Thermo-mechanical analysis of continuous and discrete media with PFEM and DEM

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Abstract. This work presents the development of coupled formulations of the Particle Finite Element Method (PFEM) and the Discrete Element Method (DEM) for the simulation of thermo-mechanical problems involving materials that can be modeled both as a continuous or a discrete medium. The thermally-coupled PFEM combines the Lagrangian and remeshing features of the PFEM for solving fluid dynamics problems with the FEM solution of the diffusion in thermodynamics problems. The result is a numerical tool that provides the possibility to apply different types of thermal boundary conditions, including to the free-surface contours. In addition, temperature dependency can be set to the mechanical and thermal properties of the materials. Concerning the constitutive models, both Newtonian and non-Newtonian constitutive laws can be employed. The thermally-coupled DEM, on the other hand, is developed by combining the classical soft-sphere approach for the mechanical behavior of particles with the solution of the energy conservation equation for the thermal behavior of the elements. Several different models of contact forces and heat transfer between particles can be employed. With these two numerical tools presented, the continuous and discrete approaches for thermo-mechanical analysis of granular materials will be explored together in the next steps of this project.

Keywords: FEM, DEM, thermally-coupled analysis, fluid dynamics, granular materials.

1 Introduction

Granular materials are characterized by a heterogeneous assembly of particles with different physical and geometric properties, whose interactions with each other dictate the macroscopic behavior. These interactions involve several different types of physics and are highly dependent on many factors that are constantly evolving, which imposes great challenges for predicting the behavior of granular media. For instance, depending on the stress state, this type of material can behave both liquid- or solid-like. Therefore, because of these unique features, many unsolved issues concerning the numerical modeling still exist. From the numerical point-of-view, two types of methods can be applied to simulate granular media, namely, continuous and discrete methods. On the one hand, continuum-based methods make use of phenomenological constitutive laws to approximate the grain-scale phenomena. In this way, the information about the microphysics of the material is missed, but the analyses are comparatively cheaper in a computational sense. On the other hand, the discrete approach simulates the grain-scale behavior with more accuracy, but at a much higher computational cost.

This work is part of an ongoing projects that seeks to explore both the continuum and the discrete approaches for simulating the thermomechanical behavior of dense granular flows. For the continuum approach, the Particle Finite Element Method (PFEM), introduced by Oñate [1], is being used due to its ability to handle large changes of topology. For the discrete approach, the selected strategy is the widely used Discrete Element Method (DEM), specifically, the soft-sphere version proposed by Cundall & Strack [2]. The final goal of the project is to combine these methods into a single multiscale framework to take advantage of the benefits of each one. In order reach this goal, a thermally-couple PFEM and DEM are being developed separately, and will be presented in the sequence.

2 Thermal PFEM

The PFEM is a continuum-based numerical method suitable for engineering problems with severe changes of topology and evolving free-surfaces. It is based on a Lagrangian FEM mesh, where the mesh nodes are treated as particles by transporting their physical properties as they move. To circumvent the excessive mesh deformation, a remeshing procedure is constantly applied by erasing the elements and combining the Delaunay triangulation with the Alpha-Shape method to generate a new mesh from the cloud of nodes. The discretized governing equations are then solved via FEM to compute the next nodal positions, $\boldsymbol{x}$, and so the process repeats. Normally, an implicit scheme is used for the time integration. For a general review of the method, see Cremonesi et al. [3].

When applied to flow problems, the momentum (eq. (1)) and mass (eq. (2)) conservation equations are solved for the velocities, $\boldsymbol{v}$, and pressure, P, respectively, in a nonlinear iteration loop within each time step. Since these equations are in a Lagrangian form, no convective term appears in the momentum equation and, therefore, no stabilization for this term is required in the FEM solution. However, because of the Delaunay triangulation, equal-order interpolation is used for $\boldsymbol{v}$ and P, so the *inf-sup* condition is not satisfied and a technique is applied to stabilize the solution. In the current implementation, the Finite Increment Calculus, presented by Oñate [4], is used for this purpose. Furthermore, as it can be seen in eq. (2), a quasi-incompressible flow is assumed, so that the pressure can be computed explicitly. For more details on the PFEM formulation for fluid dynamics, see Oñate et al. [5].

