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NOTETAKER CHECKLIST FORM

(Complete one for each talk.)

Name: Malgorzata Marciniak **Email/Phone:** mmarciniak@lagcc.cuny.edu 5734620411

Speaker's Name: Vanessa Robins

Talk Title: Insights from the persistent homology analysis of porous and granular materials

Date: 10 / 04 /2018 **Time:** 9 :30 am / pm (circle one)

Please summarize the lecture in 5 or fewer sentences:
Persistent homology is implemented for the analysis of 3 dimensional images obtained by X-ray micro CT. The code package, diamorse, for computing skeletons, partitions, and persistence diagrams from 2D and 3D images is available on GitHub. This software enables to explore the connections between topology, geometry and physical properties of sandstone rock cores and granular packings.

CHECK LIST

(This is **NOT** optional, we will **not pay** for **incomplete** forms)

- ☑ Introduce yourself to the speaker prior to the talk. Tell them that you will be the note taker, and that you will need to make copies of their notes and materials, if any.
- ☑ Obtain ALL presentation materials from speaker. This can be done before the talk is to begin or after the talk; please make arrangements with the speaker as to when you can do this. You may scan and send materials as a .pdf to yourself using the scanner on the 3rd floor.
  - **Computer Presentations**: Obtain a copy of their presentation
  - **Overhead**: Obtain a copy or use the originals and scan them
  - **Blackboard**: Take blackboard notes in black or blue **PEN**. We will **NOT** accept notes in pencil or in colored ink other than black or blue.
  - **Handouts**: Obtain copies of and scan all handouts
- ☑ For each talk, all materials must be saved in a single .pdf and named according to the naming convention on the "Materials Received" check list. To do this, compile all materials for a specific talk into one stack with this completed sheet on top and insert face up into the tray on the top of the scanner. Proceed to scan and email the file to yourself. Do this for the materials from each talk.
- ☑ When you have emailed all files to yourself, please save and re-name each file according to the naming convention listed below the talk title on the "Materials Received" check list. (*YYYY.MM.DD.TIME.SpeakerLastName*)
- ☑ Email the re-named files to notes@msri.org with the workshop name and your name in the subject line.

Insights from the persistent homology analysis of porous and granular materials

Vanessa Robins

Applied Mathematics, RSPE, ANU

ARC Future Fellowship
FT140100604

ARC Discovery Projects
DP1101028, DP0666442

overview

- X-ray micro CT image acquisition, reconstruction, analysis
  - Segmentation into phases, e.g. “rock” and “pore”
  - Geometry via the Signed Euclidean Distance Function

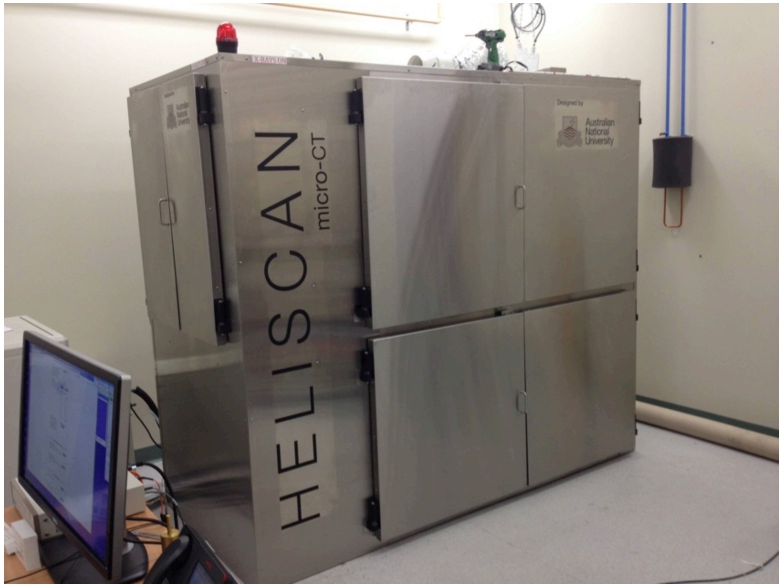
- Persistent homology from images
  - via (discrete) Morse theory

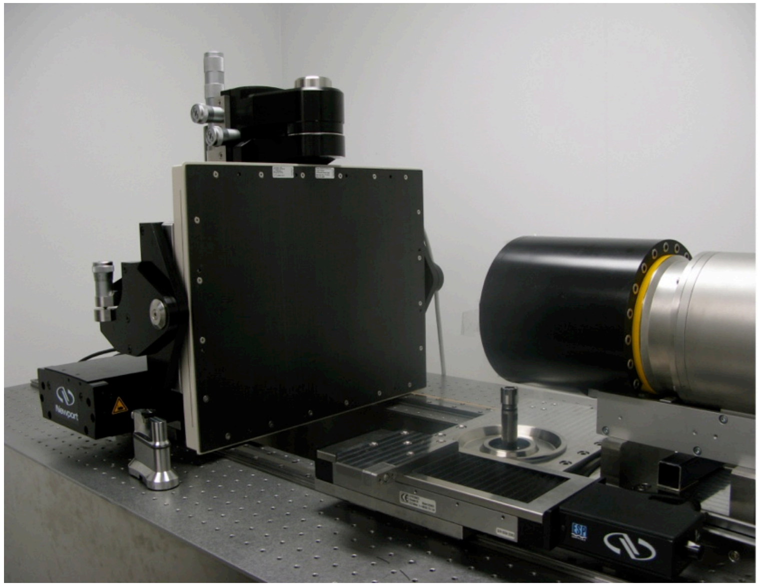
- Connecting persistent homology to physical properites.
  - consolidation of sandpacks versus sandstones
  - percolating length scales in porous materials
  - permeability of 2D and 3D models
  - trapping in two-phase fluid flow experiments

Above covers work with the Applied Maths micro CT group and
Adrian Sheppard, Anna Herring, Moh Saadatfar, Olaf Delgado-Friedrichs, Peter Wood

ANU lab-scale micro-CT facility

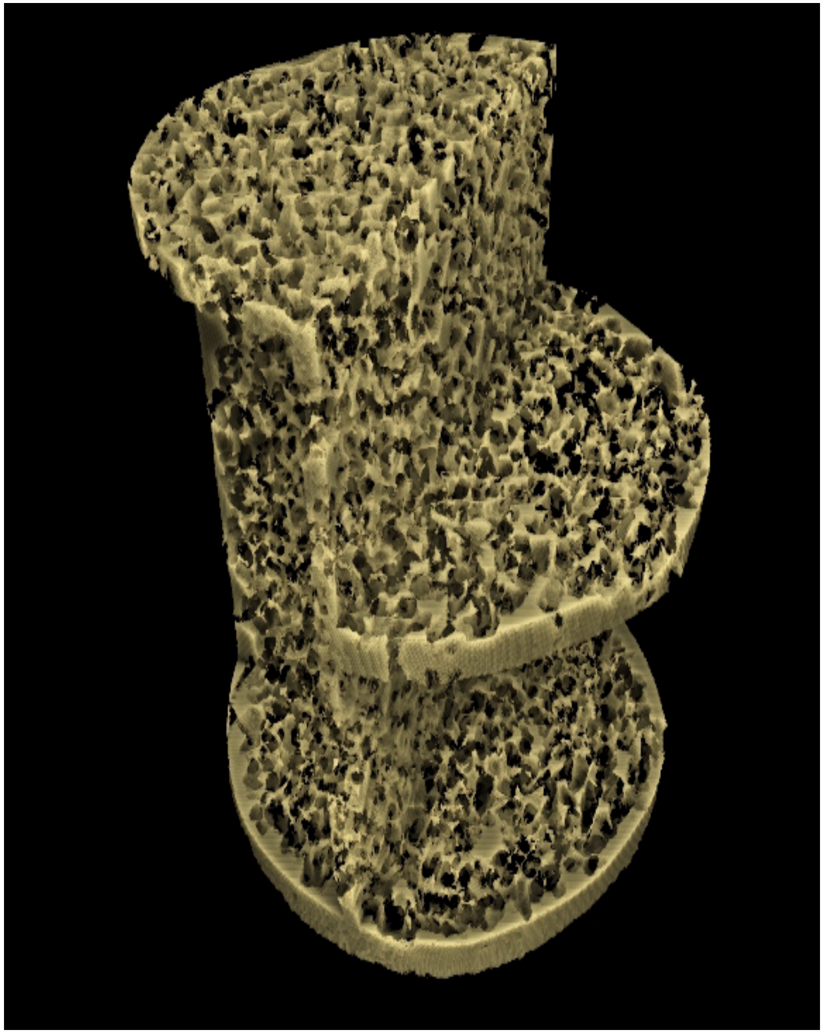
- In continual development since 2000, over 30 staff and students involved in past 15 years (lead by Mark Knackstedt, Tim Senden, Adrian Sheppard)
- x-ray sources and detectors “off the shelf”
- standard resolution down to ~2 microns on samples up to ~150 mm long
- latest machines achieve submicron resolution on ~ 2 mm samples.
- in-house acquisition protocols (Heliscan), and reconstruction,
- image segmentation and quantitative analysis (mango, diamorse) and visualisation software (Drishti)
- samples include porous and granular materials, fossils, insects, plants.



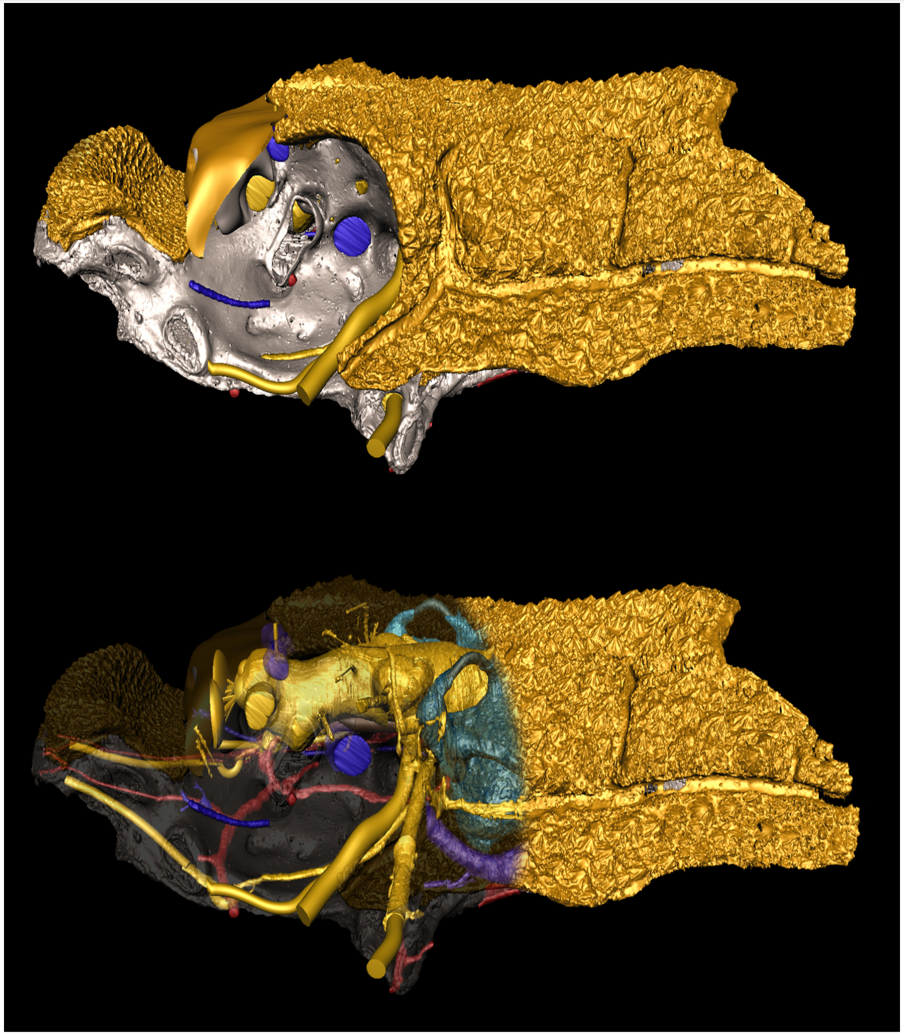


Sheppard et al. “Techniques in Helical Scanning” *Nuclear Instruments and Methods in Physics Research B* vol 324 (2014): 49–56.

