FAU

EAM ENGINEERING OF ADVANCED MATERIALS

DEM simulation of particles of complex shapes using the multisphere method: application for additive manufacturing

Eric J. R. Parteli

Institut für Multiscale Simulation, Universität Erlangen-Nürnberg, Nägelsbachstraße 49b, 91052 Erlangen

Introduction – We develop a numerical tool for modeling the transport mechanism of powder particles during additive manufacturing[1]. In this type of manufacturing process, objects are created by selectively melting particles of a powder bed through a laser or electron beam (Fig. 1). Understanding the mechanical behavior of the powder as a function of material properties, size distribution and particle shape is essential for the optimization of the production process. We adapt a software (LIGGGHTS[2]) for particle-based simulations using the Discrete Element Method (DEM) in order to account for the complex geometries of the powder particles, as well as for the dynamic boundary conditions for the granular material which are inherent to the manufacturing process.

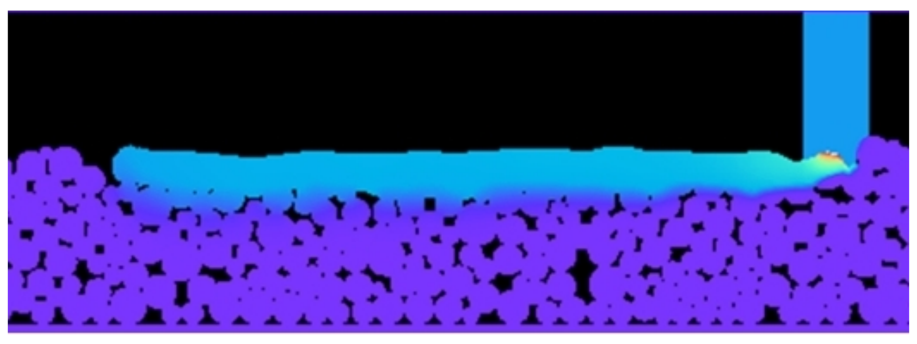

Fig. 1 – Snapshot of a Lattice-Boltzmann simulation of particle melting in additive manufacturing due to a moving electron beam (courtesy: Andreas Bauereiß, WTM, Uni Erlangen-Nürnberg).

Particle model – Powder particles of complex shapes are modeled as sphere clumps (rigid bodies) using the *multisphere method*[2,3]. Constituent spheres of a rigid body interact with spheres belonging to neighbouring particles through viscoelastic forces according to the Hertz-Mindlin model[2-4]. Indeed, one problem with the multisphere method is that the mass and moment of inertia of the resulting sphere clumps are incorrectly computed as a result of the (artifactual) contribution of the sphere-sphere overlaps (Fig. 2). Here we present an analytical (exact) method to compute the mass and moment of inertia of rigid bodies in DEM using the multisphere method.

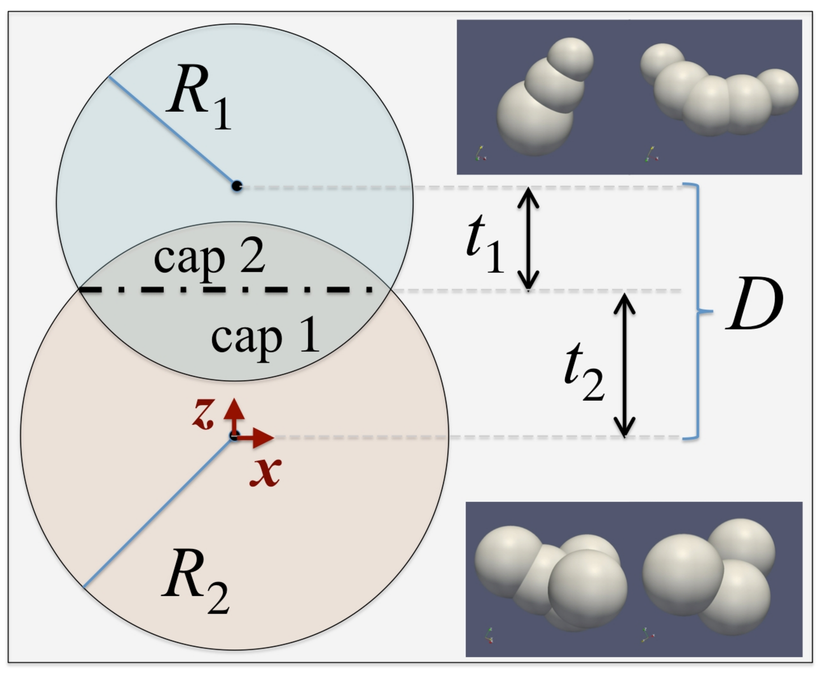

Fig. 2 – Schematic diagram of two spheres (density ρ_p, center-of-mass positions $\mathbf{r}_1$, $\mathbf{r}_2$) within a rigid body.

