Towards a general multiscale methodology for the simulation of thermal behavior of granular media

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Abstract. This work presents a continuum-discrete hierarchical multiscale methodology based on data-driven computations of the microscale response to simulate heat conduction in static granular materials. The effective thermal conductivity tensors of the continuous method at the macroscale is obtained from a database of microscale results. The microscale database is created by generating and homogenizing several Representative Volume Elements (RVEs) in order to relate the thermal conductivity of the granular material to its microstructural properties. In this study, these properties are the local porosities and anisotropies, which are inputs of the database to obtain the conductivity. An easy yet efficient protocol for RVE generation and homogenization is also presented.

Keywords: hierarchical multiscale analysis, discrete element method, representative volume elements, heat conduction, granular materials.

1 Introduction

Granular media are ubiquitous in nature and are the most processed material in the industry after water. The thermal behavior of these materials is relevant in several situations, including static and dynamic systems, such as granular mixing with rotating drums [1], additive manufacturing by selective laser sintering [2], packed and moving beds of catalytic reactors [3], latent heat storage systems [4], and landslides powered by heat-induced shear failures [5].

Typically, two different approaches are employed for the numerical modeling of granular media: continuous and discrete methods. On the one hand, continuum-based methods are more computationally efficient but less effective for representing microscale effects from grain interactions. On the other hand, discrete methods, which represent the granular media as a collection of individual particles, enable a more accurate simulation of granular behavior. However, it comes with a much higher computational cost, mainly due to the substantial number of particles needed to represent real-world scenarios. Therefore, hybrid methodologies combining both approaches were developed to overcome their limitations. One of them is the continuum-discrete hierarchical multiscale approach [6,7]. In this hybrid strategy, a continuous method is used to model the granular medium at the macroscale and the constitutive behavior arises from the homogenization of the discrete response at the microscale based on Representative Volume Elements (RVEs). Several researches were developed with this methodology, but only a few explored the thermal behavior of granular materials [8–10]. However, these multiscale methods still lack computational efficiency as the discrete response needs to be solved at several RVEs. Therefore, data-driven computations of the discrete response has been employed recently to reduce the computational cost [11].

This work combines the continuum-discrete hierarchical multiscale concept with a data-driven offline computation of the discrete response to simulate heat conduction across granular media. The continuous method used to solve the macroscale problem is the Finite Volume Method (FVM) [12], although other methods could be employed, such as the Finite Element Method (FEM) [13]. The Discrete Element Method (DEM) [14] is used at the microscale to generate RVEs where homogenization takes place. An easy yet efficient protocol for RVE generation and homogenization is presented. The microscale results are stored in a database that relates the thermal conductivity of the granular material with its microstructural properties, in this study, porosity and anisotropy. The thermal conductivity is then obtained by interpolating the database sample points. The methodology is validated by comparing the results of the proposed microscale-informed continuum model with a full DEM model.

2 Methodology

The proposed method aims to simulate the heat flux through granular materials with a fast hierarchical continuum-discrete multiscale approach. The solution of the continuous numerical method is obtained by using the effective thermal conductivity tensors derived from the solution of discrete domains representative of the local microstructure (see Fig. 1). Based on knowledge of local porosity, η, and a measure of local anisotropy, f, the effective thermal conductivity tensor, $\boldsymbol{K}$, is obtained from a database that relates these three parameters. The database is created by generating several RVEs based on the DEM. Each RVE is generated with a different pair of porosity/anisotropy values and the corresponding thermal conductivity tensor is computed by a homogenization.

