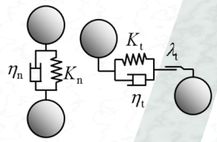
Massively parallel stress chain characterization for billion particle DEM simulation of accretionary prism formation

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1. Introduction

- The Discrete Element Method (DEM) simulation begins to handle over billion particles to reproduce a laboratory experiment as it is.
- To analyze the complex granular phenomena from the huge simulation data, stress chain analysis is a powerful approach.
- Calculation of the stress chain should be performed using HPC to analyze the billion particles with a practical time and storage system.
- We develop a new algorithm to parallelize the stress chain characterization to perform the stress chain analysis during a course of simulation.



$$\ddot{\boldsymbol{x}}_i = \sum_j (\boldsymbol{F}_{c_n} + \boldsymbol{F}_{c_t})_{ij} + \boldsymbol{g}, \quad \dot{\boldsymbol{\omega}}_i = \sum_j \boldsymbol{M}_{ij} / I_i$$

$$\boldsymbol{Fc}_{\mathrm{n}} = \eta_{\mathrm{n}} \boldsymbol{v}_{\mathrm{n}} + K_{\mathrm{n}} \boldsymbol{x}_{\mathrm{n}}$$

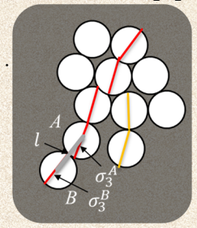
$$\boldsymbol{Fc}_{\mathrm{t}} = \min\left[\eta_{\mathrm{t}} \boldsymbol{v}_{\mathrm{t}} + K_{\mathrm{t}} \boldsymbol{x}_{\mathrm{t}}, \lambda_{\mathrm{t}} \left|\boldsymbol{Fc}_{\mathrm{n}}\right| \boldsymbol{v}_{\mathrm{t}} / \left|\boldsymbol{v}_{\mathrm{t}}\right|\right]$$

2. Real-scale sandbox simulation

- We developed the DEM code utilizing an iterative load-balancer, efficient implementation of action-reaction law and overlapping communication with space filling curve [3].
- One of the our geoscience targets is a real-size-scale sandbox simulation that used 2.4B particles at most to handle 100 μm particle size in the 1 m × 1 m × 0.02 m domain size using 4096 nodes of K computer (e.g. background image and Fig. 2).
- This is the world largest scale DEM simulation result.
- The simulation of the horizontal shortening of the granular layer shows characteristic structures of accretionary prisms such as thrusts and decollements.
- Probing the stress state with a stress chain is important to understand the mechanism behind the formation of accretionary prism which generates great earthquakes.

3. Parallel algorithm of charactering stress chain

We apply the procedure proposed by Peters et.al. *Phys rev E* 2005 [4]



i) First, calculate the most compressive principal stress vector ($\boldsymbol{\sigma}_3$) from the second rank stress tensor defined by,

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

ii) Filter out the particles with $|\boldsymbol{\sigma}_3| < average$ and create the group of contact particles $\Omega_{\mathbb{C}}$ which satisfies

$$\cos\left(\frac{\pi}{4}\right) < \frac{|l\sigma_1^A|}{|l||\sigma_1^A|} \leq 1 \quad \text{and} \quad \cos\left(\frac{\pi}{4}\right) < \frac{|l\sigma_1^B|}{|l||\sigma_1^B|} \leq 1$$

$\boldsymbol{x}$: Particle position, $\boldsymbol{f}$: Contact force, c: Index of contact particle pair, $\mathbf{r}$: Vector from the center to contact, V: Volume of particle, $\boldsymbol{l} : \boldsymbol{x_A} - \boldsymbol{x_B}$.

iii) Identify the stress chains longer than a given number of particles which is four in our case.

Parallel algorithm is needed.

To count the length of particle connections in $\Omega_{\mathbb{C}}$ by parallel computing, we develop the iterative method: Algorithm 1. In this method, the length number L_i is iteratively updated by the sum of maximum L_{c1} and second maximum L_{c2} of the adjacent particles. The length of the chain can be found by the number at the edge of chain L_{i_ed} which is an integration of connecting n-th particles, as shown in Fig. 1.

