

A DISCRETE ELEMENT METHOD FOR POLYHEDRAL PARTICLES

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Key words: DEM, Convex Polyhedral Particles, Half Space Representation, Contact Force

Abstract. The following paper presents a new approach for the Discrete Element Method (DEM) with polyhedral particles. The geometry of convex polyhedra is represented by a set of half spaces. An algorithm for contact detection for these particles is developed. Furthermore a model for the interaction forces of polyhedra in contact is suggested. The model includes elastic and damping forces in normal direction, as well as Coulomb friction in tangential direction. The feasibility of DEM with sharp edged particles is demonstrated by some engineering applications.

1 INTRODUCTION

The Discrete Element Method (DEM) is a numerical method for calculating the mechanical behaviour of particle systems, which have a range from powders to large rock formations. The method mainly consists of calculating the motion and the interaction of the particles. A major difference in various implementations of the discrete element method consists in the choice of the particles. While spherical particles provide a very high numerical efficiency, nonspherical particles give a better approximation to the real particles in many cases. Among the nonspherical particles, convex polyhedra are able to reproduce many characteristics often found in real particles like irregular shape or sharp edges. These features play an important role in many processes like grinding, polishing or lapping.

In the present paper an approach for modelling convex polyhedra by a set of halfspaces is presented. Based on this geometry representation, an algorithm for contact detection is developed. This algorithm does not only detect the contact, but also provides a complete geometric description of the overlapping region [1]. This information is directly used to calculate the interaction forces [2].

2 GEOMETRY REPRESENTATION

Lee et al. [3] have suggested a method to represent convex particles by a set of half spaces. The particle is defined as the space that belongs to all half spaces. In the following part index notation and Einstein's summation convention will be used, i.e. the subscript index denotes the spatial direction. This doesn't include superscript indices, which are only used to specify the variables in this paper.

Each half space is described by an equation of the form

$$(x_i - c_i - a_i)a_i \leq 0 \tag{1}$$

where c_i is the center of mass of the particle, a_i is a vector from the center of mass to the boundary face in normal direction and x_i is an arbitrary point inside the halfspace. In a local coordinate system located at the center of mass of the particle, equation (1) reduces to

$$(x_i - a_i)a_i \leq 0. \tag{2}$$

All further geometrical information can be calculated from this database as described in the following.

The first step is to find possible corner points of the polyhedron. This is done by calculating the intersection points of all combinations of three boundary faces out of all faces. We consider the set of half spaces to be given in a coordinate system \tilde{x}_i , with the origin inside the particle. With the vectors of the three faces \tilde{a}_i^j , where the superscript j indicates the number of the used plane, this leads to the system of equations

$$\begin{aligned} (\tilde{x}_i - \tilde{a}_i^1)\tilde{a}_i^1 &= 0 \\ (\tilde{x}_i - \tilde{a}_i^2)\tilde{a}_i^2 &= 0 \\ (\tilde{x}_i - \tilde{a}_i^3)\tilde{a}_i^3 &= 0, \end{aligned} \tag{3}$$

which can be arranged to

$$\begin{bmatrix} \tilde{a}_1^1 & \tilde{a}_2^1 & \tilde{a}_3^1 \\ \tilde{a}_1^2 & \tilde{a}_2^2 & \tilde{a}_3^2 \\ \tilde{a}_1^3 & \tilde{a}_2^3 & \tilde{a}_3^3 \end{bmatrix} \begin{pmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \tilde{x}_3 \end{pmatrix} = \begin{pmatrix} \tilde{a}_i^1 \tilde{a}_i^1 \\ \tilde{a}_i^2 \tilde{a}_i^2 \\ \tilde{a}_i^3 \tilde{a}_i^3 \end{pmatrix}. \tag{4}$$

The expressions in the right hand side vector are scalar products. Equation (4) is solved for all combinations of faces.

In the second step the points have to be checked whether they belong to all half spaces. Only in this case they are corner points of the polyhedron.

To calculate geometrical characteristics like volume, mass or moments of inertia, the faces have to be triangulated using the afore calculated corner points. Each triangle forms a tetrahedron with the origin of the coordinate system, while the polyhedron is the sum of these tetrahedra. Thus the calculation becomes trivial.