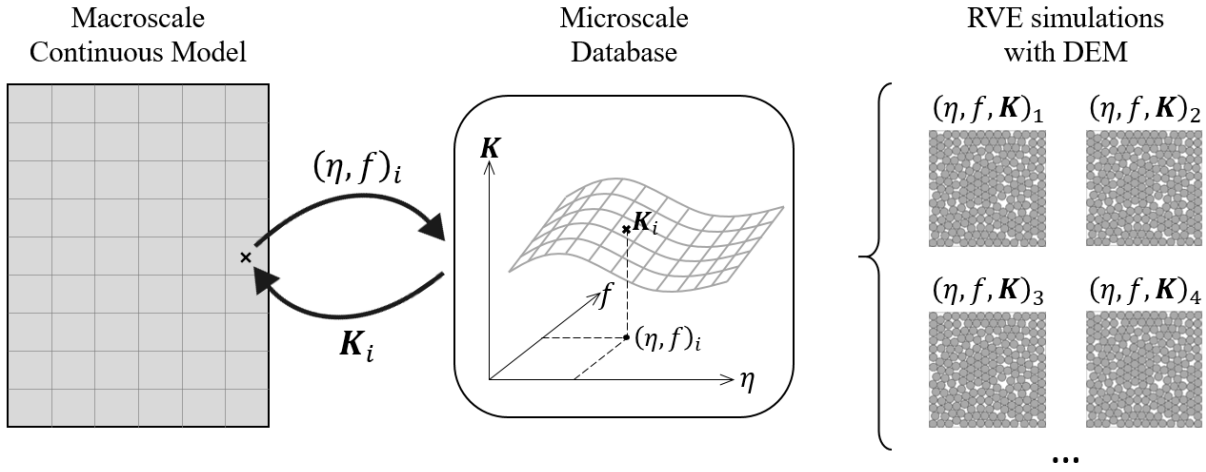


Figure 1. General overview of the proposed continuum-discrete multiscale method.

2.1 Micro and macroscale formulations

In this work, for simplicity, we focus on two-dimensional analysis only. However, the proposed approach is general and can be safely used for three-dimensional problems.

At the microscale, cylindrical DEM particles (rods) with unit length are used with simple linear models of contact forces. The normal contact force, $\boldsymbol{F}_n$, acting on a particle by one of its neighbors is calculated with Eq. (1), where k_n is the normal contact stiffness, δ_n is the contact overlap, and $\boldsymbol{n}$ is the unit outward normal of the contact. The tangential contact force, $\boldsymbol{F}_t$, is calculated incrementally and subjected to Coulomb's friction condition, as shown in Eq. (2). In that equation, $\boldsymbol{F}_t^{prev}$ is the tangential force of the previous time step, k_t is the tangential contact stiffness, $\Delta\boldsymbol{u}_t$ is the increment of relative tangential displacement at the contact, $\boldsymbol{t}$ is the unit vector along the tangential direction of the contact, and φ is the contact friction angle.

$$\boldsymbol{F}_n = -k_n \delta_n \boldsymbol{n} \tag{1}$$

$$\boldsymbol{F}_t = \begin{cases} \boldsymbol{F}_t^{prev} - k_t \Delta \boldsymbol{u}_t & \text{if } |\boldsymbol{F}_t| \leq |\boldsymbol{F}_n| \tan(\varphi) \\ |\boldsymbol{F}_n| \tan(\varphi)\, \boldsymbol{t} & \text{otherwise} \end{cases} \tag{2}$$

The normal and tangential stiffnesses are calculated with Eq. (3), where E and ν are, respectively, the Young's modulus and Poisson's ratio of contacting particles, and R_1 and R_2 are their radii.

$$k_n = 2E\, R_1 R_2/(R_1 + R_2), \quad k_t = \nu k_n \tag{3}$$

In addition, a non-viscous damping force, $\boldsymbol{F}_d$, is added to each particle in the opposite direction of its velocity, $\boldsymbol{v}$. It is calculated with Eq. (4), where μ is the damping coefficient and $\boldsymbol{F}_c$ is the resulting contact force of the particle given by the sum of the normal and tangential contact forces with all its neighbors.

$$\boldsymbol{F}_d = -\mu |\boldsymbol{F}_c|\, \boldsymbol{v}/|\boldsymbol{v}| \tag{4}$$

The torque caused by each neighbor is simply given by the tangential force and its lever arm with respect to the particle longitudinal axis. Rolling resistance is not taken into account.

