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Morse theory and persistent homology for topological analysis of 3D images of complex materials

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Outline

1. Introduction to skeletons and watersheds
2. Morse theory: topo-geometric structure of a scalar function $f(\mathbf{x})$
3. constructing the **discrete Morse complex** from 2D/3D grayscale images
4. Defining **skeletons** and consistent **partitions** from the Morse complex
5. Using **persistence homology** for simplification and analysis

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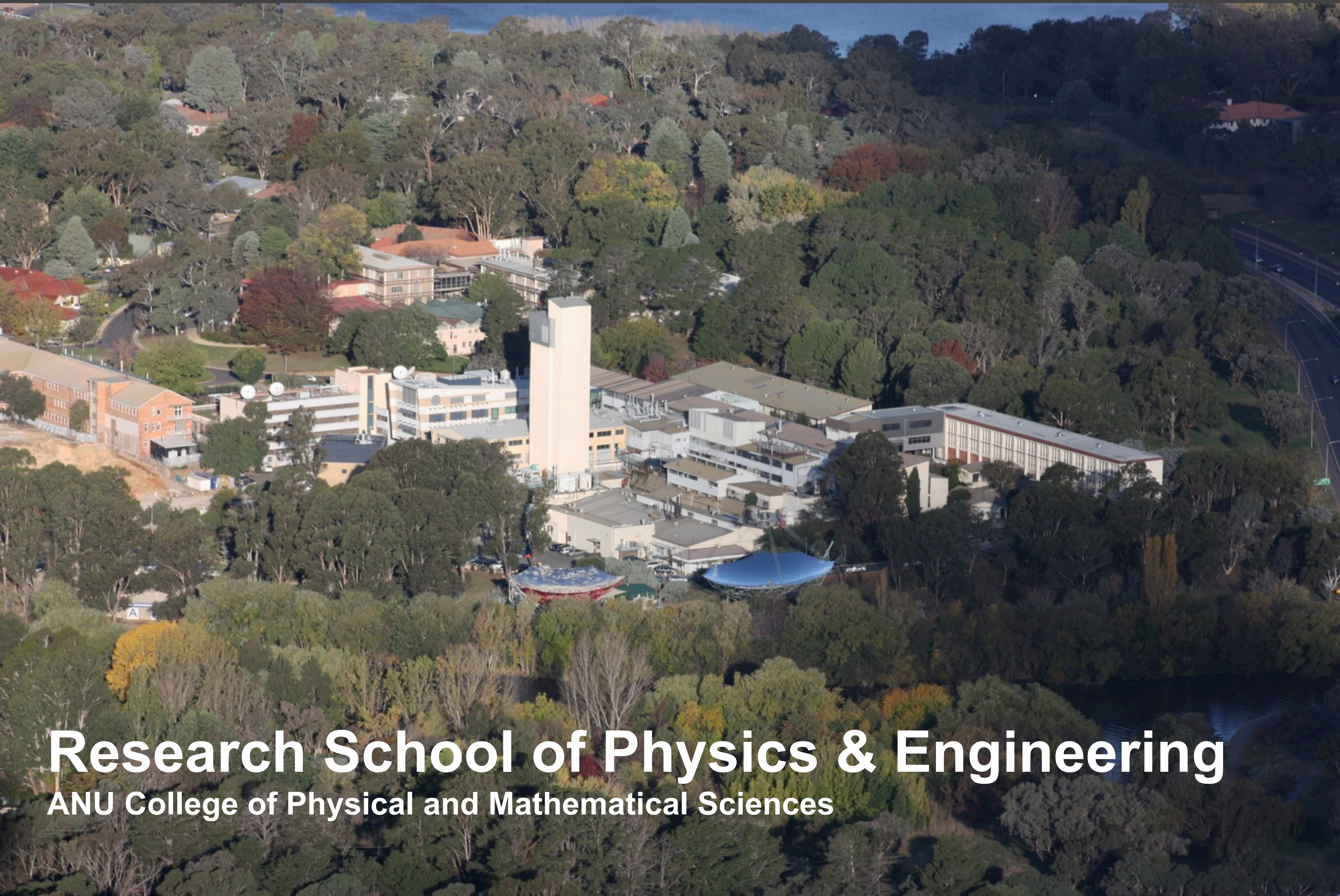
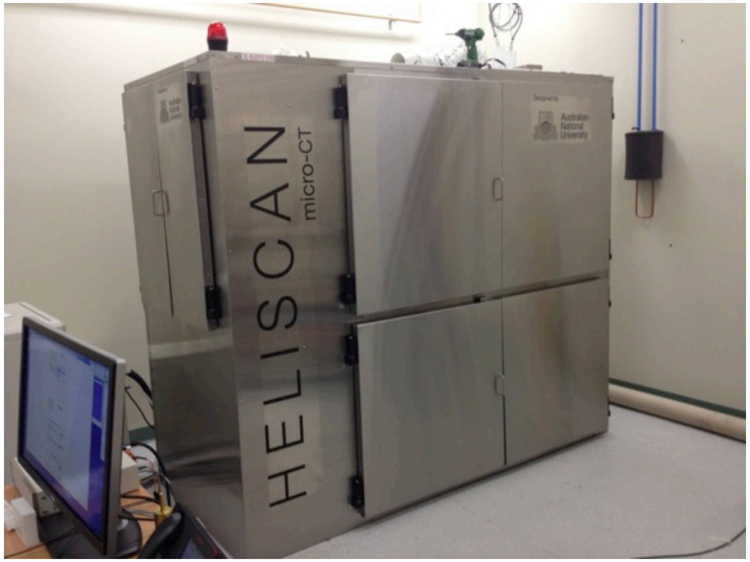


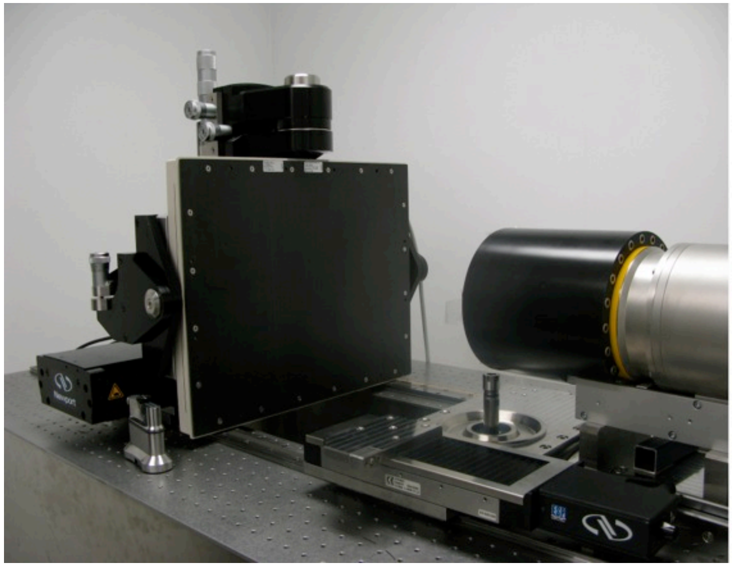
Research School of Physics & Engineering

ANU College of Physical and Mathematical Sciences

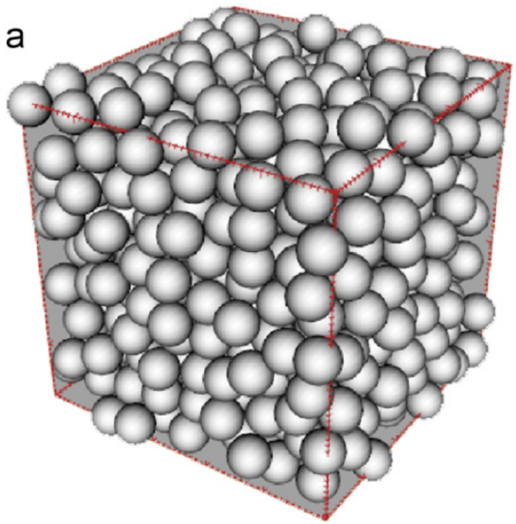
ANU micro-CT facility

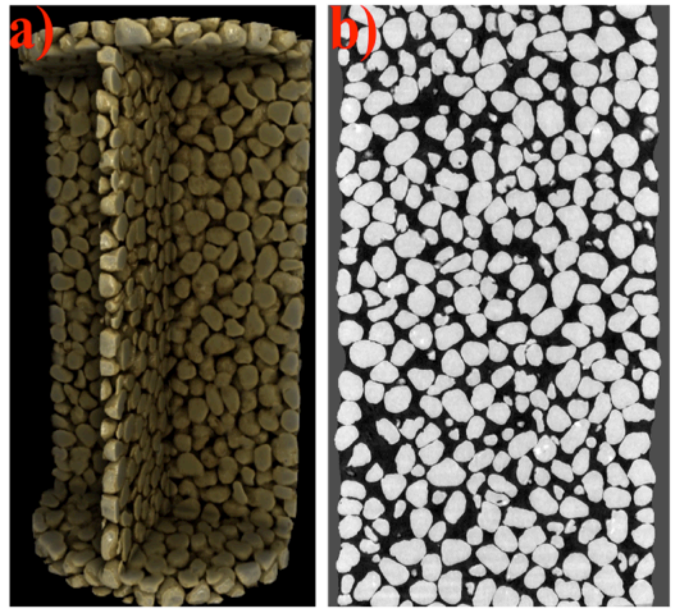
- In continual development since 2000
- Sources and detectors “off the shelf” (Hamamatsu, Varian, Perkin Elmer et al.)
- resolution down to 2 microns, submicron system under construction
- routine image sizes 3000x3000x10000 voxels (180 GB)

