Topological Data Analysis with applications to porous and granular materials

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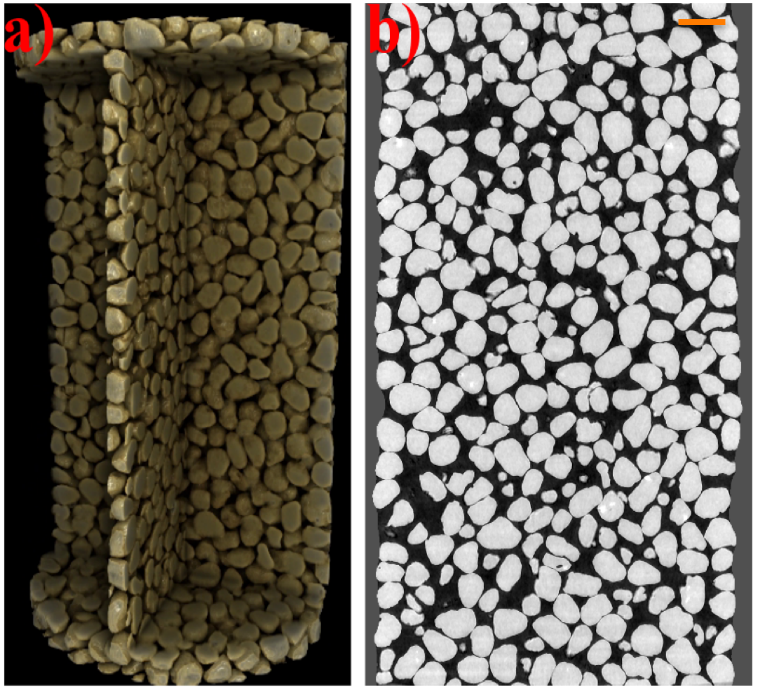
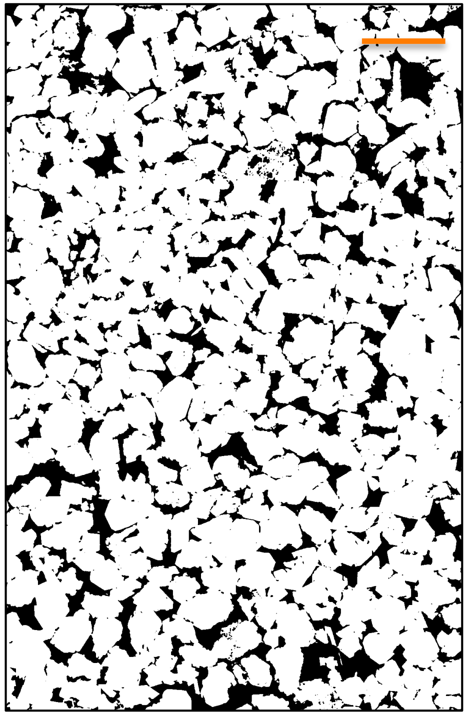
ARC Future Fellowship
FT140100604

ARC Discovery Projects
DP1101028, DP0666442

granular and porous materials

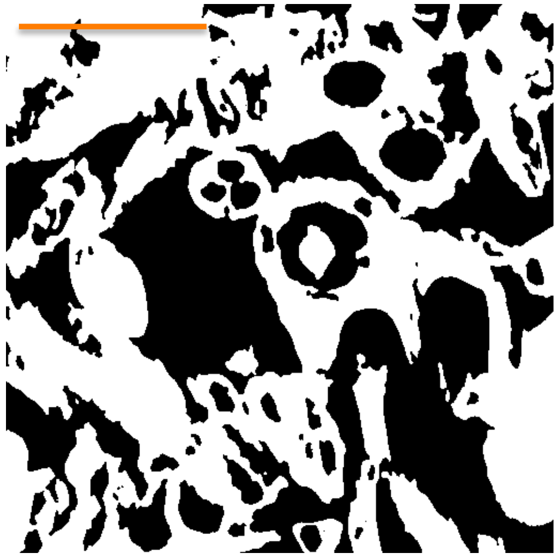


Ottawa sand



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, mechanical response to load.

figures obtained at the ANU micro CT facility

Topology from data?

- Challenge: compute topological invariants from finite noisy data with structure on different length-scales.
  - e.g. connected components (clustering)
  - Euler characteristic, Betti numbers, homology groups.

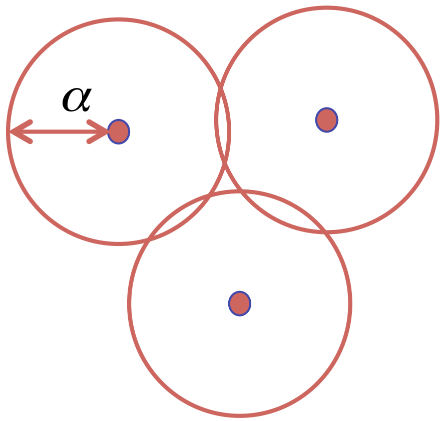
- Requirements:
  - a cell complex
  - efficient algorithms
  - statistical methods for the analysis of topological invariants

- Applications:
  - Spherical bead packings and other granular and porous materials
  - Glass transition, Materials informatics (for MOFs, etc.)
  - Histology image analysis, protein structure, distribution of galaxies in the universe, dynamical systems/ time series analysis, ...

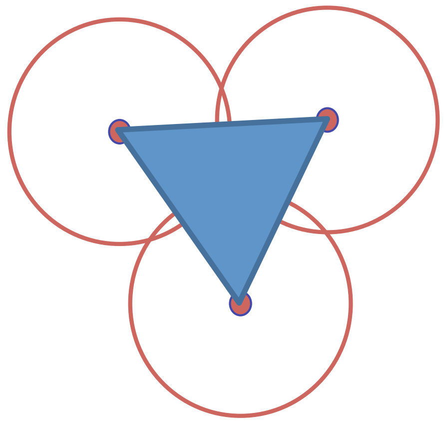
How to build a complex

- Points are $X = \{x_1, x_2, x_3, \ldots, x_n\}$ in (M,d) a metric space
- The Rips complex $R(X,\alpha)$ has a k-simplex $[a_0, a_1, \ldots, a_k]$ for a_i *in X*, if $d(a_i, a_j) < 2\alpha$ for all pairs $i,j= 0,\ldots,k$.
- The Cech complex $C(X,\alpha)$ has a k-simplex $[a_0, a_1, \ldots, a_k]$ for a_i *in X*, when $\Pi\ B(a_i,\alpha)$ is non-empty.

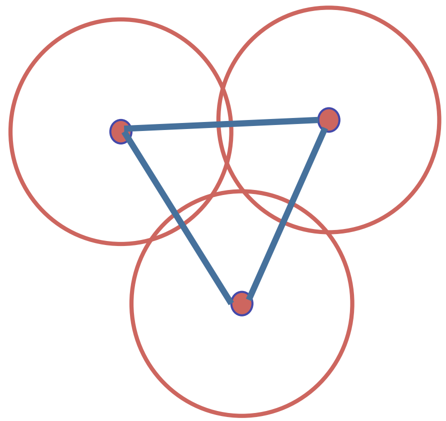
- Cech complex is homotopic to the union of balls so it captures the geometry of X more accurately, but Rips is simpler to build.



$X\alpha = U\ B(x,\alpha)$



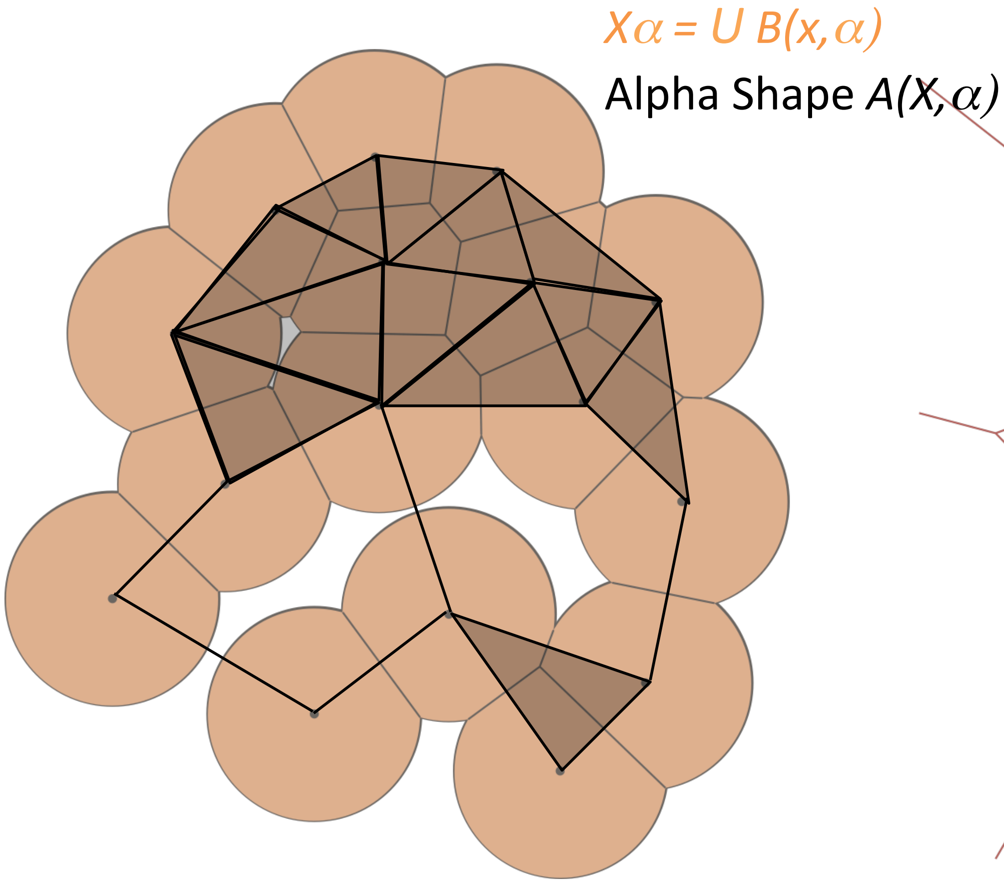
Rips $R(X,\alpha)$

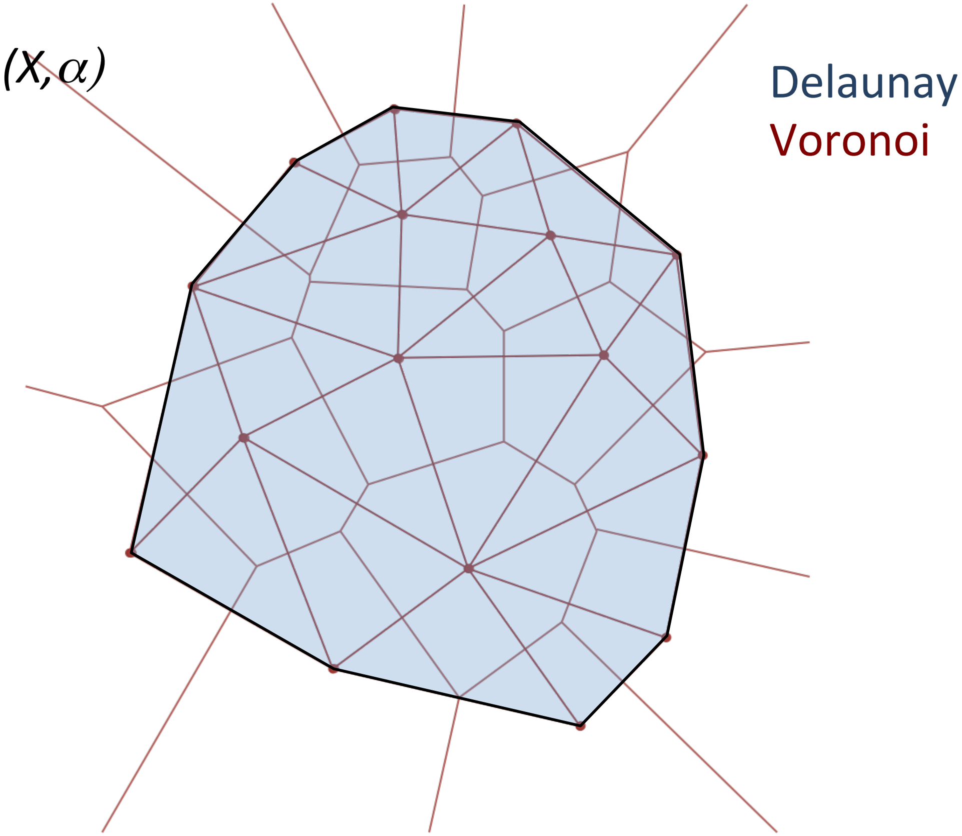


Cech $C(X,\alpha)$

How to build a complex

- If your metric space is R^2, R^3, or R^4, the best geometric complex is the Alpha Shape, $A(X,\alpha)$. [H. Edelsbrunner (1983,1994,1995)].
- $A(X,\alpha)$ is a subset of the Delaunay Triangulation.
- A k-simplex $[a_0, a_1, \ldots, a_k]$ is in $A(X,\alpha)$ if its circumsphere is empty and circumradius < α.

