# The theory and applications of persistent homology

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# Outline

1. Introduction
2. Homology and persistent homology
3. Applications of persistent homology
4. Software for persistent homology

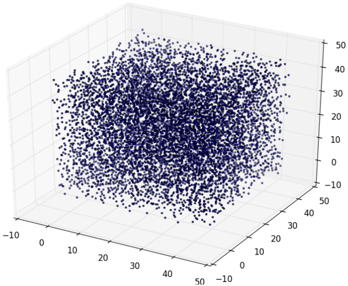
# Introduction

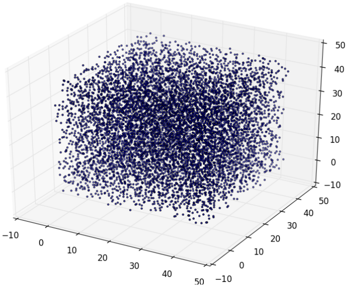
# Persistent homology

- Topological Data Analysis (TDA)
  - Data analysis using topology from mathematics
  - Characterize the shape of data quantitatively
    - Connected components (islands), rings (holes), cavities
- Persistent homology (PH) is one of the most important tools for TDA
  - Uses the concept of "homology"
  - Gives the good descriptor of the shape of data (persistence diagram)
- Developed rapidly in 21st century
  - Mathematical theories and algorithms
  - Software
  - Applications to materials science, life science, etc.

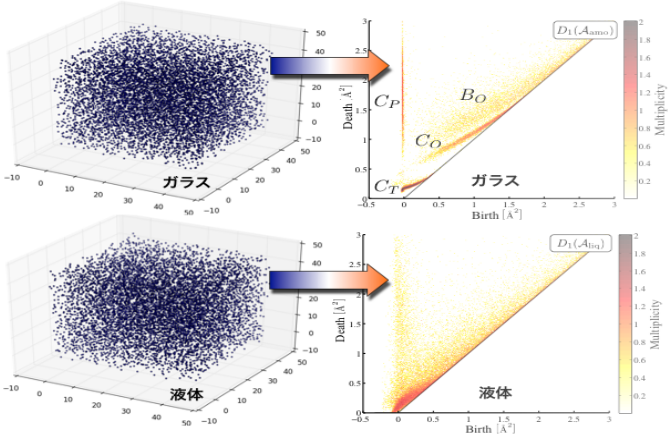
- Mathematics and data analysis
  - Probability - statistics and machine learning
  - Analysis - Fourier analysis and numerical analysis
  - Algebra - Symmetry analysis (for crystals)
  - Geometry and topology - *TDA*
- TDA is good for:
  - heterogeneous data
  - disordered data
  - data without complete randomness
- Mathematics and materials
  - Liquid and gas - random - probability theory and statistical models
  - Crystals - ordered - group theory
  - Amorphous, polycrystalline, and porous media - disordered - *topology*

# Example 1



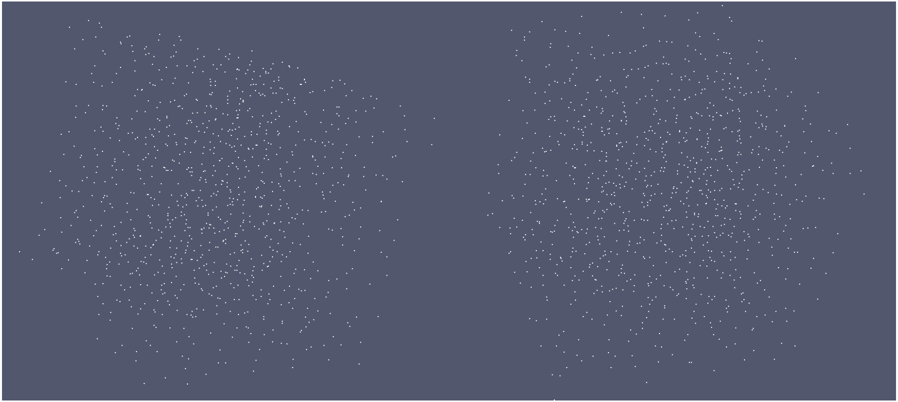

Atomic configurations of amorphous silica and liquid silica. Do you identify?



