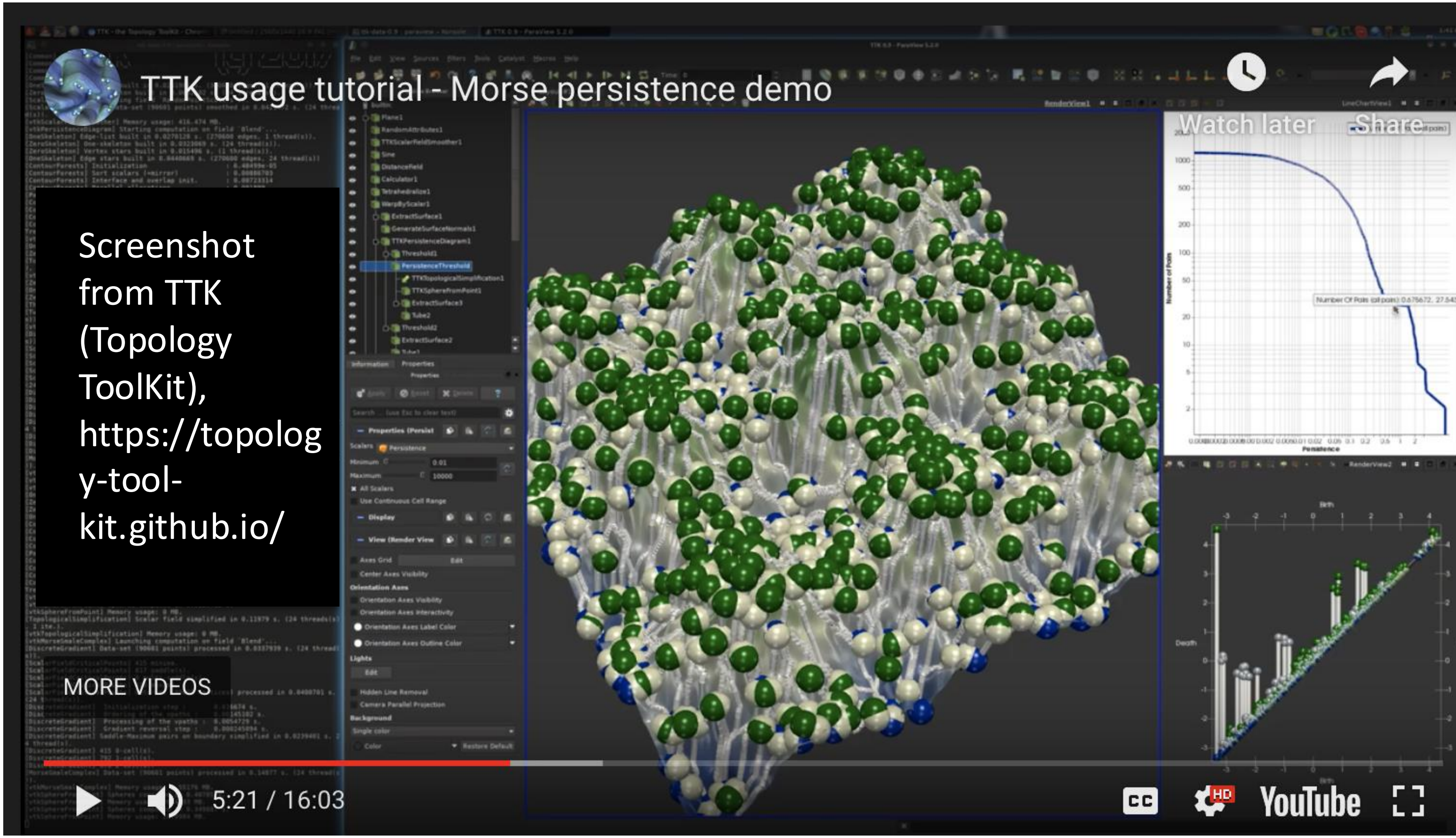
An Introduction to Morse Theory

Henry Adams (Colorado State University)
Enrique Alvarado (Washington State University)

Morse Theory Overview

- Morse theory provides a cellular model for the sublevelsets of an energy landscape.
- Nearby critical points of low persistence can be cancelled.

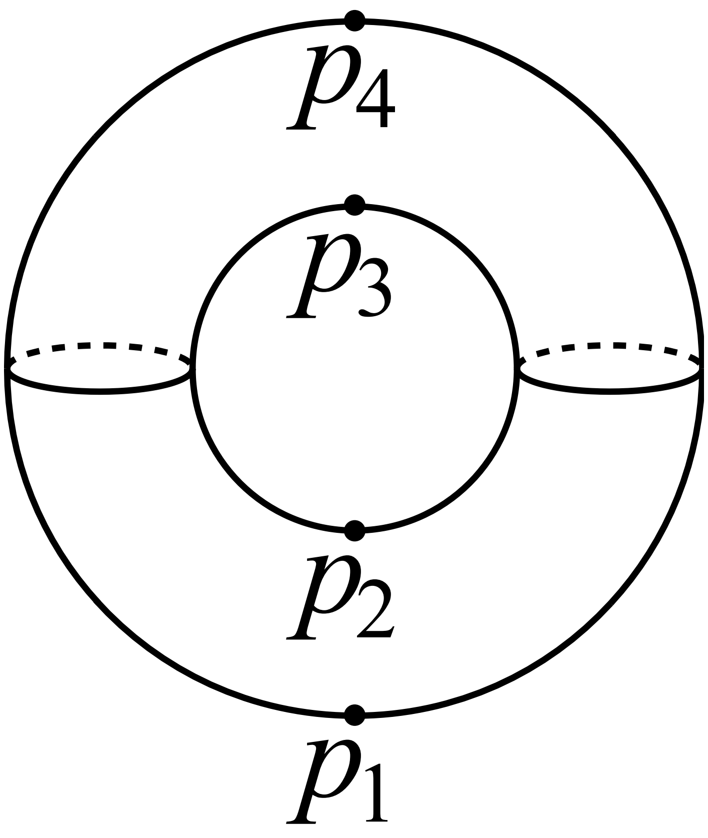
Morse Theory Overview

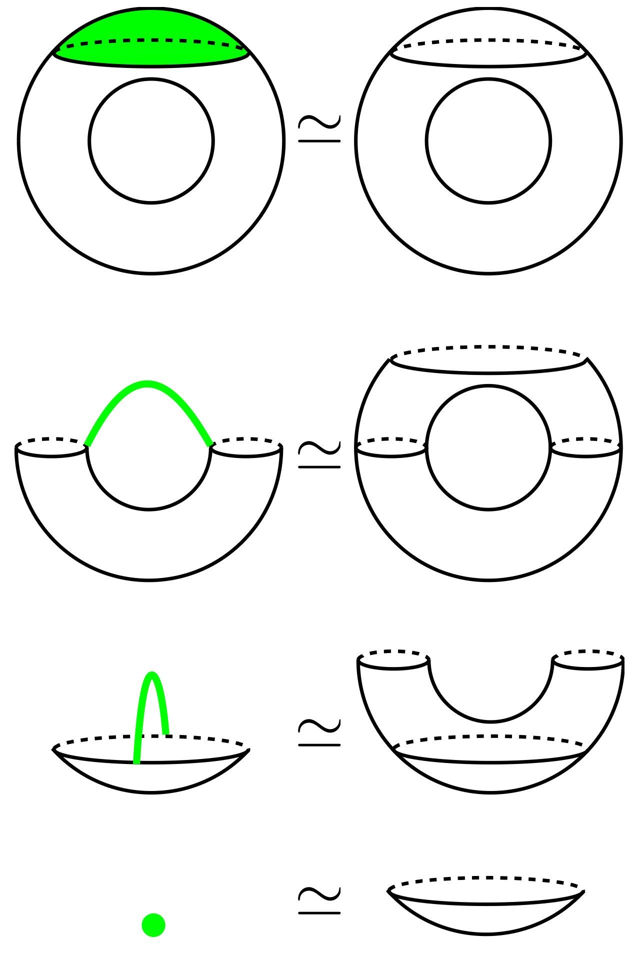


- Morse theory provides a cellular model for the sublevelsets of an energy landscape.
- Nearby critical points of low persistence can be cancelled.

Morse Theory Overview

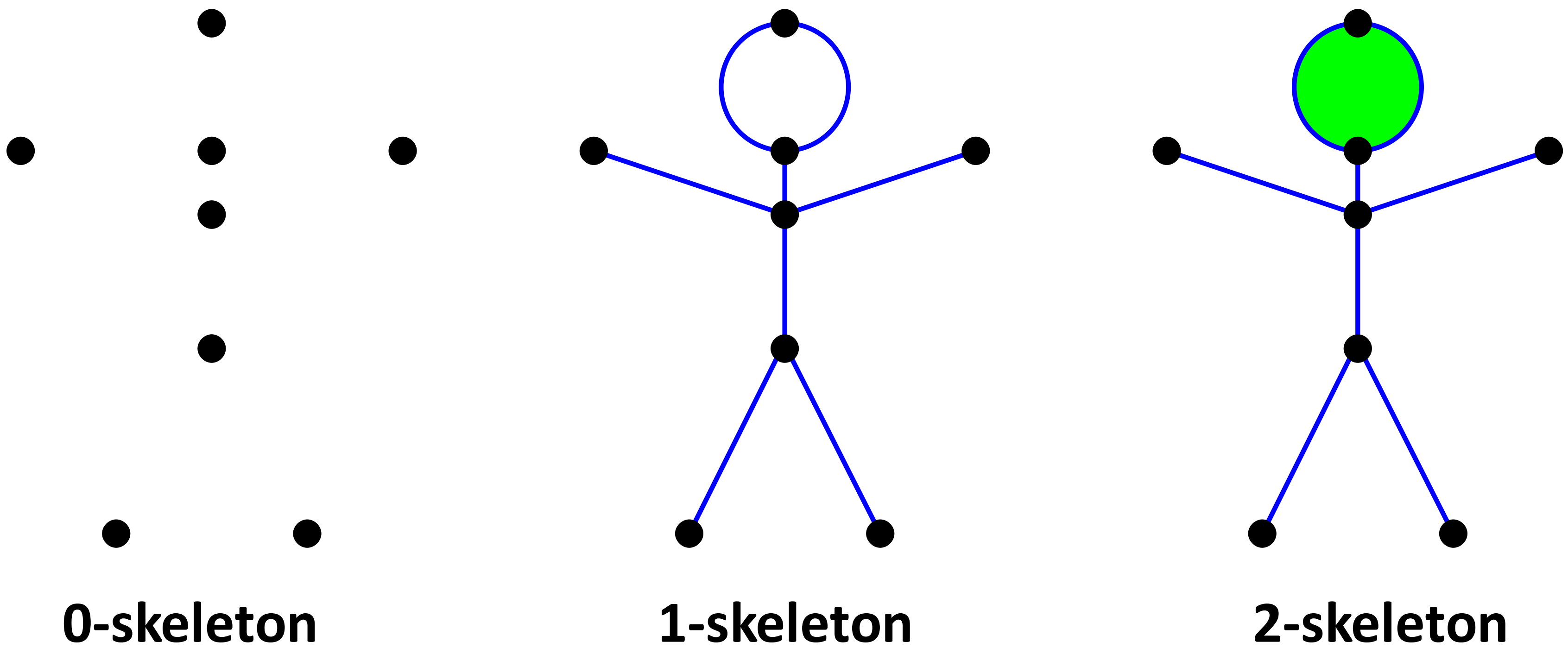
- Morse function $f: M \to \mathbb{R}$
- M is homotopy equivalent to a CW complex with one cell of dimension i for each critical point of f of index i