$$\rho \frac{\partial \boldsymbol{v}}{\partial t} = \nabla \cdot \boldsymbol{\sigma} + \rho \boldsymbol{b} \tag{1}$$

$$\frac{\partial P}{\partial t} + \kappa \nabla \cdot \boldsymbol{v} = 0 \tag{2}$$

To consider the thermal effects in this work, the energy conservation equation (eq. (3)) is included and solved for the temperature in the same Lagrangian FEM mesh. Again, no convective term exists as the heat convection in the fluid is automatically done by the motion of the nodes, so only the thermal diffusion is computed.

$$\rho c_p \frac{\partial T}{\partial t} = k \nabla^2 T + G \tag{3}$$

The computational implementation of this numerical method was done in the open-source framework *Kratos Multiphysics* [6], and a graphical interface was created in *GiD* [7] for pre and post processing.

2.1 Thermo-mechanical coupling scheme

The coupling between the fluid dynamics and the thermal diffusion problems within the PFEM framework is done according to Fig. 1, which depicts the scheme of a single time step. The solution of the mechanical problem (fluid dynamics) corresponds to the new nodal velocities and positions, by assuming a constant temperature. Then, based on the new configuration, the temperature field is obtained from the solution of the thermal problem. This strategy belongs to a class of staggered schemes because both physics are solved in two different linear systems. Particularly, it is called external scheme because the thermal problem is solved after the convergence of the mechanical one, in contrast to an internal staggered scheme in which both problems are solved together in the same iteration loop. Moreover, no iterations are performed for the thermal problem in each time step because the thermal response is assumed to evolve much slower than that of the mechanical problem.

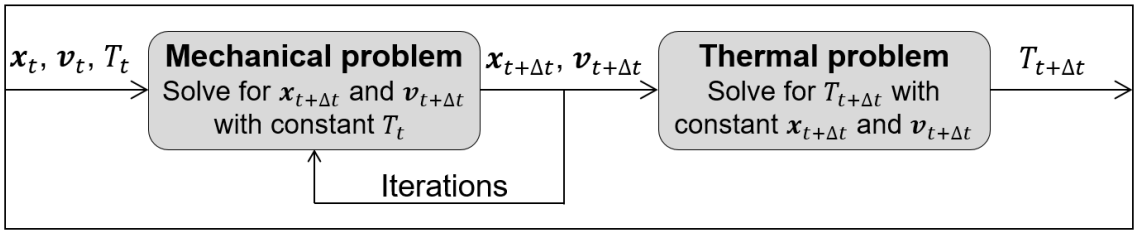

Figure 1. PFEM coupling scheme between the mechanical and thermal problems in the time step [t,t+Δt].

2.2 Main features of the method

The thermally-coupled PFEM, resulting from the above described methodology, obviously inherits all the features from the original method related to the solution of flow problems. In addition, it brings some new interesting features related to the solution of the thermal problem.

One of the new features is the possibility to apply different types of thermal boundary conditions (B.C.) to the model: prescribed temperature (Dirichlet B.C.), prescribed heat flux (Neumann B.C.), and heat transfer by convection and / or radiation (Robin B.C.). In fact, all these boundary conditions can be applied to the free-surface of the domain, which is constantly updated and tracked. Furthermore, internal heat generation can also be imposed to the elements. Regarding the constitutive models, it is possible to employ both Newtonian and non-Newtonian constitutive laws, including Herschel-Bulkley, frictional-viscoplastic models, and the μ(I)-rheology. The latter was proved to be the most appropriate for simulating the behavior of dense granular flows [8]. Moreover, temperature dependency can also be set, by means of input tables, to the material properties and parameters required by the constitutive models.

2.3 Examples

To demonstrate the capabilities of the new numerical tool, two examples are presented.