For the thermal behavior, particles are assumed isothermal and the heat flux happens only by conduction through the contact area between neighbors. The heat transferred to a particle from one of its neighbors is calculated with a thermal pipe model following Eq. (5). K is the thermal conductivity of particles, A_p is the cross-sectional area of the thermal pipe (in 2D: the in-plane contact length), L_p is the length of the pipe (distance between particles' longitudinal axes), and ΔT is the temperature difference between the particle and its neighbor.

$$Q = -KA_p \Delta T / L_p \tag{5}$$

At the macroscale, the continuum is considered a granular medium where heat conduction occurs only through the solids. Therefore, the thermal behavior in a domain Ω of boundaries Γ is ruled by the volume-averaged heat diffusion equation:

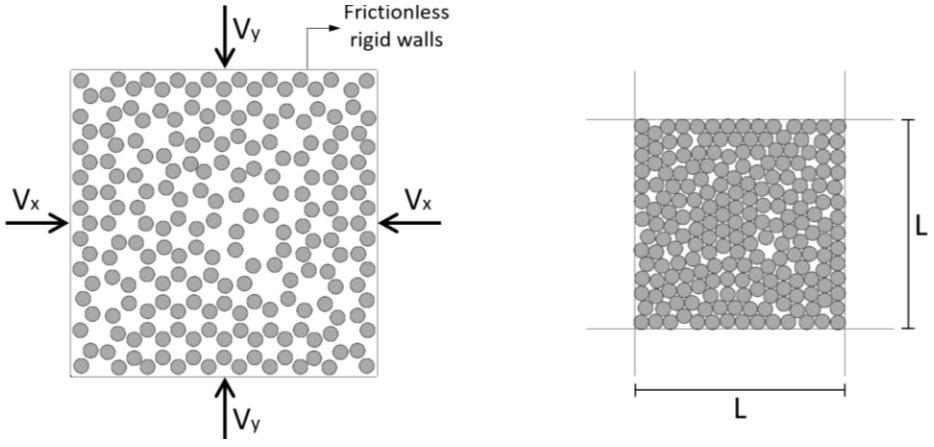
$$\begin{aligned} \rho c_p (1-\eta) \frac{\partial T}{\partial t} &= \nabla \cdot (\boldsymbol{K} \nabla T) \ \text{ in } \Omega \\ T &= \bar{T} \ \text{ in } \Gamma_{\mathrm{D}} \\ -\boldsymbol{K} \nabla \mathrm{T} \cdot \boldsymbol{n} &= \bar{q} \ \text{ in } \Gamma_{\mathrm{N}} \end{aligned} \tag{6}$$

where ρ and c_p are the density and heat capacity of the grains, respectively. The porosity η is defined as the ratio of void volume to averaging volume. As mentioned, the effective thermal conductivity tensor $\boldsymbol{K}$ depends on the microscale structure of the granular medium and is obtained from a database of microscale results. On Dirichlet boundaries, Γ_{D}, $\bar{T}$ is the imposed temperature, while on Neumann boundaries, Γ_{N}, the heat flux $\bar{q}$ is given. In this work, Eq. (6) is discretized and solved via FVM. The implementation is done using the open-source library OpenFOAM [15].

2.2 Generation of RVEs

An RVE is a DEM assembly with a number of particles large enough to be statistically representative to capture the material constitutive behavior and adequately small to render it computationally effective. For this work, a convergence study indicated that 500 particles suffice, which is similar to that proposed by [7].

Our protocol for generating RVEs consists of randomly positioning the particles in a region delimited by frictionless flat walls, which have assigned the same material parameters as the particles (expect for the friction angle) and are used to compress them without considering gravity (see Fig. 2). The size of the delimited region where particles are disposed is such that the final shape of the RVE is approximately a square. During compression, the walls move at a relatively slow speed (about the mean particle radius per second) to avoid excessive dynamic effects. The compression speed is kept constant, but it can be set differently in the horizontal and vertical directions to vary the final anisotropy of the RVE. When a desired porosity is reached, the walls stop moving and the simulation continues until the system is in equilibrium. The final position of particles and walls are used for homogenizing the anisotropy and thermal conductivity, as it will be described in the next section.