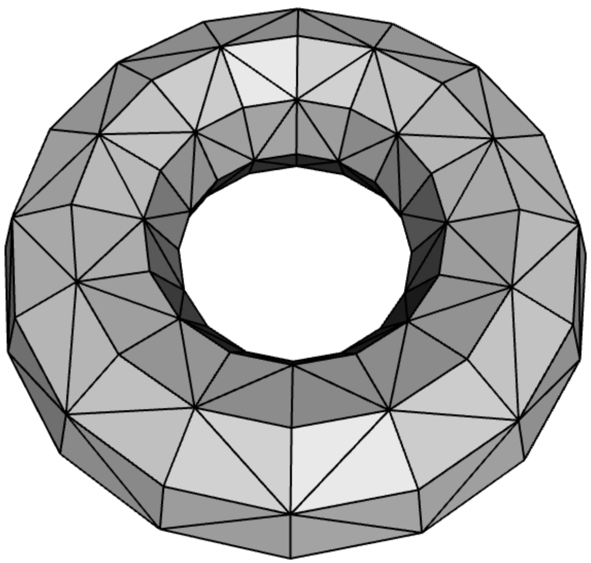
CW complexes

Stick figure example

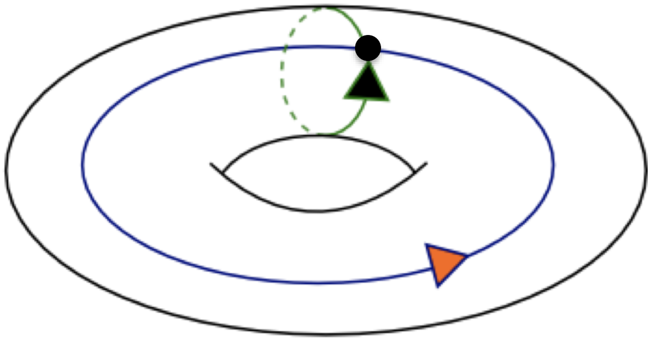


- A CW complex is formed by inductively attaching 0-cells, 1-cells, 2-cells, 3-cells, … along their boundaries.

CW complexes



CW complex with hundreds of vertices, edges, 2-cells

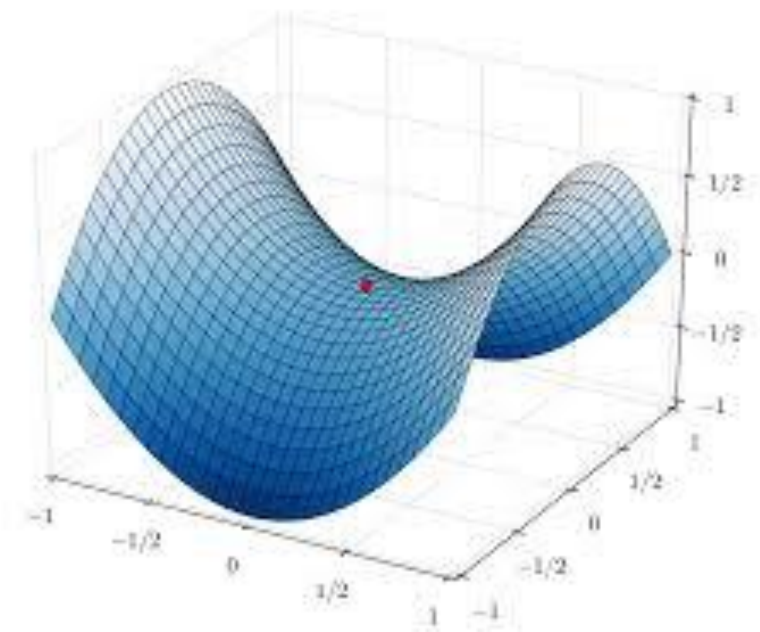


CW complex with one vertex, two edges, one 2-cell

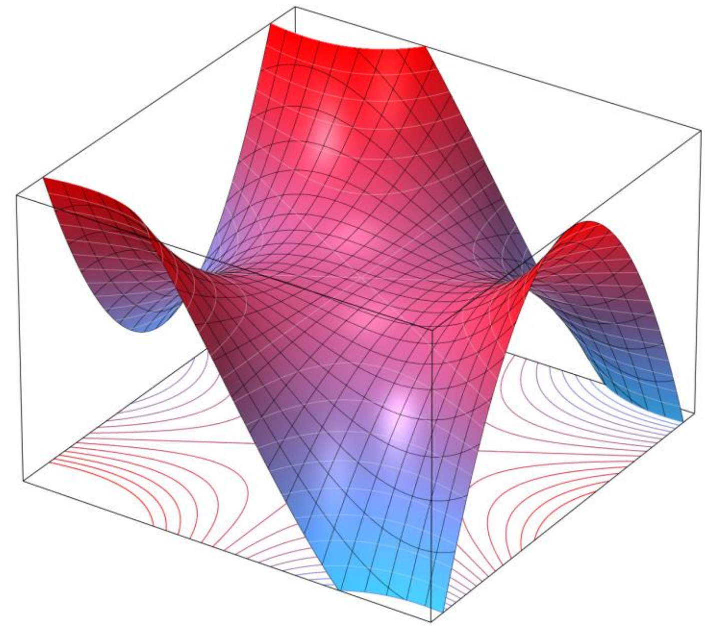
- A CW complex is formed by inductively attaching 0-cells, 1-cells, 2-cells, 3-cells, … along their boundaries.

Morse Theory

- Let M be a manifold. A smooth function $f: M \rightarrow \mathbb{R}$ is a *Morse function* if all of its critical points are non-degenerate (the Hessian matrix of second derivatives is non-singular).



A non-degenerate saddle point



A degenerate monkey saddle

Images from Wikipedia

Morse Theory

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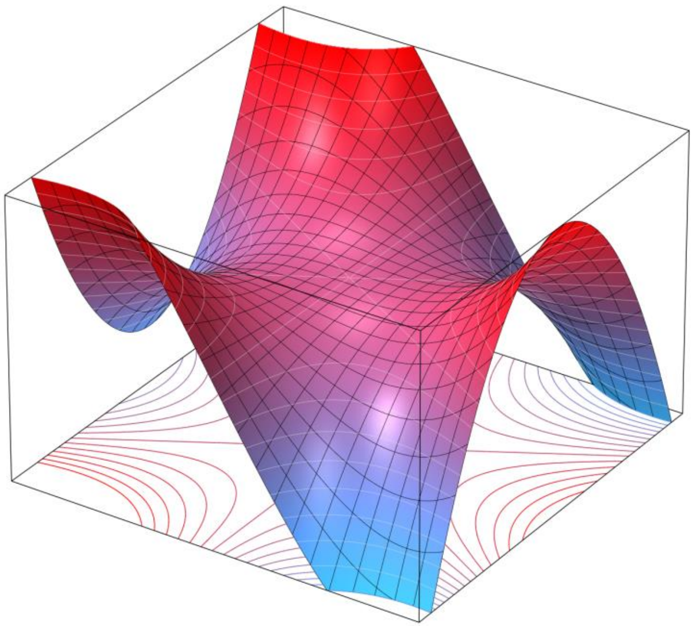
$$\begin{bmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1}(x) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(x) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_d}(x) \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(x) & \frac{\partial^2 f}{\partial x_2 \partial x_2}(x) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_d}(x) \\ \vdots & \ddots & \vdots & \\ \frac{\partial^2 f}{\partial x_d \partial x_1}(x) & \frac{\partial^2 f}{\partial x_d \partial x_2}(x) & \cdots & \frac{\partial^2 f}{\partial x_d \partial x_d}(x) \end{bmatrix}$$



