Discrete element modeling for predicting 3D-printed concrete process parameters

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Abstract. This work presents a computational model for the simulation of the rheological behavior of 3D-printed fresh concrete. Our approach is based on the discrete element method (DEM) for description of the particles' overall dynamics, combined with the Discrete Fresh Concrete (DFC) model [1] to account for particle-particle and particle-wall interactions at the level of the (contact) constitutive equation. Using the DFC model, we hope to be able to represent the interaction among coarse aggregate particles within a fine mortar matrix. This is an on-going research that is part of a master's dissertation, and only the theoretical framework will be presented by now. Numerical results shall appear soon.

Keywords: 3D concrete printing, particles, discrete element methods (DEM)

1 Introduction

Recently, the construction industry has undergone a revolutionary advancement with the introduction of 3D Concrete Printing (3DCP). It offers several advantages over traditional construction methods, including: (1) greater flexibility in architectural design; (2) significant reduction in construction time and material waste; and (3) enhanced sustainability, and cost-effectiveness. However, there are still some uncertainties and technological challenges that need to be addressed before 3DCP can be widely adopted in the construction industry, including: (1) current 3D printing technologies require improved materials in order to reach their full potential; (2) concrete rheological characteristics need to be considered when developing new 3D printing technologies; and (3) the required pumping and extrusion pressure during the 3DCP process.

To address the challenges associated with 3DCP, numerical simulation may be an effective tool. Considering that fresh concrete has a rather discrete (and two-phase) nature at the level of the coarse aggregates, the discrete element method (DEM) stands as a natural approach. First introduced by Cundall in the 1970s [2, 3] and further refined by Cundall and Strack [4], DEM can be understood as a model for the representation and study of granular materials. It proposes to numerically solve the differential equations of motion for systems composed by a large number of rigid solids ("discrete elements" or "particles") [5]. In DEM simulations, these individual particles are treated as discrete entities, and their interactions are governed by simple mechanical laws, such as contact forces, frictional forces, and others. By tracking the motion of each (and all) individual particles and considering their interactions, DEM provides valuable insights into complex phenomena at any desired time instant. This includes individual particle trajectories, forces interacting, interactions among neighboring particles, and many other factors that are challenging to obtain through experimental techniques.

This article presents an approach that combines the DEM formulation for modeling particle dynamics with the DFC model equations to account for particle-particle and particle-wall interactions in fresh printable concrete. The DFC model, introduced by Cusatis and Ramyar [1], is based on stress-strain relationships to represent the contact interactions, and, when used in the DEM framework, provides an accurate description of the interactions among coarse aggregate particles within a fine mortar matrix. They idealize each particle as spheres with two phases: (i) a rigid inner sphere (representing the aggregate) and (ii) a soft outer layer, covering the first (representing the mortar), with a known thickness. Our approach adopts the DEM formulation developed by Campello [5–7] and Quintana-Ruiz and Campello [8] for the mechanical part of the problem. This is an on-going research that is part

of a master's dissertation, and only the theoretical framework will be presented by now. Numerical results shall appear soon.

2 Methodology

In this work we incorporate the DFC model, developed by Cusatis and Ramyar [1], to describe contact between particles (and between particle and wall) in our in-house DEM code. Our main objective is to simulate the rheological behaviour of printable fresh concrete for 3D concrete printing. It is important to mention that this research is in initial development phase, and we anticipate further advances as we continue our work. The results of this study will be presented at the congress.

2.1 Particle's Dynamics and Discrete Fresh Concrete

2.1.1 Particle's Dynamics

In this study, we adopt a Lagrangian DEM description. Let us consider a system of N_P spherical "biphasic" particles, consisting of a rigid inner sphere covered by a thin layer of soft mortar on the outside, each characterized with essential properties, including mass m_i, radius R_i, aggregate radius r_i, mortar thickness h_i (Fig. 1) and rotation inertia j_i (relative to particle's center). To mathematically describe their motion, we represent the position vector of each particle as $\boldsymbol{x_i}$, the velocity vector as $\boldsymbol{v_i}$, the incremental rotation vector as $\boldsymbol{\alpha}_i^{\Delta}$ (rotation vector relative to two consecutive configurations) and the spin vector as $\boldsymbol{\omega_i}$. Following classical (Newton-Euler) dynamics, the equations of motion for the ith particle are