sample applications



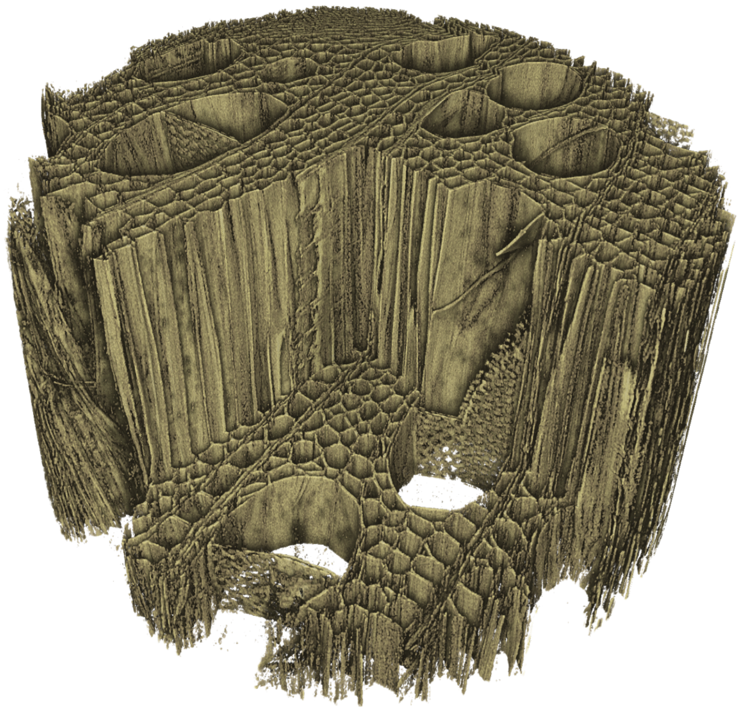
rock core



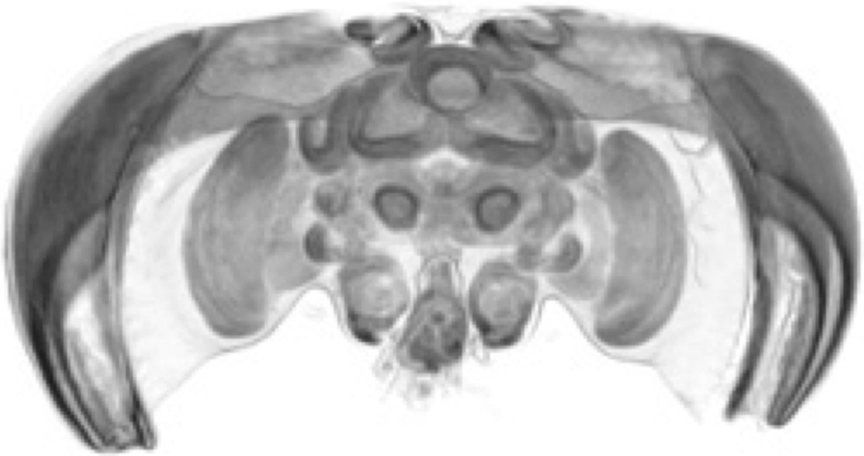
400 MYO placoderm fish

figures obtained at the ANU micro CT facility, volume rendering using Drishti

sample applications



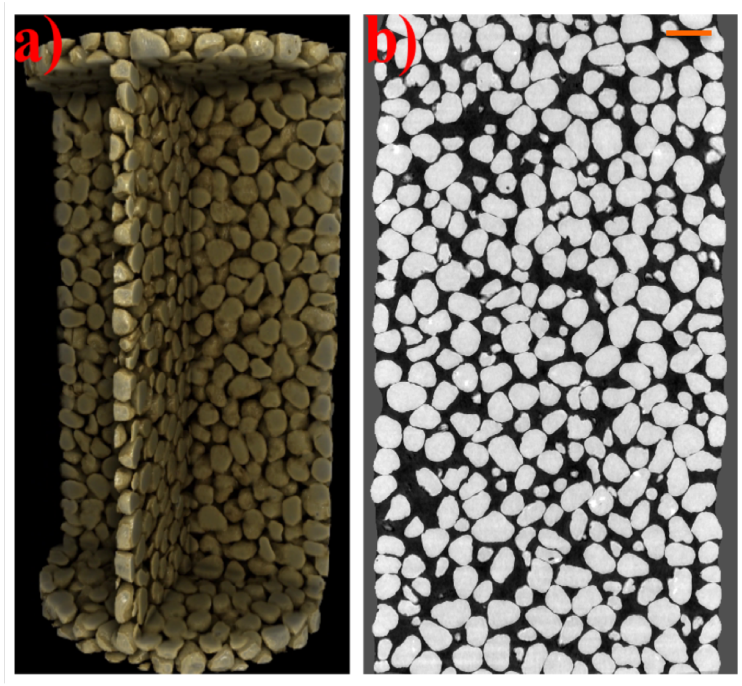
English willow
(from a professional cricket bat)



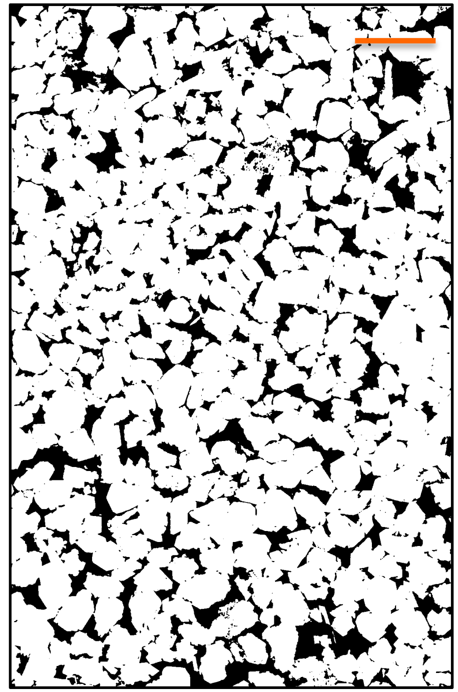
bee brain cavity
(imaged with osmium staining)

figures obtained at the ANU micro CT facility, volume rendering using Drishti

granular and porous materials

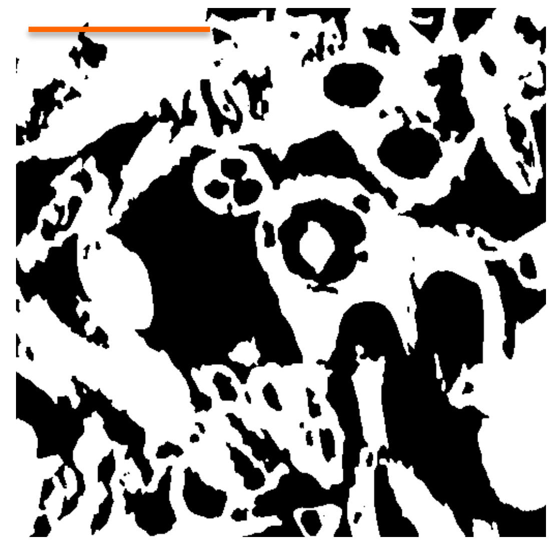


Ottawa sand



Clashach sandstone

1mm scale bars



Mt Gambier limestone

Want accurate geometric and topological characterisation from x-ray micro-CT images

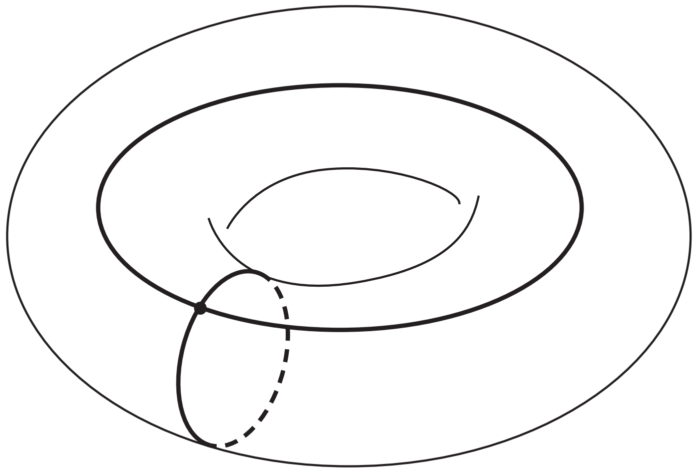
- pore and grain size distributions, structure of immiscible fluid distributions
- adjacencies between elements, network models

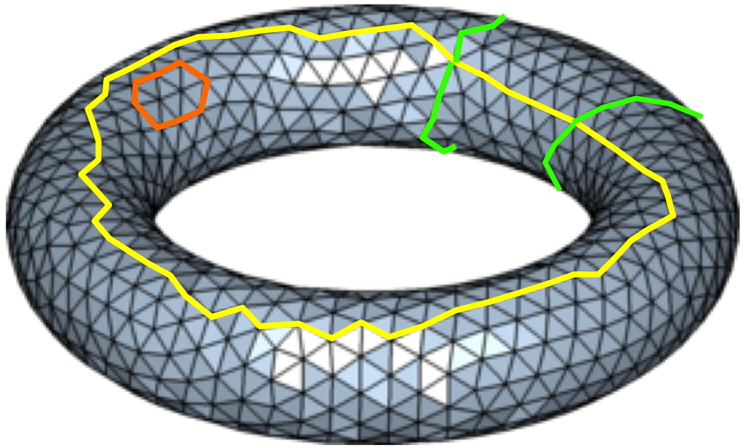
Understand how these quantities correlate with physical properties such as

- diffusion, permeability, trapping capacity, mechanical response to load.

figures obtained at the ANU micro CT facility

homology





$\beta_0 = 1,\ \beta_1 = 2,\ \beta_2 = 1$

Manifold | Cell complex

C_i = formal sums of i-dimensional cells

$\partial : C_i \rightarrow C_{i-1}$ is the boundary operator. $\partial\,\partial = 0$

Boundaries are the image space of ∂

Cycles are the null space of ∂

Two cycles are homologous when their difference is a boundary.

The homology group is $H_i(X) = \text{null } \partial \,/\, \text{im } \partial$

Betti numbers, β_i, are the ranks of the homology groups

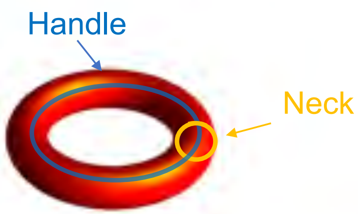
image credit: torus mesh from http://persson.berkeley.edu/distmesh/

homology

Theorems: [1] homology is independent of the way a space is 'cut up' into cells.
[2] homology is invariant up to homotopy
(deformation that maintains connectivity)

for a subset of R^3, the possible non-zero Betti numbers are

$$(\beta_0, \beta_1, \beta_2) =$$
(Objects, Loops, Cavities)



Solid Object:	(1,1,0) $\chi = 0$	(1,2,0) $\chi = -1$	(1,3,0) $\chi = -2$
Hollow Object:	(1,2,1) $\chi = 0$	(1,4,1) $\chi = -2$	(1,6,1) $\chi = -4$

the Euler characteristic $\chi = \beta_0 - \beta_1 + \beta_2$ is another topological invariant

Topological property:

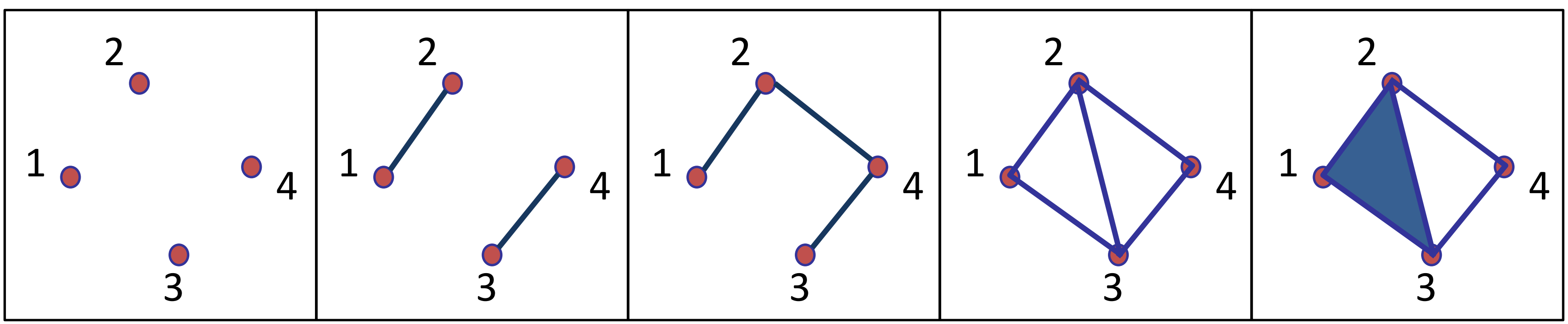
Betti numbers are independent of the "size" of the topological feature so small "noisy" features contribute as much as large ones.

persistent homology

idea is to measure topology of a growing sequence of spaces (a filtration)

$$X_0 \subset X_1 \subset X_2 \cdots \subset X_n$$

$$H(X_0) \rightarrow H(X_1) \rightarrow H(X_2) \cdots H(X_n)$$



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{1, 2, 3, 4, [12], [34], [24], [13], [23], [123] }

persistent homology

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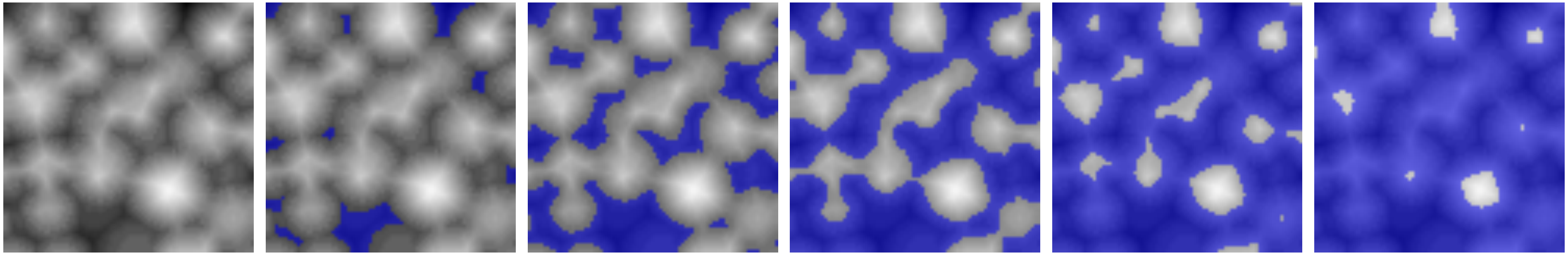
$$H(X_0) \to H(X_1) \to H(X_2) \cdots H(X_n)$$



this is the lower-level set filtration of a real-valued function:

$$X_h = \{x \text{ such that } f(x) \leq h\}$$

Each homology class is born at a parameter value *h = b* and dies (becomes a boundary) at a value *h = d*.
This gives us a set of intervals *(b,d)* for the filtration.

