New Method for Analyzing the Hole-Structure of a Crystal: Merge Trees of Periodic Filtrations

Teresa Heiss-Synak (ISTA ➛ ANU)
joint work with Herbert Edelsbrunner

ICERM Geometry of Materials, Apr 11, 2025
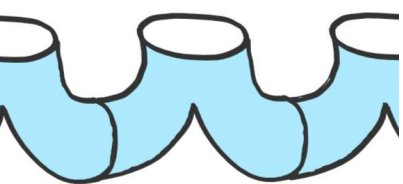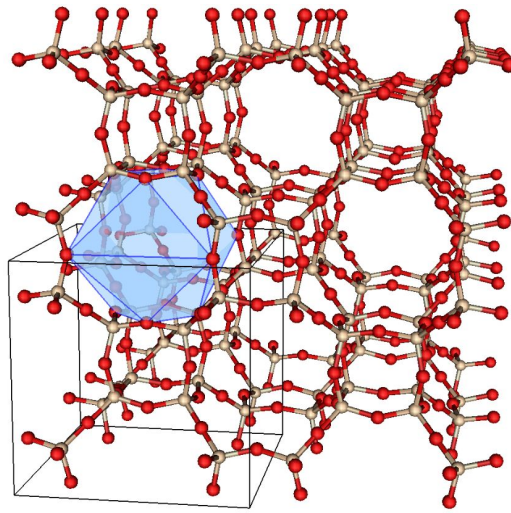
Overview
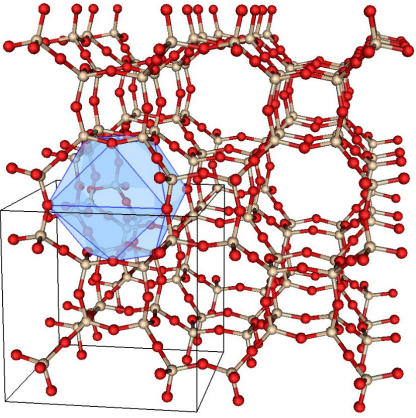
1) Motivation, Applications: Why compute the hole-structure of a (crystalline) material?
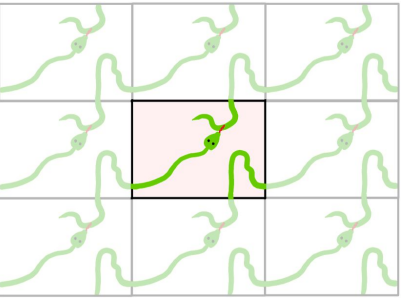
2) Step 1: How to compute 0-dim holes = connected components

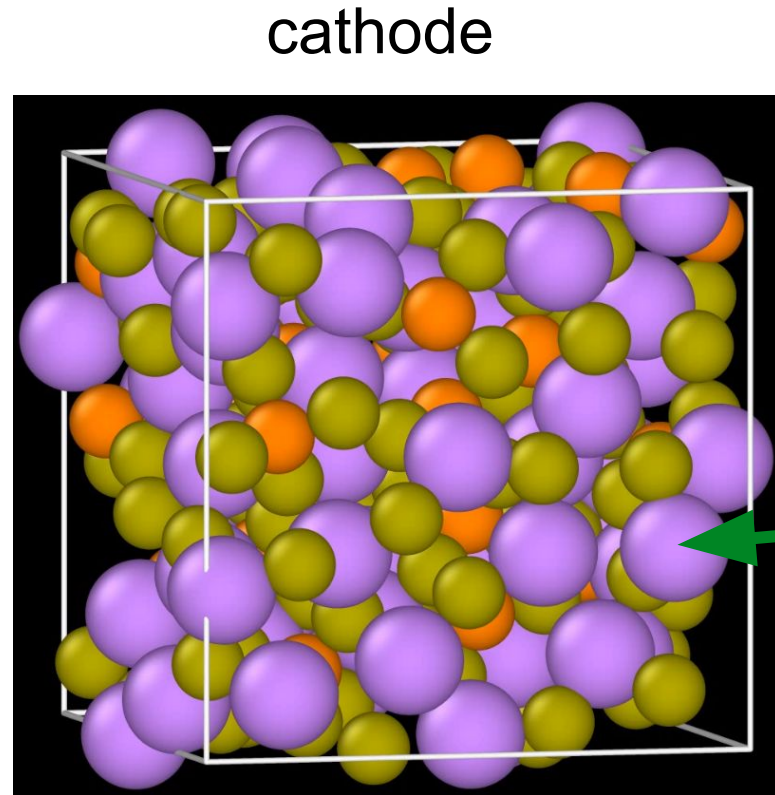3) Step 2: Hot to extend to higher dim holes

Motivation, Applications

Materials Science

Example applications that show that:

Physical / chemical properties of materials are often determined by their holes and connected components.

Application: More efficient batteries

cathode

anode

Collaboration with
Chemistry Professor
Morten M. Smedskjaer
& Topology Professor
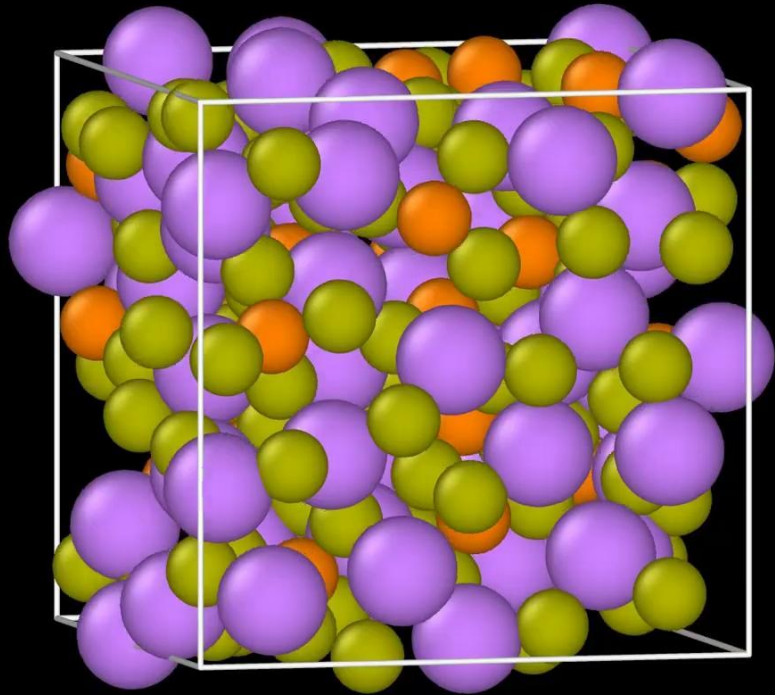Lisbeth Fajstrup
Aalborg University

Li-ions (purple)

Application: More efficient batteries

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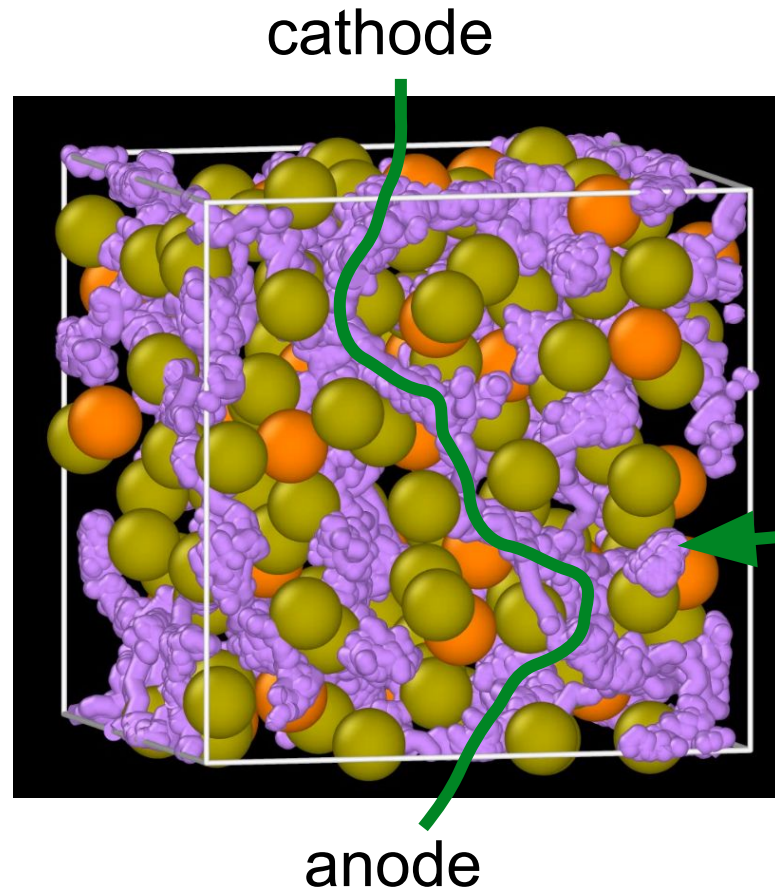& Topology Professor
Lisbeth Fajstrup
Aalborg University
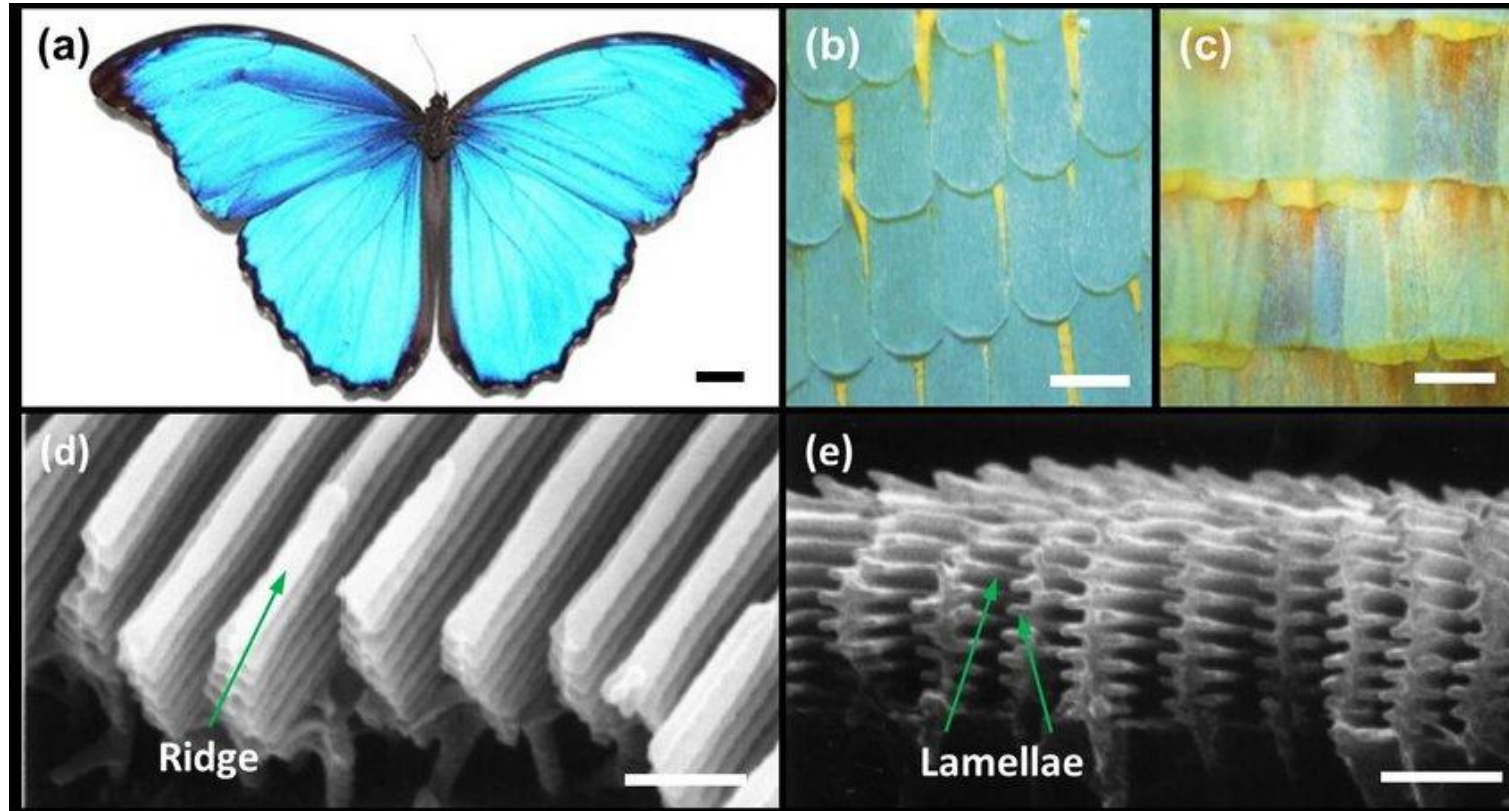
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Tunnels!
Connectedness!