$$\begin{aligned} m_i\dot{\boldsymbol{v}}_i &= \boldsymbol{f}_i^{con} + \boldsymbol{f}_i^{env}, \\ j_i\dot{\boldsymbol{\omega}}_i &= \boldsymbol{m}_i^{rol}, \end{aligned} \tag{1}$$

where $\boldsymbol{f}_i^{con}$ are the forces due to mechanical contacts with other particles or walls and $\boldsymbol{f}_i^{env}$ are the forces due environment (in this study, we take only the gravitational contribution $m_i\boldsymbol{g}$, where $\boldsymbol{g}$ is the gravity acceleration vector). Still in eq. (1), $\boldsymbol{m}_i^{rol}$ are the moments induced by rolling resistance effects. It is important to mention that there are works in the literature that incorporate additional forces into the model, such as frictional forces, adhesive forces, drag forces, among others [5–8]. The forces due to mechanical contacts with other particles or walls, $\boldsymbol{f}_i^{con}$, are calculated as the sum of the forces acting on particle i due to the contact with all other particles or objects. This is described in eq. (2), where $\boldsymbol{f}_{ij}^{con}$ is the force acting on particle i due to the contact with particle j, and N_i^c is the number of particles and objects in contact with particle i.

$$\boldsymbol{f}_i^{con} = \sum_{j=1}^{N_i^c} \boldsymbol{f}_{ij}^{con} \qquad \text{with} \qquad \boldsymbol{f}_{ij}^{con} = -\frac{4}{3}\sqrt{r^*}E^*\delta_{ij}^{3/2}\boldsymbol{n}_{ij} - d^{con}\dot{\delta}_{ij}\boldsymbol{n}_{ij}, \tag{2}$$

with

$$r^* = \frac{r_i r_j}{r_i + r_j} \qquad E^* = \frac{E_i E_j}{E_j(1-\nu_i^2) + E_i(1-\nu_j^2)} \qquad \boldsymbol{n}_{ij} = \frac{\boldsymbol{x}_j - \boldsymbol{x}_i}{||\boldsymbol{x}_j - \boldsymbol{x}_i||}, \tag{3}$$

where r^* and E^* are the effective radius and effective elasticity modulus of particle pair $i-j$ (with E_i and ν_i the elasticity modulus and Poisson coefficient of particle i and the E_j and ν_j the elasticity modulus and Poisson coefficient of particle j), respectively; $\boldsymbol{n}_{ij}$ is the unit vector that points from the center of particle i to center of particle j; and $\dot{\delta}_{ij}$ is the overlap velocity of the pair. Still in eq. (2), δ_{ij} is the overlap between particles and d^{con} is the damping constant, which is given by

$$\delta_{ij} = r_i + r_j - ||\boldsymbol{x}_i - \boldsymbol{x}_j||, \tag{4}$$

and

$$d^{\text{con}} = 2\xi^{\text{con}}\sqrt{2E^* m^* \sqrt{r^*}\delta_{ij}^{1/4}} \qquad \text{with} \qquad m^* = \frac{m_i m_j}{m_i + m_j}, \tag{5}$$

where ξ^{con} is the damping rate and m^* is the effective mass of pair $i-j$. For the rolling resistance, is used a rotational spring-damper-slider model. Accordingly, for every contacting pair $i-j$, we initially consider an elastic trial stick state (i.e., one in which there is no rolling) where the rolling resistance moment is

$$\boldsymbol{m}_i^{\text{rol}} = \sum_{j=1}^{N_i^c} \boldsymbol{m}_{ij}^{\text{rol}} \qquad \text{with} \qquad \boldsymbol{m}_{ij}^{\text{roltrial}} = -k_{\text{rol}} \Delta\theta_{ij}^{\text{trial}} - d^{\text{rol}}\omega_{ij} \qquad \text{with} \qquad d^{\text{rol}} = 2\xi^{\text{rol}}\sqrt{j^* k_{\text{rol}}}, \tag{6}$$

where $\boldsymbol{m}_{ij}^{rol}$ is the rolling resistance moment acting on particle i due to its rolling on particle j, k_{rol} is the stiffness of the rotational spring, $\Delta\theta_{ij}^{trial}$ is the pair's trial rotation, d^{rol} is the rolling damping constant, ξ^{rol} is the rolling damping rate, and j^* is the rotational inertia of pair $i-j$.