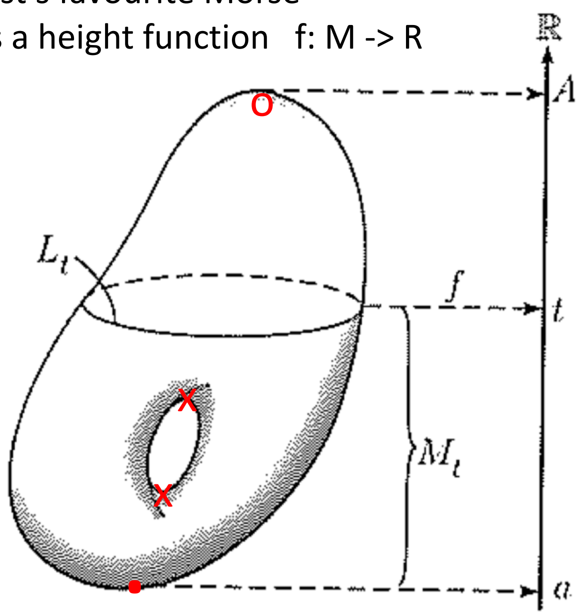
Morse theory

Suppose f: M -> **R** is a real valued function on a manifold, M.

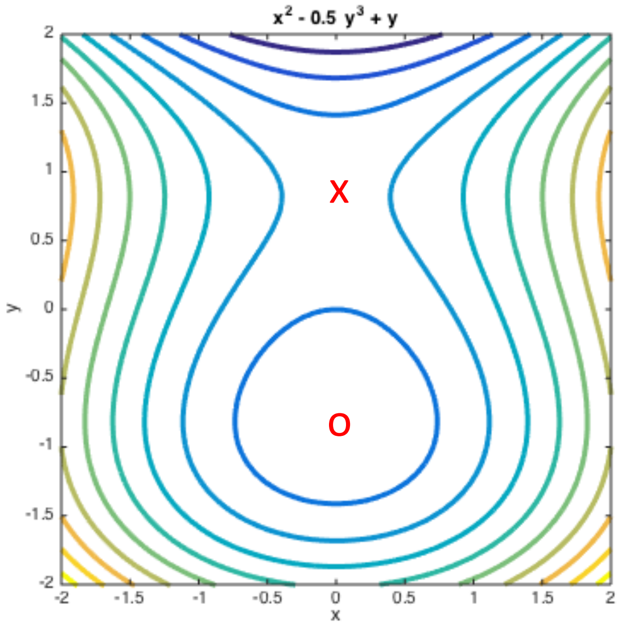
A filtration of M is defined by the lower-level sets of f:

$M_t = \{ x \text{ in } M \text{ such that } f(x) \leq t \}$

A topologist's favourite Morse function is a height function f: M -> R



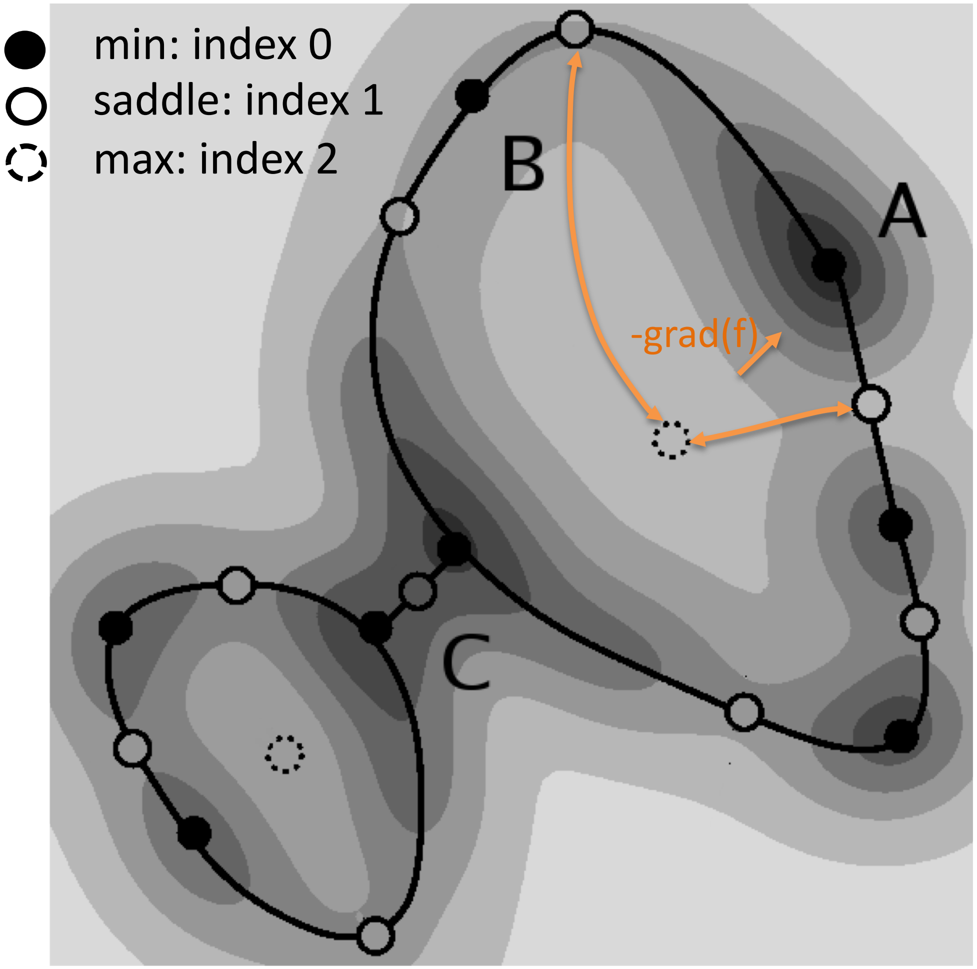
We will study f: R^n -> R, here illustrated as level sets in a contour plot:



Key insight of Morse theory: The topology of lower level sets, M_t, changes only when t passes through a critical value of f

Morse complex

The index of an isolated critical point is the number of descending directions



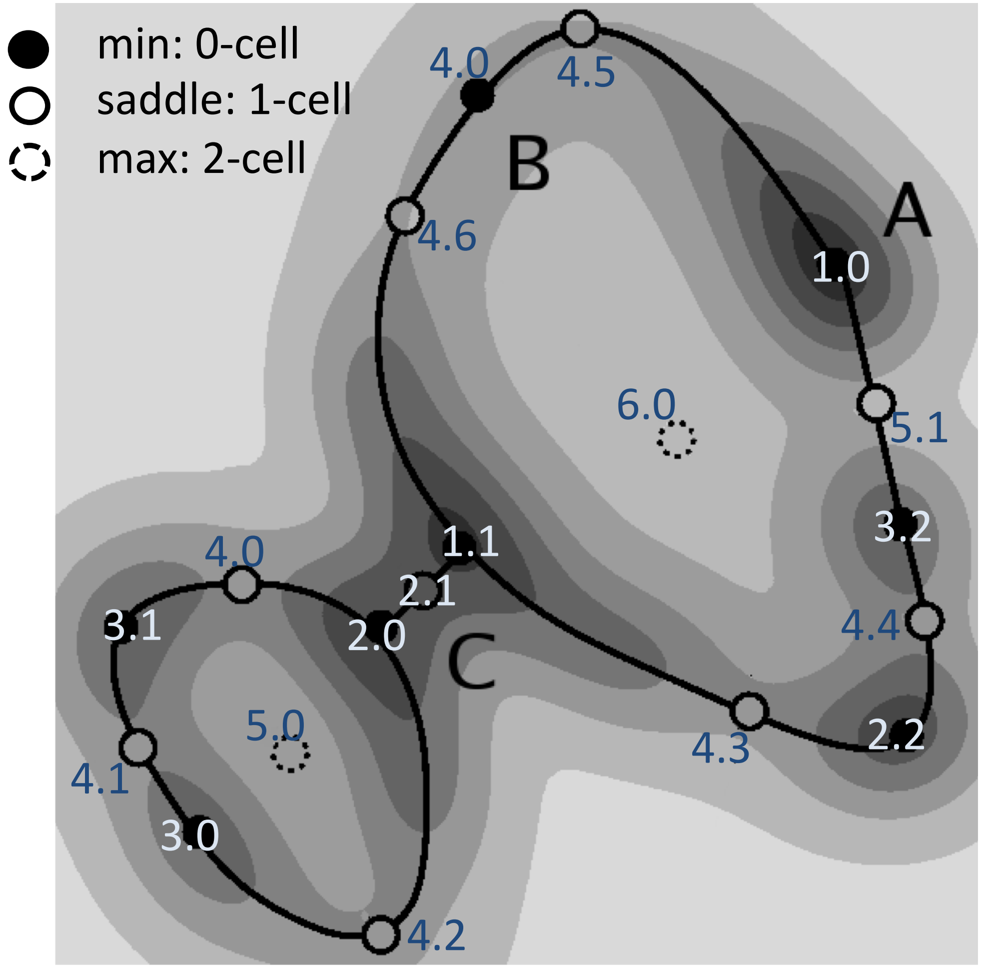
negative gradient flowlines show where a drop of water would flow

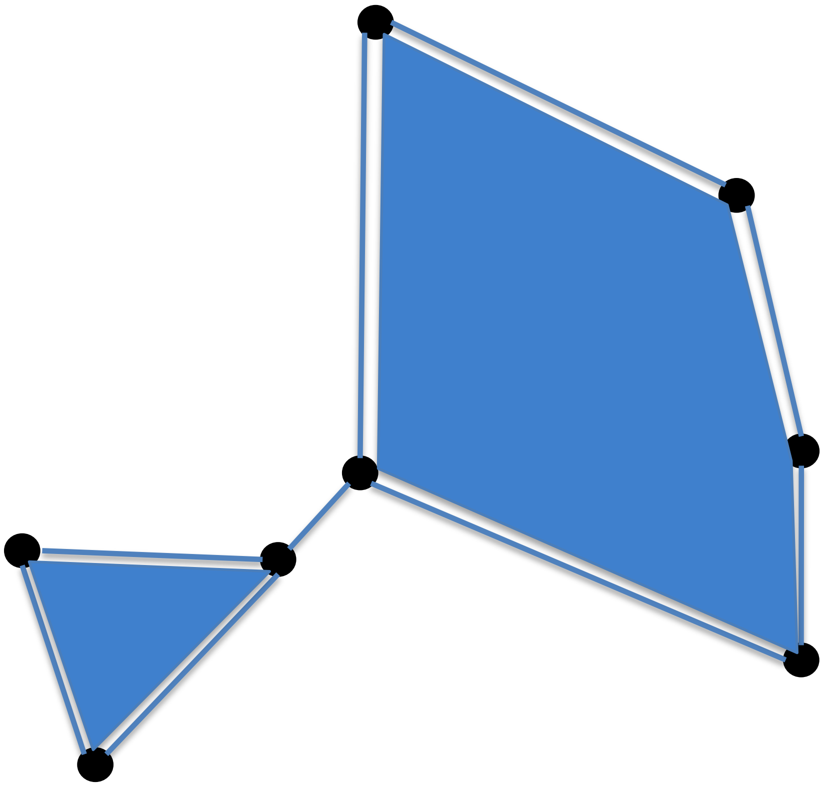
unstable manifold of an index-i critical point is an i-cell.