(a) (b)

Figure 2. RVE generation process: (a) initial configuration and (b) final configuration with a target porosity.

2.3 Homogenization in RVEs

The anisotropy measure is obtained from the fabric tensor, which is computed as:

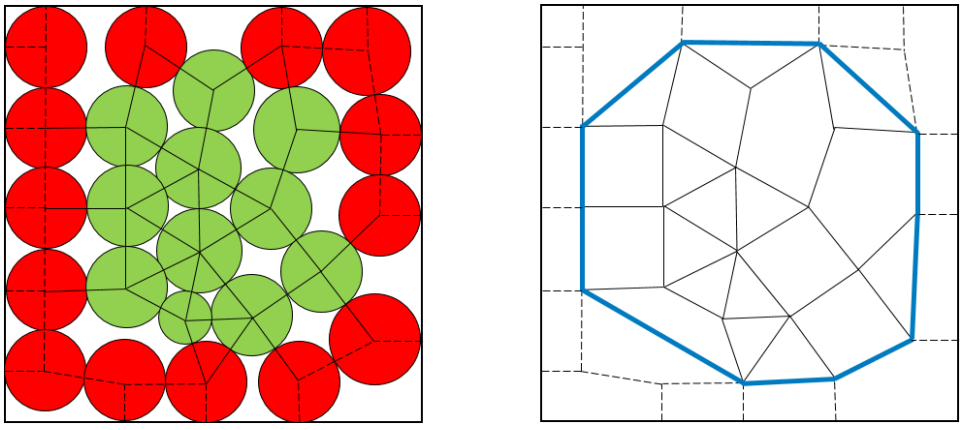
$$\boldsymbol{F} = \frac{1}{N}\sum_1^N \boldsymbol{n} \otimes \boldsymbol{n} \tag{7}$$

where N is the total number of contacts in the RVE and $\otimes$ is the dyadic product. Since this tensor always has a trace of 1.0, the diagonal components, F_{xx} and F_{yy}, are related and can be synthetized into a single scalar, f, given by the difference $f = F_{xx} - F_{yy}$. Because in the analyzes carried out in this work the off-diagonal components are negligible, f will be taken as the sole parameter to quantify the anisotropy in the RVE.

The thermal conductivity is homogenized into an effective thermal conductivity tensor. In particular, following the thermal pipe model for heat conduction presented in Eq. (5), the homogenization of thermal conductivity takes the form of Eq. (8), where V_{RVE} is the volume of the RVE.

$$\boldsymbol{K} = \frac{1}{V_{RVE}}\sum_1^N KA_pL_p\boldsymbol{n} \otimes \boldsymbol{n} \tag{8}$$

To mitigate the effects of flat walls, the particles in contact with the walls are not taken into account during the homogenization process. It means that only contacts involving a particle that is not touching a wall are considered and the homogenization volume V_{RVE} is reduced accordingly. To this end, a convex hull delimiting the chain of considered contacts is created. The volume (area with unit length in 2D) of the convex hull is taken as the volume for homogenizing the thermal conductivity and for computing the porosity to stop the RVE compression. This strategy is illustrated in Fig. 3. All implementations to generate RVEs and perform homogenizations were made in the open-source framework *KratosMultiphysics* [16].



(a) (b)

Figure 3. Strategy for mitigating the effects of flat walls illustrated for a simple assembly of particles: (a) RVE showing particles touching walls (red), particles not touching walls (green), discounted contacts (dashed lines), and considered contacts (continuous lines). (b) The convex hull delimiting the chain of considered contacts is shown in thick blue lines.