The first example, shown in Fig. 2a, is the natural convection of a fluid with temperature dependent density in a square cavity of unitary sides. The initial temperature of the fluid is 273.65 K, the left and right walls are kept at 274.15 K and 273.15 K, respectively, while the others are insulated. The fluid has a viscosity of 0.71 Pa.s, bulk modulus of 10^9 Pa, thermal conductivity of 1 W/m.K, and specific heat of 1 J/kg.K. The density at the initial temperature is 1000 kg/m^3, and it varies linearly with a rate of 100 kg/K.m^3. Initially, the mesh is composed of 2498 triangular elements. The upper left image shows the beginning of the fluid motion due to density change at 5s, and the image to its right shows the temperature distribution after an approximate steady state is reached in about 20s. The isothermal lines of the steady state are given in the lower left image and they are clearly in agreement with the solution presented by Davis [9], in the lower right.

The second example, shown in Fig. 2b, is the simulation of the melting behavior of a block of a Bingham material that has temperature dependent yield shear stress and viscosity. The temperature of the walls are kept fixed (as the same of the initial material temperature) and a radiative heat flux is imposed to the evolving free-surface. As the material temperature increases, the yield shear stress decreases up to a point when the material starts to flow and behave fluid-like. The model parameters are skip for this example since it is not intended to validate the correctness of the results, but to show an interesting simulation made possible by the developed method.

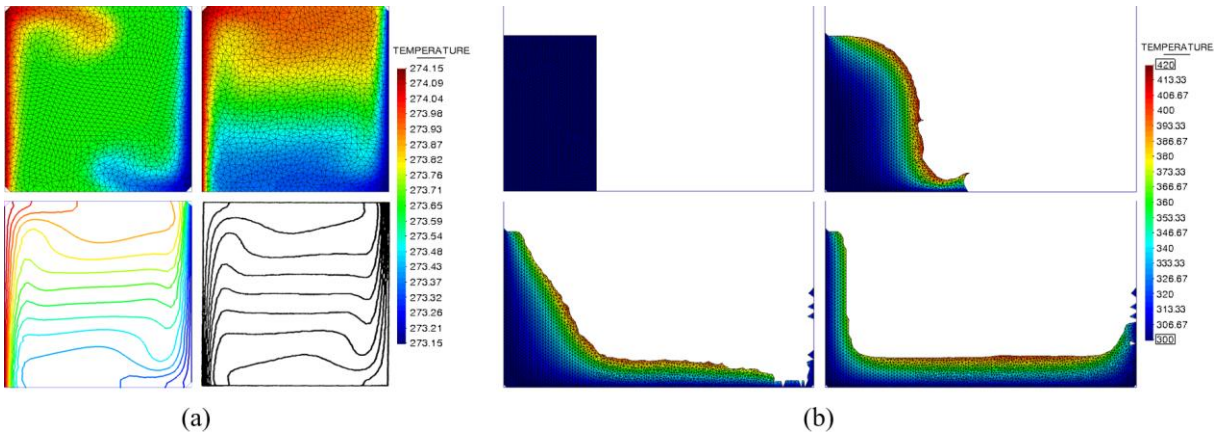

Figure 2. (a) Buoyancy-driven flow in a square cavity. (b) Melting due to radiation applied to the free-surface.

3 Thermal DEM

The DEM represents the material as a collection of individual particles interacting with each other. No constitutive model is needed in this approach. Instead, the macroscopic behavior of the material relies on the models that govern the particles interactions. Therefore, it is best suited for granular media, as it can simulate the behavior of grains with more accuracy, capturing micro-scale effects that constitutive laws are unable to represent.

The motion of each particle is determined by the equations of Newton's second law (eq. (4) and eq. (5)). These equations are solved numerically to obtain the translational, $\boldsymbol{v}$, and rotational, $\boldsymbol{\omega}$, velocities, as well as the coordinates and angular orientations. The force, $\boldsymbol{F}$, and torque, $\boldsymbol{M}$, acting on a particle are needed to be calculated in each time step, and they can result from different contributions, including contact and non-contact interactions with the surrounding objects, body weight, etc. A vast number of models have been proposed to mathematically describe each of these contributions, as the bulk mechanical behavior highly depends on the adopted models [10].