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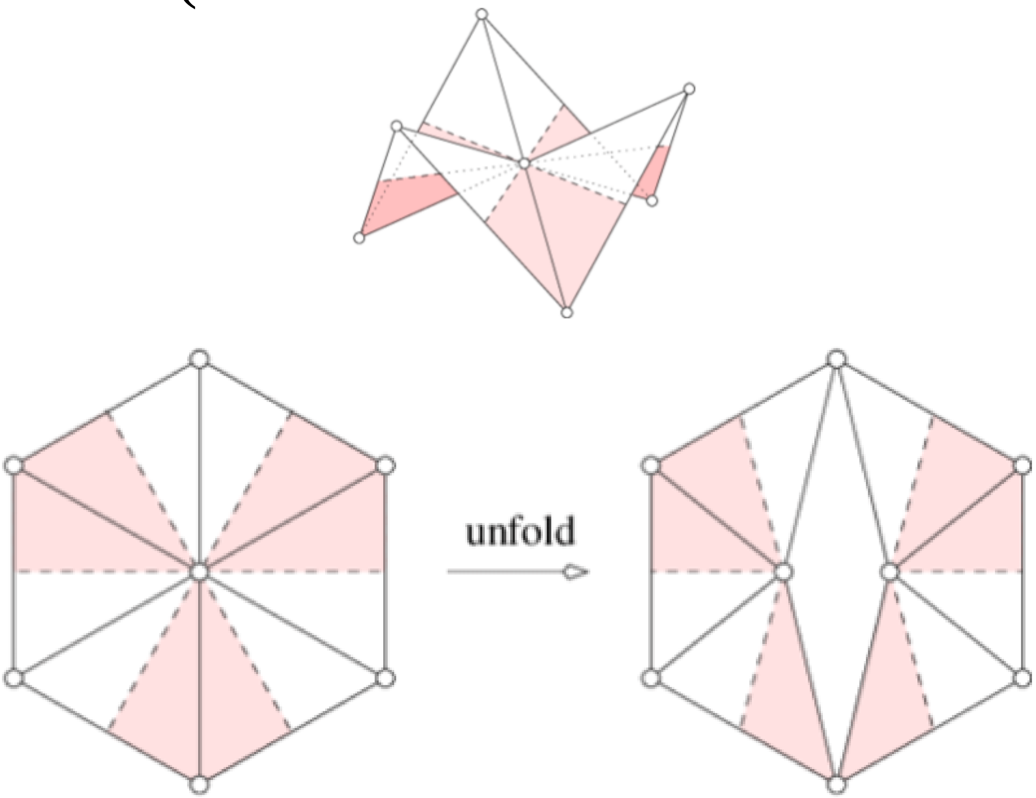
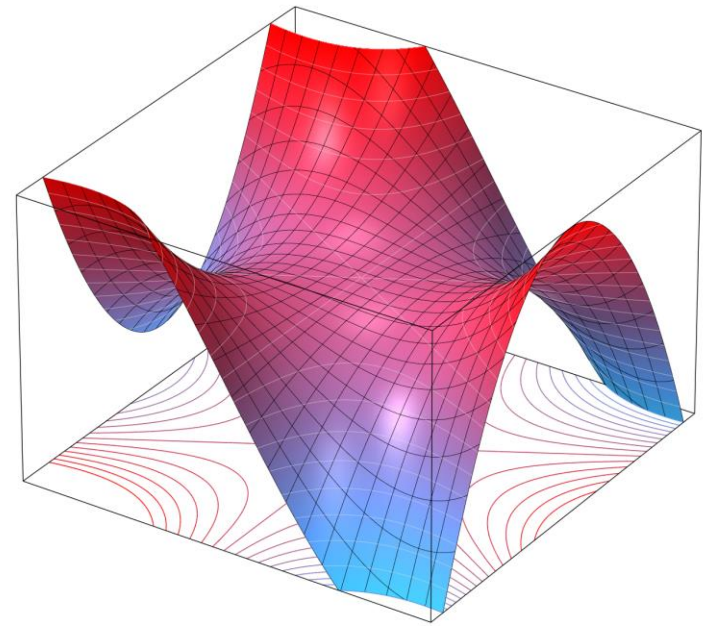


Resolving a monkey saddle into two standard saddles



A degenerate monkey saddle

Images from *Computational Topology: An Introduction* by Edelsbrunner and Harer

Morse Theory

- Let M be a manifold. A smooth function $f: M \to \mathbb{R}$ is a *Morse function* if all of its critical points are non-degenerate (the Hessian matrix of second derivatives is non-singular).
- Morse Lemma. If *p* is a non-degenerate critical point of *f*, then locally there is a coordinate chart so that

$$f(x) = -x_1^2 - \ldots - x_i^2 + x_{i+1}^2 + \ldots + x_m^2 + f(p)$$

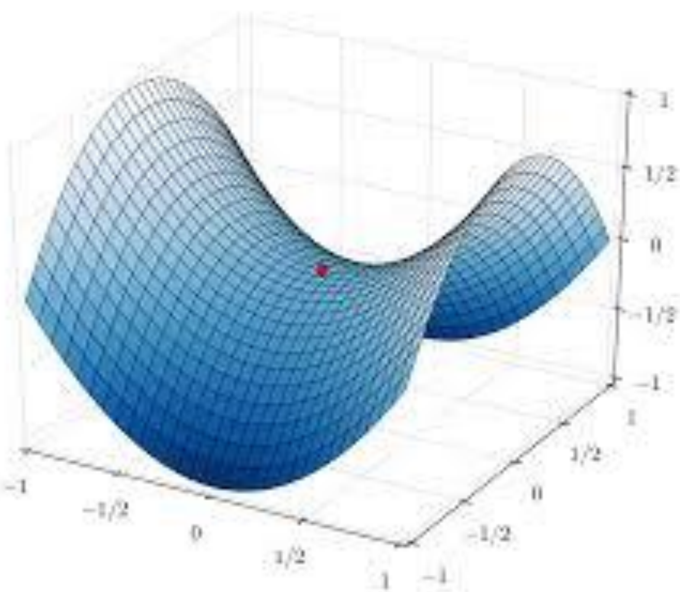


Image from Wikipedia

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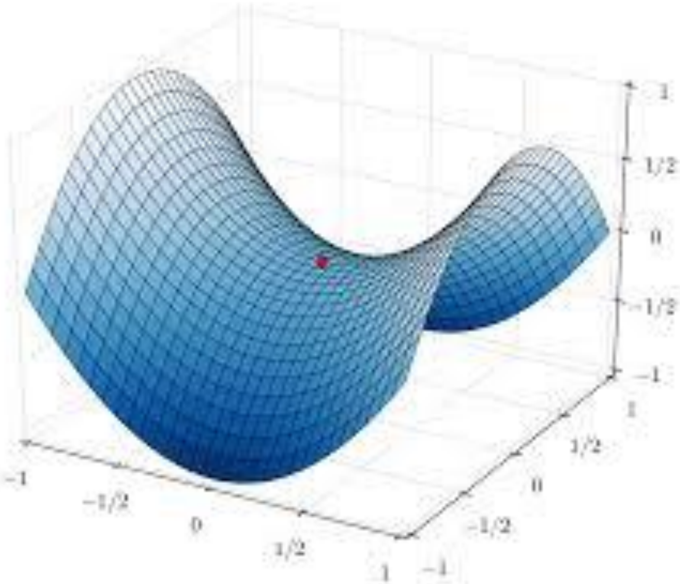

Example with *i*=1 (*m*=2).

The *index i* of a critical point is the number of “linearly independent decreasing directions.”

Image from Wikipedia

Morse Theory

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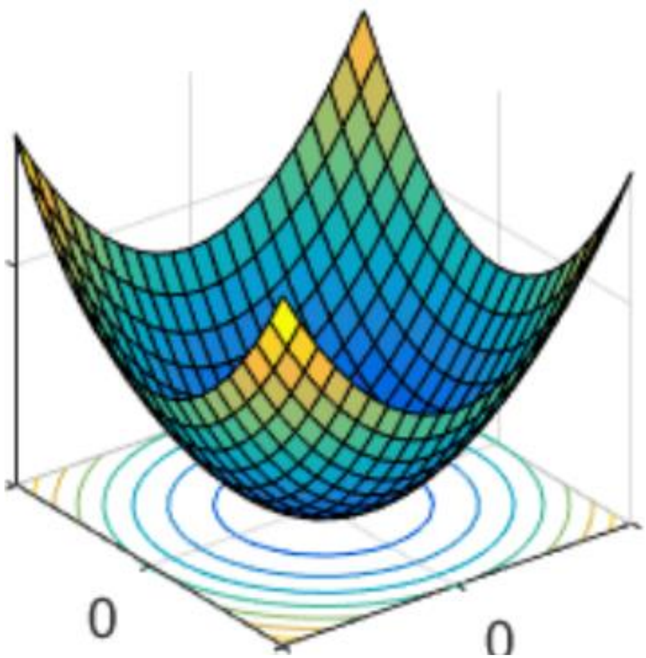

Example with i=0 (m=2).

The *index i* of a critical point is the number of "linearly independent decreasing directions."

