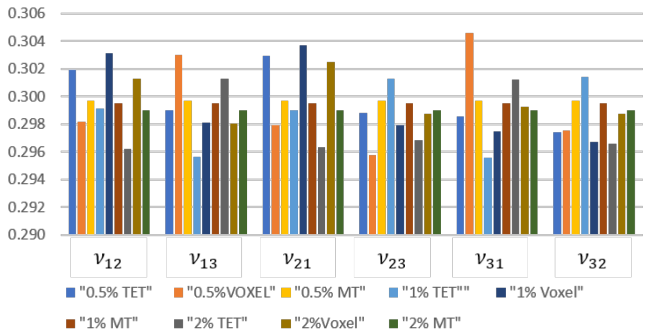
Figures 10, 11, and 12 show the results of aspect ratio 5 cases. Similar to previous findings, the difference between MFH and FEMBH results gets closer as the RVE sizes increase. The increase in aspect ratio also affects the effective modulus values increasingly.



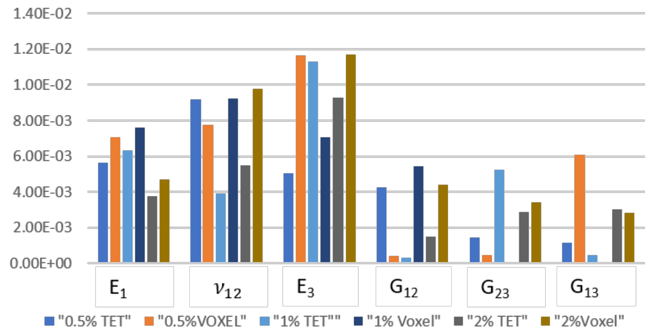

(a) Elasticity modulus




(b) Shear modulus

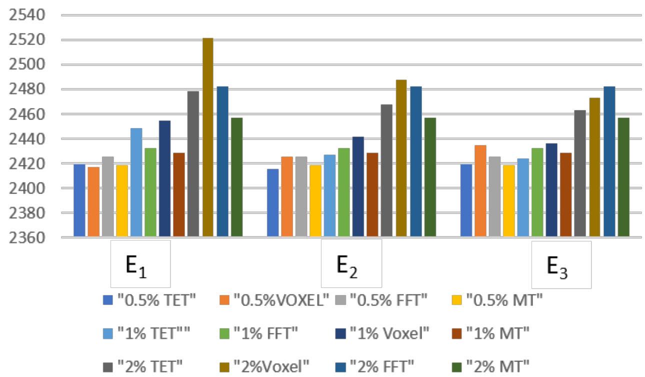



(c) Poisson's ratio

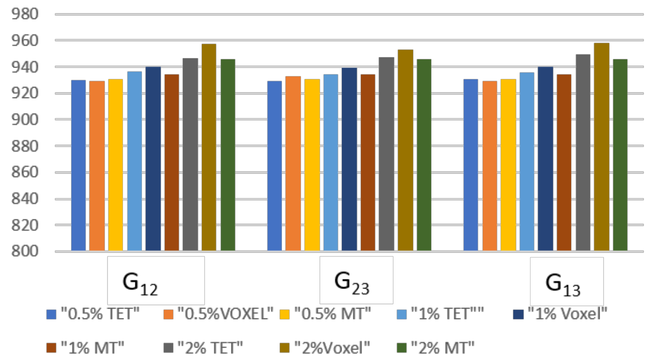



(d) Mismatch

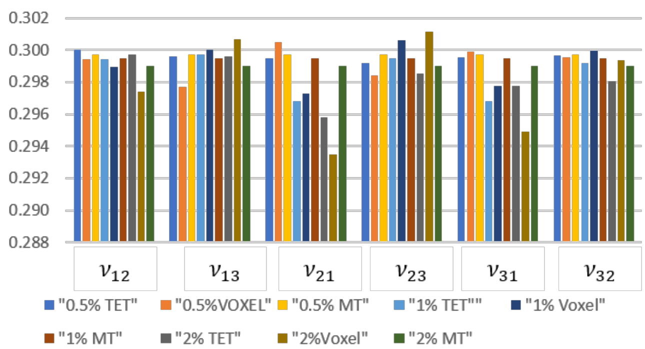
Fig. 10: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 5, RVE = 1.5).