The volume V , the surface A and the center of mass \tilde{c}_i of the polyhedron can be calculated as

$$V = \sum_{k=1}^m V^k = \sum_{k=1}^m \frac{1}{6} |(\epsilon_{ikl} \tilde{p}_k^{k1} \tilde{p}_l^{k2}) \tilde{p}_i^{k3}| \quad (5)$$

$$A = \sum_{k=1}^m \frac{1}{2} |\epsilon_{ikl} (\tilde{p}_k^{k3} - \tilde{p}_k^{k2}) (\tilde{p}_l^{k1} - \tilde{p}_l^{k2})| \quad (6)$$

$$\tilde{c}_i = \frac{1}{V} \sum_{k=1}^m V^k \tilde{c}_i^k, \quad (7)$$

where m is the number of tetrahedra respective triangles. \tilde{p}_i^{k1} , \tilde{p}_i^{k2} and \tilde{p}_i^{k3} are the corner points of the tetrahedron respective triangle k . ϵ_{ikl} is the Levi-Cevita permutation tensor and $\epsilon_{ikl} a_k b_l$ denotes the cross product of the vectors a_k and b_l . V^k and \tilde{c}_i^k are defined as

$$V^k = \frac{1}{6} |(\epsilon_{ikl} \tilde{p}_k^{k1} \tilde{p}_l^{k2}) \tilde{p}_i^{k3}| \quad (8)$$

$$\tilde{c}_i^k = \frac{1}{4} (\tilde{p}_i^{k1} + \tilde{p}_i^{k2} + \tilde{p}_i^{k3}). \quad (9)$$

3 CONTACT DETECTION

In order to detect the contact, the overlapping region is defined as that region belonging to all half spaces of the two polyhedra in contact, [3]. The same algorithm as for the description of a particle can be applied. This way an exact geometric representation of the overlapping region is obtained, which can be used for the calculation of the interaction forces. A separate treatment of the different contact types, like corner to face, edge to edge or face to face, is not necessary. In the following the contact algorithm is described in detail.

- To each particle j a radius r^j is assigned, which defines a sphere completely surrounding the polyhedron. In a first step of the contact algorithm it is checked whether these spheres are in contact. This means the inequality

$$|c_i^2 - c_i^1| < r^1 + r^2 \quad (10)$$

has to be fulfilled, where c_i^j are the centers of the particles. Otherwise the contact detection is terminated.

- In order to speed up the algorithm all corner points of one particle are checked whether they are close enough to the other particle for being in contact. This is performed by the following algorithm, which is visualized in figure 1:

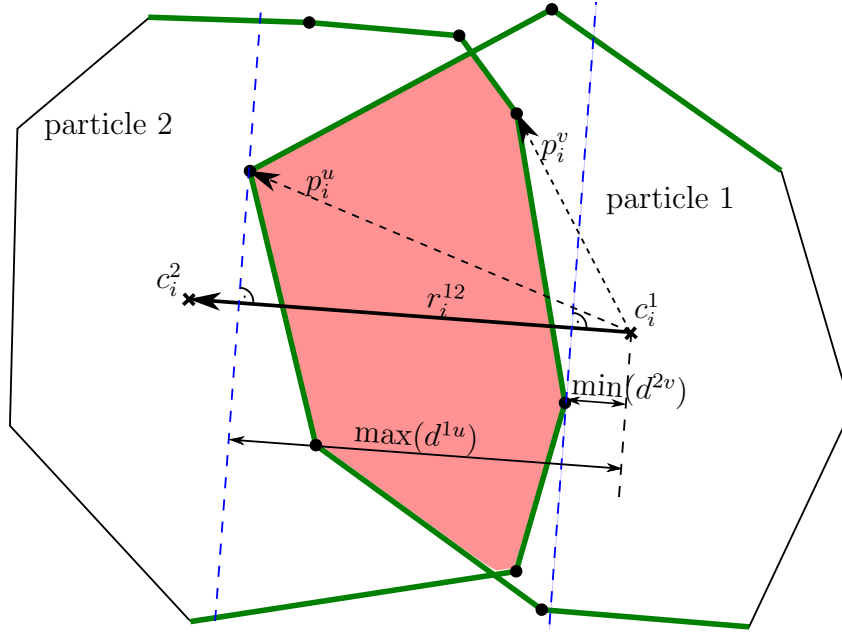


Figure 1: An area (dotted lines) is defined which encloses the overlapping region (red). All points (black) and planes (green) of the polyhedra in this area are taken into account for contact calculation. All other points and planes are excluded from the calculation (2D simplification).

