

Massively parallel stress chain characterization for billion particle DEM simulation of accretionary prism formation

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ABSTRACT

Herein, a novel algorithm for characterizing stress chains using a large parallel computer system is presented. Stress chains are important for analyzing the results of large-scale discrete element method (DEM) simulations. However, the general algorithm is difficult to parallelize especially when selecting networks longer than several particles. Therefore, we propose a new parallel algorithm to count the number of particles that are tightly connected, based on iterative operations with nearest-neighbor computations and communications. The new algorithm is examined via a real-scale numerical sandbox experiment using 2.4 billion particles. We successfully compute the stress chains with a reasonable computational cost comparable to the single-step DEM computation time. The visualization of the stress chains from the large-scale DEM simulation result reveals the existence of arcuate stress structures that may control accretionary prism formation, which is an important scientific discovery.

KEYWORDS

Parallel algorithm, Stress chain, Scientific visualization, Discrete Element Method, Dynamic load-balancing, Accretionary prism

1 INTRODUCTION

Discrete element method (DEM) simulations have begun to handle simulation sizes of over a billion particles due to the development of parallelization techniques for shared and distributed-memory systems [1, 2, 3]. For example, in our previous work, we performed a real-scale sandbox experiment using 2.4 billion particles as a scaled analog model of accretionary prism formation [1]. Large-scale DEM simulations generate huge amounts of data to reproduce such complex granular phenomena. A stress chain analysis is a powerful tool to record scientific discoveries from such a dataset. Stress chains are one of the most prominent features of granular dynamics as they control the majority of the load applied to the system and probe the non-continuum features of granular materials. Because stress chains are constructed using only particles that form a strong network of contact forces, we can significantly reduce the number of particles

that must be analyzed. Therefore, identifying stress chains is critical for extracting the catachrestic features of complex 3D granular dynamics from huge DEM simulation datasets. Several approaches have been proposed to quantify stress chains [4]; however, such approaches are difficult to parallelize. Therefore, we propose a new algorithm suitable for parallel computing to characterize the stress chains during simulation and to applying them to a real-scale numerical sandbox simulation.

2 Parallel algorithm for characterising stress chains from a DEM simulation result

Our algorithm to quantitatively identify stress chains is based on the method proposed by Peter et. al. [4]. We first calculate the most compressive principal stress vector (σ_3) for all DEM particles from the stress tensor defined by,

$$\sigma_{IJ} = \frac{1}{V} \sum_{c=1}^{m_c} f_I^c r_J^c \quad (1)$$

where $1 < c < m_c$ denotes all particle pairs in contact with each other, V is the volume of a particle, f_I is the I -th component (in xyz -direction) of the force between two contacting particles, and r_J is the J -th component of the radius vector from the center of a particle to its point of contact with its paired particle. The particles that have $|\sigma_3^i|$ less than the average are filtered out to isolate the strong network. In addition, we select only those groups of contact particles that are in a co-linear arrangement defined by the stress vectors (i.e. σ_3^i and σ_3^j) aligned within a 45° angle. Identifying the group of candidate particles $i \in \Omega_c$ to form stress chains via above procedures in parallel using the particle number as a loop counter is a straightforward process.

Finally, we count the length of the particle connection of $i \in \Omega_c$ to identify the stress chains that are longer than a given number of particles, which is four in our case. We developed the algorithm to parallelize this process in an iterative manner with a counter n . A length number L_i is introduced for each candidate particle $i \in \Omega_c$. These length numbers are updated using the sum of the maximum L_{c1} and the second maximum length number L_{c2} of the adjacent particles, where $c \in N_i$ and N_i denotes the group of particles connected to the i -th particle. Because the length number at the edge of the chain $L_{i,ed}$ shows the integration of the connecting particles, the length of the chain can be obtained with certain magic

numbers $\mathbf{M}$ as shown in Fig. 1. The iterative operations are based on nearest-neighbor communications and can be parallelized using the same shared (OpenMP) and distributed-memory implementations (MPI) as the DEM code. Algorithm 1 summarizes the proposed algorithm.