This section shows how the conventional DEM works, and the contact model from eq. (2) to eq. (6) will be replaced by a model based on constitutive equations, which is the DFC.

2.1.2 Discrete Fresh Concrete (DFC)

The DFC model uses DEM principles with stress-strain relationships to more accurately represent the behavior of fresh concrete. Specifically, the model is designed to accurately represent mortar-to-mortar contact, i.e., between the outer layers of each particle. As a result, the equations of motion (eq. (1)) for the ith particle can be reformulated as

$$\begin{aligned} m_i \dot{\boldsymbol{v}}_i &= \boldsymbol{f}_i^{dfc} + \boldsymbol{f}_i^{env} \\ j_i \dot{\boldsymbol{\omega}}_i &= \boldsymbol{m}_i^{dfc}, \end{aligned} \tag{7}$$

where $\boldsymbol{f}_i^{dfc}$ are the forces on particle i due to mechanical contact between particles (or between particle and wall), $\boldsymbol{f}_i^{env}$ are the forces on particle i due environment that may arise from the possible existence of gravitational, electric and/or magnetic fields, $\boldsymbol{m}_i^{dfc}$ are the moments on particle i induced by other particles or walls. The calculation of the forces and moments acting on the particle due to its interactions with other particles and walls are

$$\begin{aligned} \boldsymbol{f}_i^{dfc} &= \sum_j A_{ij}\boldsymbol{\sigma}_{ij} \\ \boldsymbol{m}_i^{dfc} &= \sum_j A_{ij}(\boldsymbol{a}_i \times \boldsymbol{\sigma}_{ij}) \end{aligned} \tag{8}$$

where $\boldsymbol{\sigma}_{ij}$ is the stress on particle i at the contact point with particle j and $\boldsymbol{a_i}$ is the vector from the center of particle i to the contact area center. The contact area A_{ij} is given by,

$$A_{ij} = \pi(H_{ij})^2. \tag{9}$$

Given that particles are spherical, the contact area formed between two particles or between a particle and a wall can be modeled as a circle with radius H_{ij}, which is calculated as follows:

$$H_{ij} = \sqrt{(R_i)^2 - (a_i)^2} \qquad \text{and} \qquad a_i = \frac{(R_i)^2 - (R_j)^2 + (L_{ij})^2}{2L_{ij}}, \tag{10}$$

where a_i is the distance from the center of particle i to the contact area center and L_{ij} is the distance between the center of particle i and j (or object), which is given by

$$L_{ij} = ||\boldsymbol{x}_j - \boldsymbol{x}_i||. \tag{11}$$

Still in eq. (8), to calculate $\boldsymbol{\sigma}_{ij}$ and $\boldsymbol{a_i}$, it is necessary to establish a local Cartesian reference system, Fig. 1c. This reference system is based on the motion of particles i and j according to the classical Lagrangian formulation. The unit vector $\boldsymbol{e}_{\boldsymbol{N}}^{ij}$ is oriented along the line segment connecting the center of the two particles, which is calculated as follows:

$$\boldsymbol{e}_{\boldsymbol{N}}^{ij} = \frac{\boldsymbol{x}_j - \boldsymbol{x}_i}{L_{ij}}. \tag{12}$$

To fully establish the local Cartesian reference system, the unit vector $\boldsymbol{e}_{\boldsymbol{M}}^{ij}$ is calculated using the direction of the tangential relative velocity between particle i and j (or object) at the point of contact $\boldsymbol{v}_{rel,t}^{P}$, and the unit vector $\boldsymbol{e}_{\boldsymbol{L}}^{ij}$ is oriented forming a right-handed coordinate system. The unit vectors $\boldsymbol{e}_{\boldsymbol{M}}^{ij}$ and $\boldsymbol{e}_{\boldsymbol{L}}^{ij}$ are given by