these flowlines define adjacencies between critical points in an (abstract) cell complex called the Morse Complex

filtration of the Morse complex

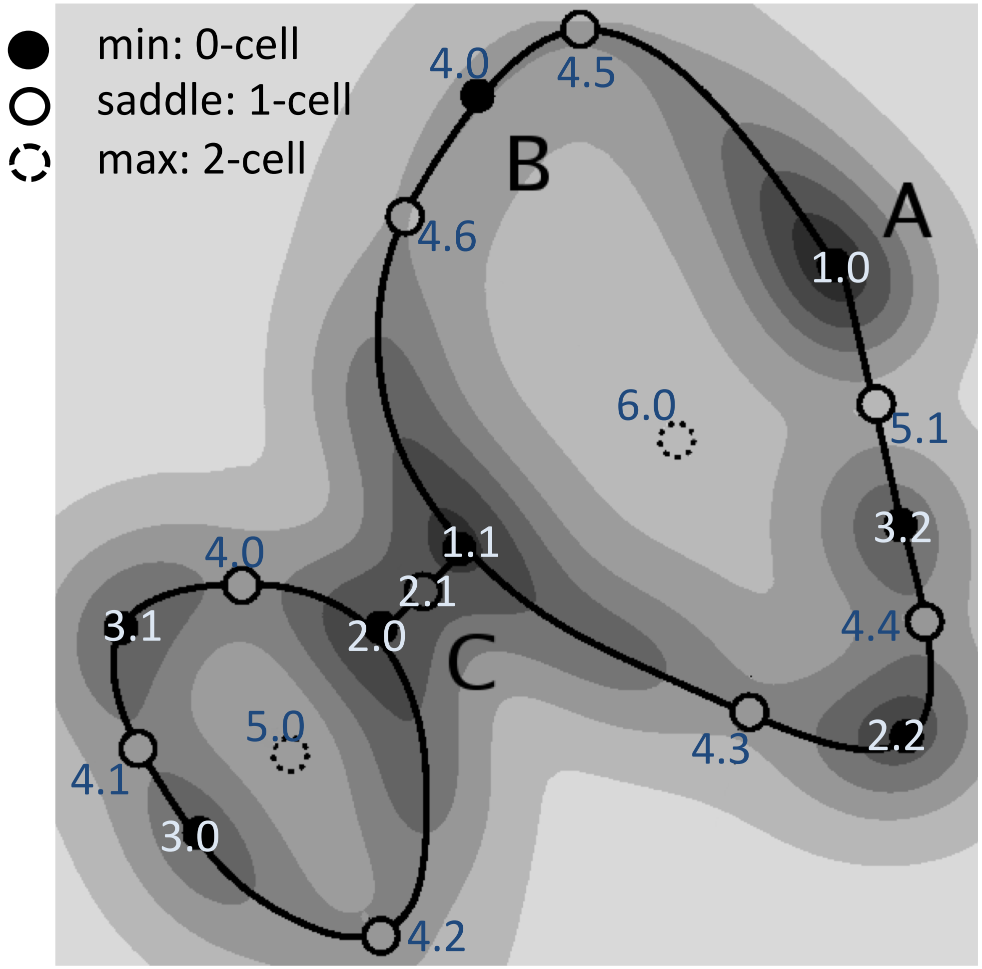
Order the critical points by function value to get a filtration of the cell complex

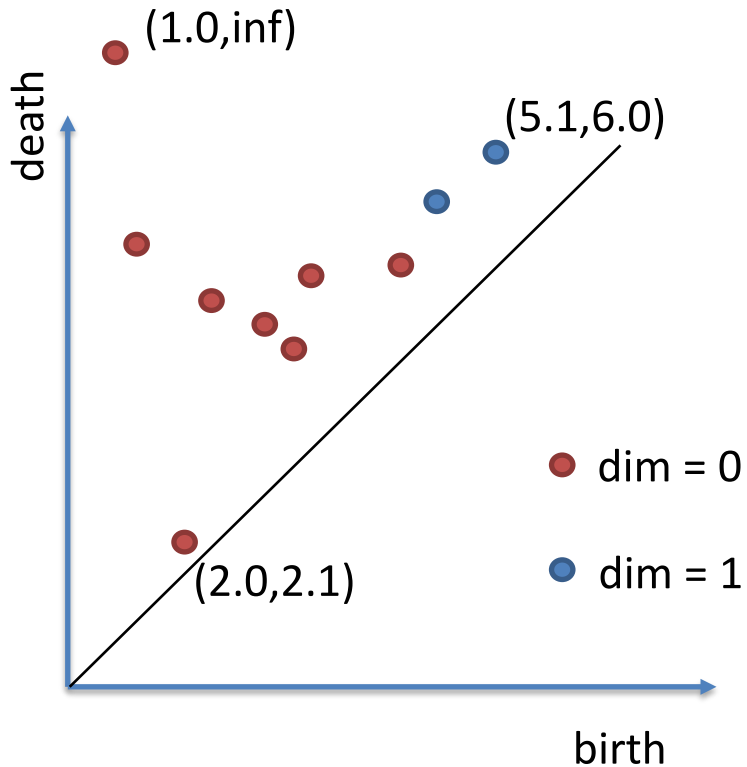




persistence diagram

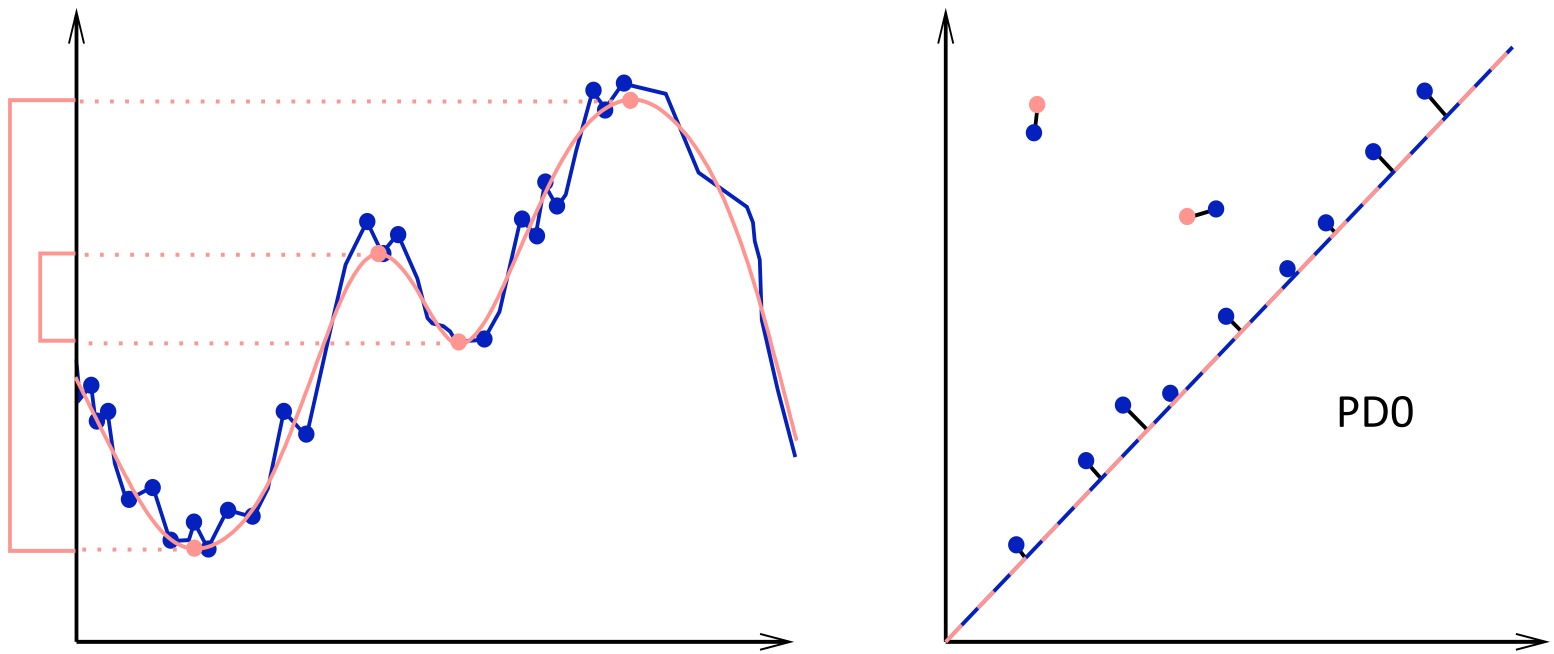
Order the critical points by function value to get a filtration of the cell complex





stability of persistence diagrams

The connection between Morse theory and persistent homology helped establish the stability of persistence diagrams [Cohen-Steiner, Edelsbrunner, Harer (2007)]



$d_H(\,PD(X), PD(Y)\,) \leq \|\, f_X - f_Y \,\|_\infty$

Figure 2: Left: two close functions, one with many and the other with just four critical values. Right: the persistence diagrams of the two functions, and the bijection between them.

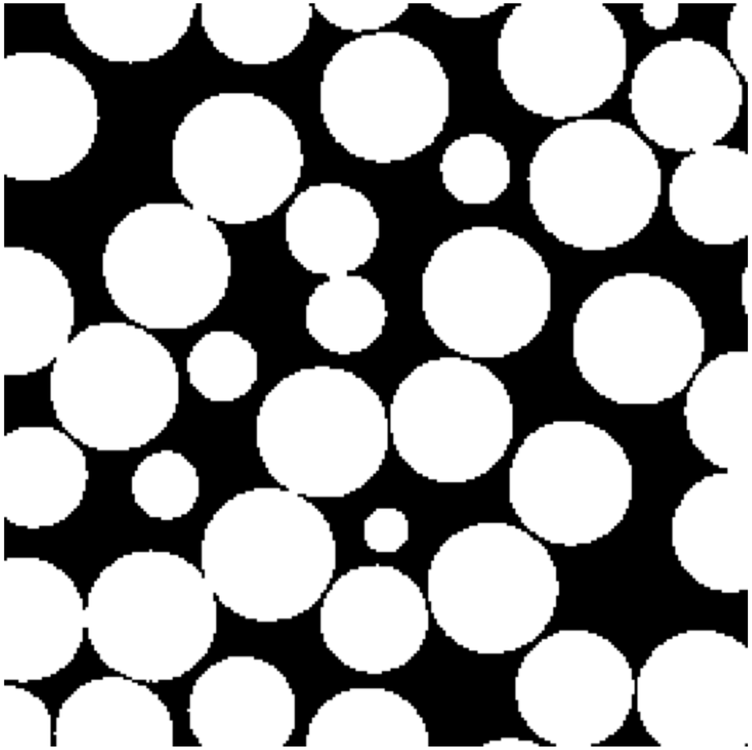
distance functions from images

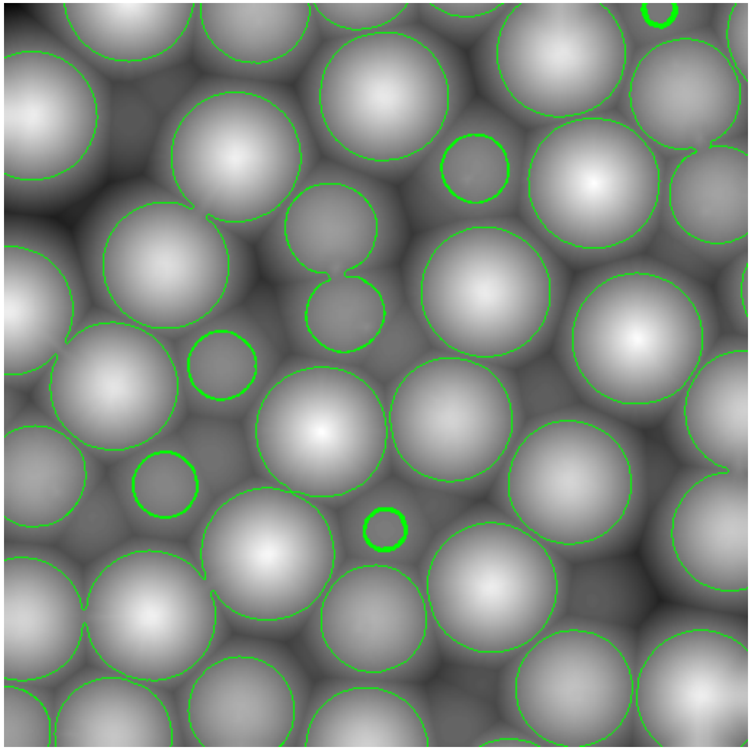
Segment an XCT image into
grain (white) and
pore (black) regions.