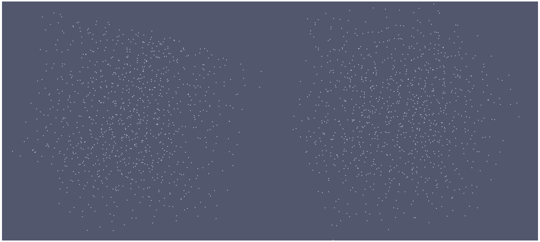

From Y. Hiraoka, et al., PNAS 113(26):7035-40 (2016)

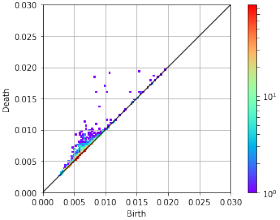
We can identify by using persistence diagram.

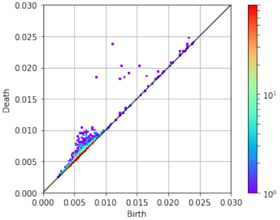
# Example 2

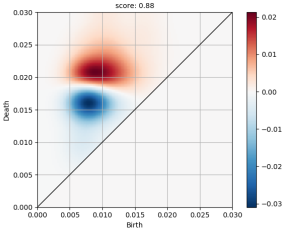


What is the characteristic difference between these two pointcloud ?





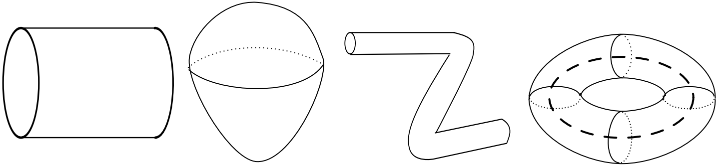




We can distill the characteristic geometric patters by the combination of PH and machine learning

# Homology and Persistent homology

# Homology

- We can mathematically formalize “connected components”, “rings” “cavities” by *homology*.
- Algebra is used for the formalization
- We can identify the “type” of “holes” by a kind of dimension (called degree)

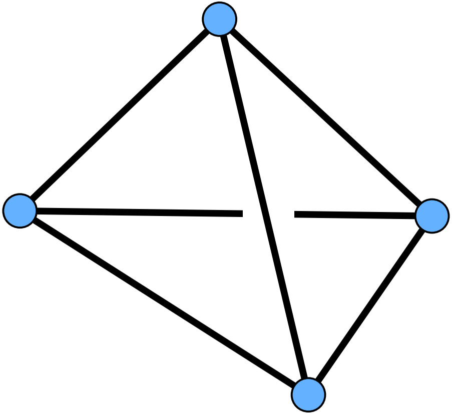


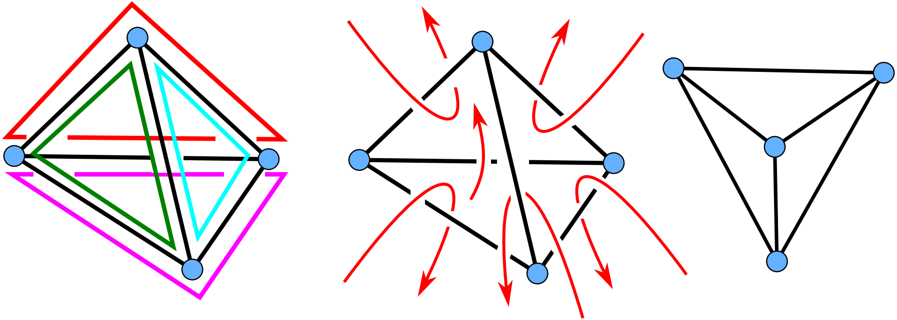
| | | | |
|---|---|---|---|
| dim 1: 1<br>dim 2: 0 | dim 1: 0<br>dim 2: 1 | dim 1: 1<br>dim 2: 0 | dim 1: 2<br>dim 2: 1 |

1 dim: You can see the inside from outside    2 dim: You cannot see

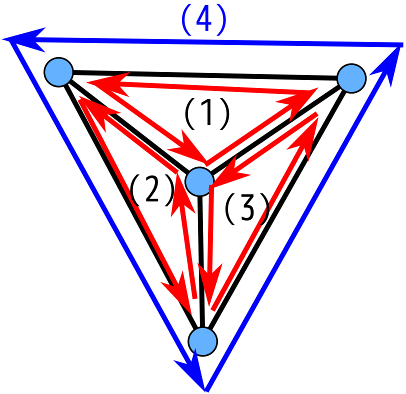
# Count the rings

How many rings in this figure?





