Insights from the persistent homology analysis of micro-CT images of porous and granular materials

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Summary: The physical properties of porous and granular materials critically depend on the topological and geometric details of the material micro-structure. This type of information is summarised by a mathematical tool called *persistent homology*. Our work with CT images has demonstrated how persistent homology highlights physically-relevant length scales and provides a summary of important structural features.

1. INTRODUCTION

Topology is the study of those aspects of shape that cannot be changed by a continuous deformation. For 3D objects, this encompasses quantities such as the number of pieces, N, number of independent loops, L, number of cavities, O, and Euler characteristic, $\chi = N - L + O$. Since these topological quantities are insensitive to size, small and large features are counted with the same weight leading to a lack of stability with respect to noise.

Persistent homology is a mathematical theory developed in the late 1990's to overcome this and address the challenge of extracting robust topological information from finite, noisy data. To do so, we must build a nested sequence of objects, ordered by some parameter. For 3D images, the data are scalar values, $f(x)$, at vertices of a regular cubical grid, C, the parameter is a threshold value, h, and the nested objects are the lower level cuts of the image function at increasing values of the threshold:

$$L_f(h) = \{\text{cells } \sigma \text{ in C such that } \; f(x) \leq h \text{ for each } x \text{ a vertex of } \sigma \; \}. \tag{1}$$

As the threshold h increases, we see that topological features such as a loop are born at some parameter value b, and then later become filled in or "die" at a larger value, d. A persistence barcode, or persistence diagram, records these parameter values as a pair (b, d) for each topological feature detected in the image. The persistence of the feature is $d-b$, and so the numbers of components, loops, cavities and Euler characteristic with persistence greater than a chosen amount, p, can be recovered by counting points with $d - b > p$ from the appropriate diagram.

A key result for applications is that persistent homology is *stable* in the sense that if two functions f, g defined on the same cell complex C have $|f(x) - g(x)| < \epsilon$ for all $x \in C$ then points in the persistence diagrams of f and g are also close in a suitable sense [1].

2. EXPERIMENTAL METHOD

To characterise the geometry and topology of two-phase structures imaged using micro-CT data, we begin with a segmented image where voxels are assigned to either "grain", G, or "pore", P. We then compute a *signed Euclidean distance function* (SEDT) $f(x)$ as the distance from a voxel x to the closest point on the interface, I, between grain G and pore P. We assign negative distances to voxels in the pore phase and positive distances to those in the grain phase.

$$f(x) = \begin{cases} -\min_{y \in I} ||x - y||^2 & \text{if } x \in P \\ \min_{y \in I} ||x - y||^2 & \text{if } x \in G \end{cases} \tag{2}$$

We compute persistent homology using an implementation based on discrete Morse theory and outlined in the papers [5]. Our code package, *diamorse*, has been optimised for micro-CT images is available from github.

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A good segmentation remains essential here to obtain an SEDT that accurately reflects the geometry and topology of the two-phase structure. Mis-identified voxels create an error in $f(x)$ that depends on the distance from x to the interface I.

3. RESULTS

We have shown that persistent homology of SEDTs derived from micro-CT images give a clear signature of the onset of crystallisation in bead packs [6], the degree of consolidation in granular materials [2], highlights the percolation threshold [4], and can correlate to physical properties such as fluid permeability and non-wetting phase trapping capacity in sandstones [3].

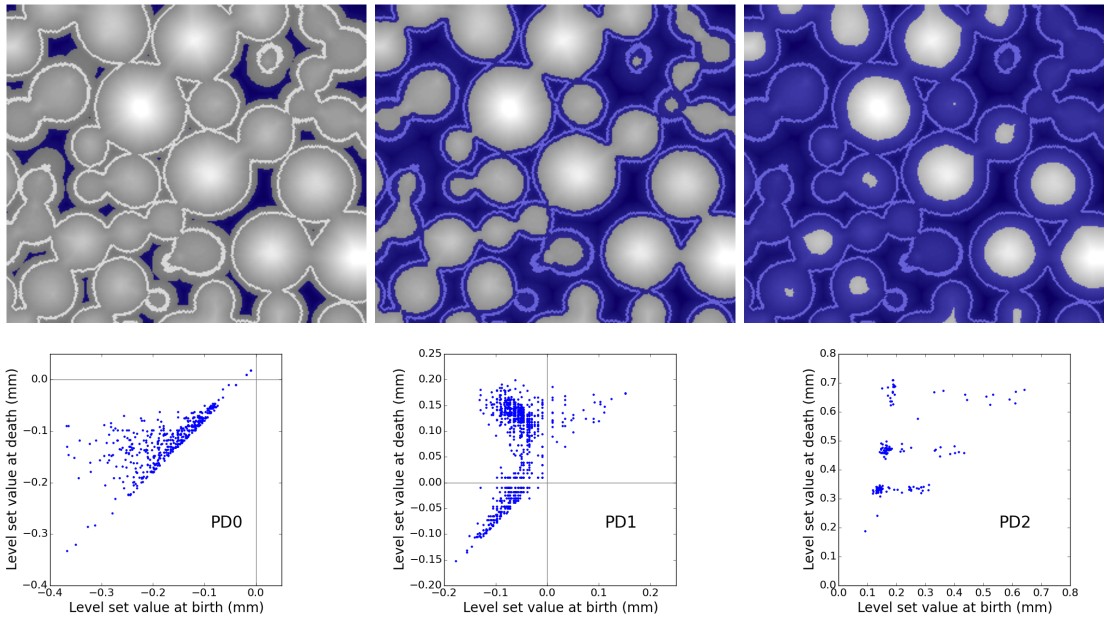

Figure 1: *Top* A sequence of lower level sets of the SEDT function $f(x)$ derived from a micro-CT image of a bead pack with three different radii. The interface between grain and pore phase is highlighted by a two-voxel wide contour around $f(x) = 0$. *Bottom* The corresponding persistence diagrams PD0, PD1, PD2, showing the persistence pairs for connected components, loops and cavities respectively.

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