Algorithm 1	
Step0.	Set the length number $L_i = 1$ for particles i ∈ $\Omega_{\mathbb{C}}$ and the iterative counter n = 0.
Step1.	Update $L_i = L_{c1} + L_{c2}$ where $L_{c1} = max\{L_c : c \in \boldsymbol{N}_i\}$ and $L_{c2} = max\{L_c : c \in \boldsymbol{N}_i \setminus c1\}$ ($L_{c2} = 0$ when $\boldsymbol{N}_i \setminus c1 = \emptyset$).
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.

Need only nearest neighbor particle interaction

Same shared and distributed-memory parallel implementation as DEM modules

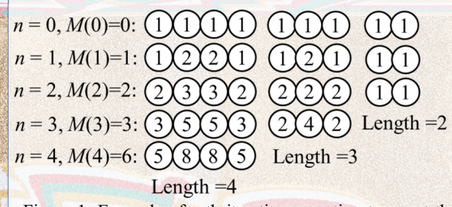


Figure 1: Example of n-th iterative operation to count the length and criteria number $M(n)$ until $n = 4$.

4. Result

- Result of real-scale sandbox experiment

Check the movie.

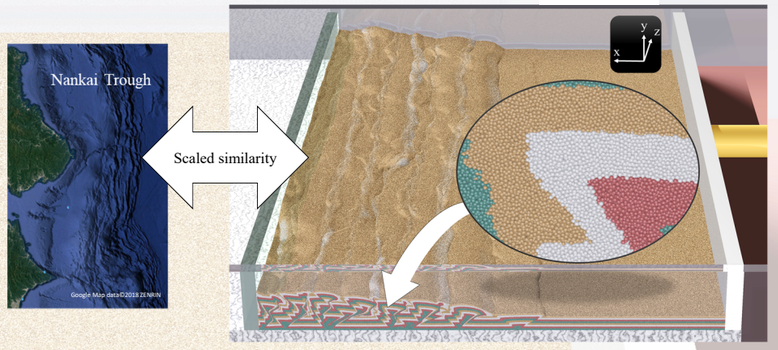


Figure 2: Snapshot of the simulation result

- The stress chain in real-scale sandbox experiment

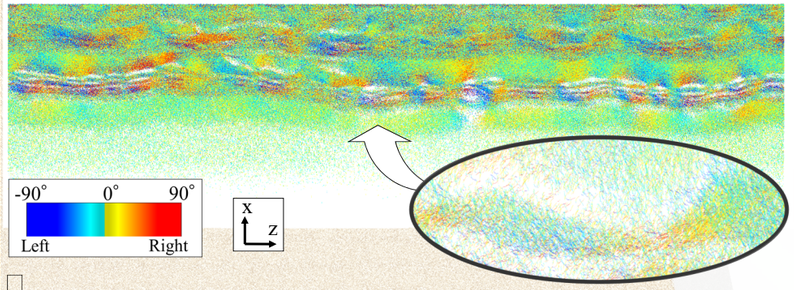


Figure 3: The Map view of stress chain in the thin layer of Fig. 2. The $\boldsymbol{\sigma}_3$ in the stress chains are visualized by the colored lines. The color shows the angle of the vector in the horizontal plane.

Stress chain analysis contributes to the scientific findings from large-scale DEM simulation: The existence of arcuate stress structures that control the formation of deformation structures in sand and possibly in accretionary prisms. [Furuichi et.al. *Scientific Reports* (2018)].

5. Conclusion

- We propose parallel algorithm for the stress chain analysis.
- The cost of the stress chain calculations was negligibly small compared to the total elapsed time when performed every ten thousand steps.
- Our iterative algorithm successfully visualizes the stress chain inside the sand layer consisting of billion particles which reveals the hidden mechanism in the accretionary prisms.

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