2.4 Microscale database from RVEs

Several RVEs need to be generated with different porosities and anisotropies, which are the inputs of the database. The porosity is controlled by stopping the compression of the RVE, while the anisotropy is controlled by using different relative wall speeds in the horizontal and vertical directions. The results of homogenized thermal conductivities can be considered as sample points of a continuous two-dimensional function Φ:

$$\boldsymbol{K} = \Phi(\eta, f) \tag{9}$$

Therefore, it is necessary to define the multi-valuated and multi-dimensional function Φ to predict the thermal conductivity for non-simulated scenarios of the inputs. To this end, the following actions are carried:

- *Preparation*: In the two-dimensional input space, obtain the Delaunay triangulation of the sampling points. This task is done only once.

- *Use*: For a given non-simulated configuration $(\hat{\eta}, \hat{f})$, obtain $\hat{\boldsymbol{K}} = \Phi(\hat{\eta}, \hat{f})$ by performing a piecewise linear interpolation using the precomputed Delaunay triangulation and the data values at sampling points. The interpolation is done individually for each component of the thermal conductivity tensor ($\boldsymbol{K}_{xx}$, $\boldsymbol{K}_{yy}$, $\boldsymbol{K}_{xy}$). This stage is done during the macroscale simulation to obtain the effective thermal conductivity considering the local microscale properties.

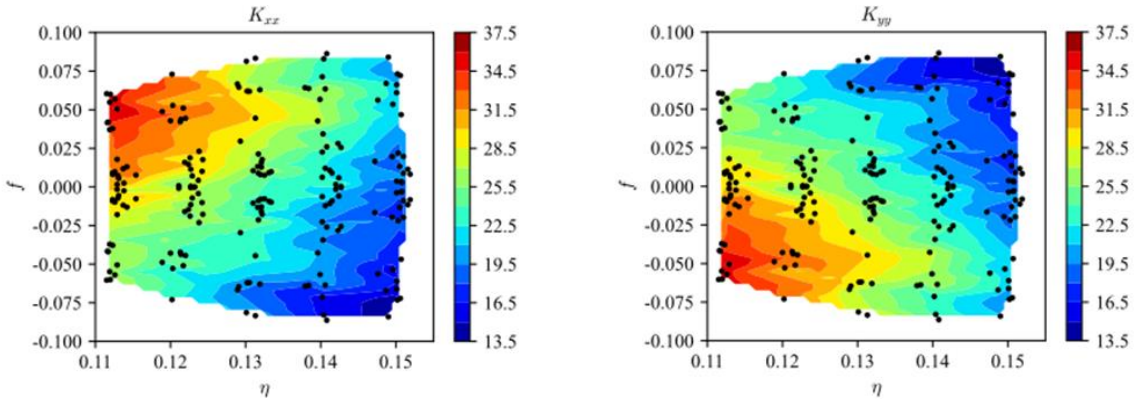
It is important to mention that the database is only valid for the granular material used for its creation (i.e. same material properties and particle size distribution) and for the range of porosity and anisotropy covered during the generation of RVEs. In addition, extrapolation operations should be avoided.

3 Results

3.1 Microscale database

A database of microscale results is created for a granular material with the following properties: density of 2650 kg/m^3, Young's modulus of 600 MPa, Poisson's ratio of 0.8, friction angle of 0.5, thermal conductivity of 100 W/mK, and heat capacity of 100 J/kgK. The particle size distribution follows the one used in [7], with a mean, minimum and maximum radius of 5.0 mm, 3.0 mm and 7.0 mm, respectively. In addition, a damping coefficient of 0.1 is applied.

One hundred RVEs were generated with a range of porosities between 11.1% and 15.2% and a range of anisotropies between –0.09 and +0.09. Figure 4 shows the interpolation map of the *xx* and *yy* components of the effective thermal conductivity tensor with respect to porosity and anisotropy. The *xy* component was also mapped but is not shown.



