AN ADAPTIVE REDUCED-DIMENSIONAL DISCRETE ELEMENT MODEL FOR DYNAMIC RESPONSES OF GRANULAR MATERIALS WITH HIGH-FREQUENCY NOISES

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Original Manuscript Submitted: 6/10/2018; Final Draft Received: 7/29/2018

We present a dimensional-reduction framework based on proper orthogonal decomposition (POD) for the nondissipative explicit dynamic discrete element method (DEM) simulations. Through Galerkin projection, we introduce a finite dimensional space with lower number of degree of freedoms such that the discrete element simulations are not only faster but also free of high-frequency noises. Since this method requires no injection of artificial or numerical damping, there is no need to tune damping parameters. The suppression of high-frequency responses allows a larger time step for faster explicit integration. To capture the highly nonlinear behaviors due to particle rearrangement, an automatic mode-update scheme is formulated such that the most efficient basis can be used to predict mechanical responses. Numerical examples including the wave propagation simulations and uniaxial extension and compression tests are used to demonstrate the capacity of the reduced-order model.

KEY WORDS: model reduction, proper orthogonal decomposition, high-frequency issue, dynamic responses, discrete element model

1. INTRODUCTION AND BACKGROUND

From simulating the mixing of granular materials, wheel-soil interaction to cutting of rock, the discrete element method (DEM) has become a valuable prediction tool for agriculture, chemical engineering, civil engineering, mining, and pharmaceutical applications (Bertrand et al., 2005; Cundall and Strack, 1979; Wellmann and Wriggers, 2012). Nevertheless, despite the computing speed increases significantly these past years, simulations run via DEM still impose significant computational demands that, in some circumstances, limit the applications of DEM in engineering practices (Guo and Zhao, 2016; Liu et al., 2016a,b; Ulven and Sun, 2018).

This high demand is due to a number of factors. First, the particulate simulations impose a linear relation between the number of particles and the degrees of freedom. If the particles in the simulations are of the physical size, then the size of the simulation domain will be constrained by both the availability of the memory and CPU time of the computer (Kuhn et al., 2015; Sun et al., 2013; Wang and Sun, 2016). Second, in the majority of implementations, DEM simulations are often incrementally updated via an explicit time integrator. This treatment is convenient because the explicit scheme does not require a Newton-Raphson solver to resolve the nonlinear system of equations. However, because the explicit scheme is only conditionally stable, the DEM simulations must be incrementally updated in a
time step smaller than the critical time step (Wang and Sun, 2018). Since the critical time step can be small when the particle assemblies contain light or stiff particles, this leads to simulations either becoming very time-consuming or being confined in a very short duration. Furthermore, even if one can afford to use the sufficient time step to maintain numerical stability, the DEM results may still be plagued by the high-frequency noises. Presumably, the issue of high-frequency noise can be suppressed by introducing numerical damping (Liu et al., 2016b). However, numerical damping may also cause energy dissipation that affects the accuracy of the predictions.

Since simulations of large-scale particulate systems remain computationally intensive, there is a demand to reduce both the computational costs and the storage requirements without sacrificing too much accuracy. One possible option is to explore the modal order reduction (MOR) for DEM simulations, which is the approach adopted in this paper.

The basic idea of modal reduction is to find a proper set of basis that spanned a low-dimensional space, which preserves the essential features of full-scale nonlinear systems (Berkooz et al., 1993; Krysl et al., 2001; Lee and Chen, 2013). In previous studies (Berkooz et al., 1993; Meyer and Matthies, 2003), the model reduction method has been interpreted, rediscovered, and reinvented in multiple disciplines. As a result, it is often referred to in different terminologies, such as the proper orthogonal decomposition (POD), Karhunen-Loève (KL) expansion, principal component analysis (PCA), empirical orthogonal eigenvectors, factor-analysis, and Galerkin projection (Krysl et al., 2001; Meyer and Matthies, 2003). Among all the MOR techniques, we propose to use the method of snapshot, a specific form of POD method to run discrete element simulation in reduced dimensional space. The POD method was first introduced in the context of turbulence flow by Lumley (1967) and has been widely used as an efficient model reduction technique in different research and engineering fields during the last few decades. In the field of fluid dynamics, the POD has become an important tool for the analysis and modeling of turbulent flows (Berkooz et al., 1993; Borée, 2003; Ilak and Rowley, 2008; Rowley, 2006; Smith et al., 2005; Wang et al., 2012). As pointed out by Aubry (1991), this success is attributed by both the optimal convergence and the space/time symmetry, which permits the access to spatio-temporal dynamics.

In the field of structural dynamics and fluid-solid interaction, the fluctuating wind pressure acting on the building models were reduced and analyzed by using the POD. The correlations between the decomposed pressures and the approaching wind are examined in the reduced-order system (Tamura et al., 1997). In addition, POD was used for the evaluation of properties and the prediction of responses to wind forces acting on high-rise buildings (Tamura et al., 1999). For data analysis, based on time-resolved particle image velocimetry (PIV) data of velocity fields, the POD was used to recover the time information between two consecutive PIV time measurements (Drueault et al., 2005). Other applications of the POD method are also found in controller design for real-time control of partial differential equations (Kunisch et al., 2004) and image processing (Liu et al., 2014). Remarkably, to the best of the authors’ knowledge, the first application of proper orthogonal decomposition on granular materials does not take place until another 30 years after Lumley (1967), in which Williams and Rege (1997) proposed to use POD to study the coherent structures within a deforming granular material simulated via discrete element method. Similar effort is suggested in Boukouvala et al. (2013), where the principal component analysis is combined with a surrogate model to extrapolate simulation results. Nevertheless, there has not yet been any effort on exploring and analyzing the possibility of applying POD to run discrete element simulations at the grain scale.

The objective of this work is to fill this knowledge gap. Our objective is threefold. First, we introduce different methodologies to generate the snapshots either in parametric space or in different temporal domains. Second, we explore the usage of POD not only as a tool to speed up simulations but also as a method to eliminate or suppress high-frequency noise in simulations without the need to introduce the artificial dampings that may ruin the quality of dynamic wave propagation simulations. Finally, we also formulate an adaptive method to update and construct the POD modes to maintain the discrepancy of reduced-order simulations for highly nonlinear problems. Numerical examples are included to demonstrate the proper ways to collect, update, and use the snapshots and the corresponding orthogonal basis for forward predictions. This systematic study may show new insight on using POD as a means to accelerate or eliminate spurious responses for explicit particulate mechanics simulations with limited computational resources.