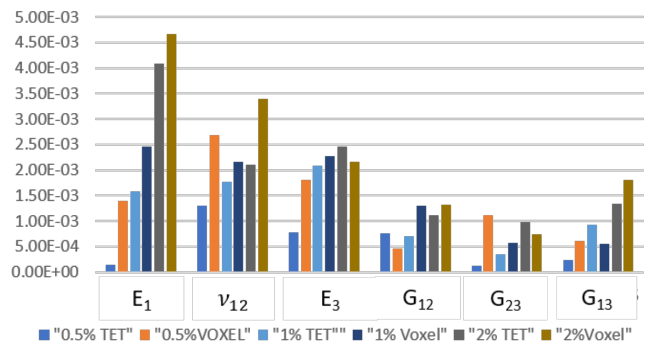

(a) Elasticity modulus




(b) Shear modulus

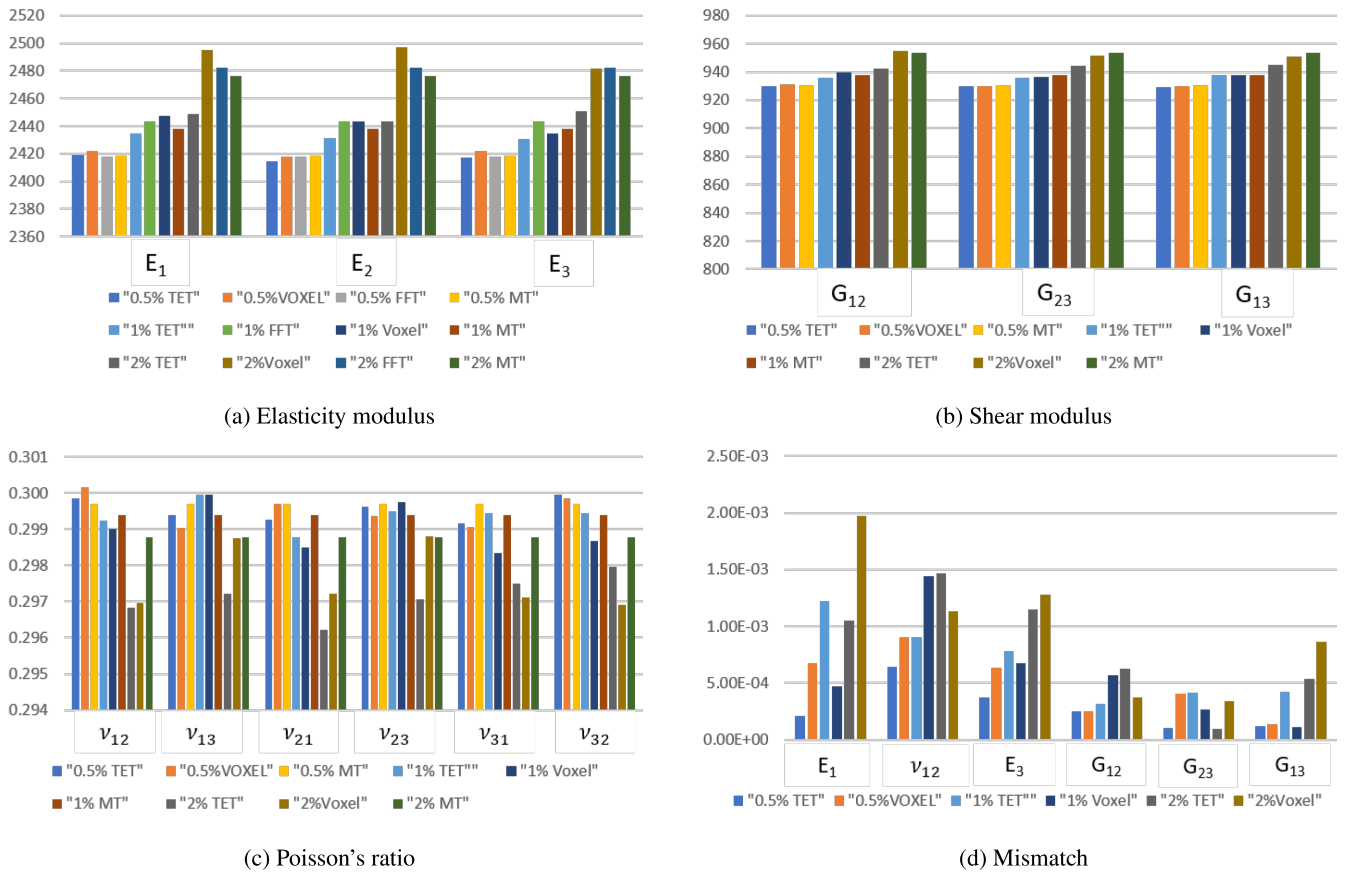



(c) Poisson's ratio




(d) Mismatch

Fig. 11: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 5, RVE = 3).



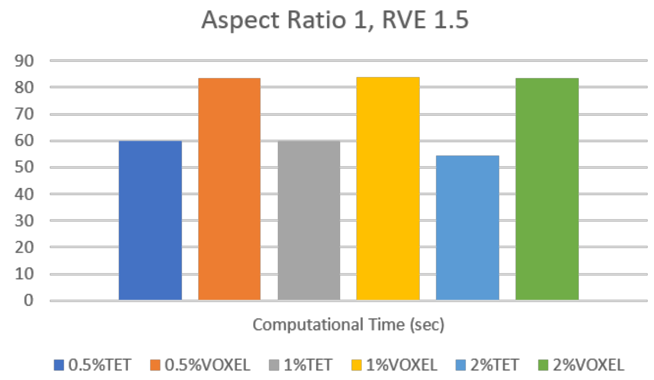

(a) Elasticity modulus (b) Shear modulus

(c) Poisson's ratio (d) Mismatch

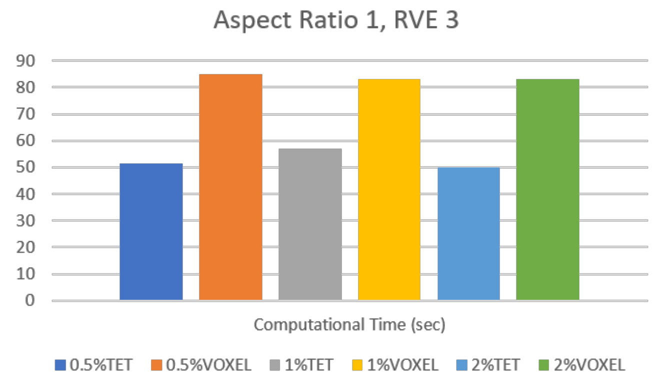
Fig. 12: Elasticity modulus and shear modulus for spherical inclusions (aspect ratio = 5, RVE = 5).

The results for elasticity modulus, shear modulus, and Poisson's ratio are obtained from FEMBH using both tetrahedral and voxel meshes, FFT method and MFH. This convergence is interpreted as an indicator of the reliability of the finite element solutions in this study. The term convergence is emphasised with the repeatability of the analyses and consistency of the results obtained from the different material homogenisation approaches. The consistent behaviour across different mesh types and RVE sizes supports the conclusion that FEMBH is capable of producing convergent solutions that reflect the detailed microstructural characteristics of the composite.

