Generation of Samples of Granular Material using Diffusion Models

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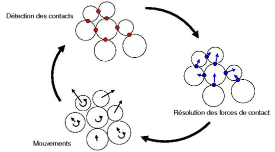
Granular Media and Discrete Element Methods

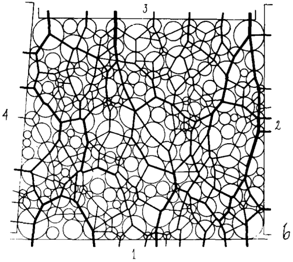
Collection of Contacting Bodies

- Granular media are collections of discrete particles
- Examples: sand, rocks, ballast
- Exhibits complex dynamics (e.g. friction, energy dissipation etc.)



One time step in DEM simulation in LMGC90[a]

[a] Frédéric Dubois and Rémy Mozul 2013.



A Force Chain Network Simulation[a]

[a] Cundall and Strack 1979.

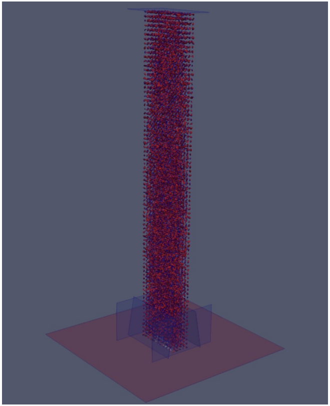
Simulation Tool

- Discrete Element Method (DEM)[a] is the standard tool for granular media simulations
- DEM simulations represent dynamnic behaviors as a time-stepping algorithm, where force-displacement relationships are defined alternatively.

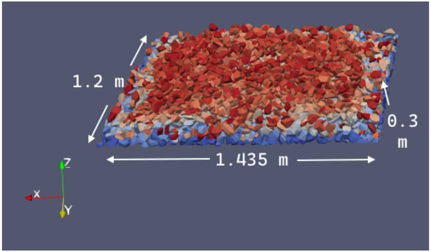
[a] Cundall and Strack 1979.

Another Challenge

Sample Setup phase is a bottleneck



Ballast Deposition in LMGC90[a]



Compressed ballast samples

- Tradition DEM requires manual setup of sample
- Limits the feasibility of extensive studies on longer samples
- Train track not long enough to capture long term effects
- Minimum time step controlled by: detection of contacts, velocities, etc.

[a] Frédéric Dubois and Rémy Mozul 2013.

Example: 3-5 hours per ballast sample of 5000 grains (around $10000/m^3$)

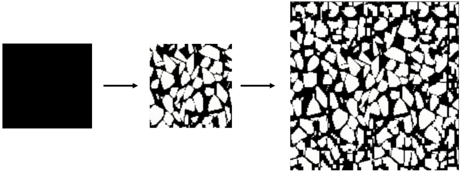
Objective

Need for Speed

Develop a faster method for generation of DEM samples that are already setup as required

Goals:

- Utilize a Generative Model to create DEM samples.
- Ensure the samples are representative of realistic media.
- Ultimately, cut down hours to fractions for sample preparation.



Creation of small patches and stitching them together

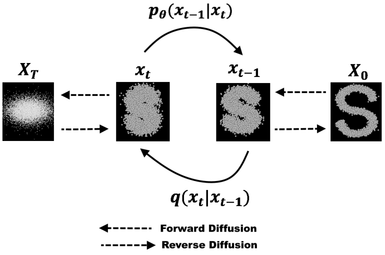
Use smaller, existing databases of small DEM samples to learn to generate larger samples.

Models of Choice: Diffusion Models

Definition

Diffusion models[a] are a class of generative models that iteratively transform noise into structured data by learning the reverse of a diffusion (noise-adding) process.

[a] Ho, Jain, and Abbeel 2020.



Process of noising and denoising[a]

[a] PhD 2022.

Main Equations

$$q(x_t|x_{t-1}) = \mathcal{N}\left(x_t; \sqrt{1-\beta_t}\, x_{t-1}, \beta_t \mathbf{I}\right)$$

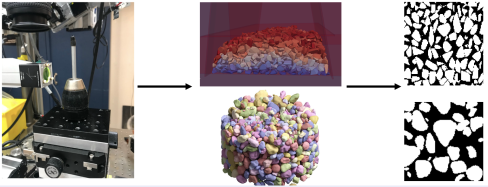
$$x_{t-1} = \frac{1}{\sqrt{\alpha_t}}\left(x_t - \frac{1-\alpha_t}{\sqrt{1-\bar{\alpha}_t}}\epsilon_\theta(x_t, t)\right) + \sigma_t z$$

Where $\alpha_t = 1 - \beta_t$, $\bar{\alpha}_t = \prod_{s=1}^{t} \alpha_s$, ϵ_θ is the neural network parameterizing the model, and $z \sim \mathcal{N}(0, \mathbf{I})$.

Step 1: Learning to create new patches

Input Data

- 10k 2D patches of 128x128 with some grains (ballast: 0.3 m length),
- Conditional information: B/W ratio, edges, number of grains, shape information.

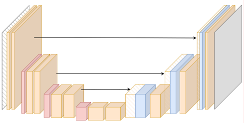


Extraction of input: 1. Tomography, 2. Digitalization, 3. Slicing (credits:[a])

[a] Vlassis et al. 2024.

Model

Noise Estimator ϵ_θ : UNet from Diffusers[a]



[a] von Platen et al. 2022; O'Sullivan 2023.

Output

- New samples with required properties
- Preserved statistics

Outputs can have different properties

Step 2: Longer samples

Idea

Stitch together smaller patches with similar statistical properties to form longer samples.