The rest of the paper is organized as follows: Section 2 outlines the governing and integration equations of DEM simulations. Then we introduce the basic procedure of the POD combined with the method of snapshots and present
the construction of the reduced-order system. In Section 3, the POD is used to eliminate the high-frequency issues of the dynamic simulations and a cantilevered beam example is given. Section 4 gives a 3D dynamic example to show the effectiveness of POD for solving a parametrized equation over the entire parameter domain. In Section 5, a POD mode-updating scheme is presented, followed by the uniaxial tension and compression numerical examples. Finally, conclusions are presented in Section 6.

As for notations and symbols, bold-faced letters denote tensors; the centerdot denotes a single contraction of adjacent indices of two tensors (e.g., \(a \cdot b = a_i b_i\) or \(c \cdot d = c_{ij} d_{jk}\); the colon denotes a double contraction of adjacent indices of tensor of rank two or higher (e.g., \(C : e^e = C_{ijkl} e_{kl}^e\)); and the symbol \(\otimes\) denotes a juxtaposition of two vectors (e.g., \(a \otimes b = a_i b_j\)) or two symmetric second-order tensors (e.g., \((\alpha \otimes \beta)_{ijkl} = \alpha_{ij} \beta_{kl}\)). Moreover, \((\alpha \otimes \beta)_{ijkl} = \alpha_{ij} \beta_{ik}\) and \((\alpha \otimes \beta)_{ijkl} = \alpha_{ij} \beta_{jk}\).

2. DIMENSIONAL MODEL REDUCTION FOR DEM SIMULATIONS

In this section, we describe the dimensional-reduction method used for the discrete element simulations. We first review the basics of the discrete element method, then describe the application of proper orthogonal decomposition for DEM simulations, followed by a detailed account of how to use the method of snapshot to select low-dimensional space empirically.

### 2.1 Explicit Integration of Discrete Element Method

In DEM simulations, the governing equation is originated from the balance principle (Ceccato et al., 2018; Cundall and Strack, 1979; Kuhn and Mitchell, 1993; Wang and Sun, 2015, 2017, 2018). Here, we consider a simplified version of DEM in which the rotational degree of freedom is neglected. As such, the governing equation reads as follows:

\[
M \ddot{u} = f_{\text{ext}} - f_{\text{int}}(u) = F_{\text{total}}(u)
\]

where \(M\) is the global mass matrix of all particles, and \(f_{\text{ext}}\) and \(f_{\text{int}}(u)\) are external and internal force vectors, respectively. \(F_{\text{total}}(u)\) denotes the total force vector.

In order to discretize the system in the time domain, the Verlet scheme is used to update the acceleration, velocity, and displacement of the particles explicitly, i.e.,

\[
\ddot{u}^t = M^{-1} F_{\text{total}}(u)
\]

\[
\dot{u}^{t+1/2} = \dot{u}^{t-1/2} + \ddot{u}^t \Delta t
\]

\[
\dot{u}^{t+1} = \dot{u}^t + \dot{u}^{t+1/2} \Delta t
\]

where \(\ddot{u}, \dot{u}, u\) are the accelerations, velocities, and displacements of particles, respectively; \(t\) is the current time step; and \(\Delta t\) is the size of time step. It should be noted that, with a few exceptions such as Miehe and Dettmar (2004), the majority of the discrete element models are integrated in time explicitly. This treatment is convenient because it does not require solving a nonlinear system of equations, and hence, there is also no need to assemble the tangent of the residuals. Nevertheless, the reduction in the asymptotic cost of the reduced dimensional system in an explicit scheme is also less significant than the implicit counterpart. More recent works, such as Ryckelynck (2009) and Lee and Chen (2013), have attempted to cut the computational cost further by replacing the full internal force calculation with different approximated procedures. This development could potentially be applied to discrete element simulations but is out of the scope of this current work.

### 2.2 Proper Orthogonal Decomposition

The objective of the proper orthogonal decomposition is to construct a Galerkin projection of a full dimensional model space \(U \in \mathbb{R}^n\) onto a reduced-order subspace \(U^m \in \mathbb{R}^m\) that preserves the features in \(\mathbb{R}^n\). The dimension \(n\)
is the total number of degrees of freedom of the full dimensional model, and \( m \) is the number of degrees of freedom of the corresponding reduced-order model such that \( m \gg n \).

Let \( U(x, t) \) be a state field on the domain \( \Omega \). In this work, \( U(x, t) \) is denoted as the displacement field due to the absence of any rotational degrees of freedom. Note that there are two important decisions that dictate the success of the POD reduced-dimensional simulations: (i) where do we collect this displacement field, and (ii) how do we construct the Galerkin projection based on the displacement field we obtained. Rather than attempting to develop a one-size-fits-all strategy, we found that a more effective approach for the POD-DEM model is deploying the right tactics depending on the given circumstance, as demonstrated in Sections 3–5.

The POD aims at finding the optimal structure \( \{ \phi_i(x) \}_{i=1}^m \) of an ensemble of snapshots of the field \( U(x, t) \), which is equivalent to obtain the optimal orthonormal basis functions \( \phi_i(x) \) by maximizing the ensemble average of the inner product between the state field \( U(x, t) \) and the basis \( \phi_i(x) \) such that (Kerschen et al., 2005; Lee and Chen, 2013):

\[
\text{max} \quad \langle |(U, \phi_i)|^2 \rangle \quad \text{subject to} \quad \|\phi_i\|^2 = 1
\]

where \( \langle f, g \rangle = \int_\Omega f(x)g(x)dx \) is the inner product in the domain \( \Omega \), \( x \) is the spatial coordinates of particles, \( \langle f \rangle = 1/T \int f(t)dt \) denotes the temporal averaging operator, \( |\cdot| = (\cdot)^{1/2} \) denotes the norm, and \( |\cdot| \) denotes the complex modulus. Then the maximization problem in Eq. (5) can be recast as a variational problem subjected to the constraint \( \|\phi_i\|^2 = 1 \)

\[
J[\phi] = \langle |(U, \phi_i)|^2 \rangle - \lambda(\|\phi_i\|^2 = 1)
\]

where \( \lambda \) is the Lagrange multiplier. Strictly speaking, the constraint \( \|\phi_i\|^2 = 1 \) is not essential if the bases are orthogonal. Nevertheless, the normalization is helpful for maintaining the condition number of the projection operator. Considering a stationary condition (Holmes et al., 2012), the aforementioned operation reduces to the following integral eigenvalue problem:

\[
\int_\Omega \langle U(x, t)U(x', t) \rangle \phi(x') dx' = \lambda \phi(x)
\]

where the kernel \( \langle U(x, t)U(x', t) \rangle = K(x, x') \) is the averaged auto-correlation function.