Image from https://www.offconvex.org/2016/03/22/saddlepoints/

Morse Theory

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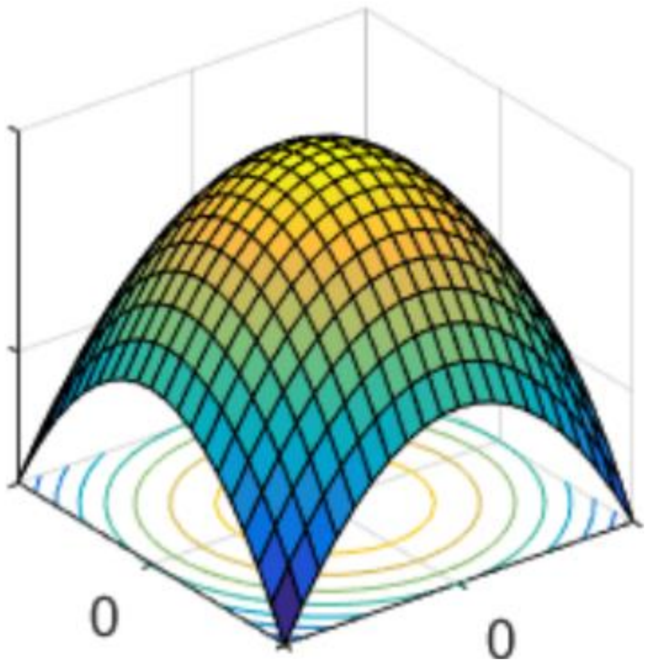
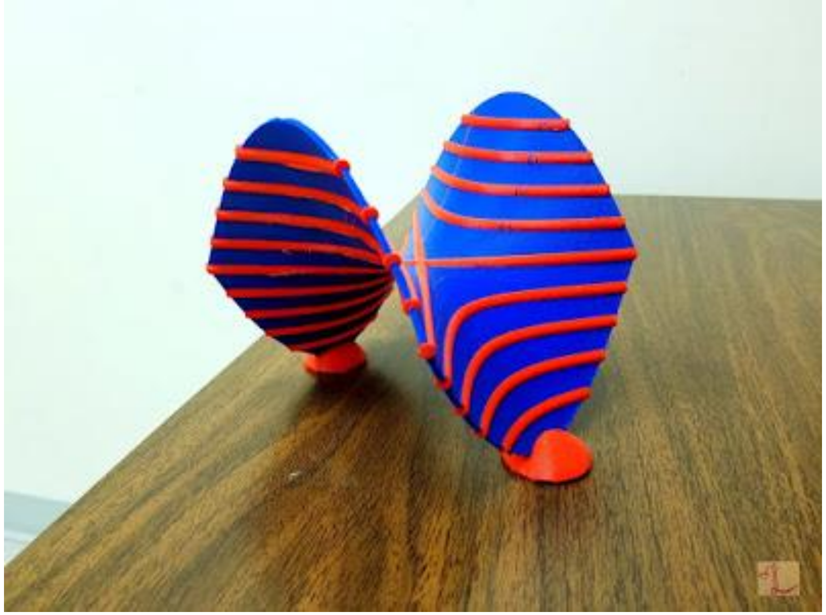


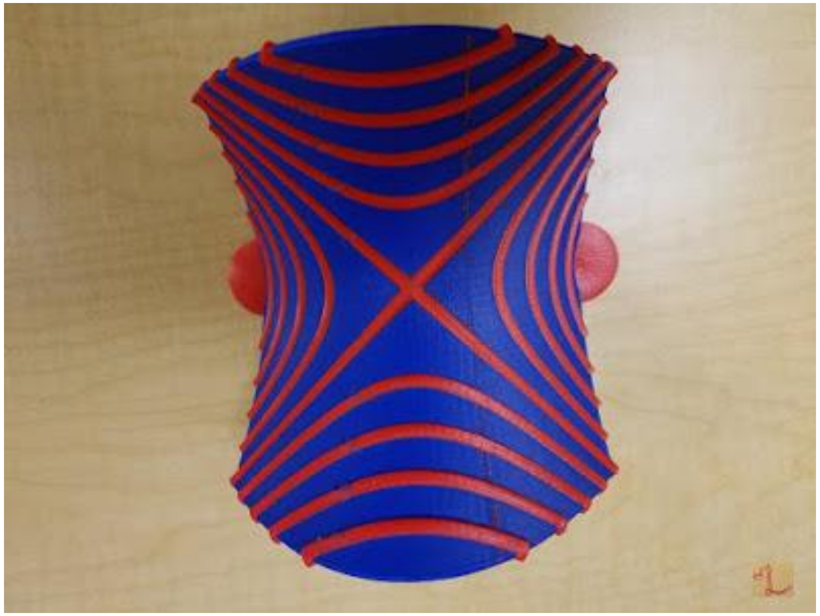
Example with i=2 (m=2).

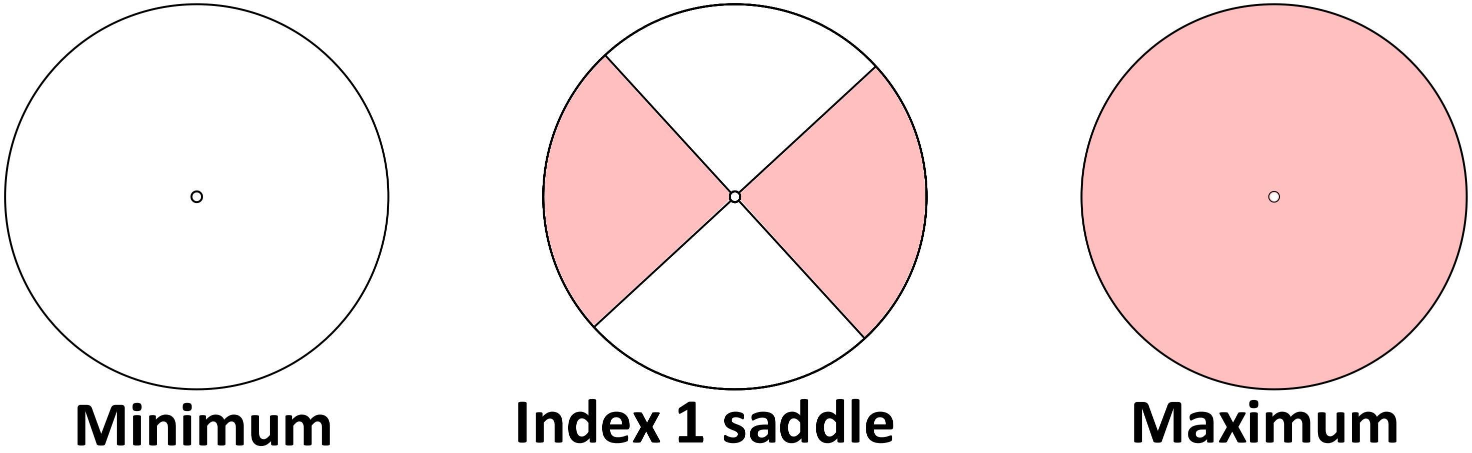
The *index i* of a critical point is the number of "linearly independent decreasing directions."

Image from https://www.offconvex.org/2016/03/22/saddlepoints/

Saddle points in 2D

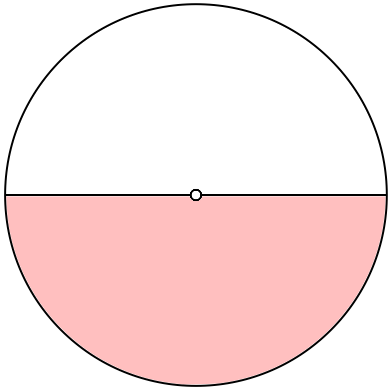




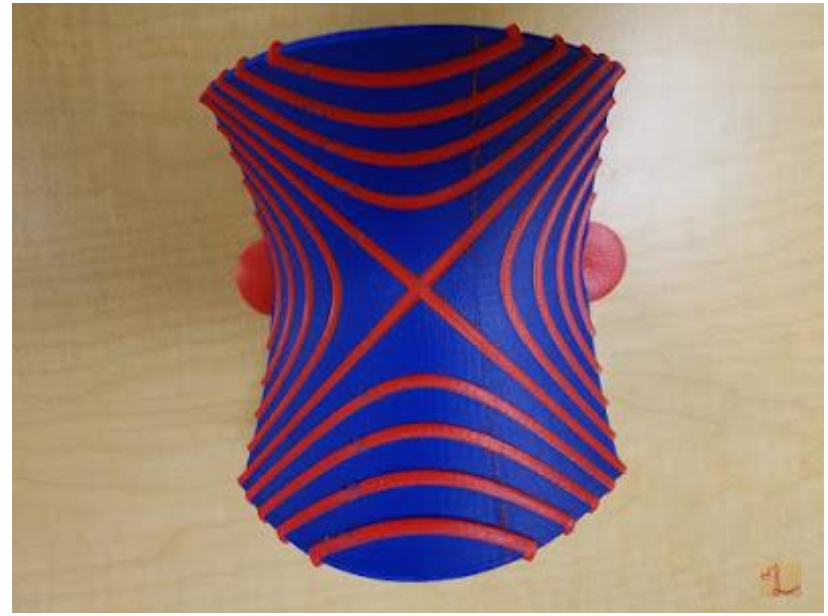


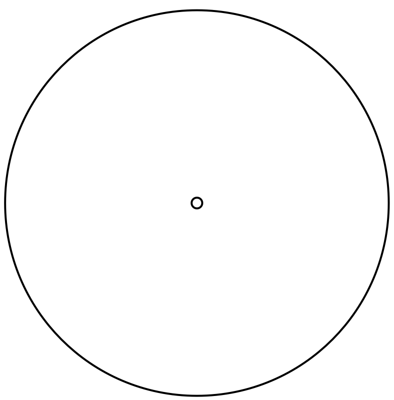
Images from http://gmumathmaker.blogspot.com