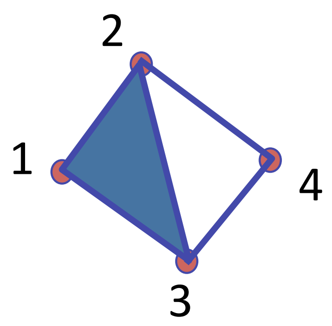




Simplicial homology

- K is a simplicial complex.
- The *k-th chain group $C_k(K, G)$* is the free abelian group with coefficients G, generated by the oriented k-simplices of K.
- The boundary operator maps each k-simplex onto the sum of the (k-1)-simplices that are its faces.

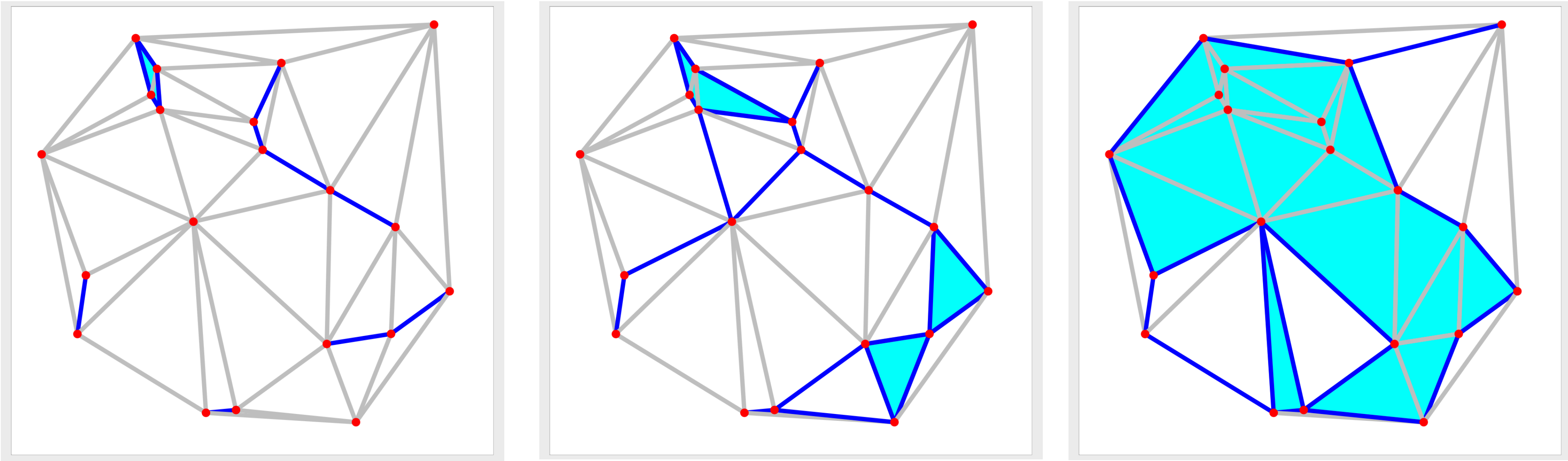
$$\partial_k : C_k \longrightarrow C_{k-1} \qquad \boxed{\partial_{k-1}\partial_k = 0}$$



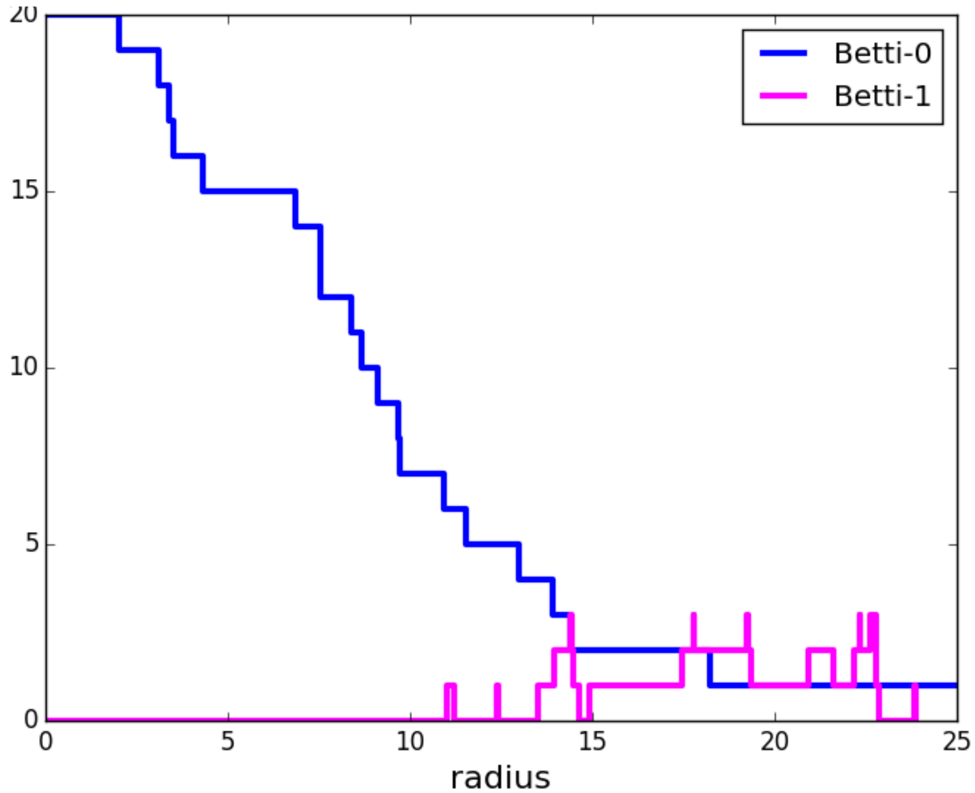
- The image of ∂_k is the boundary group, B_{k-1}
- The kernel of ∂_k is the cycle group, Z_k
- The homology group is $H_k = Z_k / B_k$
- The structure theorem for finitely generated abelian groups tells us that if G = Z, (integers) then

$$H_k(K,Z) = \underbrace{Z \oplus \ldots \oplus Z}_{\beta_k \text{ copies}} \oplus Z_{t1} \oplus \ldots \oplus Z_{tm}$$

- β_k is the Betti number and t_i are the torsion coefficients



$\beta_0=9, \ \beta_1=0$ $\beta_0=3, \ \beta_1=2$ $\beta_0=1, \ \beta_1=2$

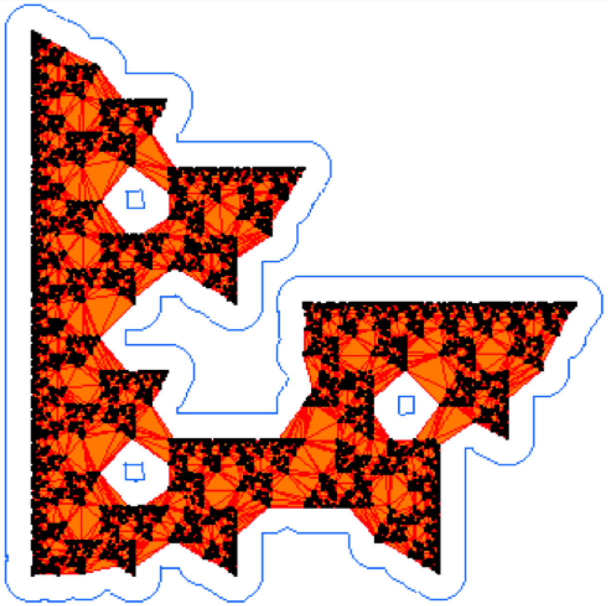


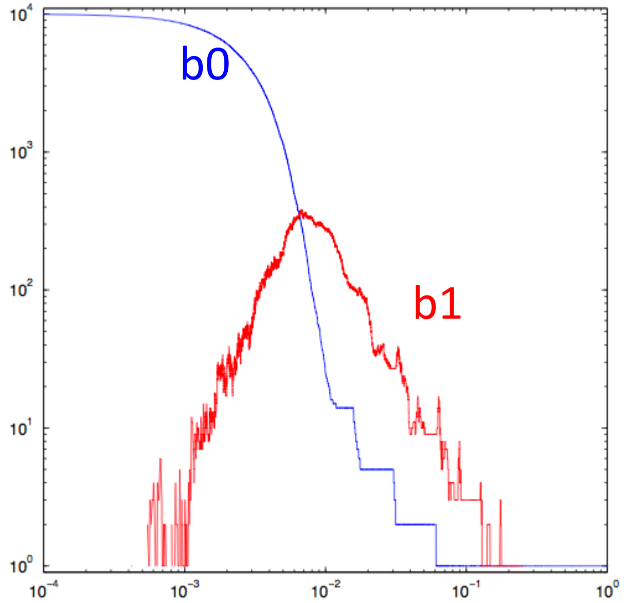
Betti number functions of A(X,α) are not stable wrt small changes in point locations.

But persistent homology intervals are.

Cohen-Steiner, Edelsbrunner, Harer (2007)

Fractal examples

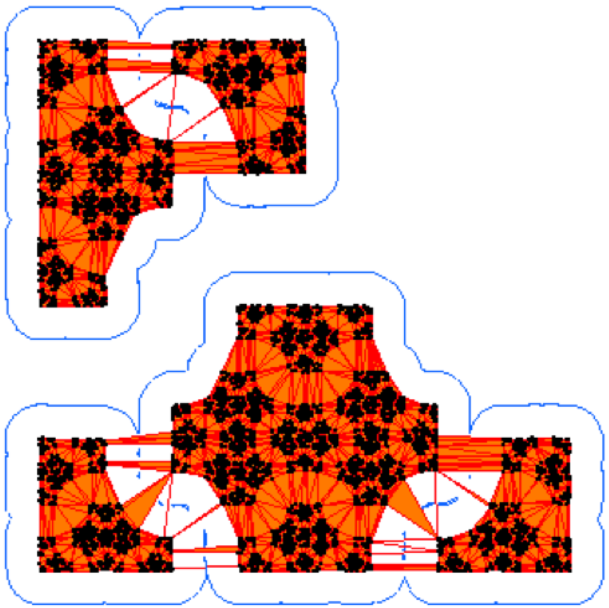


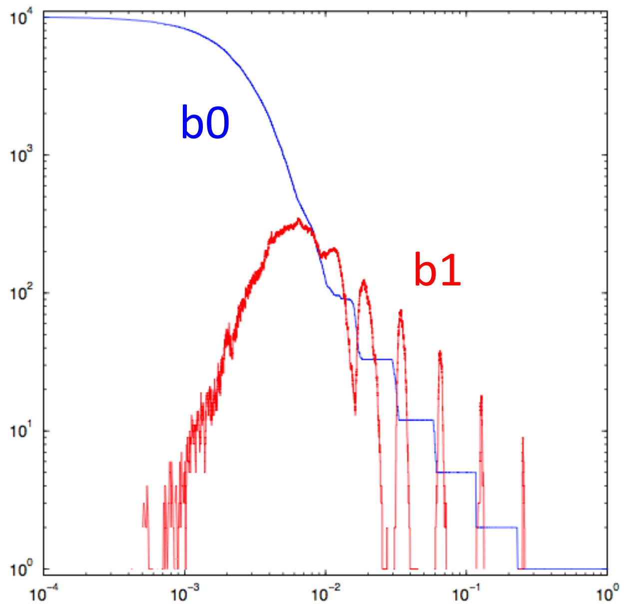


b0 is number of components

b1 is number of holes

Problem with counting holes that do not persist for smaller radii.