- First the vector between the centers of the particles r_i^{12} is calculated.

$$r_i^{12} = c_i^2 - c_i^1 \quad (11)$$

- The distance d^{1u} of a corner u of particle 1 to the center of particle 1 in direction of r_i^{12} is

$$d^{1u} = \left| \frac{r_i^{12} p_i^u}{r_i^{12} r_i^{12}} \right|, \quad (12)$$

where p_i^u is the vector from the center of particle 1 to the corner u .

- In the same way the distance d^{2v} of a corner v of particle 2 to the center of particle 1 in direction of r_i^{12} reads

$$d^{2v} = \left| \frac{r_i^{12} p_i^v}{r_i^{12} r_i^{12}} \right|, \quad (13)$$

where p_i^v is the vector from the center of particle 1 to the corner v .

- All corners of particle 1 that fulfill the inequality

$$d^{1u} > \min(d^{2v}) \quad (14)$$

are considered valid.

- All corners of particle 2 that fulfill the inequality

$$d^{2v} < \max(d^{1u}) \quad (15)$$

are considered valid.

- If no valid corners are found the contact detection is terminated.
- All boundary planes of the particles that contain at least one valid corner are considered as valid for contact detection.
- New points are found by the intersection of two planes of one particle and one plane of the other particle. All possible combinations of valid planes have to be considered. The system of equations for one combination reads

$$\begin{bmatrix} a_1^{1g} & a_2^{1g} & a_3^{1g} \\ a_1^{2g} & a_2^{2g} & a_3^{2g} \\ a_1^{3g} & a_2^{3g} & a_3^{3g} \end{bmatrix} \begin{pmatrix} x_1^g \\ x_2^g \\ x_3^g \end{pmatrix} = \begin{pmatrix} (c_i^1 + a_i^{1g}) a_i^{1g} \\ (c_i^2 + a_i^{2g}) a_i^{2g} \\ (c_i^3 + a_i^{3g}) a_i^{3g} \end{pmatrix}, \quad (16)$$

where a_i^{jg} are the vectors of the faces in global coordinates and c_i^j is the center of the particle the face belongs to.

- The points belonging to the overlapping region have to be found.
 - All corners of particle 1 are checked whether they are inside particle 2.
 - All corners of particle 2 are checked whether they are inside particle 1.
 - All new points are checked whether they are inside particle 1 and particle 2.
- All planes that include at least 3 points of the overlapping region are part of the region.
- Volume and center of mass of the overlapping region can be calculate as described above for the particles. For this purpose a new coordinate system is introduced that results from translating the coordinate system of the first particle to a point c_i^o inside the overlapping region, which is defined by

$$c_i^o = \frac{1}{n} \sum_{w=1}^n p_i^{ow}, \quad (17)$$

where p_i^{ow} are the corners of the overlapping domain and n is the number of valid corners.

For a more detailed description of the geometry representation and contact detection the reader is referred to [1].

4 INTERACTION FORCES

4.1 Elastic normal force model

The most important part of the interaction forces is the elastic normal force F_i^n . The force is characterized by defining its magnitude, its direction and its application point. The magnitude F^n of the force is defined as

$$F^n = E^* k \sqrt{Vd} \quad (18)$$

$$\frac{1}{E^*} = \frac{1 - \nu_1^2}{E_1} + \frac{1 - \nu_2^2}{E_2}, \quad (19)$$

where E_i and ν_i are the Young's modulus and the Poisson's ratio of particle i , respectively. d is the indentation depth and V is the volume of the overlapping region. The constant k is defined as $k = 0.62$. This model is related to the Hertzian contact. Like in the Hertzian contact model, the deformation zone has to be small with respect to the particle size. A comparison of the proposed new force law (18) with FEM results shows good agreement, independent of the geometries and materials in contact [2].