Application: Photonic crystals

Collaboration with
Engineering Prof
Rose Cersonsky
UW–Madison

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Application: Methane Adsorption

Topological Descriptors Help Predict Guest Adsorption in Nanoporous Materials

Aditi S. Krishnapriyan*, Maciej Haranczyk, and Dmitriy Morozov

THE JOURNAL OF PHYSICAL CHEMISTRY C

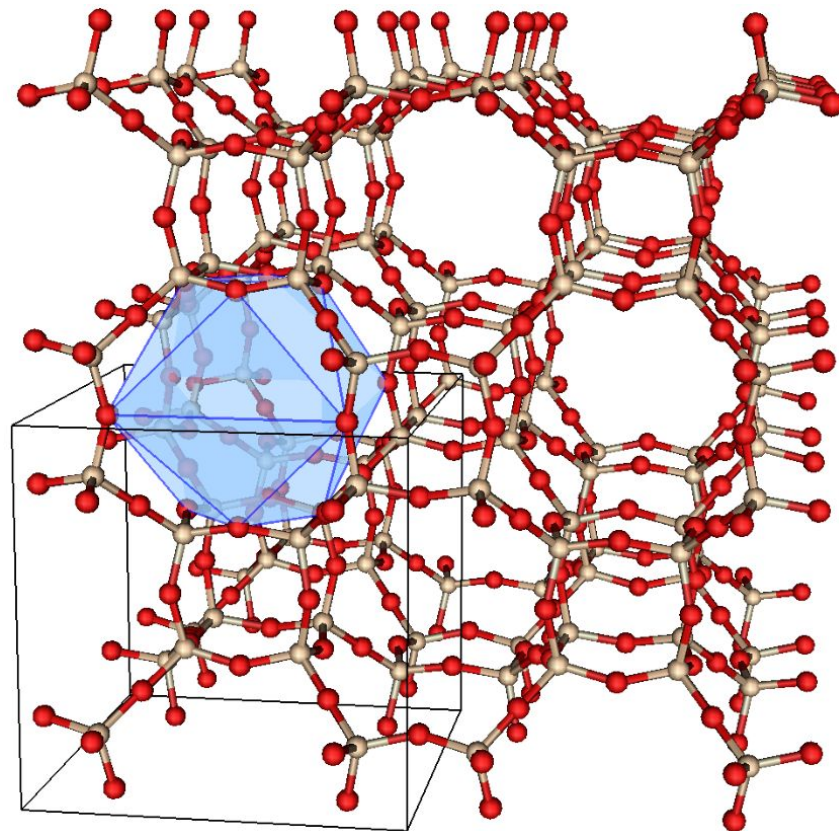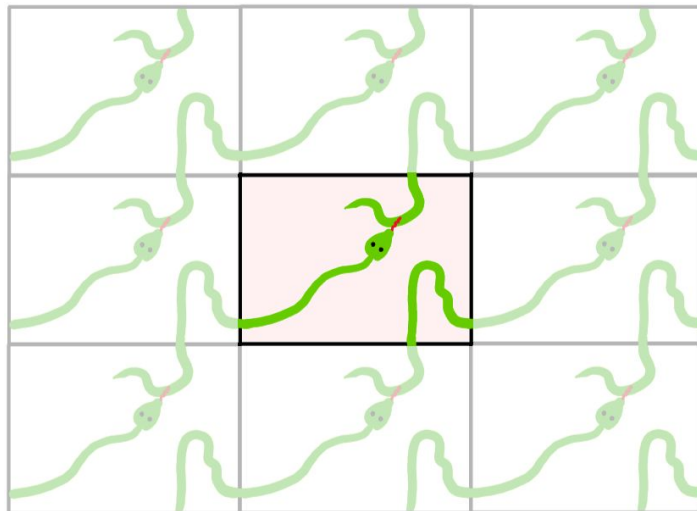Go to The Journa

The Journal of Physical Chemistry C
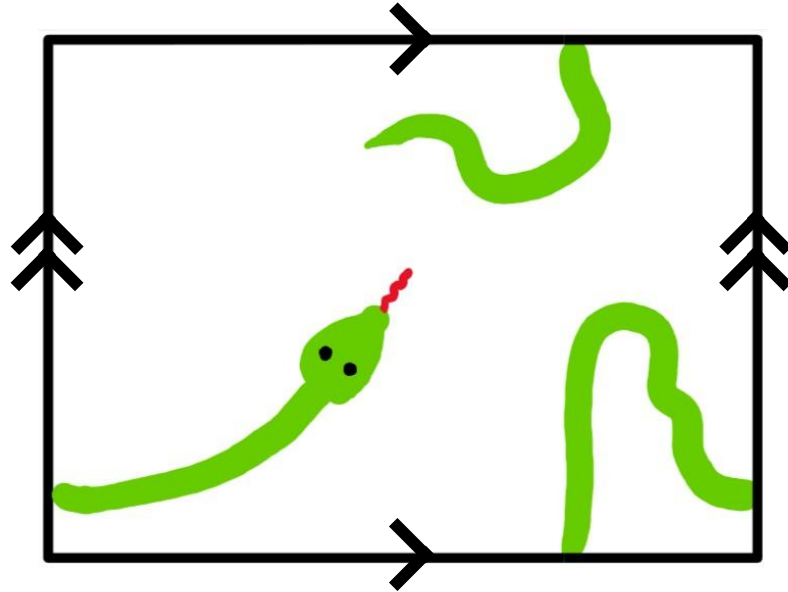
partly motivated
my research

Voids / Cavities!

Merge Tree for Periodic Data

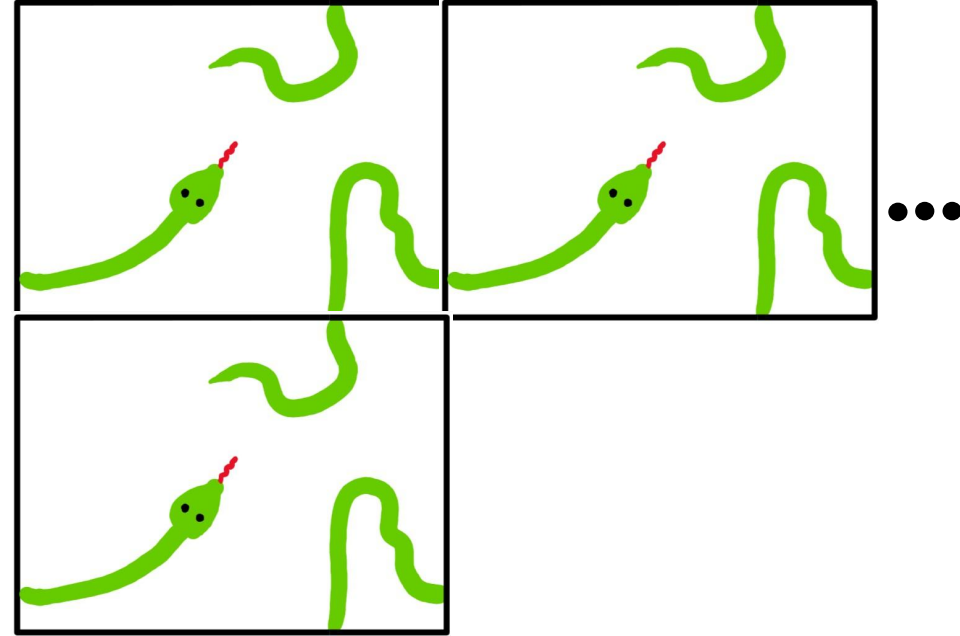[1] Herbert Edelsbrunner and Teresa Heiss. Merge trees of periodic filtrations. ArXiv preprint arXiv:2408.16575, 2024
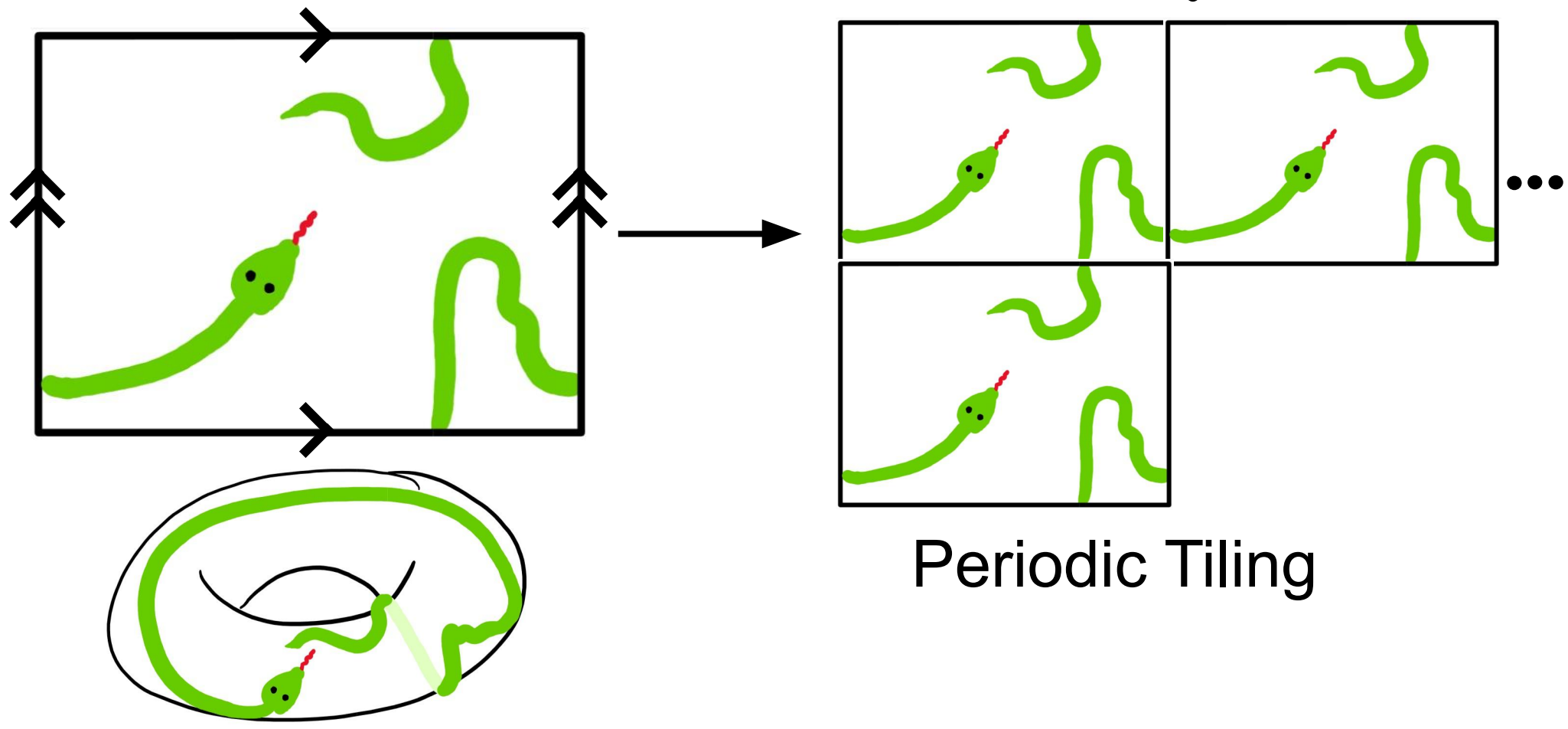
Periodic Data

Game Snake with periodic boundary conditions
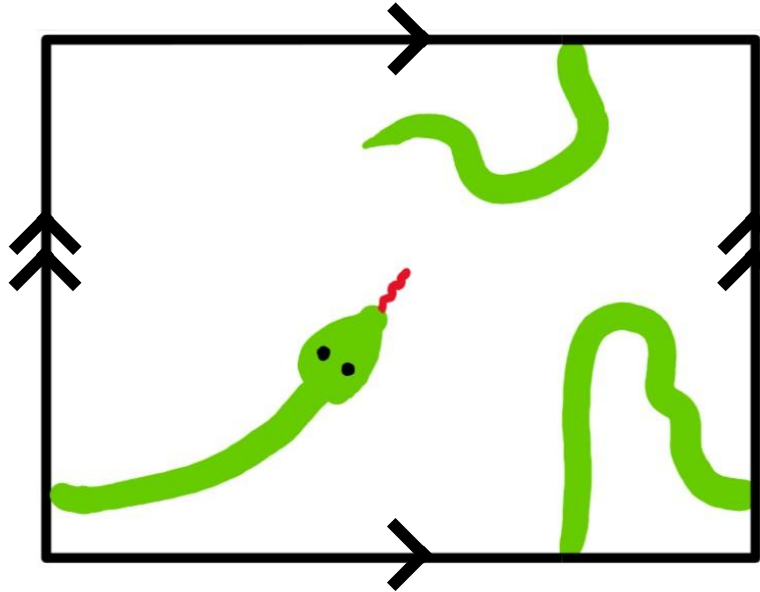
Or Pac-Man

