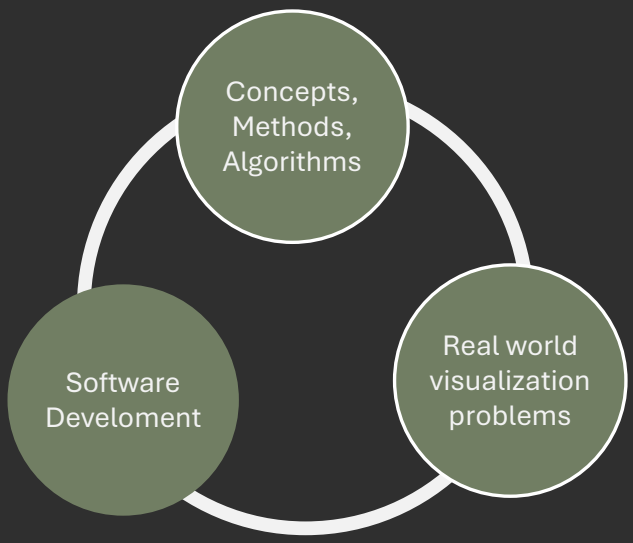
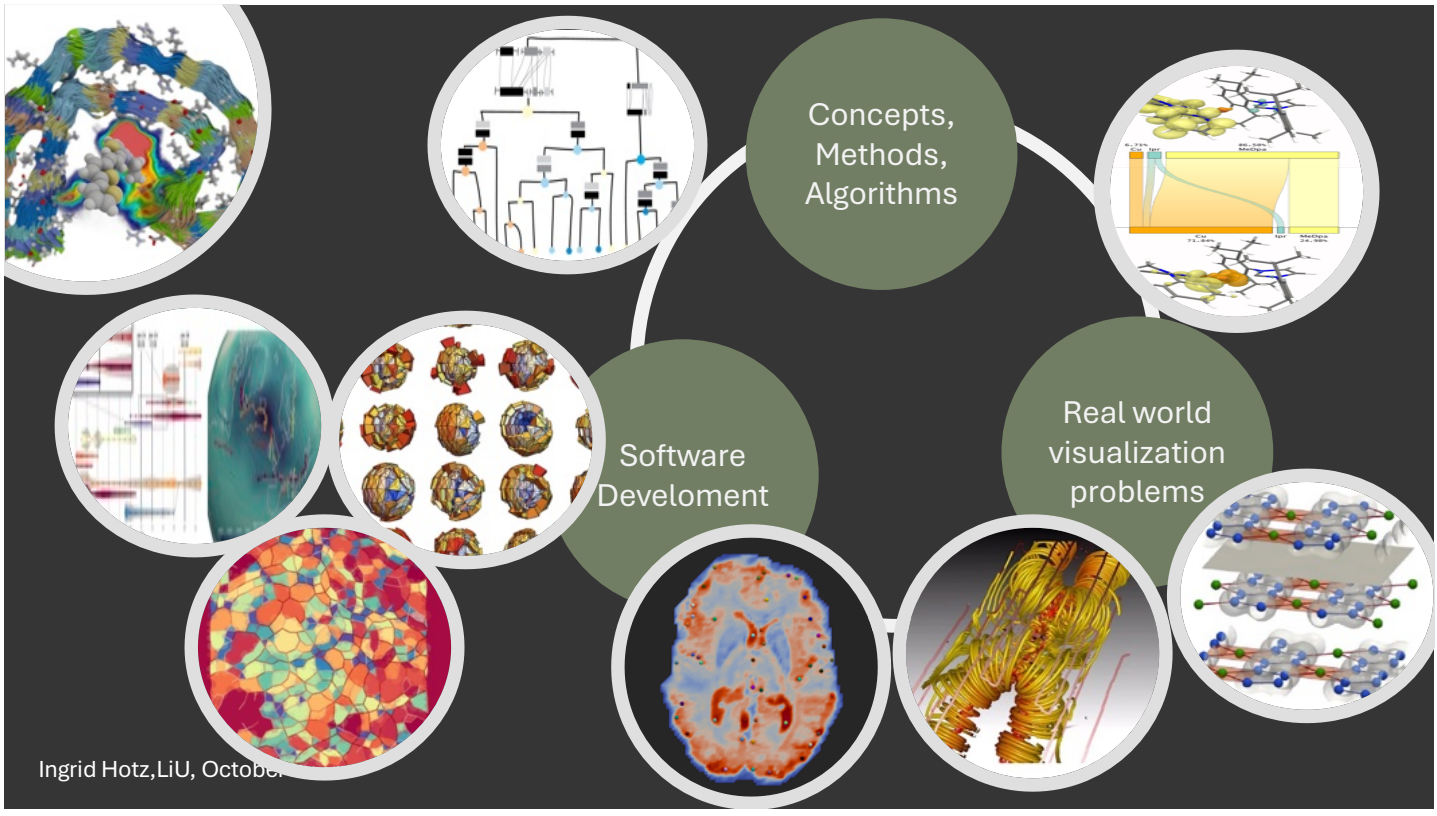
Topological data analysis in visualizaiton



Ingrid Hotz, LiU
Lund, October 3, 2024

Combining automatic analysis with the expert's knowledge through effective explorative visualization



Topology
Study of shape invariants under continuous deformation

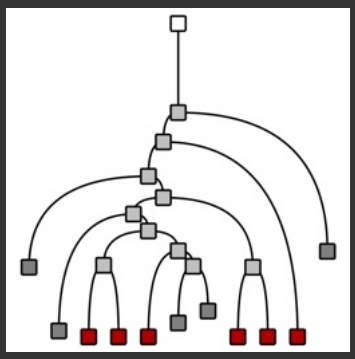
Image: http://math.arizona.edu/~models/Topology/image/coffee_cup_to_donut.jpg

A topologist does not know the difference between a coffee cup and a donut.

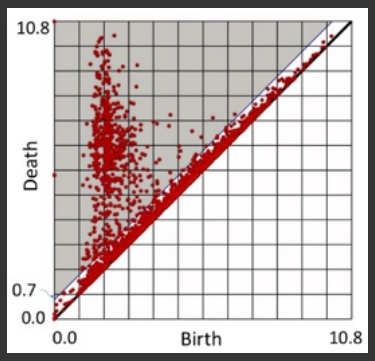
Algebraic topology	Computational topology	Topology in Visualiaiton
Concepts, theorems	Algorithms, Practical solutions to topological problems	Semantic abstractions Answer domain specific questions
Classify shapes Investigate spaces via algebraic invariants	Reliable, robust, efficient Strong guarantees $(\ldots < \epsilon)$	Mapping to the domain needs

Ingrid Hotz,LiU, October 2024

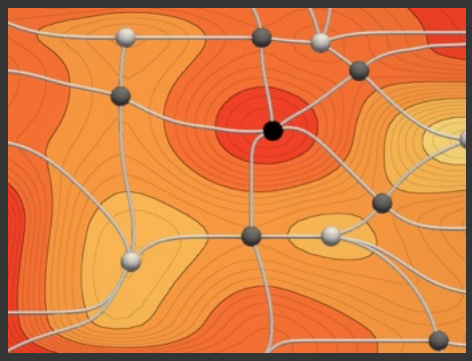
Topological Descriptors frequently used in Visualizaion