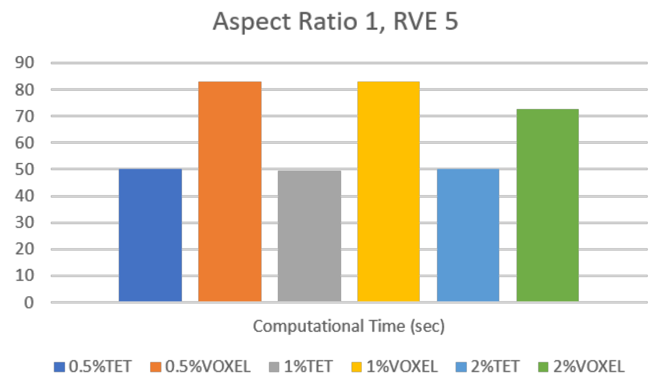
Additionally, the computational times of each method are compared to examine the effectiveness/benefit ratio. The computational times for each analysis are given as bar graphs in Figures 13, 14, and 15. The results show that as RVE sizes increase, the computational time for getting results increases, especially in aspect ratio 5 and RVE 5 case.




(a) RVE size = 1.5

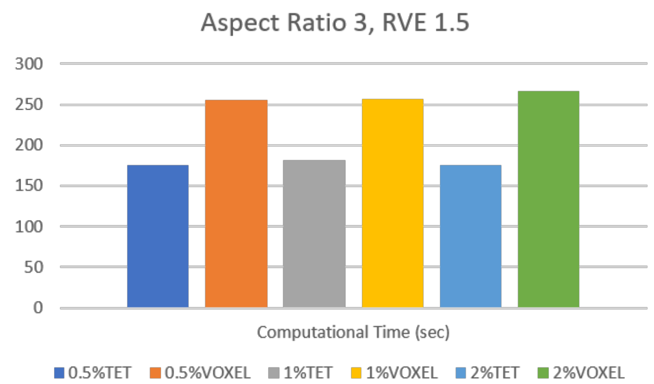



(b) RVE size = 3

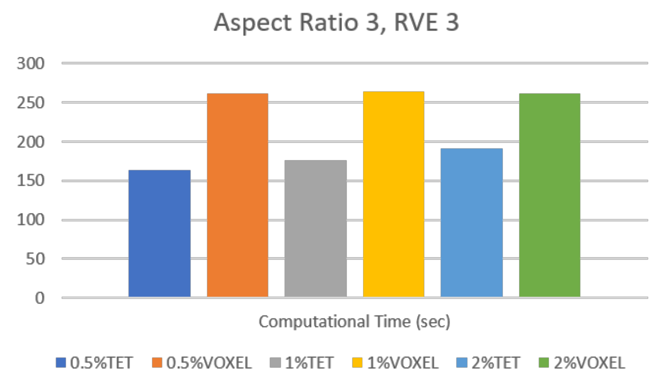



(c) RVE size = 5

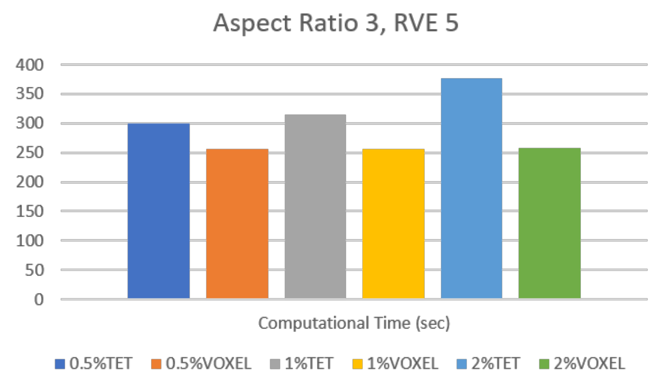
Fig. 13: Computational times for aspect ratio 1 case.