Periodic Tiling

Periodic Data

Periodic Tiling
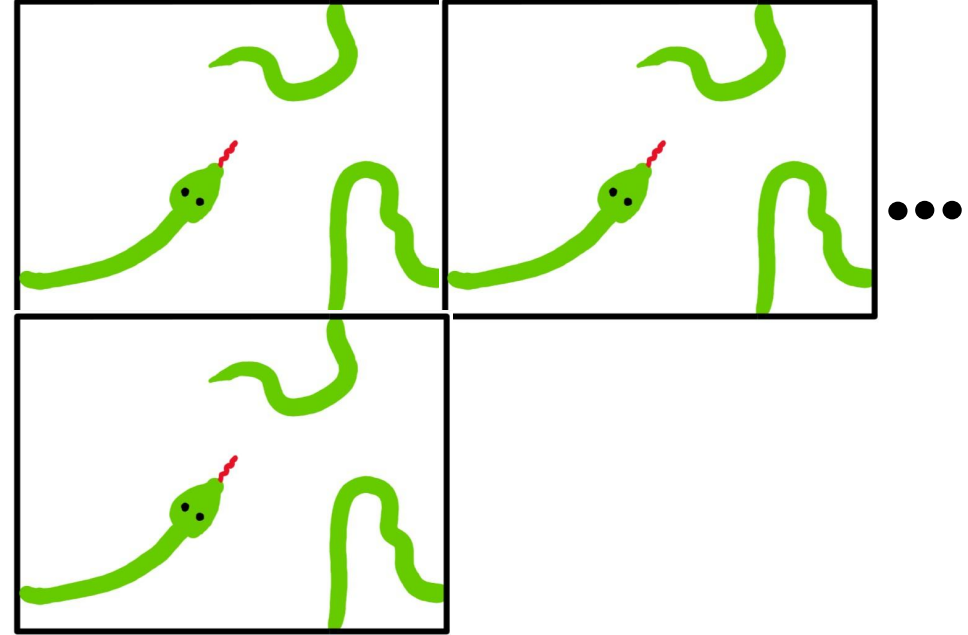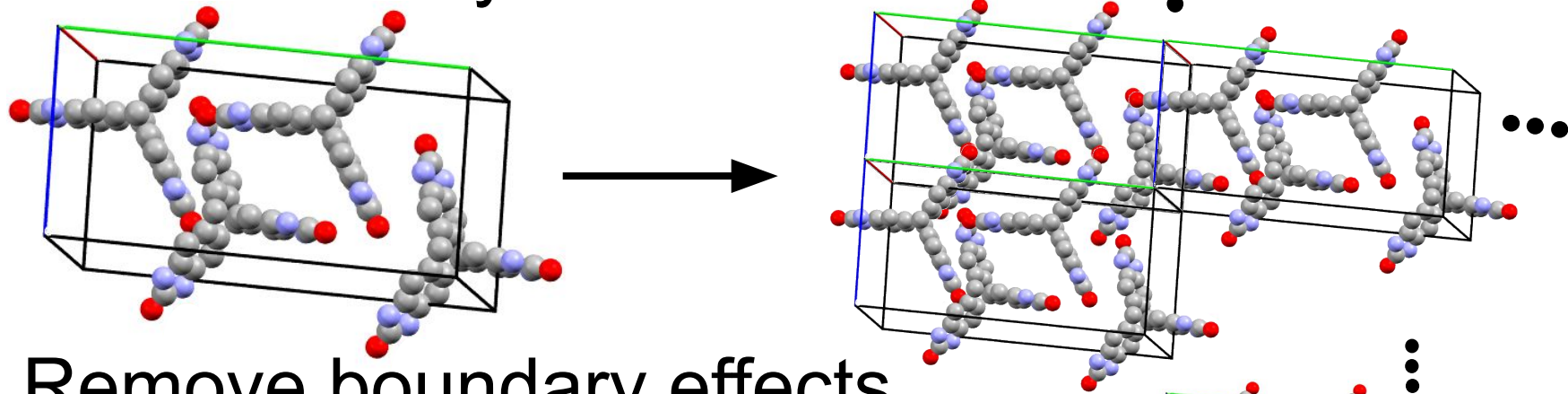
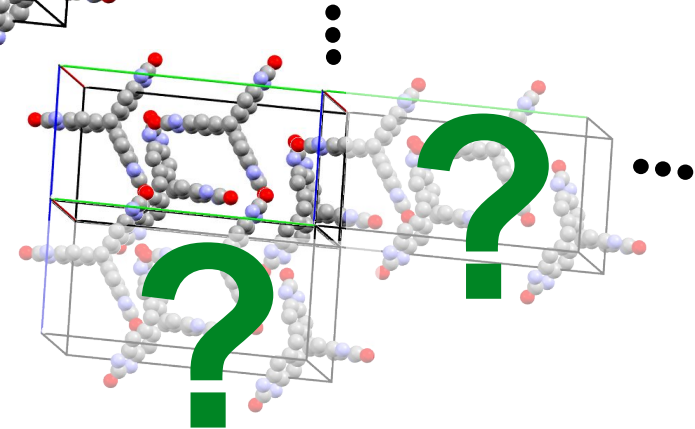# Periodic Data

Torus

Covering space

Periodic Data in Applications
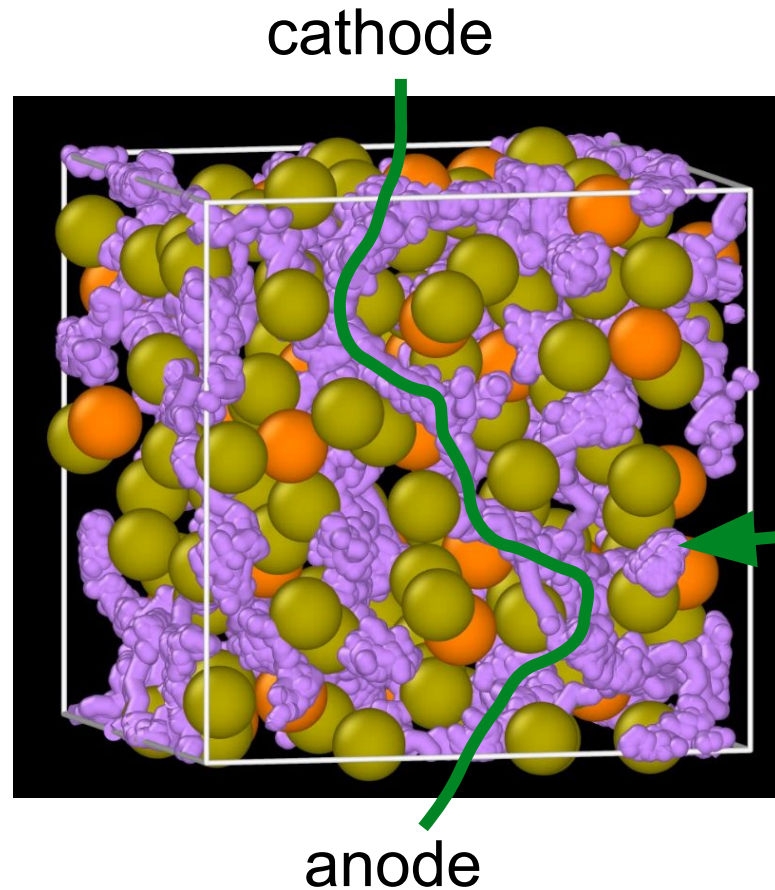
- Atoms of a crystalline material

- Remove boundary effects

  e.g. molecular dynamic
  simulations of
  non-periodic material,
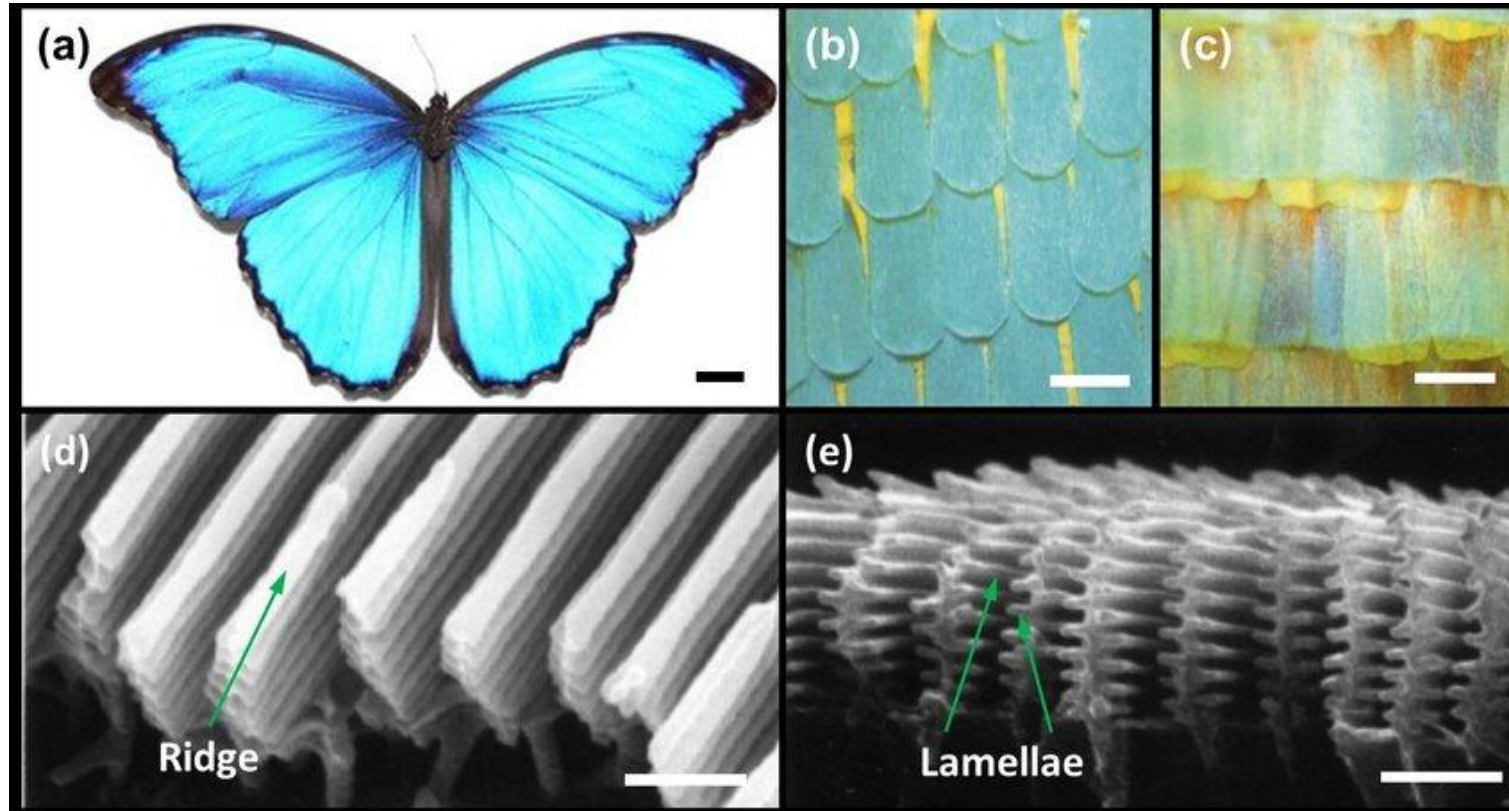 cosmology data

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Application: Photonic crystals

Collaboration with Engineering Prof Rose Cersonsky UW–Madison

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THE JOURNAL OF PHYSICAL CHEMISTRY C

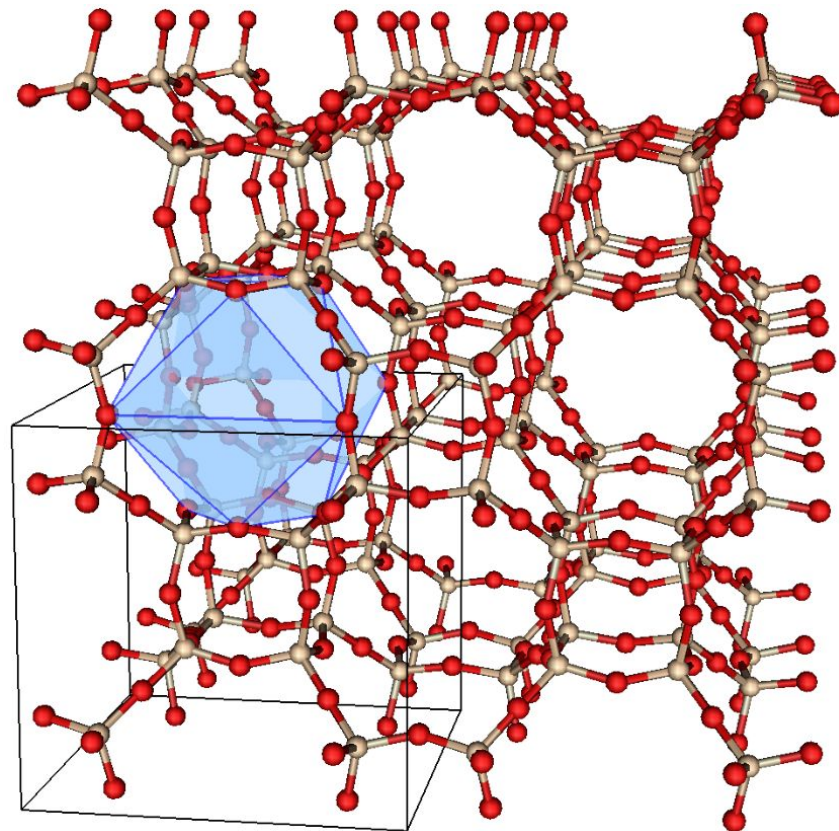Go to The Journa

The Journal of Physical Chemistry C

partly motivated
my research

Voids / Cavities!

TDA for Periodic Data: Problem

Plan: Compute Persistent Homology on torus? Not enough info!