Contour tree
Merge tree



Persistence diagrams
Barcodes



Mores-Smale complex
Extremal structures

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Merge Tree

Hydrogen: Electron Density Field s
Set of nested isosurface

$\{(x, y, z) \in D | s(x, y, z) = C_i\} = s^{-1}(C_i)$
for a scalar function s and iso values
$C_i \in \mathbb{R}, i = 1 \dots n$

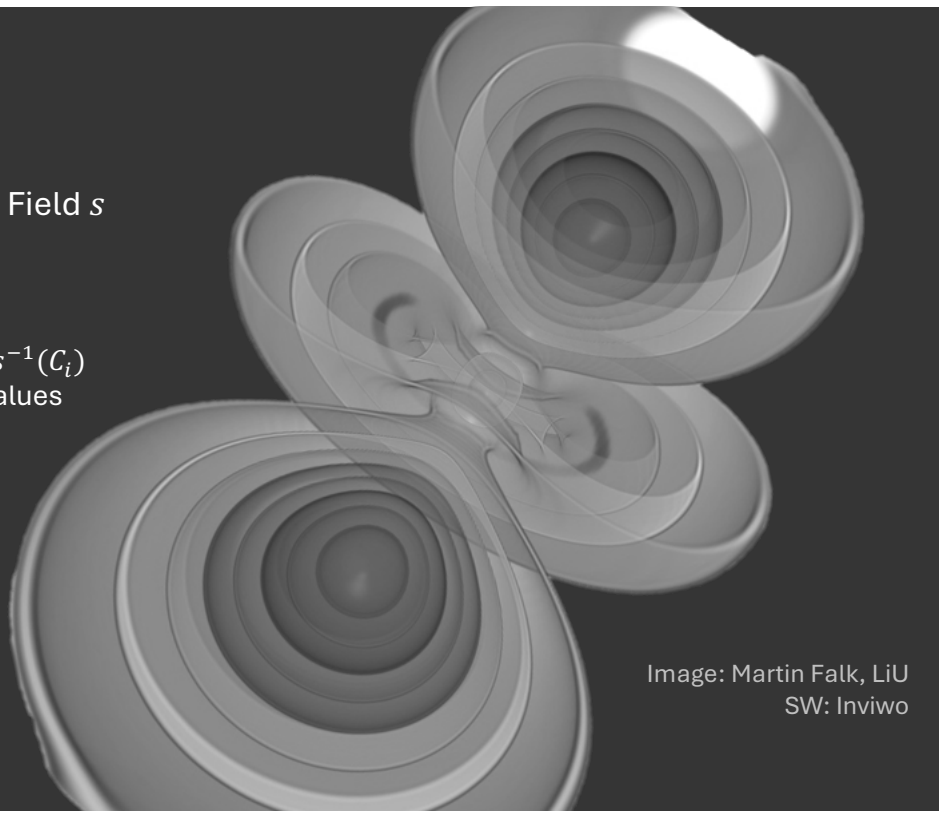
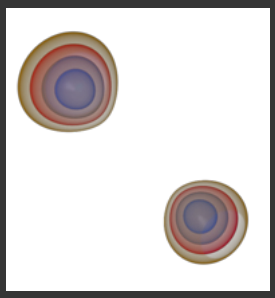


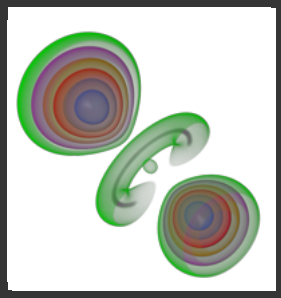
Image: Martin Falk, LiU
SW: Inviwo

Ingrid Hotz,LiU, October 2024

Merge Tree

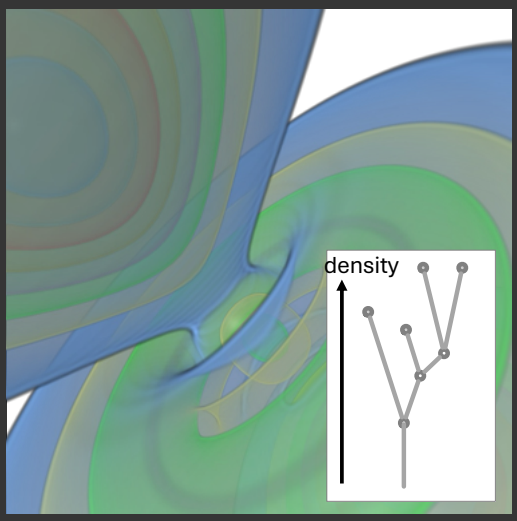
Electron Density Field Hydrogen
Isosurface representation





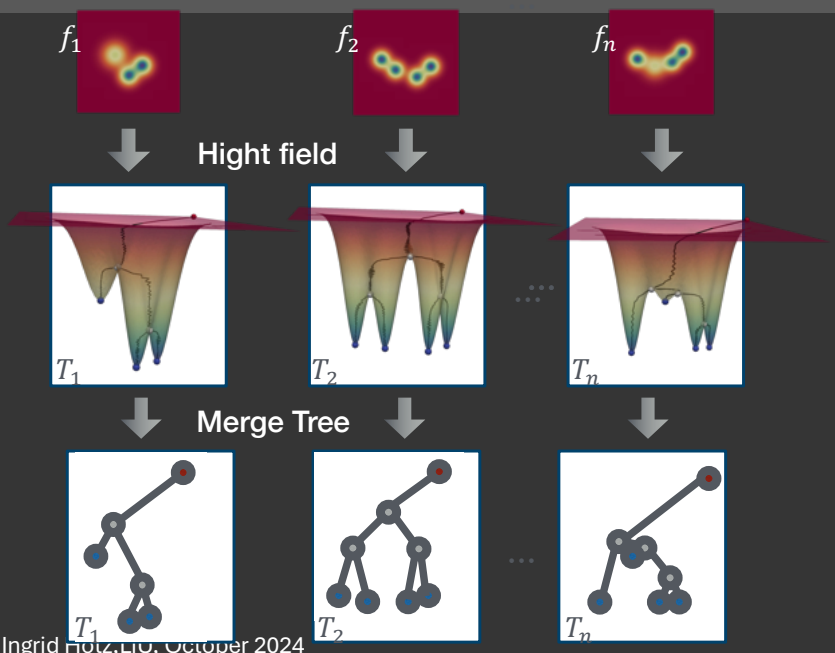
Chosen iso value

c_1



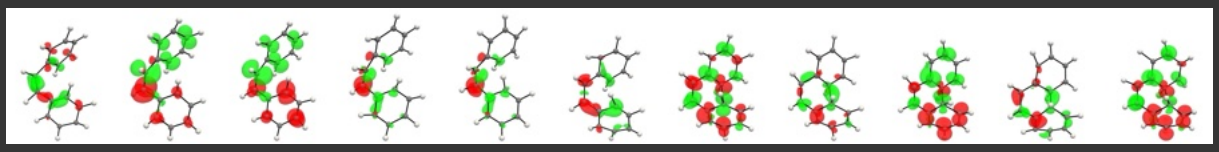
Images: Martin Falk, LiU

Utilizing the merge tree for data summarization



- Abstraction
- Spatial segmentation and feature definitions
- Support multi scale analysis