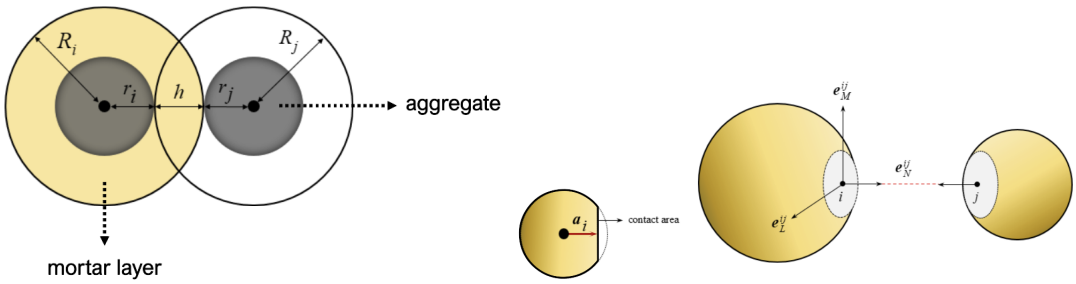
$$\boldsymbol{e}_{\boldsymbol{M}}^{ij} = ||\boldsymbol{v}_{rel,t}^{P} - (\boldsymbol{v}_{rel,t}^{P} \cdot \boldsymbol{e}_{\boldsymbol{N}}^{ij})\boldsymbol{e}_{\boldsymbol{N}}^{ij}||, \qquad \boldsymbol{e}_{\boldsymbol{L}}^{ij} = \boldsymbol{e}_{\boldsymbol{N}}^{ij} \times \boldsymbol{e}_{\boldsymbol{M}}^{ij}. \tag{13}$$

where, $\boldsymbol{v}_{rel,t}^{P}$ is calculated from the relative velocity at contact point $\boldsymbol{v}_{rel}^{P}$, which are given by

$$\boldsymbol{v}_{rel,t}^{P} = \boldsymbol{v}_{rel}^{P} - (\boldsymbol{v}_{rel}^{P} \cdot \boldsymbol{e}_{\boldsymbol{N}}^{ij})\boldsymbol{e}_{\boldsymbol{N}}^{ij}, \qquad \boldsymbol{v}_{rel}^{P} = \boldsymbol{v}_j + \boldsymbol{\omega}_j \times \boldsymbol{a}_j - \boldsymbol{v}_i + \boldsymbol{\omega}_i \times \boldsymbol{a}_i, \tag{14}$$

Given the distance a_i, the vector $\boldsymbol{a_i}$ is calculated as follow:

$$\boldsymbol{a_i} = a_i \boldsymbol{e}_{\boldsymbol{N}}^{\boldsymbol{ij}}. \tag{15}$$



(a) (b) (c)

Figure 1. (a) general configuration of two interacting particle; (b) contact area; (c) local Cartesian reference system

Still in eq. (8), $\boldsymbol{\sigma_{ij}}$ is the sum of stiffness stresses $\boldsymbol{\sigma}_s$ with the viscous stresses $\boldsymbol{\sigma}_v$, which is given by

$$\boldsymbol{\sigma_{ij}} = \boldsymbol{\sigma_s} + \boldsymbol{\sigma_v} \qquad \text{with,} \qquad \boldsymbol{\sigma_s} = \begin{bmatrix} \sigma_{Ns} \\ \sigma_{Ms} \\ \sigma_{Ls} \end{bmatrix} \qquad \text{and} \qquad \boldsymbol{\sigma_v} = \begin{bmatrix} \sigma_{Nv} \\ \sigma_{Mv} \\ \sigma_{Lv} \end{bmatrix} \tag{16}$$

where, to calculate $\boldsymbol{\sigma_s}$ and $\boldsymbol{\sigma_v}$ we consider the current configuration of the particle pair, which is defined by the relative position between them. In a generic configuration (Fig. 1a), the contact between two particles starts when $L_{ij} < r_i + r_j + 2h$ and the equilibrium configures when $L_{ij} = L_{ij0} = r_i + r_j + h$, where h is the mortar layer. Which means that, when two particles are in contact and $L_{ij} > L_{ij0}$, they are in tension (and we called it soft contact) and this is the case when particles are with attractive forces. Similarly, when $L_{ij} < L_{ij0}$ and $L_{ij} > r_i + r_j$, compression appears (also called it soft contact), causing repulsive forces. In addition, when $L_{ij} = L_{ij0}$, we are in zero (or neutral) configuration, and then no force is applied. Finally, when $L_{ij} = r_i + r_j$, the aggregates of particles i and j are in contact (and we called it hard contact). When in tension ($L_{ij} > L_{ij0}$) or compression, i.e. soft contact, ($L_{ij} < L_{ij0}$ and $L_{ij} > r_i + r_j$), $\boldsymbol{\sigma_s}$ and $\boldsymbol{\sigma_v}$ are

