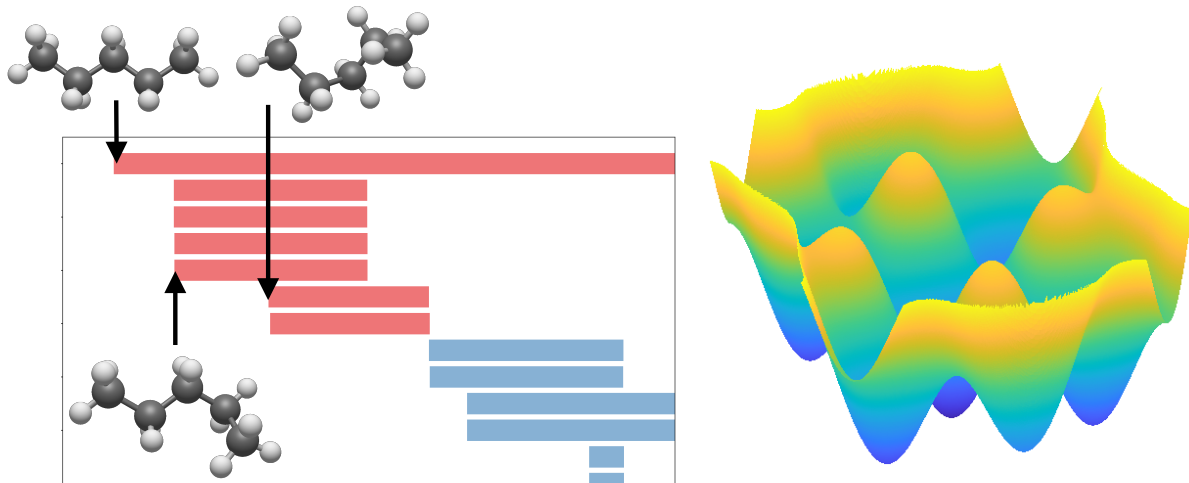


# Representations of Energy Landscapes by Sublevelset Persistent Homology: An Example with n-alkanes



Henry Adams, ~~Colorado State University~~, DELTA NSF #1934725  
University of Florida

Joint with Joshua Mirth, Yanqin Zhai, Johnathan Bush, Enrique G Alvarado, Howie Jordan, Mark Heim, Bala Krishnamoorthy, Markus Pflaum, Aurora Clark, YZ

# Representations of energy landscapes by sublevelset persistent homology: An example with $n$ -alkanes

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 Joshua Mirth,  Yanqin Zhai,  Johnathan Bush,  Enrique G. Alvarado,  Howie Jordan,  Mark Heim, 

Bala Krishnamoorthy,  Markus Pflaum,  Aurora Clark,  Y Z, and  Henry Adams

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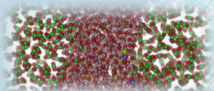
## COLLECTIONS

Note: This paper is part of the JCP Special Collection in Honor of Women in Chemical Physics and Physical Chemistry.

 This paper was selected as an Editor's Pick

# DELTA

## Descriptors of Energy Landscapes Using Topological Analysis



3N Energy Landscape (Simulation/Experiment)

Dimensionality Reduction

Topology of Reduced Energy Landscapes

Predictive Machine Learning

Optimized Synthetic Conditions

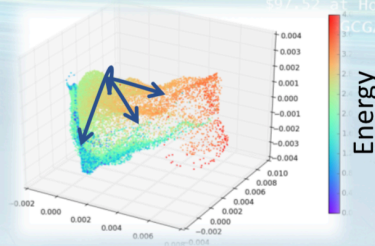
Phase Behavior

Tuning Catalytic Pathways

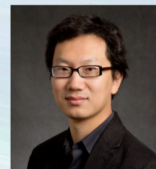
Accelerated Sampling

- PCA
- Non-linear Methods
- Generalized Collective Coordinates

- Morse Theory
- Persistent Homology
- Catastrophe Theory
- Singularity Theory



NSF #1934725



WASHINGTON STATE UNIVERSITY

Colorado State University

Rensselaer

AUBURN UNIVERSITY

University of Colorado Boulder

UNIVERSITY OF ARKANSAS ILLINOIS

INAUGURAL

# INTERVIEW

SERIES



AATRN

Applied Algebraic Topology  
Research Network

SEP  
30TH  
1PM ET

HERBERT EDELSBRUNNER  
INTERVIEWED BY  
DMITRIY MORZOV

NOV  
18TH  
5PM ET

VANESSA ROBINS  
INTERVIEWED BY  
ELIZABETH BRADGEY

GUNNAR  
INTERVIEWED BY  
CARLSSON VON DE SIENA  
FEB 3RD  
11AM ET

MASSIMO  
INTERVIEWED BY  
FERRI  
APR 21ST  
11AM ET

FOR 100M COORDINATES,  
BECOME AN AATRN MEMBER  
AT

[topology.ima.umn.edu](http://topology.ima.umn.edu)

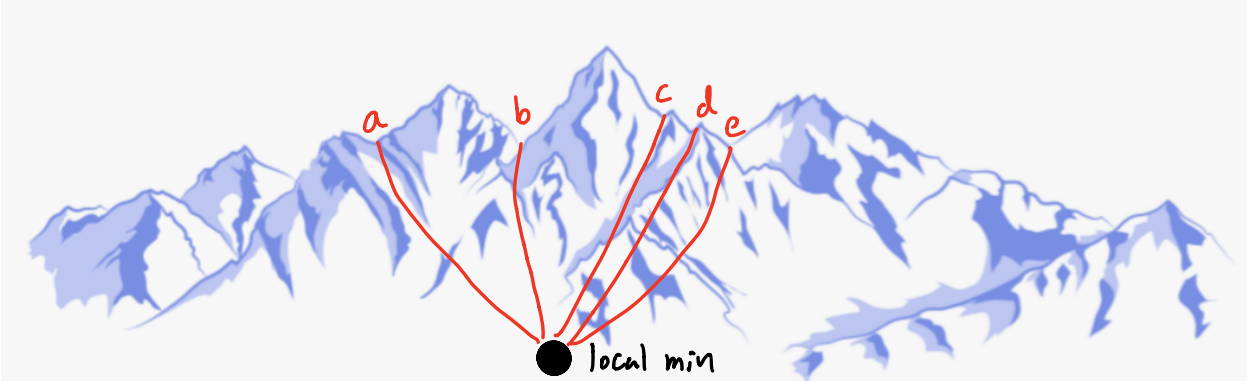
AATRN: Applied Algebraic  
Topology Research Network