The solution of the aforementioned integral eigenvalue problem is thus given by a series of orthogonal eigenfunctions \( \phi_i \) and the corresponding eigenvalues \( \lambda_i \) \((\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \cdots \geq 0)\), called POD modes (POM) and POD values (POV) respectively. The total energy \( e \) contained in the relevant data can be computed by \( e^{\text{total}} = \sum \lambda_i \), and the energy captured by the first \( m \) POM is given by (Deokar et al., 2017; Kerschen et al., 2005; Volkwein, 2013):

\[
e^m = \sum_{i=1}^m \lambda_i
\]

Then, the low-dimensional approximation subspace of \( U \) spanned by POM can be expressed as follows:

\[
U(x, t) \approx U^m(x, t) = \sum_{i=1}^m \xi_i(t) \phi_i(x)
\]

where \( U^m(x, t) \) is the optimal approximation subspace of first \( m \) POD modes \( \phi_i \), and \( \xi_i(t) \) are the uncorrelated coefficients that determined by

\[
\langle \xi_i(t) \xi_j(t) \rangle = \delta_{ij} \lambda_i
\]

\[
\xi_i(t) = \langle U(x, t), \phi_i(x) \rangle
\]

When using the POD for discrete element simulations, caution must be paid for the enforcement of essential boundary conditions. Whereas, Eq. (9) may satisfy a homogeneous boundary condition, enforcing an inhomogeneous boundary condition using the coefficient for the reduced basis does not always yield satisfactory results (Kalashnikova and Barone, 2012; Krysl et al., 2001). Presumably, improvements can be achieved by (i) choosing a coordinate frame such that the inhomogeneous boundary condition can be re-expressed as a homogeneous one, or (ii) enforcing the boundary conditions through penalty or Lagrangian multipliers. These options will be considered in future studies.
2.3 Method of Snapshots

The method of snapshots formulated by Sirovich (1987) is widely used for computing the POD modes. Suppose that we denote the snapshot \( u(t_0) = u(x, t_0) \) at time \( t_0 \). After running a dynamic simulation, conducting an experiment for a small period of time \( t = t_n = s \cdot \Delta t \), we may collect \( s \) number of snapshots of the displacement field and store them in the snapshots matrix \( X \)

\[
X = [u_1(x) \ u_2(x) \ \cdots \ u^n(x)] = \begin{bmatrix} u(x_1, t_1) & \cdots & u(x_1, t_n) \\ \vdots & \ddots & \vdots \\ u(x_n, t_1) & \cdots & u(x_n, t_n) \end{bmatrix}
\]

(12)

where \( X \) is a \( n \times s \) matrix, and \( n \) is the number of degrees of freedom and \( s \) is the number of snapshots. In general, we can collect those snapshots from any source that makes sense and is sufficiently relevant to the forward predictions we are planning to make. Nevertheless, it is important to keep in mind that our choices of the snapshot (and the number of basis we use) will be crucial to determine whether the reduced-dimensional basis is effective. Since the discrete snapshots data do not necessarily have a zero mean, the averaged auto-correlation function mentioned above can be written as follows (Kerschen et al., 2005):

\[
C = E[(u - \bar{u})(u - \bar{u})^T]
\]

(13)

where \( C \) denotes the co-variance matrix, \( E[\cdot] \) is the exception, and \( \bar{u} \) is the mean of the displacement vector \( u \). Assume that the whole simulation is stationary and ergodic, a reliable estimate of the corresponding discrete covariance matrix can be given by

\[
C = \frac{1}{n}X^T X
\]

(14)

where \( C \in \mathbb{R}^{n \times n} \). Then the integral eigenvalue problem in Eq. (11) is equivalent to solve the eigenfunction (Lee and Chen, 2013):

\[
C \Phi = \Lambda \Phi
\]

(15)

where \( \Lambda \) denotes the diagonal matrix containing all the eigenvalues in descending order and \( \Phi = [\phi_1 \ \phi_2 \ \cdots \ \phi_n] \) is matrix of POM. Generally, if \( n > s \), it is more efficient to compute POM and POV by replacing the correlation matrix \( C = (1/n)X^T X \in \mathbb{R}^{s \times s} \) with \( \hat{C} = (1/n)X^T X \in \mathbb{R}^{s \times s} \) such that

\[
\phi_i = \frac{1}{\sqrt{\lambda_i}} X \psi_i, \quad i = 1, 2, \ldots, m = \text{rank}(C)
\]

(16)

where \( \Phi_m = [\phi_1 \ \phi_2 \ \cdots \ \phi_m] \) are the eigenvectors of \( C \) and \( \Psi_m = [\psi_1 \ \psi_2 \ \cdots \ \psi_m] \) are the eigenvectors of \( \hat{C} \). However, computing POM and POV directly from the matrix \( C \) or \( \hat{C} \) is still expensive and instead the singular value decomposition (SVD) is adopted (Ceccato et al., 2018; Chatterjee, 2000):

\[
X = D \Sigma V^T
\]

(17)

where \( C \in \mathbb{R}^{n \times s} \) is the same snapshot matrix we have above, \( D = [d_1 \ d_2 \ \cdots \ d_n] \in \mathbb{R}^{n \times n} \) is an orthonormal matrix containing the eigenvectors of \( C \), and \( V \in \mathbb{R}^{s \times s} \) is an orthonormal matrix containing the eigenvectors of \( \hat{C} \). \( \Sigma \in \mathbb{R}^{n \times s} \) is a pseudo-diagonal matrix with the main diagonal containing singular values of \( X \) with descending order (\( \Sigma_{ii} = \sqrt{\lambda_i}, \ \lambda_1 \geq \lambda_2 \geq \lambda_{\min(n,s)} \geq \cdots \geq 0 \)).