9



time

Photoinduced dynamics of molecules

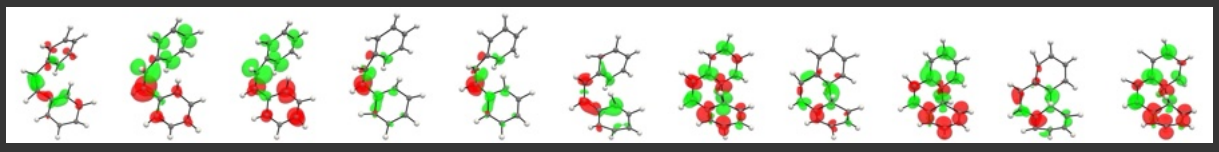
Theoretical Chemist
- Nanna List KTH

Data analysis and visualization experts
- Florian Wetzel, Tu Kaiserslautern
- Christoph Garth, Tu Kaiserslautern
- Talha Bin Masood, LiU
- Ingrid Hotz, Liu

International collaboration between
- TU Kaiserslautern, Germany
- Linköping University, Sweden

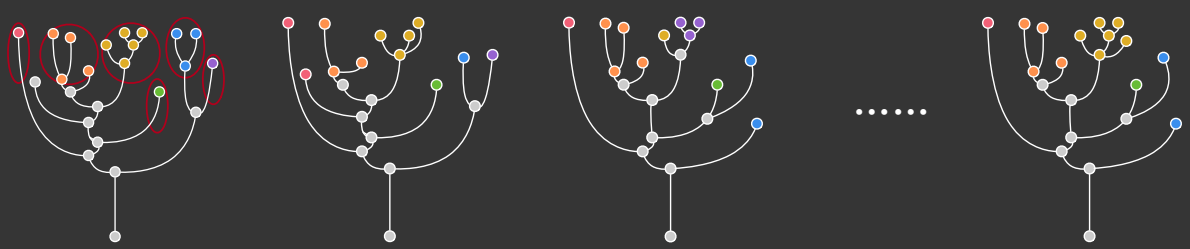
Ingrid Hotz,LiU, October 2024

10



time

Photoinduced dynamics of molecules



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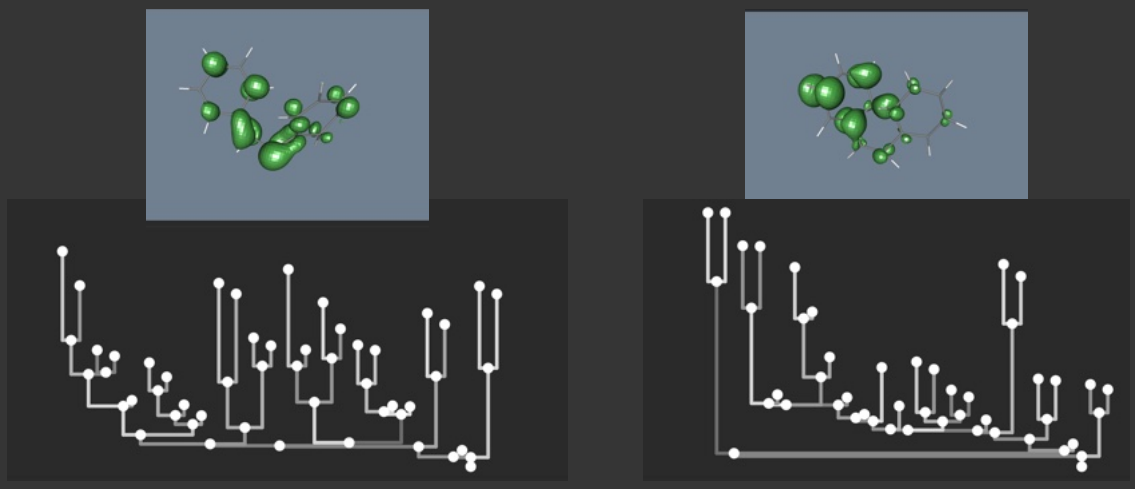
Electronic structures
Utilizing the merge tree for summarization and comparison

[Exploring Electron Density Evolution using Merge Tree Mappings. Wetzels et al, 2024]

Compute 'Edit Distance distance' between two merge trees
→induces mappings between edges in the merge trees.



Edit Distance distance between two merge trees T_1 , T_2

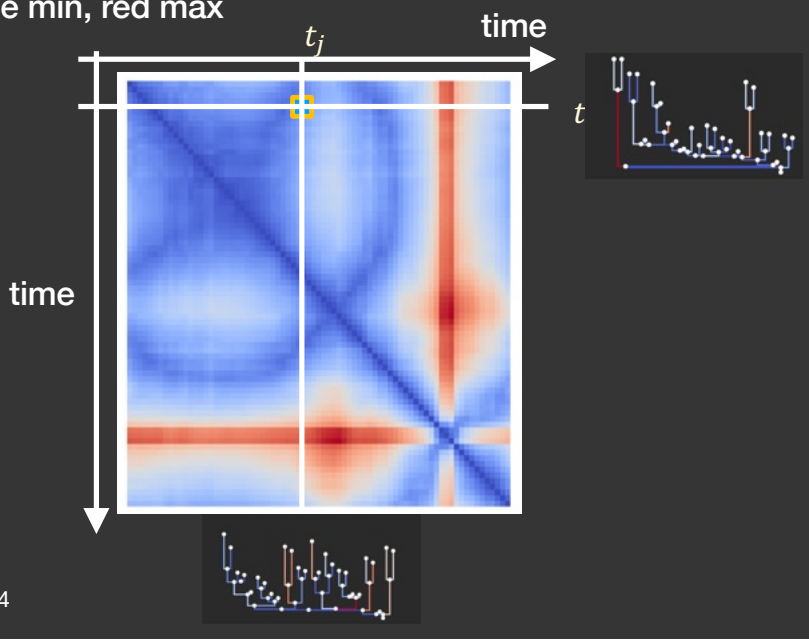
is defined to be the minimal cost of an edit sequence transforming T_1 into T_2

$$\delta_E(T_1, T_2) = \min\{c(S) | T_1 \xrightarrow{S} T_2\}.$$

The deformation edit distances are a metric for (abstract) merge trees

Tree Edit Distance (TED) distance matrix

Color: $d(t_i, t_j)$, blue min, red max



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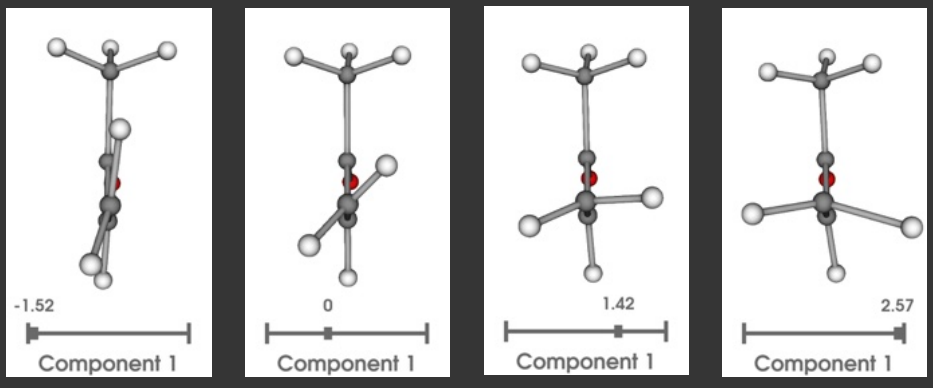
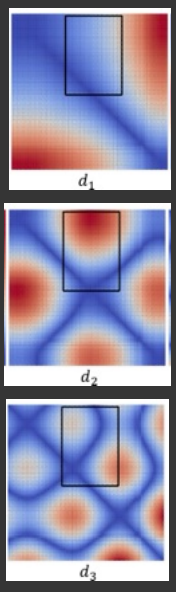
Correlation with nuclear structure $\{p_1, \cdots, p_n\}$,