[www.aatrnet.net](http://www.aatrnet.net)

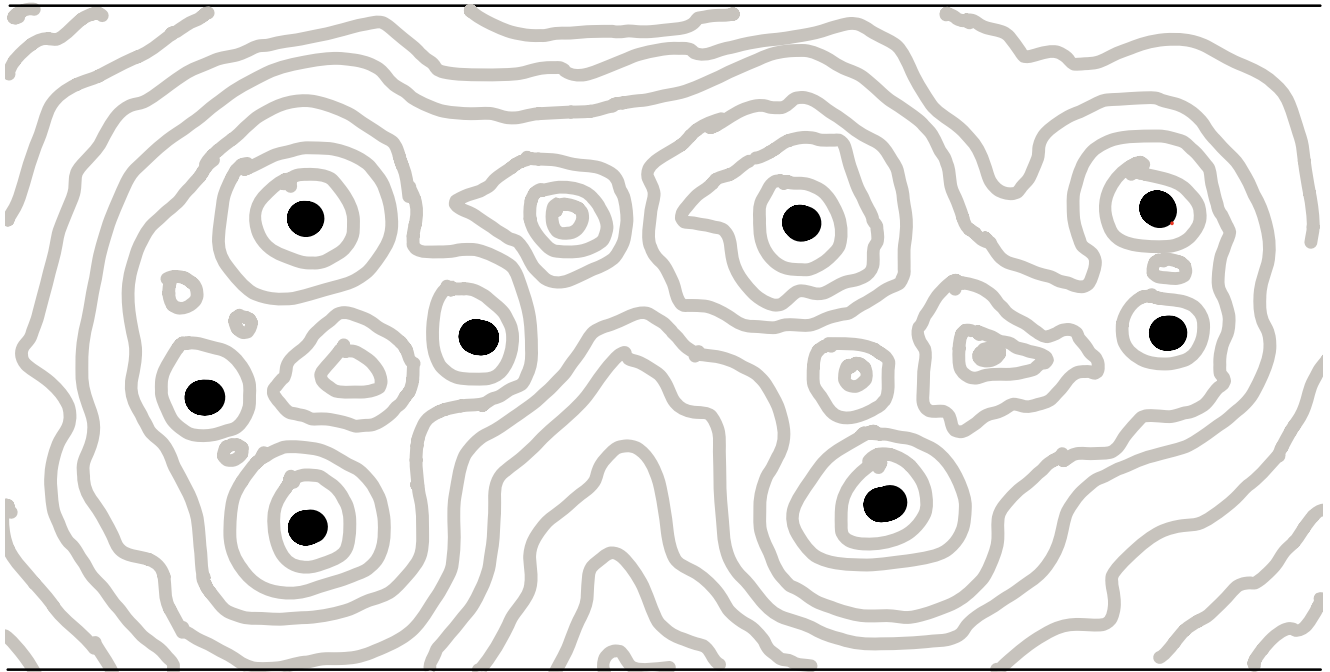
1-2 live talks per week

YouTube: 7,500 subscribers,  
20 hours watched per day

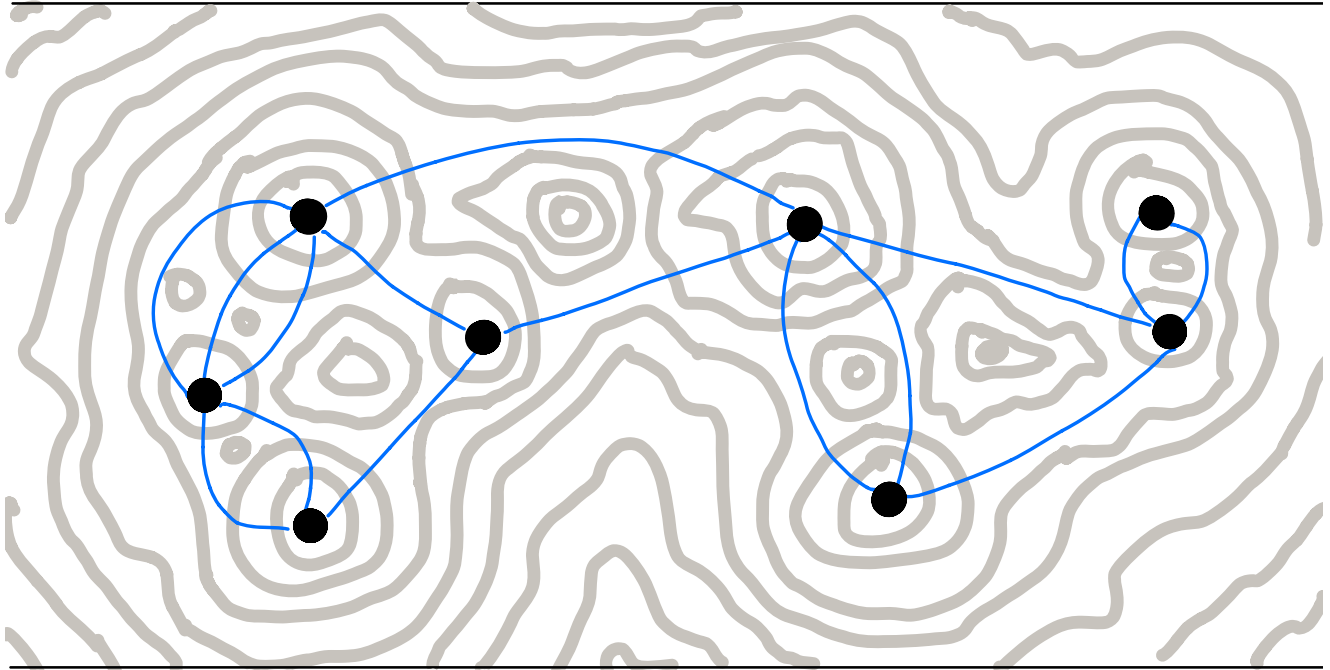
iMSi, Chicago, Aug 2025



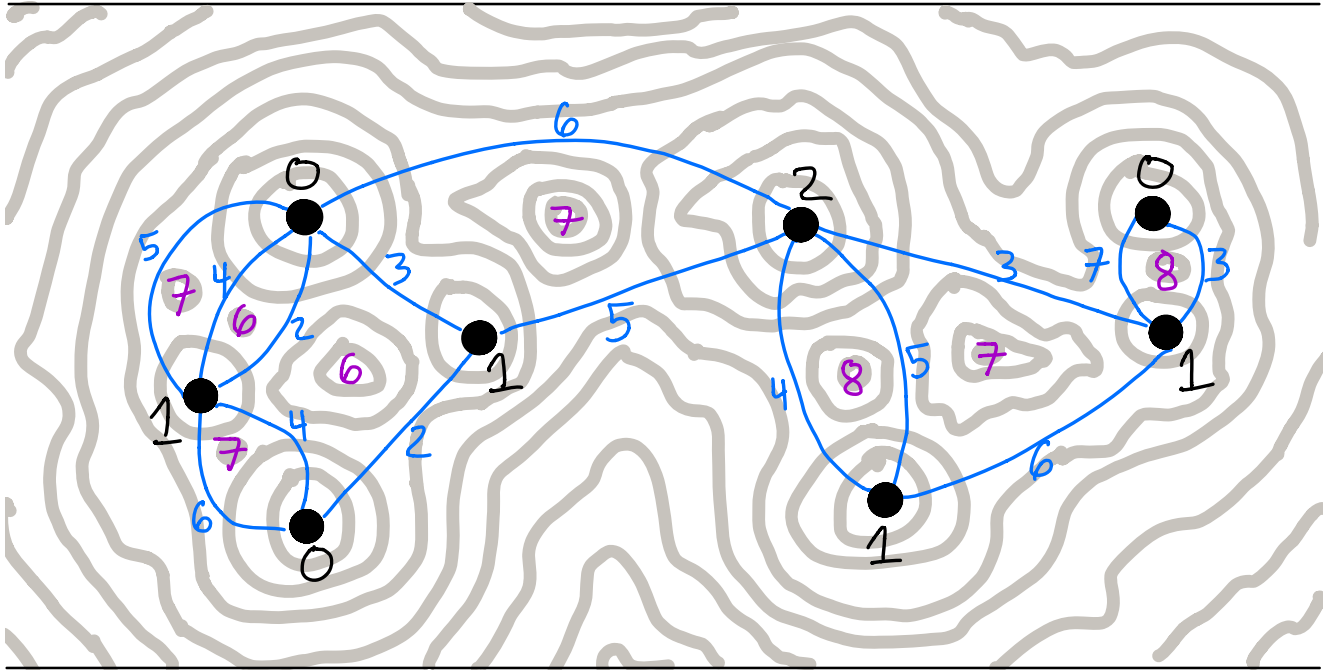
# Merge trees and sublevelset persistent homology