1 component, 1 hole

1 component, 1 hole

1 component with 1 hole
and its copies in
2 space directions
$\Theta(R^2)$ copies in $B_R(0)$

1 component with 0 holes
and its copies in
1 space direction
$\Theta(R^1)$ copies in $B_R(0)$
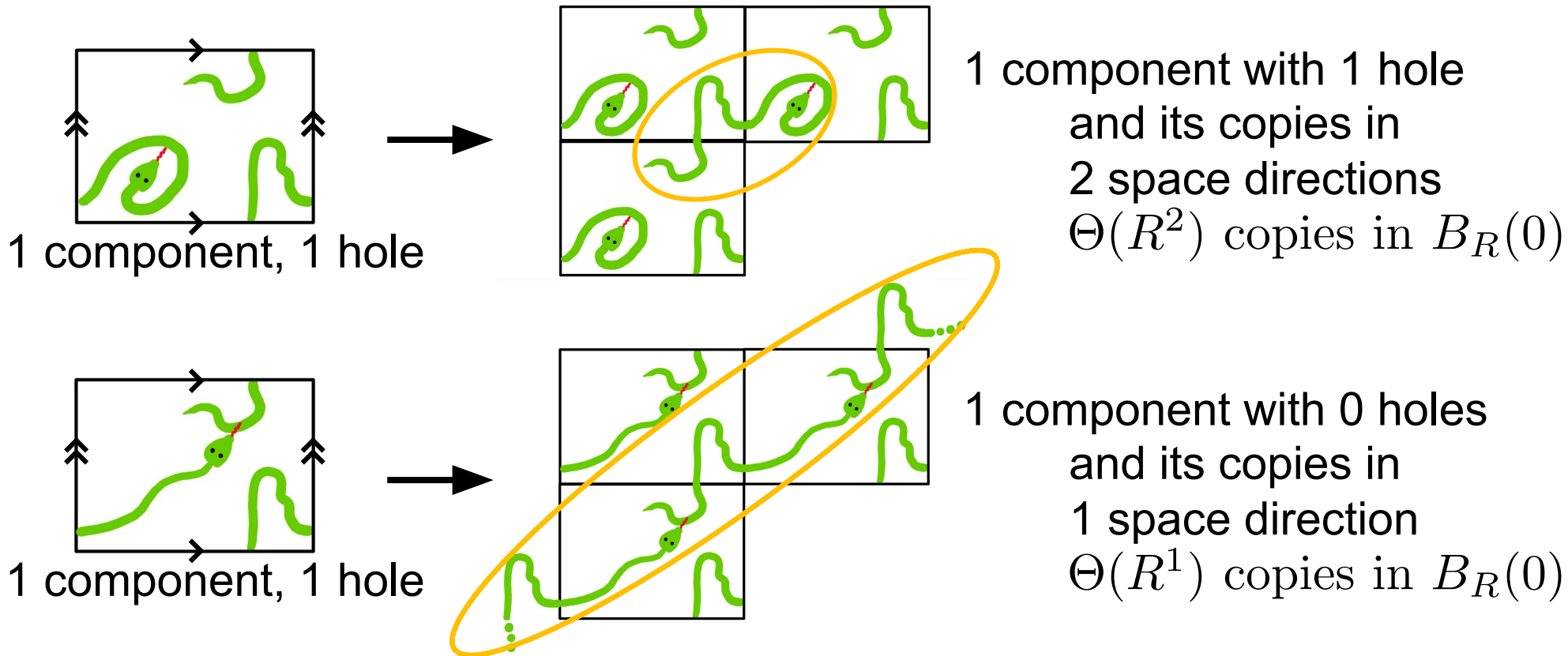
Frequency

How many components in the covering space map to γ?

often: Answer $= \infty$

$R \to \infty$

cR^3

growth rate

cR^2

density

cR

c

γ

therefore:

... within a ball of radius R?

Periodic Merge Tree

Plan: Track components on torus, assign each a frequency

input

Periodic Merge Tree

Plan: Track components on torus, assign each a frequency

input

Periodic Merge Tree

Plan: Track components on torus, assign each a frequency
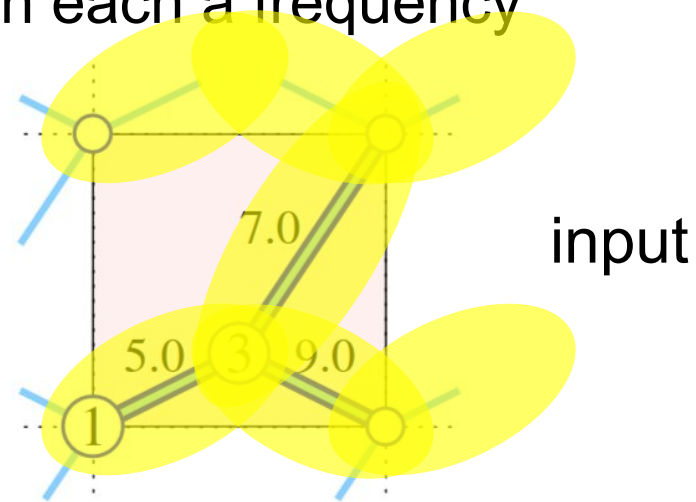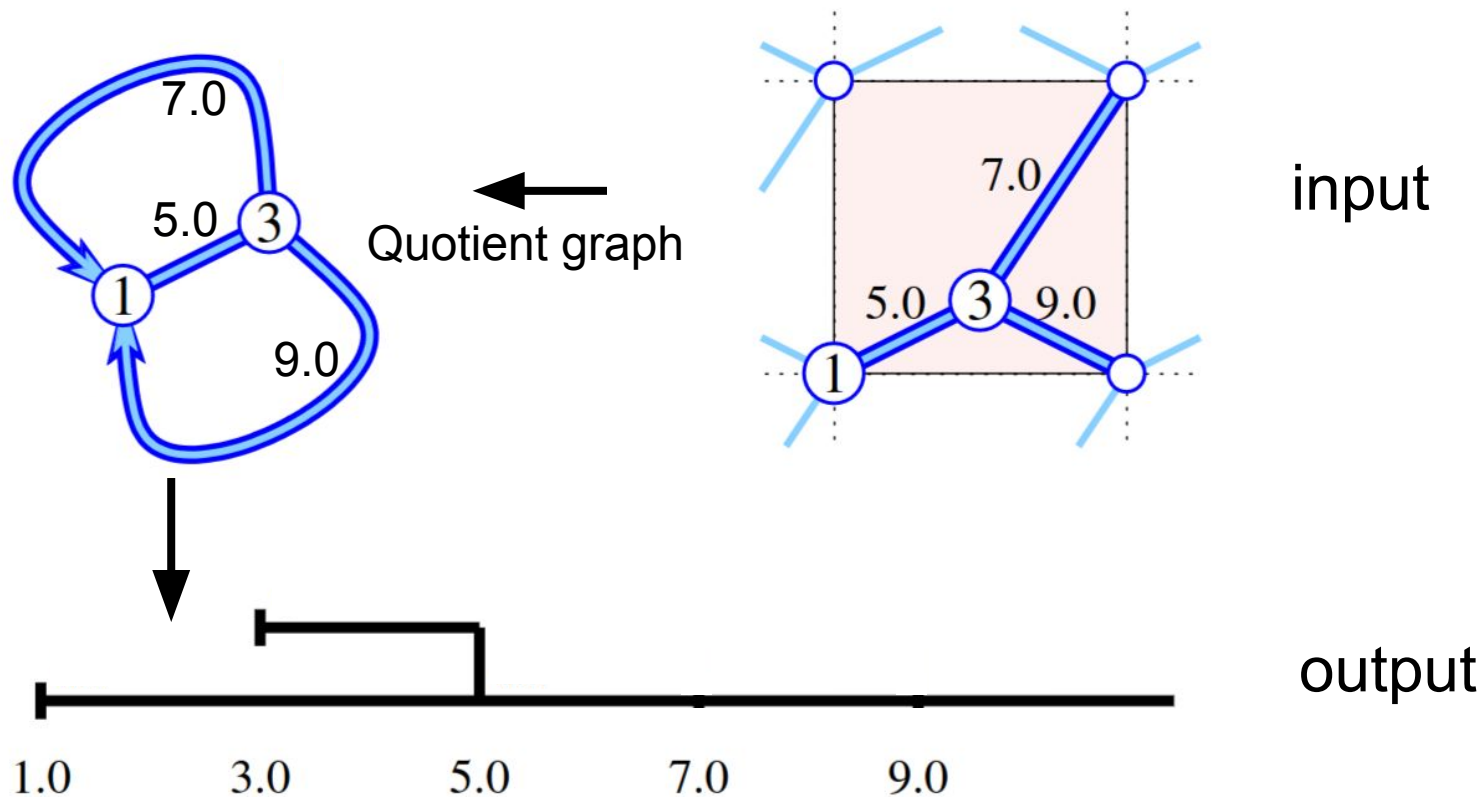

Quotient graph

input

output

Periodic Merge Tree

Plan: Track components on torus, assign each a frequency

Periodic Merge Tree

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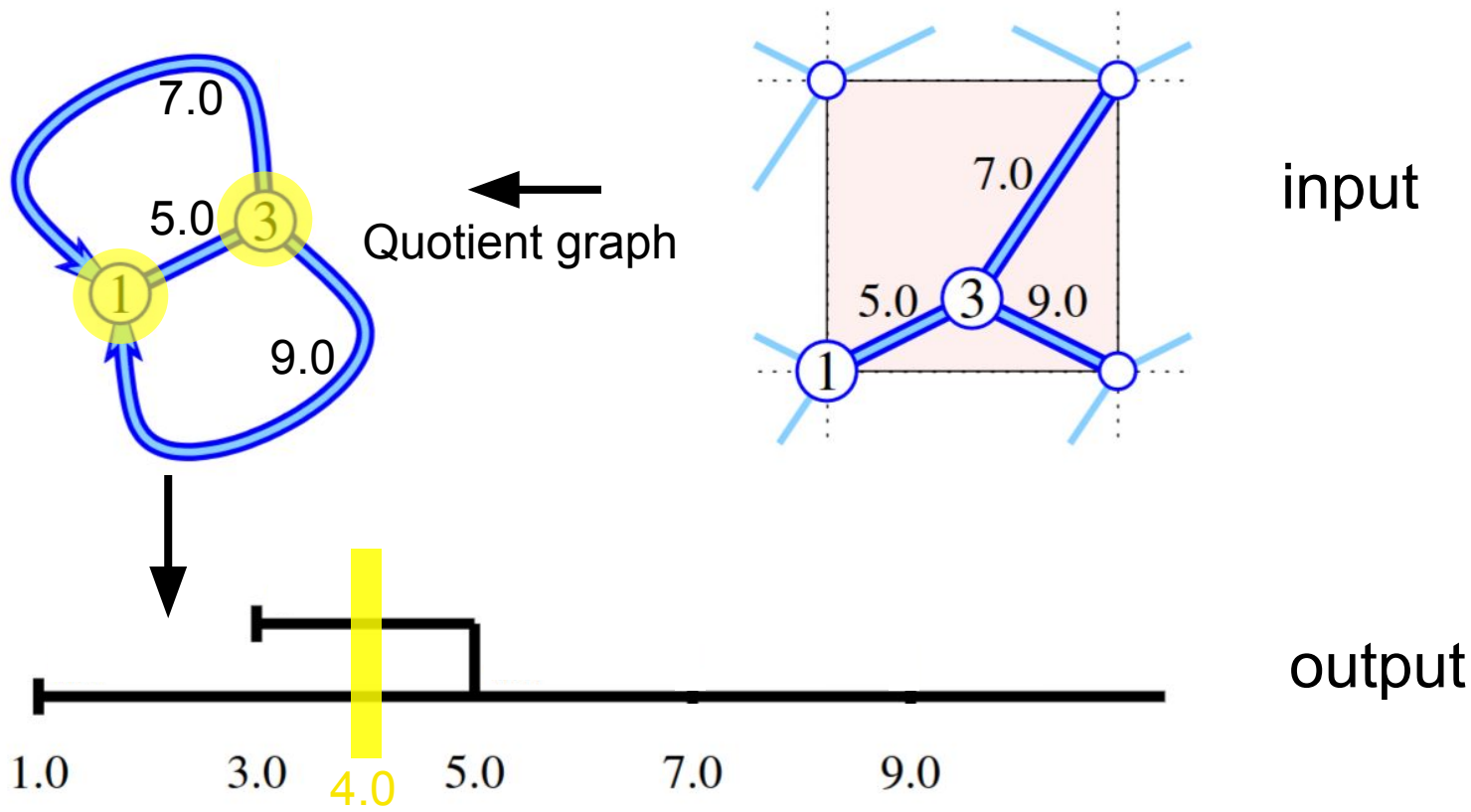# Periodic Merge Tree