- Focus on three main principal components $c_1,\ c_2, c_3$
- Distance metrices $d_i(m_1, m_2) = |c_1^i - c_2^i|, i = 1,2,3$





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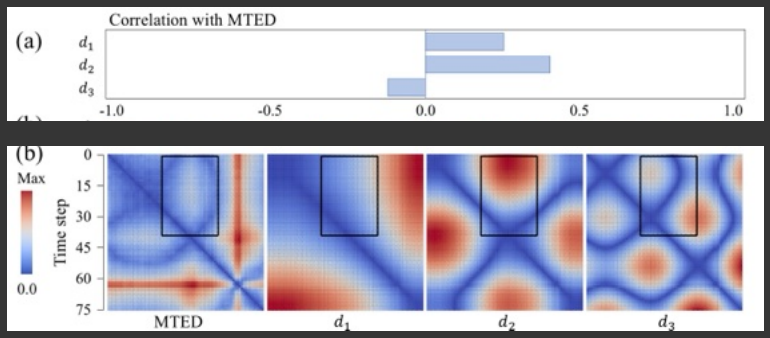
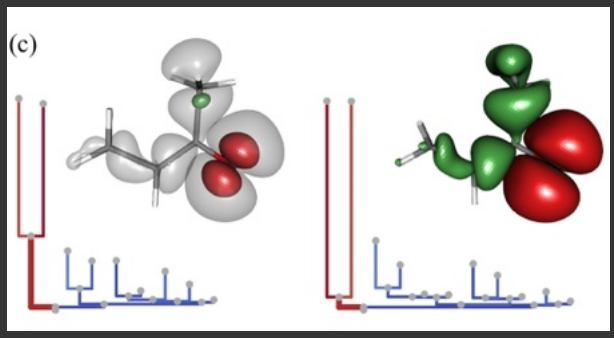
Visualization interface

- Four distance matrices based on the TED, d_1, d_2, d_3
- Correlation bars between the values of TED and each of d_1, d_2, d_3 for selected submatrices.
- Timeline View for nuclear structures
- Merge Tree View.
- Spatial contours evolutions/changes for two selected time-steps





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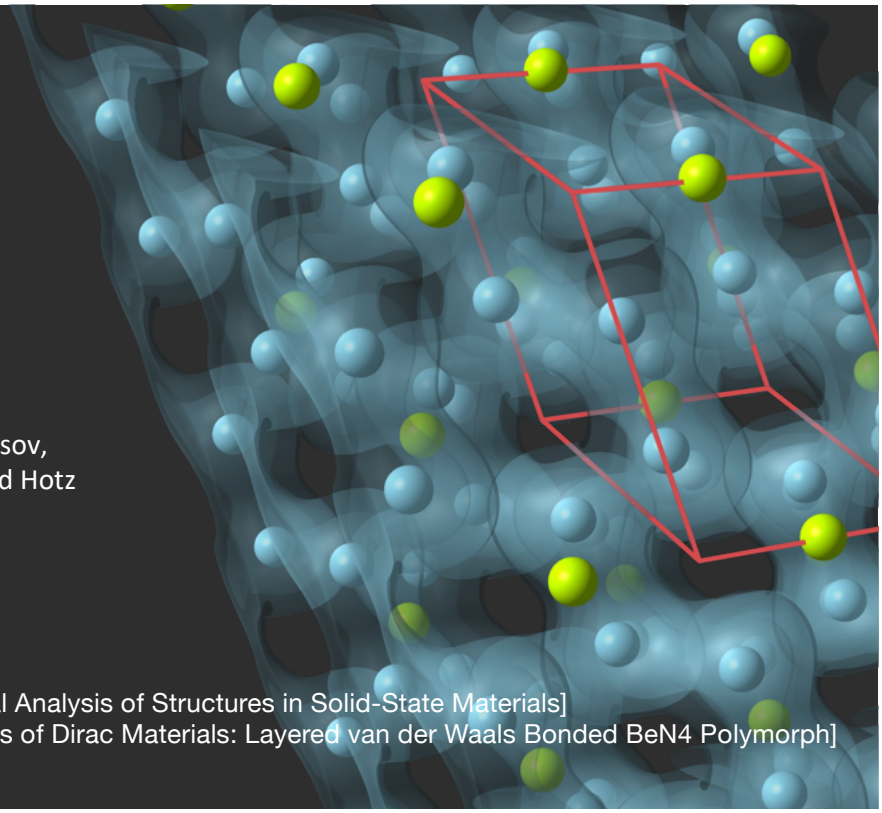
Analysis of Structures in Solid-State Materials

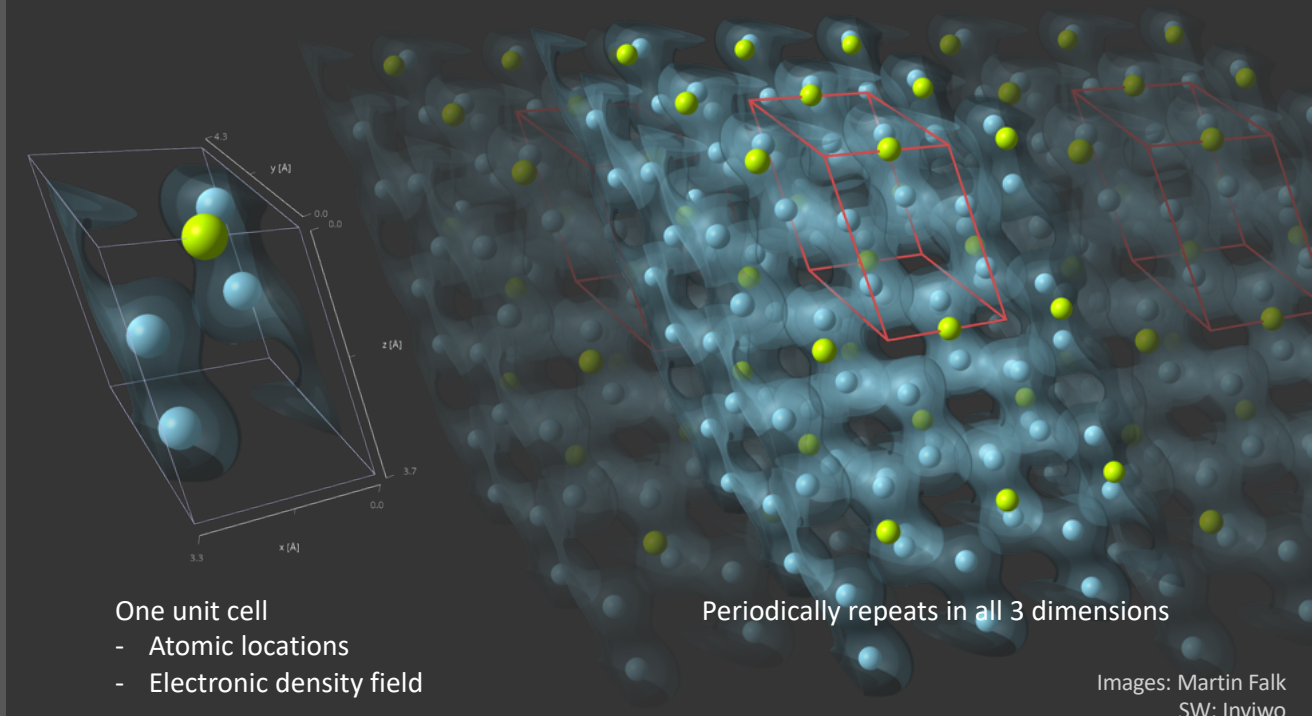
Signe Sidwall Thygesen, Alexei I. Abrikosov,
Peter Steneteg, Talha Bin Masood, Ingrid Hotz