Saddle points in 2D

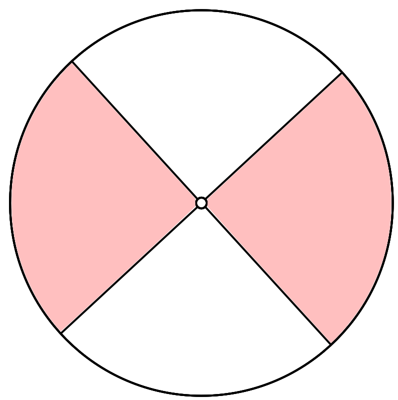


Regular point

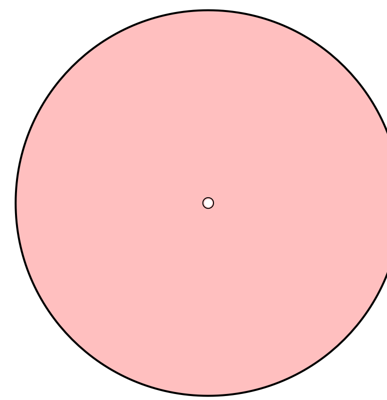




Minimum



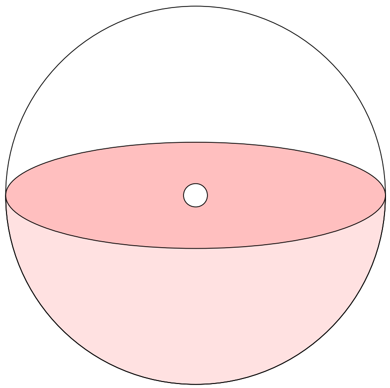
Index 1 saddle



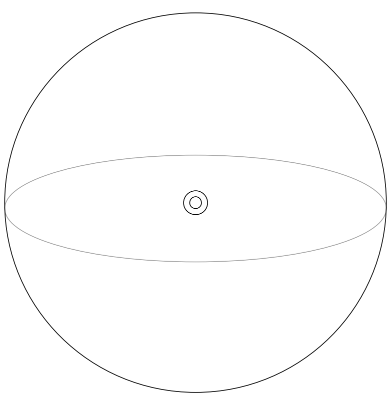
Maximum

Images from http://gmumathmaker.blogspot.com

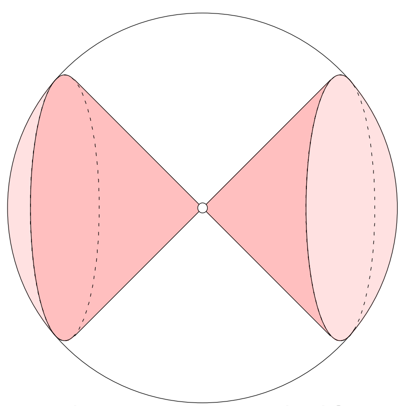
Saddle points in 3D



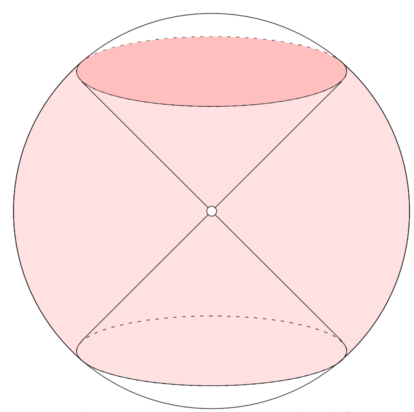
Regular point



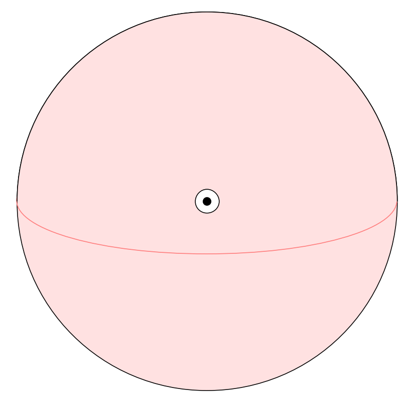
Minimum



Index 1 saddle



Index 2 saddle

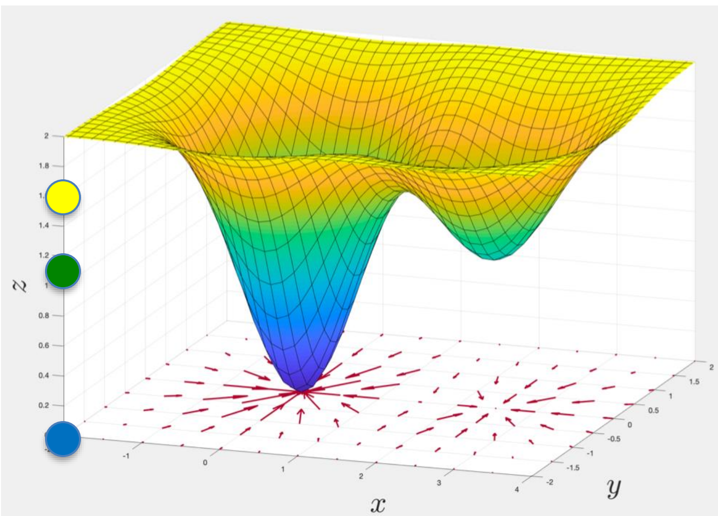


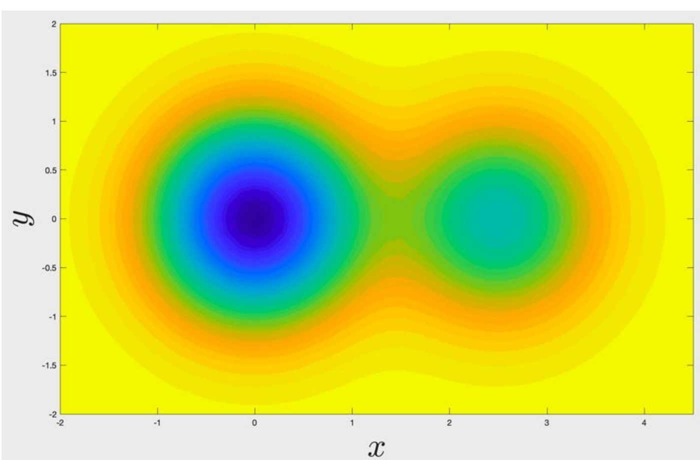
Maximum

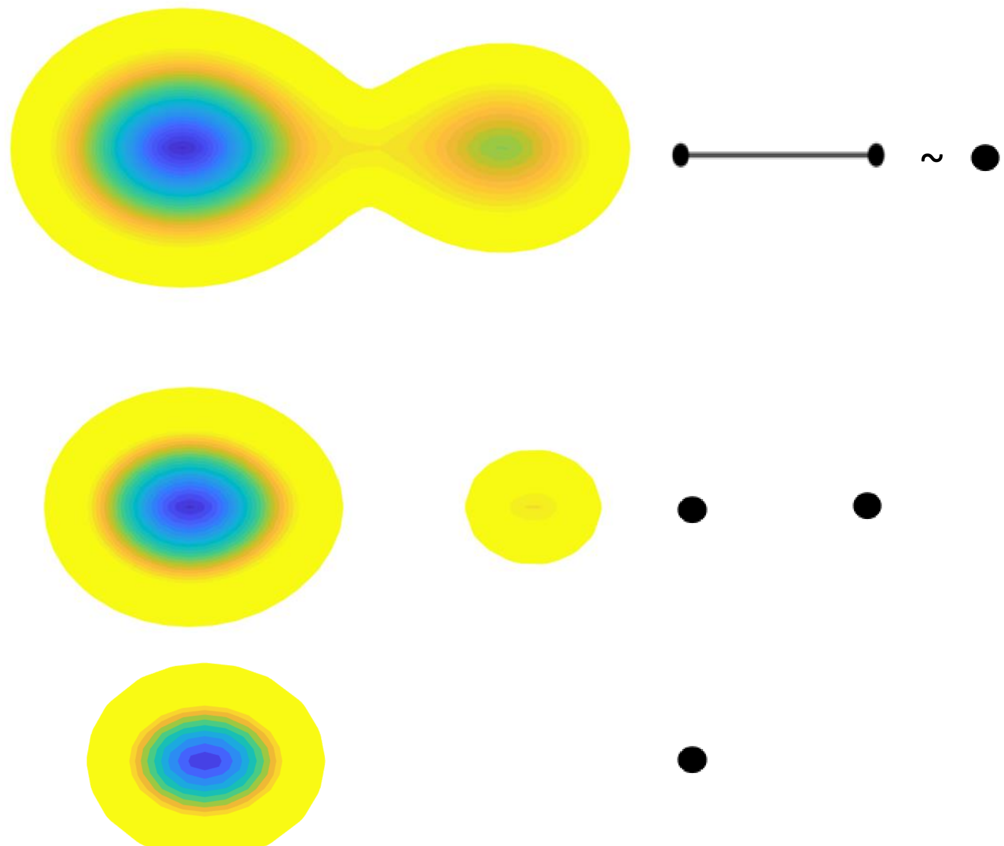
Images from *Computational Topology: An Introduction* by Edelsbrunner and Harer

Morse Theory

- Let $M_a = f^{-1}(-\infty, a]$ be the sublevelset at height *a*.
- <u>Morse Theorem 1</u> If there are no critical points with values in [*a*, *b*], then M_a and M_b are *homotopy equivalent*.