Persistent homology

Let Xa = U B(x,a) so $i : Xa \hookrightarrow Xb$ for *a < b*.

The cell complexes, R(X,a), C(X,a) and A(X,a) also have this inclusion property.

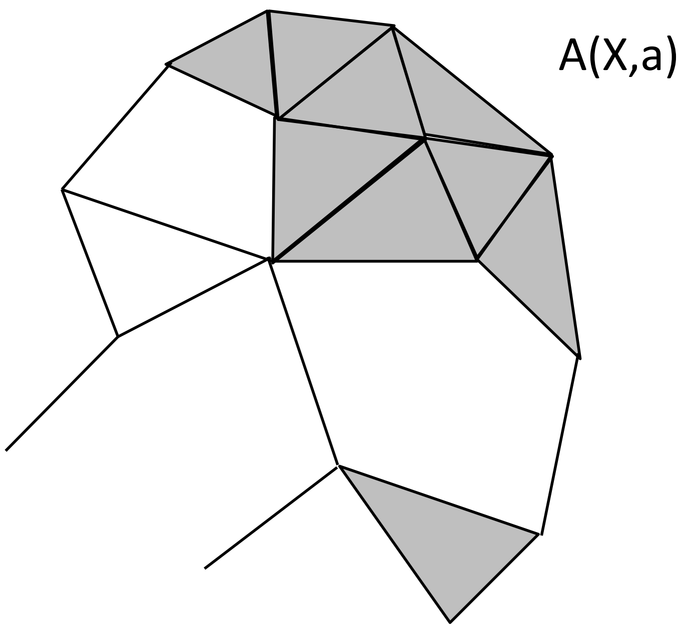
Homology is a functor so *i* becomes a group homomorphism:

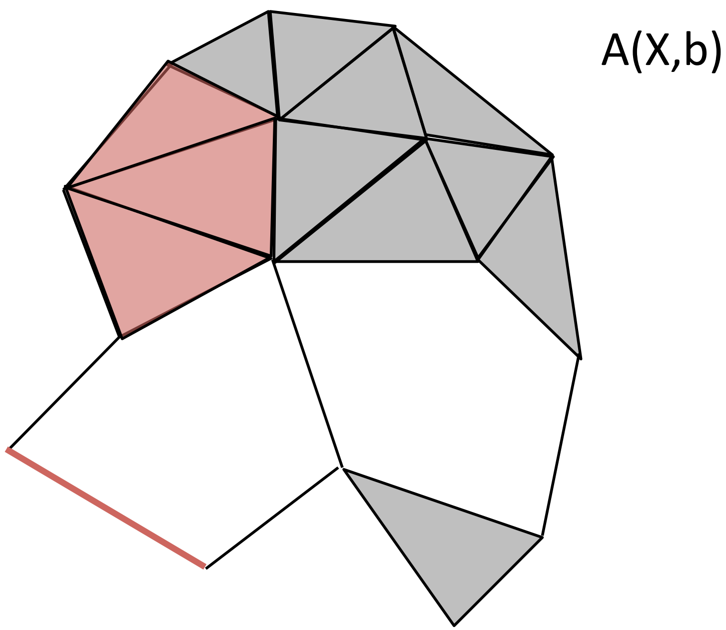
$$i* : H_k(Xa) \to H_k(Xb)$$

The persistent homology group is the image of *i* :*

$$H_k(a,b) = i*(H_k(Xa)) = Z_k(Xa)/(B_{k+1}(Xb) \cap Z_k(Xa))$$

[VR Topology Proceedings 1999]





Persistent homology

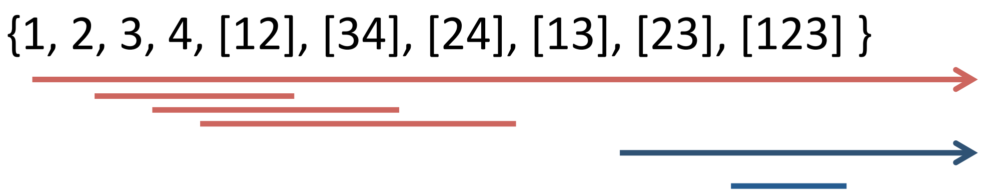
Algorithmic definition

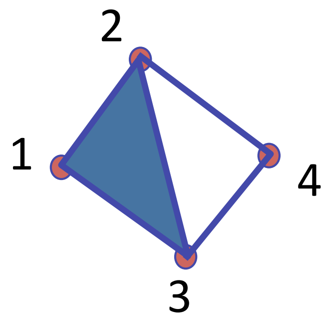
When adding a single k-simplex, σ^k, to a cell complex that already contains all faces of σ^k exactly one of two changes in topology can happen:

- σ^k creates a k-cycle (it is marked +ve)
- σ^k makes a (k-1)-cycle a boundary (it is marked –ve)

[Delfinado and Edelsbrunner, 1993]

A persistent homology class is found by pairing each –ve *k*-simplex with the most recently added and as-yet-unpaired +ve *(k-1)*-simplex in its boundary class. [Edelsbrunner, Letscher, Zomorodian, DCG 2002].





Persistent homology

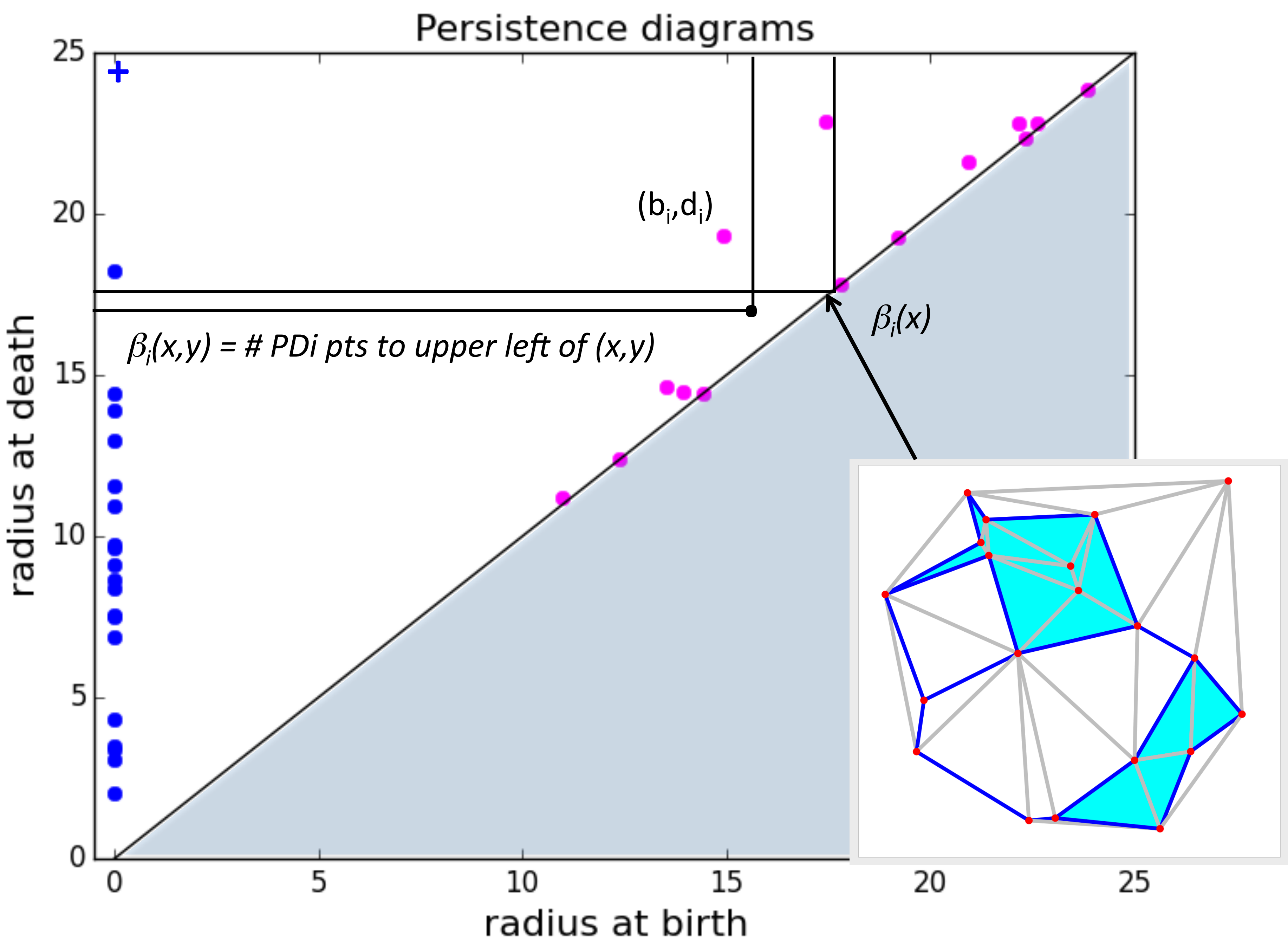
- A more algebraically sophisticated view of persistent homology is given by G. Carlsson (e.g. AMS Bulletin, 2009).
- A filtration is a directed space:

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

- The functorial property of homology means the induced maps on homology groups also form a directed space.
- If the coefficient group is a field (e.g. R, or Z_2) we can form a graded module of this homology sequence and an algebraic structure theorem tells us that

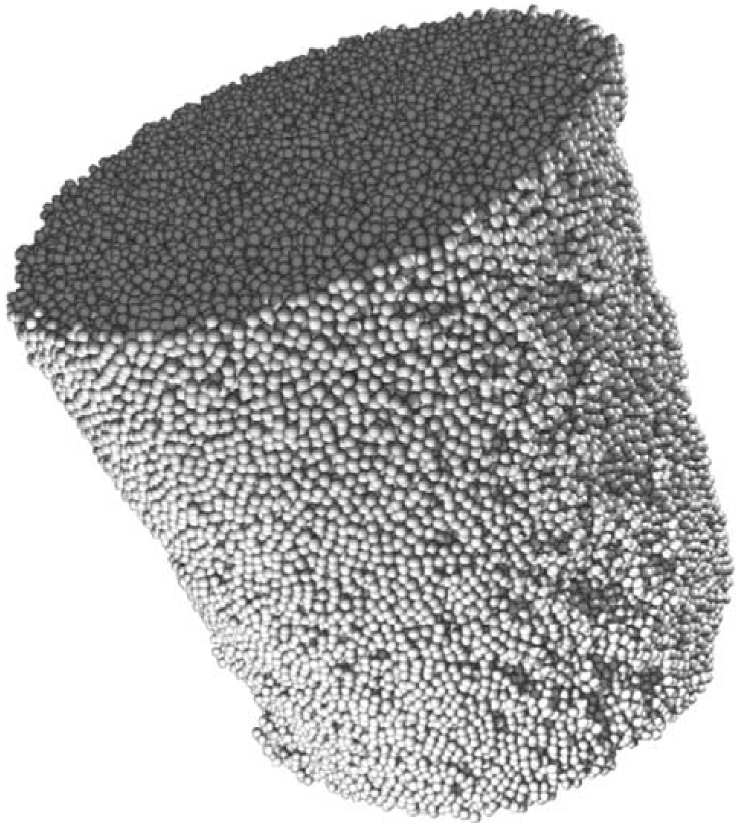
$$PH_k(X) = \bigoplus_{i=1}^{N} I[b_i, d_i]$$