The application point is simply defined as the center of mass of the overlapping region. The normal force direction n_i^f is defined as the normalized vector obtained by integrating the surface normal n_i^A over the part A of the surface of the overlapping region that belongs to one particle (see figure 2). For polyhedra this means, n_i^f is obtained as the sum of the surface normals n_i^{Aj} over all parts A^j of A , weighted by the area.

$$n_i^f = \frac{\int_A n_i^A ds}{\left| \int_A n_i^A ds \right|} = \frac{1}{\sum_j A^j} \sum_j A^j n_i^{Aj} \quad (20)$$

Thus the force vector F_i^n is obtained as

$$F_i^n = F^n n_i^f. \quad (21)$$

If A is part of particle 1, then F_i^n is applied to particle 2 and $-F_i^n$ is applied to particle 1. For a detailed explanation see [1]. The indentation depth d is defined as the extension of the overlapping region in direction of the force. It can be calculated as the difference between the maximum and the minimum of the projection of the coordinates of the corners of the overlapping region p_i^c on the normal vector n_i^f .

$$d = \max \left(n_i^f p_i^c \right) - \min \left(n_i^f p_i^c \right) \quad (22)$$

4.2 Damping

Material damping in normal direction is modeled with a viscous approach. Including the damping term in equation (18) for the normal force gives

$$F^n = E^* k \sqrt{Vd} (1 + c\dot{d}), \quad (23)$$

where c is a constant for the damping and \dot{d} is the magnitude of the relative velocity between both particles in the direction of the normal force.

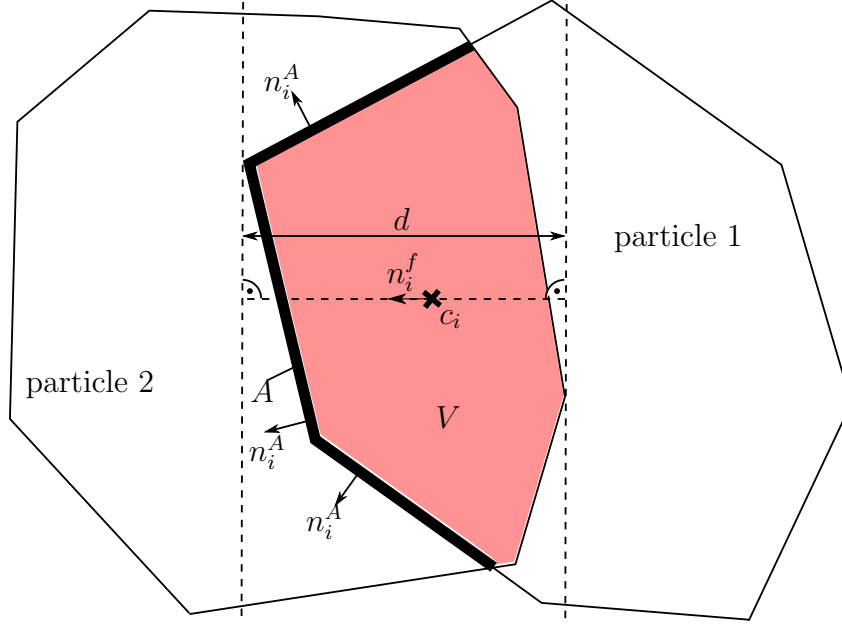


Figure 2: The overlapping region (red) is used as the database for the calculation of the contact forces. The force application point is defined by the center of mass c_i . The magnitude is defined by the volume V and the indentation depth d . The direction n_i^f is defined by integrating the surface normal n_i^A over the surface belonging to particle 1 (bold black line) (2D simplification).

4.3 Friction

The magnitude of the friction force is assumed by the relation to the normal component

$$F^f = \left((2\mu^{s*} - \mu^k) \frac{x^2}{x^4 + 1} + \mu^k - \frac{\mu^k}{x^2 + 1} \right) F^n. \quad (24)$$

μ^{s*} is calculated from the static and kinetic friction coefficients μ^s and μ^k as

$$\mu^{s*} = \mu^s \left(1 - 0.09 \left(\frac{\mu^k}{\mu^s} \right)^4 \right). \quad (25)$$

x is defined as

$$x = \frac{v^t}{v^s}, \quad (26)$$

where v^t is the magnitude of the tangential velocity and v^s is the velocity at transition from static to kinetic friction. The resulting behavior of the friction force with respect to the tangential velocity is shown in figure 3.