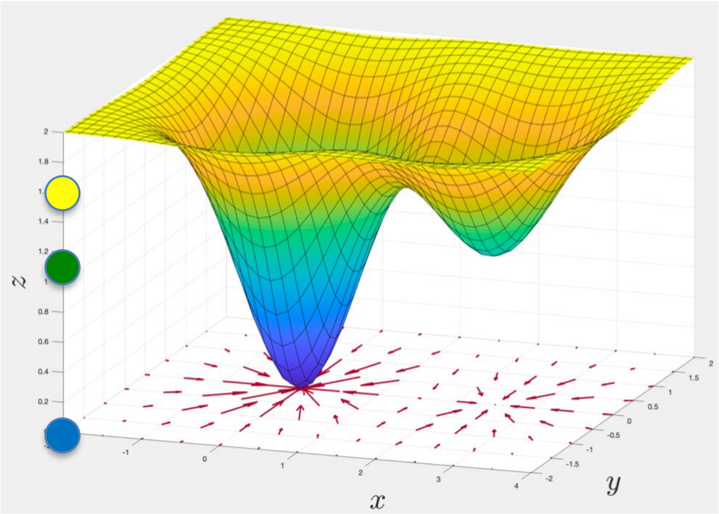


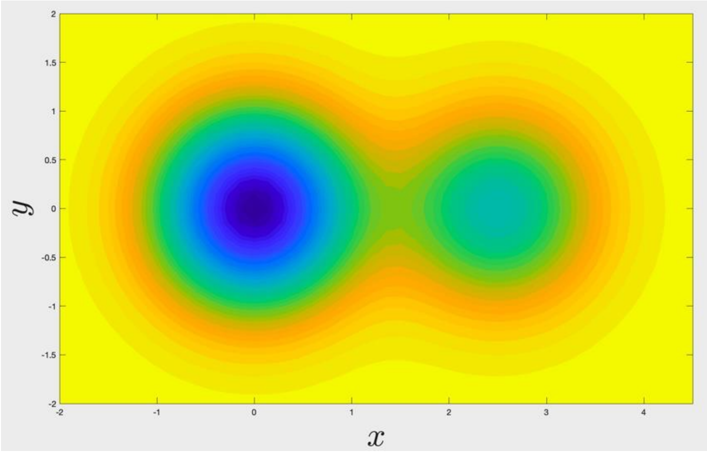


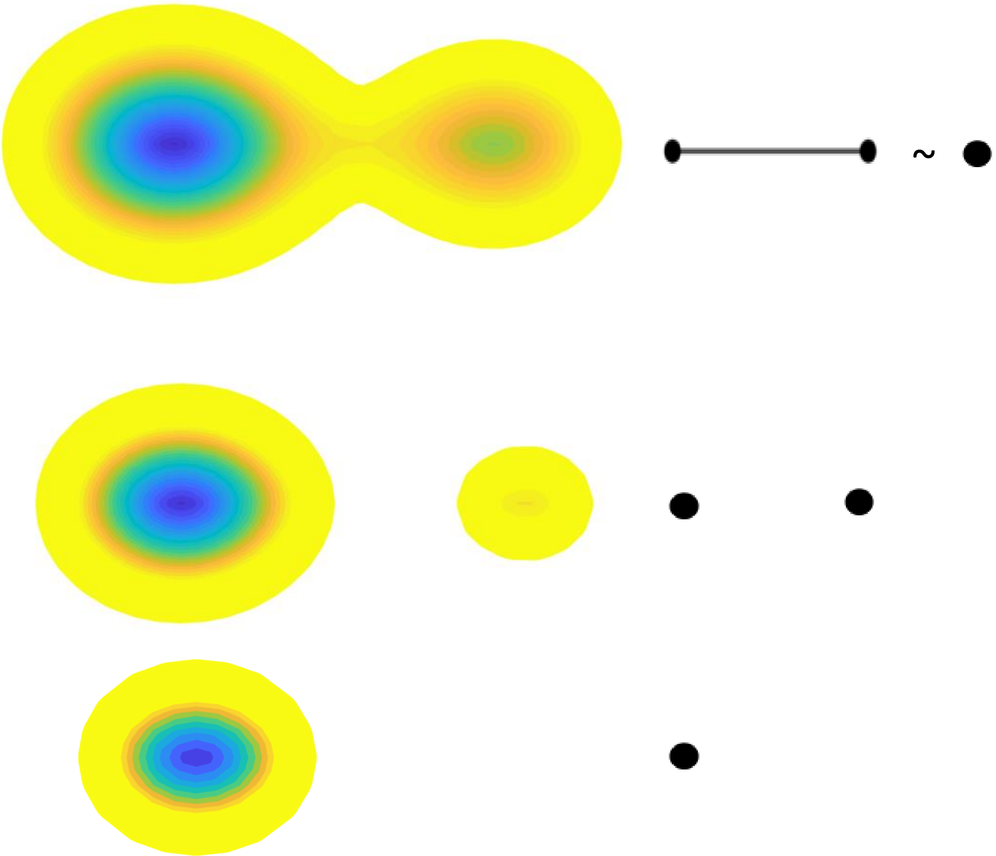


Morse Theory

- Let $M_a = f^{-1}(-\infty, a]$ be the sublevelset at height *a*.
- Morse Theorem 2 Upon passing a critical point of index *i*, the shape of the sublevelset changes by attaching a single *i*-cell.

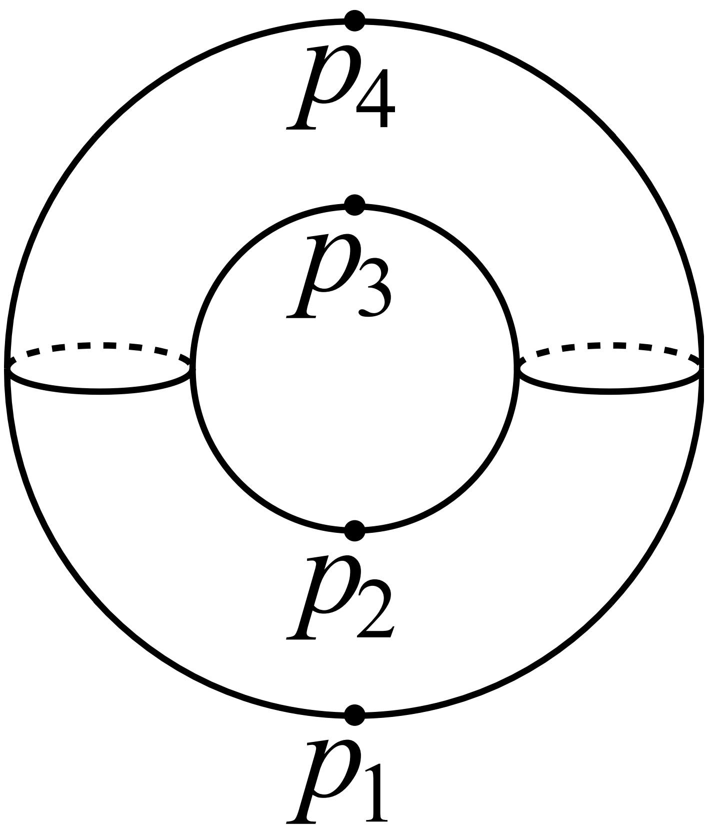


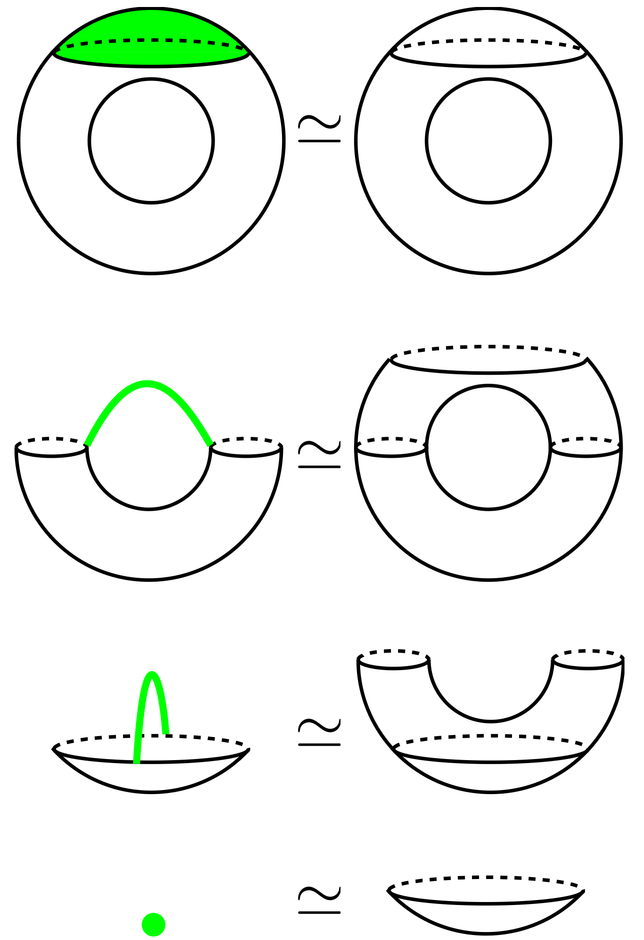




Morse Theory

- Let $M_a = f^{-1}(-\infty, a]$ be the sublevelset at height a.
- <u>Morse Theorem 2</u> Upon passing a critical point of index i, the shape of the sublevelset changes by attaching a single i-cell.





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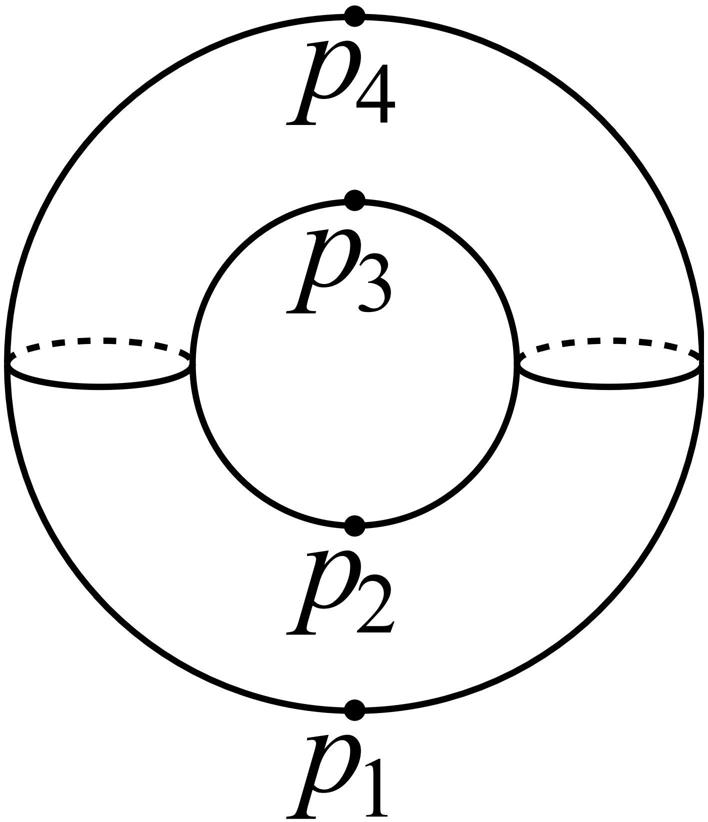