Compute the
Signed Euclidean Distance Transform:

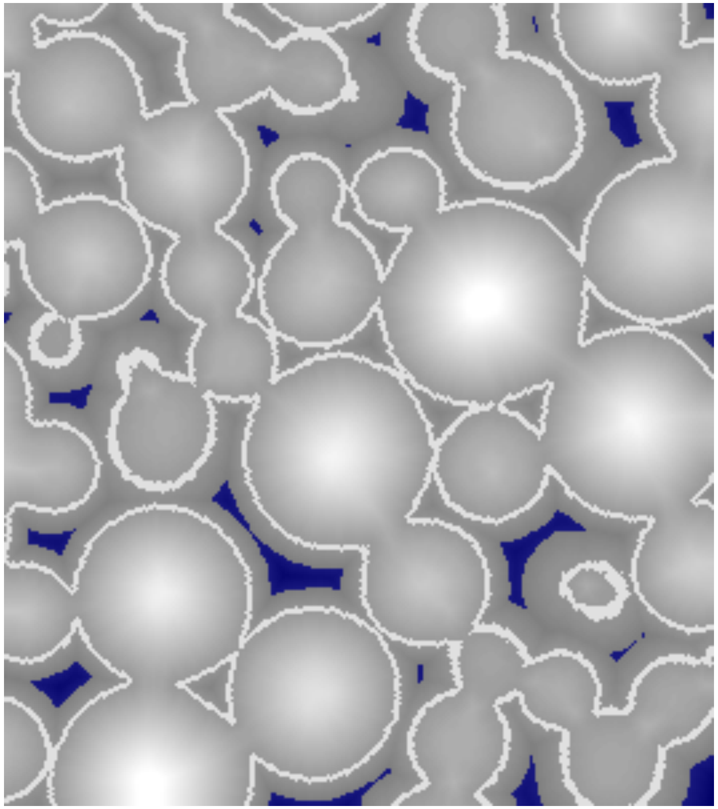
SEDT(x) = - dist(x, W) if x is in B

SEDT(x) = dist(x,B)   if x is in W

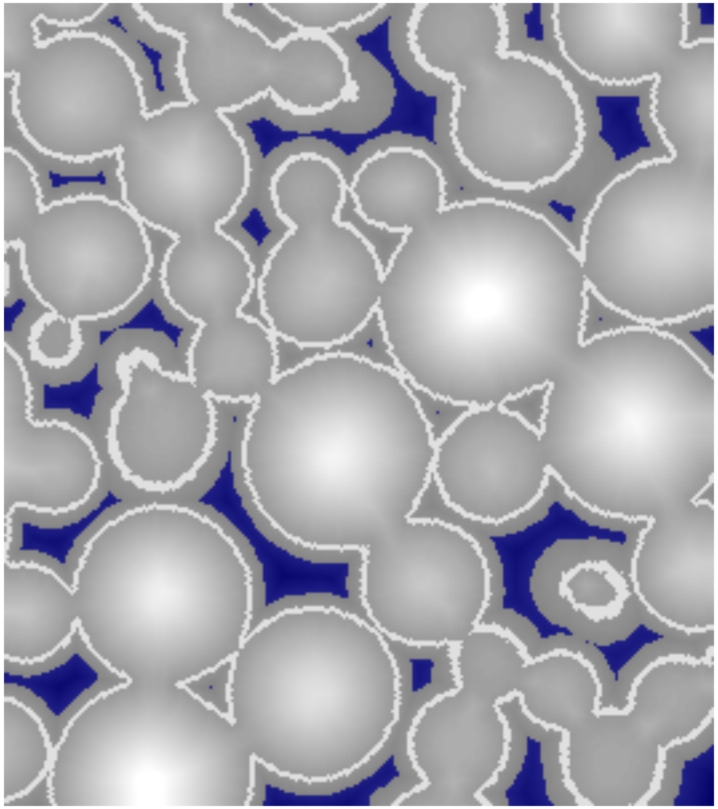




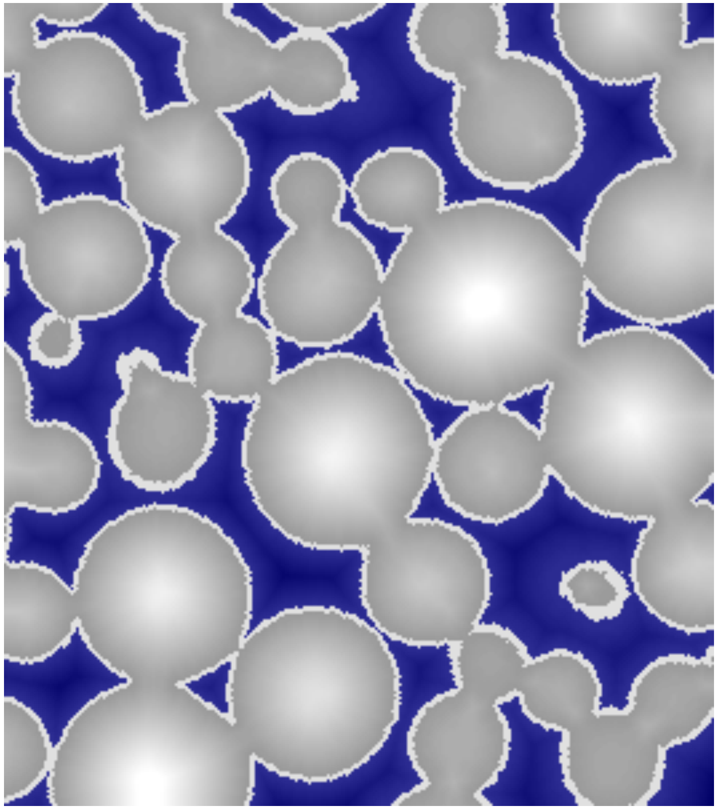
lower level set filtration



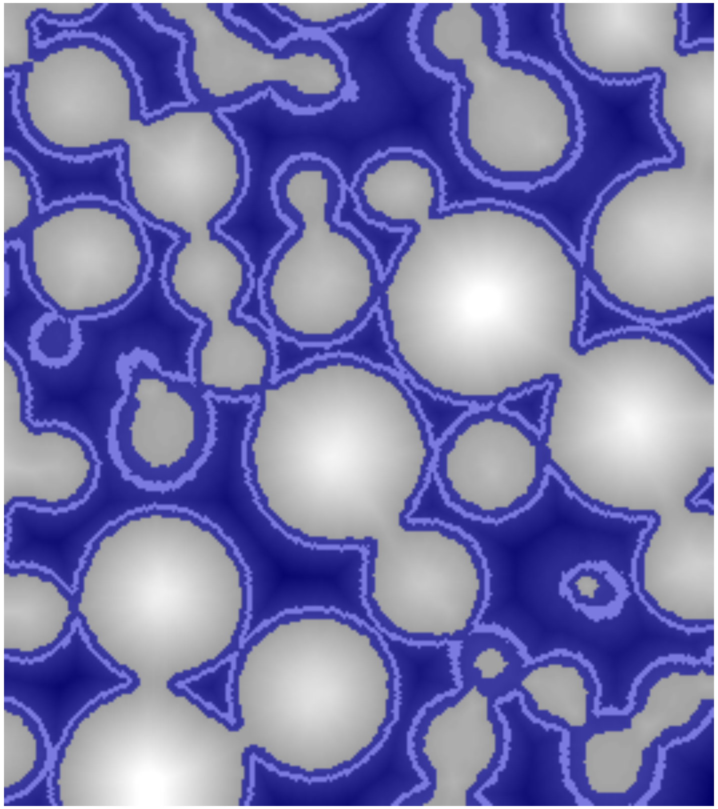
lower level set filtration



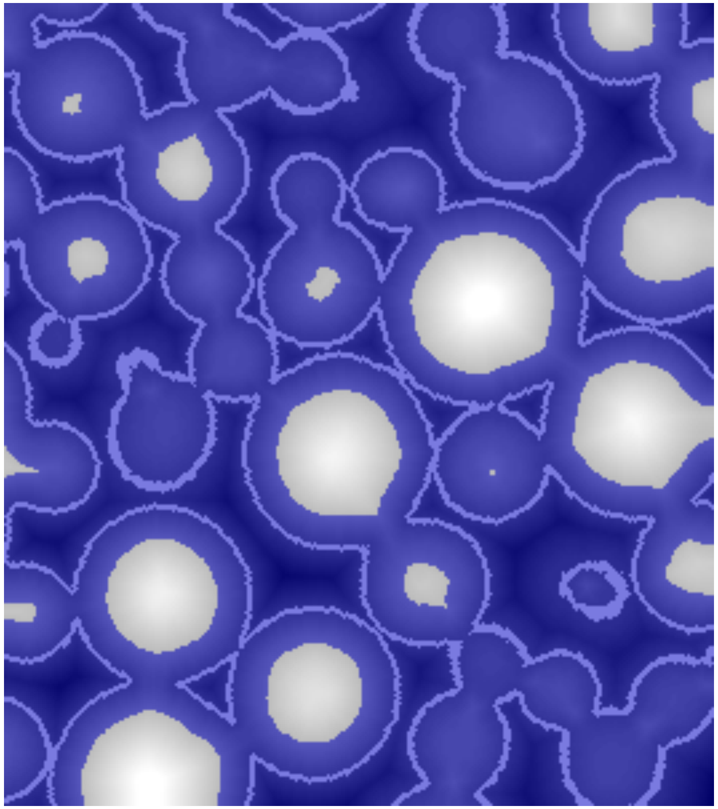
lower level set filtration



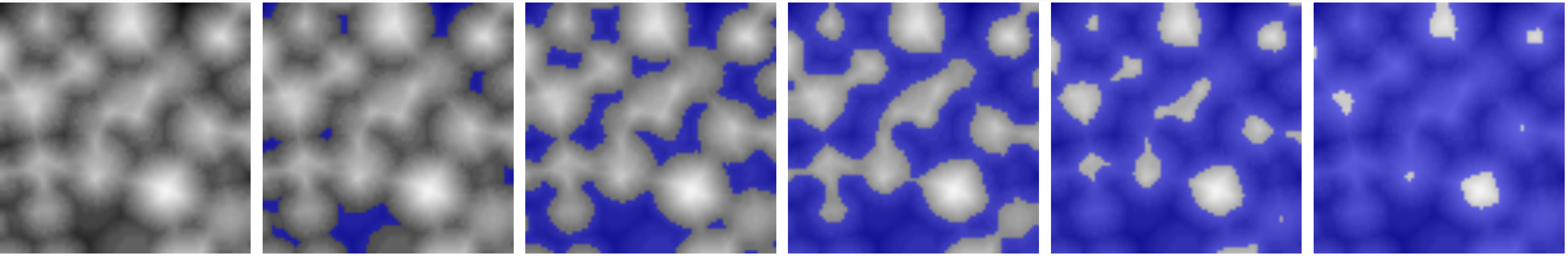
lower level set filtration

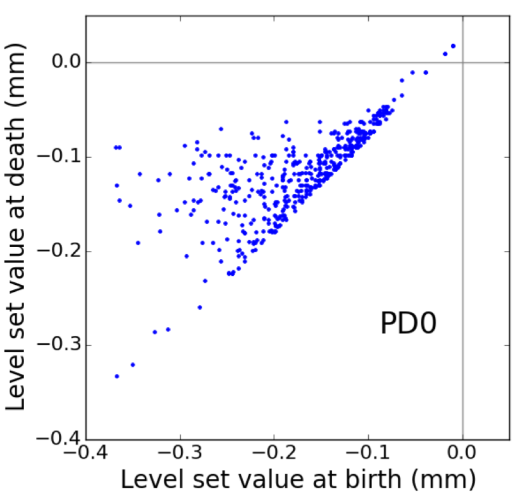


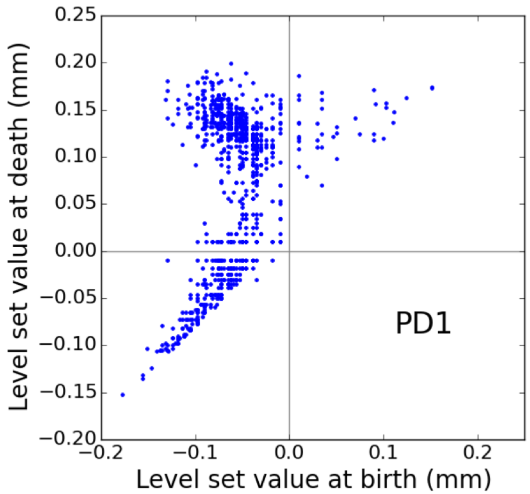
lower level set filtration

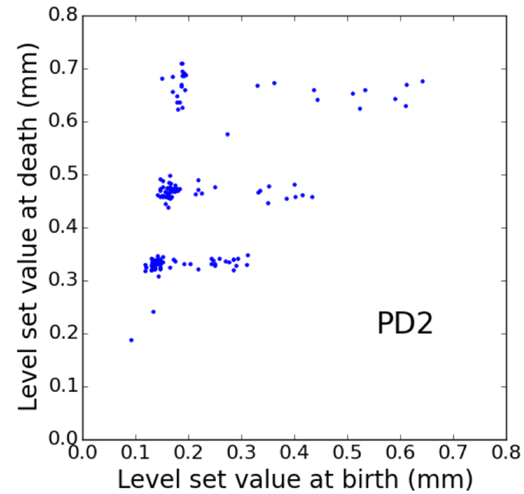


persistence diagrams of an SEDT









b < 0, d < 0

- birth = pore radius
- death = max pore throat

b < 0, d > 0

- birth = min throat in loop
  death = min grain-contact radius

b > 0, d > 0

birth = max grain contact

death = grain radius.

