Entropy Measures for the Micro-topology of Dense Granular Flow

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1 Problem Summary

- Regime of behavior: Dense granular flow of 2-dimensional material (i.e., "steady-state" or "critical state" flow)
- Phenomena of interest: Probability distributions of the local void topology (void cell valence) and particle topology (coordination number)
- Hypothesis: these probability distributions can be estimated by applying a maximum entropy principle.

2 Background

Dense granular flow at the "critical state"

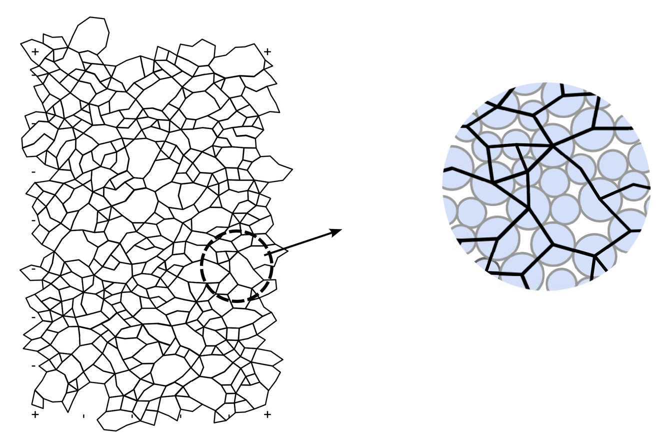
- Characterized by constant bulk characteristics: constant volume, constant mean stress, constant shear stress, constant fabric anisotropy, etc.
- Yet, at the micro-scale, change is rapid and pervasive.
- Our focus is on the continually changing contact topology.

Topology of two-dimensional flow

Bulk measures of topology:

$$\text{Mean coordination no.} = \overline{n} \quad \text{Mean void valence} = \overline{l}$$

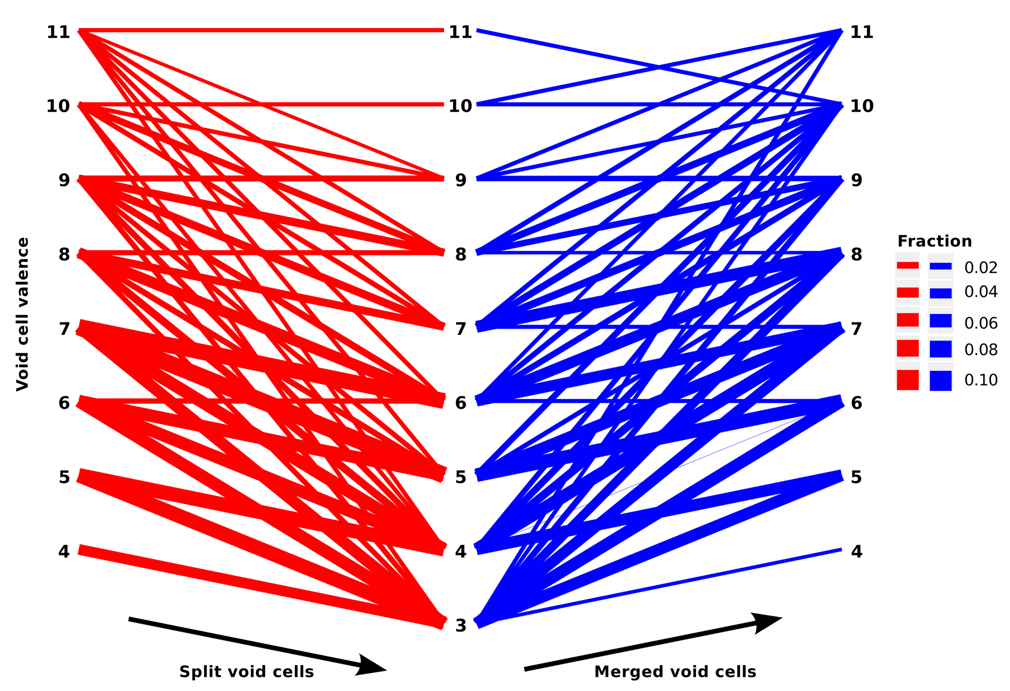
The particle graph is a planar graph that represents the contacts (edges), particles (vertices), voids (faces, polygons).



The particle graph continually changes:

- New contacts "split" existing polygons
- Lost contacts "merge" existing polygons

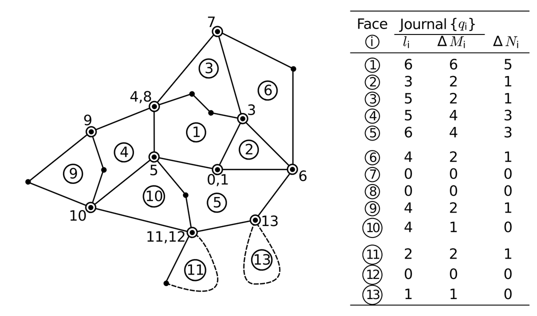
These changes of topology will completely alter the particle graph during small increments of deformation.