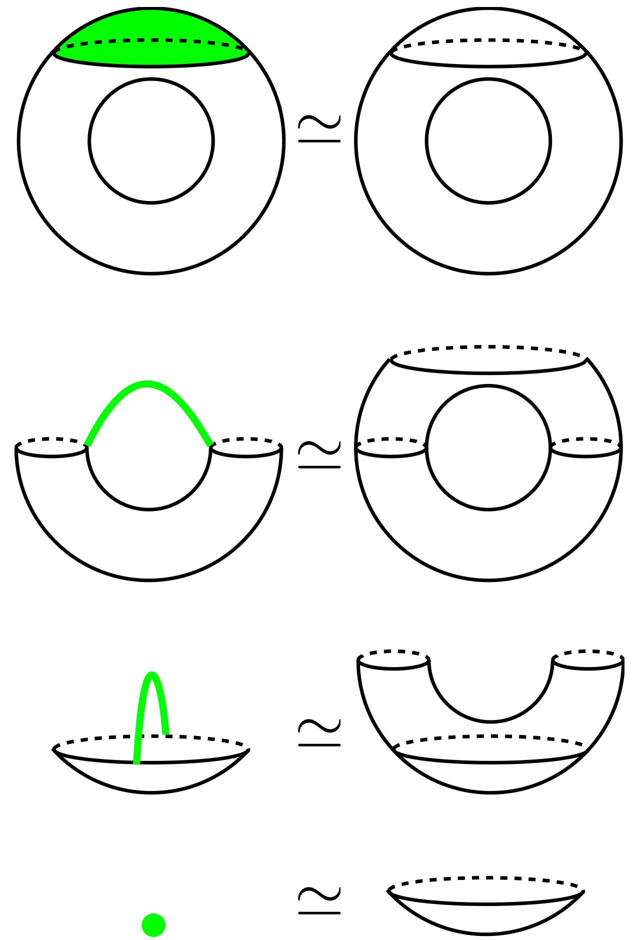

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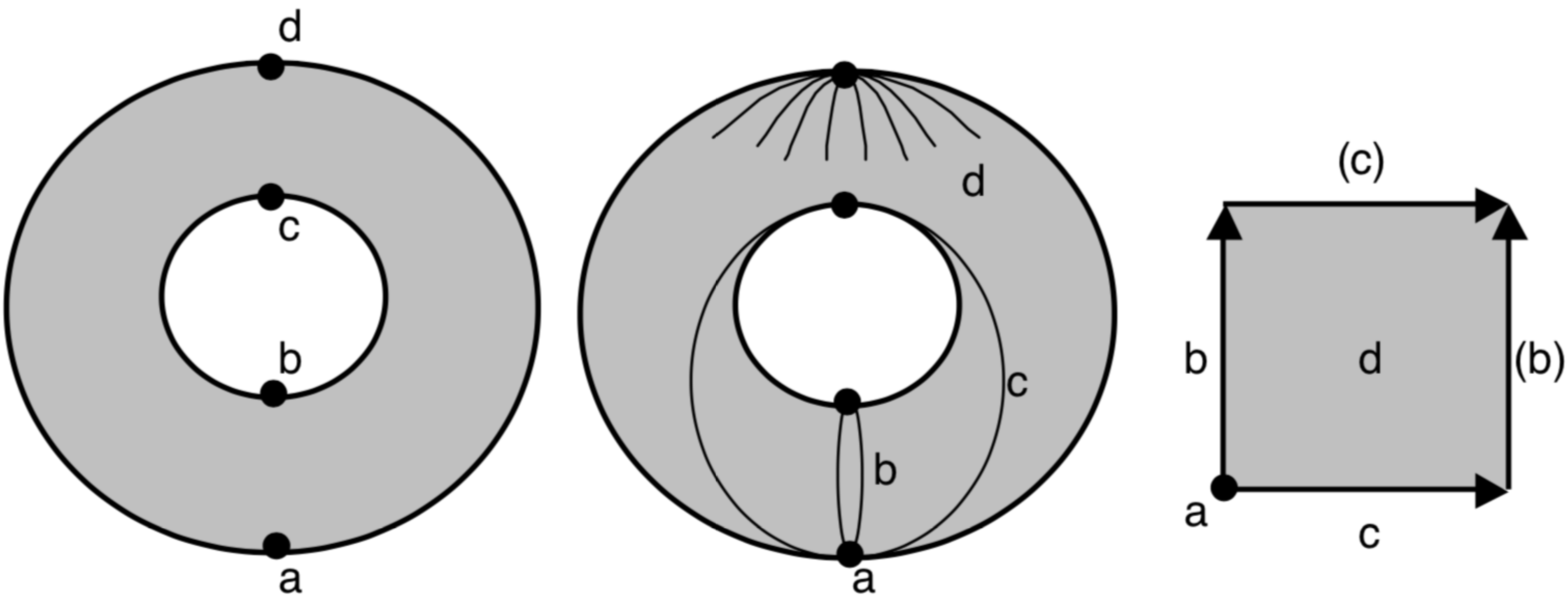
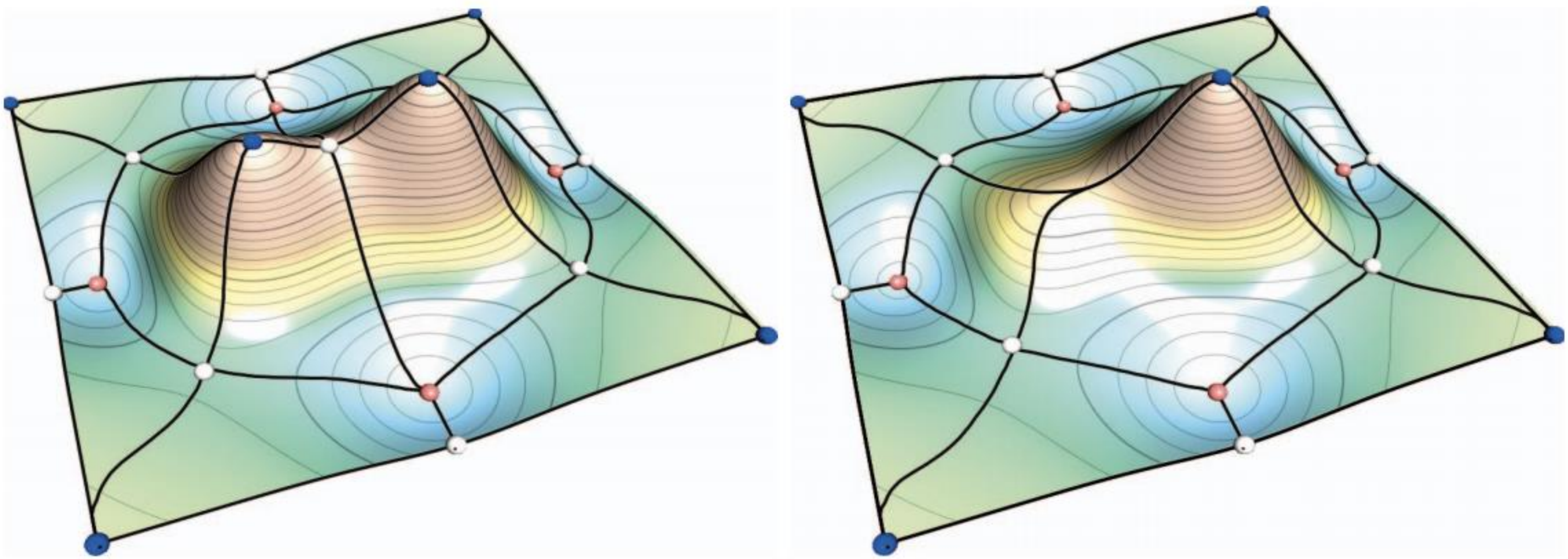


Image from *Using the CW complex to represent the topological structure of implicit surfaces and solids* by John C Hart

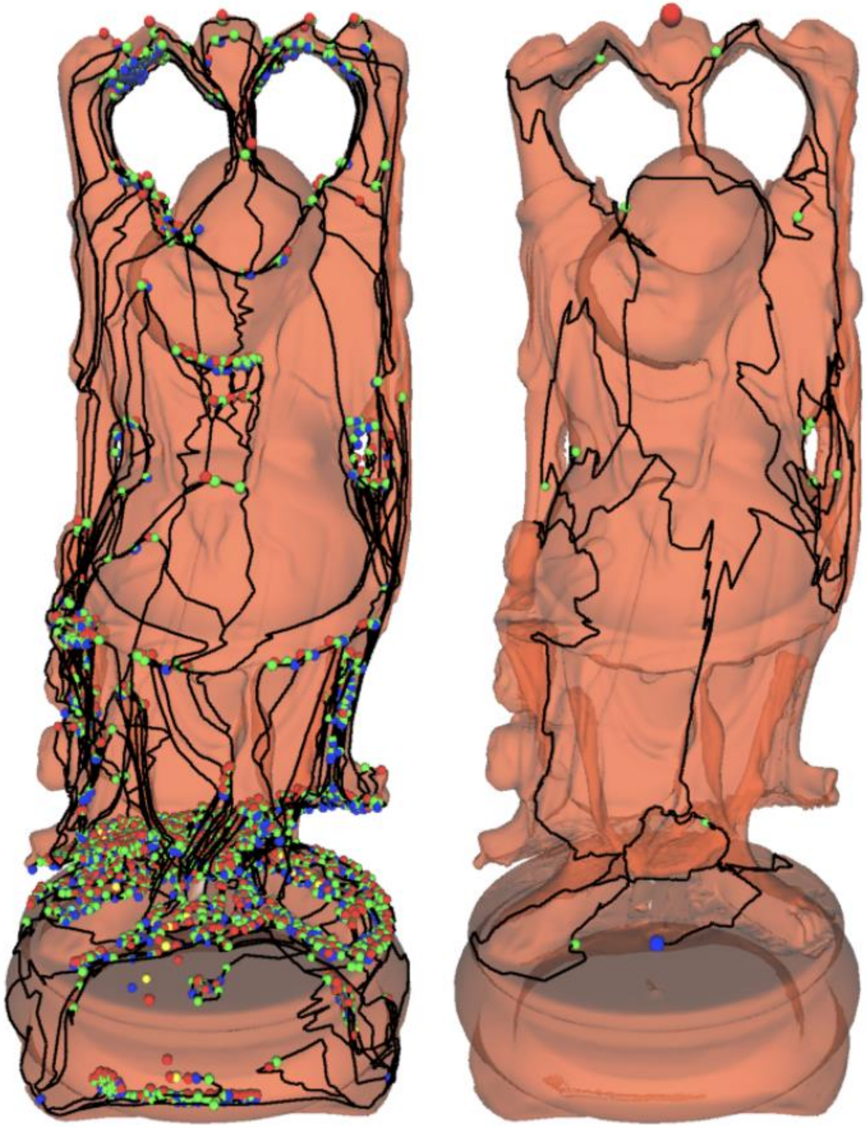
Topological Simplification



(a) Before cancellation (b) After cancellation

A structure-preserving visual representation of scalar fields
by Carlos Correra, Peter Lindstrom, Peer-Timo Bremer.