The direction of the friction force F_i^f is opposite to the direction of the relative tangential velocity v_i^t , which leads to the equation

$$F_i^f = -F^f \frac{v_i^t}{|v_i^t|}. \quad (27)$$

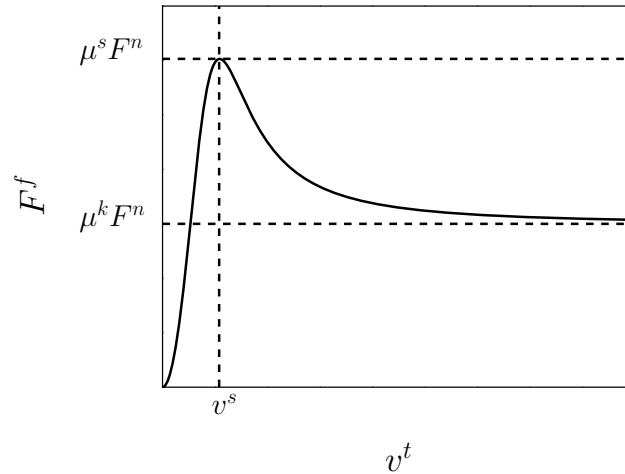


Figure 3: Magnitude of the friction force with respect to the magnitude of the tangential velocity

The presented friction model is controlled by the coefficients of friction μ^s and μ^k as well as the model parameter v^s which defines the transition from static to kinetic friction. The model gives a good approximation of the original Coulomb law for dry friction. Static friction is approximated by very slow sliding rates. The jumps in the classical Coulomb friction model are smoothed in order to avoid numerical instabilities. Thus, the evaluation of equilibrium conditions is avoided to calculate the friction force. No information about other forces than the normal contact force on the particle or about previous timesteps is needed. Therefore the model is well suited for implementation in discrete element method. For a more detailed description of the interaction forces the reader is referred to [2].

5 EXAMPLES

The presented models are implemented in the open source DEM code LIGGGHTS. In this section the capabilities of the code are demonstrated with three examples, representing typical applications where the simulation of sharp edged particles is inevitable

5.1 Particle flow through a hopper

In the first example a particle flow through a hopper is simulated. In this example the particle motion is highly influenced by the particle shape, as a rolling movement is restrained by the polyhedral shape. To simulate the particle flow through a hopper into a silo, random particles are placed on a regular grid above the hopper. The walls of hopper and silo are modeled by non-moving particles. Under gravity the particles drop into the hopper. The results at several time steps are shown in figure 4.

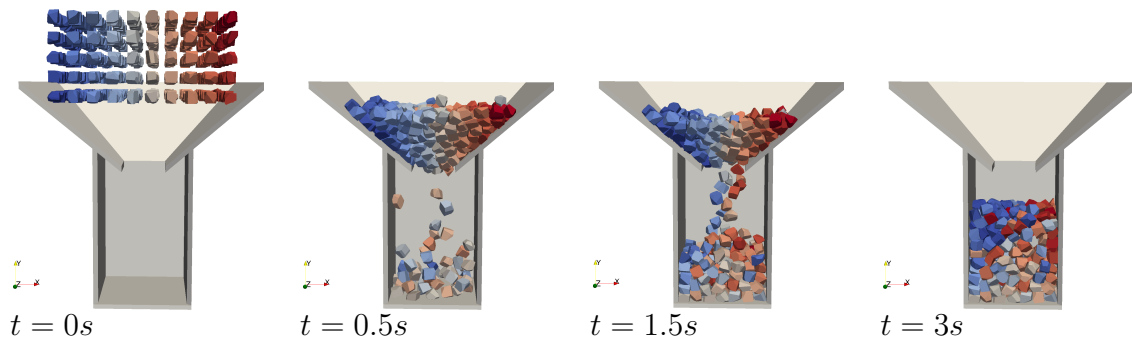


Figure 4: 800 Particles (coloured by id) falling into a hopper at different time steps

5.2 Mixer

The second example deals with the particle movement in a mixer. The mixer is filled by placing particles on a regular grid inside the mixer. After the particles dropped down to the bottom of the mixer, the mixer starts rotating. In this example again the particle shape has a strong influence, as rolling is hindered. The results at several time steps are shown in figure 5.