Collaboration: Igor Abrikossov, LiU



[Thygesen et al. 2023. Level of Detail Visual Analysis of Structures in Solid-State Materials]
[Bykov et al. 2021. High-Pressure Synthesis of Dirac Materials: Layered van der Waals Bonded BeN4 Polymorph]

The data



One unit cell
- Atomic locations
- Electronic density field

Periodically repeats in all 3 dimensions

Images: Martin Falk
SW: Inviwo

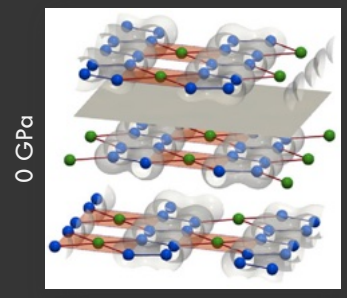
The collaboration and context – visualization challenge

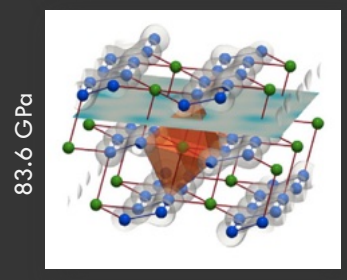
Data per unit cell

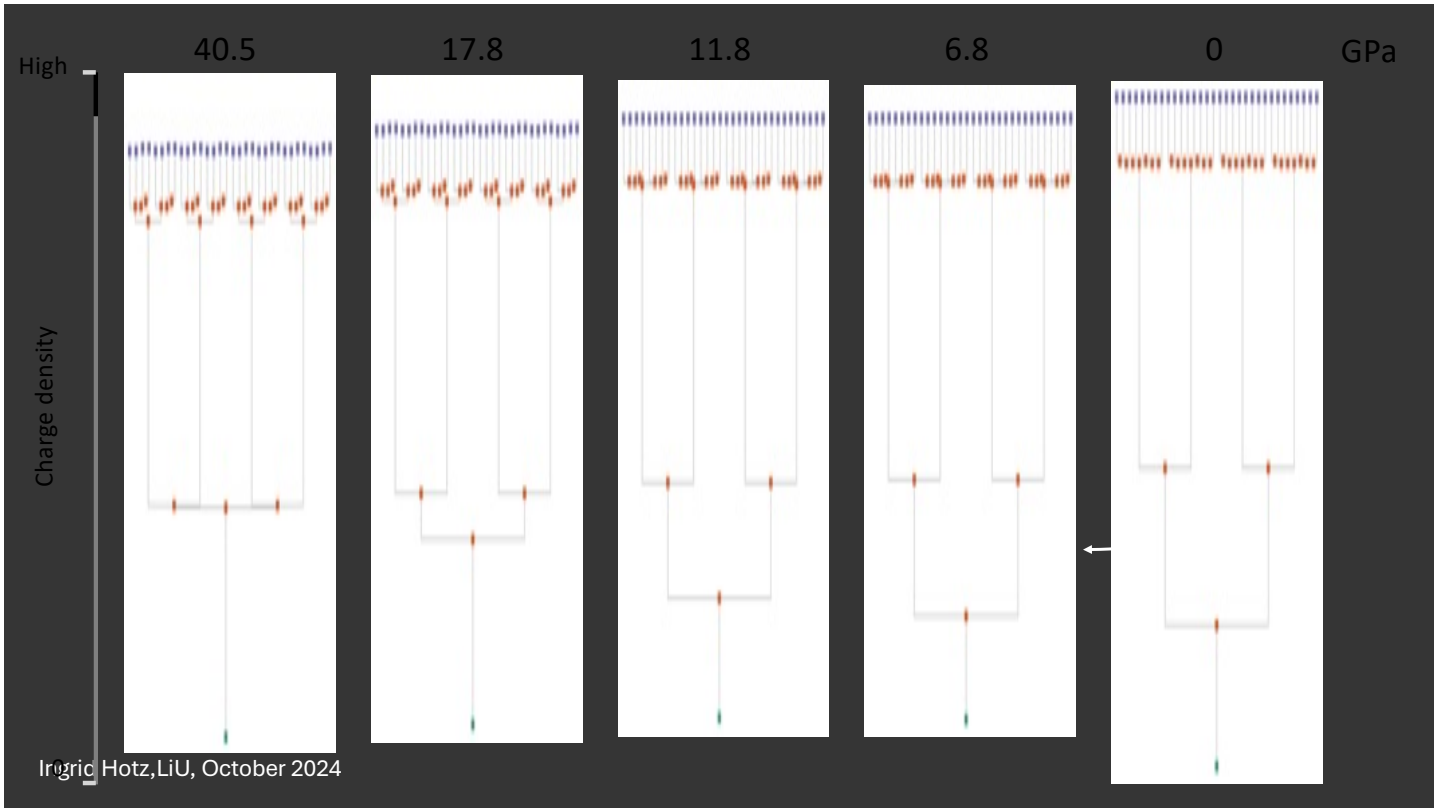
- Charge density for BeN_4 at 7 different pressure points (0 to 83.6 GPa)
- Atomic positions