Topological Simplification



(a) (b)

Left: 3,605 critical points.

Right: One minimum, one maximum, 12 saddles (minimal possible for genus 6 surface).

Fair Morse functions for extracting the topological structure of a surface mesh by Ni et al.

Topological Simplification

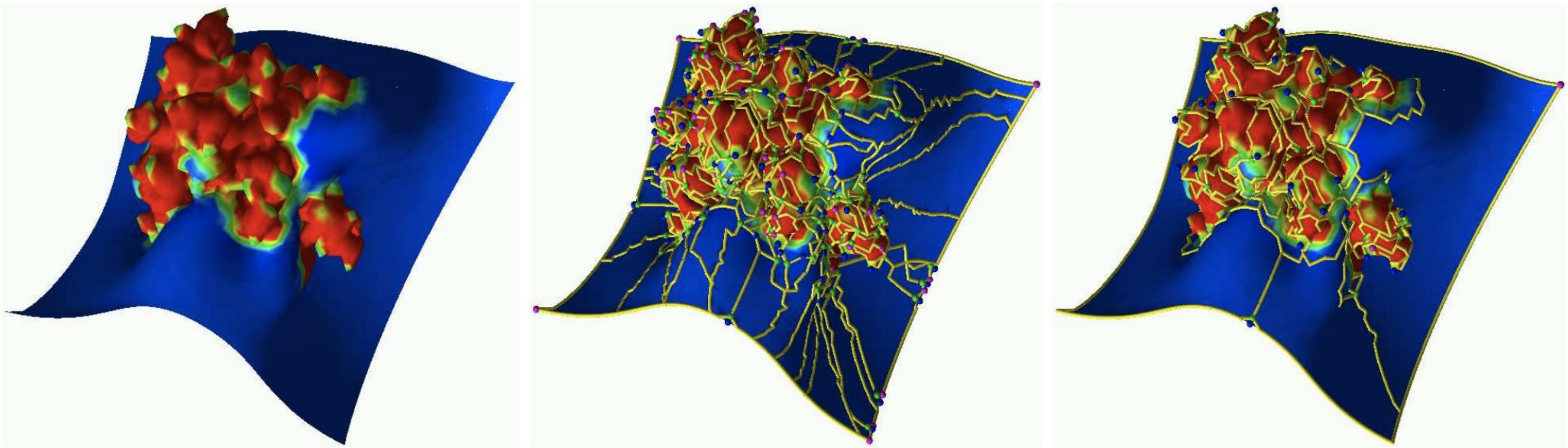


Fig. 16. Interaction energy between glucose and ethane under the three translational degrees of freedom. Left: isosurface of the electrostatic interaction pseudo-colored with the corresponding van der Waals potential. Middle: full MS complex with 564 critical points. Right: simplified MS complex with 166 critical points highlighting good candidate binding sites.

Topological hierarchy for functions on triangulated surfaces by Peer Timo-Brener, Herbert Edelsbrunner, Bernd Hamann, and Valerio Pasucci

Topological Simplification

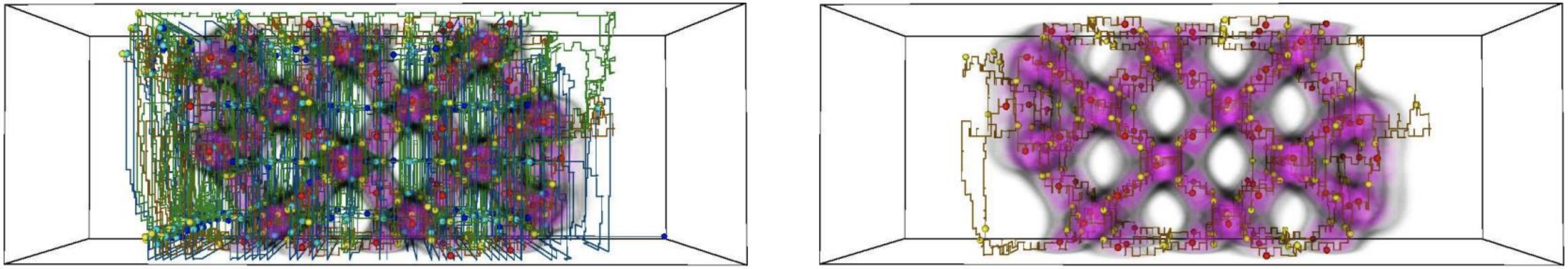


Fig. 14. Topological simplification of the silicium data set. Cancellation of low-persistence critical pairs reveals the shape of the silicium lattice structure.

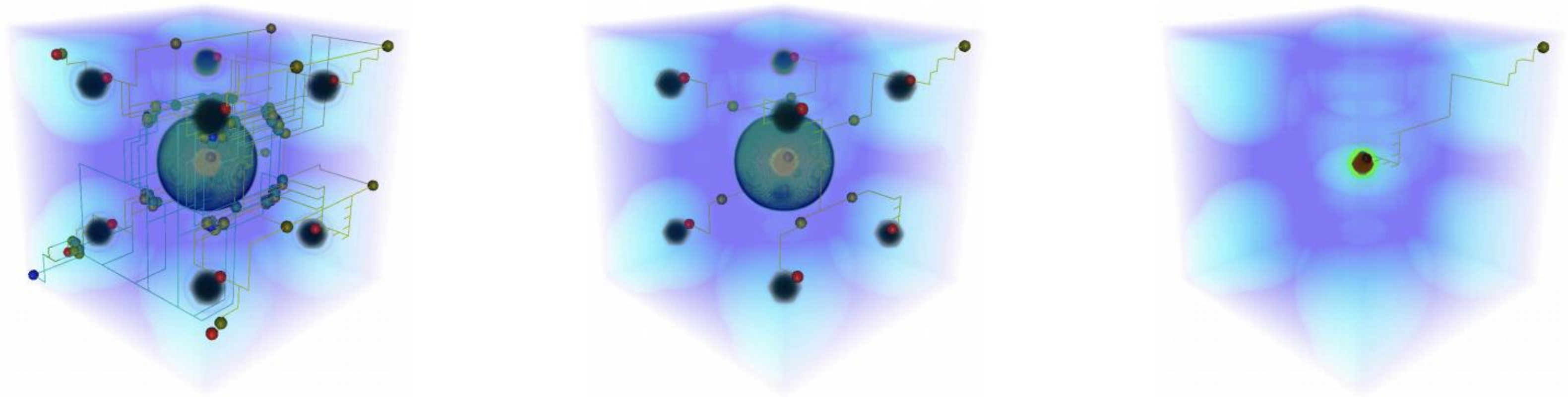


Fig. 15. Noise in a synthetic function introduces features with negligible persistence. Left: The function consists of various spikes with the central one being the largest. Each spike is visualized as a sphere in the volume-rendered image. Middle: All nine spikes are clearly visible after removing noise that created the thin shells surrounding the spheres. Right: Further simplification destroys all maxima except the one representing the crucial features.

A topological approach to simplification of three-dimensional scalar functions
by Attila Gyulassy, Vijay Natarajan, Valerio Pasucci, Peer Timo-Brener, Bernd Hamann

Topological Simplification

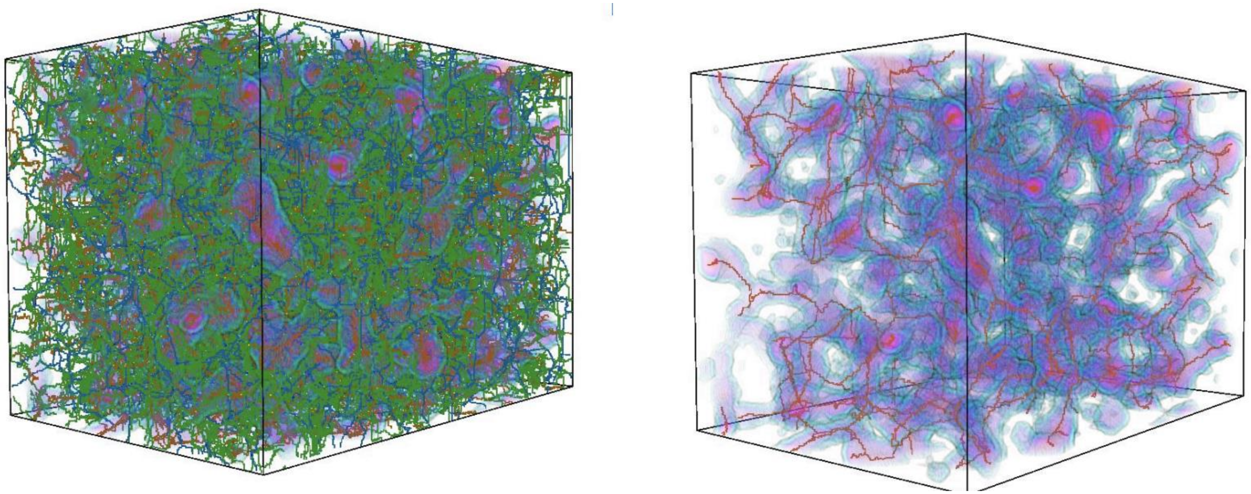


Figure 7. The initial computation of the MS complex for the full dataset (left) is simplified revealing the graph structure (right) of the porous solid.

Multiscale Morse Theory for science discovery by Valerio Pasucci and Ajith Mascarenhas