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \boldsymbol{F}_i \tag{4}$$

$$\boldsymbol{I}_i \frac{d\boldsymbol{\omega}_i}{dt} = \boldsymbol{M}_i \tag{5}$$

The exchange of thermal energy between DEM particles is simulated by numerically solving the energy balance equation for each element (eq. (6)) in order to compute its temperature, T. For simplicity, the particles are normally considered to be isothermal, which is an assumption that is valid when the *Biot* number is much smaller than unity, so that the temperature gradient in the interior of the body can be neglected. In this way, in every time step, it is enough to compute the total rate of heat transfer, Q, towards or outwards each particle to obtain its temperature variation. The net heat transfer may be originated from many different mechanisms, by means of conduction, convection, radiation, internal sources, etc. As with forces, each of these mechanisms can be modeled in several different ways. For a comprehensive review of the heat transfer models in DEM, see Peng et al. [11].

$$m_i c_{p,i} \frac{\partial T_i}{\partial t} = Q_i \tag{6}$$

A computer application was created for the implementation of thermo-mechanical analyses with DEM [12]. This program is written in the MATLAB script language with the purpose of offering a modular environment for readily testing many thermo-mechanical interaction models in small-scale problems. Once the models are tested and validated, they will be implemented in *Kratos Multiphysics*, where problems of larger scale can be simulated.

3.1 Thermo-mechanical coupling scheme

The coupling between the mechanical and thermal behaviors of the particles is simple and follows the scheme in Fig. 3. The equations of motion and energy balance are solved simultaneously at every time step. A two-way coupling between both physics happens by the dependency of the thermal solution on the particle kinematics, while the mechanical solution can also depend on the thermal state, as in the case of variable material properties.

An important aspect of the DEM is that, within a time step, no mechanical or thermal disturbance can propagate further than a particle's immediate neighbors. As a consequence, an explicit time integration strategy is required with a very small step to ensure a stable solution. In general, the stability condition for the mechanical problem is much more restrictive than for the thermal problem and, therefore, it controls the time step size.

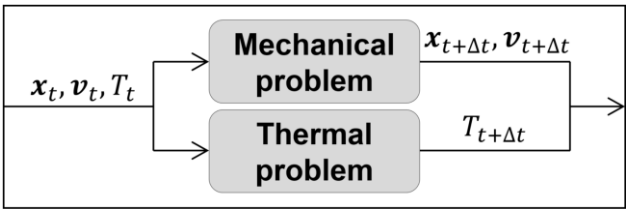

Figure 3. DEM coupling scheme between the mechanical and thermal problems in the time step [t,t+Δt].

3.2 Main features of the method

The computational tool developed in this work allows for three separated types of DEM analysis: mechanical, thermal, and thermo-mechanical. The first two isolate their respective physics ignoring the other, and the latter considers both of them simultaneously, as described in the previous section. The separation of the thermal analysis is intended to provide great savings in computational effort and simulation time. It assumes that all particles are rested in static equilibrium, so forces, torques and motion are not computed. As a consequence, the algorithm for searching the neighbors of all particles (known as the most expensive task in a DEM simulation) is performed only once. Furthermore, the critical time step to ensure the stability can be much larger. Therefore, this analysis type is very useful for simulating packed beds, for example. By taking advantage of this feature, a future implementation is to allow the thermal and thermo-mechanical analyses to be used at the same time in different regions of the model, depending on the motion regime.

Regarding interaction models, the program includes the most used contact force models for the normal and tangential directions, and for rolling friction resistance. However, the focus of this work is on the heat transfer models. Initially, only the heat conduction of particle-particle and particle-wall interactions is being considered, as it can be regarded as the dominant mechanism of heat transfer in dense granular systems. Two types of heat conduction can be found in the literature: direct and indirect conduction. The former happens through the contact area between the bodies, while the latter happens through the thin wedge of interstitial fluid between contacting or non-contacting particles that are very near. Some models to simulate these heat conduction mechanisms are currently implemented according to the formulations provided in Tab. 1 and Tab. 2 for the direct and indirect conductions, respectively. All of these models, as well as most models for heat exchange in DEM, are developed for spherical particles. For more details, the indicated references should be consulted. Some particular considerations for our implementation is included in the program's documentation.

In those tables, d is the distance between the centers of particles; ρ is the density; k is the thermal conductivity; c_p is the heat capacity; R is the radius; $\tilde{R}$ is the average radius of both particles; R_c and R_c^{max} are the current and maximum contact radii; t_c is the expected collision duration; V_{ij} is a volume related to the Voronoi cell where a particle is located; Sub-indices *i*, *j* and *f*, refer to the two contacting particles and the interstitial fluid.