Finally, we obtain \( \Phi_m \) of the first \( m \) POM corresponds to the first \( m \) columns of \( D \)

\[
\Phi_m = [\phi_1 \ \phi_2 \ \cdots \ \phi_m] = [d_1 \ d_2 \ \cdots \ d_m]
\]

(18)

where \( m \) is the aforementioned truncation number determined by Eq. (8). The orthogonal POM matrix \( \Phi_m \) satisfies the condition \( \Phi_m^T \Phi_m = I \).
2.4 Explicit Dynamics in the Reduced-Order System

If the selected snapshot \( X \) is representative enough of the actual response, the full-dimensional displacement field \( U \in \mathbb{R}^n \) can be projected onto the low-dimensional subspace \( U^m \in \mathbb{R}^m \) through \( \Phi_m \)

\[
U \approx U^m = \sum_{i=1}^{m} \xi_i \phi_i = \Phi_m \xi
\]

(19)

where \( \Phi_m \) denotes the basis of the objective subspace and \( \xi \) denotes the corresponding coefficients that are also interpreted as the reduced-order displacements satisfying \( \xi = \Phi_m^T U \). Integration equations (2)–(4) can thus be rewritten in the reduced-order scheme

\[
\ddot{\xi} = \Phi_m (\Phi_m^T M \Phi_m)^{-1} [\Phi_m^T F_{\text{total}}(u)]
\]

(20)

\[
\dot{\xi}^{t+\frac{1}{2}} = \dot{\xi}^{t-\frac{1}{2}} + \dot{\xi}^{t} \Delta T
\]

(21)

\[
\xi^{t+1} = \xi^{t} + \dot{\xi}^{t+\frac{1}{2}} \Delta T
\]

(22)

The \( \Delta T \) here is the stable time step of reduced-order integration, and it is subjected to the relationship \( \Delta T < 2/\omega_{\text{max}} \), where \( \omega_{\text{max}} \) is computed from \( |\Phi_m^T K \Phi_m - \omega^2 \Phi_m^T M \Phi_m| = 0 \), and \( \Phi_m^T K \Phi_m \) is the stiffness matrix of the subspace (Ceccato et al., 2018). Thus, a larger stable time step is permissible for the integration of the reduced-order system.

3. APPLICATION 1: POD FOR ELIMINATING HIGH-FREQUENCY ISSUES IN THE NUMERICAL SIMULATION

In dynamic particulate mechanics simulations, high-frequency modes may lead to the spurious numerical results and also cause stability and convergence issues in explicit scheme (Deokar et al., 2017). In the case where concurrent multiscale coupling takes place in a handshake domain, the high frequent component may destabilize the numerical simulations and must be eliminated in the transition zone (Badia et al., 2007; Chamoin et al., 2010; Sun et al., 2017; Sun and Mota, 2014). Hence, the numerical dissipation approach is frequently introduced to the explicit time integration algorithms in order to damp out the spurious oscillations occurring in high-frequency domain. There exists a substantial amount of literature on the numerical dissipation scheme algorithms (Fung, 2003; Hulbert and Chung, 1996; Maheo et al., 2013). However, numerical damping also causes energy dissipation that affects the accuracy of the simulations (Deokar et al., 2017; Maheo et al., 2013).

Instead of proposing another ad hoc damping model that may inevitably cause non-physical energy dissipation, we propose a procedure that leverages the POD to resolve the high-frequency issue while using an energy-preserving time integrator [cf. Martys and Mountain (1999); Simo et al. (1992)] for discrete element simulations.

3.1 POD-based Model Reduction Approach

The procedure of the POD-based approach is similar to the one proposed for dynamic finite element simulations first proposed by Deokar et al. (2017). The step-by-step procedure is in the following. First, we run the dynamic simulations with the numerical damping scheme for a certain amount of time steps to collect the snapshots data and then construct the matrix of snapshots \( X \). Second, we compute the POM \( \Phi_m \) and truncate the POD basis based on a predefined tolerance of error. Then, we construct the corresponding reduced-order system using the reduced basis obtained from the POM \( \Phi_m \). Finally, the reduced-order system can be simulated by using the explicit integration algorithm without the numerical damping (\( \lambda = 0 \)).

Since (i) the snapshots are obtained from a dissipation scheme that filter out high-frequent responses, and (ii) the solution space is spanned by the basis function generated from the proper orthogonal decomposition of the matrix of snapshots \( X \), it is therefore not possible for the particulate system to exhibit spurious oscillation modes that are orthogonal to the basis of the solution, regardless of whether numerical damping is used. One important upshot of this
POD-based Discrete Element Simulations

3.2 Numerical Example: Dynamic Vibrations of Cantilevered Beam

The numerical modeling of vibrations in granular materials is an important tool to understand seismic soil-structure interaction, foundation vibration, and seismic wave propagation (Borja and Sun, 2008; Liu et al., 2016b; Zeghal and Oskay, 2002). Here, we consider the dynamic responses of a cantilevered beam composed of granular cohesive-frictional materials. The setup of the simulation is illustrated in Fig. 1.

The left-hand side of the beam is totally fixed while the right-hand side was subjected to a vertical sinusoidal cyclic loading with the maximum displacement $u_{s,\text{max}} = 8.0 \times 10^{-5}$ m and the loading frequency $f = 2.5$ kHz. We use the concrete particle model (CPM) in Šmilauer et al. (2010) and neglect any physical damping. The configuration of other material parameters is shown in Table 1. In order to ensure the numerical stability of the explicit integration scheme, the time step is set to $\Delta t = 7.545 \times 10^{-7}$ s, and the time duration of the whole simulation is $6000\Delta t = 4.527 \times 10^{-3}$ s.