Algorithm 1

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- Step0. Set the length number $L_i = 1$ for particles $i \in \Omega_C$ and the iterative counter $n = 0$.
- Step1. Update $L_i = L_{c1} + L_{c2}$
where $L_{c1} = \max\{L_c: c \in N_i\}$ and $L_{c2} = \max\{L_c: c \in N_i \setminus c1\}$
($L_{c2} = 0$ when $N_i \setminus c1 = \emptyset$).
- Step2. If $L_{i,ed} < M(n)$, then the length of the chain is the iteration counter n .
- Step3. Update the counter with $n = n + 1$ and return to Step 1.
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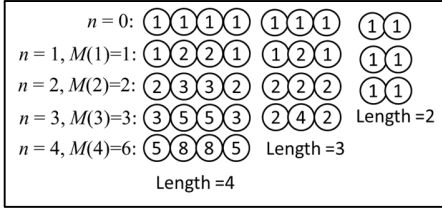


Fig 1: Example of the n -th iterative operation to count the length and criteria number $M(n)$ until $n = 4$.

3 Results

We implemented the parallel stress chain algorithm in a parallelized DEM code with a dynamic load balancer available for various supercomputer systems, including those with heterogeneous architectures [1, 3, 5]. Our geoscientific target is a real-scale sandbox simulation that used 2.4 billion particles to handle 100- μm sized particles in a $1 \times 1 \times 0.02$ m domain using 4096 nodes (32,768 cores) of the K computer (Fig. 2). Sandbox experiments have been extensively studied to investigate accretionary prisms, which generate large earthquakes such as those occurring in the Nankai Trough. Using our new algorithm, the stress chains in the sand layer are successfully characterized as shown in Fig. 3. The cost of the stress chain calculations was comparable to five computation time steps of the DEM kernel and was negligibly small compared to the total elapsed time when performed every ten thousand steps.

The 3D stress structures in such sandbox experiments have not been directly measured due to technological limitations. Therefore, this is the first visualization result of the stress chains in the billions of particles inside a sandbox and illustrates important scientific findings [1]. For example, despite the nearly uniform initial conditions, macroscale fault undulations similar to those observed in accretionary prism trenches appeared. Our stress chain analysis revealed that the formation of stress arches (i.e., pairs of red and blue chains in Fig. 3) causes these undulations. Similar multiscale behavior is expected to generate complex 3D stress states inside accretionary prisms without geological-scale perturbations.

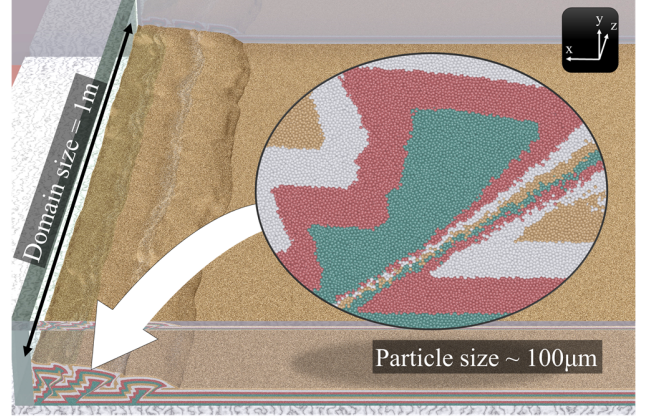


Figure 2: Snapshot of the sandbox simulation using 4096 nodes on the K computer.

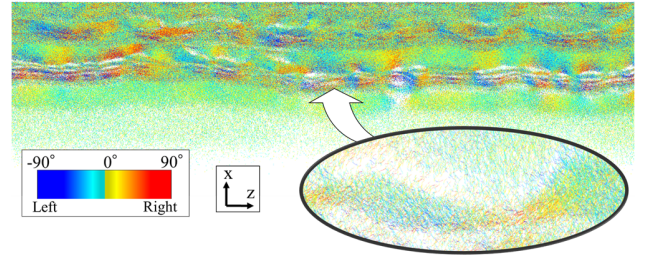


Figure 3: A Map view of the stress chains in a thin layer of Fig. 2. The σ_3 of the stress chains are visualized by the colored lines. The color shows the angle of the vector in the horizontal plane. Complex lateral stress structure spontaneously occurs in the granular deformations.

4 Conclusion

We developed a parallel algorithm to perform a stress chain analysis. In principle, without our technique, it is possible to compute the stress chains in post processing on a single node. However, this computation is impossible in practice owing to the huge size of the output data and the large amount of computational time required. Our iterative algorithm successfully visualizes the stress chain during in-situ processing using 4096 nodes. The stress chain inside a sand layer comprising billions of particles helps reveal the hidden mechanisms in accretionary prisms.

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