

# <sup>1</sup> PeriDEM – High-fidelity modeling of granular media consisting of deformable complex-shaped particles

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## Software

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## **Summary**

<sup>10</sup> Accurate simulation of granular materials under extreme mechanical conditions, such as crushing,  
<sup>11</sup> fracture, and large deformation, remains a significant challenge in geotechnical, manufacturing,  
<sup>12</sup> and mining applications. Classical discrete element method (DEM) models typically treat  
<sup>13</sup> particles as rigid or nearly rigid bodies, limiting their ability to capture internal deformation and  
<sup>14</sup> fracture. The PeriDEM library, first introduced in ([Jha et al., 2021](#)), addresses this limitation  
<sup>15</sup> by modeling particles as deformable solids using peridynamics, a nonlocal continuum theory  
that naturally accommodates fracture and significant deformation. Inter-particle contact is  
handled using DEM-inspired local laws, enabling realistic interaction between complex-shaped  
particles.

<sup>16</sup> Implemented in C++, PeriDEM is designed for extensibility and ease of deployment. It relies on  
a minimal set of external libraries, supports multithreaded execution, and includes demonstration  
examples involving compaction, fracture, and rotational dynamics. The framework facilitates  
granular-scale simulations, supports the development of constitutive models, and serves as a  
foundation for multi-fidelity coupling in real-world applications.

## **Statement of Need**

<sup>21</sup> Granular materials play a central role in many engineered systems, but modeling their behavior  
under high loading, deformation, and fragmentation remains an open problem. Popular open-  
source DEM codes such as YADE ([Smilauer et al., 2021](#)), BlazeDEM ([Govender et al., 2016](#)),  
Chrono DEM-Engine ([Zhang et al., 2024](#)), and LAMMPS ([Thompson et al., 2022](#)) are widely  
used but typically treat particles as rigid, limiting their accuracy in scenarios involving internal  
deformation and breakage. A recent review by Dosta et al. ([Dosta et al., 2024](#)) compares  
several DEM libraries. Meanwhile, peridynamics-based codes such as Peridigm ([Littlewood et  
al., 2024](#)) and NLMech ([Jha & Diehl, 2021](#)) are designed to simulate deformation and fracture  
within a single structure, with limited support for multi-structure simulations.

<sup>31</sup> PeriDEM fills this gap by integrating state-based peridynamics for intra-particle deformation with  
DEM-style contact laws for particle interactions. This hybrid approach enables direct simulation  
of particle fragmentation, stress redistribution, and dynamic failure propagation—capabilities  
essential for modeling granular compaction, attrition, and crushing.

<sup>35</sup> Recent multiscale approaches, including DEM-continuum and DEM-level-set coupling methods  
([Harmon et al., 2021](#)), aim to bridge scales but often rely on homogenization assumptions. Sand  
crushing in geotechnical systems, for example, has been modeled using micro-CT-informed FEM  
or phenomenological laws ([Chen et al., 2023](#)). PeriDEM offers a particle-resolved alternative  
that allows bottom-up investigation of granular failure and shape evolution, especially in  
systems where fragment dynamics are critical.

## 41 Background

42 The PeriDEM model was introduced in (Jha et al., 2021), demonstrating its ability to model  
43 inter-particle contact and intra-particle fracture for complex-shaped particles. It is briefly  
44 described next.

### 45 Brief Introduction to PeriDEM Model

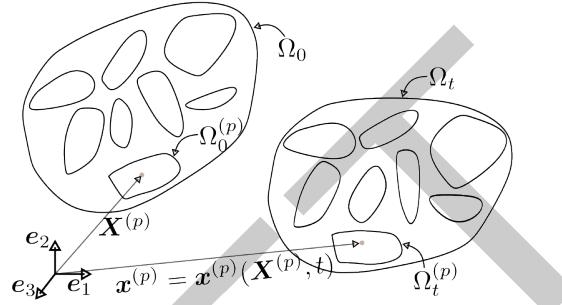


Figure 1: Motion of particle system.