# Merge trees and sublevelset persistent homology

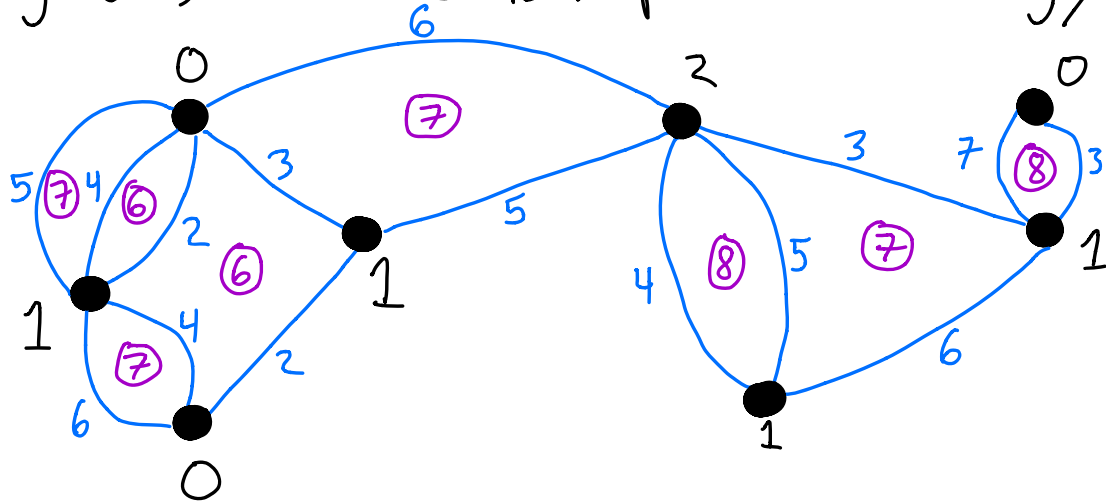


# Merge trees and sublevelset persistent homology

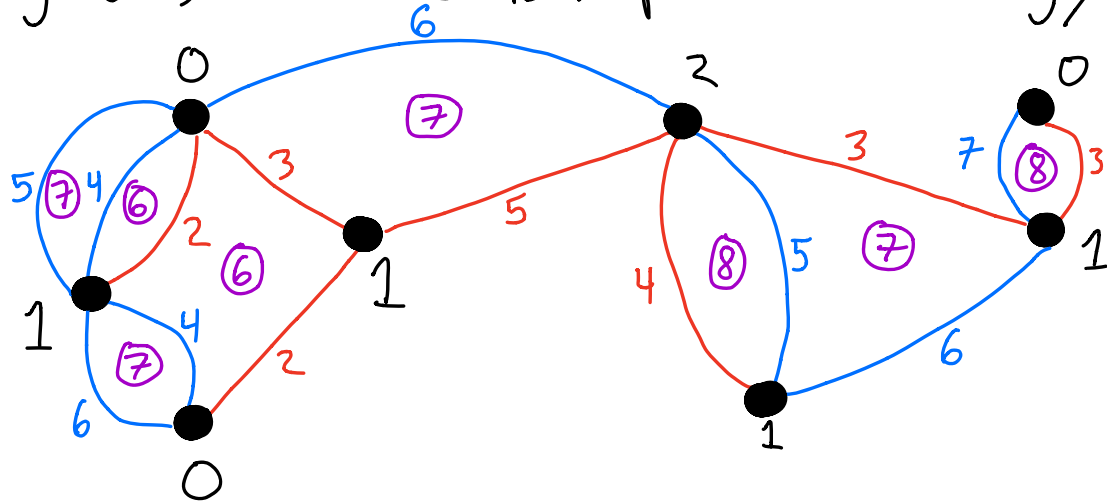




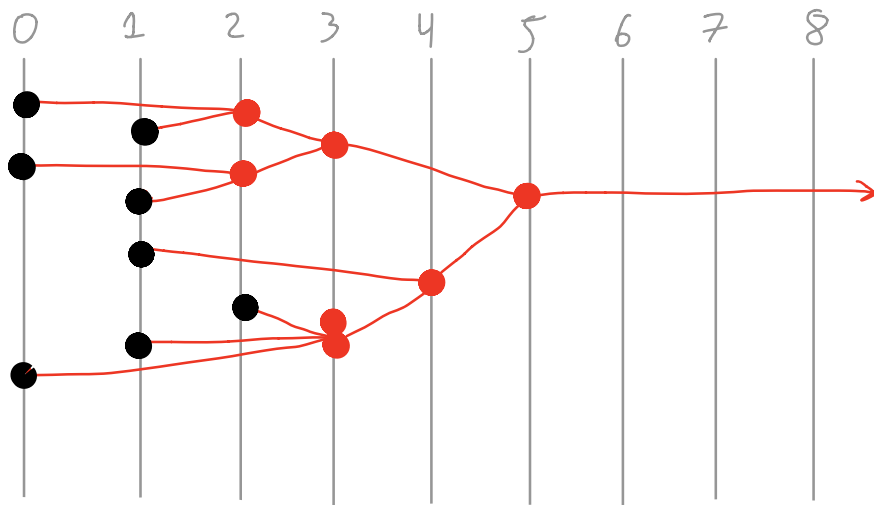
# Merge trees and sublevelset persistent homology



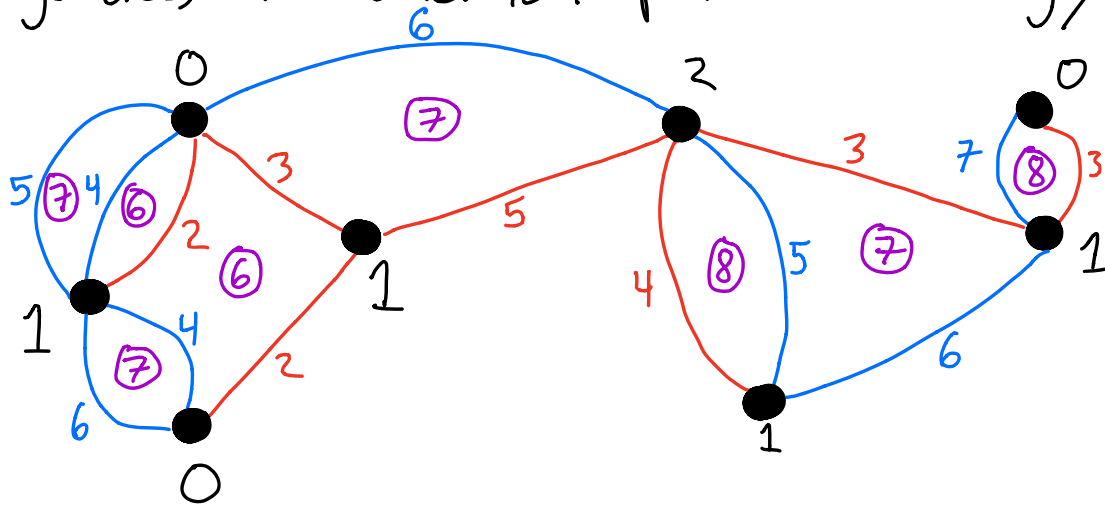