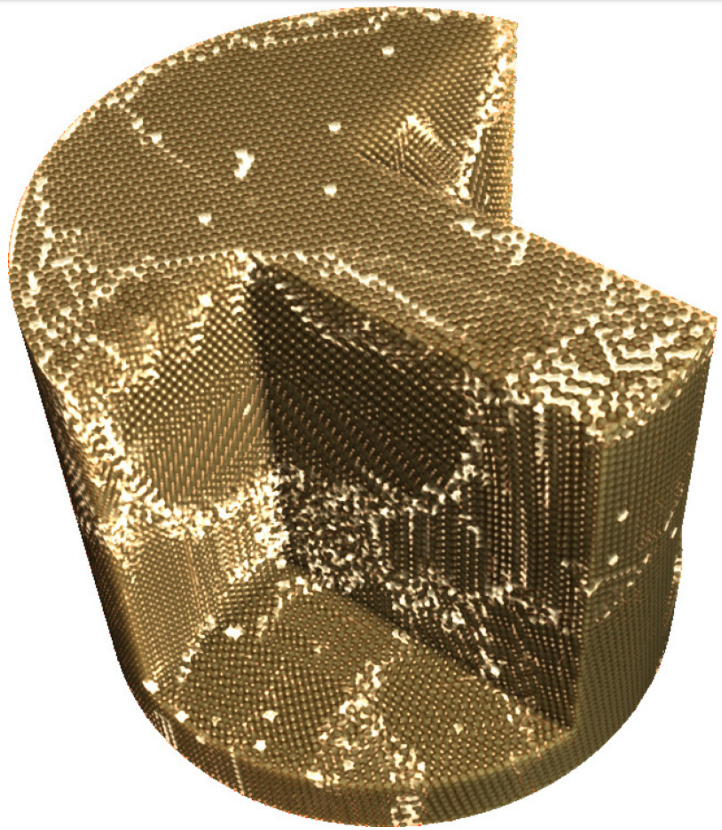
- This collection of intervals is called the barcode.
- If we plot the (b,d) values on 2D axes, it is called the persistence diagram.
- The function $\beta_k(a,b) = rank\ H_k(a,b)$ is the persistent homology rank function



Persistence diagrams
radius at death
radius at birth
0
5
10
15
20
25
0
5
10
15
20
25
(b_i,d_i)
β_i(x,y) = # PDi pts to upper left of (x,y)
β_i(x)

spherical bead packing



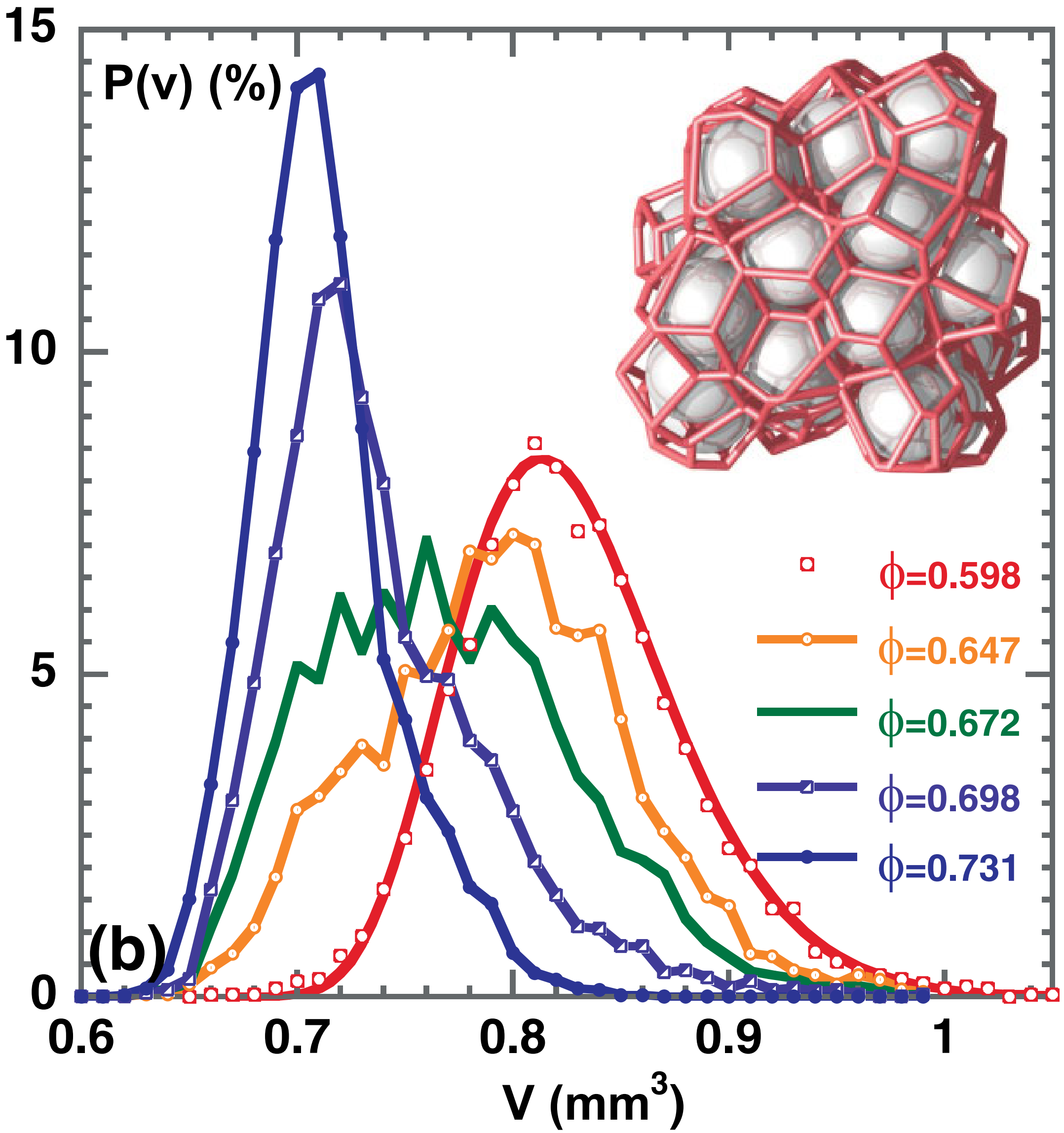


Disordered packing
(random close pack, maximally jammed)
Bernal limit has vol frac Φ = 64%
Well-defined distribution of local volumes

Partially crystallized packing, Φ=70%
a fully crystallized packing has Φ=74%
(i.e layers of hexagonally close packed spheres)

data from M Saadatfaar, ANU x-ray CT of ~150K beads, (1.00 +/- 0.025)mm diameter.

spherical bead packing



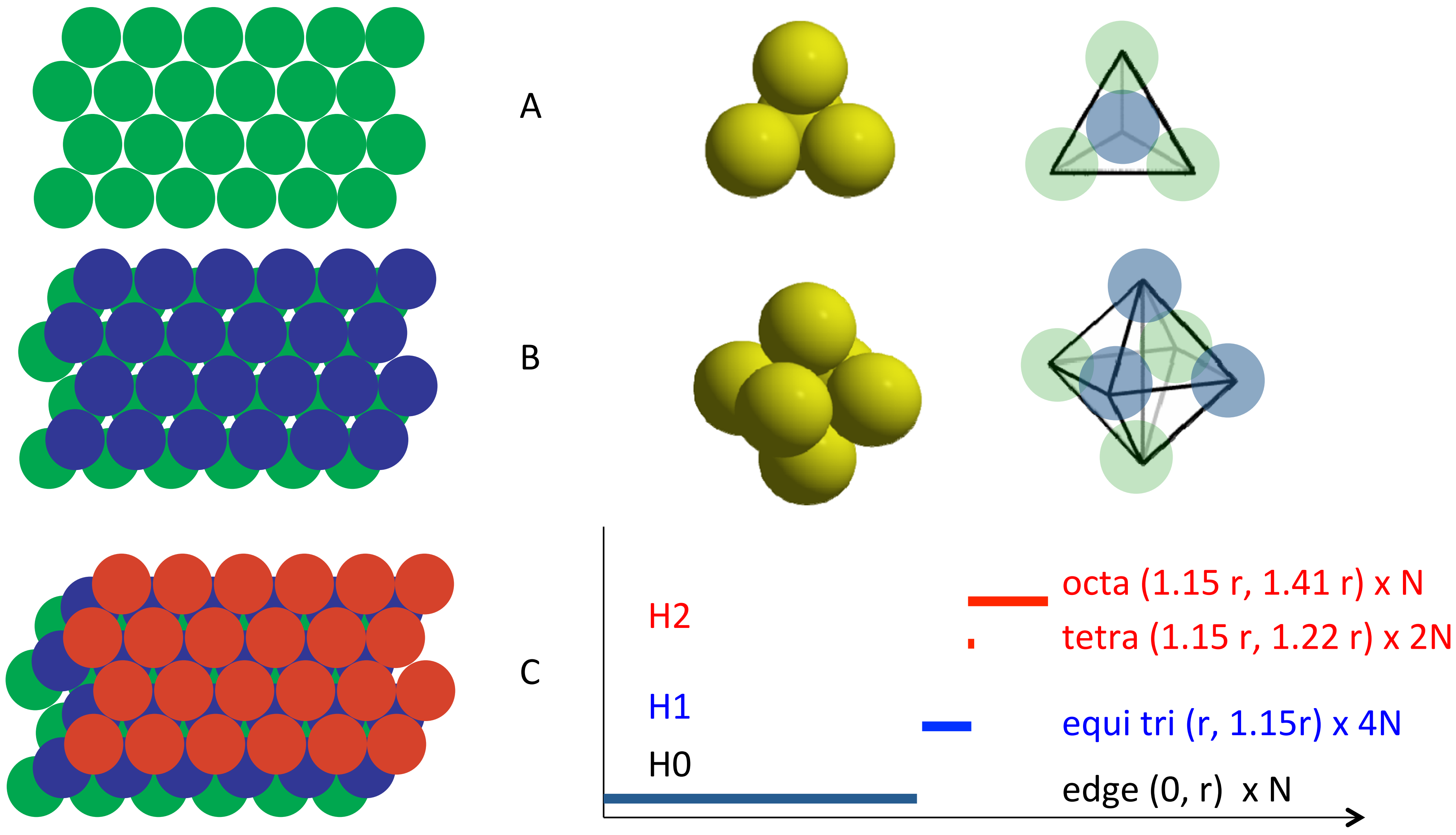
Distributions of Voronoi cell volumes from packings with different global volume fractions ϕ.