46 Consider a fixed frame of reference and  $\{e_i\}_{i=1}^d$  are orthonormal bases. Consider a collection  
47 of  $N_P$  particles  $\Omega_0^{(p)}$ ,  $1 \leq p \leq N_P$ , where  $\Omega_0^{(p)} \subset \mathbb{R}^d$  with  $d = 2, 3$  represents the initial  
48 configuration of particle  $p$ . Suppose  $\Omega_0 \supset \cup_{p=1}^{N_P} \Omega_0^{(p)}$  is the domain containing all particles; see  
49 Figure 1. The particles in  $\Omega_0$  are dynamically evolving due to external boundary conditions and  
50 internal interactions; let  $\Omega_t^{(p)}$  denote the configuration of particle  $p$  at time  $t \in (0, t_F]$ , and  
51  $\Omega_t \supset \cup_{p=1}^{N_P} \Omega_t^{(p)}$  domain containing all particles at that time. The motion  $x^{(p)} = x^{(p)}(\mathbf{X}^{(p)}, t)$   
52 takes point  $\mathbf{X}^{(p)} \in \Omega_0^{(p)}$  to  $x^{(p)} \in \Omega_t^{(p)}$ , and collectively, the motion is given by  $x = x(\mathbf{X}, t) \in$   
53  $\Omega_t$  for  $\mathbf{X} \in \Omega_0$ . We assume the media is dry and not influenced by factors other than  
54 mechanical loading (e.g., moisture and temperature are not considered). The configuration of  
55 particles in  $\Omega_t$  at time  $t$  depends on various factors, such as material and geometrical properties,  
56 contact mechanism, and external loading. Essentially, there are two types of interactions  
57 present in the media:

- 58     ▪ *Intra-particle interaction* that models the deformation and internal forces in the particle  
59       and
- 60     ▪ *Inter-particle interaction* that accounts for the contact between particles and the boundary  
61       of the domain in which the particles are contained.

62 In DEM, the first interaction is ignored, assuming that particle deformation is insignificant  
63 compared to inter-particle interactions. On the other hand, PeriDEM accounts for both  
64 interactions.

65 The balance of linear momentum for particle  $p$ ,  $1 \leq p \leq N_P$ , takes the form:

$$\rho^{(p)} \ddot{\mathbf{u}}^{(p)}(\mathbf{X}, t) = \mathbf{f}_{int}^{(p)}(\mathbf{X}, t) + \mathbf{f}_{ext}^{(p)}(\mathbf{X}, t), \quad \forall (\mathbf{X}, t) \in \Omega_0^{(p)} \times (0, t_F), \quad (1)$$

66 where  $\rho^{(p)}$ ,  $\mathbf{f}_{int}^{(p)}$ , and  $\mathbf{f}_{ext}^{(p)}$  are density, and internal and external force densities. The  
67 above equation is complemented with initial conditions,  $\mathbf{u}^{(p)}(\mathbf{X}, 0) = \mathbf{u}_0^{(p)}(\mathbf{X})$ ,  $\dot{\mathbf{u}}^{(p)}(\mathbf{X}, 0) =$   
68  $\dot{\mathbf{u}}_0^{(p)}(\mathbf{X})$ ,  $\mathbf{X} \in \Omega_0^{(p)}$ .

69    **Internal force - State-based peridynamics**

70    The internal force term  $f_{int}^{(p)}(\mathbf{X}, t)$  in the momentum balance governs intra-particle deformation  
71    and fracture. In PeriDEM, this term is modeled using a simplified state-based peridynamics for-  
72    mulation that accounts for nonlocal interactions over a finite horizon. The specific constitutive  
73    structure used—including damage-driven bond weakening, volumetric strain contributions, and  
74    neighbor-weighted quadrature—is discussed in detail in (Jha et al., 2021, sec. 2.1 and 2.3).  
75    This formulation allows unified simulation of deformation and fracture in individual particles.

76    **DEM-inspired contact forces**

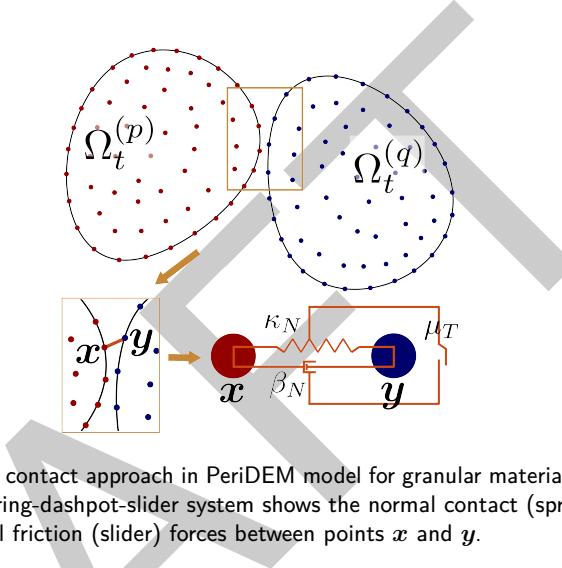


Figure 2: High-resolution contact approach in PeriDEM model for granular materials? between arbitrarily-shaped particles. The spring-dashpot-slider system shows the normal contact (spring), normal damping (dashpot), and tangential friction (slider) forces between points  $x$  and  $y$ .