Plan: Track components on torus, assign each a frequency

Periodic Merge Tree

Plan: Track components on torus, assign each a frequency
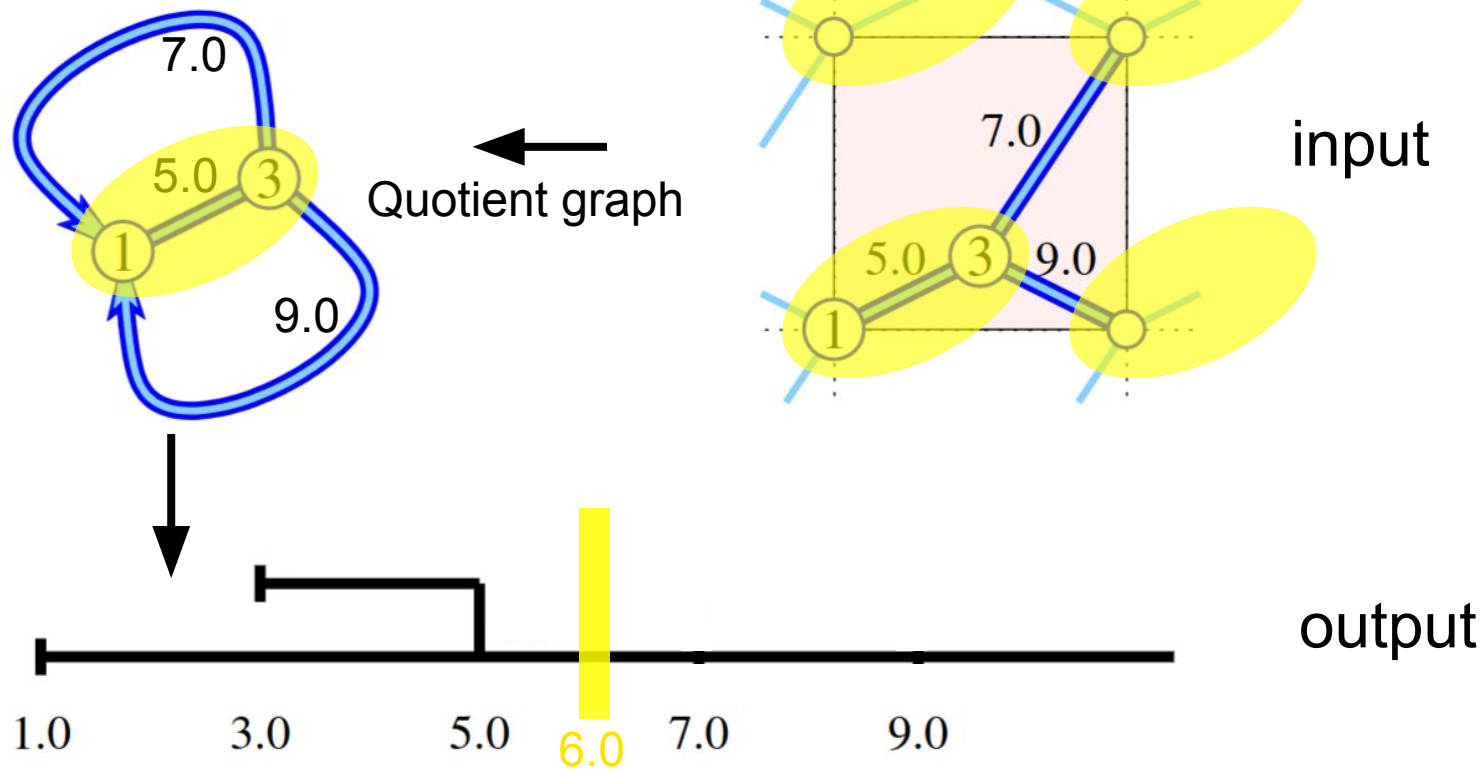
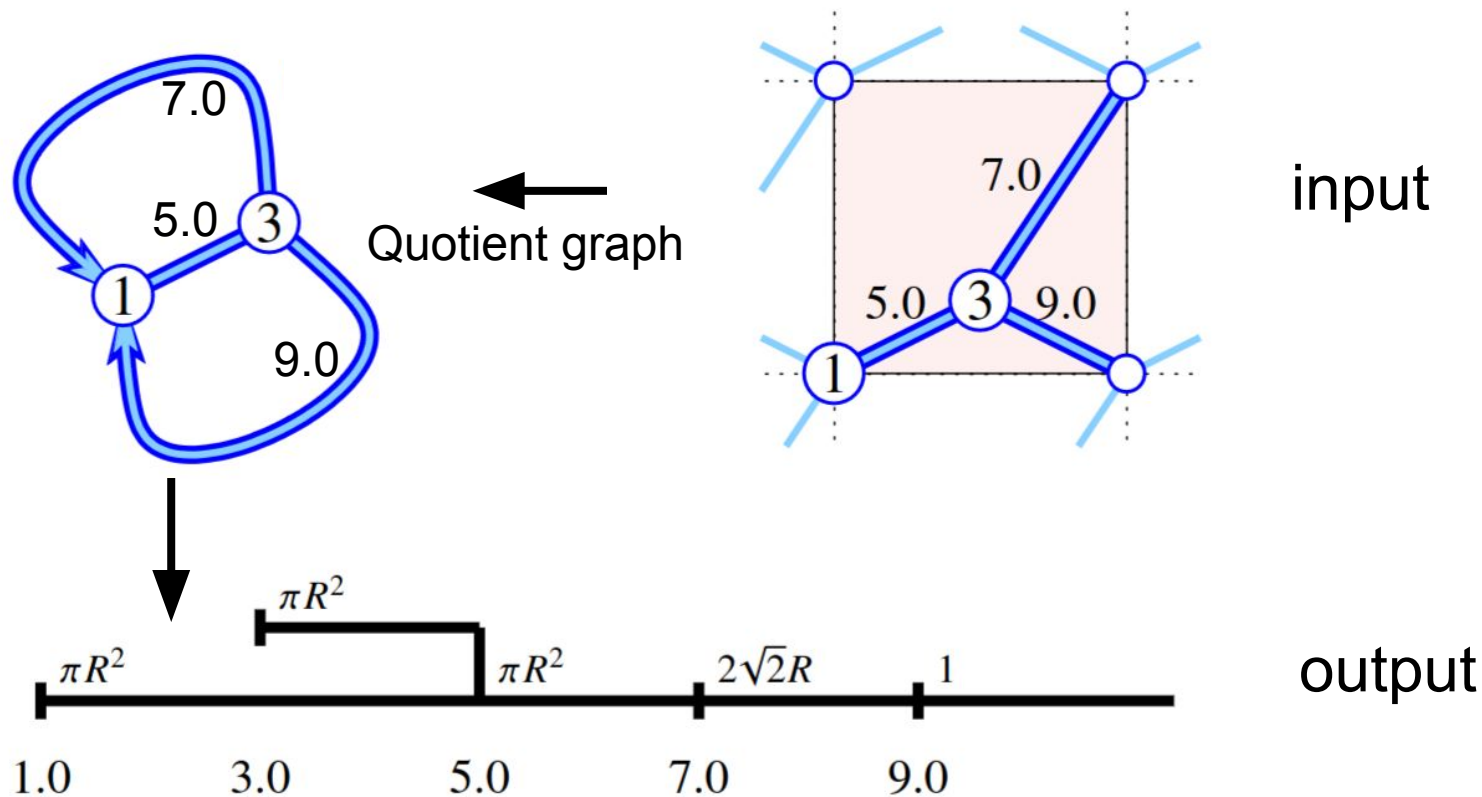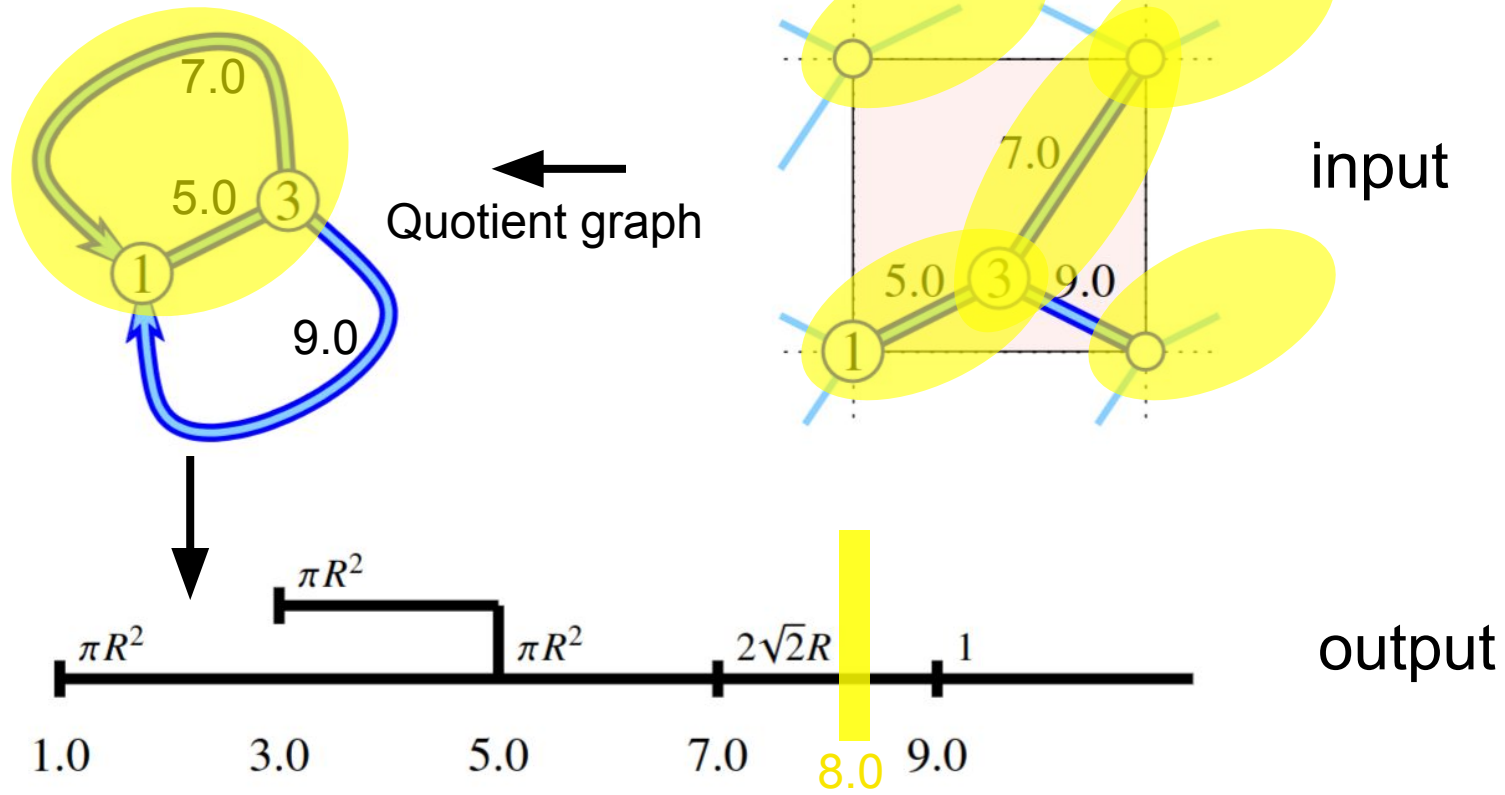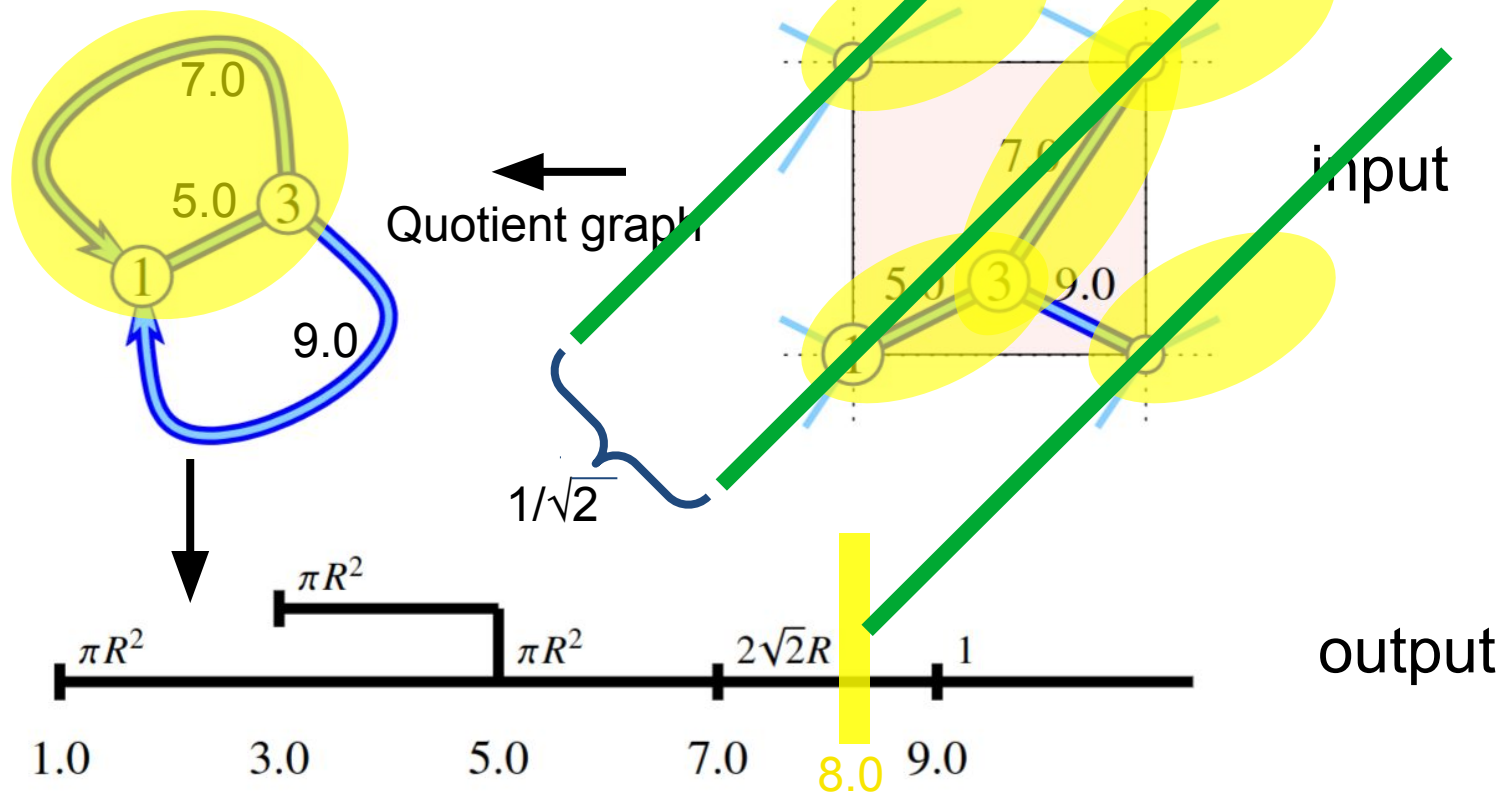