As mentioned in Section 3.1, we first ran simulations with numerical dissipation to collect the snapshots for the forward predictions. In particular, we use the following numerical damping scheme to generate snapshots (Šmilauer et al., 2015):

$$
(\ddot{u}_i)_{\text{damped}} = \ddot{u}_i \left[ 1 - \lambda \cdot \text{sgn} \left( \frac{1}{2} \frac{\Delta t}{\Delta x_i^2} + \frac{1}{2} \frac{\Delta t}{\Delta y_i^2} \right) \right]
$$

(23)

**FIG. 1:** Sample of a dry granular cantilevered beam with boundary conditions

<table>
<thead>
<tr>
<th>TABLE 1: Parameter configuration</th>
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<tbody>
<tr>
<td><strong>Parameters</strong></td>
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<tr>
<td>Length of the beam (m)</td>
</tr>
<tr>
<td>Radius of the beam (m)</td>
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<tr>
<td>Number of particles</td>
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<tr>
<td>Number of DOFs</td>
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<tr>
<td>Particle density (kg/m$^3$)</td>
</tr>
<tr>
<td>Young’s modulus (Pa)</td>
</tr>
<tr>
<td>Poisson ratio</td>
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<tr>
<td>Initial cohesion (Pa)</td>
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where $\lambda$ is the numerical damping coefficient and is set to $\lambda = 0.3$ following the treatment in Šmilauer et al. (2015). The subscript $i$ refers to the $i$th degree of freedom and $t$ denotes the current time step $t$. A cyclic motion is prescribed at one end of the cantilever beam, while the other end is fixed. Snapshot data are then obtained via solving the dynamic problem with the numerical dissipation scheme for a total time of $1000\Delta t = 7.545e^{-4}$ s. Then, the Galerkin projection operator is constructed by sorting the bases according to the magnitude of their corresponding singular values, then concatenates the first $m$ bases together to form the POM matrix $\Phi_m$.

Figure 2 shows the first 100 POD values (square of the singular value) of the snapshot matrix $X$. Figure 2 provide a guidance on whether it is possible to identify a low-dimensional space that captures the essential behaviors, patterns, or physics of the full-scale simulations. In particular, if after the ranking the singular values of the snapshot matrix are of similar magnitude, then this trend may indicate that one must increase the dimension of the reduced space to reproduce patterns exhibited in the full-scale simulations. On the other hand, if the singular values drop significantly against the descending rank, then it is more likely that one may use a lower dimensional space for the reduced-dimensional simulations.

Figure 3 shows the shapes of the first six POD normalized modes and the corresponding POD values. As expected, the modes corresponding to the higher POD value exhibit simpler patterns. As the POD value drops, the corresponding mode shape becomes less representative, in an empirical sense. On the basis of this rationale, we introduce a cutoff POD value below which the corresponding modes are not incorporated in the reduced dimensional simulations.

Following this step, we construct the Galerkin projection operator such that one may now run reduced-order DEM simulations with an energy- and momentum-preserving time integrator. To evaluate the reduced-order simulations, we also conducted simulations with a nondissipative time integrator and without the Galerkin projection. Ultimately, the three types of simulations conducted (i) with a nondissipative time integrator and without the Galerkin projection, (ii) with a dissipative time integrator but without the Galerkin projection, and (iii) with a nondissipative time integrator and with the Galerkin projection. In case (iii), 10 POD bases are used to construct the Galerkin projection. Figure 4 shows the motion time-history of a particle in the cantilever beam of these three different simulations (cases i–iii). As shown in Fig. 4, the numerical nondissipation solution contains high-frequency oscillations, which are particularly clear in acceleration and velocity plots. Although those oscillations can be presumably damped out by using a numerical dissipation scheme, the undesirable side effect (shown in Fig. 4) is that the dissipation may also significantly reduce the amplitude of the wave. Although this issue might be resolved via some careful tuning and calibration, the POD approach appears to be a simpler resolution. As the evidence shown in Fig. 4, the numerical simulations conducted by strategy (iii) clearly suppress the high-frequency responses. Yet, the amplitude of the wave does not reduce due to the Galerkin projection.

Errors are computed to estimate the accuracy of the reduced-order systems constructed by different numbers of POM. Table 2 demonstrates the comparison of the reduced-order systems using the root-mean-square error (RMSE):

![FIG. 2: First 100 POD values (square of the singular values) of the snapshot matrix $X$](image-url)
FIG. 3: Shapes of the first six normalized POD bases $\Phi_m, m = 1, 2, ..., 6$ (POVs) used to form the Galerkin projection and the corresponding POD values

(a) Mode 1: $\text{POV} = 1.867 \times 10^{-3}$
(b) Mode 2: $\text{POV} = 5.438 \times 10^{-4}$
(c) Mode 3: $\text{POV} = 2.086 \times 10^{-5}$
(d) Mode 4: $\text{POV} = 3.243 \times 10^{-6}$
(e) Mode 5: $\text{POV} = 2.217 \times 10^{-6}$
(f) Mode 6: $\text{POV} = 8.367 \times 10^{-7}$

FIG. 4: Historical responses of particle P at $(x, y, z) = (0.0106, 0.0087, 0.0129)$ in the direction of $z$-axis: (a) acceleration, (b) velocity, and (c) displacement; and total kinetic energy of all particles: (d) energy
where $u^{\text{full}}(t)$ denotes the full DEM solution of displacement vector at time $t$ while $u^{\text{POD}}(t)$ is the POD solution, and $p$ is the number of total time steps. The dimension of the dynamic system $\mathbb{R}^{6021}$ can be significantly reduced to $\mathbb{R}^{10}$ with an acceptable RMSE.

This result is not surprising, because all the high-frequency modes are orthogonal to the solution space of the reduced-order simulations. Whether these encouraging results can be further generalized to other cases is not absolutely clear. Nevertheless, this numerical experiment demonstrates that the proposed approach is effective in eliminating the high-frequency issues and obtain accurate responses of accelerations, velocities, and displacements while conserving total energy and the physics of low-frequency modes. This result is interesting in the sense that it showcases that the applications of POD method is not only limited to speed-up simulations. POD may also be used to obtain desirable discrete element solutions by controlling, manipulating, and selecting the image (and kernel) of the solution spaces for a given problem.

4. APPLICATION 2: REDUCED-DIMENSIONAL DYNAMIC SIMULATIONS FOR GENERATING RESPONSE SURFACES

In the previous example, the POD method employs the space spanned by the numerical solution of a related problem to obtain the reduced dimensional space for nondissipative simulations. However, the POD application is not limited to generate non-dissipative simulations. In fact, a more common application of POD in another domain of interest is to reduce the time required to generate a response surface for a particular set of explanatory valuables. This type of application is important for a wide spectrum of particulate mechanics-related energy applications, such as granular mixing and separations and powder manufacturing.

Because of the nonlinear nature of the problems, it is relatively difficult to obtain a response surface reliable enough for predictions. Presumably, this issue can be resolved if one conducts a large number of physical experiments. In practice, this is proven to be inefficient and sometimes wasteful of time and resources. Although well-calibrated discrete element simulations may provide an alternative to cutting costs, this alternative by itself can also be very expensive if the simulation domain contains a large number of particles.