77    The external force term  $f_{ext}^{(p)}(\mathbf{X}, t)$  includes body forces, wall-particle interactions, and contact  
78    forces from other particles. Contact is modeled using a spring-dashpot-slider formulation applied  
79    locally when particles come within a critical distance. This approach introduces nonlinear normal  
80    forces, damping, and friction without relying on particle convexity or simplified geometries.  
81    Figure 2 illustrates the local high-resolution contact approach between deformable particles.  
82    The full formulation of contact detection, force assembly, and its implementation is provided  
83    in (Jha et al., 2021, sec. 2.2).

84    **Implementation**

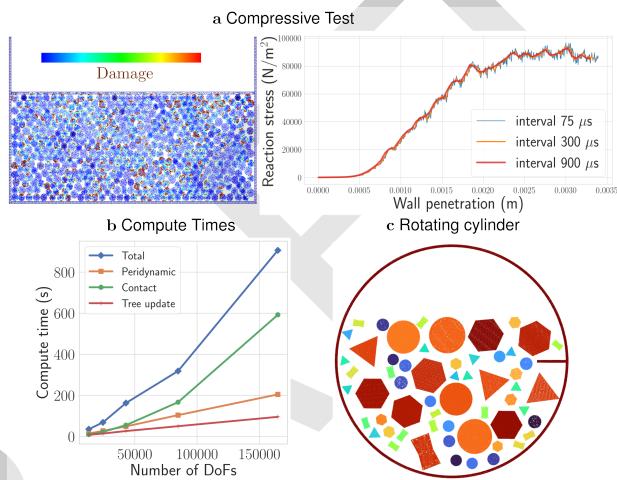
85    PeriDEM is implemented in C++ and hosted on GitHub. It depends on a minimal set of  
86    external libraries, most of which are bundled in the external directory. Some of the key  
87    dependencies include Taskflow (Huang et al., 2021) for multithreaded parallelism, nanoflann  
88    (Blanco & Rai, 2014) for efficient neighborhood search, and VTK for output and post-processing.  
89    The numerical strategies for neighbor search, peridynamic integration, damage evaluation,  
90    and time stepping follow those introduced in (Jha et al., 2021, sec. 3), where additional  
91    implementation details and validation are discussed. The core simulation model is implemented  
92    in `src/model/dem`, with the class `DEMModel` managing particle states, force calculations, and  
93    time integration.

94    This work builds on earlier research in the analysis and numerical methods for peridynamics;  
95    see (Jha & Lipton, 2018a, 2018b, 2019; Jha & Lipton, 2020; Lipton et al., 2019).

## 96 Features

- 97     ▪ Combines peridynamics and DEM to model intra-particle deformation and inter-particle
- 98         contact
- 99
- 100     ▪ Simulates deformation and breakage of single particles under complex loading conditions
- 101
- 102     ▪ Supports arbitrarily shaped particles for realistic granular systems
- 103
- 104     ▪ Ongoing development of MPI-based parallelism and adaptive modeling strategies to
- 105         improve efficiency without sacrificing accuracy

## 106 Examples



**Figure 3:** (a) Nonlinear response under compression, (b) exponential growth of compute time due to nonlocality of internal and contact forces, and (c) rotating cylinder with nonspherical particles.

107 Examples are described in [examples/README.md](#). One key case demonstrates compression  
 108 of 500+ circular and hexagonal particles in a rectangular container by moving the top wall.  
 109 The stress on the wall as a function of penetration becomes increasingly nonlinear as damage  
 110 accumulates and the medium yields; see [Figure 3a](#). Preliminary performance tests show an  
 111 exponential increase in compute time with the number of particles, due to the nonlocal nature of  
 112 both peridynamic and contact forces, highlighting a computational bottleneck. This motivates  
 113 the integration of MPI and the development of a multi-fidelity framework. Additional examples  
 114 include attrition of non-circular particles in a rotating cylinder ([Figure 3c](#)).

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 118 the continued development and enhancement of the PeriDEM library.

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