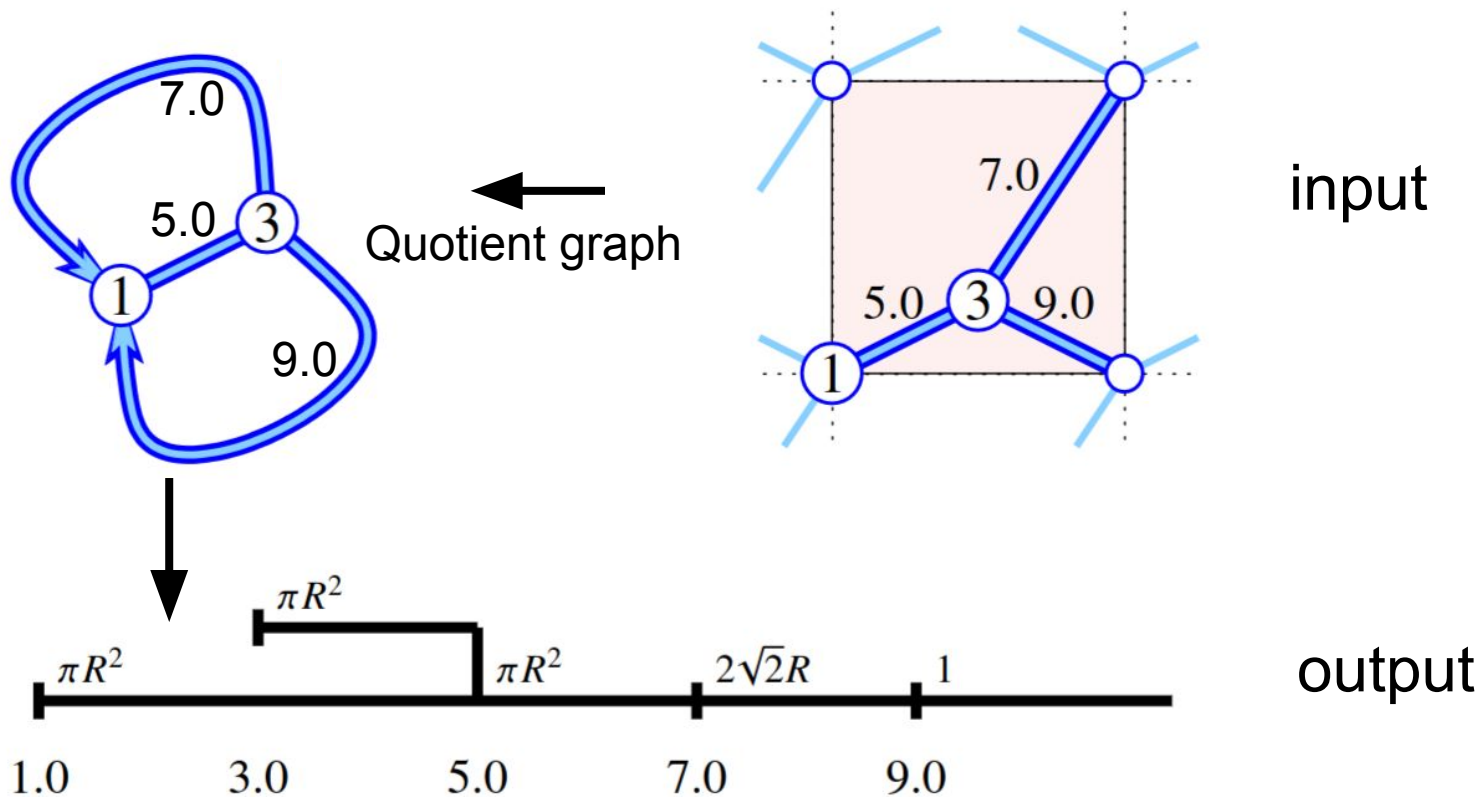Quotient graph

input

output

Periodic Merge Tree

Plan: Track components on torus, assign each a frequency

Periodic Merge Tree

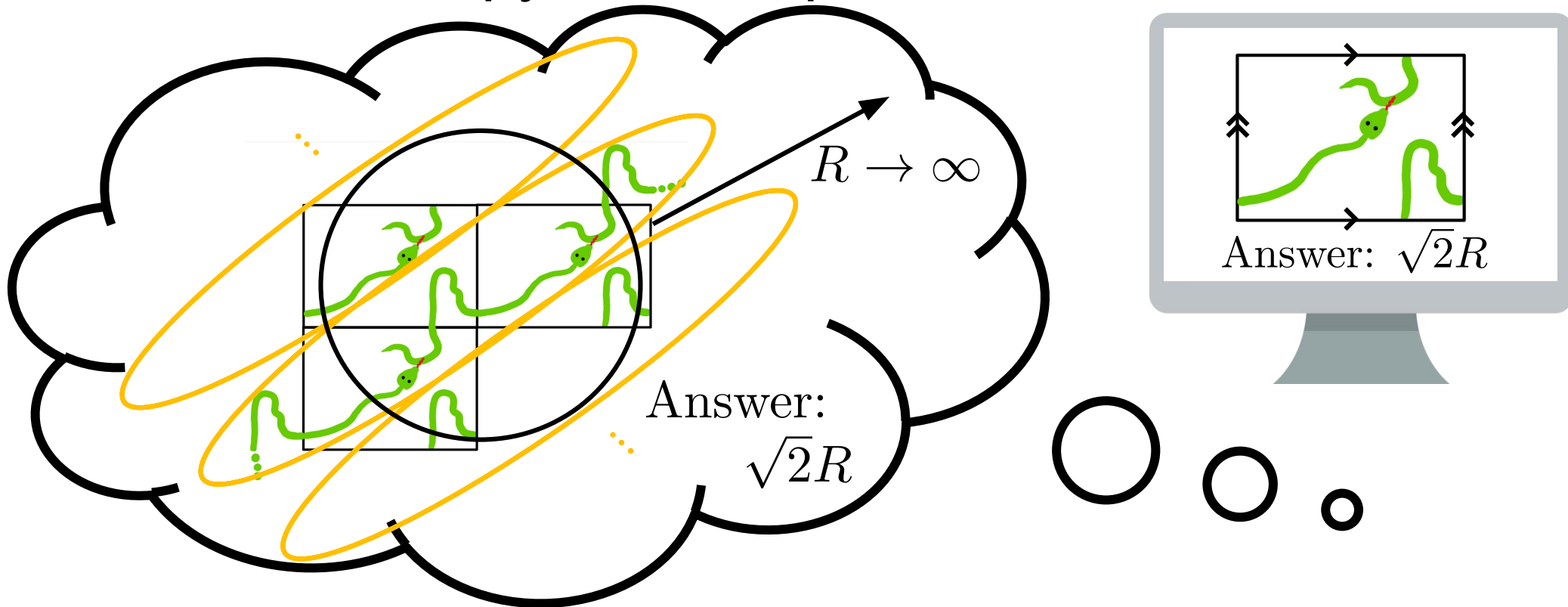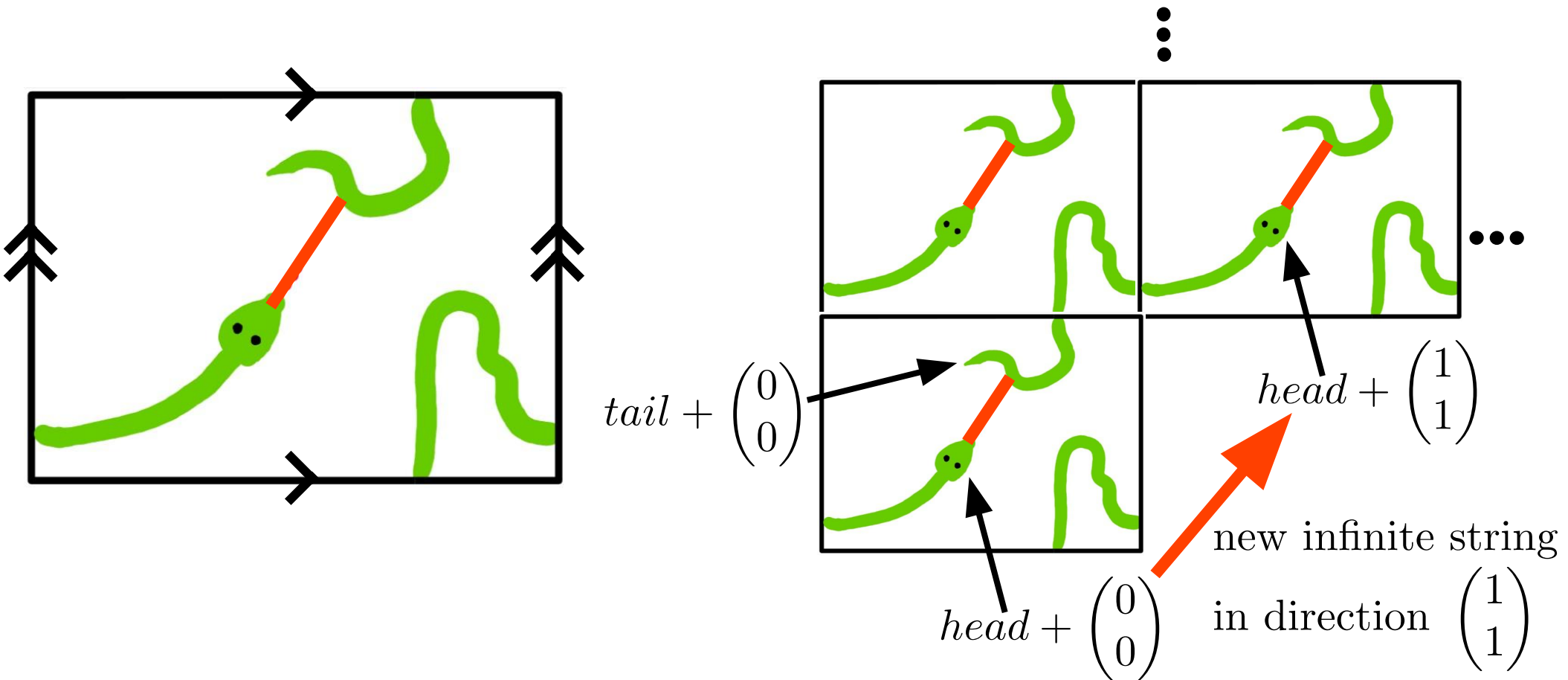Plan: Track components on torus, assign each a frequency

Quotient graph

input

output

Computation: Periodic Merge Tree

No need to copy tile multiple times!

$R \to \infty$

Answer: $\sqrt{2}R$

Answer: $\sqrt{2}R$
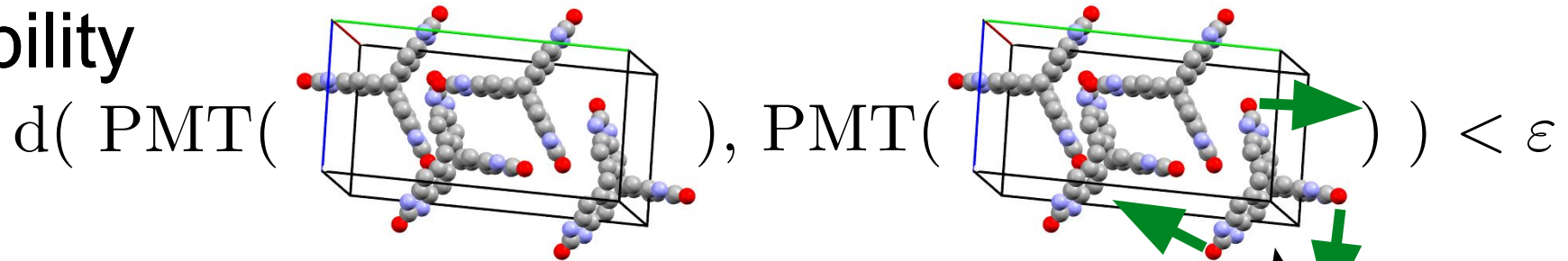
Computation: Periodic Merge Tree

- No need to copy tile multiple times!

- Implemented by Chiara Martyka and Jiaqi Zheng

- Loglinear running time!