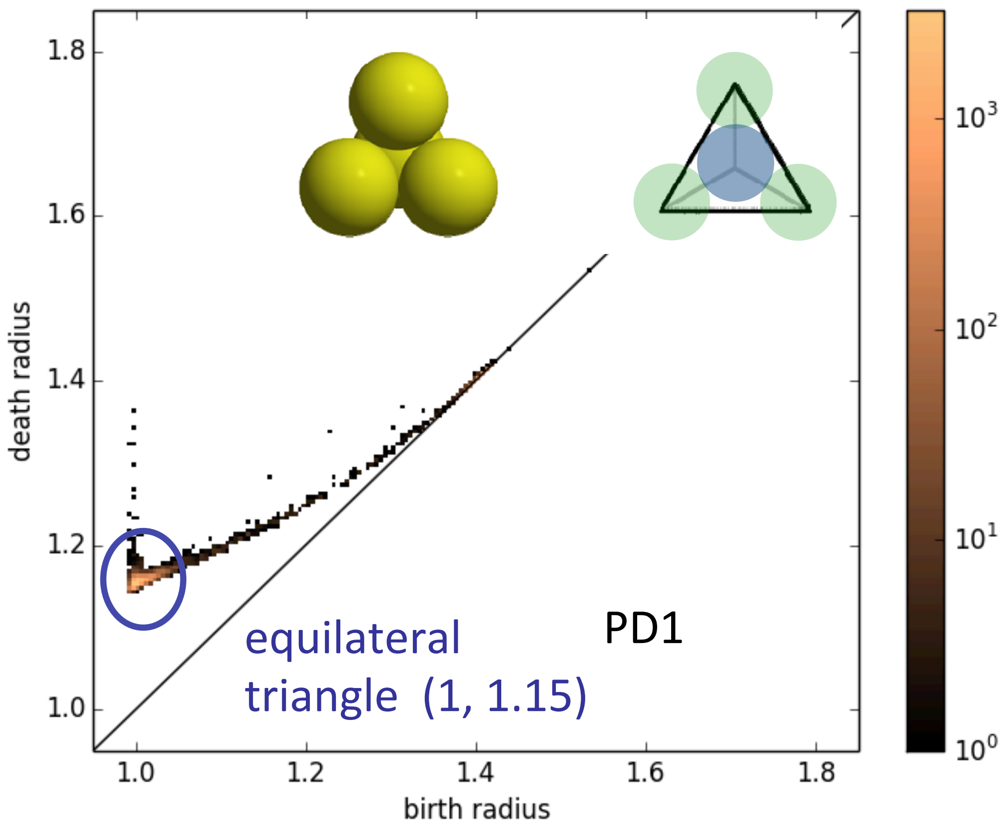
fig from:
Francois, Saadatfar, et al
Phys. Rev. Lett. **111** (2013).

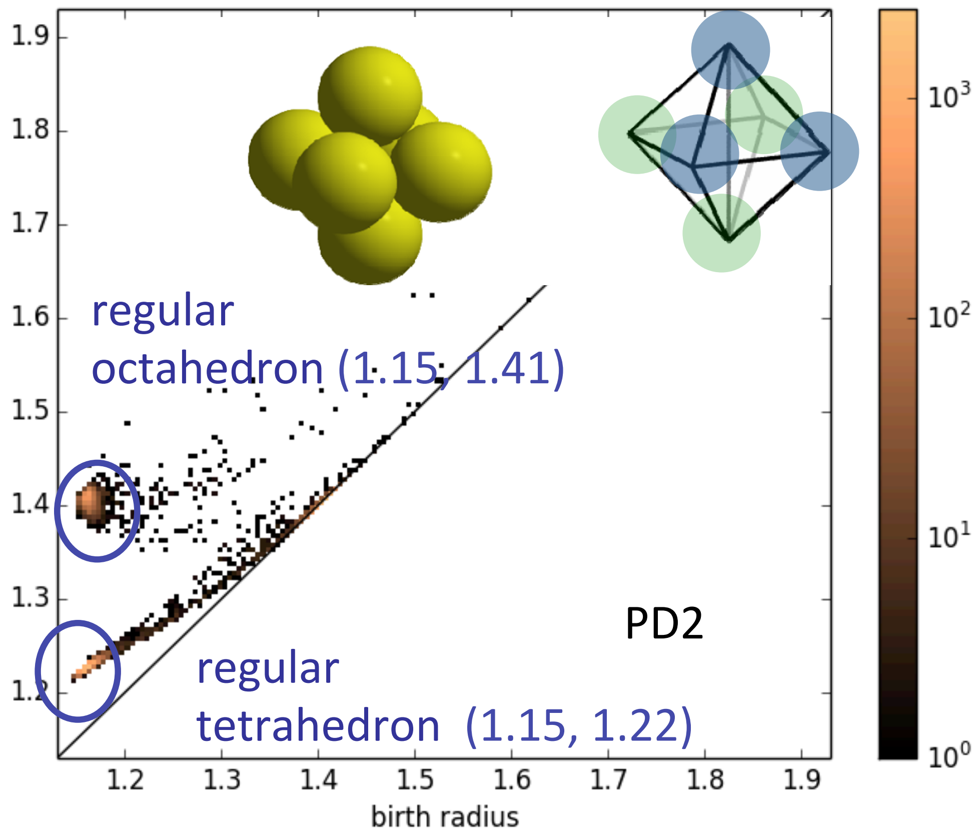
and see earlier work by
Edwards;
Aste;
Anikeenko and Medvedev.

spherical bead packing

A maximally dense packing is built from layers of hexagonally packed spheres
Locally, these give pores related to regular tetrahedra and octahedra

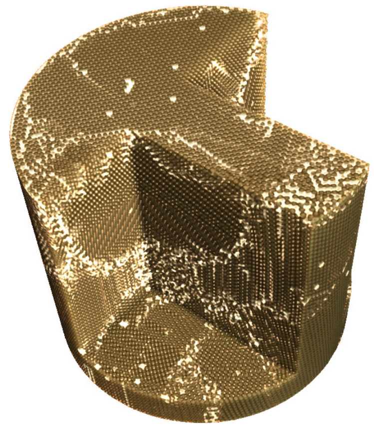


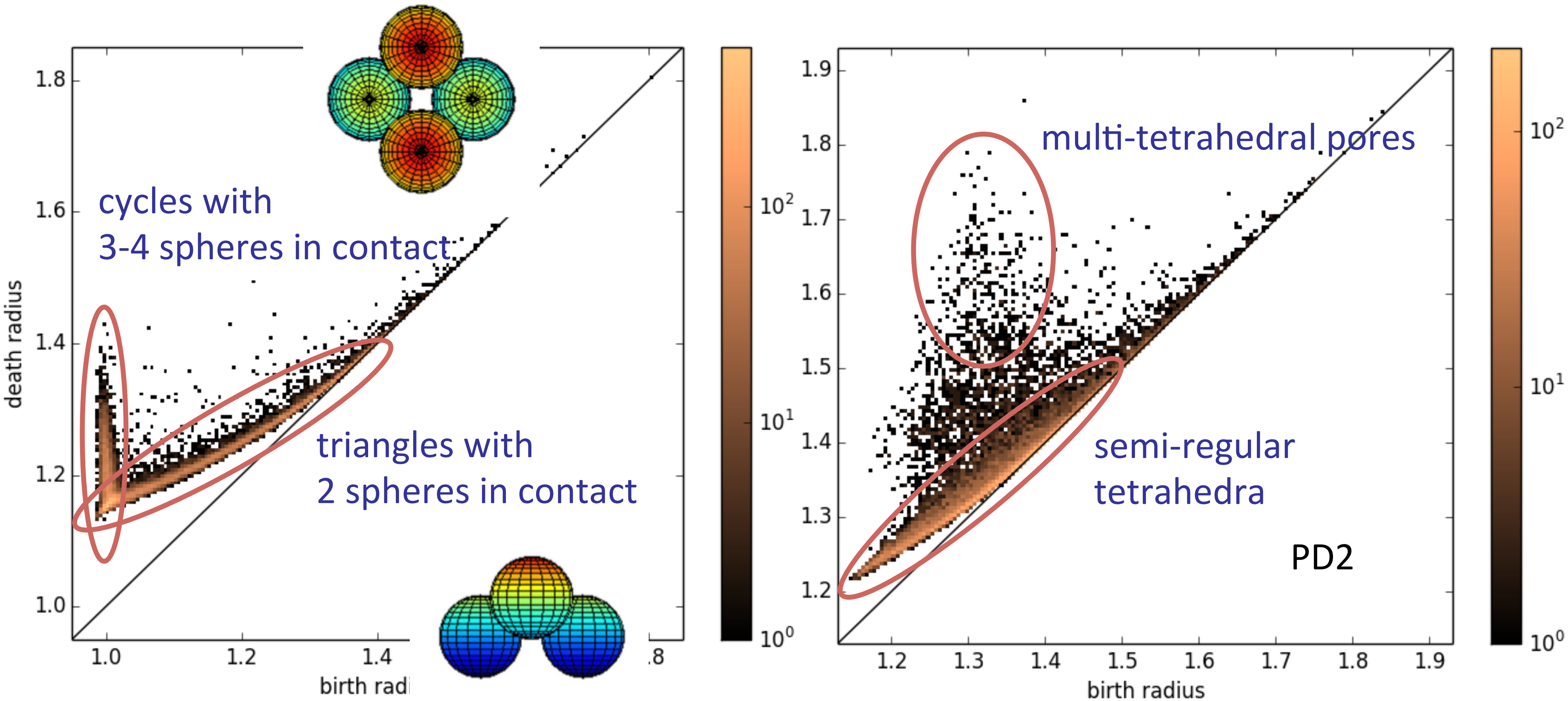


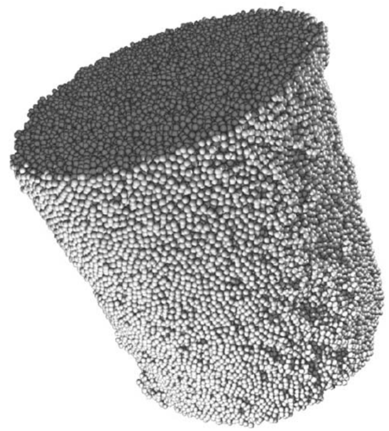


Persistence diagrams for a subset (14mm^3) of the partially crystallised packing with high volume fraction = 72%.

axis units now normalised by bead radius = 0.5mm





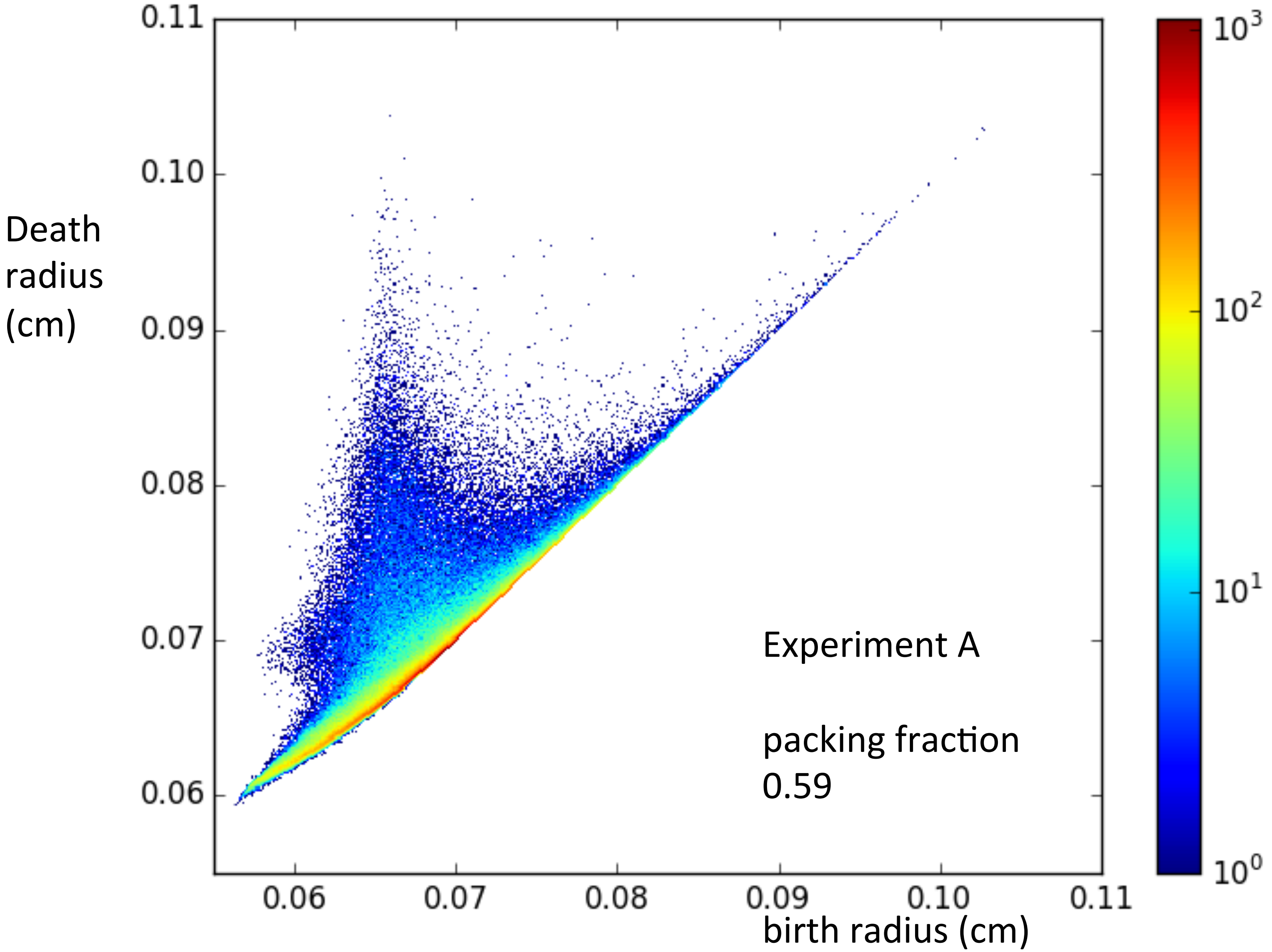


Persistence diagrams for a subset (14mm^3) of the random close packing with volume fraction = 63%.

