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PARALLELIZATION OF DEM SOLVER FOR NON-SPHERICAL SOLIDS: A PATHWAY TO SCALABLE CFD-DEM SIMULATIONS

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Abstract: *Granular matter formed from non-spherical solids appears in both natural and industrial settings. These include, among others, landslides, mixing, and fluidization. The commonly used predictive method for granular matter is the discrete element method (DEM). However, DEM was initially designed for spherical particles and faces many challenges in modeling the non-spherical ones , which are prevalent. Therefore, various approaches, including multi-sphere clusters, super-quadrics and polyhedral models, were developed to approximate the irregular shapes. The polyhedral approach offers the highest level of fidelity, but comes with the biggest computational costs, particularly for non-convex particles. Hence, optimization and parallelization of codes with polyhedron-based DEM solvers are of great interest. In this work, we present recent advances in the development of our custom polyhedron-based DEM solver, focusing on parallel computing. With improvements in the solver architecture and boosted computational efficiency, the DEM code scales well at least up to 32 cores and allows for efficient coupling with computational fluid dynamics (CFD) to simulate complex particle-laden flows.*

Keywords: Discrete element method, non-spherical particles, MPI, CFD-DEM, OpenFOAM.

1. Introduction

The omnipresence of granular matters in nature and, consequently, industry requires ways to predict their behavior according to a given situation, e.g. prediction of landslides, mixing, or separation. One possible way is to use the discrete element method (DEM), which is capable of describing the movement of individual particles while considering collisions either reciprocal or with system boundaries (Cleary, 2010). DEM was initially proposed for spherical particles due to their simple definition and the existence of an analytic solution for collisions (Antypov and Elliott, 2010). However, irregular particle shapes are prevalent in nature and particle morphology tends to play a crucial role in the granular matter behavior. This fact poses a number of challenges in modeling systems with non-spherical particles, starting from shape approximation, including applied contact model, and ending with computational efficiency. Furthermore, when solids are transported by and densely dispersed in a fluid, the shape of the particles also plays a key role in the resulting flow properties (Xiong et al., 2021). Therefore, coupling a non-spherical DEM solver with computational fluid dynamics (CFD) might provide a deeper insight into such systems.

Today, the DEM treatment of arbitrarily shaped solids might be divided into three main approaches: (i) multi-sphere model, (ii) super-quadrics model and (iii) polyhedral model (Zhong et al., 2016). Each approach varies in level of fidelity of the shape approximation. At the same time, models (i) and (ii) are more suited to approximate smoothly curved surfaces, while benefiting from the sphere contact model with minor adjustments. The polyhedral model is the most general approach and is best suited for solids with sharp

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edges or corners (Chen, 2012). Nevertheless, its non-trivial shape definition demands estimation of geometric properties. Furthermore, significant modifications to the contact model with respect to the particle overlap characterization are required. Thus, overall computational efficiency of the polyhedral model is low compared to other approaches.

In this work, we present recent improvements in parallel computing of a polyhedron-based in-house developed DEM solver that is primarily designed for particle-resolved direct numerical simulation in CFD-DEM applications (Isoz et al., 2022). As such, it was implemented in the OpenFOAM C++ library, which uses message-passing interface (MPI) parallelization. In particular, the framework architecture was improved with a focus on computational time scaling. Scaling results of the DEM solver are presented in detail and conclusions regarding CFD-DEM applications are hinted at.

2. Framework fundamentals

Movement of the particles The presented DEM solver is being developed primarily for polyhedron-based solids, described with stereolithographic templates (STL files). Each solid $\mathcal{B}_i$ is added to the computational domain Ω and prescribed with standard material properties such as Young's modulus Y, Poisson's ratio ν and density ρ. The particles are considered to be rigid and homogeneous. Geometrical properties, such as the mass or the moment of inertia, are estimated from the body projection $\mathcal{B}_i^{\mathrm{h}}$ onto finite volume mesh $\Omega^h \approx \Omega$.