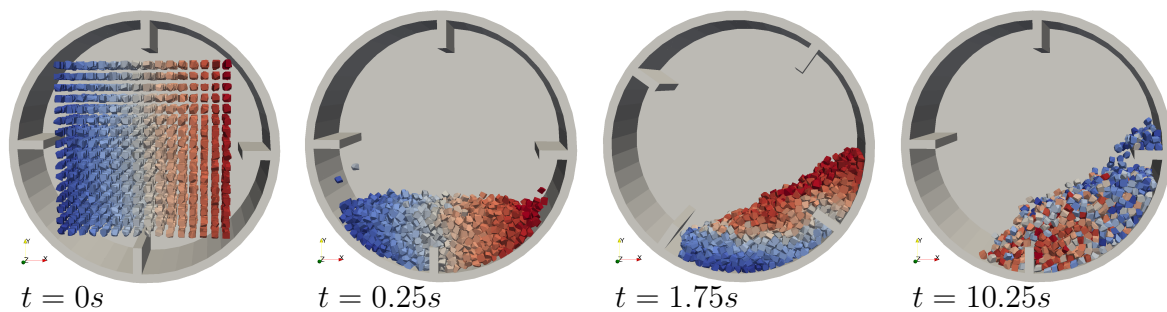


Figure 5: Movement of 2048 particles (coloured by id) in a mixer at several time steps

5.3 Lapping

In the third example the lapping process is simulated. In the lapping process the forces acting on the workpiece are of special interest. Here the model for the interaction forces provides good results. The workpiece is simulated by non-moving particles. The tool is modeled by rigidly connected particles. In the lapping direction the tool has a fixed speed. Perpendicular to the workpiece the tool can move freely, as a result of the applied lapping pressure and the interaction forces between tool and abrasive particles. The other degrees of freedom of the tool are fixed. The slurry is simulated by particles placed between workpiece and tool. For the calculation of the hydrodynamic forces on these particles laminar flow is assumed between tool and workpiece. In figure 6 a detail

of the simulation is shown at several time steps. It shows two abrasive particles rolling over each other and building a force bridge between tool and workpiece. Thus the tool gets pushed away.

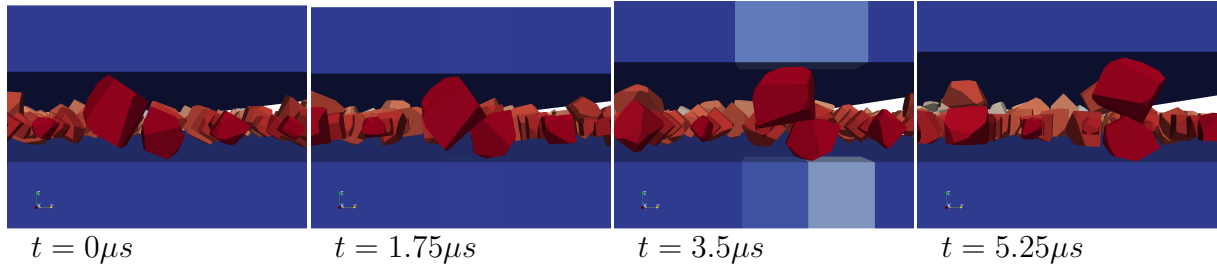


Figure 6: Lapping process at several time steps. Particles coloured by id. Workpiece (lower part) and tool (upper part) coloured by force

6 CONCLUSIONS

In the present paper an approach for implementing polyhedral particles in DEM was presented. Convex polyhedra are able to give a good approximation to various types of real particles. The geometry of the particles was described by a set of half spaces. The algorithm provides outstanding flexibility to generate particles with various numbers of faces, sharpness of edges and aspect ratios. An algorithm was presented which uses this geometry description for contact detection very efficiently and also provides a complete description of the overlapping region. This information is further used to calculate the interaction forces by an elastic law which is based on a generalized Hertzian contact model. This law yields contact forces which are calculated in a unique manner valid for all possible interpenetration geometries. This accelerates the numerical simulations very much. The elastic forces were completed by models for normal damping and tangential friction. The friction model avoids the evaluation of equilibrium conditions for static friction. Thus the numerical demands of the friction model are very low and it is well suited for implementation in DEM. The capabilities of the presented methods were demonstrated by several examples.

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