$$\boldsymbol{\sigma_s} = \begin{bmatrix} E_{Nm}\varepsilon_N^{ij} \\ 0 \\ 0 \end{bmatrix} \qquad \boldsymbol{\sigma_v} = \begin{bmatrix} \beta\eta(\dot{\gamma})\dot{\varepsilon}_N^{ij} \\ \eta(\dot{\gamma})\dot{\varepsilon}_M^{ij} \\ \eta(\dot{\gamma})\dot{\varepsilon}_L^{ij} \end{bmatrix}, \tag{17}$$

otherwise, when hard contact develops, i.e. $L_{ij} = r_i + r_j$, $\boldsymbol{\sigma_s}$ and $\boldsymbol{\sigma_v}$ are

$$\boldsymbol{\sigma_s} = \begin{bmatrix} E_{Na}\varepsilon_N^{ij} \\ \alpha_a E_{Na}\varepsilon_M^{ij} \\ \alpha_a E_{Na}\varepsilon_L^{ij} \end{bmatrix} \qquad \boldsymbol{\sigma_v} = \begin{bmatrix} \beta\eta(\dot{\gamma})\dot{\varepsilon}_N^{ij} \\ \eta(\dot{\gamma})\dot{\varepsilon}_M^{ij} \\ \eta(\dot{\gamma})\dot{\varepsilon}_L^{ij} \end{bmatrix}, \tag{18}$$

where E_{Nm} is the mortar normal elastic modulus, E_{Na} is the aggregate normal elastic modulus, α_a is the normal-shear coupling parameter and

$$\dot{\varepsilon}_N^{ij} = \frac{\boldsymbol{v}_{\text{rel}}^P \cdot \boldsymbol{e}_N^{ij}}{L_{ij}}, \qquad \dot{\varepsilon}_M^{ij} = \frac{\boldsymbol{v}_{\text{rel}}^P \cdot \boldsymbol{e}_M^{ij}}{L_{ij}}, \qquad \dot{\varepsilon}_L^{ij} = \frac{\boldsymbol{v}_{\text{rel}}^P \cdot \boldsymbol{e}_L^{ij}}{L_{ij}}, \tag{19}$$

are the strain rates in direction N, M and L. Still in eq. (17) and eq. (18), $\eta(\dot{\gamma})$ is the apparent viscosity, which is given by

$$\begin{aligned} \eta(\dot{\gamma}) = \eta_0 = \kappa_0\eta_\infty \quad &\text{if} \quad \dot{\gamma} \leq \dot{\gamma}_0 \\ \eta(\dot{\gamma}) = \eta_\infty|\dot{\gamma}|^{n-1} \quad &\text{if} \quad \dot{\gamma}_0 < \dot{\gamma} \end{aligned} \tag{20}$$

and

$$\dot{\gamma} = \sqrt{\beta\dot{\varepsilon}_N^2 + \dot{\varepsilon}_M^2 + \dot{\varepsilon}_L^2} \quad \text{and} \quad \dot{\gamma}_0 = \sigma_{\tau 0}/\eta_0 \tag{21}$$

where $\sigma_{\tau 0}$ is the shear yield stress, $\kappa_0 = 100$ is a constant, η_∞ is the mortar plastic viscosity and n refers to Newtonian ($n = 1$), shear-thickening ($n > 1$), and shear-thinning ($n < 1$) flow.

The interaction between particle and surfaces, considers any surface as padded and characterized by a thickness p. The interaction between particle and surface is identical to the particle-particle model. The differences in this case are: (i) the center to center distance L_{ij} is replaced by the shortest distance between particle and surface; (ii) the zero-configuration becomes $L_0 = r_i + h/2 + p$; and (iii) the distance of particle i from the center of contact area becomes $a_i = L_{ij} - p$. For more comprehensive details of the DFC formulation, readers may refer to (Cusatis and Ramyar) [1].