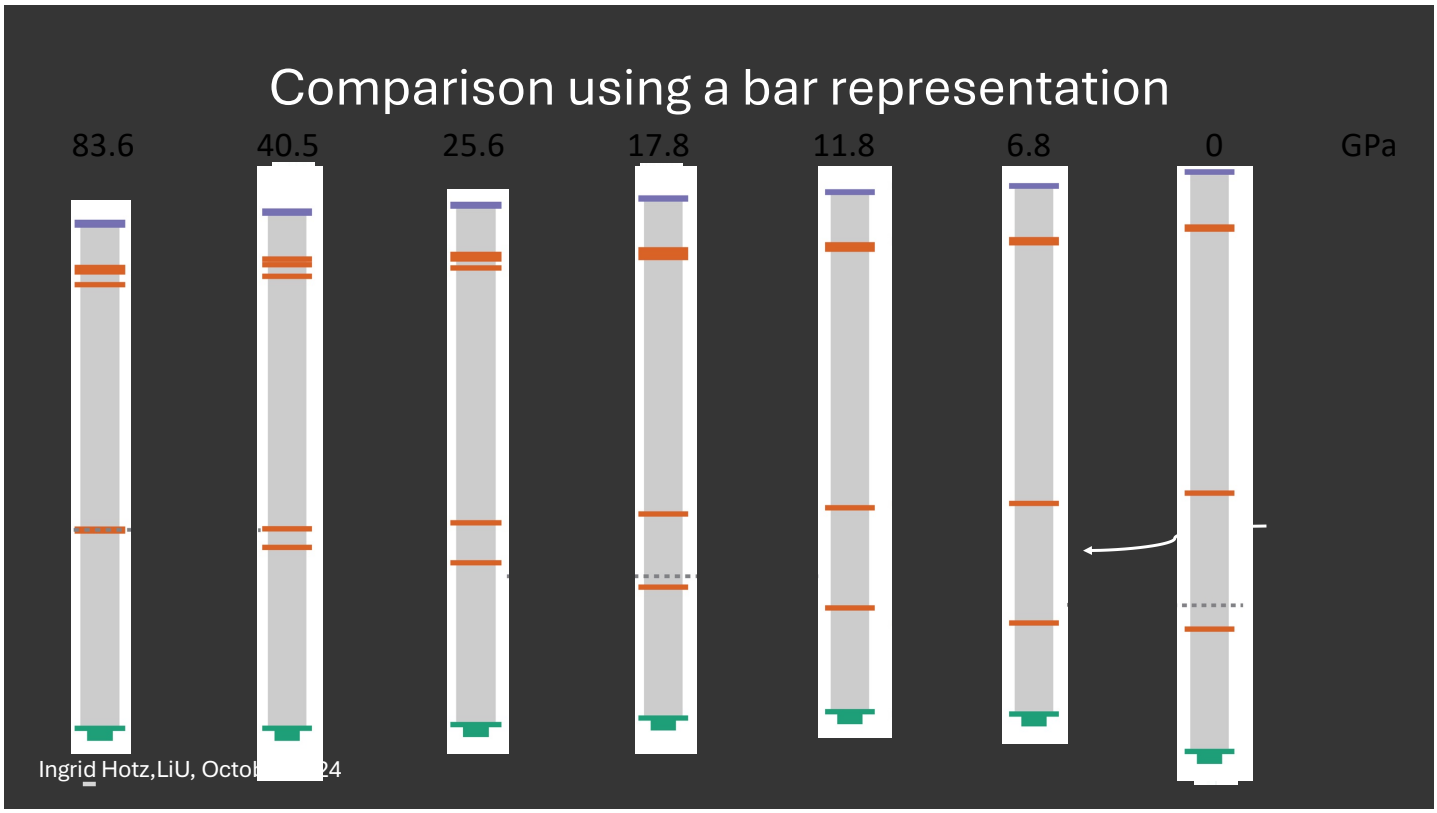
Questions:

- Can you produce nicer pictures for our publication
- Strengthen the **evidence of layers** based on charge density data?
- Provide **"data summary"** that facilitates **automatic and visual distinction** between layered vs unlayered configurations?

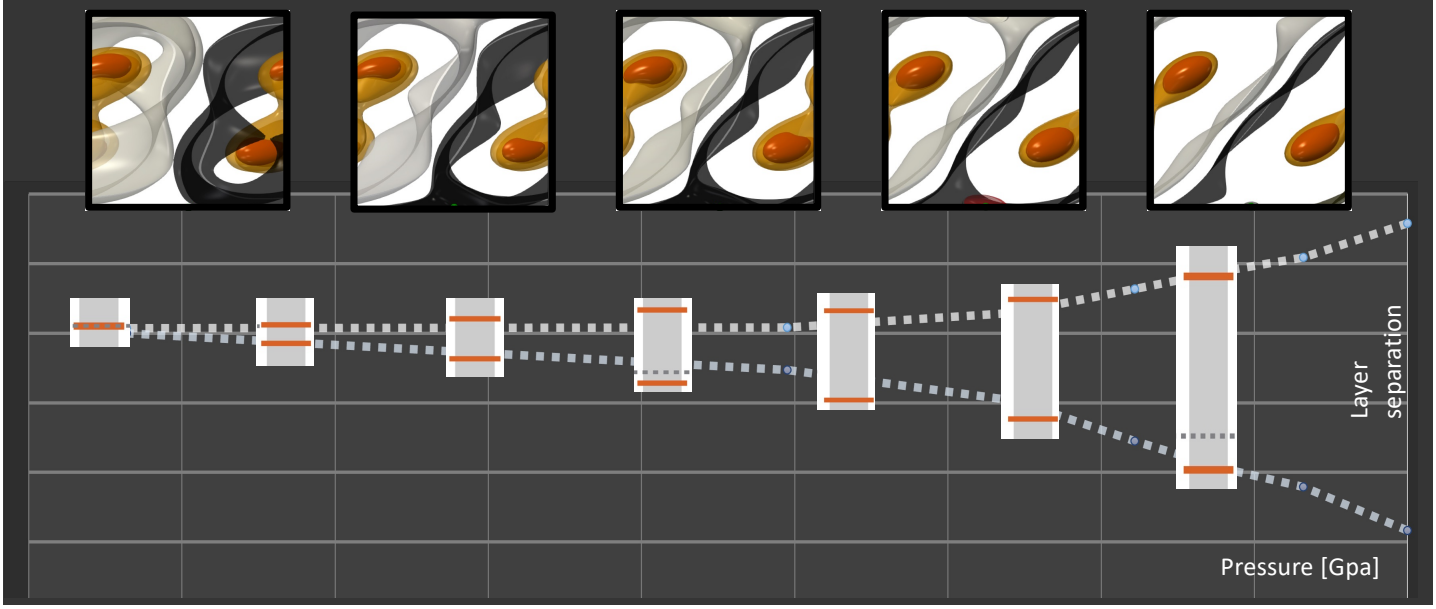





High
40.5
17.8
11.8
6.8
0
GPa
Charge density
Ingrid Hotz,LiU, October 2024


Comparison using a bar representation
83.6
40.5
25.6
17.8
11.8
6.8
0
GPa
Ingrid Hotz,LiU, Octob 24

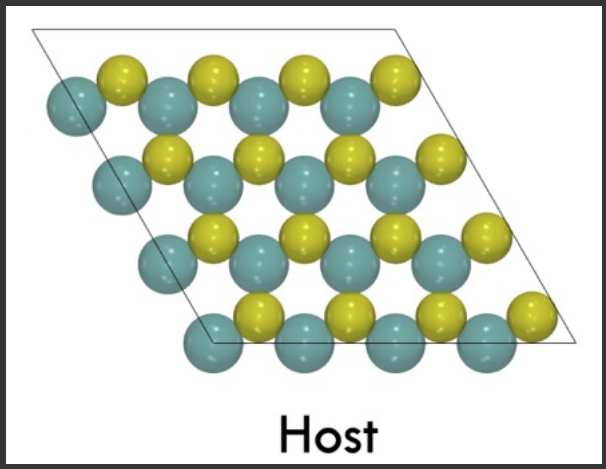
Black and white isosurfaces show the separations of layers briefly before thy merge



Automatic Defect Analysis and Qualification (ADAQ) Database

Ongoing Work

Atoms in the unit cell (top view)