In order to avoid the repeating work when solving a group of similar problems that can be described by parametrized equations, the POD method can also be used as a predictive tool to capture the responses over a parameter domain. In this circumstance, one may collect the experimental results or simulation results of a similar nature and again use the space of these solutions to find the reduced dimensional space that enables fast simulations. The strategy of the snapshot collection and the resultant reduced-order three-dimensional wave propagation simulations are demonstrated in subsequent sections.

4.1 Parametrized Equations and Collection of Snapshots

In many engineering applications, a series of boundary value problems with a similar model can be expressed via parametrized equations, in which boundary conditions, loading features, and material properties are denoted by the parameter $\mu$ (Hesthaven et al., 2016). In this section, considering the models made by different materials, the particle density is of interest. Then, the governing equation (1) can be simply rewritten as follows:
\[ M(\mu) \frac{d\mathbf{u}(t)}{dt^2} = \mathbf{F}_{\text{total}}(\mathbf{u}(t)) \]  

where \( \mu \) denotes the density \( \rho \) of particles and \( \rho \in \{3600, 4000, 4400, 4800, 5200\} \). The parametrized equation describes a group of dynamic problems with the material of five different densities.

In order to capture the response of the dynamic system for the entire parameter domain \( \rho \in [3600, 5200] \), we adopt a uniform sampling strategy to construct the snapshot matrix \( X \)

\[
X = [\mathbf{u}(t_1, \rho_1), \ldots, \mathbf{u}(t_s, \rho_1), \mathbf{u}(t_1, \rho_2), \ldots, \mathbf{u}(t_s, \rho_2), \ldots, \mathbf{u}(t_s, \rho_5)]
\]

where \( \mathbf{u}(t, \rho) \) is the displacement vector of the system with parameter \( \rho \) at time \( t \), and \( \{\rho_1, \rho_2, \rho_3, \rho_4, \rho_5\} \) is equal to the aforementioned five known densities. Hence, \( s \) snapshots of each system are collected and the total size of \( X \) is \( n \times 5s \).

### 4.2 Numerical Example: Three-Dimensional Wave Propagation in a Granular Bed

In this section, the dynamic response of a thick granular plate (length \( L = 0.2 \) m, width \( W = 0.12 \) m, thickness \( T = 0.024 \) m), composed of particles of the same size but different densities under the sinusoidal cyclic shear loading, is of interest. Our goal in this demonstration example is to study the relationship between the mechanisms of the wave propagation and the density of the particles while using the reduced-order simulations to both suppress the high-frequency responses and speed up the simulations.

The model shown in Fig. 5 contains 1795 particles of concrete particle model and material parameters are same as those used in section 3.2. Three edges of the model are totally fixed and a sinusoidal cyclic shear loading with the maximum shear displacement \( u_{s,\text{max}} = 1.0e^{-3} \) m and the loading frequency \( f = 1.5e^3 \) Hz is applied to the middle of the free edge along the \( z \)-axis. To ensure the numerical stability, the time step is set as \( \Delta t = 6.524e^{-7} \) s and the time duration of the whole simulation is 6000\( \Delta t = 3.914e^{-3} \) s.

Similarly, to filter out the high-frequency issues, we adopt the same approach as outlined in Section 3.1. In the offline stage, the numerical dissipation scheme is used and a total number of \( 5 \times 10^3 \) snapshots are collected from the simulations of five known densities via uniform sampling. Figure 6 shows the first 100 POD values. Then, the POM matrix \( \Phi_m \) of rank 23 is used for the Galerkin projection and the first nine modes of them are plotted in Fig. 7. Through the Galerkin projection, the original full-dimensional dynamic problem (\( \mathbb{R}^{5385} \)) can be projected onto a low-dimensional subspace (\( \mathbb{R}^{23} \)) and the corresponding reduced-order system is constructed according to Eqs. (20)–(22).

To evaluate the quality of the forward predictions of the reduced-order model, we use a technique called k-fold validation (Wang and Sun, 2018). In this numerical experiments, we consider the collection of snapshot and the construction of the Galerkin projection as a unsupervised learning process. To validate the quality of the Galerkin...
FIG. 6: First 100 POD values

(a) Mode 1: $\text{POV} = 2.940 \times 10^{-5}$
(b) Mode 2: $\text{POV} = 2.338 \times 10^{-6}$
(c) Mode 3: $\text{POV} = 1.518 \times 10^{-7}$
(d) Mode 4: $\text{POV} = 3.607 \times 10^{-8}$
(e) Mode 5: $\text{POV} = 1.079 \times 10^{-8}$
(f) Mode 6: $\text{POV} = 6.829 \times 10^{-9}$

(g) Mode 7: $\text{POV} = 5.315 \times 10^{-9}$
(h) Mode 8: $\text{POV} = 2.785 \times 10^{-9}$
(i) Mode 9: $\text{POV} = 1.179 \times 10^{-9}$

FIG. 7: Shapes of the first nine normalized POD bases $\Phi_m$, $m = 1, 2, ..., 9$ that form the Galerkin projection

projection, the simulation results obtained from domains consistent of particles of density $\rho = 3600, 4000, 4400, 4800,$ and $5200 \text{ kg/m}^3$ are used as the training data. Meanwhile, a forward prediction is conducted on a domain with density $\rho = 4200 \text{ kg/m}^3$. The forward prediction is denoted as the POD prediction in Figs. 8 and 9. For comparison, a benchmark solution of $\rho = 4200 \text{ kg/m}^3$ is obtained by using the original POD method, where we only collect the snapshot from its own simulation ($\rho = 4200 \text{ kg/m}^3$) when constructing $\Phi_m$. It is notable that all the solutions are solved by a nondissipation time integrator in this stage. As the magnitude of responses in the $x$ and $y$ directions are relatively small, only the responses in the $z$ direction are plotted in Figs. 8 and 9.
As shown in Figs. 8 and 9, it is clear that the change of particle density ($\rho = 4000, 4200, 4400$) kg/m$^3$ leads to the non-negligible change of dynamic responses. For the forward prediction case with $\rho = 4200$ kg/m$^3$, the historical displacements field in Fig. 10 and the closer looks in Fig. 9 show a good agreement between the POD predictions and POD benchmark solutions. In addition, results obtained by the reduced-order system and the corresponding RMSEs are computed and shown in Table 3.