The movement of individual solids is governed by Newton's second law of motion,

$$m_i \frac{\mathrm{d}^2 \boldsymbol{x}_i}{\mathrm{d}t^2} = \boldsymbol{f}_{\mathrm{g}} + \boldsymbol{f}_{\mathrm{c}}, \quad I_i \frac{\mathrm{d}\boldsymbol{\omega}_i}{\mathrm{d}t} = \boldsymbol{t}_{\mathrm{c}}\,, \tag{1}$$

here m_i is the mass of $\mathcal{B}_i$ and $\boldsymbol{x}_i$, $\boldsymbol{\omega}_i$, I_i are its centroid position, angular velocity and the matrix of its inertial moments at time t, respectively. The solver considers $\mathcal{B}_i$ to be affected by gravity (g) and by contact (c) with other bodies or boundaries of Ω. Thus, $\boldsymbol{f}$ and $\boldsymbol{t}$ in (1) represent the forces and torques acting on $\mathcal{B}_i$, respectively. The equations are solved using the finite difference method, assuming that the forces and torques are constant during each time step.

Contact The contact treatment affects the overall efficiency of any DEM solver, and there are many approaches to its solution. The presented solver utilizes the *soft*-DEM approach, which estimates contact force according to the magnitude of particle's overlap during contact. The resulting force defined by the Hertz-Mindlin model (Soltanbeigi et al., 2021) was originally proposed for spheres, for which the overlap can be characterized by the overlap length. However, such a treatment is not suitable for arbitrarily shaped solids. Thus, we reformulated the contact model to use the overlap volume introduced in (Chen, 2012). For collision of bodies $\mathcal{B}_i$ and $\mathcal{B}_j$ the normal contact force is implemented as

$$\boldsymbol{f}_{\mathrm{c}}^{\mathrm{n}} = \left(\frac{Y^{\mathrm{red}} V_{ij}^{\mathrm{o}}}{\ell_{\mathrm{c}}} + \gamma^{\mathrm{red}} \sqrt{\frac{Y^{\mathrm{red}} M^{\mathrm{red}}}{(\ell_{\mathrm{c}})^3}} \frac{\mathrm{d}V_{ij}^{\mathrm{o}}}{\mathrm{d}t} \right) \boldsymbol{n}_{\mathbf{c}}\,, \quad \ell_{\mathrm{c}} = 4 \frac{\|\boldsymbol{\ell}_i\|\ \|\boldsymbol{\ell}_j\|}{\|\boldsymbol{\ell}_i\| + \|\boldsymbol{\ell}_j\|}\,, \tag{2}$$

where γ represents the damping coefficient, M represents the mass of the colliding pair, $\boldsymbol{n}_{\mathrm{c}}$ stands for the contact normal, ℓ_{c} represents the characteristic length of the contact, with $\boldsymbol{\ell}$ representing the distance between particle's centroids and the contact centre and V_{ij}^{o} represents the overlap volume shared by the two solids $\mathcal{B}_i$ and $\mathcal{B}_j$. At last, the material properties with superscript red denote the harmonic average of the material properties of individual solids.

The tangential contact force is evaluated as

$$\begin{gathered} \Delta \boldsymbol{f}_{\mathrm{c}}^{\mathrm{t}} = k^{\mathrm{t}}\, \Delta \boldsymbol{\xi}^{\mathrm{t}} - 2\gamma^{\mathrm{n}} \sqrt{k^t M^{\mathrm{red}}}\, \boldsymbol{u}_{\mathrm{r}}^{\mathrm{t}}, \quad k^{\mathrm{t}} = 8\, G^{\mathrm{red}} \frac{\bar{A}_{\mathrm{c}}}{\ell_{\mathrm{c}}}\,, \quad \Delta \boldsymbol{\xi}^{\mathrm{t}} = \boldsymbol{u}_{\mathrm{r}}^{\mathrm{t}}\, \Delta t, \\ \boldsymbol{u}_{\mathrm{r}} = \boldsymbol{u}_i - \boldsymbol{u}_j + (\boldsymbol{\omega}_i \times \boldsymbol{\ell}_i - \boldsymbol{\omega}_j \times \boldsymbol{\ell}_j)\,, \quad \boldsymbol{u}_{\mathrm{r}}^{\mathrm{t}} = \boldsymbol{u}_{\mathrm{r}} - (\boldsymbol{u}_{\mathrm{r}} \cdot \boldsymbol{n}_{\mathbf{c}})\, \boldsymbol{n}_{\mathbf{c}}\,, \end{gathered} \tag{3}$$