- Based on Kruskal's min spanning tree algorithm:
  Process edges greedily in order of filtration value,
  for every edge FIND components of both vertices,
  if not same: take UNION and add edge to tree.
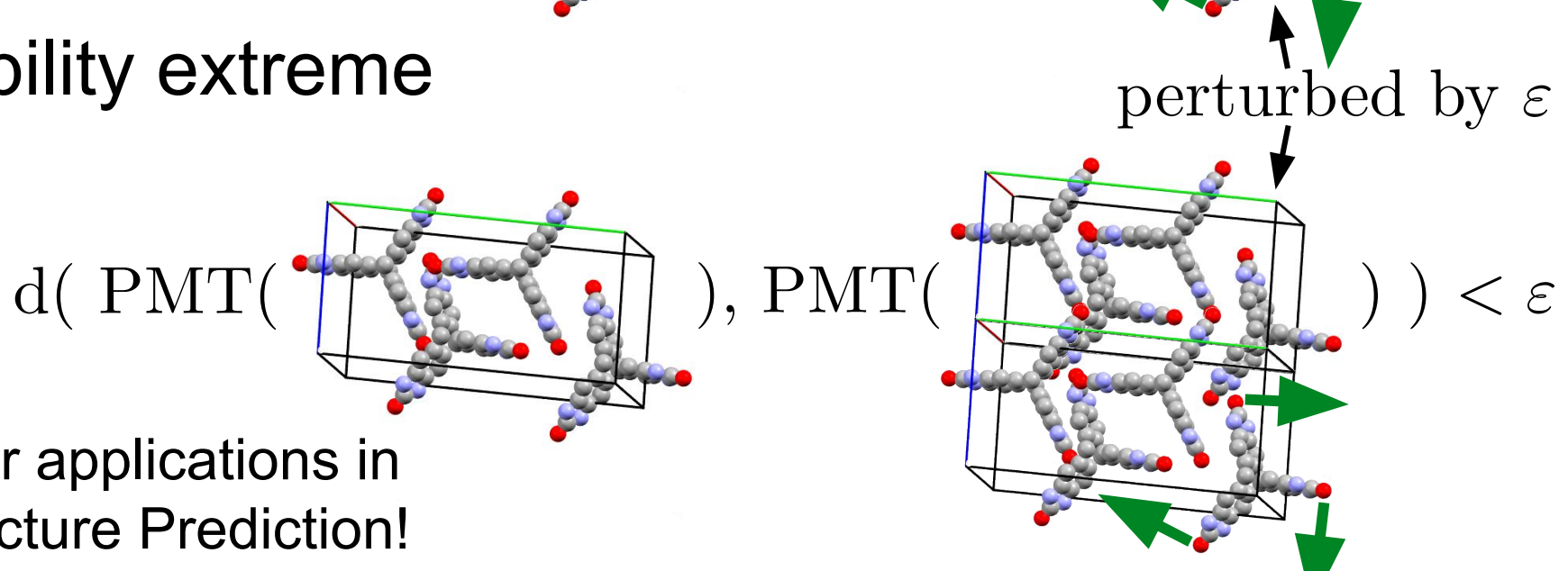
Difference to Kruskal's algorithm

$$tail + \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$head + \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$head + \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

new infinite string
in direction $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Properties: Periodic Merge Tree

1) Stability

$$d(\ \mathrm{PMT}(\quad),\ \mathrm{PMT}(\quad)\ ) < \varepsilon$$

2) Stability extreme

perturbed by ε
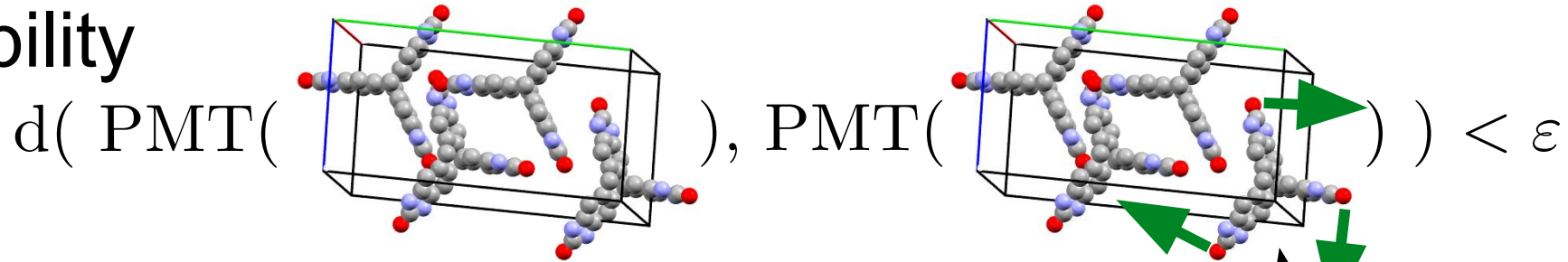
$$d(\ \mathrm{PMT}(\quad),\ \mathrm{PMT}(\quad)\ ) < \varepsilon$$

Important for applications in
Crystal Structure Prediction!

Properties: Periodic Merge Tree

1) Stability

$$d(\ PMT(\quad\quad),\ PMT(\quad\quad)\ ) < \varepsilon$$

perturbed by ε
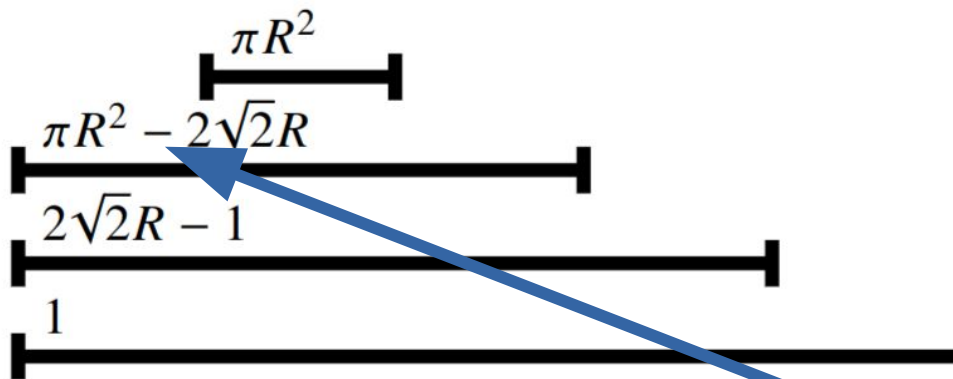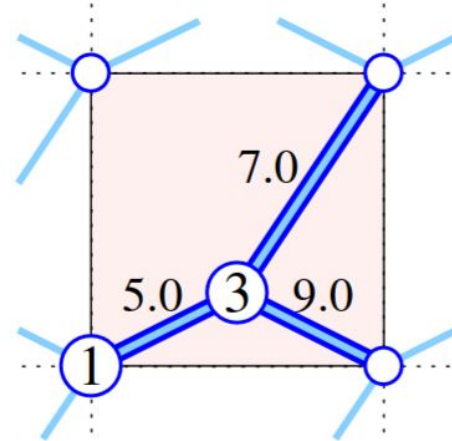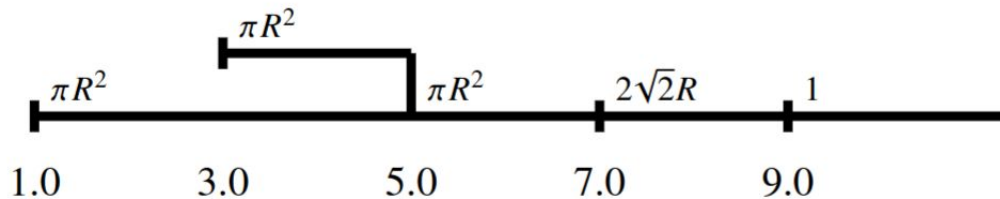
2) Stability extreme
   (important for applications in
   Crystal Structure Prediction)
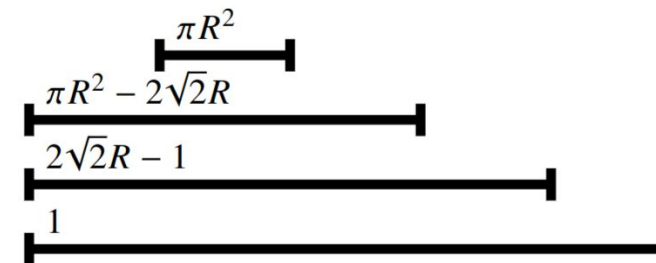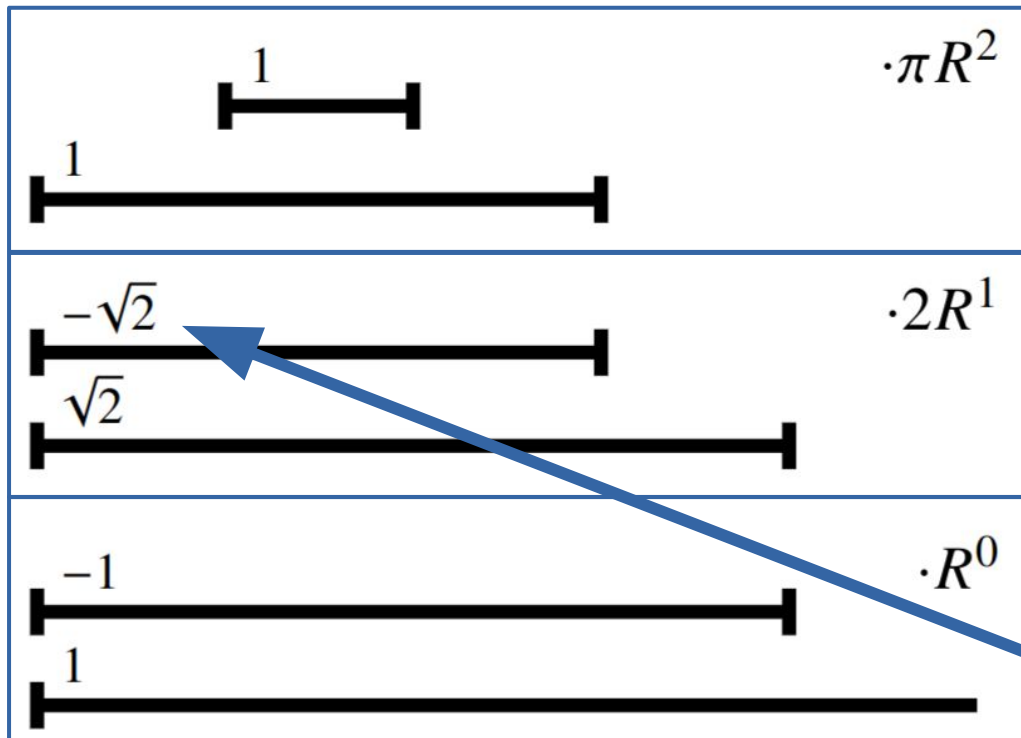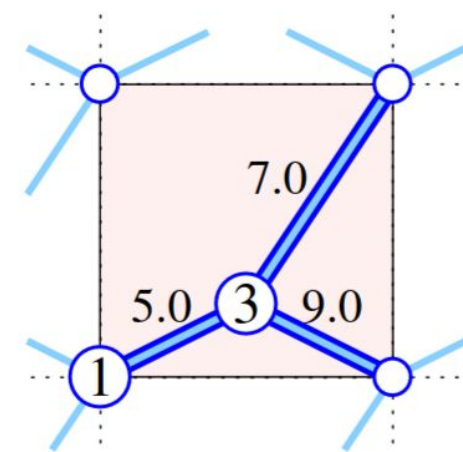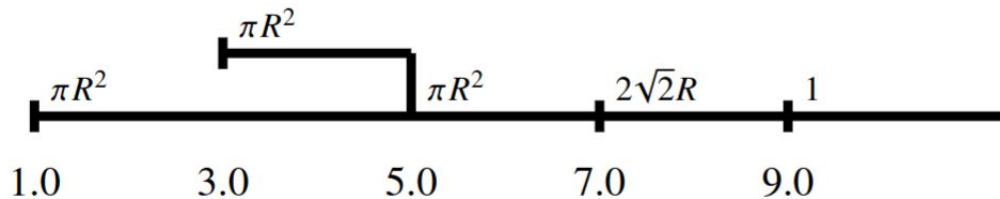
3) No unwanted boundary-effects

4) Efficient algorithm: loglinear complexity

Periodic 0-th Barcode

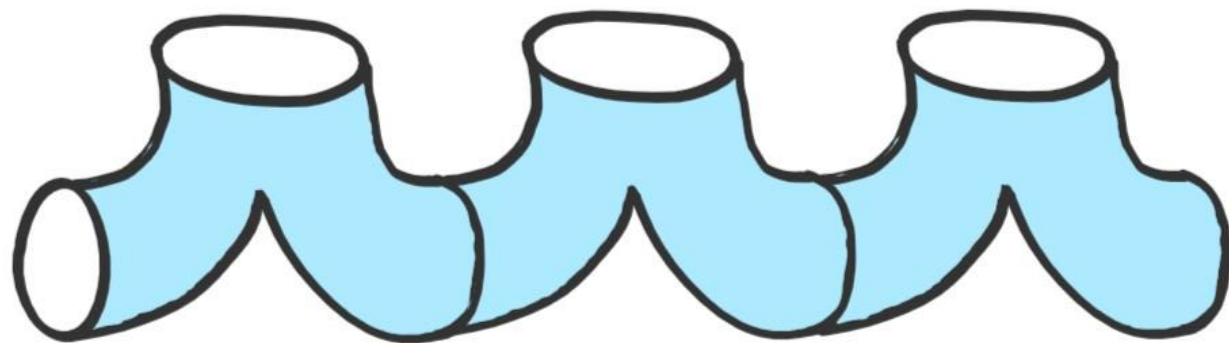Note the negative numbers

Periodic 0-th Barcode

πR^2

πR^2 πR^2 $2\sqrt{2}R$ 1

1.0   3.0   5.0   7.0   9.0

$\cdot\pi R^2$

1

1

$\cdot 2R^1$

$-\sqrt{2}$

$\sqrt{2}$

$\cdot R^0$

-1

1

7.0

5.0   ③   9.0

①

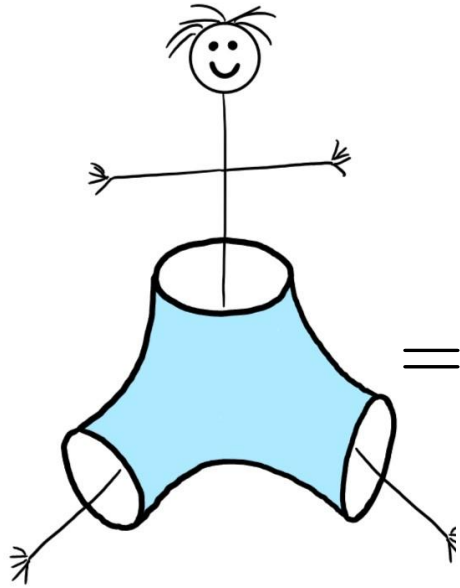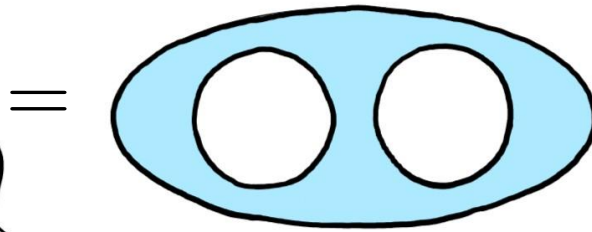πR^2