3 Numerical Solution Scheme

To solve the mechanical problem, we integrate the governing equations (eq. (7)) numerically by means of an explicit (forward Euler) scheme. We obtain the values of position, velocity, spin and incremental rotations at time t_{i+1} based on the known values at time t_i. Then, we increment time by Δ_t and transfer the information from $i+1$ to i ($i \leftarrow i+1$). Subsequently, the procedure is repeated until the final simulation time t_F is reached. The eq. (22), eq. (23), eq. (24) and eq. (25) represent the calculation of the particle's velocity, spin, position and incremental rotation at time t_{i+1}, respectively.

$$\boldsymbol{v_i}(t + \Delta t) = \boldsymbol{v_i}(t) + \frac{1}{m_i}\int_t^{t+\Delta t} (\boldsymbol{f}_i^{dfc} + \boldsymbol{f}_i^{env})dt \approx \boldsymbol{v}_i(t) + \frac{\Delta t}{m_i}[\boldsymbol{f}_i^{dfc}(t) + \boldsymbol{f}_i^{env}(t)], \tag{22}$$

$$\boldsymbol{\omega_i}(t+\Delta t) = \boldsymbol{\omega_i}(t) + \frac{1}{j_i}\int_t^{t+\Delta t} (\boldsymbol{m}_i^{dfc})dt \approx \boldsymbol{\omega_i}(t) + \frac{\Delta t}{j_i}[\boldsymbol{m}_i^{dfc}(t)], \tag{23}$$

$$\boldsymbol{x}_i(t+\Delta t) = \boldsymbol{x}_i(t) + \boldsymbol{v}_i(t+\Delta t)\Delta t, \tag{24}$$

$$\boldsymbol{\alpha}_i^{\Delta}(t+\Delta t) = \boldsymbol{\omega}_i(t+\Delta t)\Delta t. \tag{25}$$

The solution process can be schematically seen in the following algorithm:

Solution Algorithm

Step 1 Initialize time variables and get initial conditions:

$t = 0$, $\Delta t =$ given

$\boldsymbol{x}_i(0)$, $\boldsymbol{v}_i(0)$, $\boldsymbol{\omega}_i(0)$, $\boldsymbol{\alpha}_i(0)$ = given $\quad (i = 1, \ldots, N_p)$

Step 2 **While** $t \leq t_{\text{final}}$, loop over all particles: **For** $i = 1, \ldots, N_p$ **Do**

Compute forces and moments at time t via eq. (8).

Update velocity, spin, position and incremental rotation vectors:

$\boldsymbol{v_i}(t+\Delta t) = \boldsymbol{v}_i(t) + \frac{\Delta t}{m_i}[\boldsymbol{f}_i^{dfc}(t) + \boldsymbol{f}_i^{env}(t)]$,

$\boldsymbol{\omega_i}(t+\Delta t) = \boldsymbol{\omega_i}(t) + \frac{\Delta t}{j_i}[\boldsymbol{m}_i^{dfc}(t)]$,

$\boldsymbol{x}_i(t+\Delta t) = \boldsymbol{x}_i(t) + \boldsymbol{v}_i(t+\Delta t)\Delta t$,

$\boldsymbol{\alpha}_i^{\Delta}(t+\Delta t) = \boldsymbol{\omega}_i(t+\Delta t)\Delta t$

Save updated variables:

$\boldsymbol{v_i}(t) \leftarrow \boldsymbol{v_i}(t+\Delta t)$,

$\boldsymbol{\omega_i}(t) \leftarrow \boldsymbol{\omega_i}(t+\Delta t)$,

$\boldsymbol{x_i}(t) \leftarrow \boldsymbol{x_i}(t+\Delta t)$,

$\boldsymbol{\alpha_i}(t) \leftarrow \boldsymbol{\alpha_i}(t+\Delta t)$,

$t \leftarrow t + \Delta t$

4 Conclusions

In conclusion, this work presents an approach that combines the Discrete Element Method (DEM) with the DFC model for modelling fresh printable concrete, in an attempt to simulate 3D Concrete Printing (3DCP). This is an on-going research that is part of a master´s dissertation, and only the theoretical framework is presented by now. Numerical results shall appear soon.

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