where G is shear module, $\bar{A}_{\mathrm{c}}$ is cross-section area of the overlap volume, $\Delta \xi^{\mathrm{t}}$ the tangential overlap, k^{t} is tangential stiffness and $\boldsymbol{u}_{\mathrm{r}}$ is relative velocity and $\boldsymbol{u}_{\mathrm{r}}^{\mathrm{t}}$ its tangential component. The contact defining parameters such as $V_{,}^{\mathrm{o}}\, \ell_{\mathrm{c}}$, $\bar{A}_{\mathrm{c}}$, $\boldsymbol{n}_{\mathrm{c}}$ are evaluated using a virtual mesh algorithm, first presented in (Studeník et al., 2022). An increment of tangential force is added to the tangential contact force from the previous time step. Furthermore, tangential force magnitude is compared to the magnitude of the normal contact force scaled by the static friction coefficient μ. If the value is smaller, it's not modified and added to the normal component $\boldsymbol{f}_{\mathrm{c}} = \boldsymbol{f}_{\mathrm{c}}^{\mathrm{n}} + \boldsymbol{f}_{\mathrm{c}}^{\mathrm{t}}$; otherwise the value is scaled to $\mu\, \|\boldsymbol{f}_{\mathrm{c}}^{\mathrm{n}}\|$.

Solver parallelization The presented approach to contact treatment of polyhedral solids poses high demands on computational efficiency, even though the applied algorithm is highly optimized. The established approach to increasing computational efficiency is to divide solved tasks among available computational resources and solve them in parallel. The OpenFOAM library provides MPI-based parallelization (Bruck et al., 1997) and is designed for general CFD applications. Therefore, it is built to decompose finite-volume domains into subdomains, where each CPU is assigned one. During the simulation, CPUs work independently to limit information exchange to only boundary data. This is the first level (L_1) of our solver parallelization, which we employ to evaluate particle properties. Nevertheless, this approach has proven ineffective for DEM. To illustrate the situation, let us consider pouring of particles and let each CPU treat only particles within its bounds and share information with neighbors about the shared ones. Eventually, the particles start piling up on the bottom CPUs, which will be overloaded with their contact treatment, while the CPUs at the top will wait idly for the next iteration, as depicted in Fig. 1.

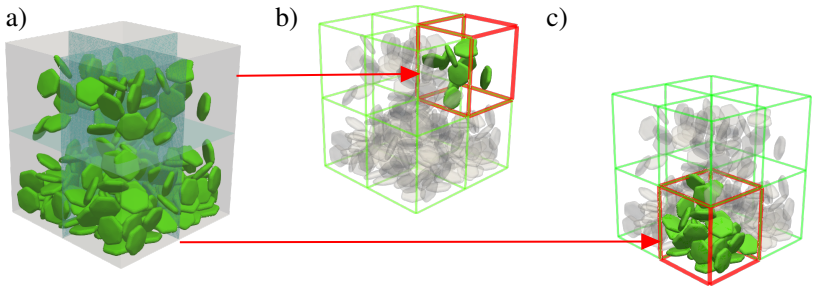

Fig. 1: Particle pouring, task distribution with standard MPI approach, outline of hexahedron domain decomposition with particles a). Illustration of uneven task distribution with b) showing an idle CPU and c) CPU overloaded with collision treatment.

Nevertheless, the L_1 MPI-imposed limitations can be mitigated by a construction of a second parallelization level (L_2). To employ all available computational resources and improve load balancing between overloaded and idle CPUs the contact solution must be distributed equally among all CPUs. However, without further treatment, the interprocessor communication tends to stall simulation speed. To avoid this, we created synchronized memory of the positions and orientations of all STL files, and each CPU can access all particle positions and each possible contact pair.