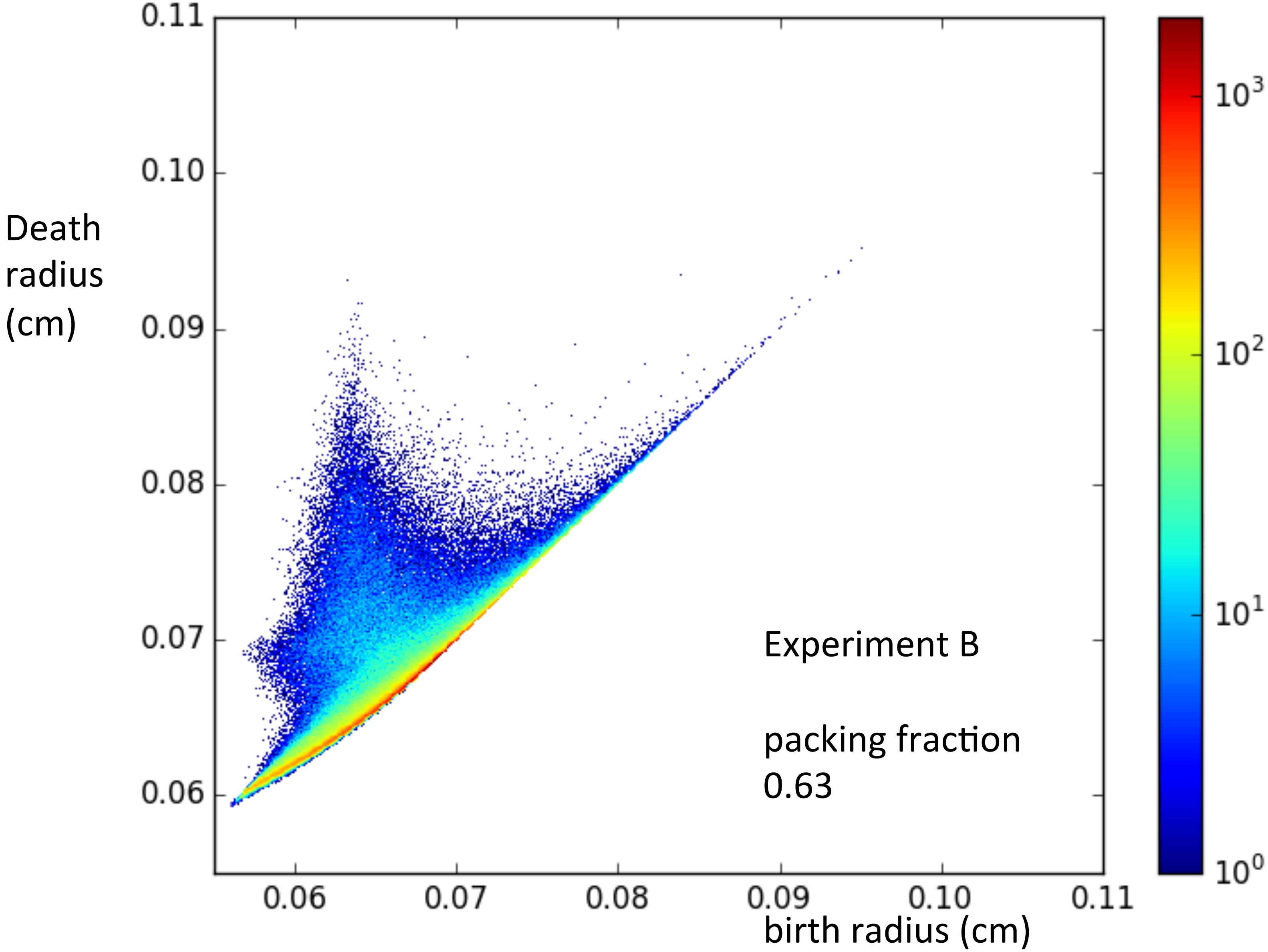
the plots are 2D histograms where colour is log10 of the number of (b,d) points in a small box