$\pi R^2 - 2\sqrt{2}R$

$2\sqrt{2}R - 1$

1

Note the negative numbers

Extension to Holes

Extension to Holes

Pair of pants

Pants on floor

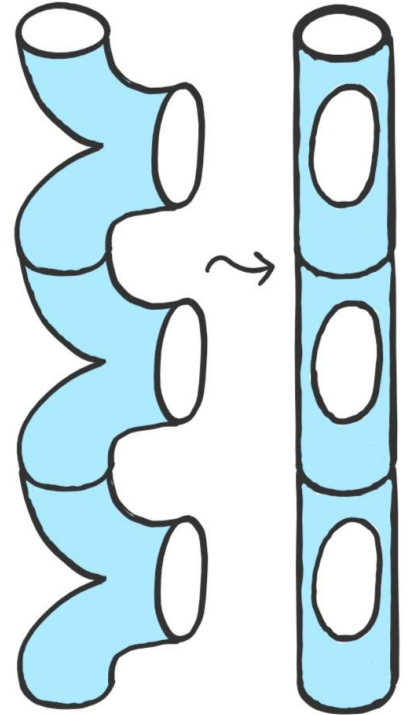Periodic pants = flute

=

No canonical cycle basis

Periodic Merge Tree of Complement
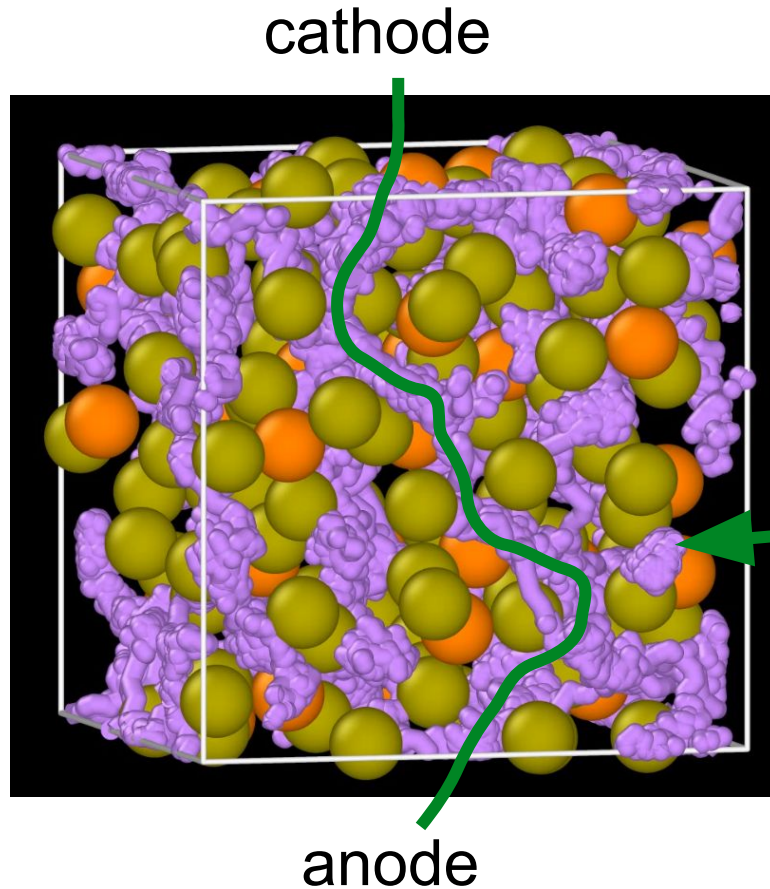
cR^3 gives the voids

cR^2 gives the infinitely long tunnels
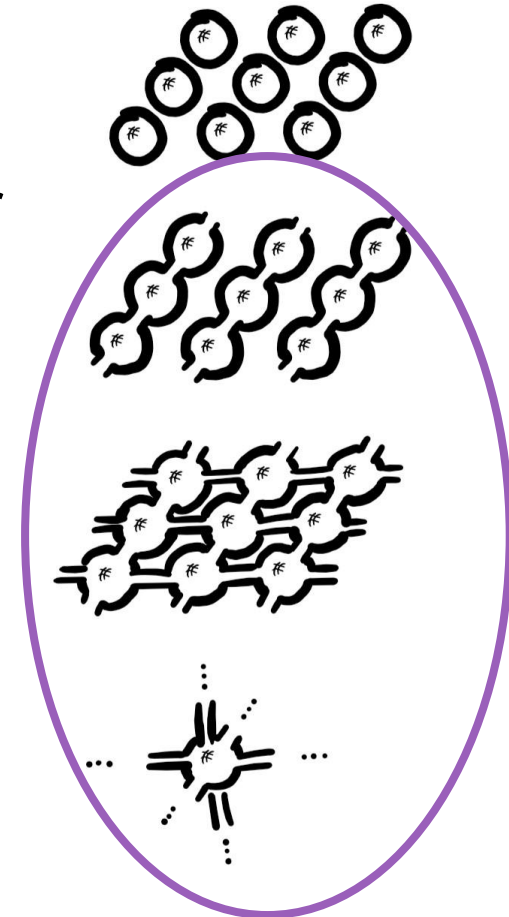
cR and more

c

Application: More efficient batteries
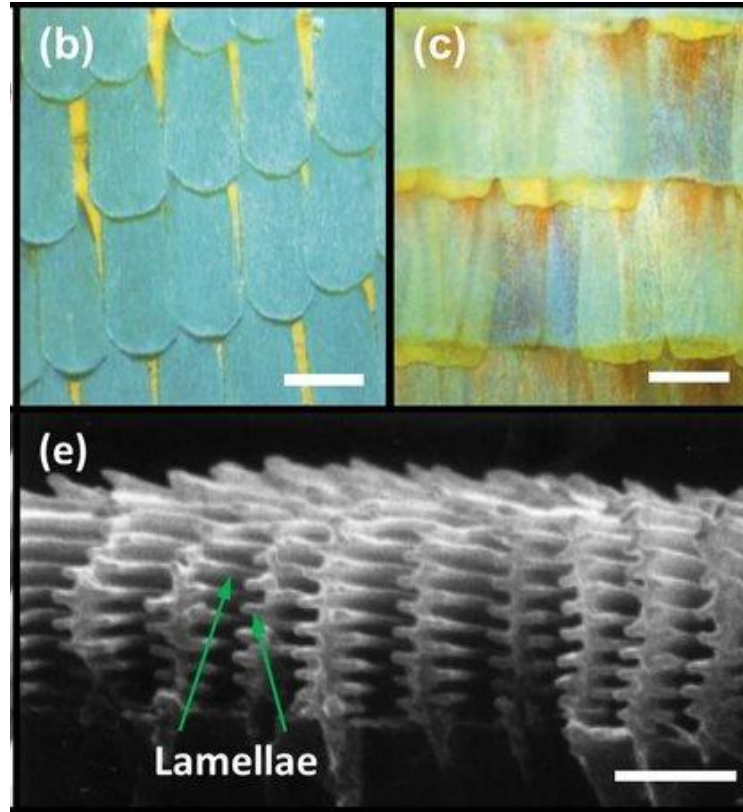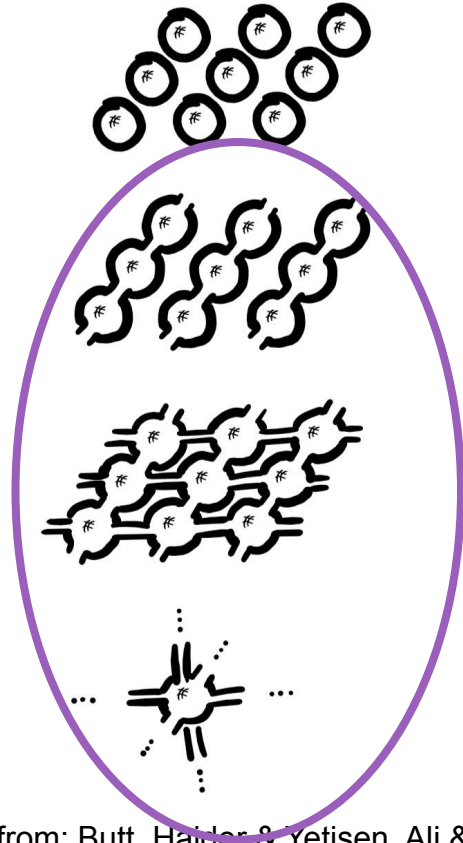

cathode

anode

Collaboration with Chemistry Professor Morten M. Smedskjaer & Topology Professor Lisbeth Fajstrup Aalborg University

Li-ion trajectories

Tunnels!
Connectedness!

Application: Photonic crystals

Collaboration with
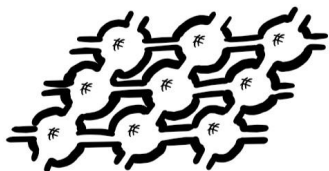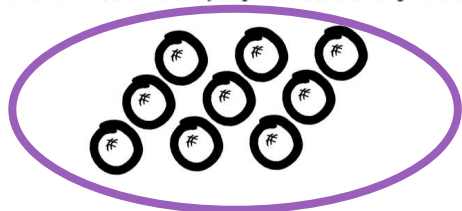Engineering Prof
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Topological Descriptors Help Predict Guest Adsorption in Nanoporous Materials

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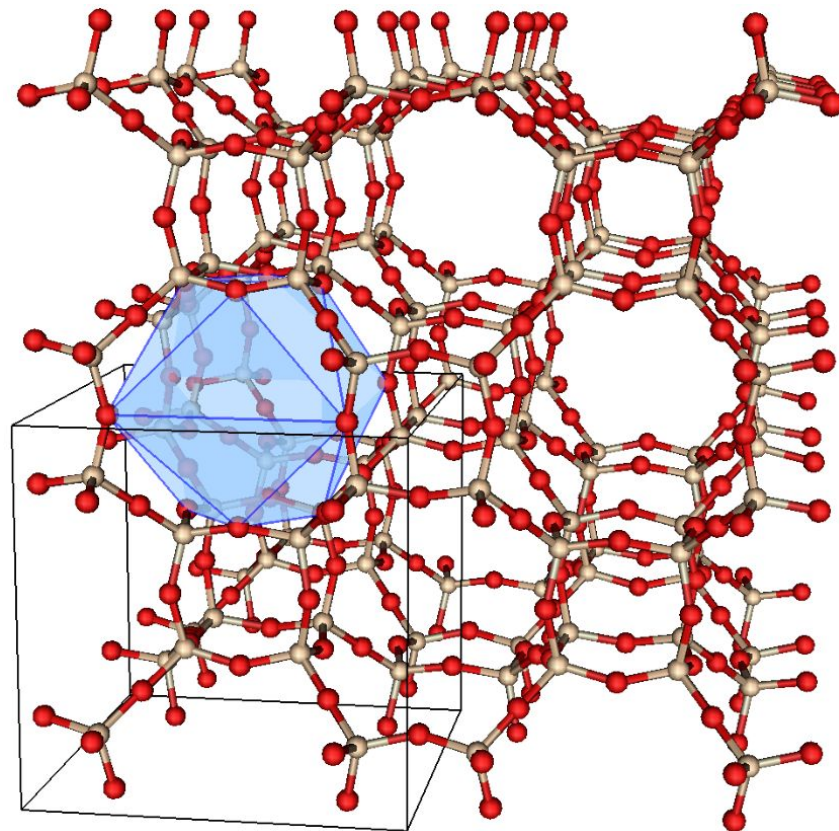
-9368

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partly motivated
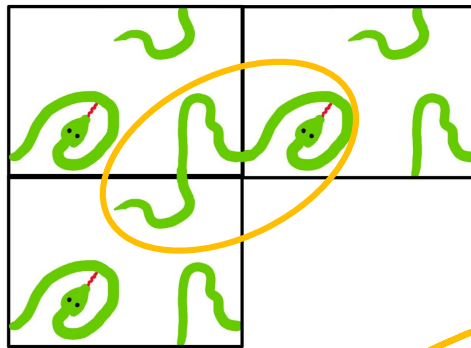my research

Voids / Cavities!
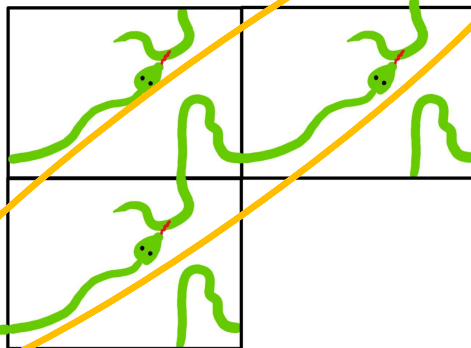
Summary: TDA for Periodic Data

Periodic Merge Tree: Track components on torus, assign each a frequency

Take-away messages:

- Rigorously measures what one wants to measure, and fulfills properties one wants

- When used on complement, gives some 1- and all 2-homology.

- Efficient to compute (log-linear)

1 component with 1 hole
and its copies in
2 space directions
$\Theta(R^2)$ copies in $B_R(0)$

1 component with 0 holes
and its copies in
1 space direction
$\Theta(R^1)$ copies in $B_R(0)$