Although this approach has proved to increase computational efficiency, MPI parallelization is not designed to work with synchronized memory. This leads to significant RAM memory requirements, as each CPU must allocate space for all particles, scaling the memory requirements according to the number of CPUs. Moreover, with synchronized memory, every interprocessor communication instance must happen among all CPUs. This limited effective use to bellow 16 CPUs, when synchronization costs start outweighing the time spared. Nevertheless, this communication-related drawback was overcome with a new memory structure arranging the overall particle information to n-dimensional arrays, with a unique range for each CPU when working in parallel. Thus, shifting processor communication from individual particles to large data structures, and leading to well-scalable simulations, as demonstrated in the results.

3. Results

To illustrate the solver properties, we designed a particle pouring test containing 1, 3 and 5 thousand of particles; 1K, 3K, and 5K, respectively. The particles are monodisperse 20-sided polyhedra with characteristic dimension $d_\mathrm{c} = 4\,\mathrm{mm}$, while the auxiliary finite volume mesh has the resolition of $d_\mathrm{c}/4$. Particles are poured into a rectangular domain with dimensions $200\,d_\mathrm{c} \times 250\,d_\mathrm{c} \times 200\,d_\mathrm{c}$. Material properties for particles are $Y = 0.5\,\mathrm{GPa}$, $\nu = 0.3$, $\rho = 4\,000\,\mathrm{kg\,m^{-3}}$, $\mu = 1$, dissipation coefficient is set to correspond to the restitution coefficient being 0.25, system boundaries have similar properties with exception of $Y = 0.1\,\mathrm{GPa}$. Particles have no initial velocity and are pulled downward by gravity set to $g = 9.81\,\mathrm{m\,s^{-2}}$. The system is studied in terms of computational time scaling with respect to the used number of CPUs or the amount of particles. Results are displayed in Fig. 2.

4. Conclusions

In this contribution, we present recent advances in parallelization of our in-house developed DEM solver. The work led to a significant increase in computational efficiency, achieving approximately 75 % of the ideal

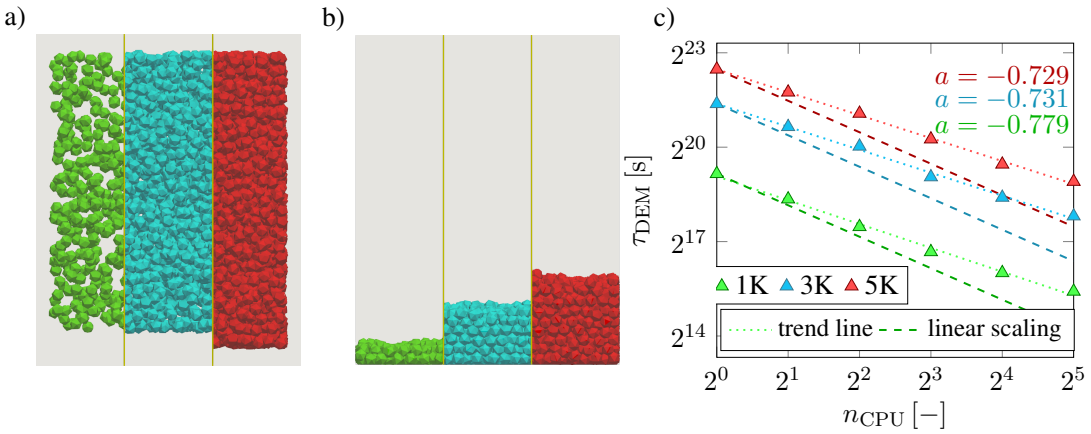

Fig. 2: Scaling of computational time for pouring polyhedral particles of different quantities; green – 1 thousand particles (1K), cyan – 3K particles and red – 5K particles. Qualitative results are shown in a) for simulation start and in b) for the end. Scaling of the current DEM implementation for given tests is compared to the linear scaling in c) with the measured trend line slope at the top right corner.

linear scaling in computational time. Significantly extended capabilities of the presented solver towards large-scale applications are demonstrated. Furthermore, with the improved parallelization of the DEM part of our CFD-DEM solver, a pathway to scalable CFD-DEM simulations is paved as the OpenFOAM, i.e. the solver CFD part, is known to scale well even on thousands of cores.

Both the DEM and CFD-DEM variants of our solvers are presently available from github.com/techMathGroup/openHFDIB-DEM

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