Table 1. Direct heat conduction models

Method	Heat Transfer Coefficient	Additional Parameters
Batchelor & O'Brien [13]	$4\bar{k}R_c$	$\bar{k} = k_i k_j / (k_i + k_j)$
Thermal Pipe [14]	$\pi (R_c)^2 \tilde{k}/d$	$\tilde{k} = (R_i + R_j)\left((R_i/k_i + R_j/k_j)\right)^{-1}$
Collisional [15]	$C\dfrac{\pi (R_c^{max})^2 (t_c)^{-1/2}}{(\rho_i c_{p,i} k_i)^{-1/2} + (\rho_j c_{p,j} k_j)^{-1/2}}$ $C = \dfrac{0.435}{C_1}\left(\sqrt{{C_2}^2 - 4C_1(C_3 - F_o)} - C_2\right)$	$C_1 = -2.300\alpha^2 + 8.909\alpha - 4.235$ $C_2 = 8.169\alpha^2 - 33.770\alpha - 24.885$ $C_3 = -5.758\alpha^2 + 24.464\alpha - 20.511$ $\alpha = \left(\dfrac{\rho_i c_{p,i}}{\rho_j c_{p,j}}\right)^2, F_o = \dfrac{k_i t_c}{\rho_i c_{p,i} (R_c^{max})^2}$

Table 2. Indirect heat conduction models

Method	Heat Transfer Coefficient	Additional Parameters
Voronoi-Based A [16]	$\displaystyle\int_{R_c}^{r_{sf}} \frac{2\pi r dr}{\left(\sqrt{\tilde{R}^2 - r^2} - rd/2r_{ij}\right)/\bar{k} + \left(d - 2\sqrt{\tilde{R}^2 - r^2}\right)/k_f}$ (Integral solved numerically)	$r_{sf} = \tilde{R} r_{ij} \left({r_{ij}}^2 - d^2/4\right)^{-1/2}$ $r_{ij} = \sqrt{3V_{ij}/\pi d}$

Voronoi-Based B [16]	$\frac{\pi}{b}\ln\left(\frac{a-b\cos\theta_0}{a-b\cos\theta_c}\right)$ $a=\left(r_c{}^{-1}-\tilde{R}^{-1}\right)/2\bar{k}+\left(k_f\tilde{R}\right)^{-1}$ $b=\left(k_f d/2\right)^{-1}$	$\theta_0=d\left(r_{ij}{}^2+d^2/4\right)^{-1/2}/2$ $\theta_c=d\left(R_c{}^2+d^2/4\right)^{-1/2}/2$ r_c is an input parameter
Surrounding Layer [17]	$\int_{R_c}^{R_e}\frac{2\pi r dr}{max\left(S,d-\sqrt{R_i{}^2-r^2}-\sqrt{R_j{}^2-r^2}\right)}$ (Integral solved numerically)	$R_e=\sqrt{\gamma^2-\left(\frac{\gamma^2-R_l{}^2+d^2}{2d}\right)^2}$ $\gamma=R_k+\delta$ $R_k=max\left(R_i,R_j\right)$ $R_l=min\left(R_i,R_j\right)$ S and δ are input parameters

3.3 Example

The implementation of the thermal DEM is not fully completed by the time of this article and, as previously mentioned, the initial implementations are being tested in a code that is able to run only small-scale simulations, due to the relatively low efficiency of the programming language used. Therefore, a simple example of a purely thermal analysis will be presented, by showing an aspect that will be the focus of the next steps of the project.