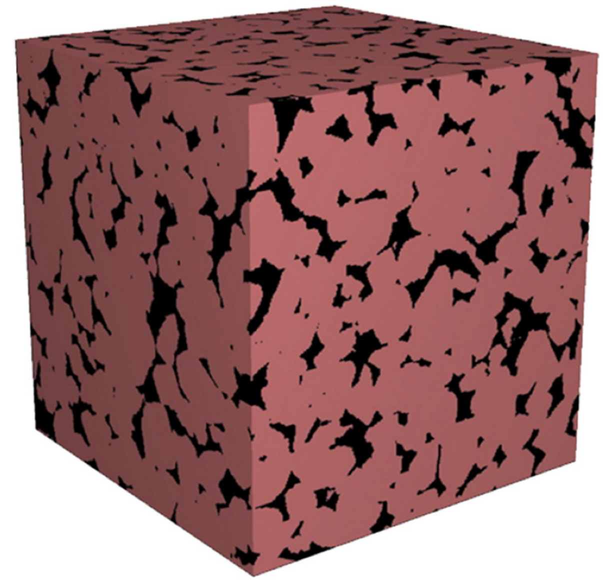


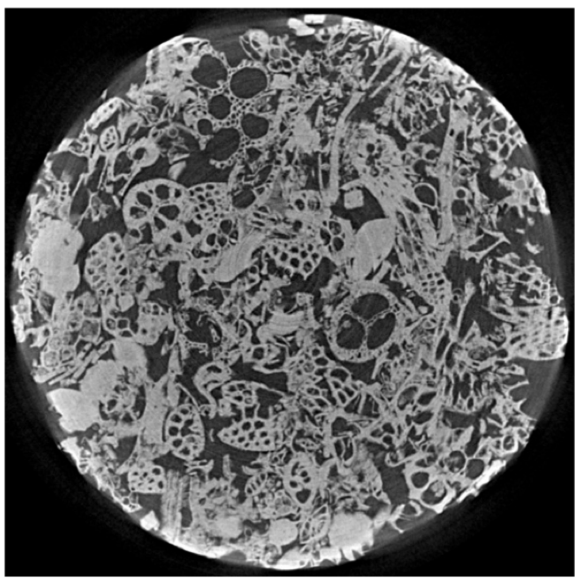


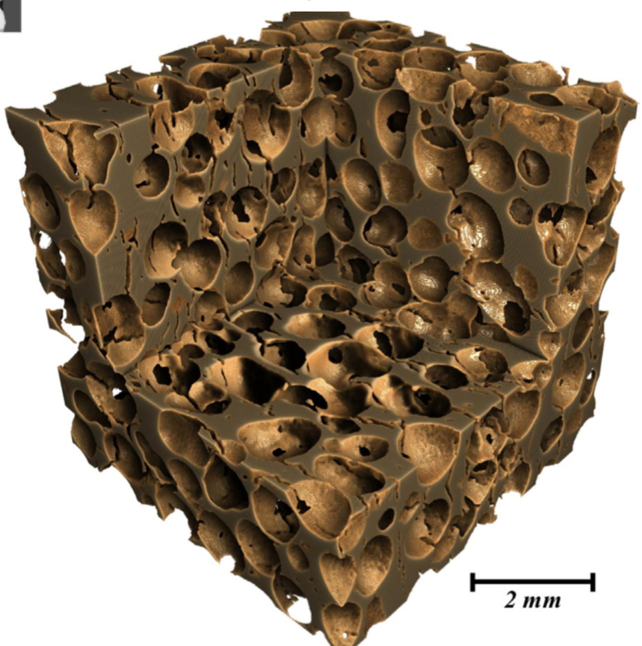
Porous materials



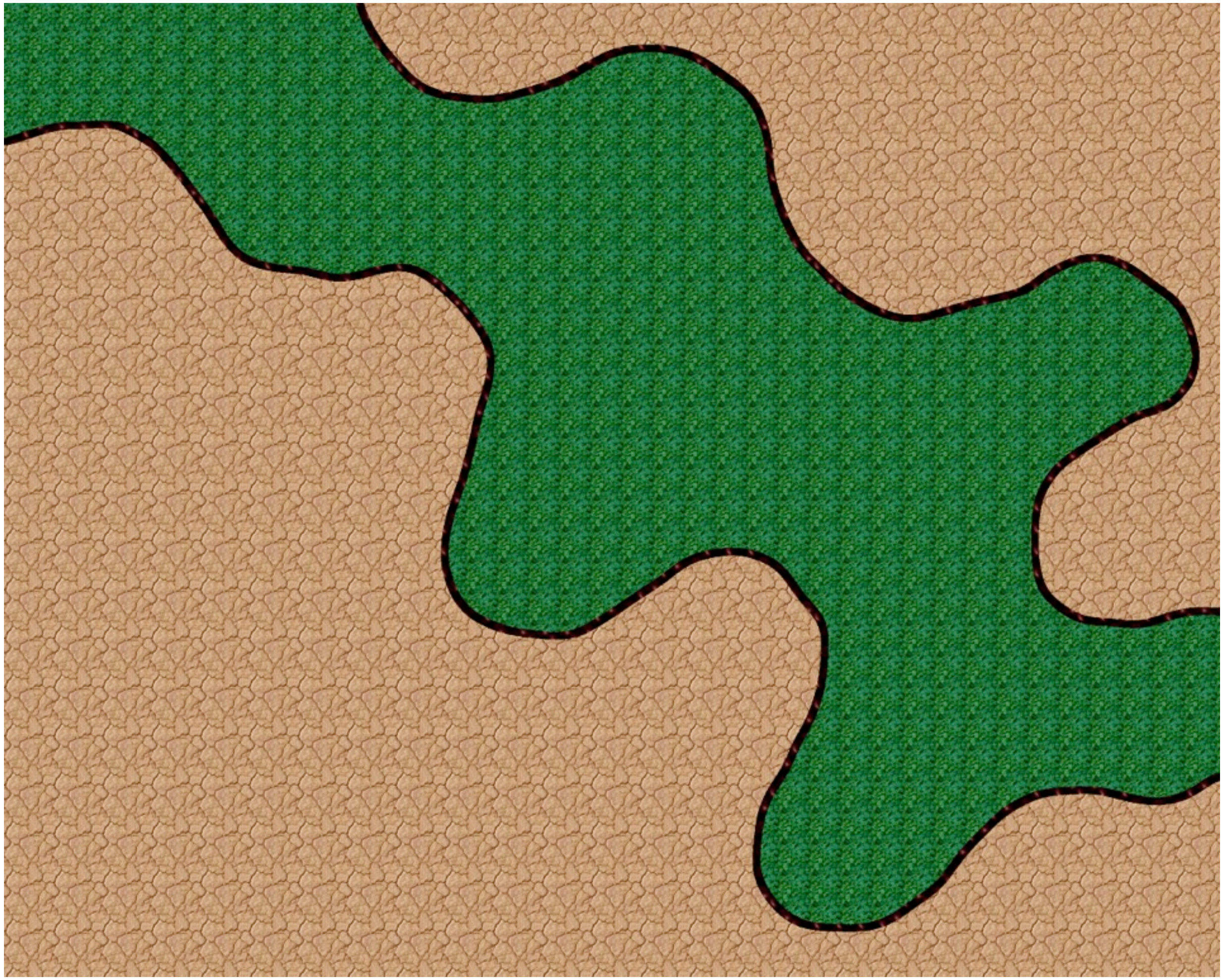




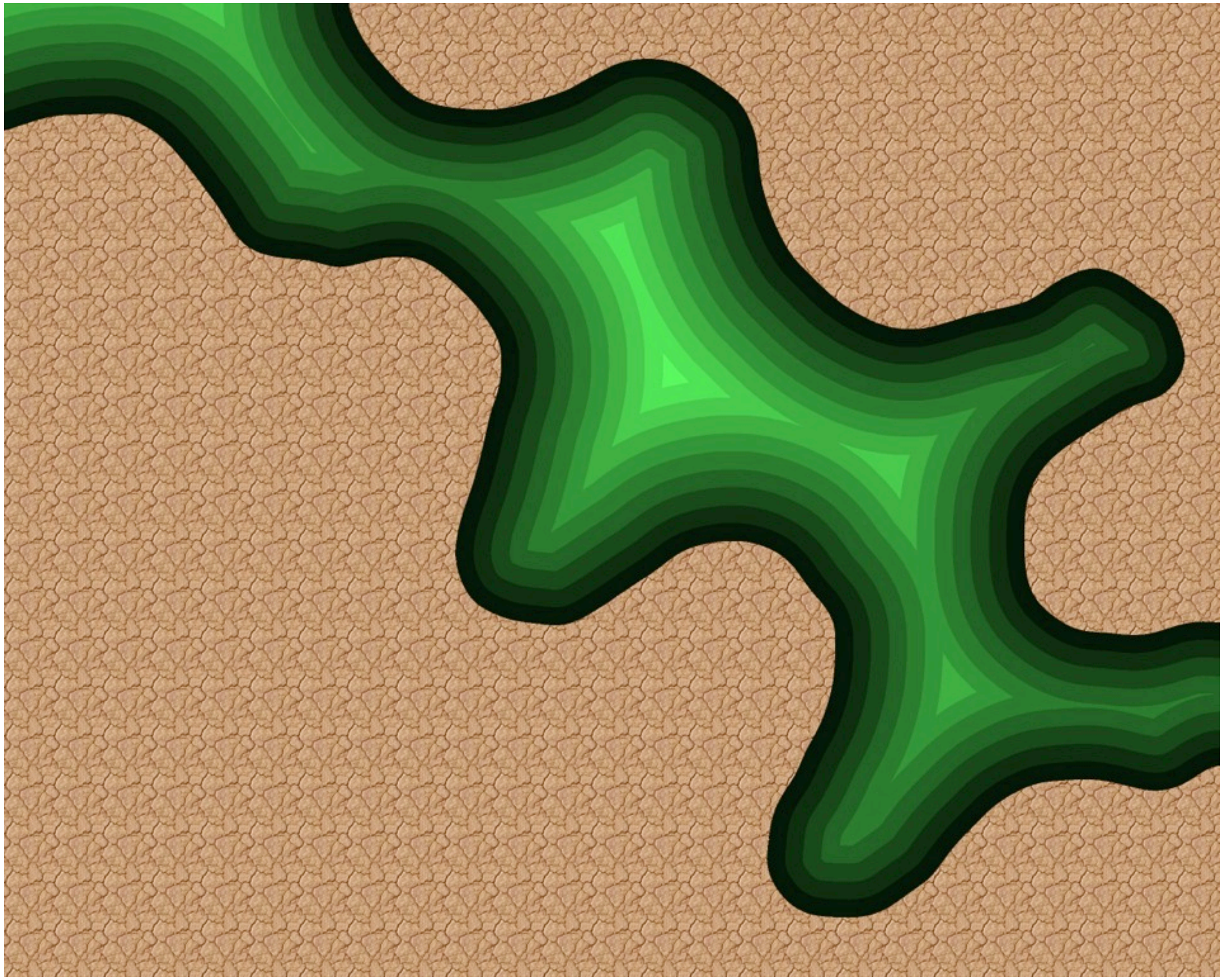




An object

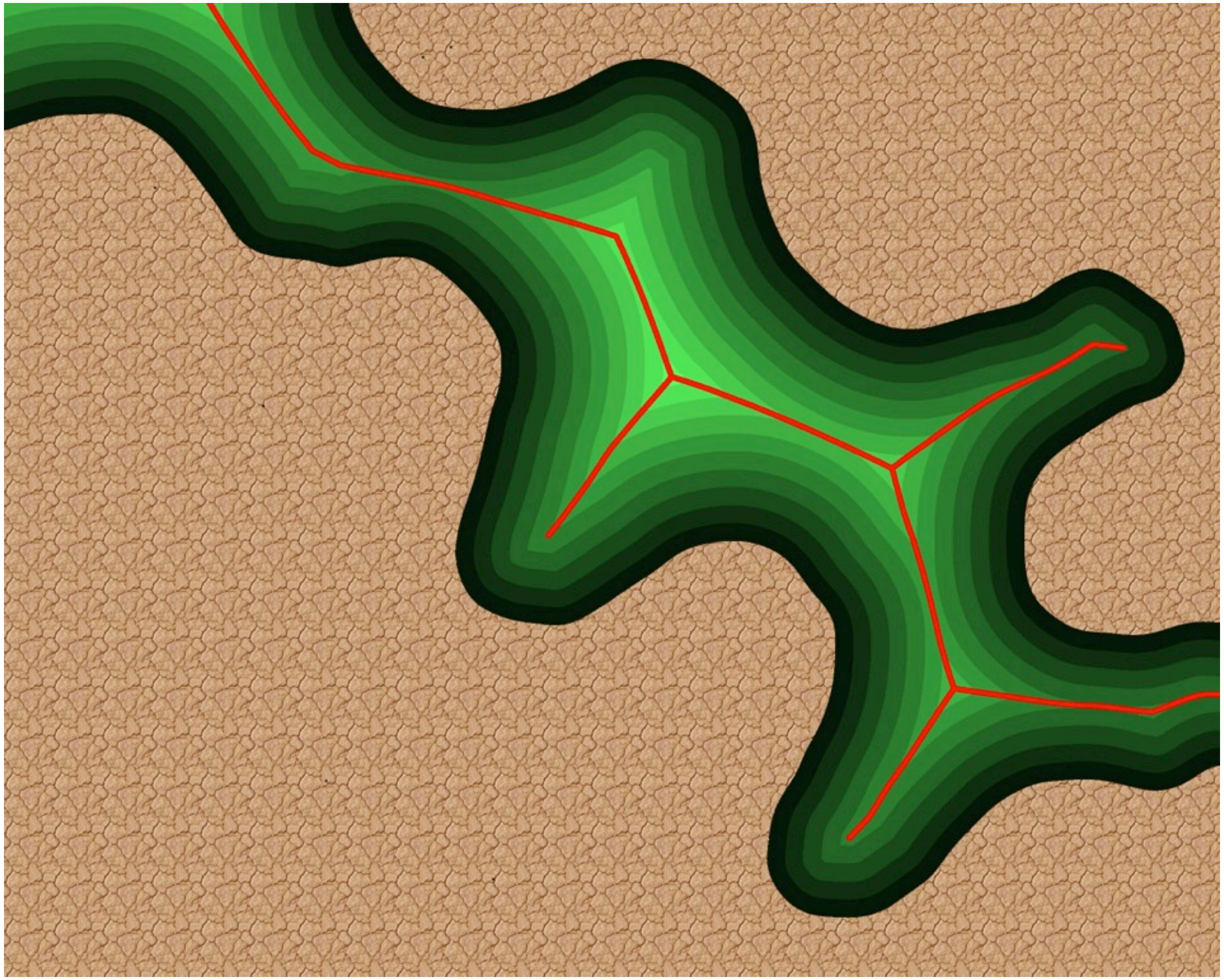


Distance transform

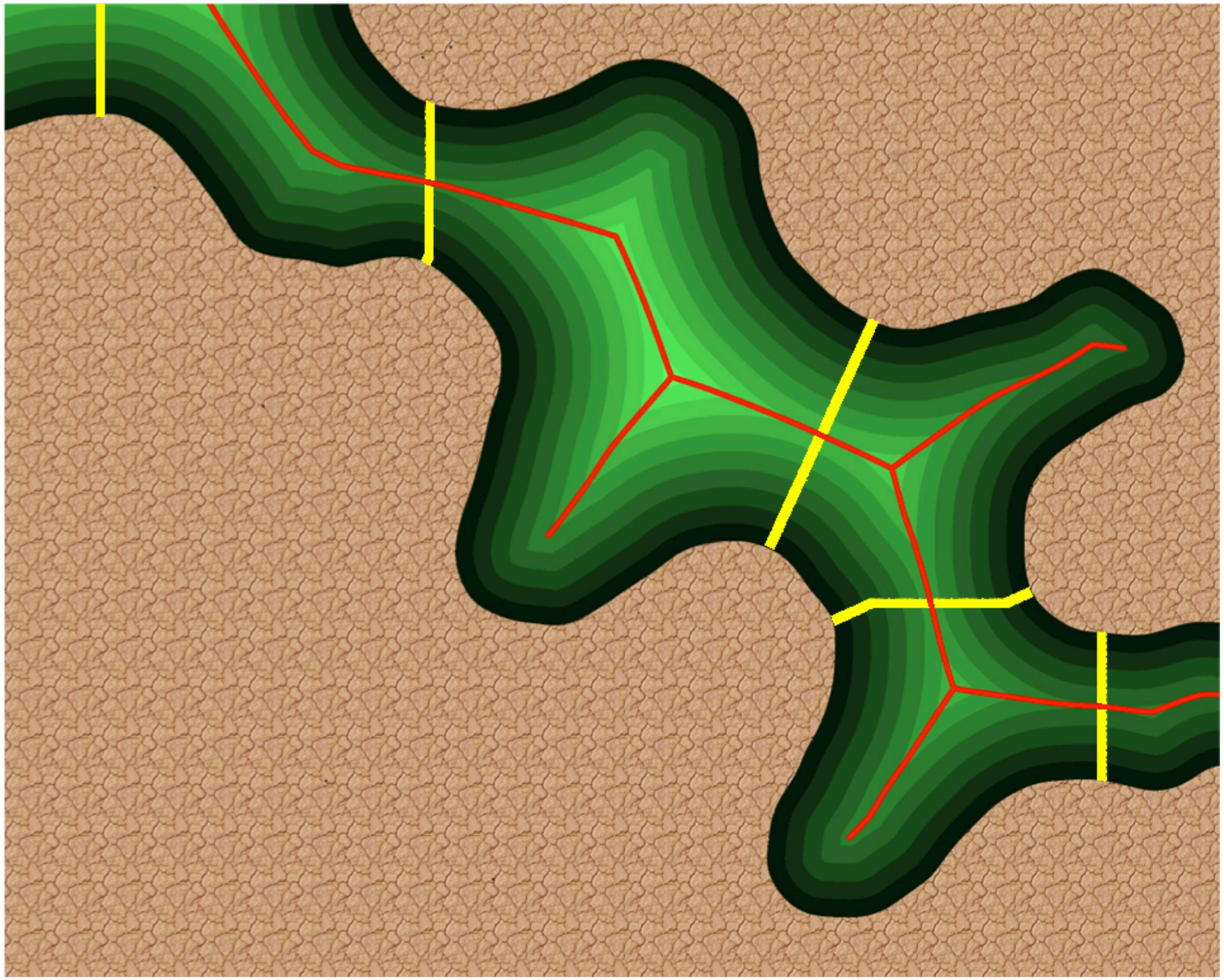


Australian art!

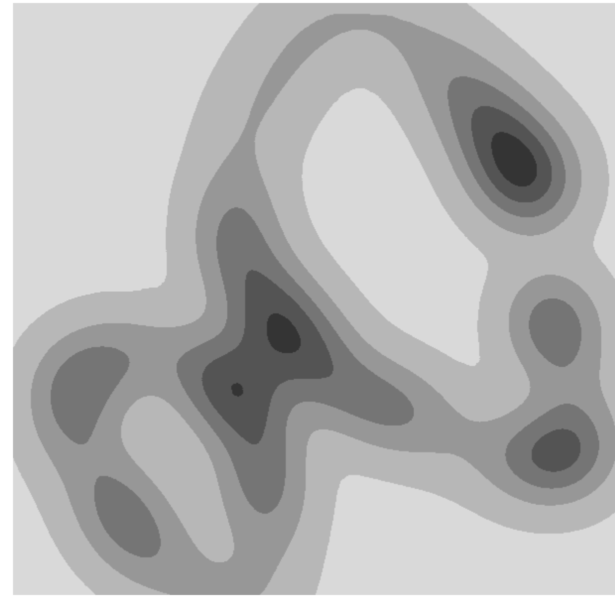
Skeleton (medial line)



Watershed partition



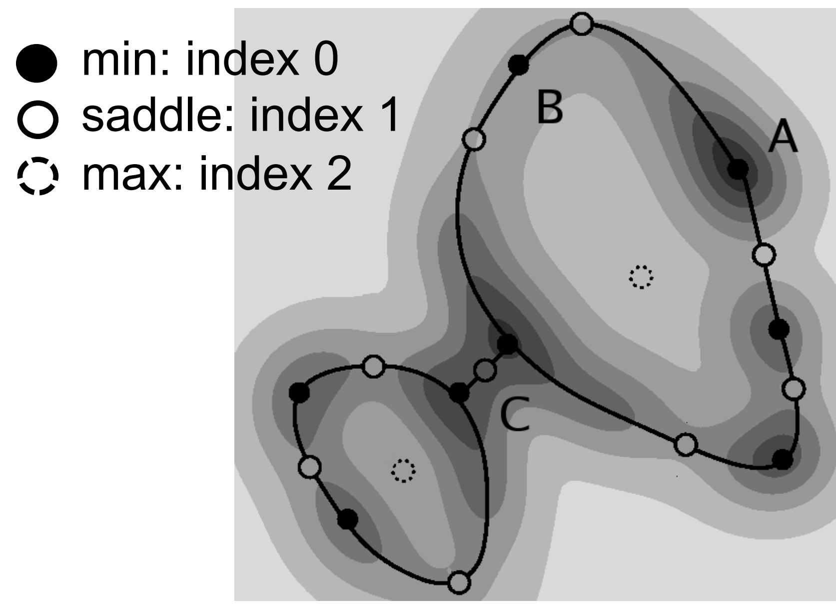
Morse theory and level cuts



The topological-geometric structure of a scalar function *f* is given by the **lower level cuts**

$$L_f(h) = \{x \mid f(x) \leq h\}$$

If we scan *h* from the lowest to highest image values, changes in the topology of *L(h)* only occur when passing a critical value of *f*.