axis units normalised by bead radius = 0.5mm

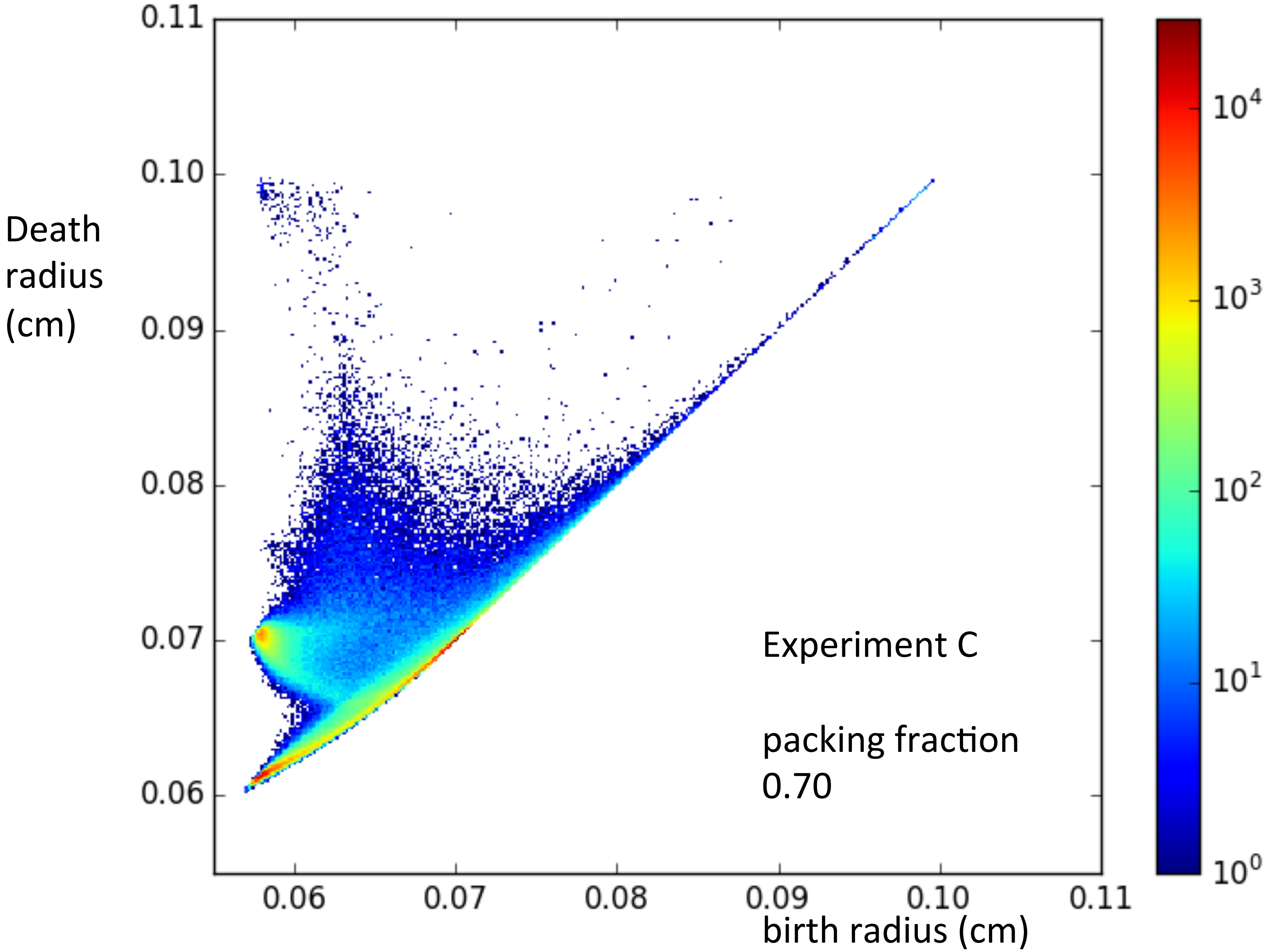
spherical bead packing PD2

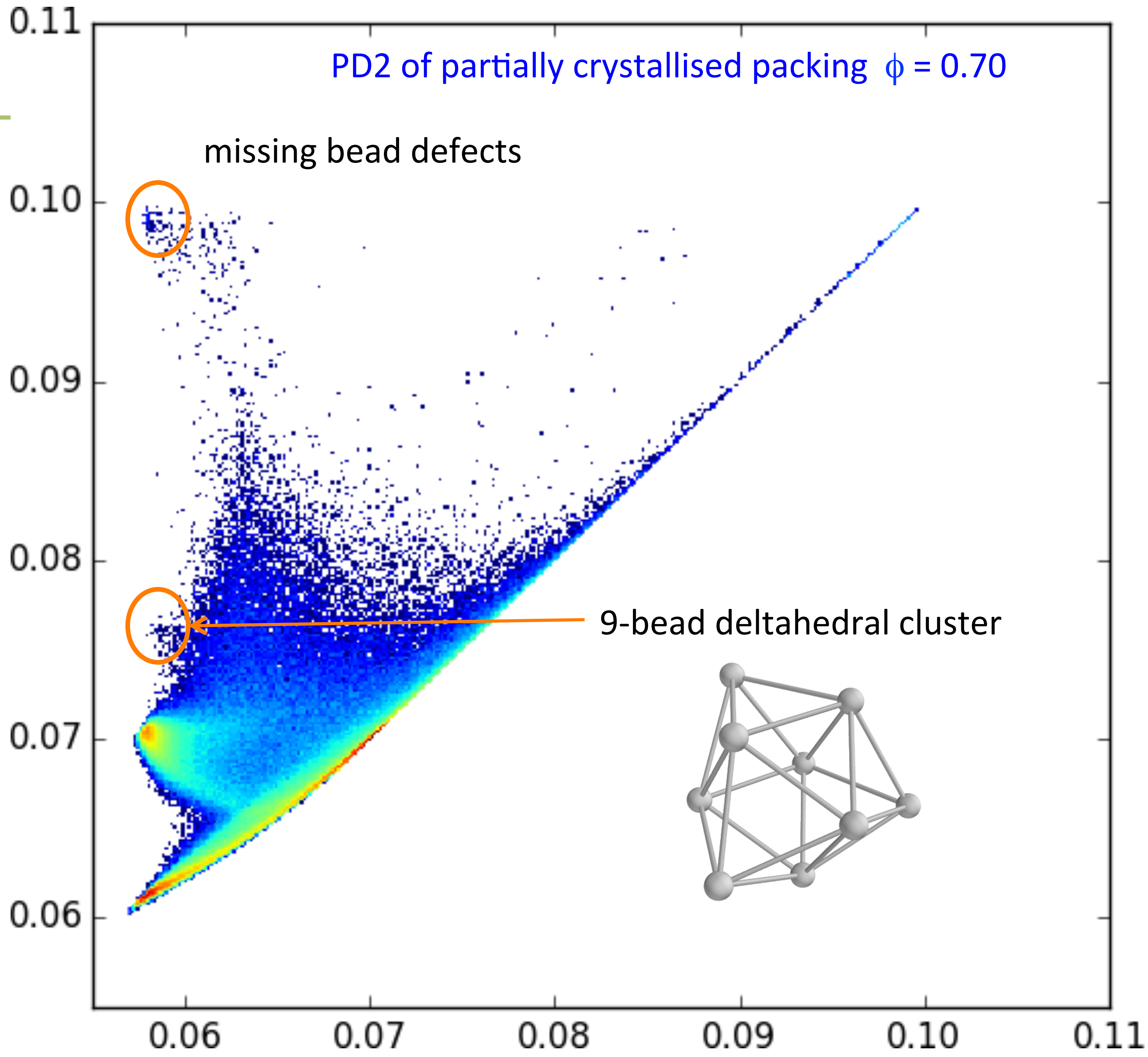


spherical bead packing PD2



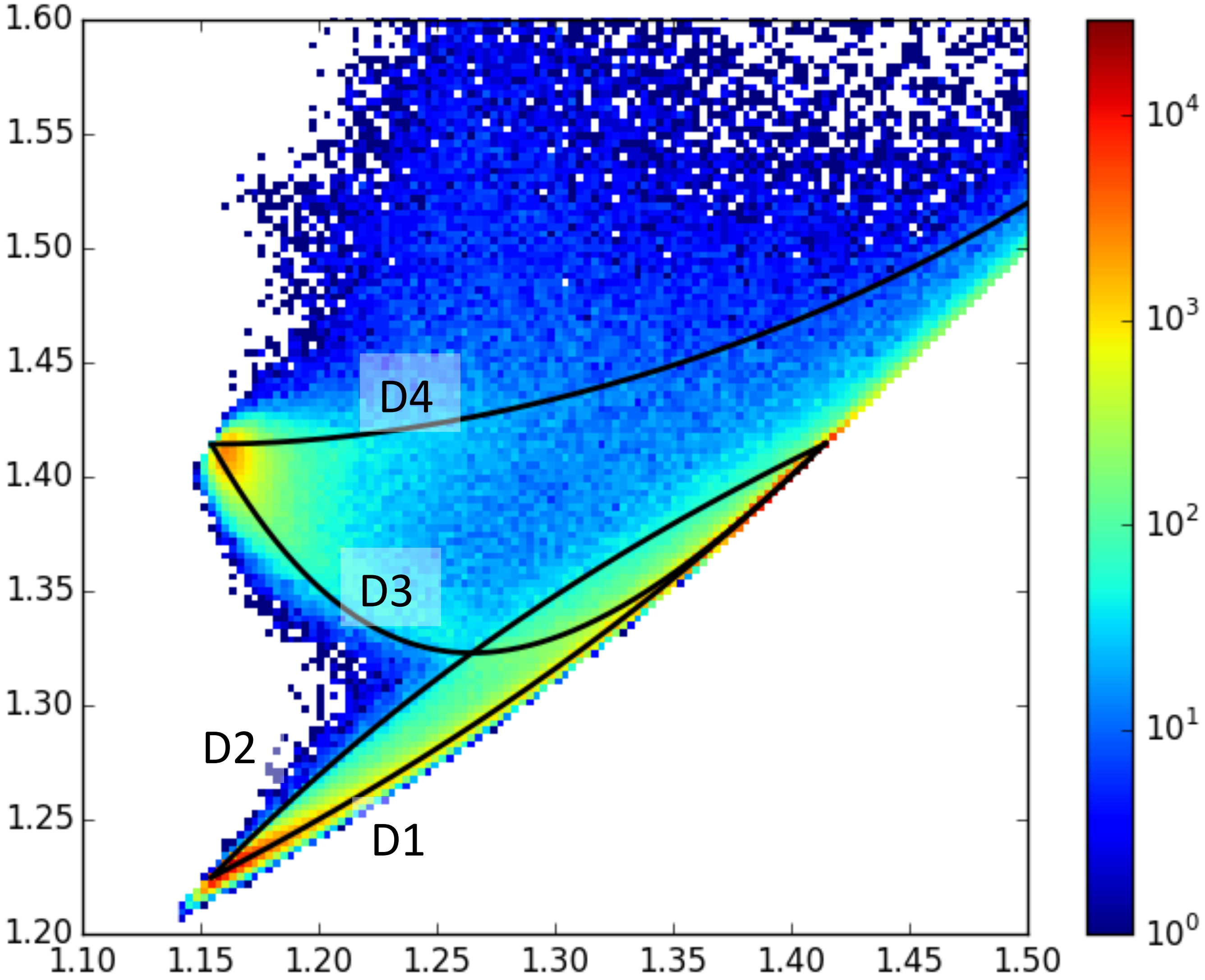
spherical bead packing PD2

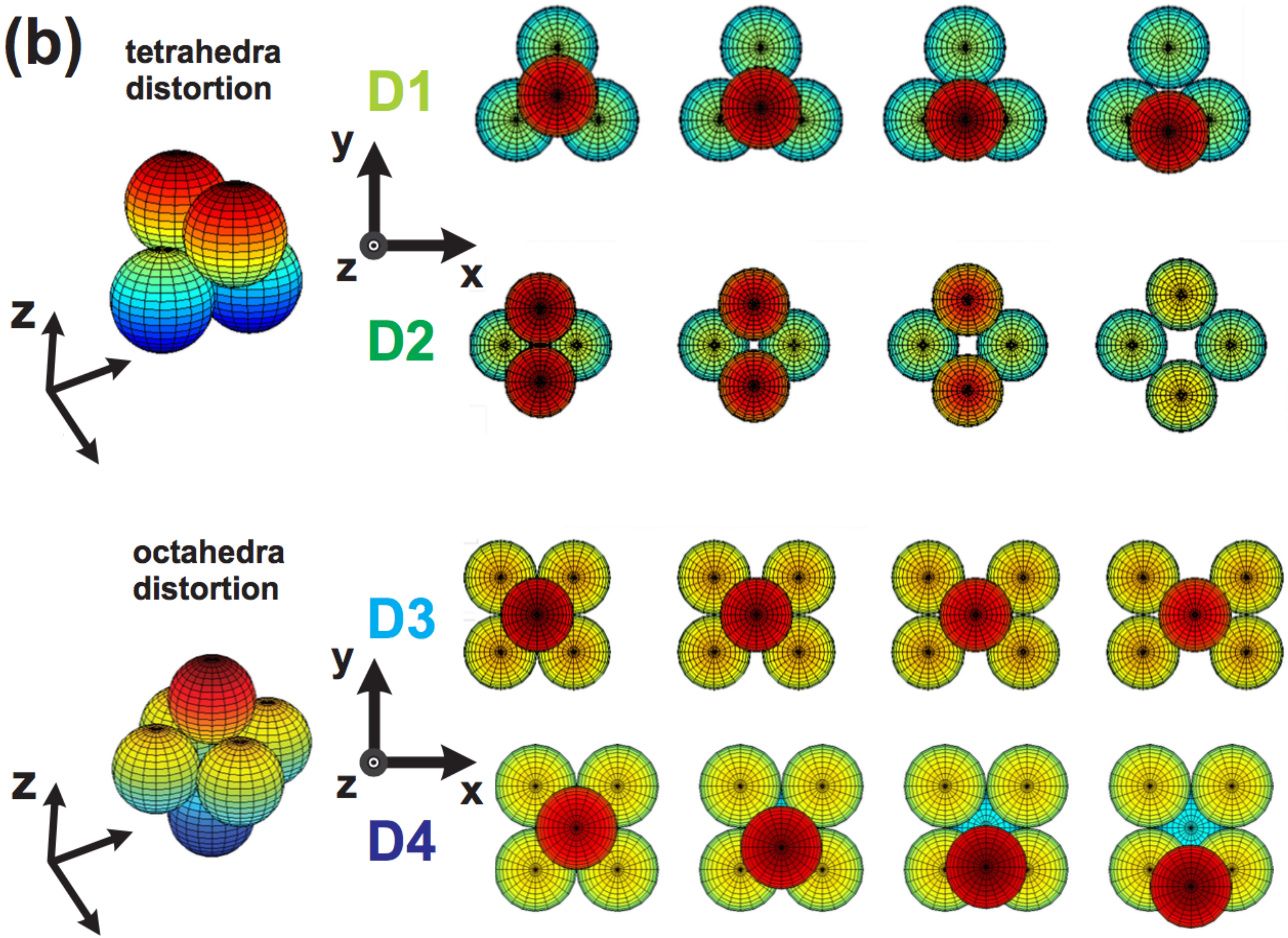



PD2 of partially crystallised packing ϕ = 0.70
missing bead defects
9-bead deltahedral cluster
0.06
0.07
0.08
0.09
0.10
0.11
10^0
10^1
10^2
10^3
10^4

PD2 of partially crystallised packing $\phi = 0.70$

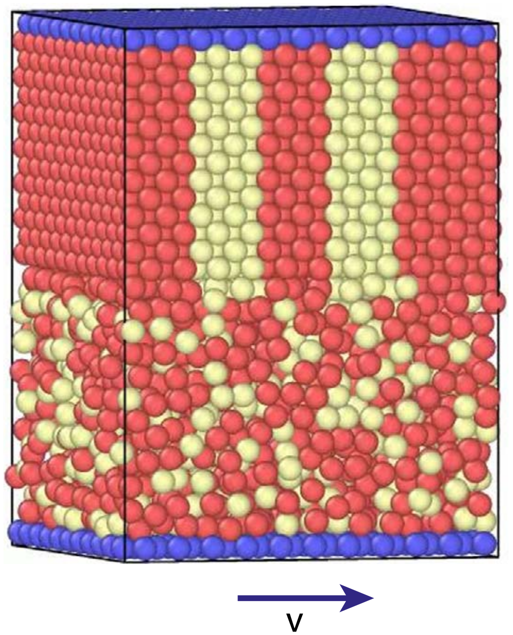
death radius (relative units)