In addition to eliminating the high-frequency oscillations, the reduced-order system constructed by the proposed method is effective in capturing the dynamic response of the simulation with any unknown density within the entire parametric domain. It should be noted that, in general, collecting more snapshots from different cases may improve the ability of the Galerkin projection to capture the essence of the dynamics of particulate responses. Nevertheless, the decision of how much training data are required for forward prediction remains a trial-and-error procedure and highly depends on the complexity of the problems.

5. APPLICATION 3: ADAPTIVE POD FOR PREDICTION OF SOFTENING BEHAVIOR

In this section, we present the strategy for the scenario in which we anticipate that there is a change of the dominating mode or physics of the numerical predictions and we attempt to incorporate this information to make better POD predictions by adaptively (and automatically) updating the Galerkin operator whenever needed during the numerical
FIG. 9: (a,c) displacement closer look, (b,d) energy closer look

FIG. 10: Historical displacement $u_z$ field of benchmark solution and POD prediction of the case $\rho = 4200$. 

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TABLE 3: Root-mean-square errors of unknown densities

<table>
<thead>
<tr>
<th>Unknown densities (kg/m³)</th>
<th>3680</th>
<th>3910</th>
<th>4200</th>
<th>4670</th>
<th>5050</th>
</tr>
</thead>
<tbody>
<tr>
<td>RMSE (%)</td>
<td>0.7048</td>
<td>0.7592</td>
<td>0.8213</td>
<td>0.9117</td>
<td>0.7787</td>
</tr>
</tbody>
</table>

simulations. In the following studies, an automatic-updating POD procedure is introduced and the numerical examples of uniaxial tests are illustrated in Section 5.2.

5.1 POM Updating

In the numerical examples presented above, the collection of snapshot data and the construction of the reduced-order system are both in the offline stage. In the online stage, the original dynamic problem is running in the obtained reduced-order system. In order to ensure the accuracy of the online process, the snapshot data must be representative of the whole simulation. However, the dynamic pattern will be variable if the constitutive law we use is nonlinear or the external loading (applied force, velocity, or displacement) is inconsistent. In that case, new snapshot data need to be updated and the corresponding reduced-order system should be recomputed. Obviously, the proper time to update new modes is determined by the real solution of the whole simulations, is always problem-dependent. Therefore, we present a predictive approach that updates the POM and the reduced-order system during the simulation automatically, and thus the online stage can be combined with the offline stage. The automatic-updating POD procedure Ceccato et al. (2018) is demonstrated below.

Assume $T_{cycle}$ is a presetting parameter of the time interval (or the number of time steps) that gives the duration of each updating cycle. At the first $N_s$ time steps of each cycle, the full-order dynamic system is carried out to collect snapshot data and, then, the reduced-order system is constructed at the end of the collecting step ($t = T_s = N_s \cdot \Delta t$). Then, during the period $T_s < t \leq T_{cycle}$, the dynamic problem shifts from full-order system to the corresponding reduced-order system. After the time interval $T_{cycle}$, the snapshots data and reduced-order system are not representative any longer and must be updated. The original system is thus carried out back to collect new snapshot data of the current dynamic response, and then the same procedure is repeated in each cycle. As shown in Fig. 11, the snapshot data are collected and updated during the simulation and the numerical integration scheme switches from the full-order system to the reduced-order system and go back periodically.

5.2 Numerical Example: Uniaxial Tests with POM Updates for Softening Behaviors

In this section, we consider the same granular model and material parameters used in Section 3. The left-hand side of the cantilevered beam is still fixed while the loading applied to the right side surface is along the $y$-axis.

In the tension test, a tension load of strain rate $\dot{\varepsilon} = 0.15$ is applied along the positive direction of the $y$-axis. The time step is set to $\Delta t = 7.545 \times 10^{-7}$ s, and the whole simulation for a time period of $T = 2.49 \times 10^{-3}$ s (3300 time steps) is of interest. First, strain-stress curves and displacement responses of particle P are obtained via original POD method without updating POM. As demonstrated in Fig. 12, the snapshots data collected in the initial period of time only capture the linear elastic response correctly; whereas, the overall response in the softening region becomes more ductile than the real response. Besides, the corresponding reduced-order system is still not representative enough for

![FIG. 11: Mode updating scheme](image-url)
In the three different mode-updating schemes, the POM and the corresponding reduced-order system are updated every $T_{\text{cycle}} = 8.30 e^{-4}$ s, $4.15 e^{-4}$ s, $2.49 e^{-4}$ s increment of time (totally update three, six, and ten times), respectively. For each cycle, 100 snapshots are collected and the number of POM is fixed to 20. The results are shown in Fig. 13.

In the compression test, a compression load of strain rate $\dot{\varepsilon} = 0.5$ is applied along the negative direction of the $y$-axis. The whole simulation duration of $T = 2.64 e^{-3}$ s (3500 time steps) is considered, which contains the softening response until the beam breaks. As shown in Fig. 14, different mode-updating schemes are used to solve the whole problem, where we set $T_{\text{cycle}} = 5.28 e^{-4}$ s, $3.78 e^{-4}$ s, $2.64 e^{-4}$ s, respectively (totally update five, seven, and ten times). In each updating cycle, 100 snapshots are collected and the number of POM is fixed to 32.

In addition to reducing the dimension of the original problem, the proposed mode-updating scheme can be used to update POM automatically and obtain accurate responses throughout the entire simulation.
FIG. 13: Historical displacements $|\mathbf{u}_p|$ of particle $P$ and strain-stress curves of the tension test with different mode-updating times

FIG. 14: Historical displacements $|\mathbf{u}_p|$ of particle $P$ and strain-stress curves of the compression test with different mode-updating times

6. CONCLUSION

We introduce the proper orthogonal decomposition method as a mean to conduct particulate mechanics simulations via the DEM model in a reduced dimensional space. In particular, we introduce three strategies to use POD to resolve a range of problems commonly encountered in discrete element simulations such that the discrete element simulations can be faster and free of spurious oscillations. By collecting snapshots from dissipative simulations, the reduced-order simulations may now be free of high-frequency noise without using damping. By reusing full-scale simulations and experimental data from similar problems, forward predictions can be made with a solution space of lower dimension and larger time step. In the case where the physics changes due to the onset of material failures, we adopt methods to update the Galerkin projection such that the essence of the responses can be captured with the same small number of degrees of freedom. Together, we show that POD could be an effective tool for the particulate mechanics simulations if a proper strategy is derived for a specific situation and the results are interpreted carefully.
ACKNOWLEDGMENTS

The first author is grateful for financial support from the China Scholarship Council (CSC) (Grant No. 201606260177). The second author is supported by the Earth Materials and Processes program from the U.S. Army Research Office under Grant Contracts No. W911NF-15-1-0442 and No. W911NF-15-1-0581 and the Dynamic Materials and Interactions Program from the Air Force Office of Scientific Research under Grant Contracts No. FA9550-17-1-0169 and No. FA9550-14-C-0058. This support is gratefully acknowledged. The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of the sponsors, including the Army Research Laboratory or the U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein. WCS would like to thank PhD student Nikolaos Vlassis for drawing Figs. A1, A2 and A3 in the article.