The contribution of the overlap to the total particle mass and moment of inertia is computed for all pairs of constituent spheres (labeled k = 1, 2) for which $|\mathbf{D}| < R_1 + R_2$, where $\mathbf{D} = \mathbf{r}_1 - \mathbf{r}_2$ (Fig. 2). The *mass* of each cap is computed through the equation,

$$m_{\text{cap}\,k} = \left[\rho_p \pi/3\right]\cdot\left[3R_k\ell_k^2 - \ell_k^3\right],$$

where $\ell_k = R_k - t_k$. Considering that $\mathbf{D}$ is parallel to the z axis (Fig. 2), the inertia tensor $\hat{\mathrm{I}}_{\text{cap}\,k}$ of each cap is diagonal, with components:

$$I_{xx,\,\text{cap}\,k} = I_{yy,\,\text{cap}\,k} = \left[\rho_p\pi/4\right]\cdot\left[4R_k^3\ell_k^2 - \frac{16R_k^2\ell_k^3}{3} + 3R_k\ell_k^4 - \frac{3}{5}\ell_k^5\right] +$$
$$+ m_{\text{cap}\,k}\left[\left(L_{\text{overlap}\,k} - L_{\text{ctrd}\,k}\right)^2 - L_{\text{ctrd}\,k}^2\right],$$

$$I_{zz,\text{cap}\,k} = \left[\rho_p\pi/2\right]\cdot\left[\frac{4}{3}R_k^2\ell_k^3 - R_k\ell_k^4 + \frac{1}{5}\ell_k^5\right],$$

where $L_{\text{centr}\,k}$ is the geometric centroid of cap k (computed relative to the center of sphere k) and $L_{\text{overlap}\,k}$ is the distance between the center of sphere k and the center of mass of the overlap volume. The inertia tensor $\hat{\mathrm{I}}_{\text{overlap}}$ for the case where $\mathbf{D}$ makes an angle φ with $\mathbf{e}_z$ reads,

$$\hat{\mathrm{I}}_{\text{overlap}} = \hat{R}\left(\hat{\mathrm{I}}_{\text{cap }1} + \hat{\mathrm{I}}_{\text{cap }2}\right)\hat{R}^{-1},$$

where $\hat{R}$ is the rotation matrix associated with the rotation of a vector by an angle φ around the axis $\mathbf{e}_D \times \mathbf{e}_z$, with $\mathbf{e}_D = \mathbf{D}/|\mathbf{D}|$. The mass and center-of-mass position of the rigid body are then computed using the equations,

$$m_{\text{body}} = \sum_{i=1}^{N_s} m_{\text{sphere}\,i} - \sum_{j=1}^{N_o} m_{\text{overlap}\,j},$$

$$\mathbf{r}_{\text{cm}} = m_{\text{body}}^{-1}\left[\sum_{i=1}^{N_s} m_{\text{sphere}\,i}\mathbf{r}_i - \sum_{j=1}^{N_o} m_{\text{overlap}\,j}\mathbf{r}_j\right],$$

where $\mathbf{r}_{\text{cm}}$ is the position of the body's center of mass.

The body's inertia tensor reads,

$$\hat{\mathrm{I}}_{\text{body}} = \sum_{i=1}^{N_s}\frac{2}{5}m_{\text{sphere}\,i}R_i^2\hat{1} - \sum_{j=1}^{N_o}\hat{\mathrm{I}}_{\text{overlap}\,j} + \hat{\mathrm{A}},$$

$$\hat{\mathrm{A}} = \sum a_k m_k \begin{bmatrix} Y_k^2+Z_k^2 & -X_kY_k & -X_kZ_k \\ -X_kY_k & X_k^2+Z_k^2 & -Y_kZ_k \\ -X_kZ_k & -Y_kZ_k & X_k^2+Y_k^2 \end{bmatrix},$$

where a_k = 1 for spheres and a_k = −1 for overlap volumes, and X_k, Y_k, Z_k are the distances from the particle's principal axes.

The inertia tensor is diagonalized through a principal axis transformation, the orthogonal transformation matrix of which ($\hat{J}$) is used to transform a vector $\mathbf{u}$ in the body's fixed frame to the inertial frame through the equation, $\mathbf{u}_{\text{in}} = \hat{J}\mathbf{u}$. Finally, the motion of the rigid body is computed by numerically solving the following equations[2],

$$m_{\text{body}}\ddot{\mathbf{r}}_{\text{cm}} = \sum_{i=1}^{N_s}\mathbf{F}_i + m_{\text{body}}\mathbf{g},$$

$$\mathbf{M} = \sum_{i=1}^{N_s}\left(\mathbf{r}_i - \mathbf{r}_{\text{cm}}\right)\times\mathbf{F}_i,$$

$$\hat{I}\dot{\vec{\omega}} + \vec{\omega}\times(\hat{I}\vec{\omega}) = \hat{J}^{-1}\mathbf{M}.$$

where $\mathbf{g}$ is gravity, $\mathbf{F}_i$ is the total force on the body's i-th constituent sphere and $\mathbf{M}$ is the total torque on the body, while $\vec{\omega}$ is the body's angular velocity.