4?    6?    3?



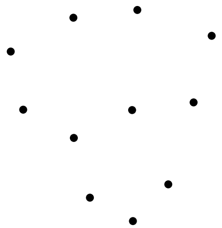

Linear algebra is the key to count the rings. Here we have $(1) + (2) + (3) = (4)$ since two arrows with opposite directions are canceled. Therefore these four rings are *linearly dependent*, and we can count the number of *linearly independent* rings by using linear algebra.

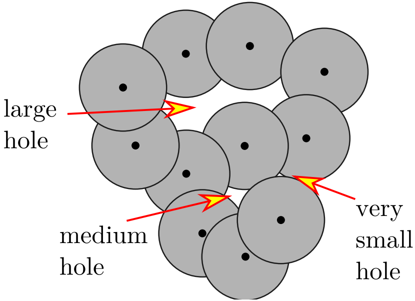
# Persistent homology

- Characterize the shape of data is difficult problem
  - for 3D data or higher dimensional data.
- Homology is used for that purpose, but we can only count the number of holes
- We need better way than homology
- Computational homology is *not* robust to noise.

$\longrightarrow$ *Use increasing sequences* (filtrations)

# $r$-Ball model

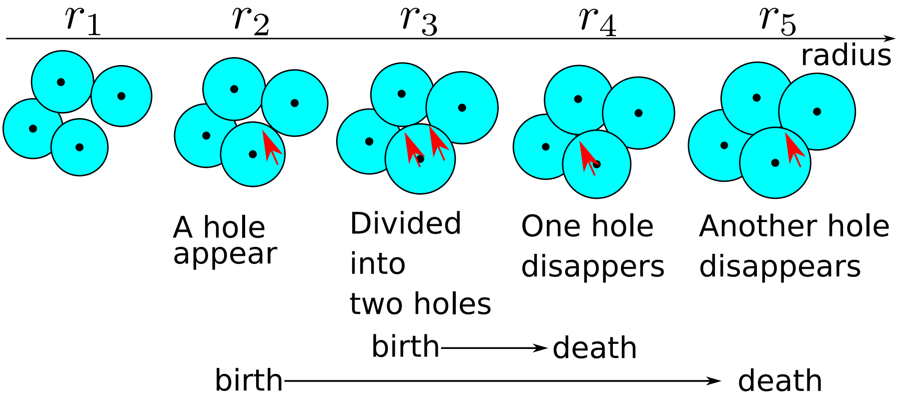





- Input data is a set of point (a pointcloud)
- There is no holes in this pointcloud, but it looks like some holes
- Put discs of radii $r$ on all points
- Three holes
  - We can count the holes by homology

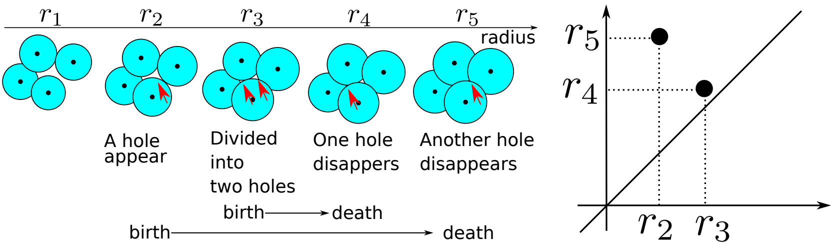
# Filtration

As the radius $r$ become larger, some holes appear and disappear. We can make pairs of appearance and disappearance of a hole by using mathematical theory of PH



# Persistence diagram

These pairs are called *birth-death pairs*. and the set of all birth-death pairs are called *persistence diagram* (PD).