# Merge trees and sublevelset persistent homology



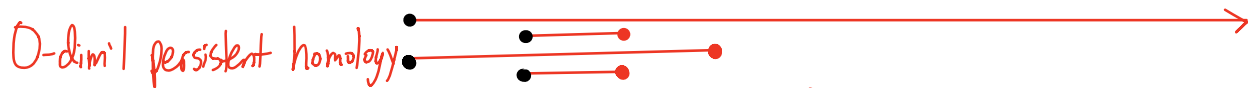
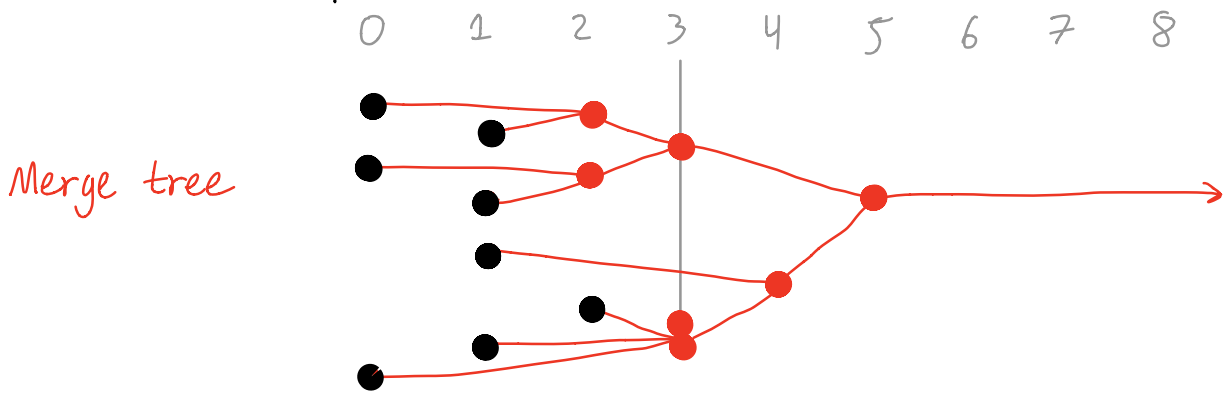
Merge tree



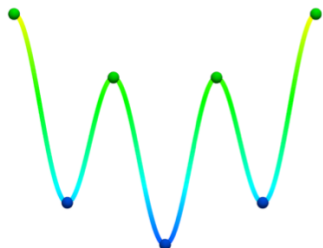
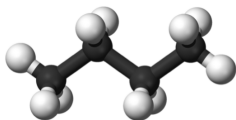
# Merge trees and sublevelset persistent homology