Modeling the transport mechanism of the particles during the manufacturing process – The boundary conditions associated with the device's complex geometry are modeled by importing triangular meshes, which are interpreted as frictional walls.

The device consists of a rake for powder application (which moves from left to right in Fig. 3) and a building tank (central area), which is filled with a powder layer and is on top of a vertically adjustable platform. Our simulations provide a helpful tool for investigating the role of particle shape and size distribution for the flowability of the powder within the geometric device.

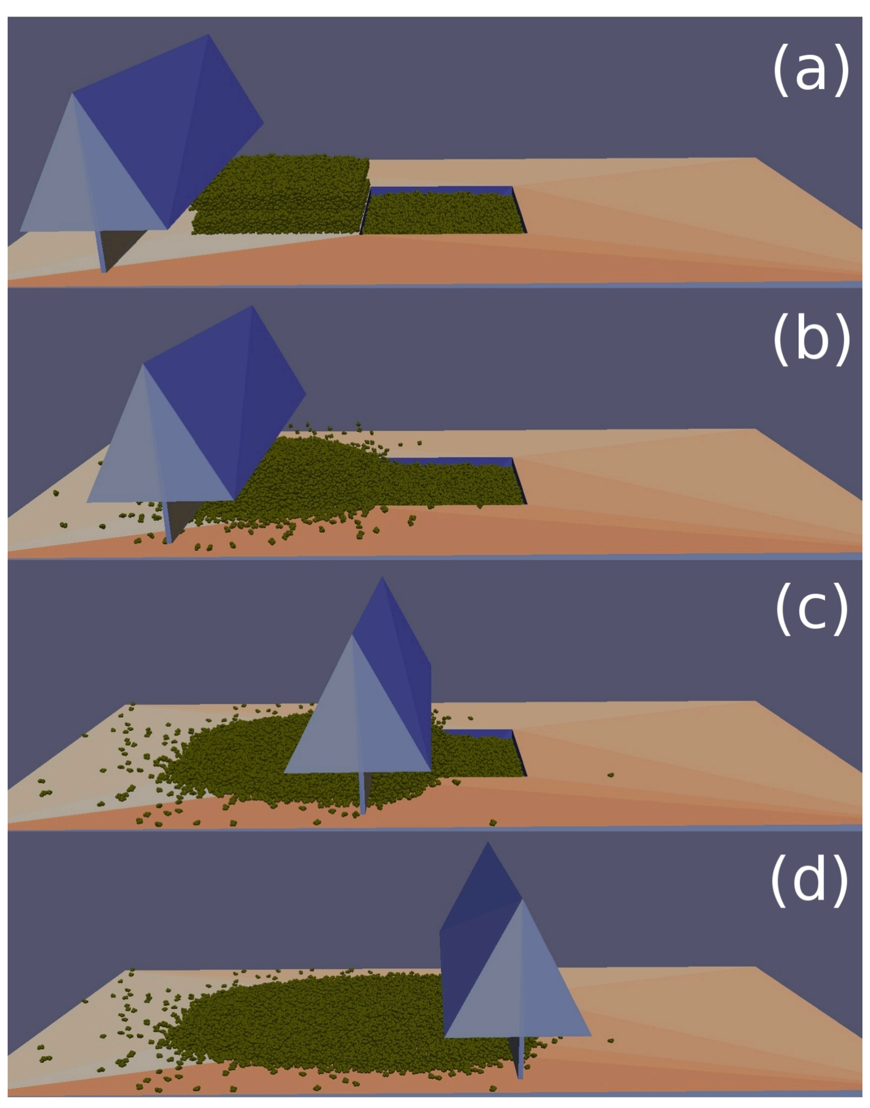

Fig. 3 – Snapshots of a simulation of particles with complex geometric shapes, built with the multisphere method, in dynamic boundary conditions which mimic the device used in additive manufacturing.

SFB 814 ADDITIVE FERTIGUNG

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REFERENCES: **[1]** www.sfb814.forschung.uni-erlangen.de; the present work is in the framework of subproject B1 of SFB 814; **[2]** www.liggghts.com; **[3]** T. Pöschel and T. Schwager, *Computational Granular Dynamics – Models and Algorithms* (Springer, Berlin), 2005 ; **[4]** E. J. R. Parteli, *AIP Conf. Proc.* **1542**, 185-188 (2013).