A **Morse function** has non-degenerate critical points whose **index** is the number of negative eigenvalues of the Hessian (matrix of second derivatives).

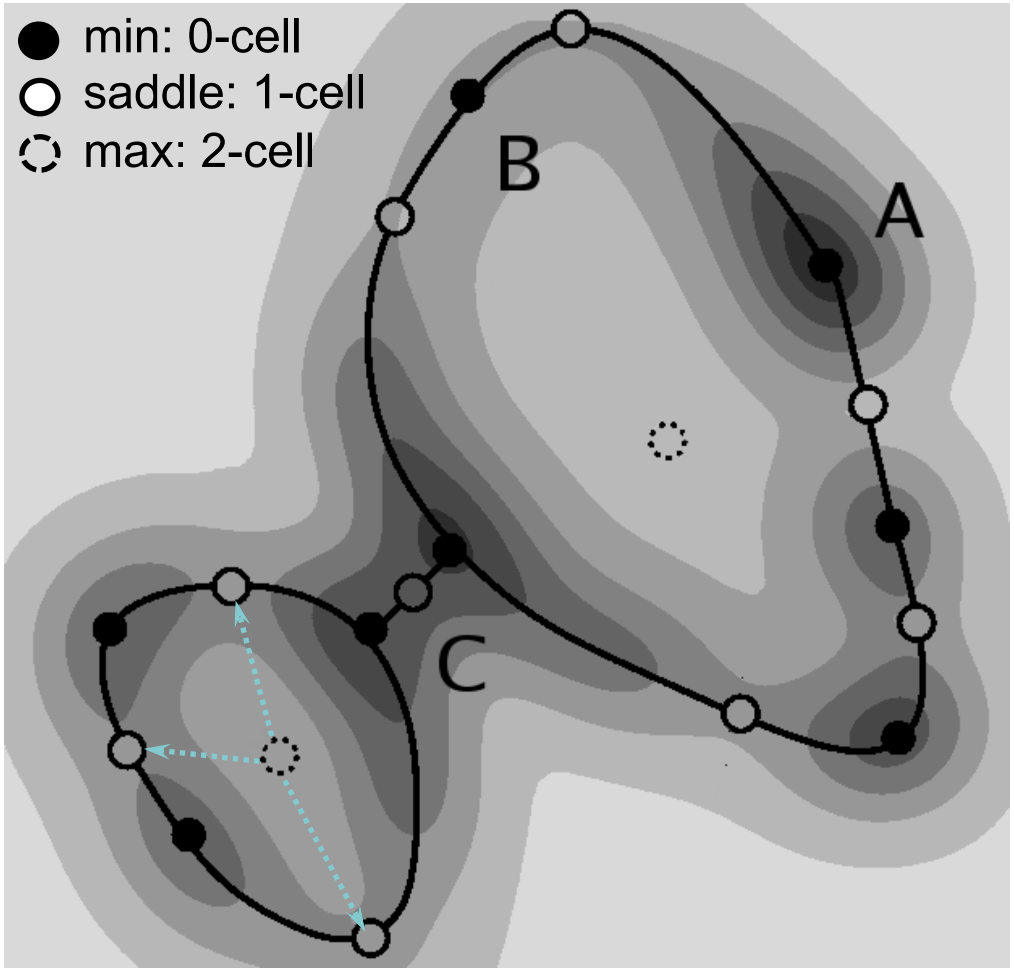
The Morse complex

for Morse functions, in continuous space

A **gradient flow-line** passes through every point; each flow-line originates and terminates at a critical point.

The **unstable manifold** of a critical point *p* is the union of all flow-lines that originate at *p*.

The unstable manifold of an index-*i* critical point forms an *i*-dimensional cell of the **Morse complex.**



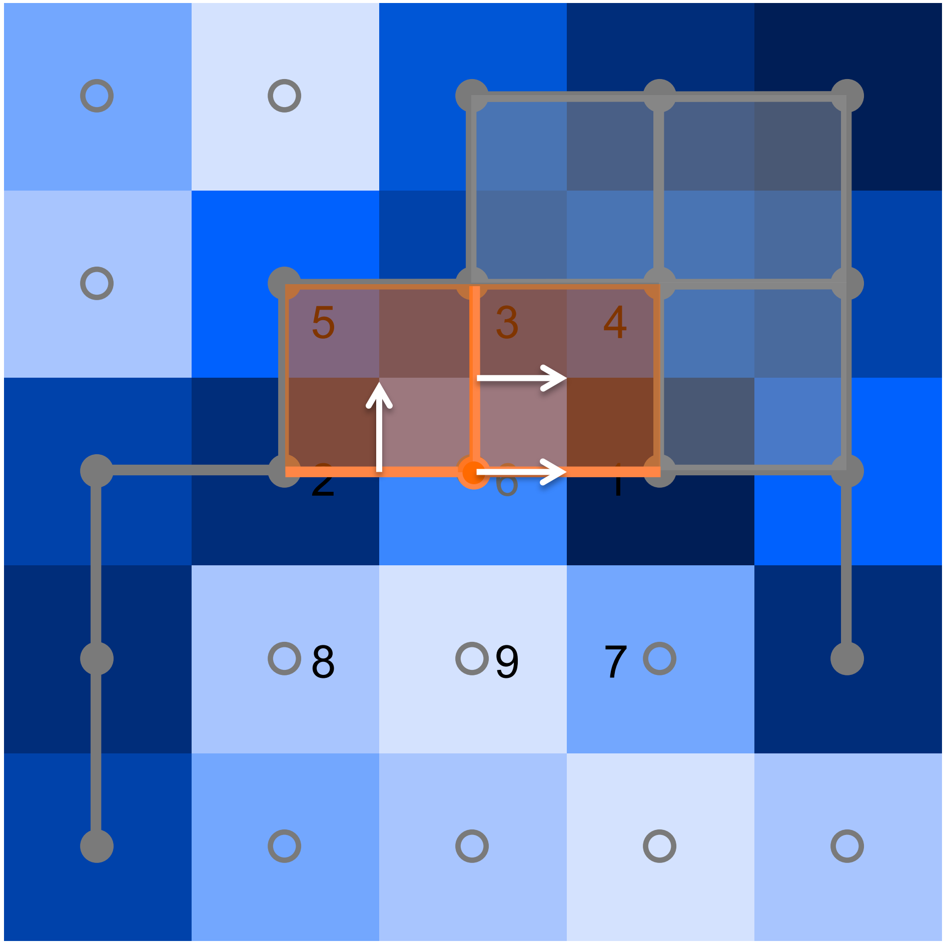
Morse theory on digital images

The goal: define all lower level cuts and capture where their topology changes

Model a digital image as a cell complex of points, lines, squares and cubes.