The example is a square box filled with a granular material simulated using the DEM and the FEM (PFEM is not needed as there is no motion). The side of the box has 0.6 m, the thermal conductivity and heat capacity of the material in both models is 2000 W/m.K and 100 J/kg.K. The density of the DEM particles is 2500 kg/m^3, while the density of the continuous FEM material is 2296.3 kg/m^3, to account for the voids. The initial temperature of the material is 400 K and the bottom and side walls are kept at 300 K while the top is insulated. In the DEM model, 4454 particles were used (avg radius: 4.83 mm; min/max radius: 2.56 mm, 7.92 mm; std dev: 0.53 mm). The initial positions were obtained by letting the particles rest under their own weight in a mechanical simulation. A Forward Euler scheme was used for the time integration with a time step of 10^{-4} s. The only heat exchange mechanism considered was the Batchelor & O'Brien model for direct conduction, as it is done by many authors. The FEM model was discretized into 8020 linear triangles and used a time step of 10^{-2} s. The simulation ran up to 10s.

Figure 4 shows the comparison between both models. The two images at the top correspond the DEM solution at 2.5s and 10s, and the images below are the FEM solution for the same time. The graph shows the evolution of the temperature at the mid-top position (a particle in DEM and a node in FEM). As expected, the FEM solution overestimates the heat conduction by a large margin as the thermal conductivity of the continuous material is not taking into account the granular nature of the medium. In order to get accurate solutions with the FEM (or PFEM), an effective thermal conductivity needs to be considered for the continuous material. The way to obtain some effective mechanical and thermal parameters from the DEM solution for the FEM/PFEM models will be assessed in the sequence of the project by using homogenization techniques so that both methods can be combined.

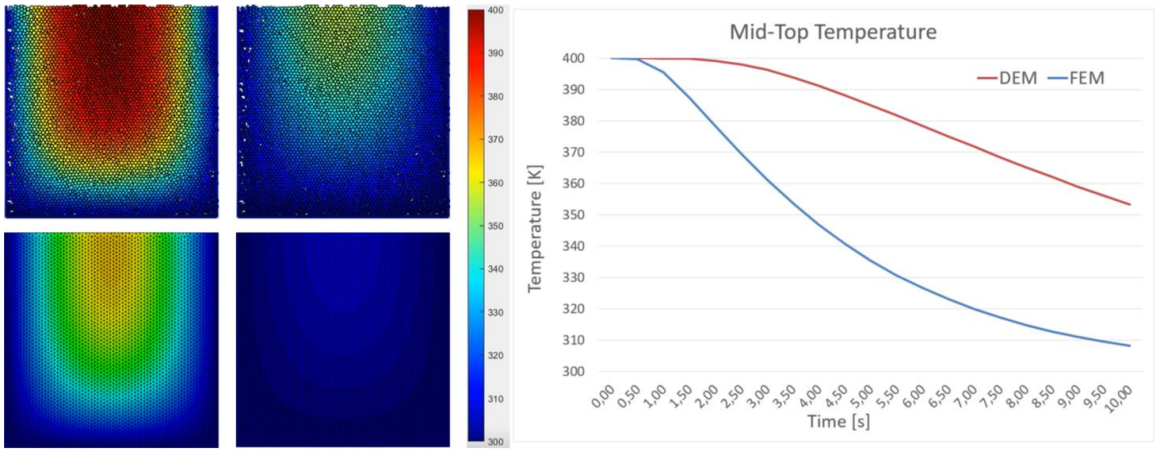

Figure 4. Comparison between discrete and continuous solutions for the heat conduction in a particulate system

4 Conclusions

This article presented the characteristics of two numerical tools developed to perform thermo-mechanical analysis by means of a continuum-based and a discrete-based approach: the thermal PFEM and thermal DEM. These tools can be applied for simulating the thermal behavior of particulate media in a static or flowing regime. However, each one has its pros and cons. The PFEM or FEM can be applied to analyze large scale problems with a feasible computational cost, in which the DEM would be impractical. On the other hand, the DEM is able to capture the grain-scale effects that govern the macroscale behavior, by the time that the continuous-based methods employ constitutive laws that, most of the times, cannot do the same. This aspect became clear in the last example, in which, the FEM solution was extremely faster but, without considering adjusted parameters, it deviates from the discrete solution by a large margin. Therefore, the objective for the sequence of the project is to combine these two techniques to explore the efficiency of the continuous method with the accuracy of the discrete one. It will be done in a multiscale sense, where DEM assemblies will placed at the integration points of the FEM mesh, so that the discrete solution will provide the effective mechanical and thermal parameters to the PFEM / FEM formulation.

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