Sulphur
Mo

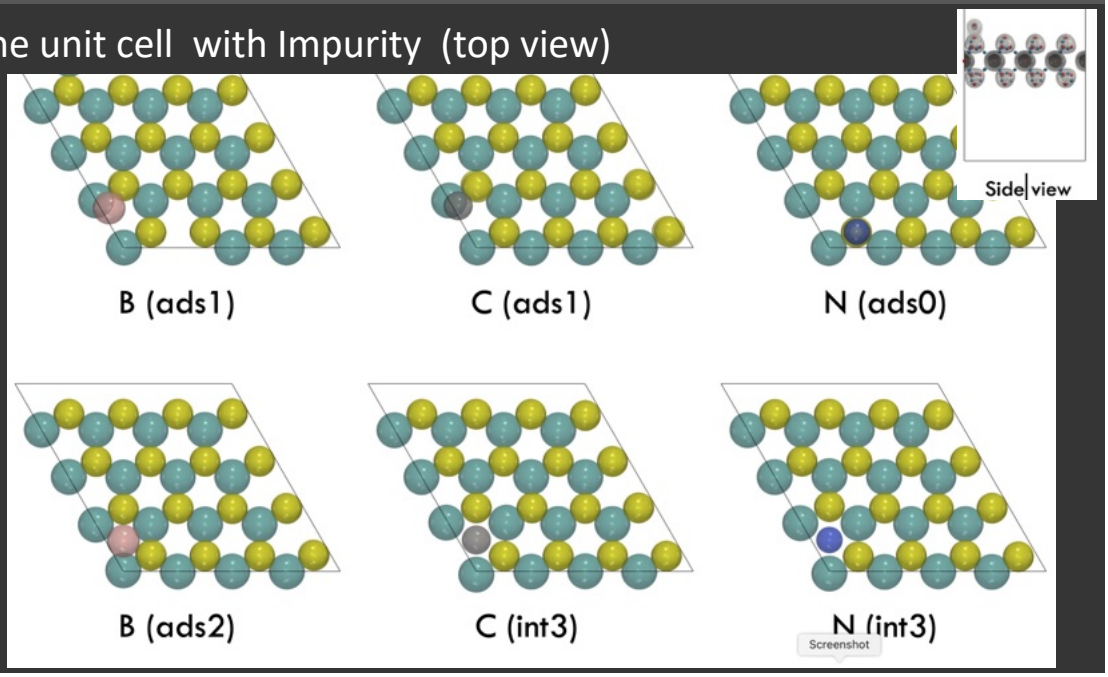
Towards supporting search and comparison in a rich dataset of defects

[Davidsson, et al.. Absorption versus adsorption: high-throughput computation of impurities in 2D materials, Springer Nature, 2023]
Images: Talha Bin Masood

Automatic Defect Analysis and Qualification (ADAQ) Database

Ongoing Work

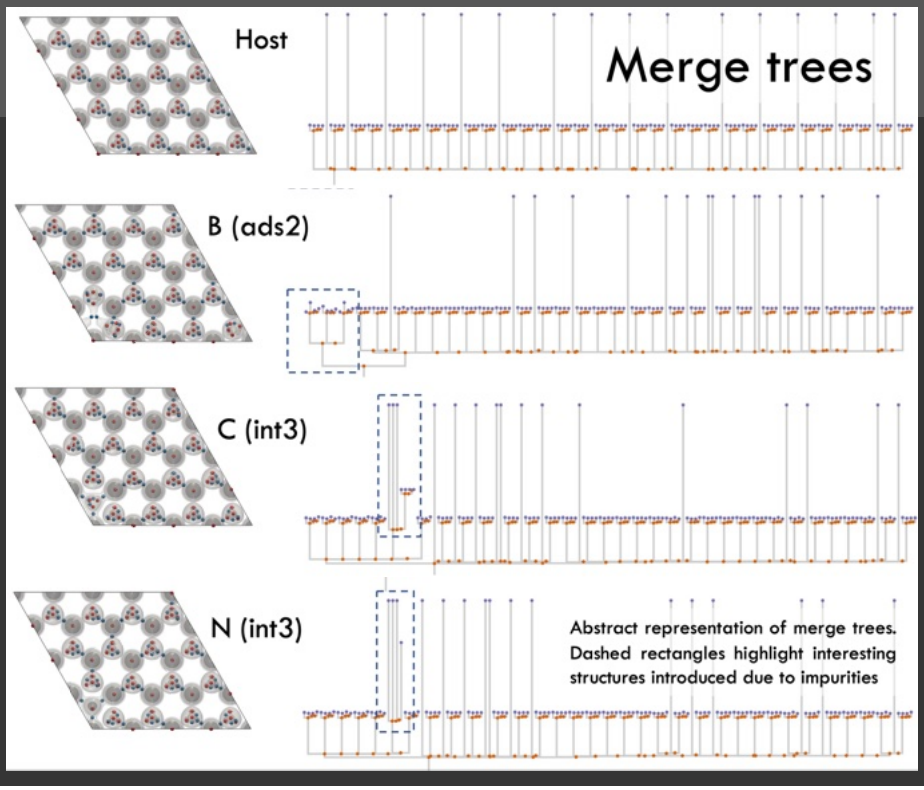
Atoms in the unit cell with Impurity (top view)



Sulphur
Mo
Boron
Carbon
Nitrogen

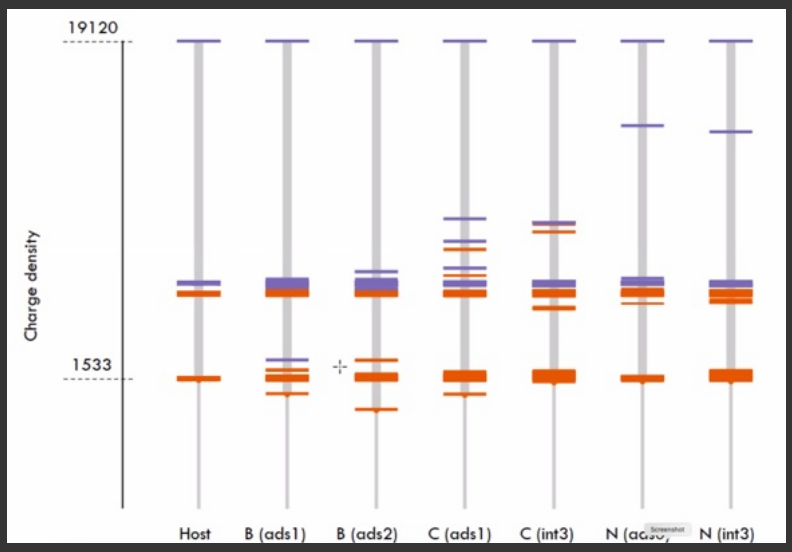
Electronic density

tz,LiU, October 2024



Automatic Defect Analysis and Qualification (ADAQ) Database

Electronic density



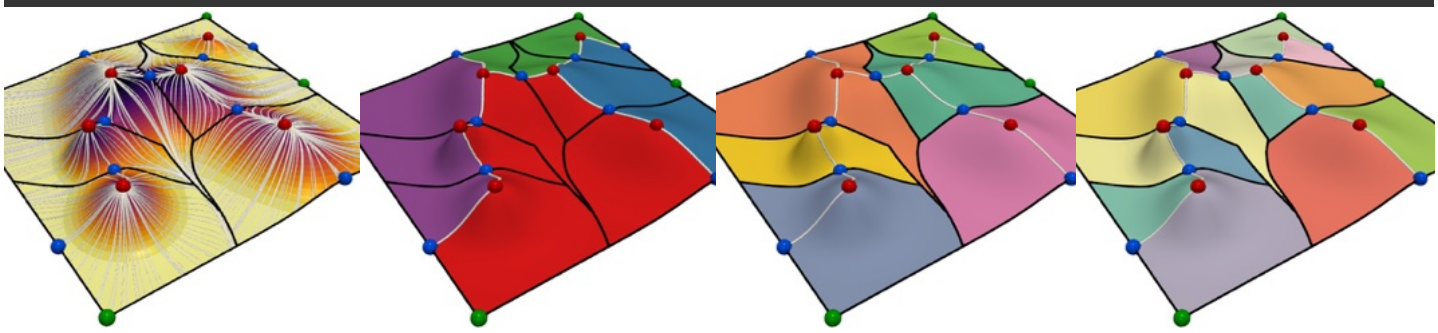
Summary bars for selected defects

tz,LiU, October 2024

Morse-Smale complex

Partitioning of the domain in regions of uniform gradient behavior

Gradient lines	Ascending manifolds (AM) partition the domain into valleys	Descending manifolds (DM) partition the domain into mountains	Morse-Smale complex Full segmentation