Construct a complex to represent each lower level cut by adding cells in grayscale order. Where possible, add cells in face-coface pairs, as simple homotopy expansions.

Unpaired cells (**critical cells)** are added only when necessary.



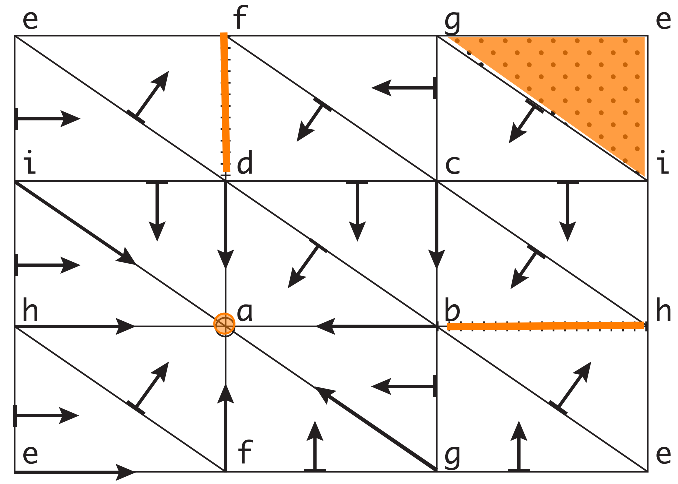
Forman's discrete Morse theory

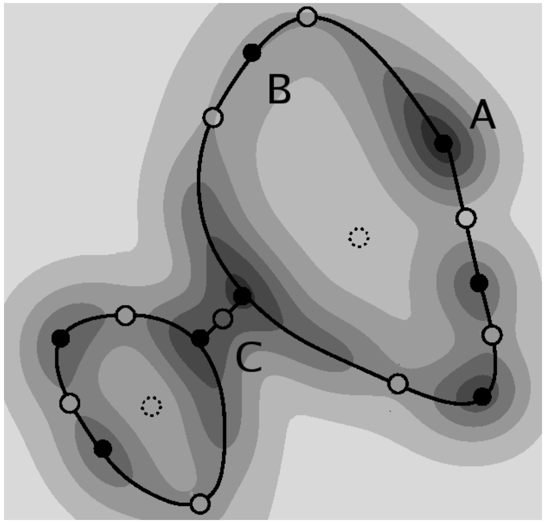
The incremental algorithm we've described allows one to construct a **discrete gradient vector field** and a **discrete Morse function** following Forman's definitions**.**

This gives **V-paths,** the discrete analogue of gradient flow lines.

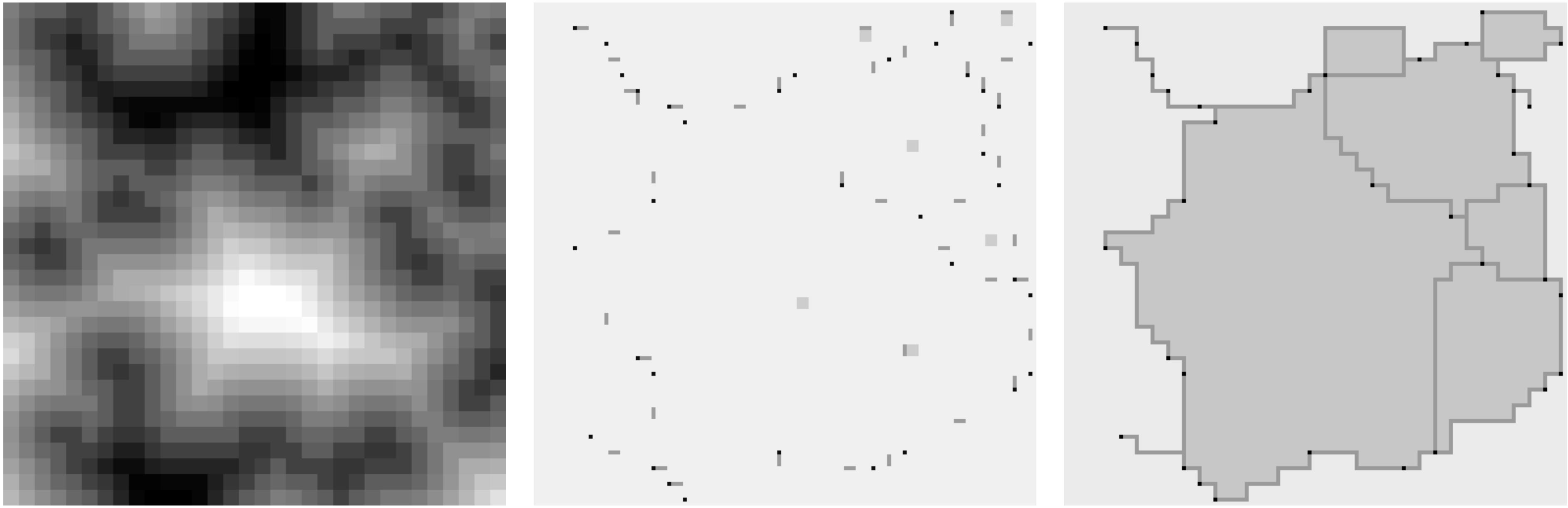
V-paths between critical cells define the **Morse chain complex.**

Each cell in the chain complex represents the **unstable set** of a critical cell *x* in the image: all cells that lie on V-paths originating at *x*.





Constructing the discrete Morse complex



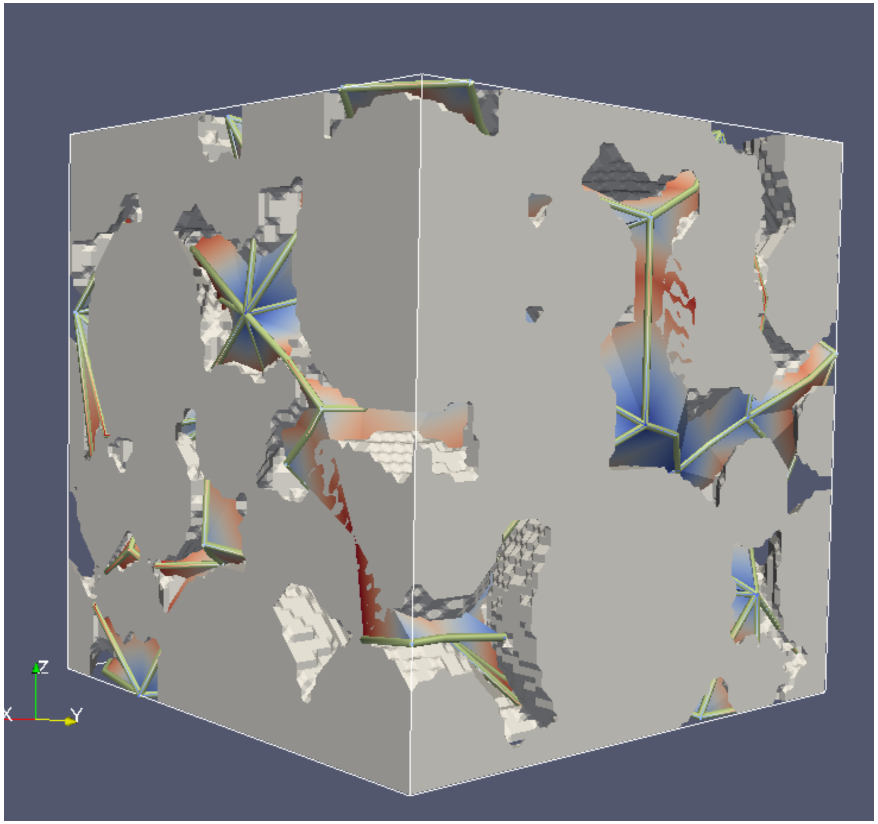
grayscale digital image (signed distance transform) — critical points — cell complex

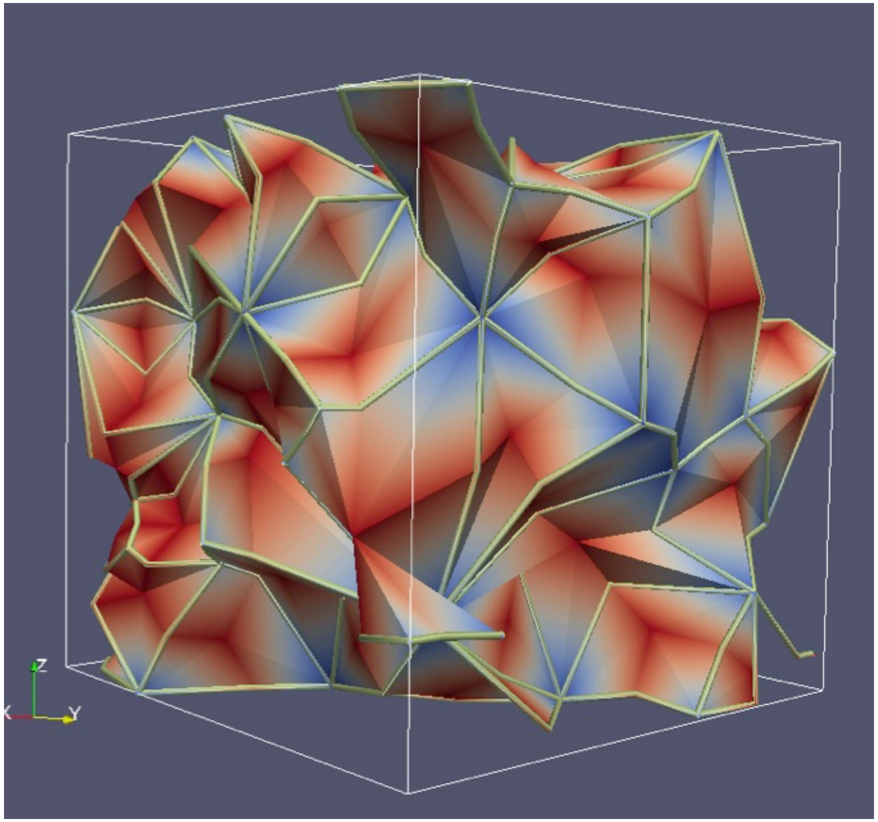
The **incremental algorithm** provides the local detail, i.e. it finds the critical points and vector field pairings.

Discrete Morse theory provides the global picture, i.e the flow lines and a combinatorial cell complex that's ideal for further computation.