3 Solution

- Objective: theory-based probability distributions of the void valences and coordination numbers
- Premise: topology is maximally disordered during granular flow
- Step 1: Categorize the individual void polygons (i.e., develop a taxonomy of void type).

  Any planar graph can be constructed from a "journal" of pairs $(l_i, \Delta M_i)$:



  Each pair describes an additional void that is appended to the previous planar graph:

$$l_i = \text{valence of the appended polygon}$$
$$\Delta M_i = \text{no. of added edges to create the polygon}$$

- Step 2: Discrete probability distribution by type:

$$\text{Probability} \quad P_{l,\Delta M} \quad \Rightarrow \quad \sum_{l=3}^{\infty} \sum_{\Delta M}^{l-1} P_{l,\Delta M} = 1$$

- Step 3: Constraints due to the average coordination number, average valence, and Euler's equation:

$$\langle \Delta M \rangle \equiv \sum_{l=3}^{\infty} \sum_{\Delta M}^{l-1} \Delta M \, P_{l,\Delta M} = \frac{\overline{n}}{\overline{n}-2}$$
$$\langle l \rangle \equiv \sum_{l=3}^{\infty} \sum_{\Delta M}^{l-1} l \, P_{l,\Delta M} = \frac{2\overline{n}}{\overline{n}-2}$$

- Step 4: Maximize the Shannon entropy, H:

$$H = \sum_{l=3}^{\infty} \sum_{\Delta M}^{l-1} P_{l,\Delta M} \ln\left(P_{l,\Delta M}\right)$$

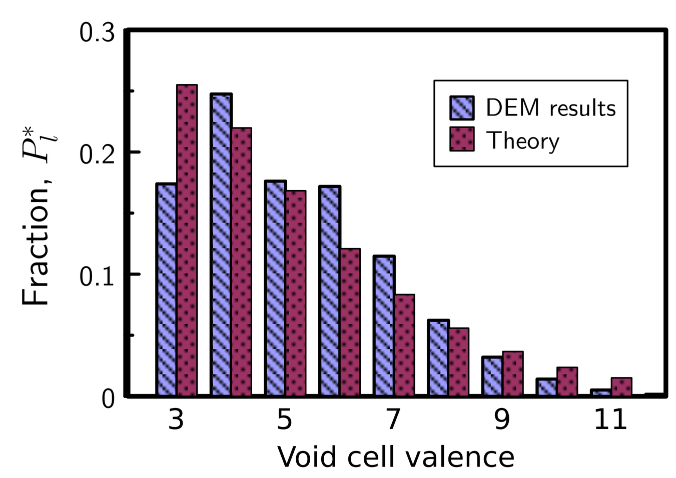
- Step 5: Using the Jaynes formalism, solve to find the void valence probabilities:

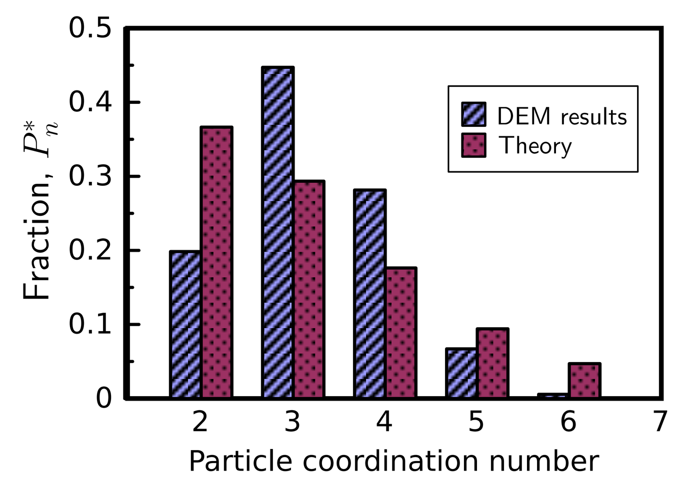
$$P_{l,\Delta M} = \frac{1}{Z\left(\lambda_1, \lambda_2\right)} \exp\left(-\lambda_1 l - \lambda_2 \Delta M\right)$$

  with a partition function $Z(\lambda_1, \lambda_2)$ and Lagrange multipliers λ_1 and λ_2 that satisfy the mean coordination number and void valence.
- Step 6: use the duality principle to derive the corresponding probability distribution of coordination numbers.

4 Verification

Comparison of predicted probability distributions with discrete element (DEM) simulations:





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