- local minima
- index 1 saddle that merges two components
- index 1 saddle that creates a loop
- index 2 critical point

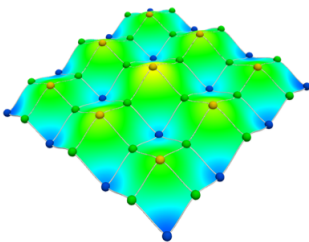
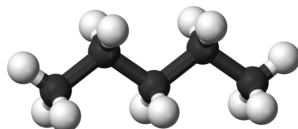


Butane



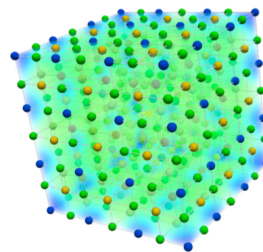
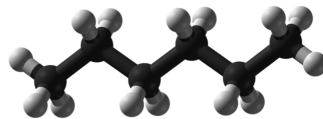
Energy  $f: S^1 \rightarrow \mathbb{R}$

Pentane



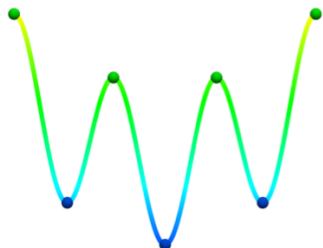
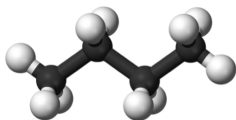
Energy  $f(\phi_1) + f(\phi_2)$

Hexane

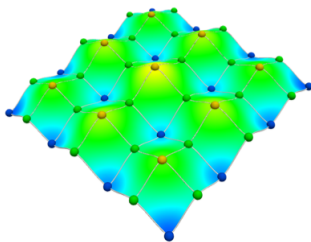
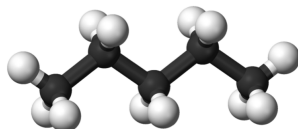


Energy  $f(\phi_1) + f(\phi_2) + f(\phi_3)$

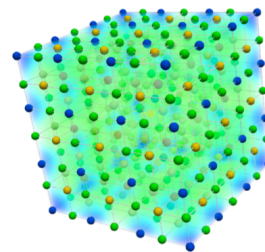
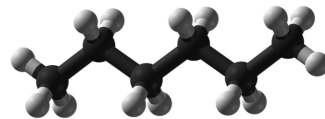
Butane



Pentane

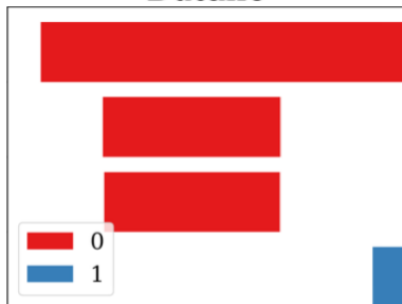


Hexane



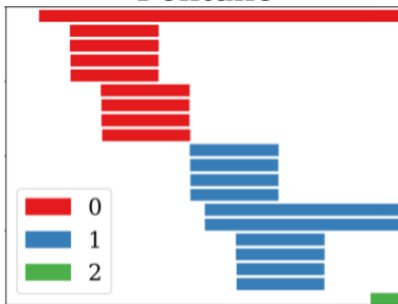
Energy  $f: S^1 \rightarrow \mathbb{R}$

Butane



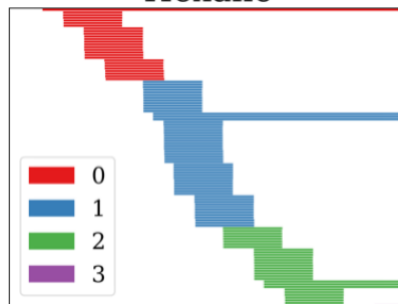
Energy  $f(\phi_1) + f(\phi_2)$

Pentane

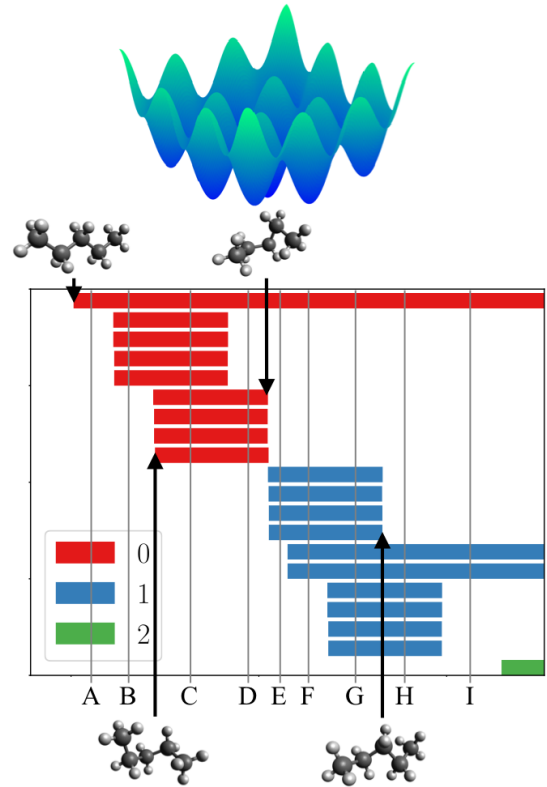
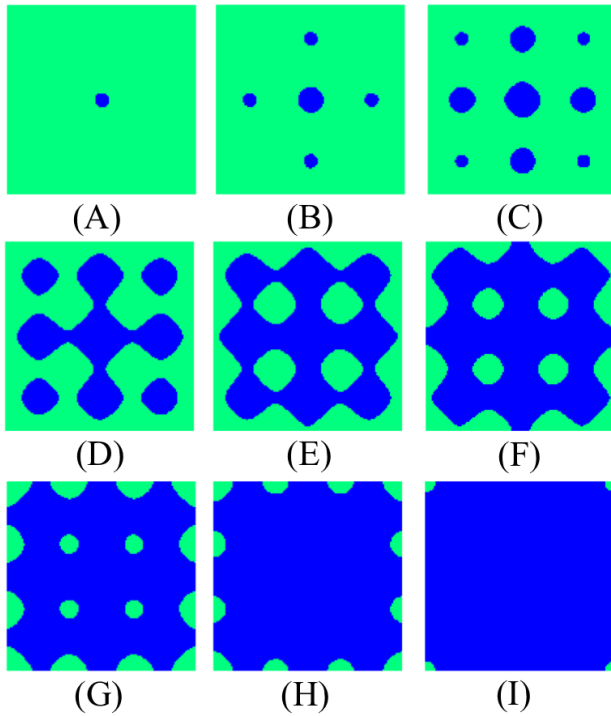