(a) RVE size = 1.5

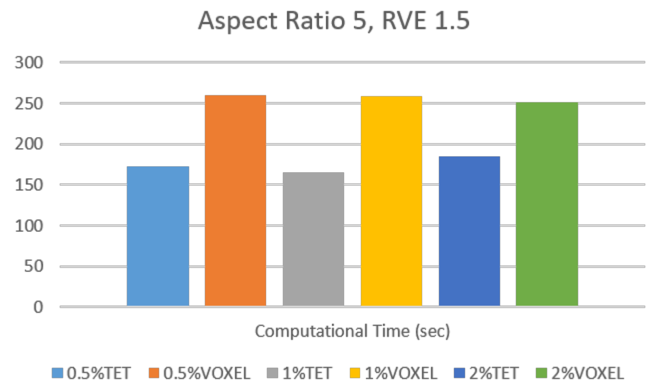



(b) RVE size = 3

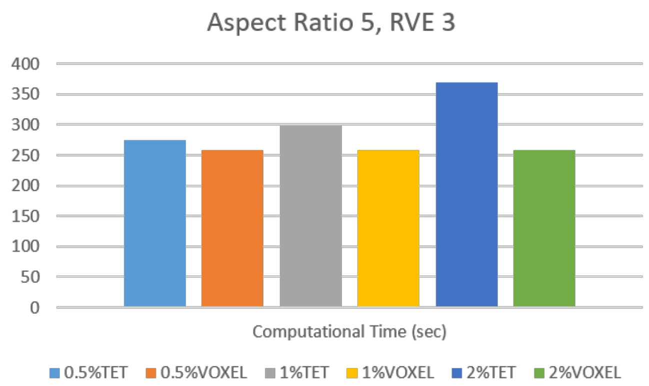



(c) RVE size = 5

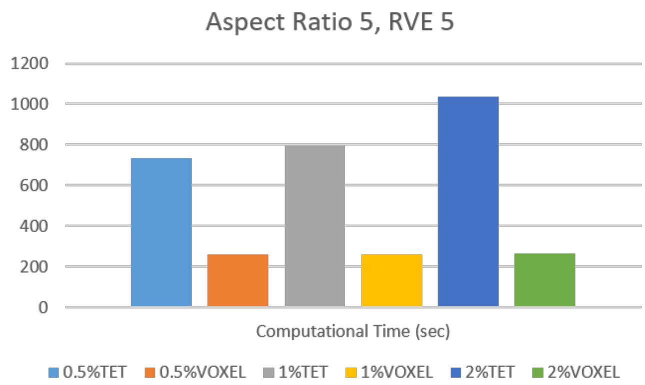
Fig. 14: Computational times for aspect ratio 3 case.




(a) RVE size = 1.5




(b) RVE size = 3




(c) RVE size = 5

Fig. 15: Computational times for aspect ratio 5 case.

Lastly, the stress distributions of the RVE model can be gathered using the FEMBH approach. Stress distribution of the aspect ratio 3 and 2% by weight inclusion reinforced model is given in Figure 16. From that figure, maximum stress values are observed in inclusion, which has a higher elasticity modulus. Inclusion carries the load that composite material is exposed to, and the matrix transfers the load to the inclusion phase. From observed stress distribution, it can be said that inclusions affect the stresses and can interact with the matrix.