porous materials PD1

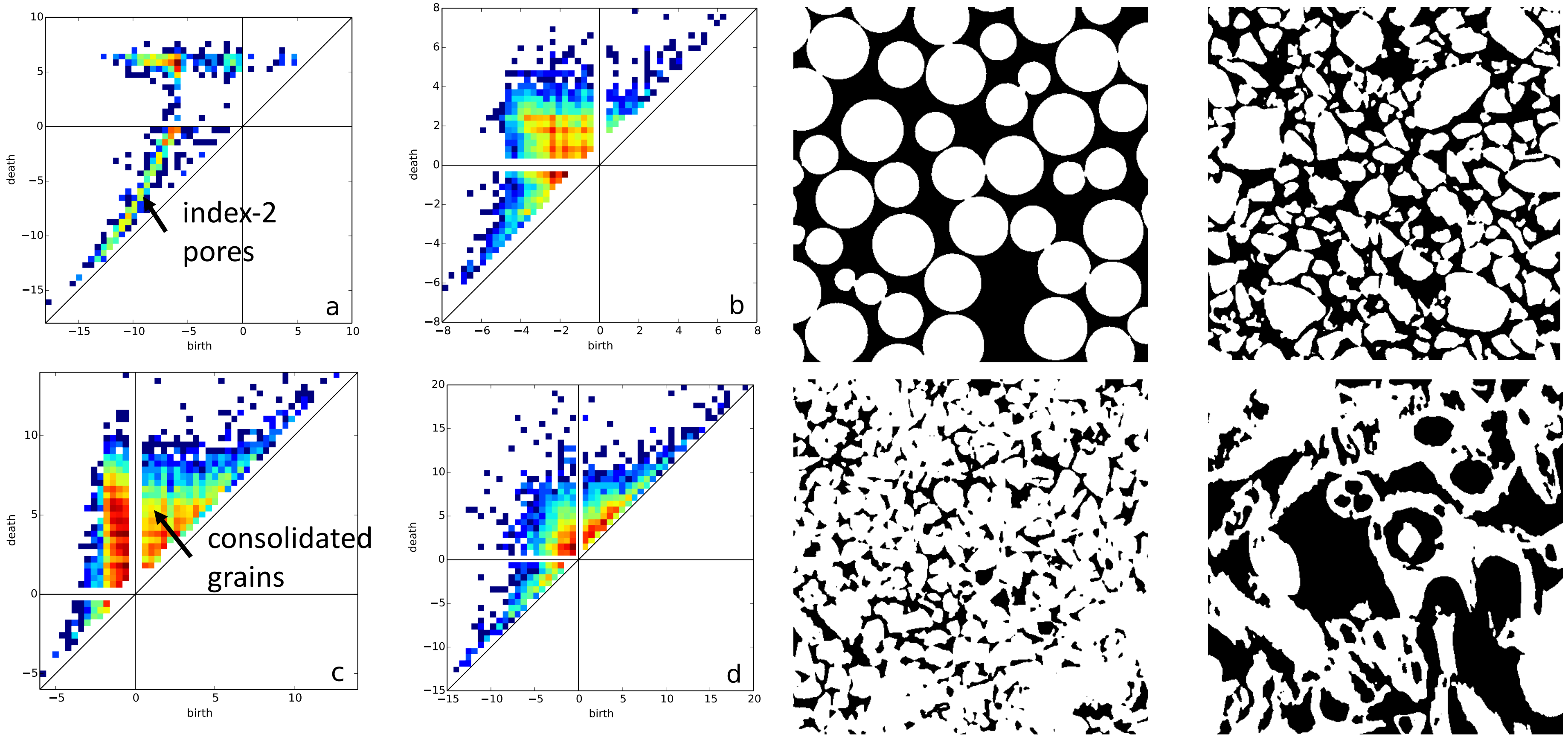
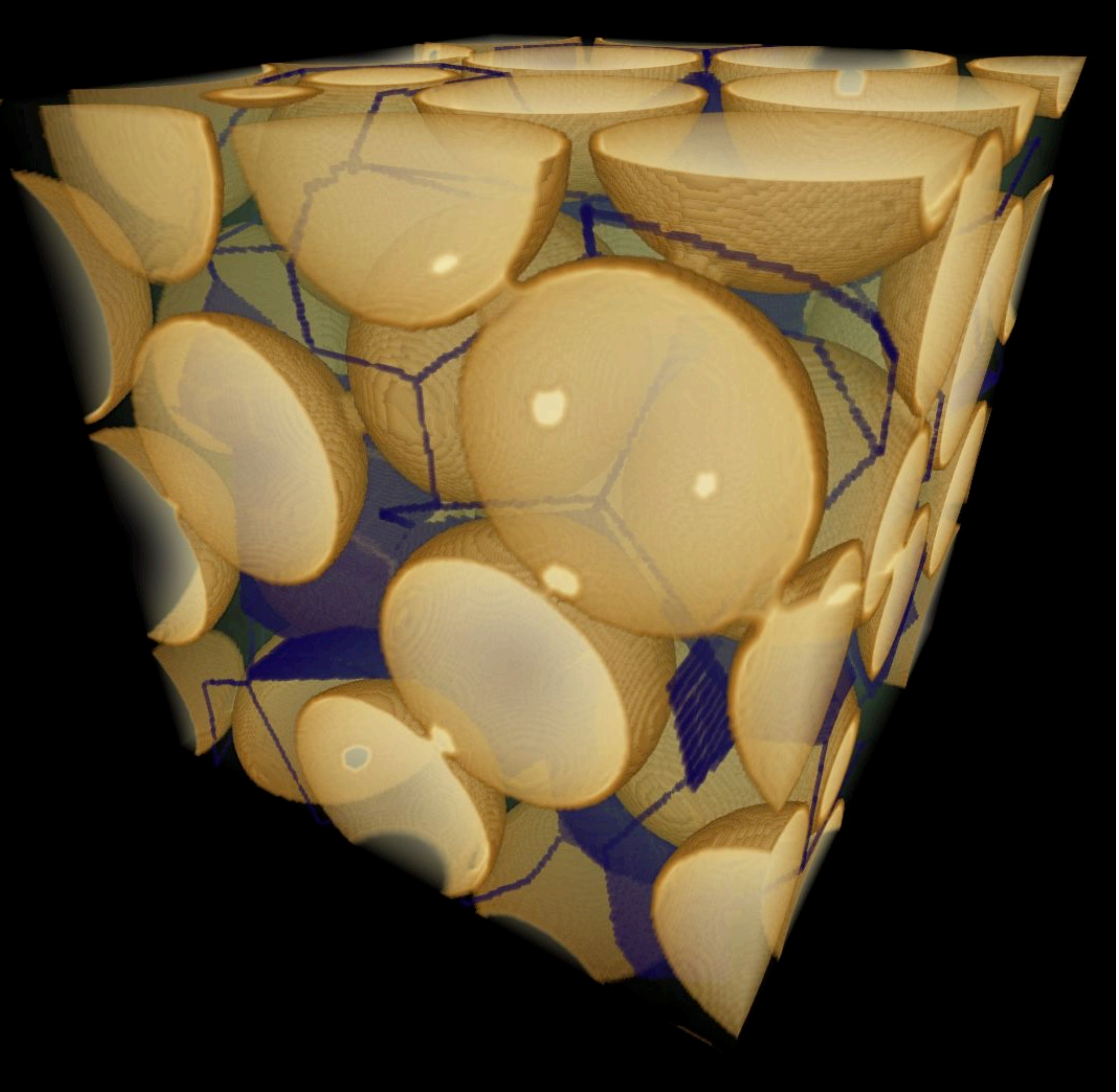


Fig. 3. Persistence diagrams (represented as 2D histograms of persistence pairs) for 1D cycles in the pore-space of four samples: (a) mono-disperse spherical bead pack, (b) polydisperse unconsolidated sand, (c) well-consolidated Castlegate sandstone, (d) fossiliferous Mt Gambier limestone.

PD1 diagrams show us the degree of consolidation of a sandstone

Delgado-Friedrichs, Robins, Sheppard. IEEE ICIP (2014)



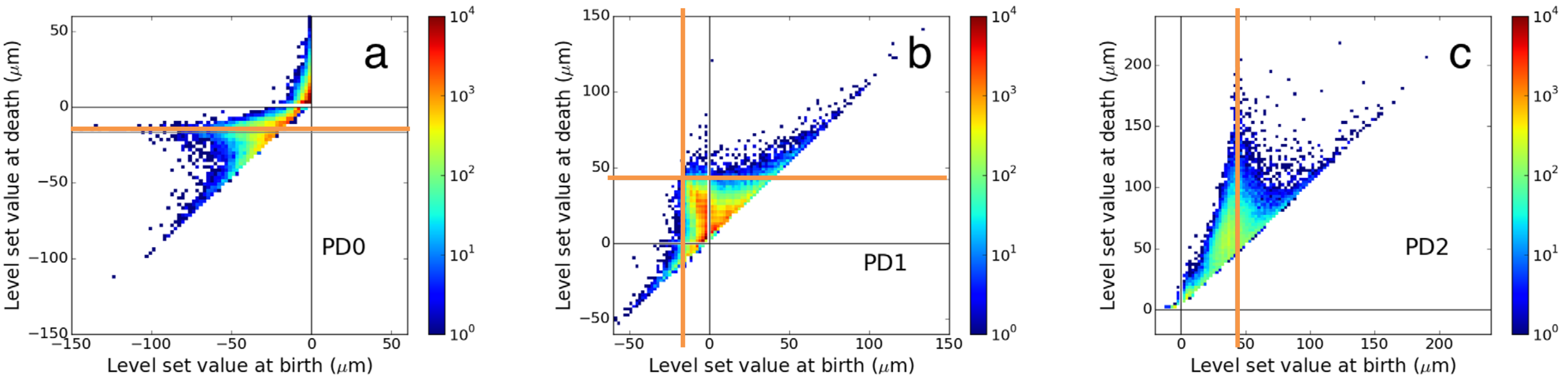
Skeleton derived from void phase of silica sphere packing.

Dark blue 2D patches show that the porespace is not well-modeled by a line skeleton.

Image by Olaf D-F using Voluminous a web-based version of Drishti, both apps developed at NCI Vizlab

percolating length scales in PDs

the percolating length is the maximal radius of a sphere that can move through the pore space
= threshold for which X_h connects opposite boundaries of the sample.