1st persistence diagram

- PH is applicable to any dimensional data
  - But it is hard to intuitively understand higher dimensional holes, 2D or 3D data is easy to analyze
  - Especially, PH is useful for 3D data
- Various increasing sequence
  - Image data
  - Especially 3D data, such as X-ray CT scan data

The following two mathematical theorems are important:

- Structural theorem for PH
  - Gives an algorithm of PDs
  - Uniqueness of a PD for a given input data
- Stability theorem for PH
  - Ensures the robustness of a PD to noises

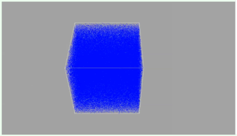
# Applications

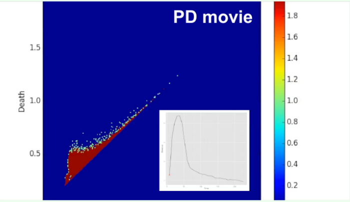
SIP (Structural Materials for Innovation) Ichinomiya, Obayashi, H. PRE (2017)

# Craze formation of polymers

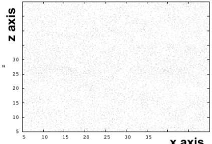
## Kremer-Grest model

**uniaxial deformation**

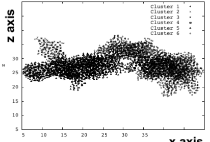





**craze position**

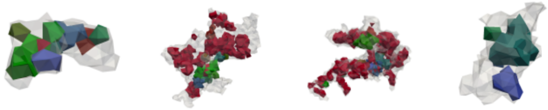



Voronoi volume (conventional)




PD method

**void coalescence during craze formation**



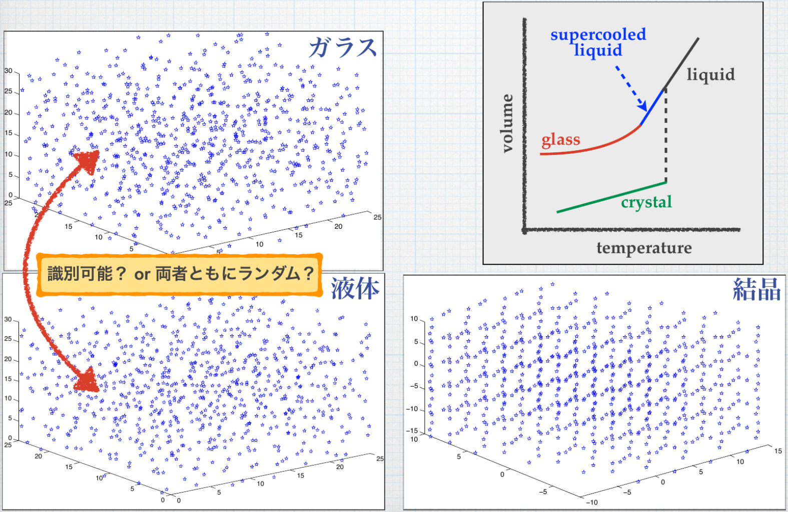
- gray voids are large voids observed after yielding
- color voids are initial micro voids generating large voids

- detect large voids from PD movie by generators with large death values
- explore initial configurations of large voids by reversing time
- large voids are generated by coalesce of micro voids (void percolation)

# Back to Example 1

- The atomic configuration of amorphous silica looks like random
  - Similar to liquid silica
- But amorphous silica has rigidity.
- Some geometric structures are important for the rigidity.
- Y. Hiraoka, T. Nakamura, et al., Hierarchical structures of amorphous solids characterized by persistent homology, PNAS 113 (26) 7035–7040, (2016)

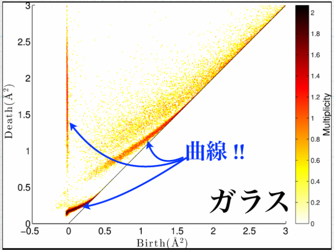
# シリカの原子配置



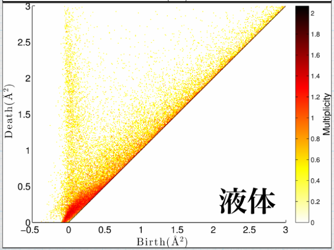
ガラス
supercooled
liquid
liquid
volume
glass
crystal
temperature
識別可能？ or 両者ともにランダム？
液体
結晶