(a) (b)

Figure 4. Components of the effective thermal conductivity tensor with respect to porosity and anisotropy: (a) *xx* component and (b) *yy* component. Black dots represent the pairs (η, f) obtained in each generated RVE.

3.2 Reference DEM model

To validate the proposed multiscale method, a full DEM model is used as a reference solution for the heat flux across a granular material (see Fig. 4). The model consists of a rectangular box 2538.4 mm wide and 507.7 mm high with flat walls as boundaries and containing 13500 particles. The material properties and particle size distribution are the same as those used for the previously created database of microscale results.

The local porosities and anisotropies of the DEM model are obtained by subdividing the domain into 10x2 square regions where these properties are calculated. This subdivision is sufficient to faithfully capture the local microstructural properties in this model. Therefore, based on this information, the components of the effective thermal conductivity tensor can be estimated from the microscale database. The map of local properties, including the inputs (porosity and anisotropy) and one output ($\boldsymbol{K}_{yy}$) of the database, are shown in Fig. 5. The other two outputs ($\boldsymbol{K}_{xx}$ and $\boldsymbol{K}_{xy}$) were computed but are not shown.

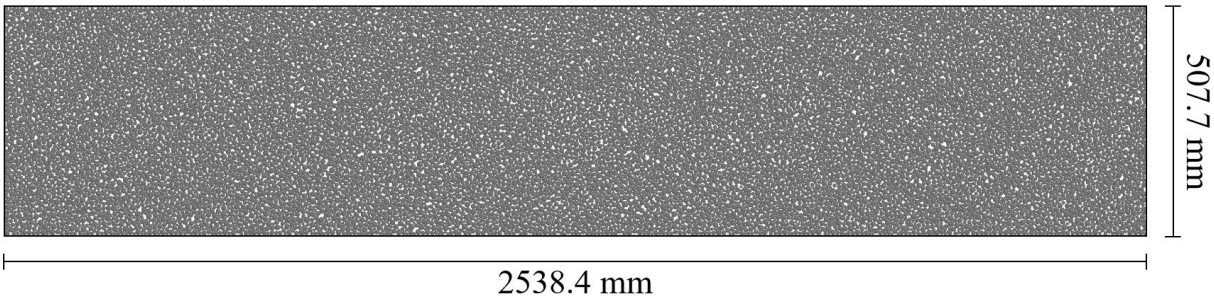


Figure 4. Full DEM model to serve as reference solution for validating the multiscale method.