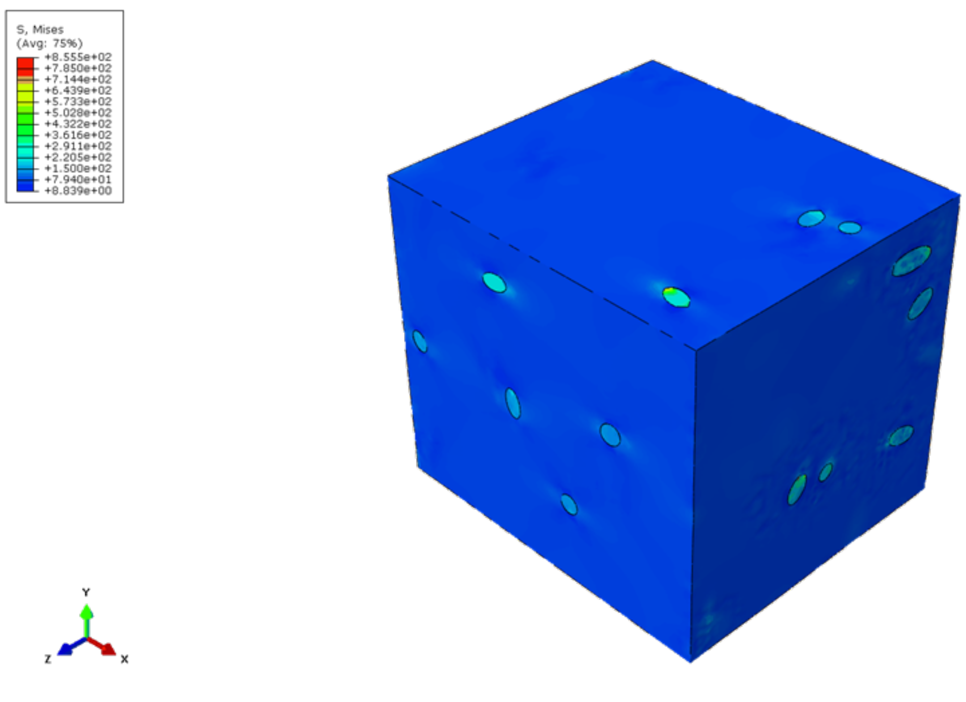



Fig. 16: Stress distribution of aspect ratio 3, 2% mass fraction model.

## 5 Final Discussions

The numerical analysis findings highlight each homogenisation technique's strengths and weaknesses. The Mori-Tanaka approach is shown to be effective for large-scale, macroscopic predictions, providing a good balance between accuracy and computational efficiency. However, it is less capable of capturing the nuanced effects of inclusion geometry on the material's mechanical properties.

In contrast, FEMBH, particularly when employing tetrahedral and voxel meshes, demonstrated a high degree of accuracy in predicting the detailed behaviour of the composite material. This method is able to account for the significant influence of inclusion geometry, including variations in aspect ratio and reinforcement orientation. The study revealed that the aspect ratio of the reinforcing particles becomes more extreme, and as the volume fraction of these particles increases, the need for higher mesh density in FEMBH models becomes critical to maintain accuracy.

However, this increased accuracy comes at a cost. FEMBH is found to be significantly more computationally demanding than the Mori-Tanaka approach, especially for composites with complex microstructures or high particle volume fractions. The use of fine mesh resolutions and the detailed modelling required for accurate FEMBH simulations necessitate substantial computational resources, making this approach less practical for large-scale analyses where computational efficiency is a priority.

## 6 Conclusions

The study began by implementing the Mori-Tanaka approach, a widely-used MFH method, which provides an effective means of predicting the macroscopic behaviour of composites. This method is particularly advantageous for its simplicity and efficiency, offering reliable predictions for materials with statistically homogeneous properties. However, the Mori-Tanaka approach is limited in its ability to capture detailed microstructural effects, particularly those arising from non-spherical inclusions or complex geometric configurations.

To address these limitations, the study also employed FEMBH, a more detailed numerical method that relies on generating RVE to simulate the composite material's microstructure. The creation of RVE is a crucial step in FEMBH, as it allows for the precise modelling of the material's microstructural characteristics, including the distribution of material properties and the application of periodic boundary conditions to mimic the repetitive nature of the microstructure.

The analysis conducted in this study focused on composites reinforced with nanoparticles, examining how the geometry of inclusions—specifically their aspect ratio and orientation—impacts the mechanical properties of the composite. Different FEMBH implementations, including tetrahedral and voxel meshes, were explored to evaluate their effectiveness in accurately predicting the behaviour of these materials.

In conclusion, this study provides a comprehensive comparison of MFH and FEMBH techniques, highlighting the trade-offs between accuracy and computational requirements. While the Mori-Tanaka approach offers a practical solution for macroscopic predictions, FEMBH stands out for its ability to model the detailed microstructural effects that are critical in nanoparticle-reinforced composites. The choice between these methods should be guided by the specific requirements of the application, with FEMBH being more suitable for cases where detailed microstructural accuracy is paramount and the Mori-Tanaka approach being more appropriate when computational efficiency is the primary concern.

Future work could explore hybrid approaches that combine the strengths of both MFH and FEMBH, potentially offering a more balanced solution that leverages the computational efficiency of MFH with the detailed accuracy of FEMBH. Additionally, further research into optimising FEMBH mesh configurations could also help reduce the computational load, making this method more accessible for large-scale applications.

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