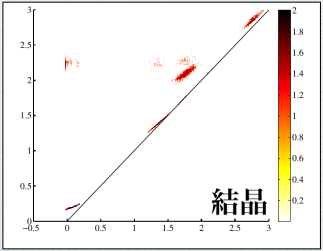
Y.H., T. Nakamura et al. PNAS (2016)

# シリカのパーシステント図



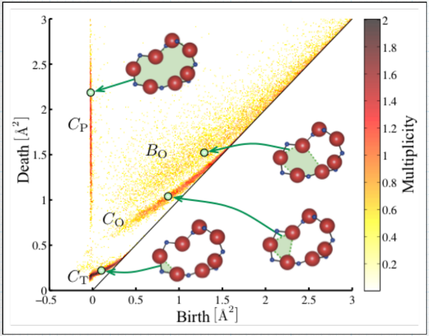

- PD1を表示（リング構造に着目）
- 結晶の規則性は 0次元的分布
- 液体のランダム性は 2次元的分布
- ガラスは 1次元的分布（曲線）!!



Y.H., T. Nakamura et al. PNAS (2016)

# ガラスの階層的幾何構造

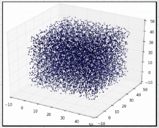



**ガラスの幾何構造**

⇕

**PD内の曲線の幾何学的な起源**

**逆問題** →

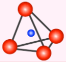


- optimal cycle
  Escolar and H. 2015.
- continuation
  Gameiro, Obayashi, H. Physica D, 2015

## 階層的リング構造

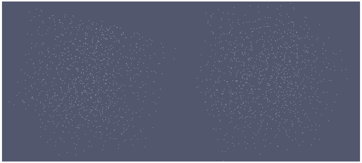
**$C_P$: primary rings generating the others** → **$C_O$: three oxygen rings**

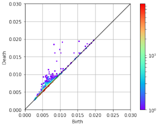
**$C_T$: triangles on tetrahedra**

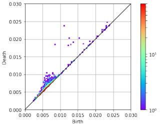


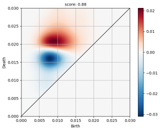
**$B_O$: oxygen rings ($\geq$ four)**

# Back to example 2



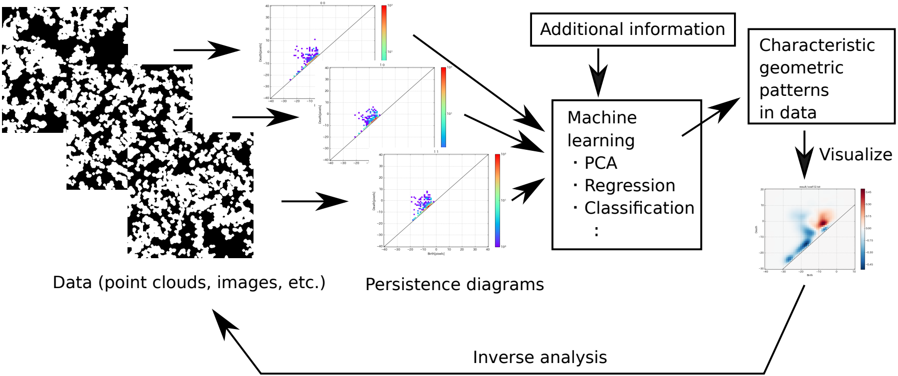



- Combination of Machine learning (ML) and PH
- We have 200 pointclouds
  - 100 pointclouds are labeled by 0, and other 100 pointclouds are labeled by 1
  - Find characteristic geometric patterns by ML and PH

# Framework



Additional information
Characteristic geometric patterns in data
Machine learning
· PCA
· Regression
· Classification
:
Visualize
Data (point clouds, images, etc.)
Persistence diagrams
Inverse analysis

- Each pointcloud is transformed into a PD
- Vectorize PDs and apply a machine learning method
- We can visualize the learned result in the form of a PD
- We can identify important birth-death pairs by comparing the learned result.
- The important pairs are mapped on the original input data by using the “inverse analysis of PDs”
- Please see the demo

# Software

# Software

Software is important for practical data analysis by PH. I introduce you *HomCloud*, data analysis software based on PH.