Morse complex of a sphere pack

Calculated from the signed Euclidean distance transform



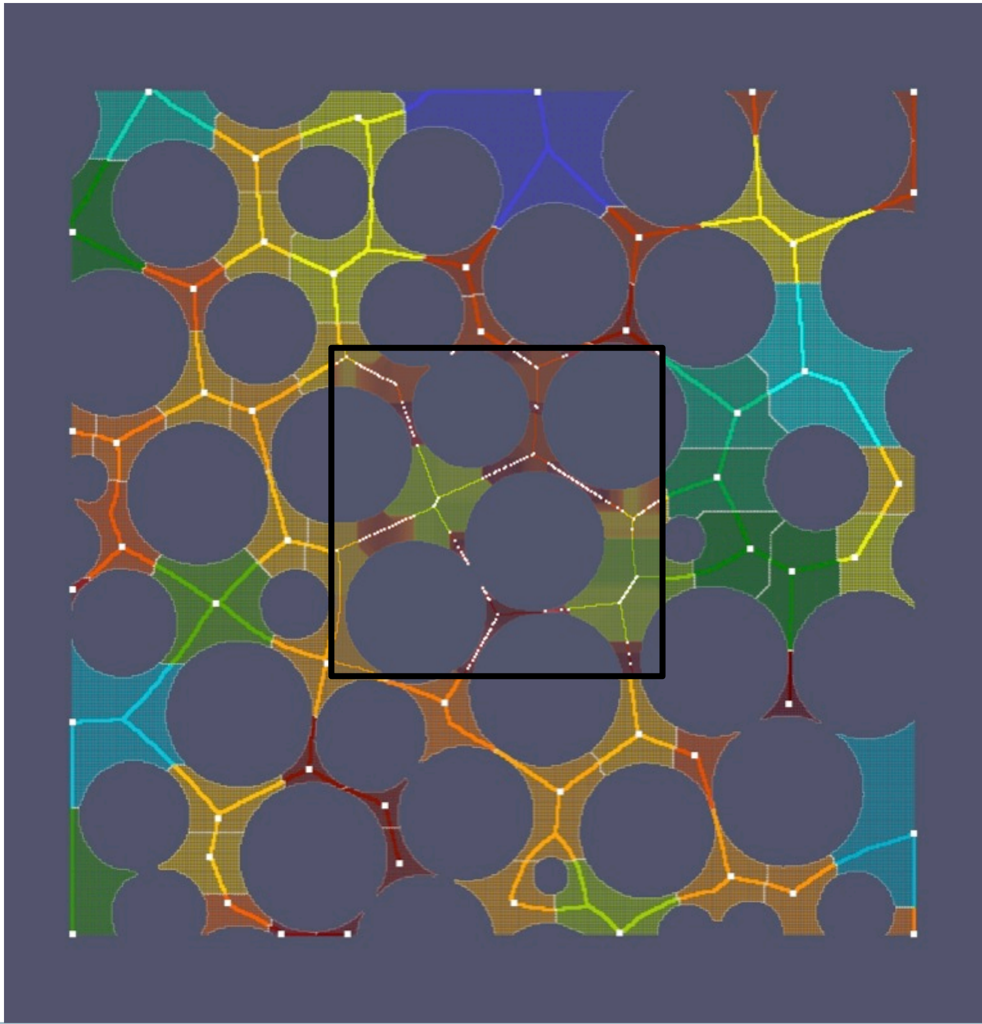


Skeletonisation and partitioning

As in the continuous case:

V-paths (flow lines) between critical points are related to **skeletons** and **watershed partitions**.

And Morse theory provides a built-in **simplification** technique for “noise” removal.

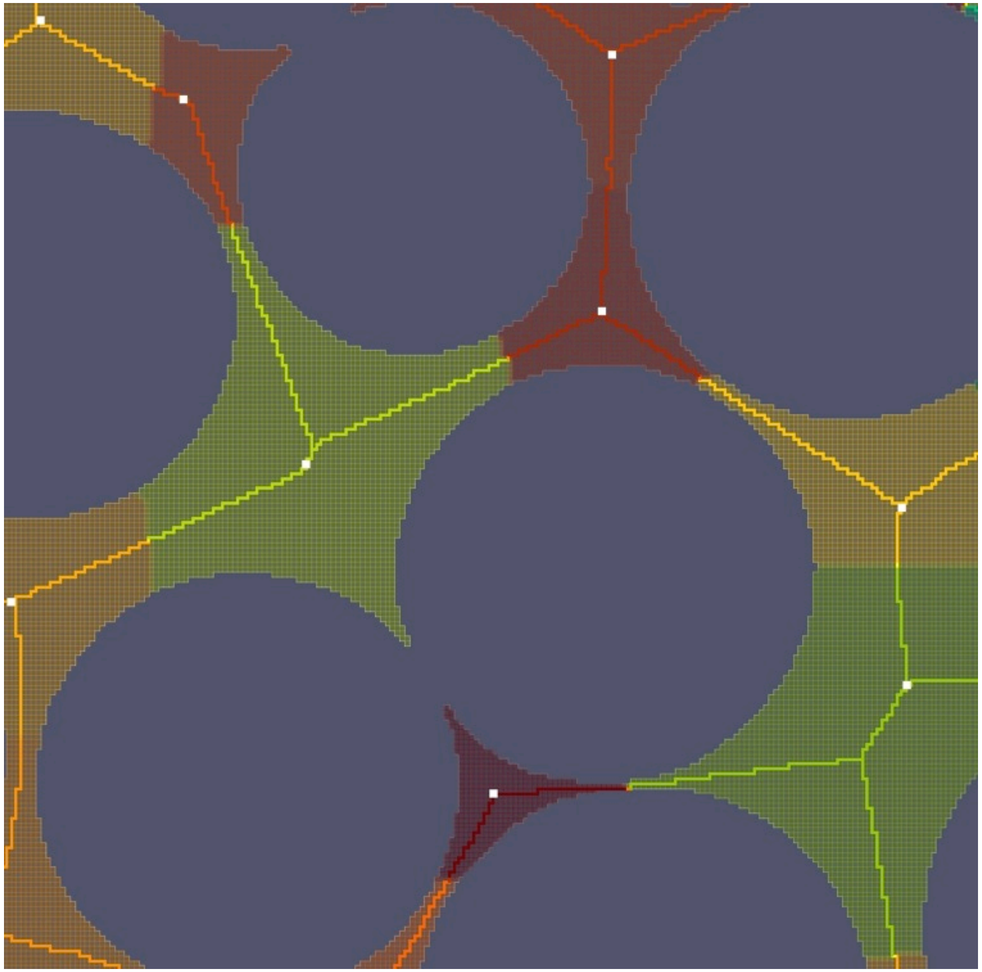


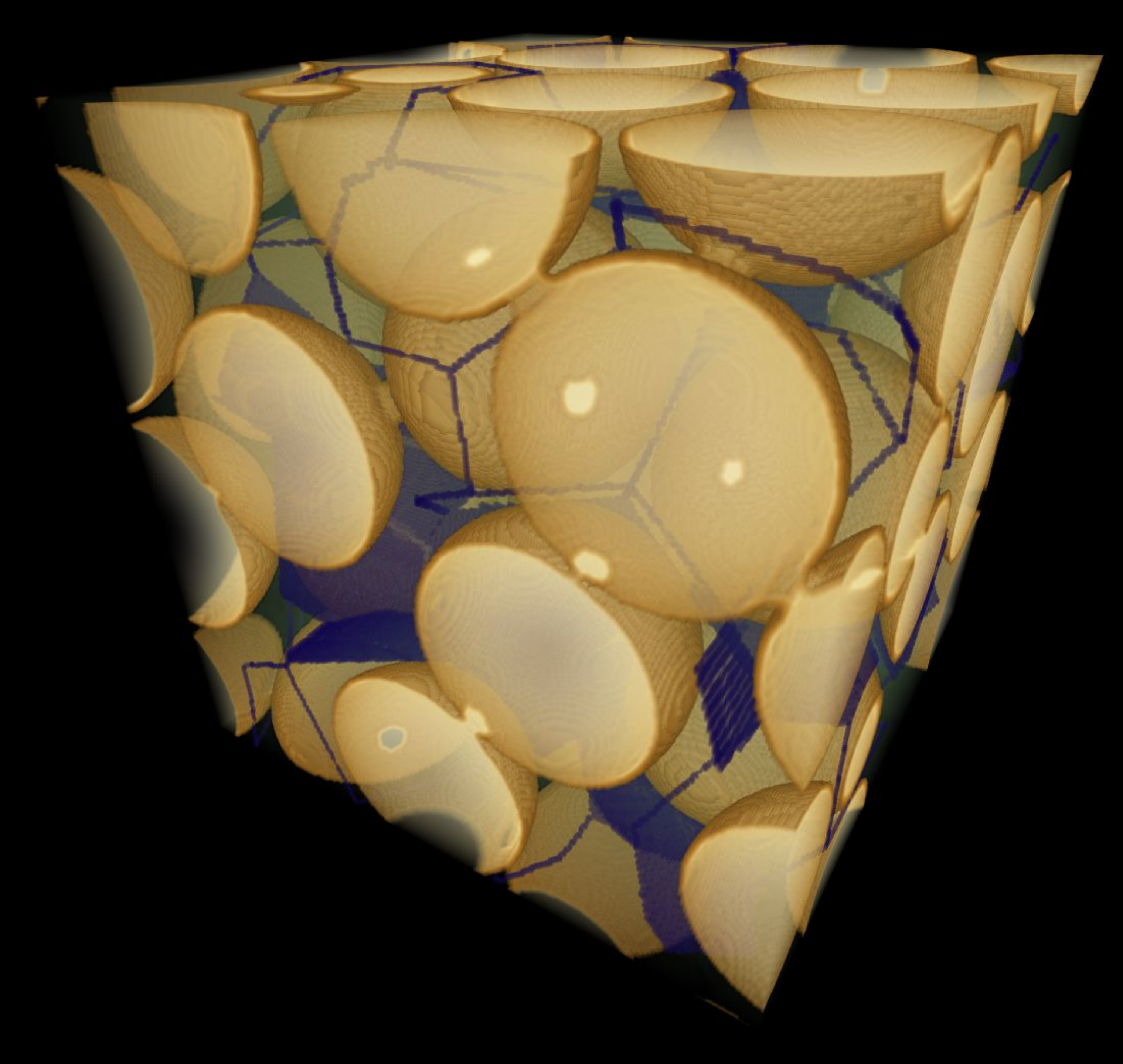
The Morse skeleton

The **Morse skeleton** *A(c)* for the lower level set at value *c* is the union of **unstable complexes** of critical points *x* with $f(x) \leq c$.

Theorem: *A(c)* is homotopic to the lower level cut at *c* by a regular collapse.

Critical 1-cells generate linear elements in the skeleton; and critical 2-cells generate sheet-like elements.





Skeleton computed from void space of sphere pack.

2D patches mean a 1D skeleton would be inaccurate.

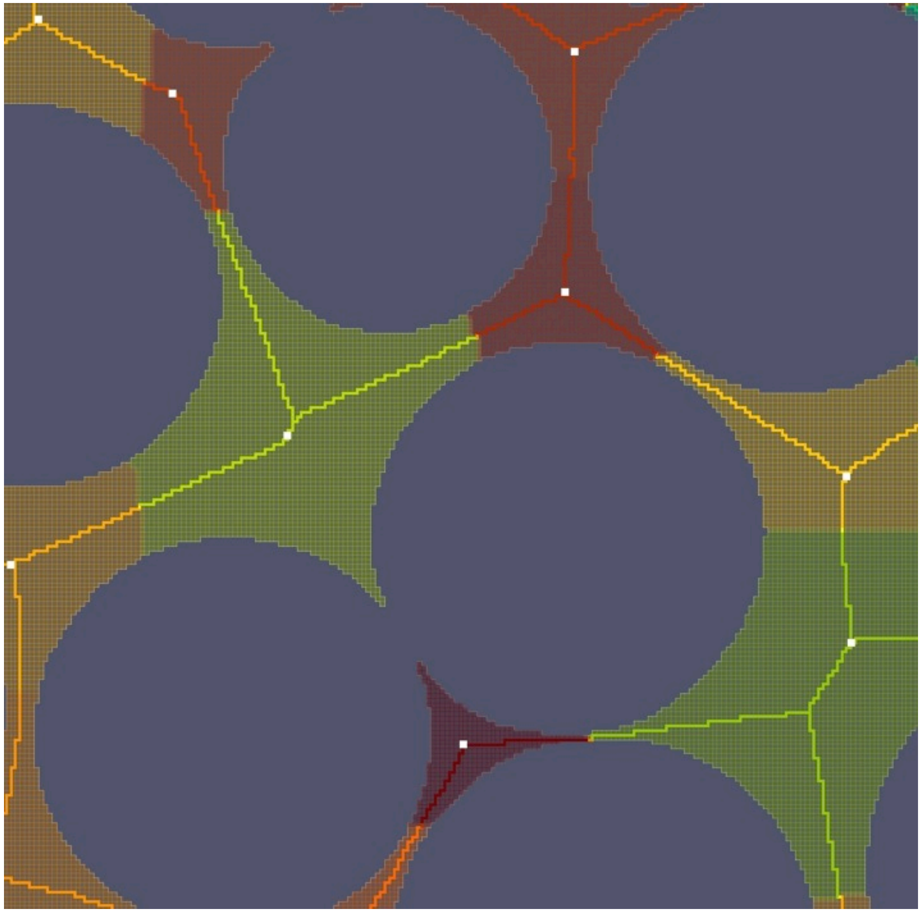
Image produced using web-based renderer, Voluminous.

Partitioning via Morse basins

Each vertex is in the **stable set** of exactly one minimum (critical 0-cell) α.

The **basin** of a minimum, $B(\alpha)$, is the maximal subcomplex that has a *regular collapse* onto α.

Morse basins are analogous to watershed basins and can be shown to be simply connected.