Energy  $f(\phi_1) + f(\phi_2) + f(\phi_3)$

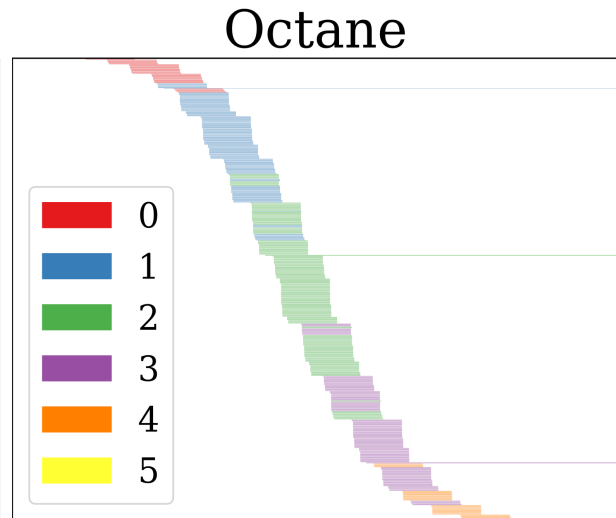
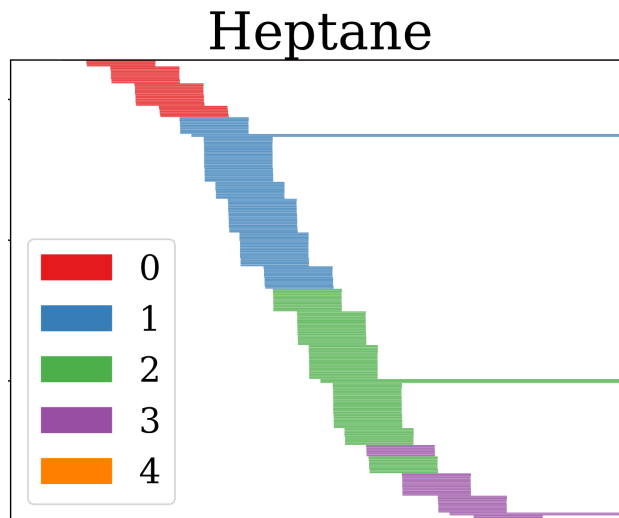
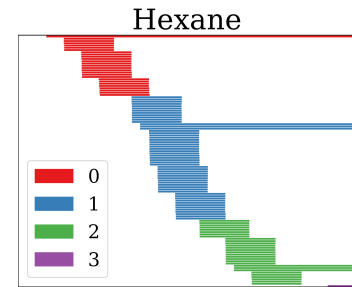
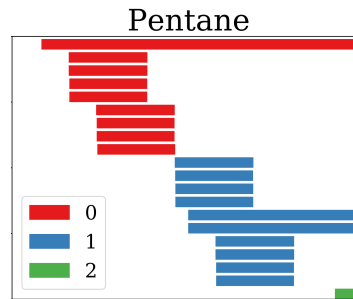
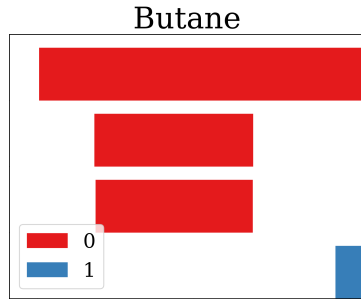
Hexane



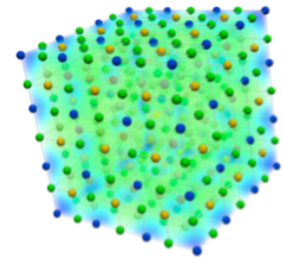
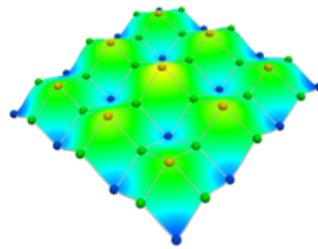
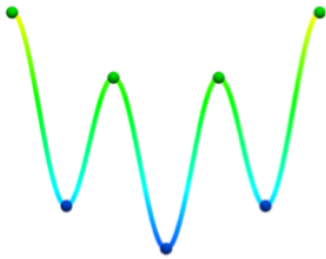
# Sublevelset persistent homology of pentane (OPLS-UA)



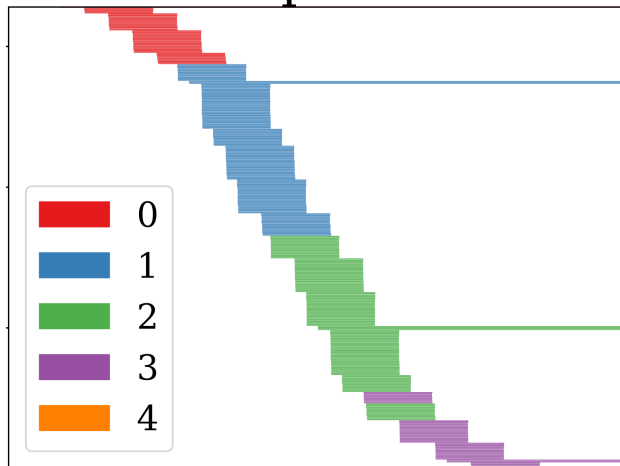
# Sublevelset persistent homology of pentane (OPLS-UA)



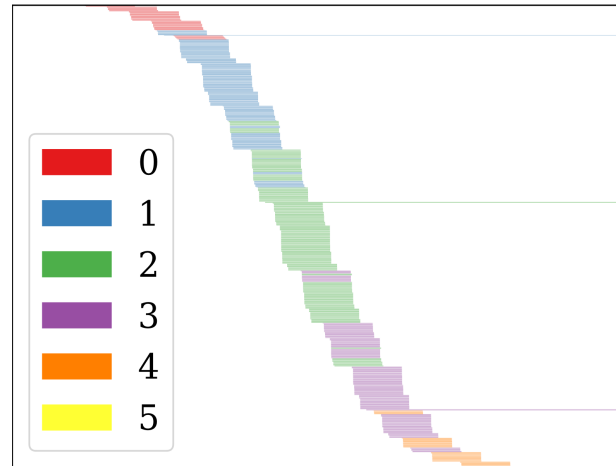
# Sublevelset persistent homology of pentane (OPLS-UA)



