Computational Materials Science 69 (2013) 46–52

Contents lists available at SciVerse ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

Simulation of continuum heat conduction using DEM domains

I. Terreros [a,*], I. Iordanoff [a,b], J.L. Charles [b]

[a] Arts et Métiers ParisTech, I2M-MPI, UMR 5295 CNRS, France
[b] Arts et Métiers ParisTech, I2M-DuMAS, UMR 5295 CNRS, France

ARTICLE INFO

Article history:
Received 31 August 2012
Received in revised form 8 November 2012
Accepted 12 November 2012
Available online 23 December 2012

Keywords:
Discrete Element Method
Heat conduction
Thermal field
Transient temperature
Continuum materials

ABSTRACT

Currently, almost all material manufacturing processes are simulated using methods based on continuum approaches such as the Finite Element Method (FEM). These methods, though widely studied, face difficulties with multibody, contact, high-strain and high-displacement problems, which are usually found in manufacturing processes. In some cases, the Discrete Element Method (DEM) is used to overcome these problems, but it is not yet able to simulate some of the physics of a continuum material, such as 3D heat transfer.

To carry out a realistic simulation of a process, its thermal field must be properly predicted. This work describes a fast and efficient method to simulate heat conduction through a 3D continuum material using the Discrete Element Method. The material is modelled with spherical discrete elements of different sizes to obtain a compact and isotropic domain adequate for carrying out mechanical simulations to obtain straightforward thermal and mechanical coupling.

Thermal simulations carried out with the proposed Discrete Element Method are compared to both the analytical and FEM results. This comparison shows excellent agreement and validates the proposed method.

1. Introduction

The importance of temperature fields in almost any manufacturing method is indisputable. Due to the very strong dependence of metallurgical phenomena on these fields, they critically influence the mechanical properties of the processed material. Consequently, the search for a realistic thermal simulation of a process, including accurate temperature predictions, is an issue of capital importance for the desired full control of manufacturing techniques.

A law for heat conduction through a continuous material was first proposed by Fourier in 1822 [1] (Eq. (1) in the case of constant conductivity where Θ is the temperature, λ is the thermal conductivity, ρ is the density of the material, and t represents the time). This equation provides analytical solutions for some geometrically simple problems [2] and has been widely solved using various numerical methods, but primarily by the Finite Element Method [3] due to its natural adaptation to partial differential equations.

$$\frac{\partial \Theta}{\partial t} = \frac{\lambda}{\rho c_p}\left(\frac{\partial^2 \Theta}{\partial x^2} + \frac{\partial^2 \Theta}{\partial y^2} + \frac{\partial^2 \Theta}{\partial z^2}\right) \quad (1)$$

In tooling processes, regions with high thermal gradients and heat fluxes are often located near the tool-piece contact. In the contact area, continuous approaches have difficulty accurately describing high strains and temperature gradients. In this area, the Discrete Element Method [4] is a good alternative to the FEM to locally solve problems related to material fracture [5], multibody system coupling [6] or dry sliding contact with a third body presence [7], among others. A long term solution consists of solving the contact area with the DEM and solving the piece and tool far from the contact with continuous approaches, such as the FEM or the NEM [8], and then coupling these methods (Fig. 1).

There are many works that describe the use of the Discrete Element Method in a mechanical field such as [9], which uses Lennard–Jones potentials [10] to describe the interaction forces between discrete elements, the work in reference [11], where discrete elements are linked in a truss, and exact results for the stress and strain fields of 2D shells are obtained, or [12], which links discrete elements by beams and describes how to carry out wear simulations for brittle elastic materials.

However, examples of the DEM in thermal fields are mostly focused on problems involving granular materials [7,13–17], with the exception of [18], in which the mathematical proof of the 2D DEM for a continuous thermal field is described.

The present work describes a method to simulate isotropic heat conduction through a 3D continuum material using the Discrete Element Method. The material is modelled with spherical discrete elements of different sizes to obtain a compact and isotropic domain adequate for carrying out 3D mechanical simulations [12]. The validity of the described method in such a discrete domain is the basis for thermo-mechanical simulations using the DEM.

* Corresponding author.
E-mail addresses: inigo.terreros@u-bordeaux1.fr (I. Terreros), ivan.iordanoff@ensam.eu (I. Iordanoff), jl.charles@i2m.u-bordeaux1.fr (J.L. Charles).

0927-0256/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.commatsci.2012.11.021

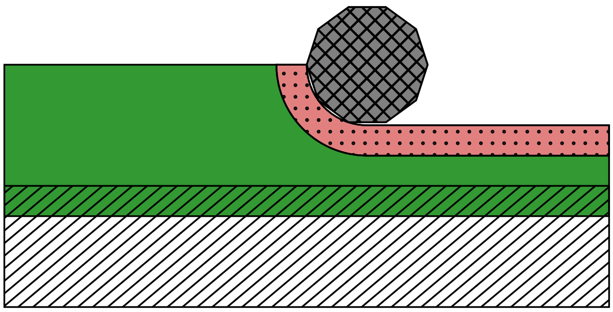

Fig. 1. Simplified example of a milling process. Discrete Element Method is used in the zone in contact with the tool (dotted) in order to simulate complex thermo-mechanical behaviours. DEM is also used beyond the contact zone (solid) in order to ease the coupling with a Finite Element Method zone (striped).