# Various software

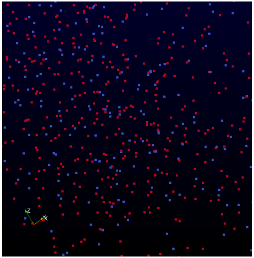
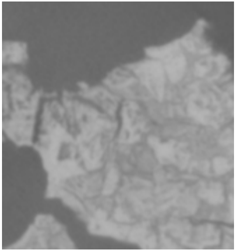
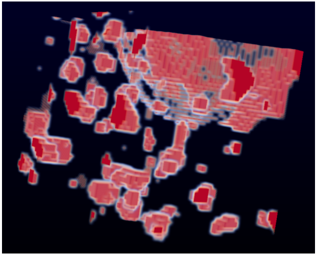
There are many software for PH.

- Gudhi
- dipha, phat, ripser
- eirine
- RIVET
- JavaPlex
- Perseus
- Dionysus

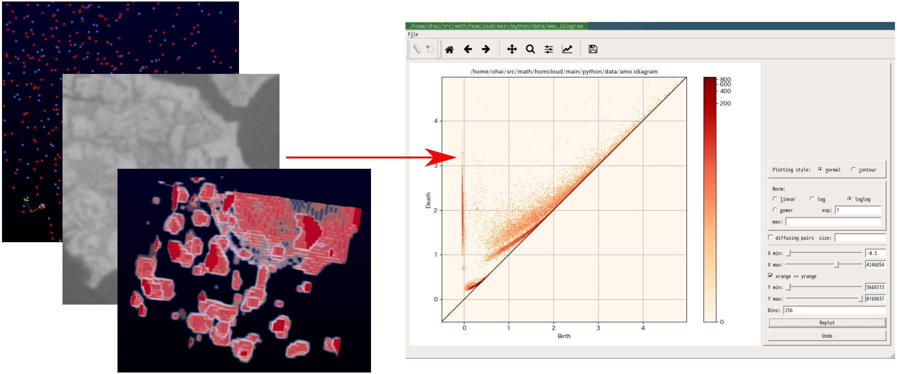
⋮

# HomCloud

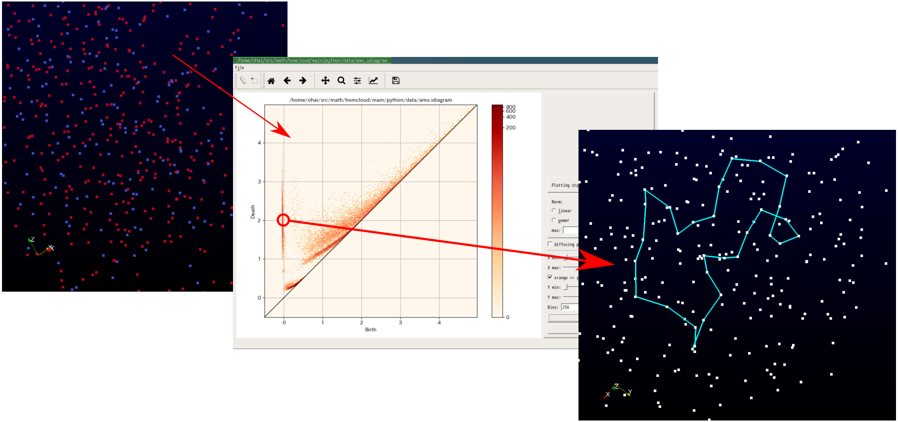
- Focus on applications, especially to materials science
    - MD simulation data
    - 2D/3D image data
    - Easy installation, user interface, machine learning, inverse analysis

We can compute PDs from 2D/3D pointclouds and $N$ dimensional bitmap data.



# 逆解析


File
/home/ohai/src/math/homcloud/main/python/data/amo.idiagram
Death
Birth
0
1
2
3
4
800
600
400
200
Plotting sty
Norm:
linear
power
max:
diffusing
X max:
xrange ==
Y min:
Y max:
Bins: 256

# HomCloud Demo

# Summary

- We can analyze the shape of data effectively and quantitatively by using PH
  - Based on topology
  - PDs are good descriptors for the shape of data
  - Useful for 3D data
- Various applications
  - Materials science
  - Life science, geology, etc.
- The fusion of theoretical studies, software development, and practical data analysis is important.

# Appendix