## Heptane

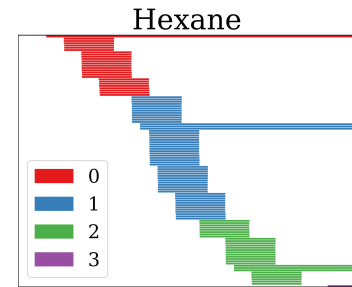
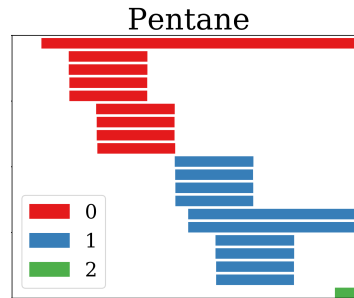
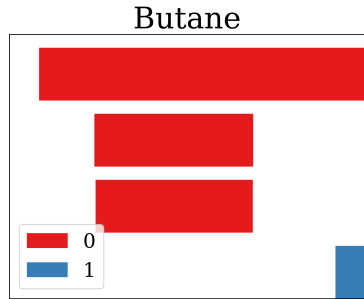


## Octane



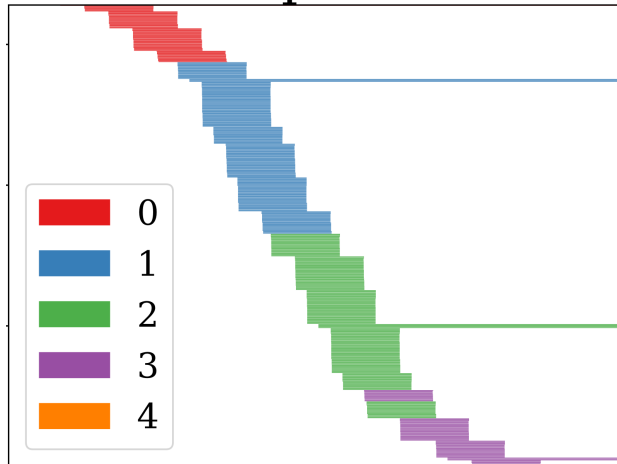


# Sublevelset persistent homology of pentane (OPLS-UA)

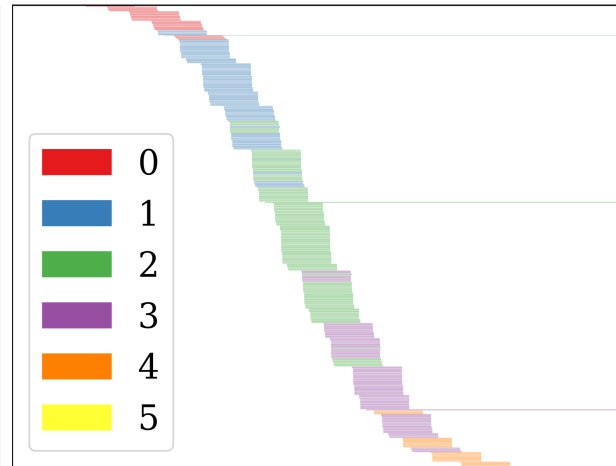


We have a complete characterization of the sublevelset persistent homology of all alkanes  $f: (S^1)^n \rightarrow \mathbb{R}$ .

Heptane

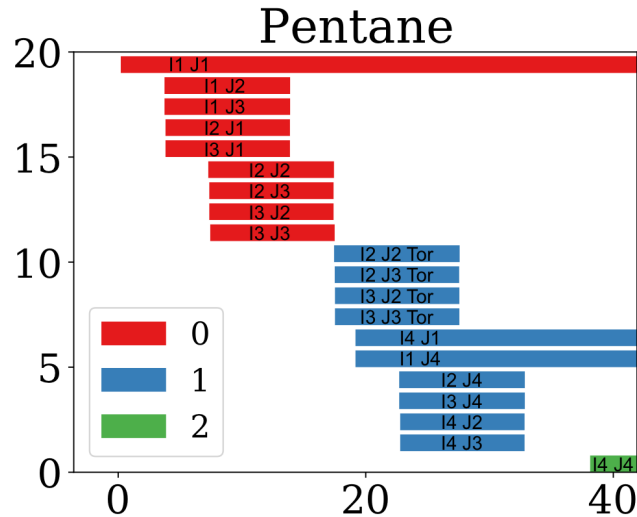
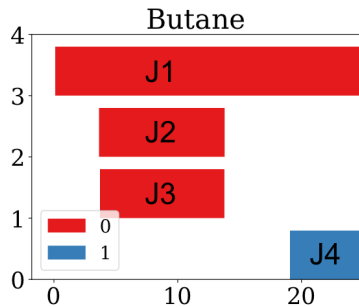
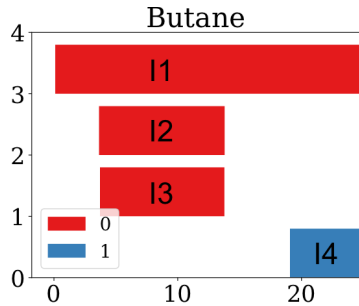


Octane



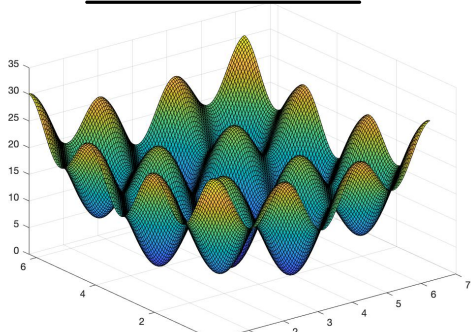
# bars is  $(6^n + 2^n)/2$

# bars in dimension  $k$  is  $\binom{n}{k} + (3^{n-1} - 1)\binom{n-1}{k}$

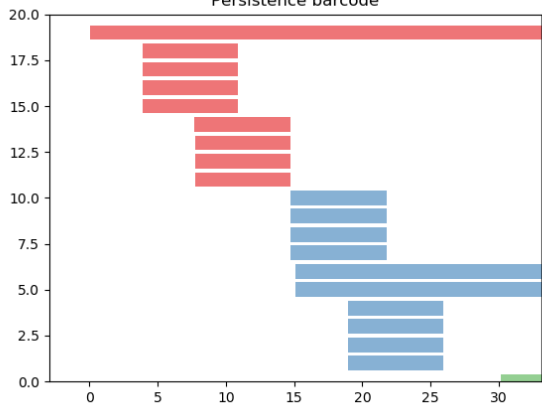


The proof of how the birth and death times pair uses "Künneth formulae in persistent homology" by Hitesh Gakhar and Jose Perea.