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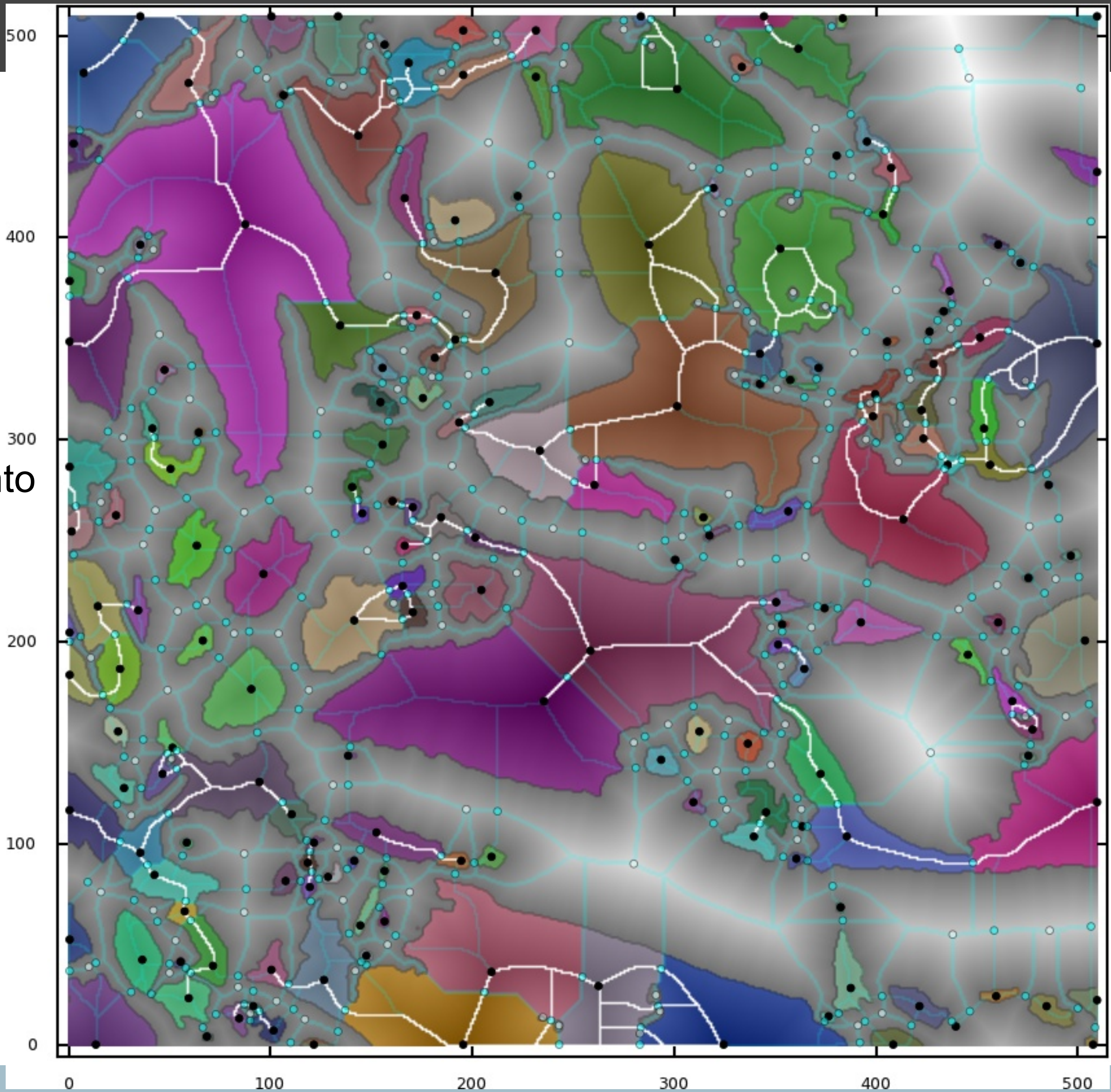
Skeleton and pore partition from SEDT on 2D slice of limestone.

Solid phase shown in grey levels;

Void space is divided into coloured pores

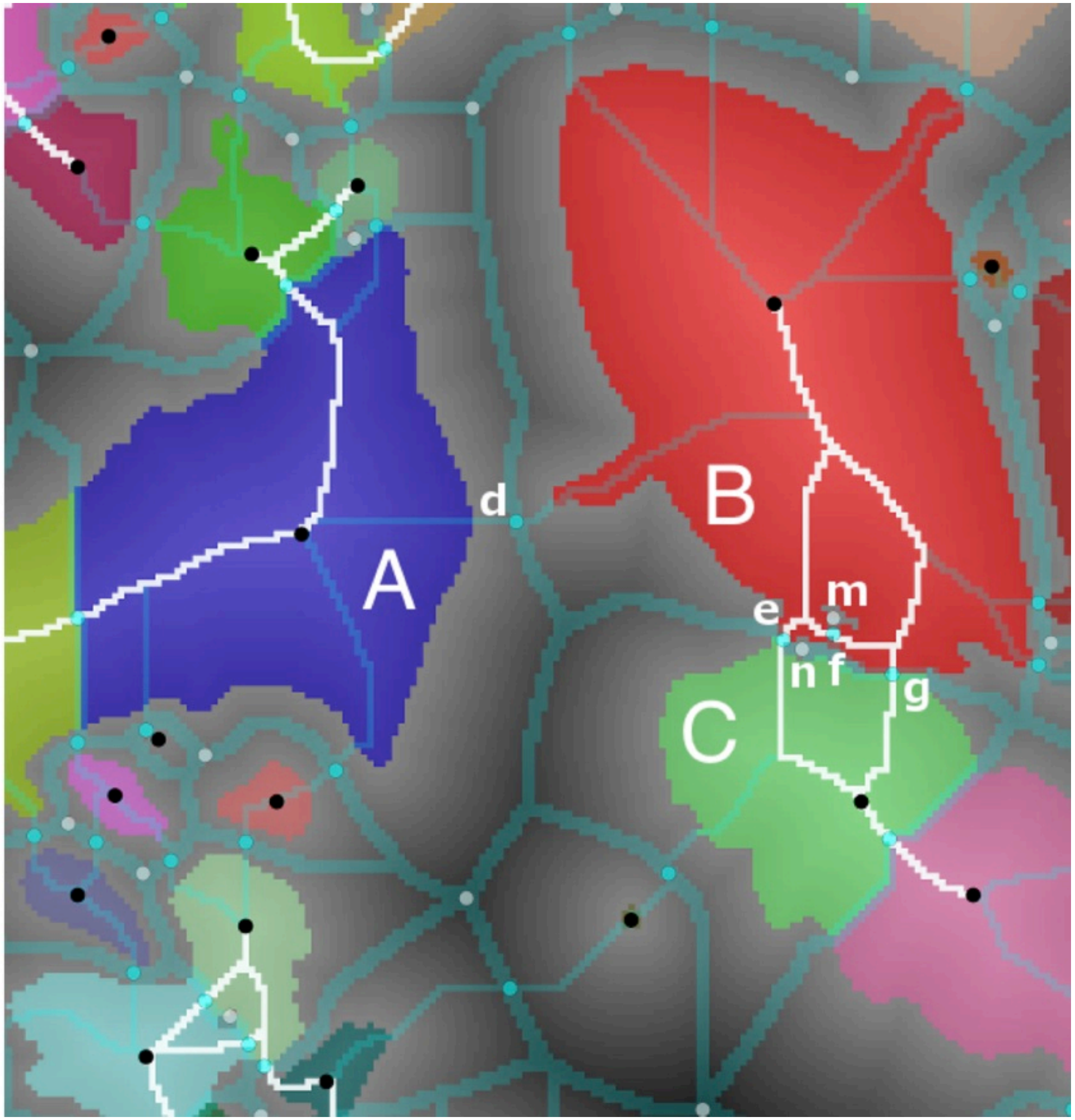
White lines are the Morse Skeleton

Blue lines are watersheds



Complexities

There is no saddle point (**critical bridge**) between A and C; they are unconnected in the dual of the Morse complex.
A and C are connected through a **canonical path.**



black points: minima

blue points: saddles

grey points: maxima

thick blue lines: basin boundaries

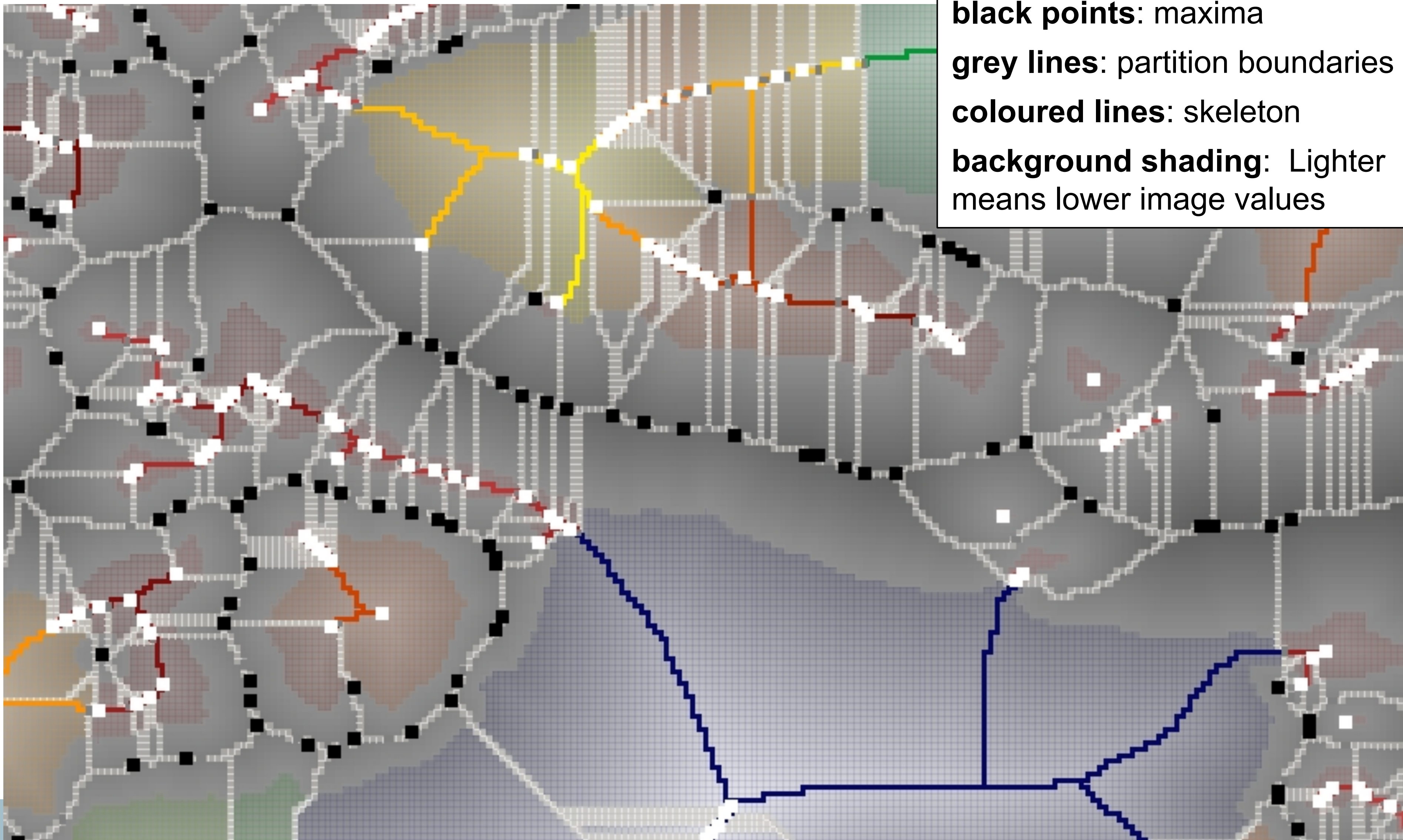
thin blue lines: non-skeleton 1-cells

white lines: skeleton

coloured regions: partition of $L_f(0)$

background shading: Lighter means lower image values

Limestone 2D Morse complex



white points: minima

black points: maxima

grey lines: partition boundaries

coloured lines: skeleton

background shading: Lighter means lower image values

Persistent homology and close pair simplification

- Each topological feature of dimension *i* is "born" with the insertion of an i-cell and "dies" with the insertion of an *i+1* cell.
- This allows us to define the **persistence** of topological features in terms of their lifetime.
- low persistence features exist for only a small range of cut values
- On the Morse chain complex filtration, reordering critical points allows the effective removal of low-persistence features