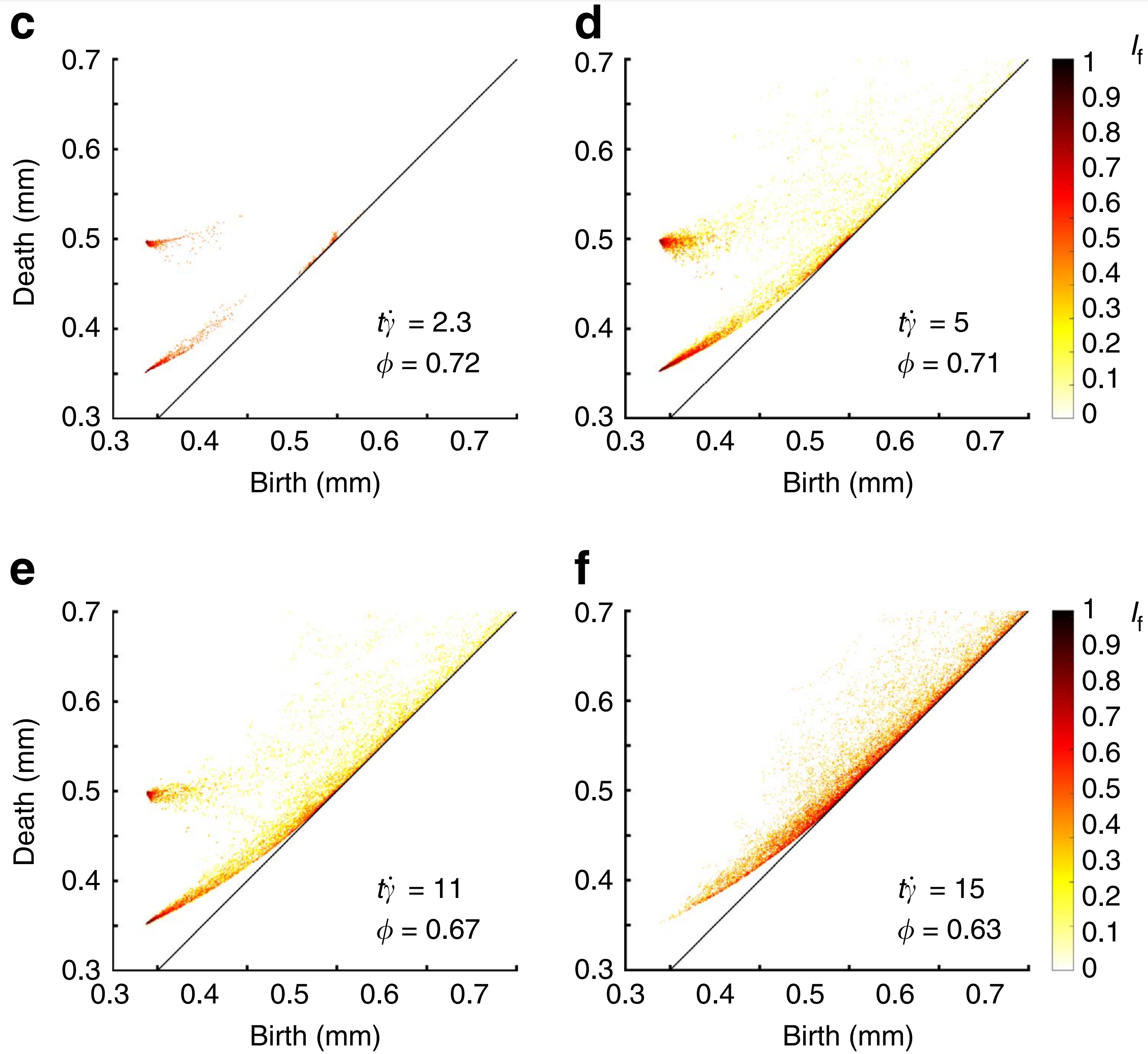


Saadatfar, Takeuchi, VR, Francois, Hiraoka,
"Pore configuration landscape of granular crystallization,"
Nature Communications, May 2017.

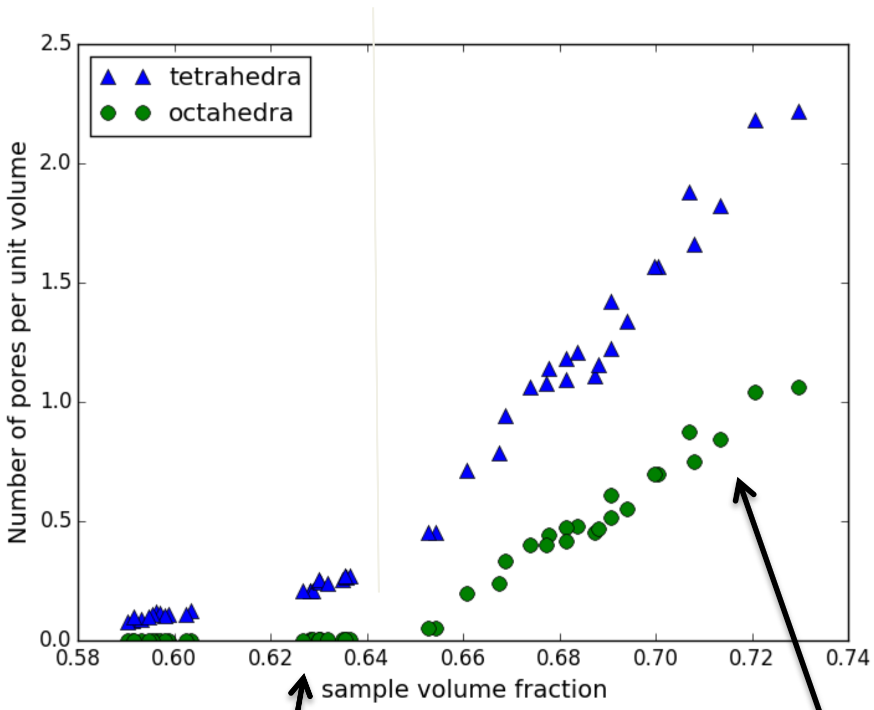
simulation data

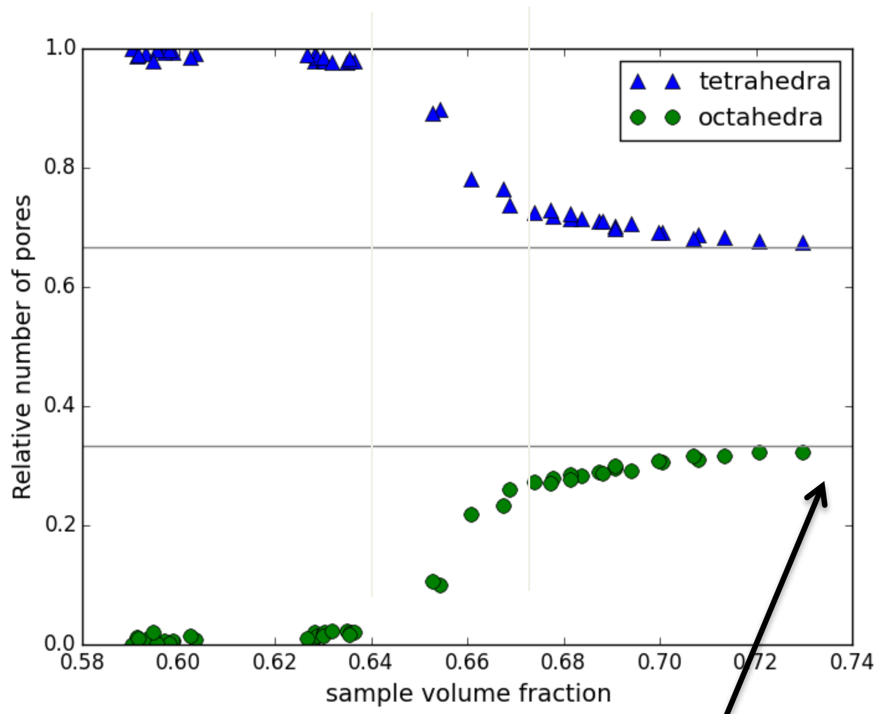


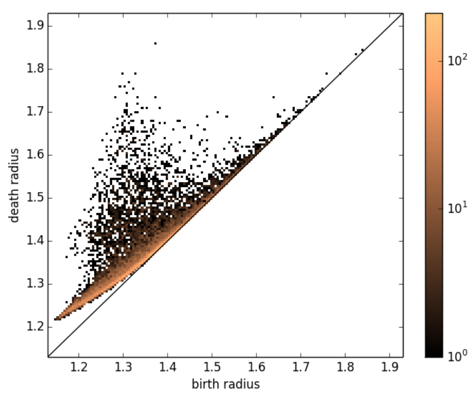
Numerical simulations of a crystalline packing subject to shear-induced “melting” show the same deformation pathways.

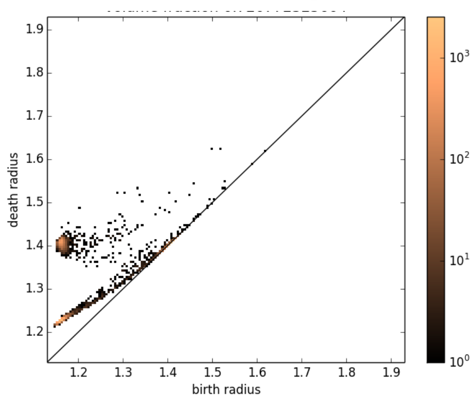


regular tet and oct pores



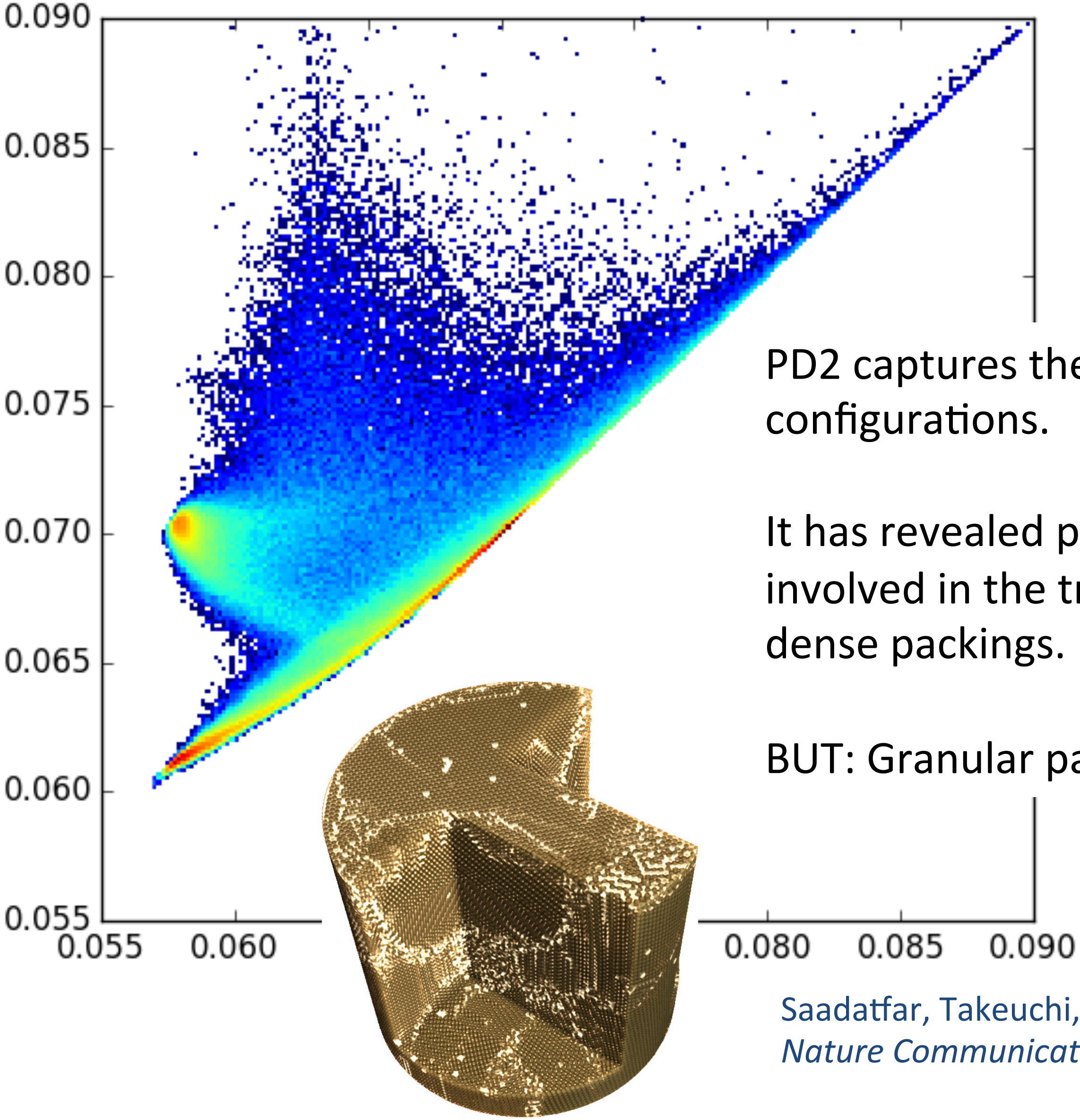






A perfect crystalline packing
has the ratio
tetra : oct of 2:1

summary of sphere packing analysis



PD2 captures the distribution of local pore configurations.

It has revealed pathways of local deformations involved in the transition from crystalline to less-dense packings.

BUT: Granular packing is much more than geometry.

Saadatfar, Takeuchi, VR, Francois, Hiraoka (2017) *Nature Communications*, vol. 8.

VR, Turner (2016) *Physica D* vol. 334.