Challenges:

1. Consistency in stitching
2. Memory constraints
3. Generation time

Possibilities:

1. Training a new conditional model
2. Using a pretrained model

Stable Diffusion Inpainting[a]

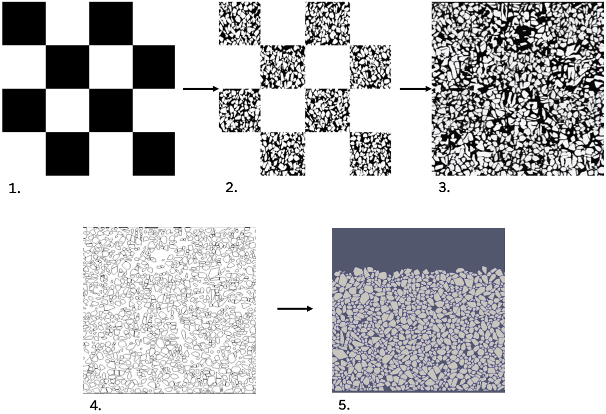
[a] *Diffusers/Stable-Diffusion-Xl-1.0-Inpainting-0.1 · Hugging Face* 2023.

Chosen Method

Stable Diffusion[a] Inpainting models are fast, cheap and most of the time, can also be fine tuned if required.

[a] Podell et al. 2023.

Step 2: Longer samples: Method

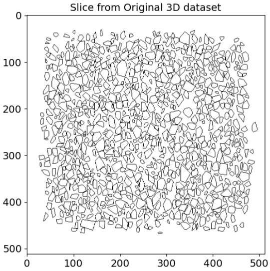


Steps in generation: 1. Create an empty canvas, 2. Partially Fill with Patches, 3. Inpaint the rest 4. Segmentation 5. DEM input and simulation

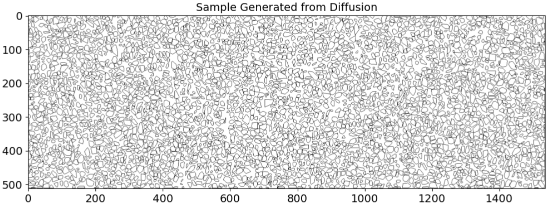
Generation in batches

- 1 second for generation of a 1536x512 pixel grid, batched generation. Stiching all the grids takes 1 second.
- Took 5 seconds to generate 80 m long 2d track (18000 grains).

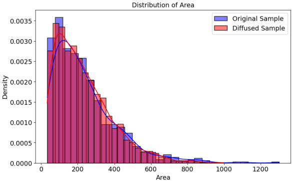
Step 2: Longer samples: Statistics



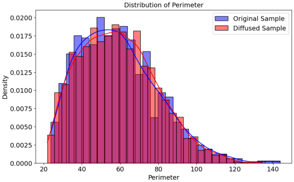
(a) 1. Original 3D Data



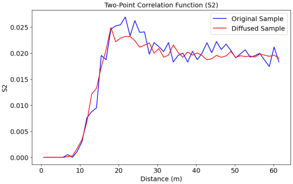
(b) 2. Generated Sample



(a) Dist. of Area



(b) Dist. of Permimeter

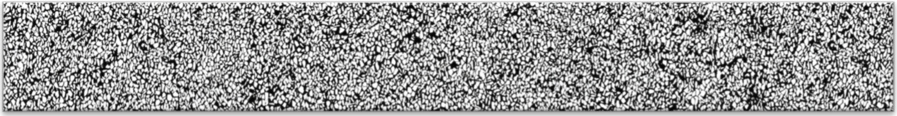


(c) Two Point Correlation

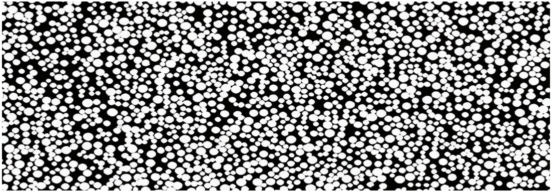
Applications

The diffusion model can be fine tuned to generate samples from different databases.

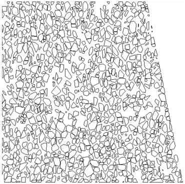
Stable Diffusion was able to generate all tested samples (packed beads, sand stacks, ballast particles).



Large Sample of Ballast



Bead Samples



Generation with a Boundary

Long Sample Simulation

Closeup Simulation

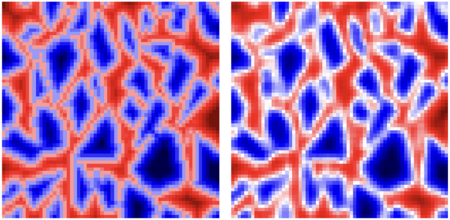
Towards 3D

Method:

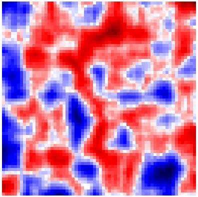
- Instead of binary, input data is **signed distance function** (zero-level set gives boundaries).
- Autoencoder to encode 3D to 2D latents (attention, convolutions, position encoding)
- Generate new latent space samples using diffusion and decode into 3D samples.

To do:

- See if the issues remain in encoded space.
- Diffusion and inpainting on 2D latents.



Middle slice of a 3D voxel: Left: original, Right: Reconstructed



Decoded middle slice of a voxel grid decoded from generated 2D latents

Conclusion

Key Achievements

- Accelerated DEM simulations using diffusion models.
- Preserved essential statistical properties in generated samples.
- Laid groundwork for extention to 3D.

Future Directions

- Develop efficient 3D DEM sample generation.
- Enhance model accuracy and versatility.

Impact: Enables faster and scalable sample setup in DEM simulations.

Thank you for your attention!

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