The paper is structured as follows: In Section 2 a description of the method is given. This method is proved in Section 3 for 3D crystal domains and in section 4 for isotropic domains. In Section 5 numerical results are shown and discussed. Finally, conclusions are inferred in Section 6.

2. General description of the method

Fig. 2 shows a typical discrete domain created exclusively with spherical discrete elements.

To find the variation of a given magnitude through a discrete domain, there are two principal steps to follow, as explained in [13]:

- First, variations due to the interaction between each discrete element and all its neighbours must be separately analysed and stored.
- Then, stored variations of each discrete element must be summed to obtain the total variation of the magnitude for the discrete element.

Mathematically:

$$G_i = \sum^{N_{neigh}} g_{ij} \tag{2}$$

where G_i is the variation of the measured magnitude for the discrete element i and g_{ij} is the variation of the magnitude of discrete element i due to its interaction with its neighbour j.

2.1. Application to heat conduction

In the particular case of heat conduction, transferred heat between two discrete elements for a given instant, W_{ij}, can be calculated using Fourier's law as follows:

$$W_{ij} = S_t \lambda \frac{(\theta_j - \theta_i)}{d_{ij}} \tag{3}$$

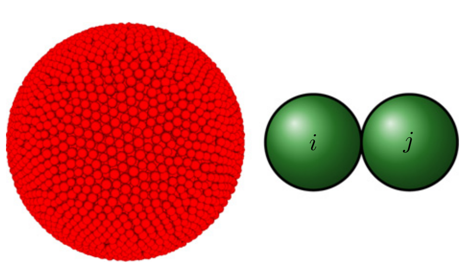

Fig. 2. A sample of a spherical discrete domain and an example of neighbour discrete elements.

where S_t is the heat transmission surface's area; $(\theta_j - \theta_j)$ is the temperature difference between discrete element i and discrete element j; λ is the material's heat conductivity and d_{ij} is the distance between discrete element i and discrete element j.

Furthermore, the thermal energy gain of a discrete element i, ΔE_i in the equation, can be calculated as a function of its rise in temperature:

$$\Delta E_i = c_p \rho_d V_i \Delta\theta_i$$

where c_p is the specific thermal capacity of the discrete element; ρ_d represents the discrete element's density; V_i is the volume and $\Delta\theta_i$ is the raise of temperature of a discrete element i.

The time derivative of the thermal energy gain represents the heat being transferred to discrete element i:

$$\frac{\Delta E_i}{\Delta t} = W_{ij} = \frac{c_p \rho_d V_i \ \Delta\theta_i}{\Delta t} \tag{4}$$

If the time step Δt is small enough to consider $(\theta_j - \theta_i)$ constant during the time step, Eqs. (3) and (4) can be combined to obtain the temperature rise of discrete element i due to its interaction with a neighbour j:

$$\Delta\theta_i = \frac{(\theta_j - \theta_i) S_t \lambda}{d_{ij} c_p \rho_d V_i} \Delta t \tag{5}$$

Finally, Eq. (2) is used to obtain $\Delta\Theta_i$, the total variation of the temperature of discrete element i, after the time step Δt:

$$\Delta\Theta_i = \sum^{N_{neigh}} \Delta\theta_i$$

3. Proof of concept on 3D crystal domains

In the work by Hahn et al. [18], a method to predict temperature fields in 2D discrete domains formed by hexagonal discrete elements is proved. In this section a proof for 3D discrete domains formed by identically-sized spherical discrete elements placed following a *simple cubic* crystal pattern will be given, following the method described in paragraph 2.1.

3.1. Proof

Fig. 3 represents an example of the domain described above. To fill all of the domain's volume, each discrete element represents a cube of continuous material whose volume equals $(2R)^3$.

Eq. (5) can be modified for the particular case of the crystal domain of Fig. 3 as follows:

First, the mass of each discrete element must equal the mass of the represented volume. Then, the discrete element's density ρ_d is linked to the material's density ρ_c by means of the volume fraction f_v following:

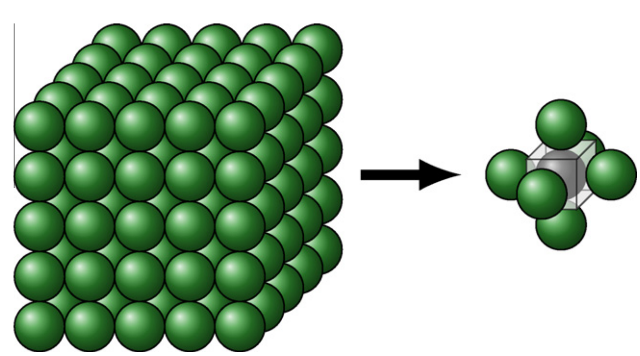

Fig. 3. 3D crystal domain and example of a random particle with six neighbours. The volume represented by each discrete element is $2R \times 2R \times 2R = 8R^3$.