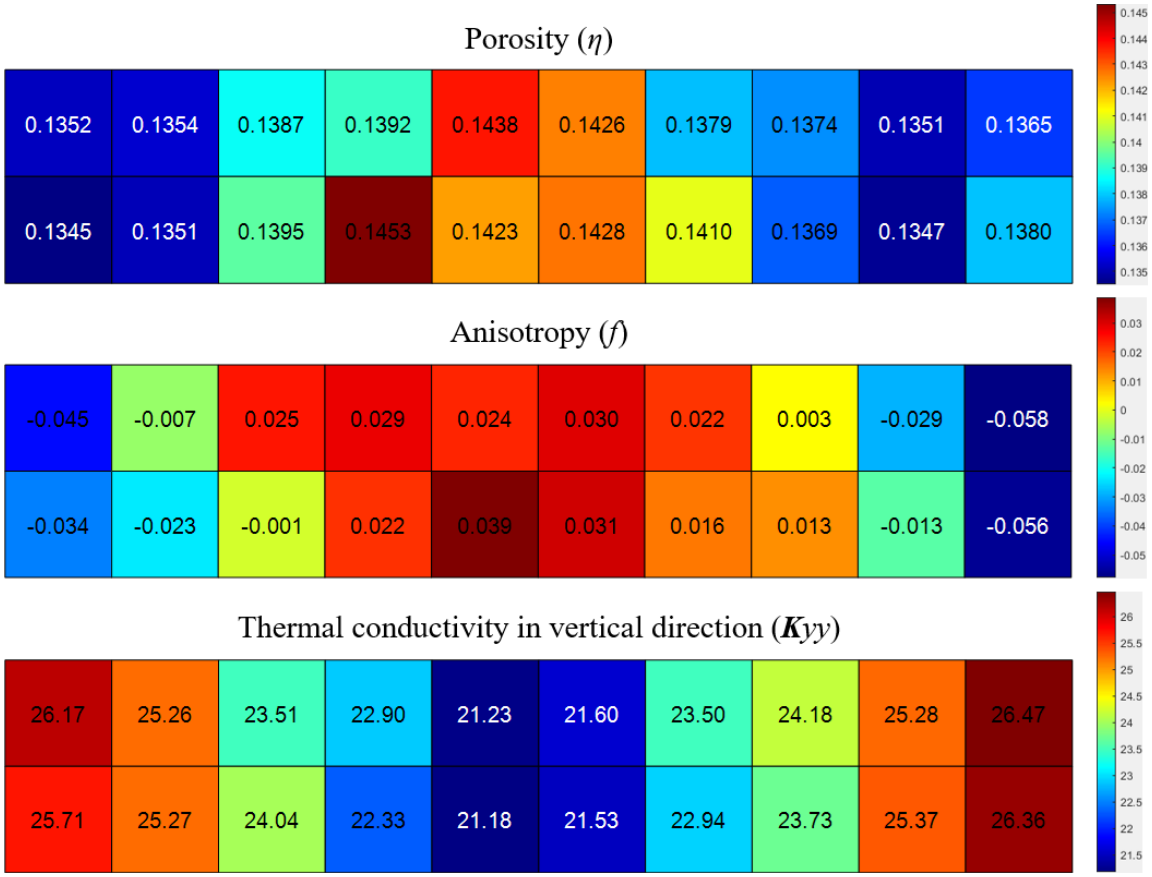


Figure 5. Maps of local properties of the reference DEM model.
Inputs: porosity (top) and anisotropy (middle); Output: thermal conductivity (bottom).

3.3 Validation of continuum-based solution

An FVM model is created by discretizing the granular domain into 1280 square cells (see Fig. 6). The density and heat capacity of the material of all cells are the same as used for the DEM particles. However, the porosity and thermal conductivity tensor of each cell are obtained from the region of local properties where the cell is located.

Both DEM and FVM models are used for a thermal analysis under the same boundary and initial conditions. The bottom wall is kept at 100°C and the others are adiabatic. The granular material (particles in DEM and cells in FVM) has an initial temperature of 0°C. The analyses ran for a total of 5000s. Figure 7 shows the temperature evolution at two points of both models, whose positions are indicated in Fig. 6. It is clear that the FVM results agree well with the DEM results. Moreover, the analysis time of the FVM model was of only a few seconds, while the DEM took several hours (around 6 hours) to conclude the simulation on the same machine.