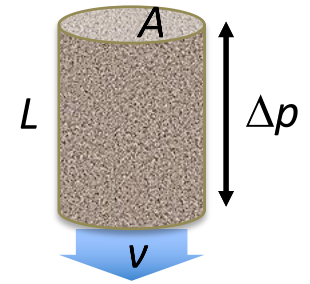
Persistence diagrams for SEDT of a sandstone micro CT image, 1280 cubed voxels
Critical percolating radii are significant features in the PDs
see: Robins, Saadatfar, Delgado-Friedrichs, Sheppard
“Percolating length scales… ” WRR (2016)

permeability

permeability k is defined by the Darcy relation between mean fluid velocity *v* measured by

- fluid flux *Q* through
- cross-sectional area *A* for
- pressure difference Δp
- over length *L* and
- fluid viscosity μ.

$$v = \frac{Q}{A} = \frac{k}{\mu}\frac{\Delta p}{L}$$



permeability is not the same as porosity (= pore vol frac)

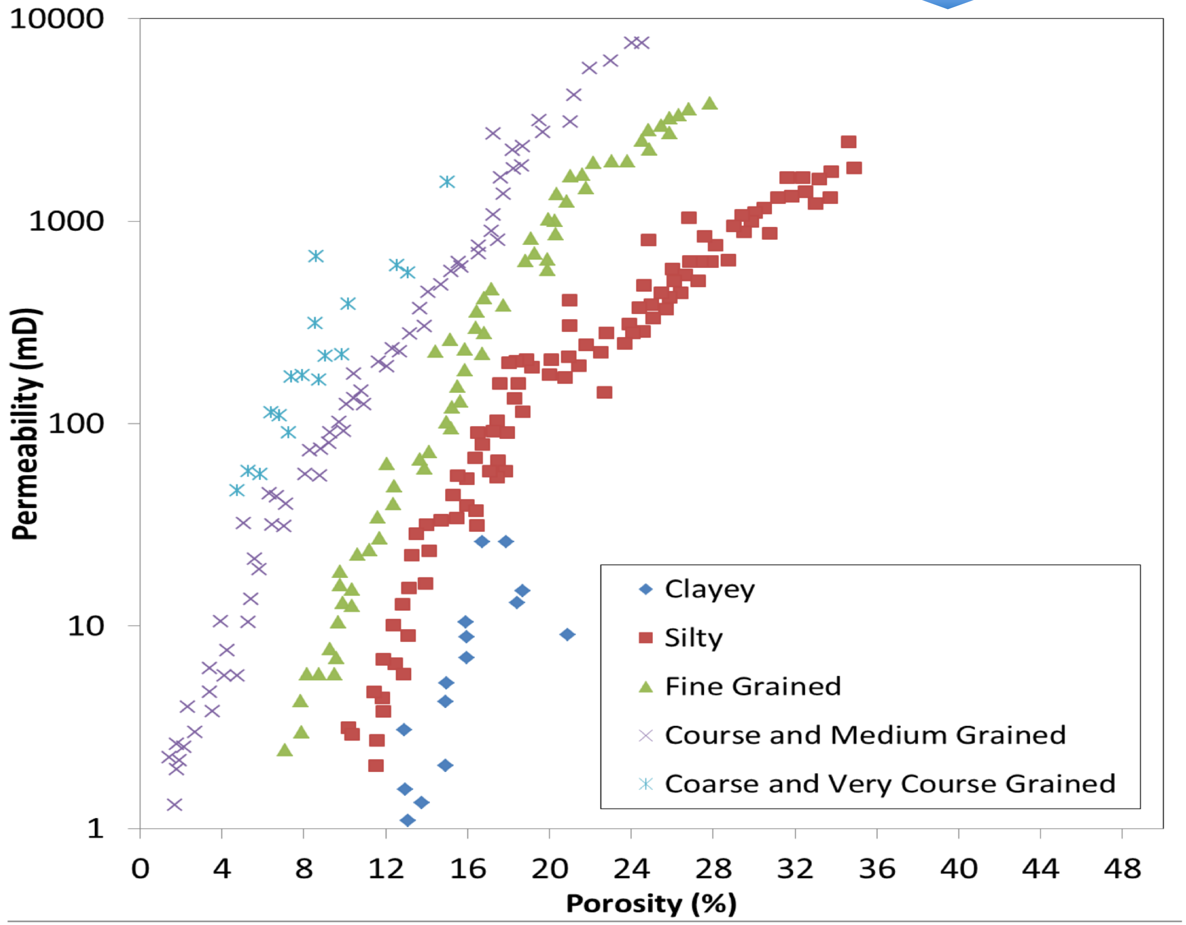


image after Tiab and Donaldson (1996)

permeability

Katz-Thompson cross-property model:
(PhysRevB 1986)

$$k = c{l_c}^2\left(\frac{\sigma}{\sigma_0}\right),$$

c geometric const (= 1/226)
l_c critical pore radius for percolation
(σ/σ_0) electrical conductivity rel to bulk

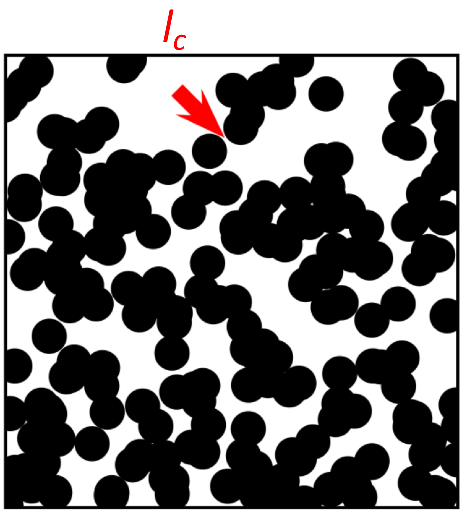


Image from Scholz et al. PRL 2012

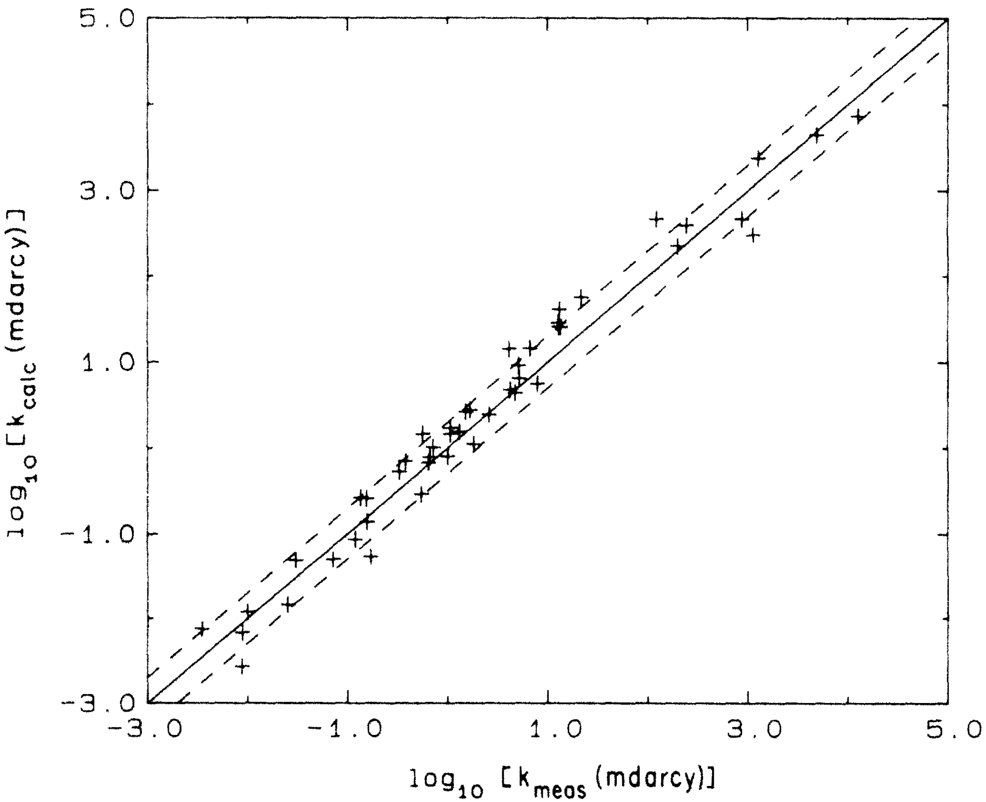


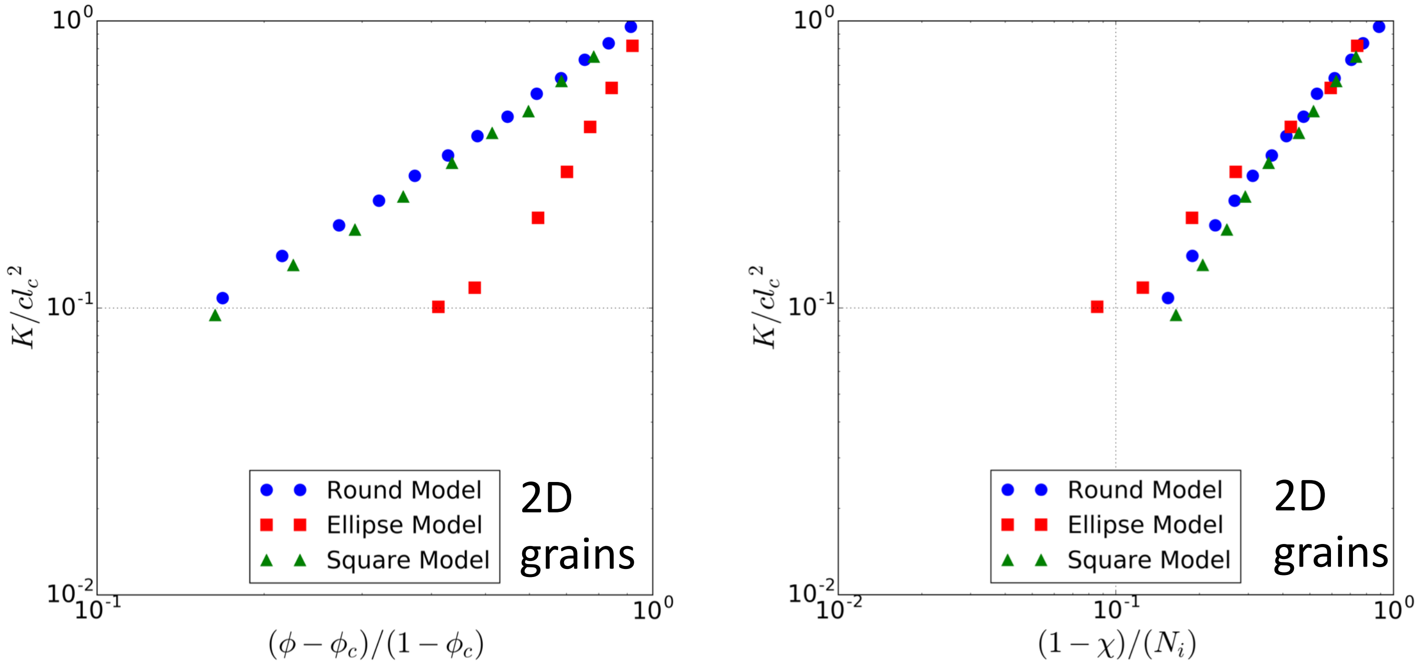
FIG. 2. Calculated permeability k_{calc} vs measured permeability k_{meas} for various sandstones and carbonates. The dashed lines indicate a factor of 2 deviation. Note that the unit of permeability is the millidarcy (md) $=10^{-11}$ cm^2.

Image from Katz, Thompson PRB 1986

permeability and topology

Scholz et al Phys Rev Lett (2012) propose (σ/σ_0) can be replaced by *$(1-\chi_0)/N = \beta_1/N$* for circular and elliptical (quasi) 2D grain models.

BUT a 3D version of the Scholz relationship does not hold
see: Liu, Herring, Robins, Armstrong
"Prediction of permeability from Euler characteristic of 3D images" SCA 2017