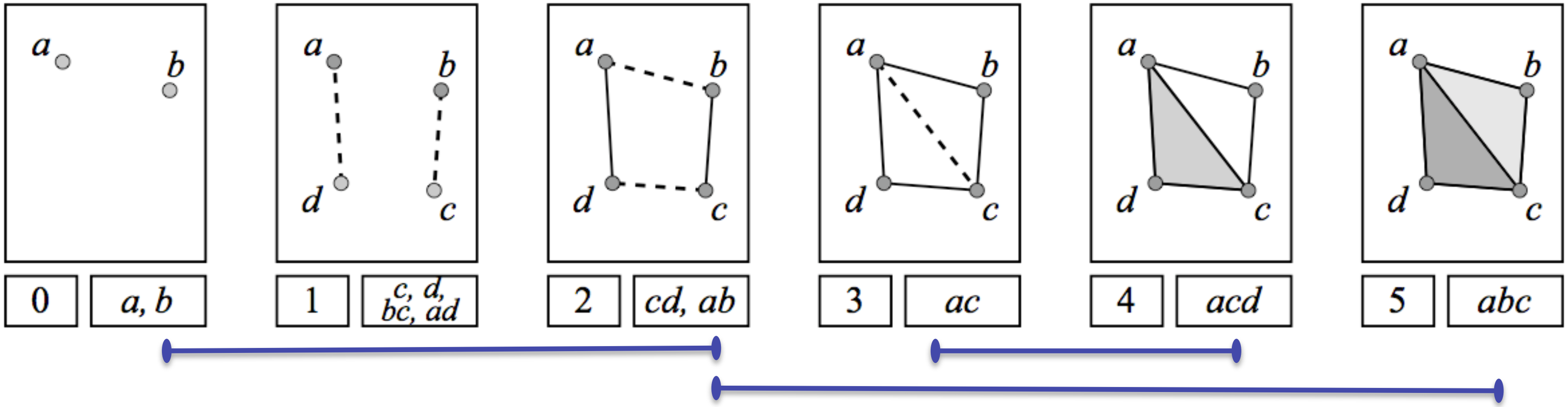


Image from Zomorodian 2009

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Limestone 2D Morse complex

pair cancellation to p=1.0

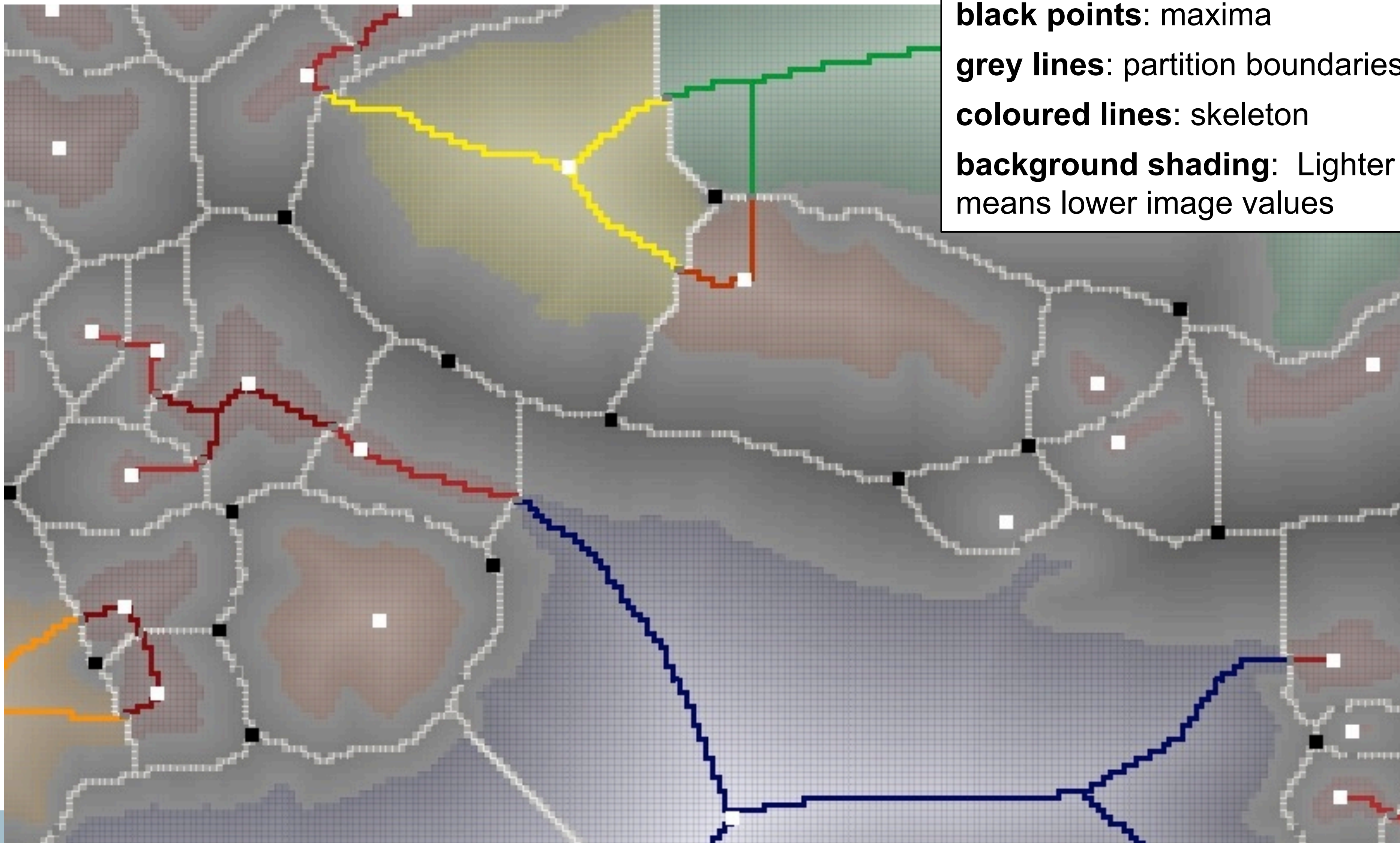
white points: minima

black points: maxima

grey lines: partition boundaries

coloured lines: skeleton

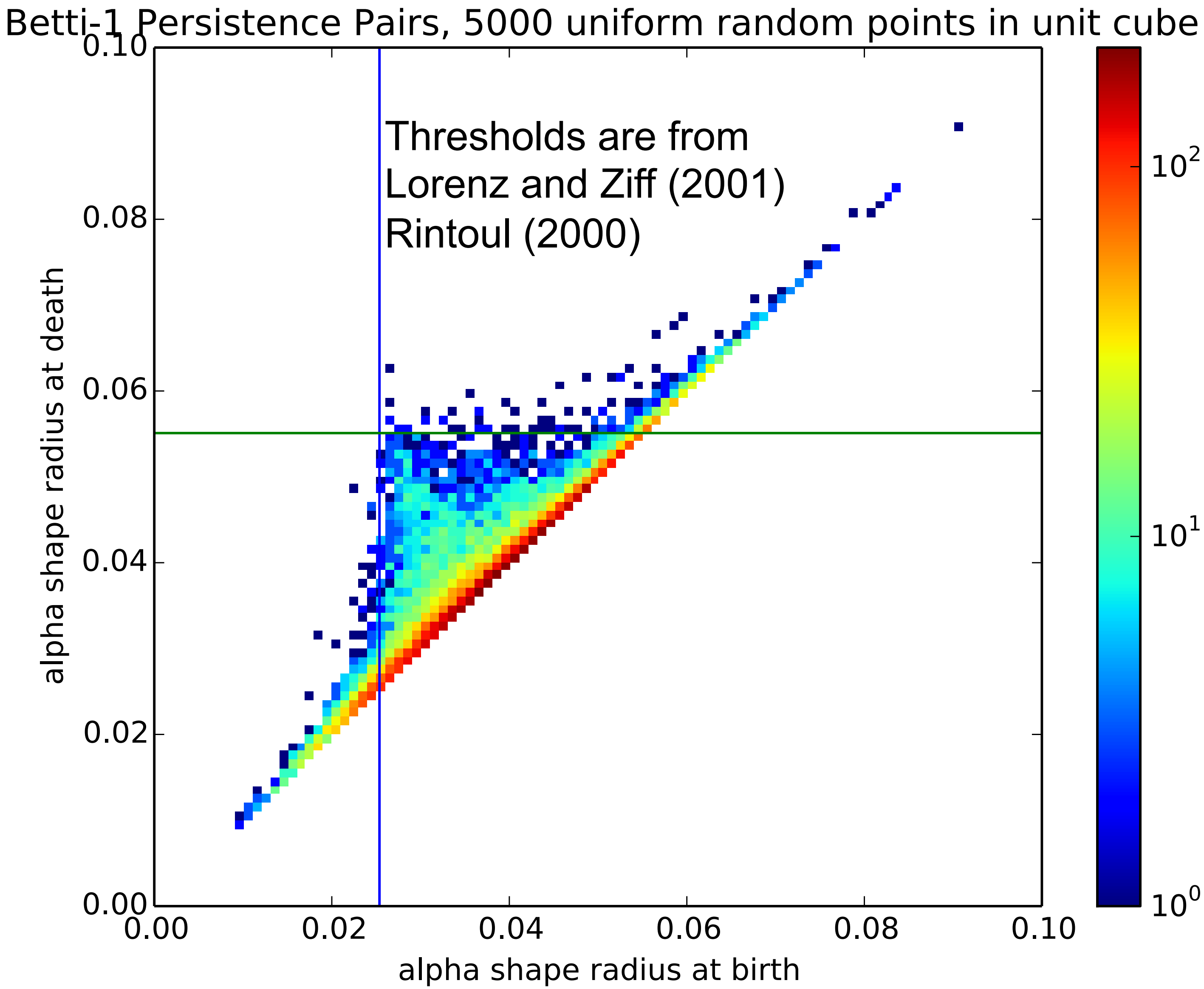
background shading: Lighter means lower image values



Summary of implementation

- All code is written in C++98 with distributed-memory parallel implementations for everything but persistent homology, using MPI for inter-process communication.
- The parallel code splits the input image into rectilinear blocks, one per process, with small overlaps (1 or 2 pixels).
- Memory consumption reduced using regularity of cubical complexes and linear arrays and binary search.
- The Morse chain complex extraction adapts Guenther (2012) in order to avoid retracing the same partial V-paths multiple times.
- Persistent homology computation uses a variation of the method by Chen and Kerber (2011).

Persistence diagram: Poisson spheres



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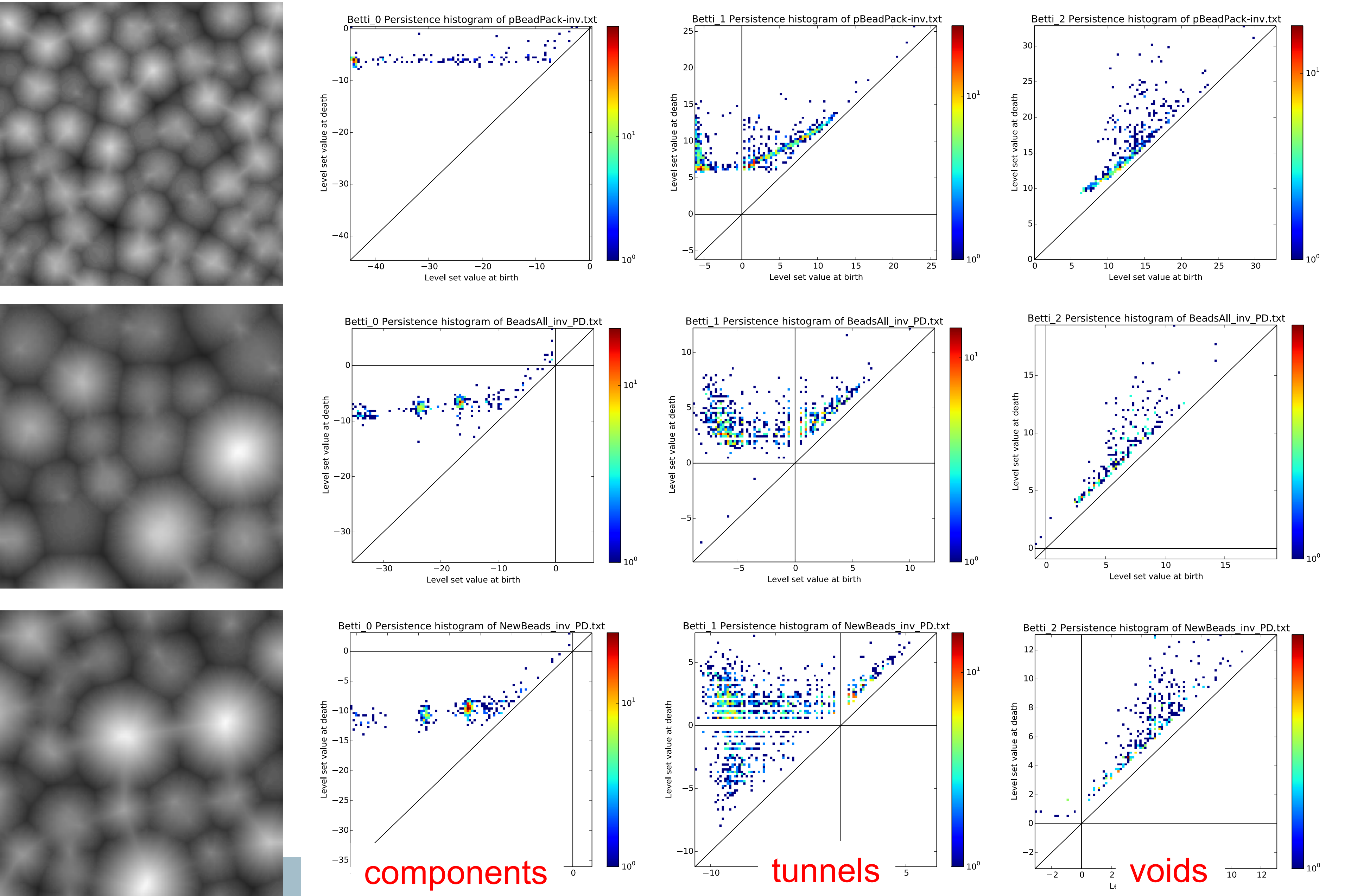
Bead packs (solid phase)