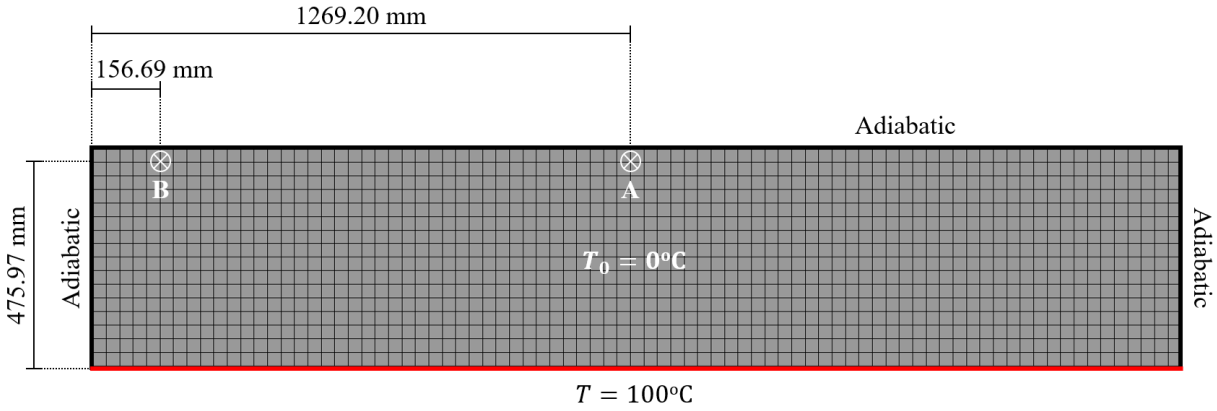
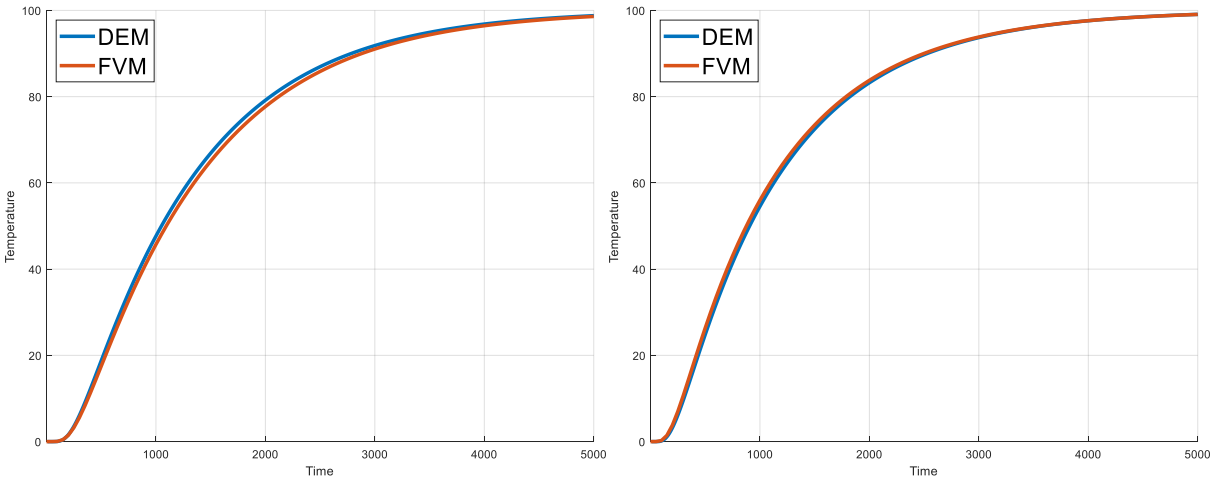


Figure 6. FVM model with boundary and initial conditions for thermal analysis.



(a) (b)

Figure 7. Comparison between continuum-based solution and reference DEM solution: temperature evolution at (a) point A and (b) point B.

4 Conclusions

The proposed multiscale methodology provides a fast and accurate way to simulate heat conduction in granular materials. In fact, the computational performance of the continuous method and the accuracy of the DEM are preserved. One of the main reasons for this is the offline computation of the microscale response based on microstructural properties. In this work, it was shown that the local thermal conductivities can be obtained from the information of local porosities and anisotropies. Therefore, it should be remarked that these microstructural properties that are input to the database of microscale results must be known a priori, possibly provided from other sources, such as in-situ analysis of soils. Moreover, the database of the analyzed material should be readily available for use when applying this methodology. Hence, creating and disseminating databases for different materials is suggested.

Future developments of the presented methodology include its extension to three-dimensional analyses and the generalization of the homogenization of the thermal conductivity tensor to consider any heat conduction model in DEM, not only the thermal pipe model. Furthermore, the method should also be expanded to include the solution of the mechanical behavior of granular materials and, thus, to allow for the simulation of dynamic systems, such as granular flows.

Acknowledgements. The authors acknowledge the support from MCIN/AEI/10.13039/501100011033 and FEDER *Una manera de hacer Europa* for funding this work via project PID2021-122676NB-I00.

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