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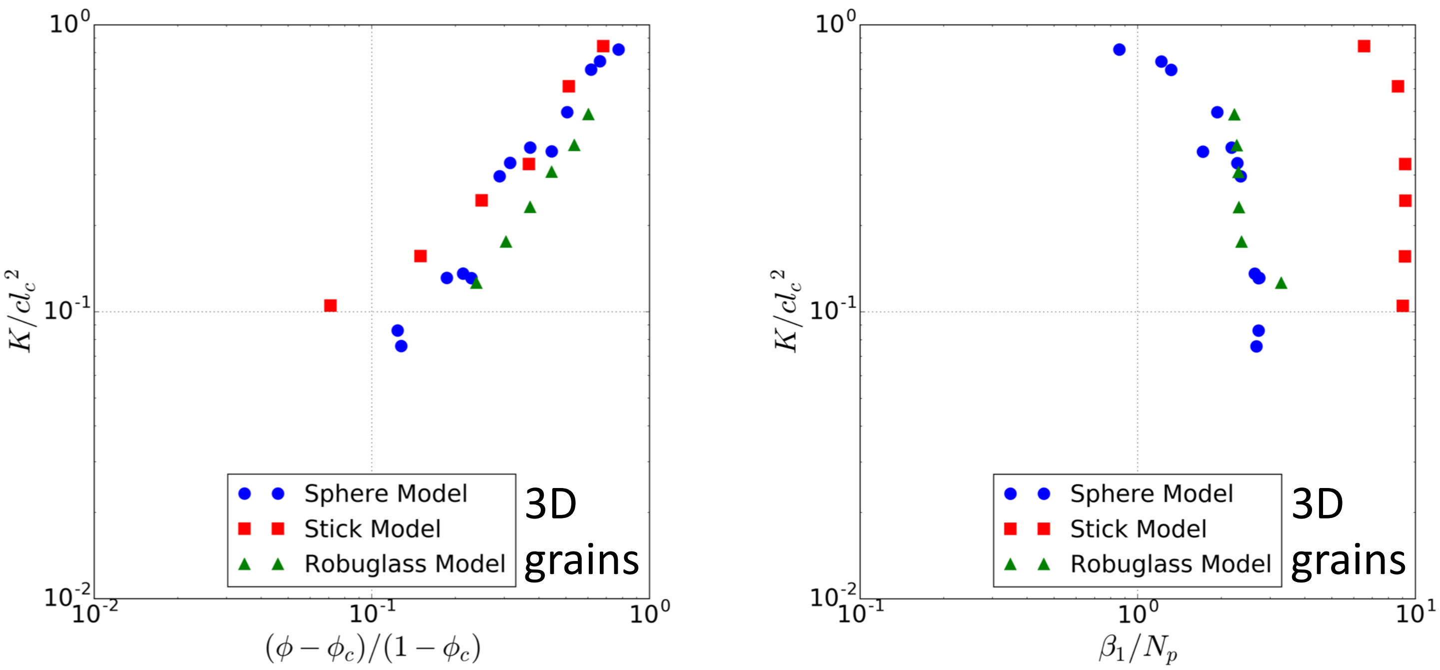
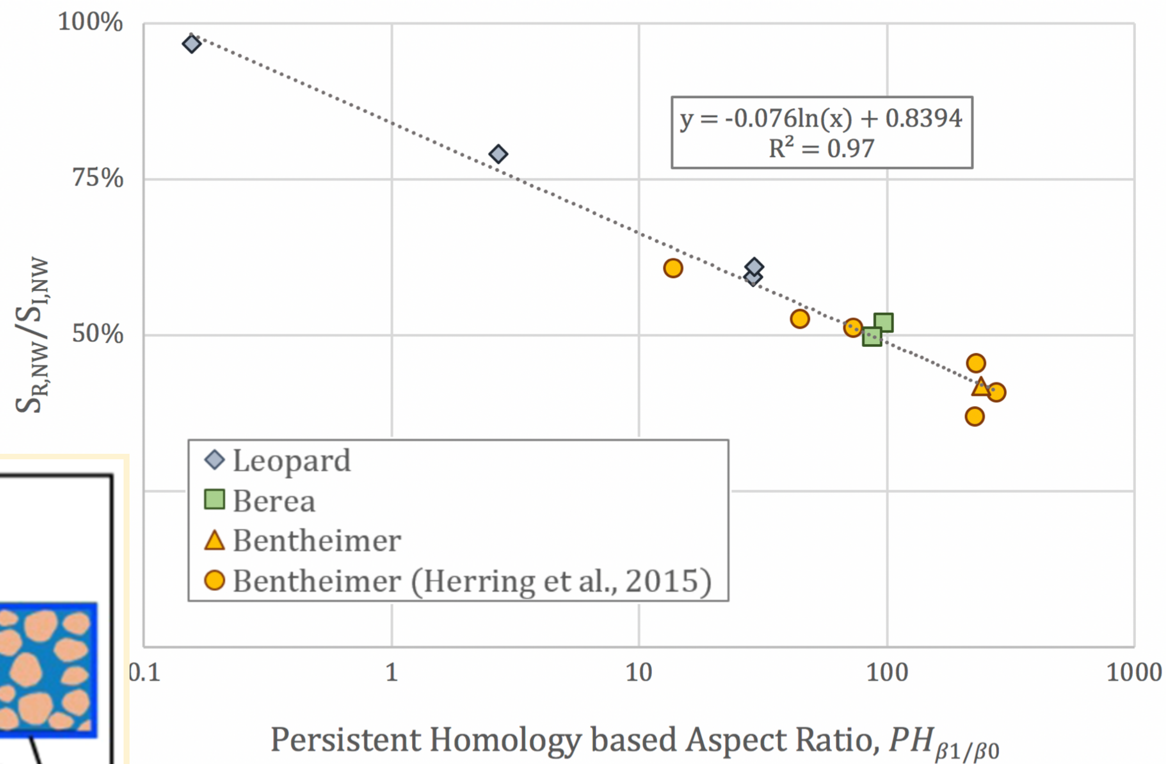
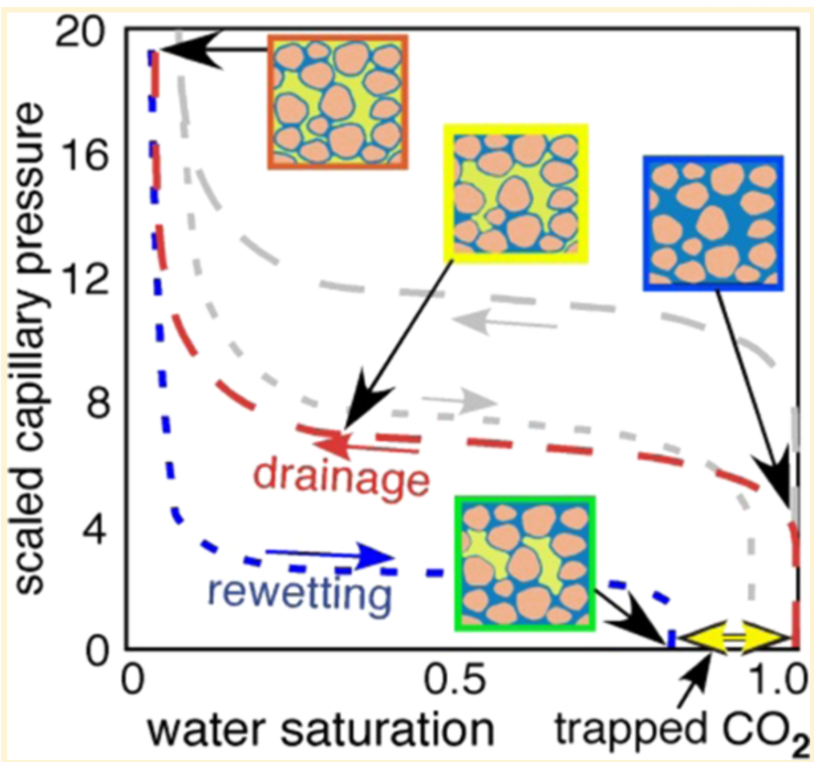


topology and trapping

Capillary trapping
occurs when a non-wetting fluid is surrounded by a wetting fluid and can no longer flow to an outlet



$$PH_{\frac{\beta_1}{\beta_0}} = \frac{\sum_i [b_i \times (d_i - b_i)]}{\sum_j [b_j \times (d_j - b_j)]} \times r^3$$



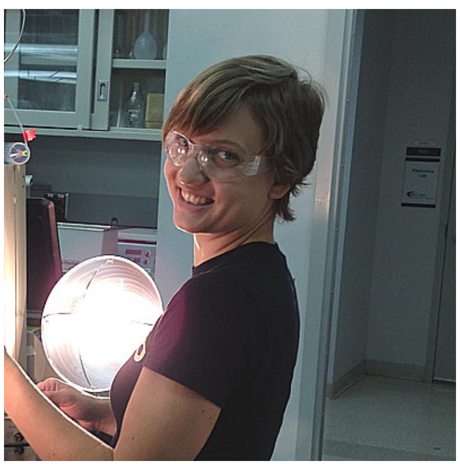
^ image from Herring, VR, Sheppard et al, WRR (submitted).

<- image from Wang, Tokunaga Env. Sci Tech (2015)

summary

1. acquire micro-CT image
2. segment into pore and grain
3. compute signed distance transform
4. build Morse complex
5. compute persistence diagrams
6. interpret!

diamorse package available at:
https://github.com/AppliedMathematicsANU/diamorse




International Conference on Tomography of Materials & Structures

ICTMS 2019

22-26 July 2019 | Cairns, **Australia**

WELCOME TO ICTMS 2019

ICTMS 2019 - INTERNATIONAL CONFERENCE ON TOMOGRAPHY OF MATERIALS & STRUCTURES
22 - 26 JULY 2019

The fourth biannual conference of IntACT (Int. Assoc. of Computed Tomography), ICTMS 2019, will bring together scientists from universities, research organisations, and industry, to discuss 3D/4D tomographic imaging and analysis methods for (non-clinical) studies of materials and structures as well as their evolution.

Australia has a strong tomography community with a long commitment to GeoX and ICTMS, with research groups active in theory, algorithms and hardware . Australian developments include lab-based micro and ultra-micro CTs (some commercialised e.g. Gatan XuM, FEI Heliscan); imaging and XRF beamlines at the Australian Synchrotron (AS), a recently commissioned neutron imaging facility, high-end TEM systems, along with numerous applications groups with sophisticated 3D analysis techniques. We hope that hosting the next ICTMS in Australia will enhance involvement in ICTMS (and intACT in general) by this community in future, and encourage increased involvement from the Asia-Pacific region simply by being more accessible. It is great timing for AS which has received a new round of funding and is expected to announce shortly the addition of a micro-CT beamline that will be nearing completion by ICTMS 2019.

Topological image analysis

Topologically consistent skeletonisation and partitioning

Solid phase shown in grey

Pore space divided into coloured pores by the basins

Blue lines are
basin boundaries

White lines are the
Morse Skeleton

Delgado-Friedrichs, Robins, Sheppard
IEEE TPAMI (2014)

Source code available from
https://github.com/AppliedMathematicsANU/diamorse

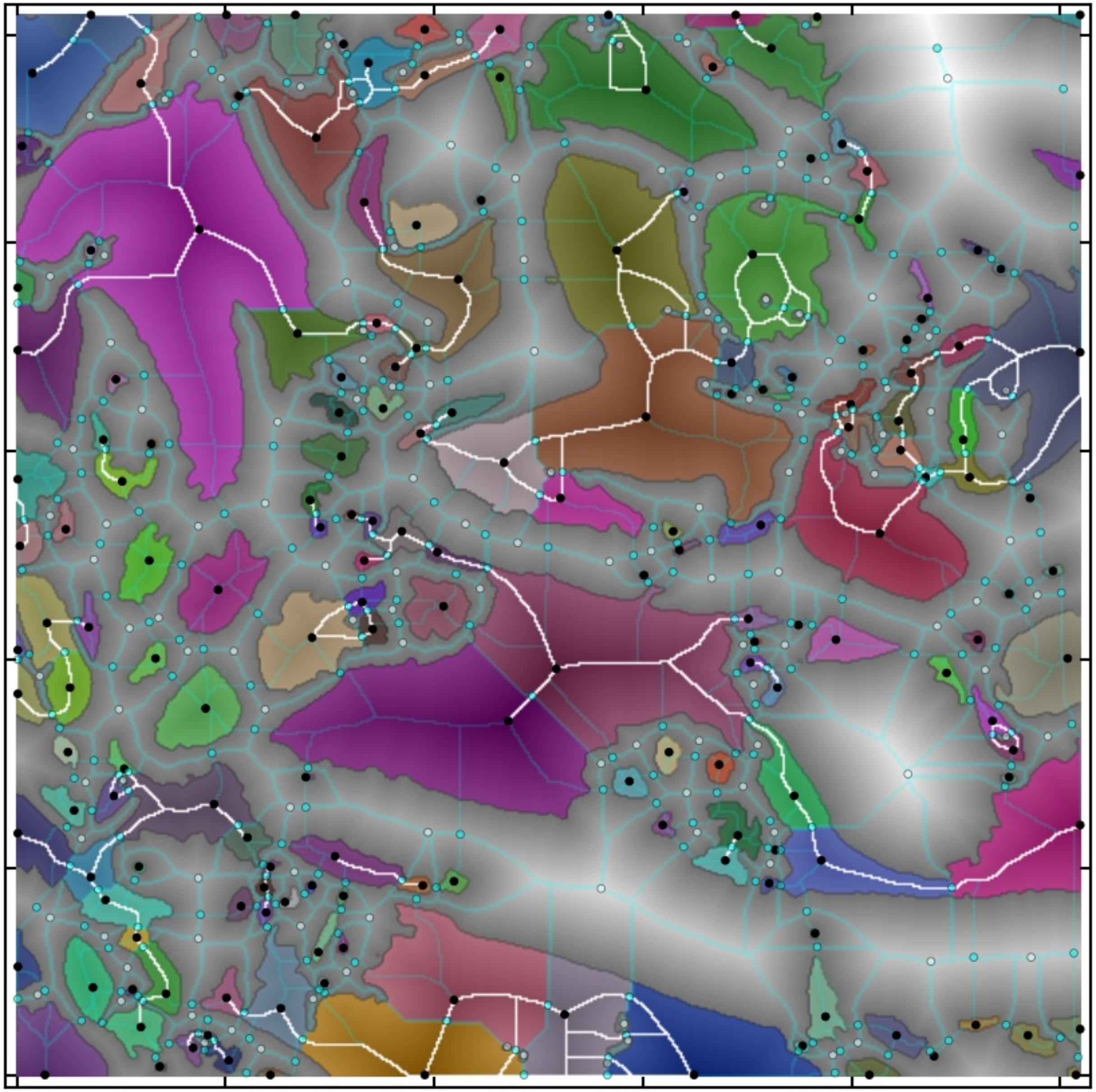


image created by Olaf Delgado-Friedrichs