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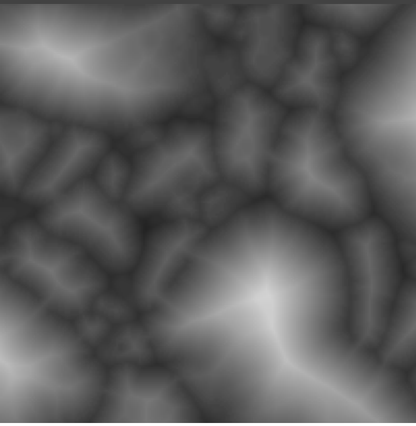
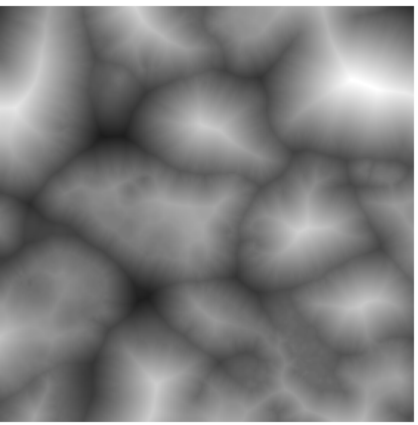
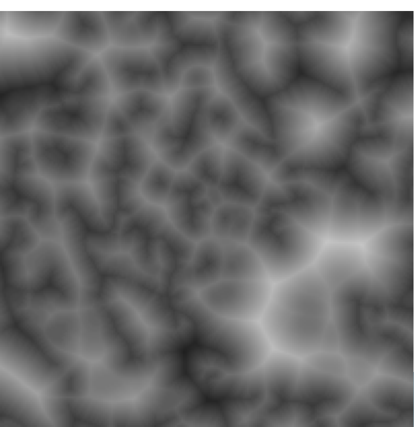
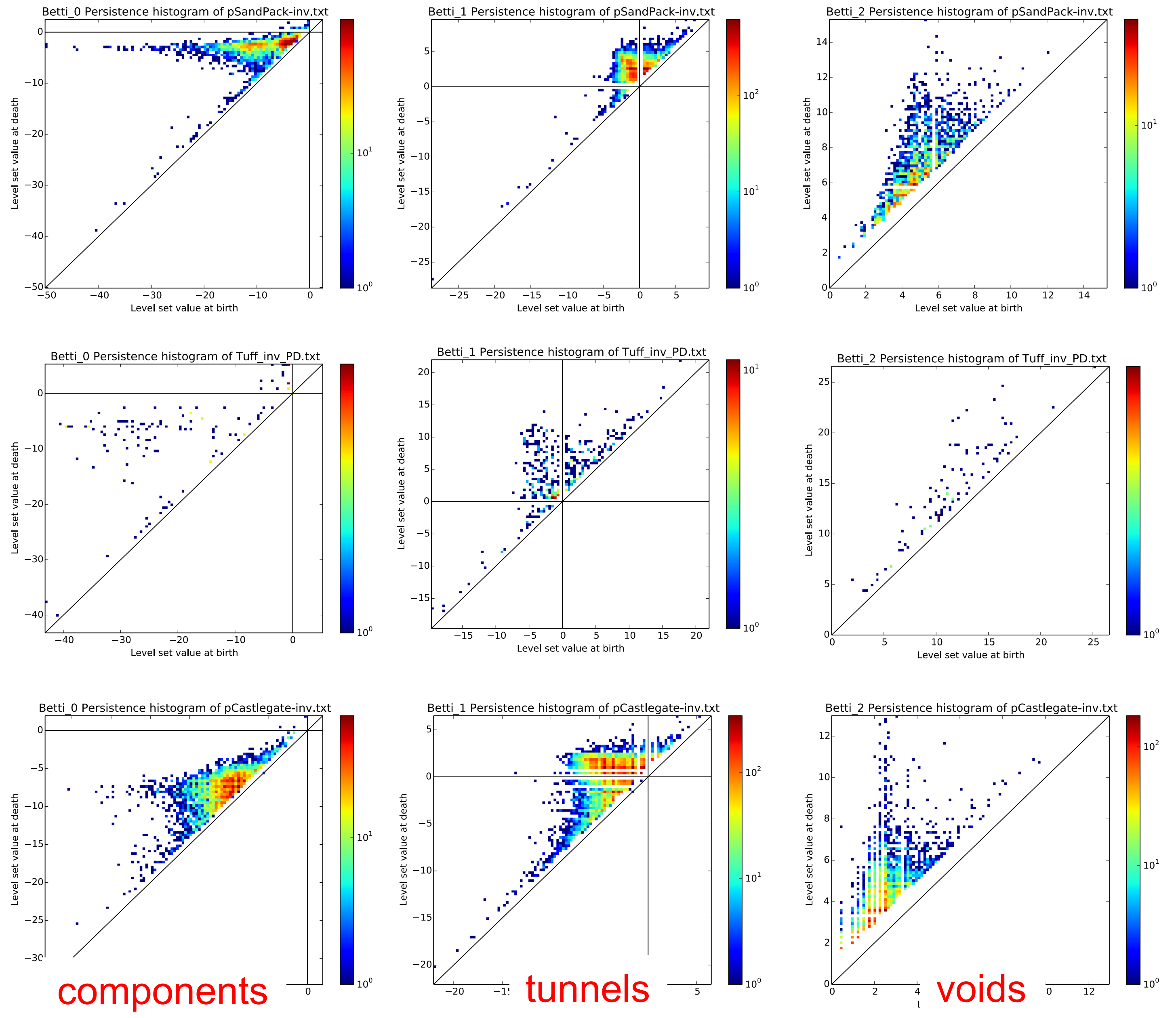
Sand, Volcanic Tuff, Sandstone









Conclusions

Discrete Morse theory of 3D grayscale image data gives:

- a good definition of critical points for functions on a 3D grid
- a single framework for watershed basins and medial axis skeletons
- topologically consistent region merging and simplification to remove “insignificant” features
- a chain complex for persistent homology computations, allowing structure characterisation

We acknowledge the support of the Australian Research Council through projects FT100100470 and DP110102964

Some observations…

Betti-0 births measure grain size as radius of max inscribed sphere.

Betti-0 deaths give maximal grain-contact resolution or overlap measure.

Sudden jump in Betti-1 births defines a percolating length scale.

Defined plateau in Betti-1 deaths is complementary percolating length scale.

Number of Betti-1 pairs with $b<0$, $d>0$ is genus of grain phase.

Betti-1 pairs with $b<0$, $d<0$ signal highly non-convex grains (ie. consolidated)

Symmetry in Betti-1 PD signals balance between pore and grain phases

Betti-2 PD measures geometry of pores.

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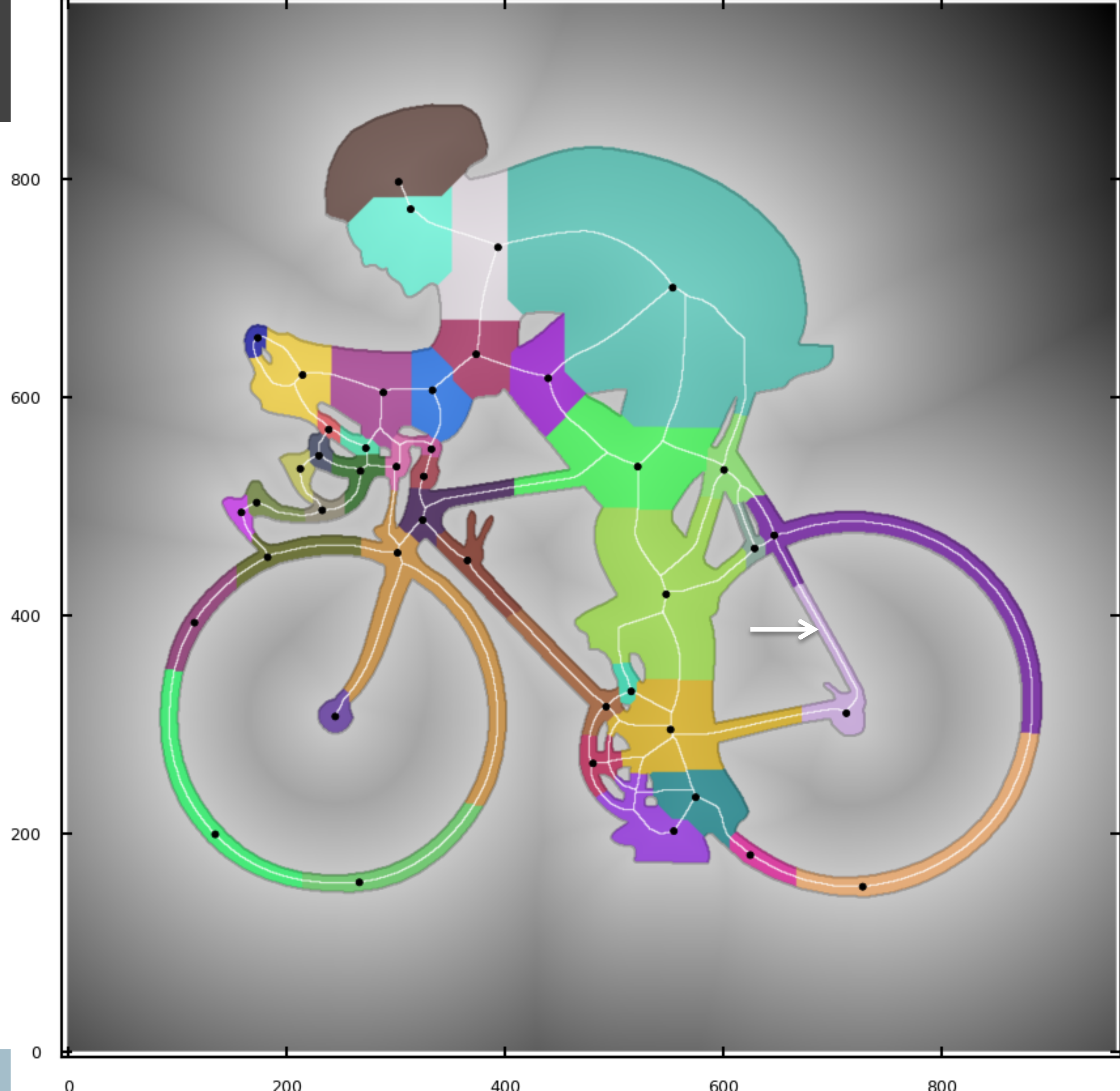
Skeleton and partition derived using simple steepest-descent pairing from ProcessLowerStar

Notice that some boundaries between watershed regions follow the grid lines too closely.



Skeleton and partition derived using newer ideas for error corrections on gradient flow.

Notice the much better geometric fidelity of the watershed boundaries.