MCMC Algorithm to Predict Ice Formation in Arctic Soils

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Introduction

- This research is motivated by thawing permafrost in Arctic Soils.
- Our goal is to generate sample geometries of ice formation in waterlogged soil using a reduced order model.

Methods

Potts Model

We build off of Peszynska et al. (2021) and represent a 2D soil slice as a lattice of values with periodic boundary conditions. Wherein:

$$x_{\langle i,j \rangle} = \begin{cases} 1 = \blacksquare = rock, \\ 2 = \blacksquare = water, \\ 3 = \square = ice, \\ 5 = \blacksquare = air \end{cases} \tag{1}$$

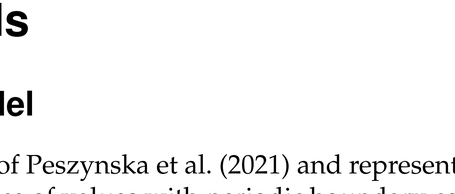
The "energy" of the particle interactions of the model can be described by the Hamiltonian:

$$E(x) = -\frac{1}{2} \sum_{i \in \Lambda} \sum_{j \in \mathcal{N}_i} w(x_i x_j) \tag{2}$$

Where $w(x_{\langle i,j \rangle}, x_{\langle r,s \rangle})$ sets tunable weights to describe the interaction strength between two particles.

Metropolis Algorithm

We use the Metropolis algorithm described in Shonkwiler and Mendivil (2009) to generate sample geometries from a random initial state.



(a) Initial State **(b)** End State

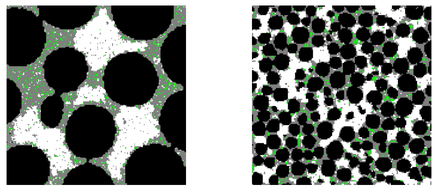
Figure 1: 50×50 single pore model before and after the Metropolis algorithm.

Results

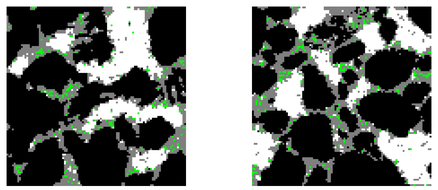
From this, we generate realistic configurations from several pore scale samples.

■■ $= 0$, ■■ $= 0$, □□ $= 0$; ■■ $= .5$, ■■ $= 0$,
■□ $= -1$, ■■ $= -1$, ■□ $= -1$, ■■ $= 0$, □■ $= -1$

Figure 2: Interaction weights $w(x_{\langle i,j \rangle}, x_{\langle r,s \rangle})$ for the models below.



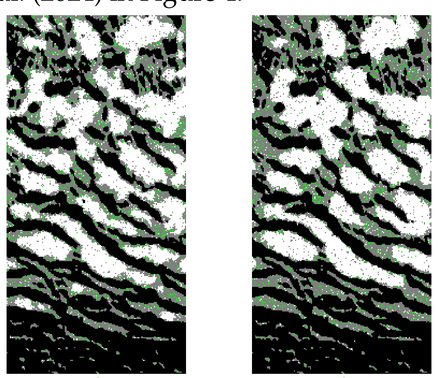
(a) Glass beads **(b)** Proppant



(c) Sandstone **(d)** Loose sand

Figure 3: Simulations on data from Peszynska et al. (2021).

We use data from Calmels et al. (2010) and post processed by Peszynska et al. (2024) in Figure 4.



(a) 10^8 trials **(b)** 10^9 trials

Figure 4: Simulations of thawing permafrost with different simulation lengths.

Reliability

In order to confirm results, models are repeated with different initial RNG seeds.

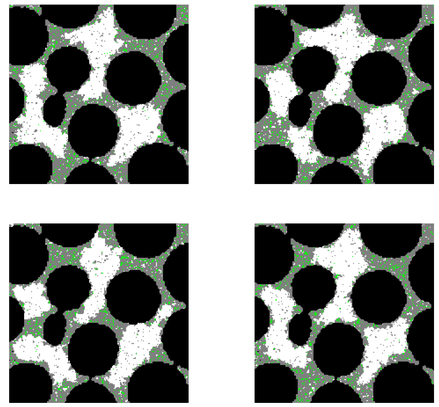


Figure 5: Multiple simulations of glass beads.

See the **QR code** to the top right for animations of the model.

Further Study

- Expanding the model to 3D simulations
- Using Machine Learning to automatically tune weights
- Fluid simulations utilizing the generated geometry

References

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