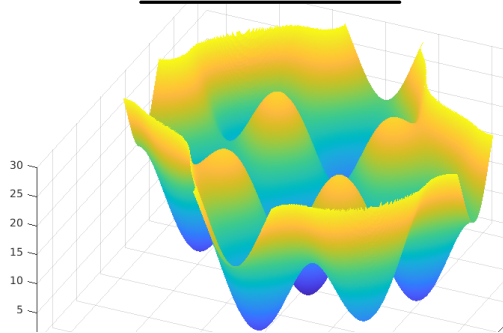
# OPLS-VA



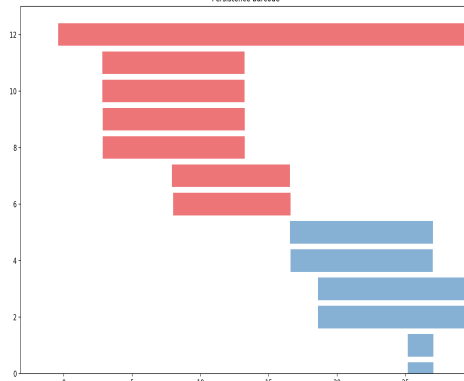
Persistence barcode



# OPLS-AA

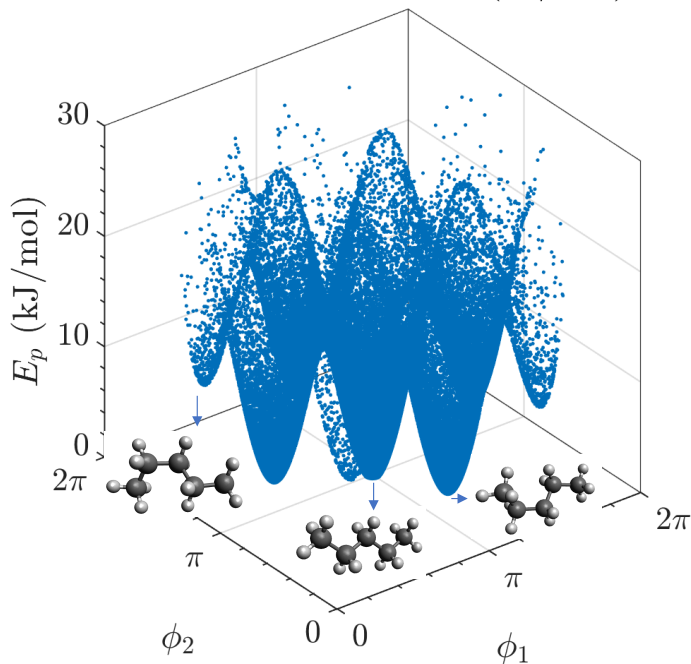


Persistence barcode

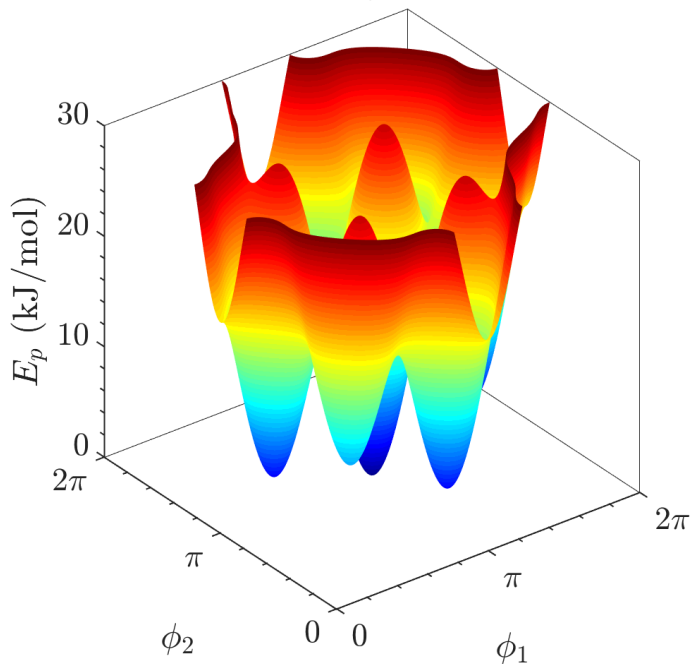


# Molecular dynamics simulation samples the EL

Numerical,  $k_B T = 16.6$  (kJ/mol)



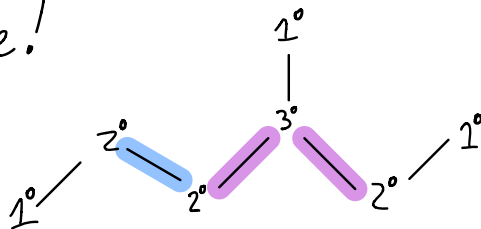
Analytical



# Ongoing and future work

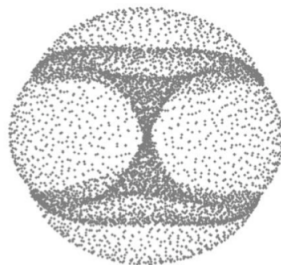
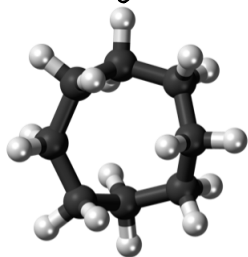
(DELTA, Aurora Clark, Biswajit Sadhu,  
Brittany Story, Ethan Berkove, Jose Perez)

- Branched alkanes – any tree!



- Alkenes and alkynes

- Cyclo-alkanes



Topology of cyclo-octane energy landscape  
Martin, Thompson, Coutsias, Watson, 2010

- Machine learning