REFERENCES


APPENDIX A. DEM MODEL

The DEM simulation framework has been implemented in the Open source code YADE (Šmilauer and Chareyre, 2010; Šmilauer et al., 2015). In this work, all the simulations were performed with YADE while the POD algorithm was implemented in a python code to update the reduced-order system for the YADE simulations.

A.1 Stiffness

In the DEM framework, basic DEM interaction defines normal stiffness $K_N$ and shear stiffness $K_T$ (Šmilauer and Chareyre, 2010). As demonstrated in Fig. A1, normal stiffness $K_N$ is computed as stiffness of two springs in configuration with lengths equal to the particle radius.

In the case of the concrete particle model, in this work we used:

$$K_i = E_i l_i = E_i \left(\frac{A_{eq}}{l_i}\right)$$  \hfill (A.1)

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where \( l_i \) are distances between contact point and particle centers, and the cross section \( A_{\text{eq}} = \pi \min(r_1, r_2)^2 \). Then, the normal stiffness \( K_N \) can be obtained from

\[
K_N = \frac{E_1 \tilde{l}_1 E_2 \tilde{l}_2}{E_1 \tilde{l}_1 + E_2 \tilde{l}_2} \quad (A.2)
\]

The shear stiffness \( K_T \) is typically determined as a given fraction of computed \( K_N \) by introducing a nondimensional constant \( \eta \)

\[
K_T = \eta K_N \quad (A.3)
\]

where the ratio \( \eta \) determines macroscopic Poisson’s ratio of the arrangement (Šmilauer and Chareyre, 2010).

### A.2 Strain Evaluation

#### A.2.1 Normal Strain

The two contacted particles with initial centers \( \overline{C}_1, \overline{C}_2 \) and radius \( r_1, r_2 \) are shown in Fig. A2. The initial contact point \( \overline{C} \) is in the middle of the overlap length and distances \( d_0, d_1, d_2 \) satisfy the relationships

\[
d_0 = d_1 + d_2 = |\overline{C}_2 - \overline{C}_1| \quad (A.4)
\]

\[
d_1 = r_1 + \frac{d_0 - r_1 - r_2}{2} \quad (A.5)
\]

Figure A2 shows the general case that the particles already overlap when the contact is created by the collision detection algorithm (Šmilauer and Chareyre, 2010). As particles undergo motion, the centers \( \overline{C}_1, \overline{C}_2 \) move to \( \overline{C}'_1, \overline{C}'_2 \) and thus the state variables and new contact point is updated

\[
n' = \frac{\overline{C}'_2 - \overline{C}'_1}{|\overline{C}'_2 - \overline{C}'_1|} \quad (A.6)
\]

\[
\overline{C}'' = \overline{C}' + n' \left( d_1 - \frac{d_0 - |\overline{C}'_2 - \overline{C}'_1|}{2} \right) \quad (A.7)
\]
Then, the normal displacement and strain are obtained from
\[ u_N = |C'_{2} - C'_{1}| - d_0 \]  
\[ \varepsilon_N = \frac{u_N}{d_0} = \frac{|C'_{2} - C'_{1}|}{d_0} - 1 \]  
(A.8)  
(A.9)
where normal displacement \( u_N \) is aligned with \( n' \).

### A.2.2 Shear Strain

As is illustrated in Fig. A3, the left plot is the initial contact configuration and the right one shows the evolution of shear displacement \( u_T \) due to both translation and rotation of the particles. In the Yade framework, the increment algorithm (Luding, 2008) was implemented to update shear displacements from the previous step \( u_T \) to the current step \( u'_T \):

\[ (\Delta u_T)_1 = -u_T \times (n \times n') \]  
\[ (\Delta u_T)_2 = -u_T \times \left[ \frac{\Delta t}{2} n' \cdot (\omega_1 + \omega_2) \right] n' \]  
\[ (\Delta u_T)_3 = -\Delta t(v_{12} - (n' \cdot v_{12})n') \]  
(A.10)  
(A.11)  
(A.12)
where Eq. (36) and (37) compute the contact move due to changes of particles’ positions \( C'_{1} \) and \( C'_{2} \) while Eq. (38) updates the mutual movement of particles and \( v_{12} \) denotes mutual velocity of particles at the contact point Šmilauer and Chareyre (2010). Finally, we obtain
\[ u'_T = u_T + (\Delta u_T)_1 + (\Delta u_T)_2 + (\Delta u_T)_3 \]  
(A.13)

### A.3 Stress Evaluation

At each time step, normal and shear forces can be computed from
\[ F_N = \begin{cases} K_N u_N n & \text{if } u_N \leq 0 \\ 0 & \text{otherwise} \end{cases} \]  
(A.14)
\[ F_T = \begin{cases} |F_N| \tan \theta |u_T| \left| \frac{u_N}{|u_T|} \right| & \text{if } |F_T| > |F_N| \tan \theta \\ K_T u_T & \text{otherwise} \end{cases} \]  
(A.15)
where \( \theta \) is the friction angle. For each particle, the total contact forces and contact torques that generated by the forces can be obtained by
\[ F_{\text{total}} = F_N + F_T \]  
\[ F_1 = F_{\text{total}}, \ T_1 = d_1(-n) \times F_{\text{total}} \]  
\[ F_2 = -F_{\text{total}}, \ T_2 = d_2 n \times F_{\text{total}} \]  
(A.16)  
(A.17)  
(A.18)

![FIG. A3: Geometry of normal strain [adapted from Šmilauer and Chareyre (2010)]](image)