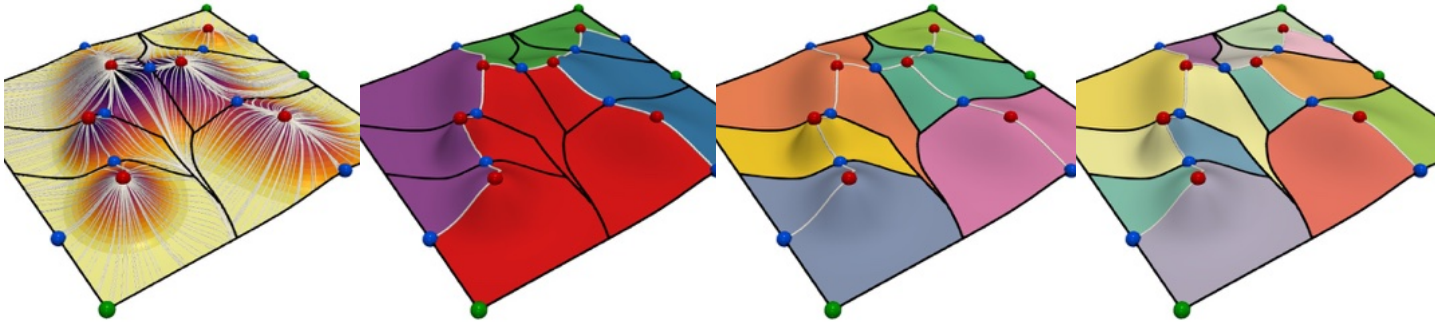
Critical points: green minima, blue saddle, and red maxima
Separatrices (black) are gradient lines forming the boundary between lines that flow towards different maxima.
Ingrid Hotz,LiU, October 2024

Images: Talha Bin Masood

Morse-Smale complex

Partitioning of the domain in regions of uniform gradient behavior

- Abstraction while maintaining more geometric information
- Spatial segmentation and feature definitions
- Support multi scale analysis



Critical points: green minima, blue saddle, and red maxima
Separatrices (black) are gradient lines forming the boundary between lines that flow towards different maxima.

Ingrid Hotz,LiU, October 2024

Images: Talha Bin Masood

Morse-Smale complex

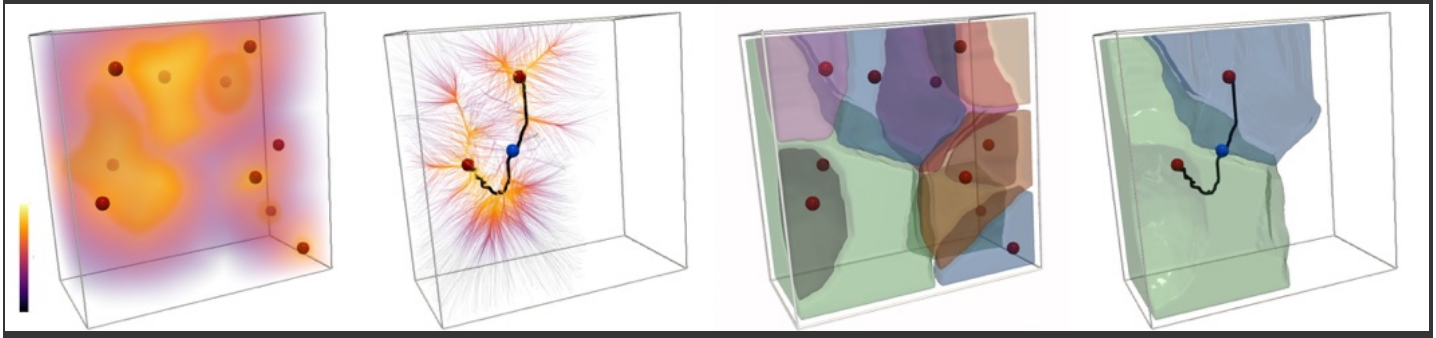
Partitioning of the domain in regions of uniform gradient behavior

Scalar field with critical points

Gradient lines

Descending manifolds (DM) partition the domain into mountains

Saddle point (blue)
Its AM (bold black line) connects the two maxima.



Ingrid Hotz,LiU, October 2024

Images: Talha Bin Masood

Project
Granular materials
Properties and scales

Discrete materials with complex mechanical behavior. Properties akin to solids, fluids, and gases depending on particle arrangement, and particle morphology.

Material scientists:
- Tejas Murthy

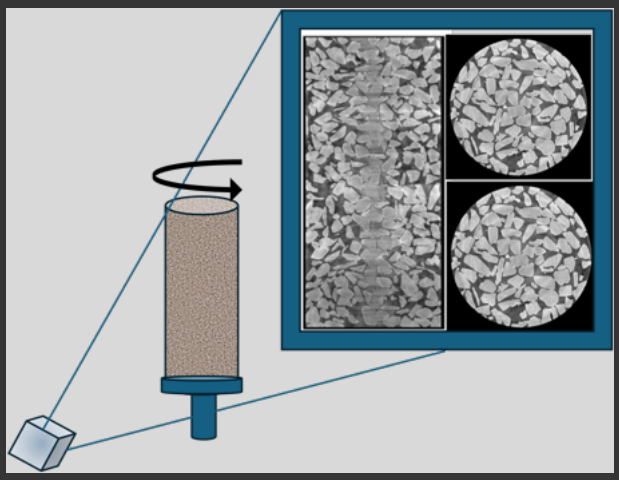
Data analysis and visualization experts
- Talha Bin Masood,
- Vijay Natarajan
- Ingrid Hotz

International collaboration between
- IISC, Bangalore, India
- Linköping University, Sweden

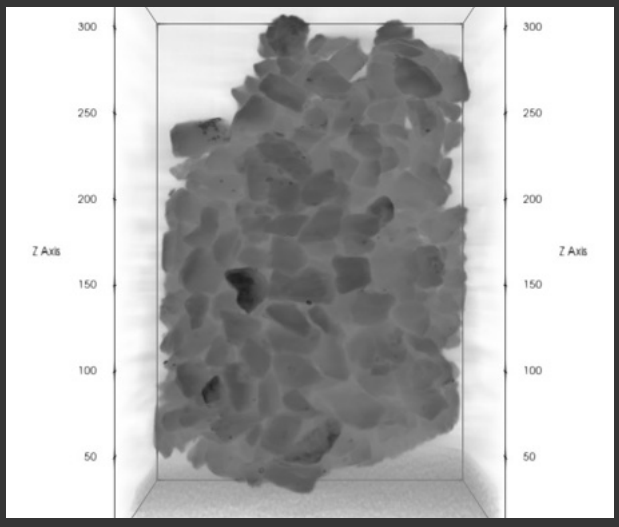
X-ray CT experiments

The specimen is placed in front of an X-ray source, mounted on a rotating table.

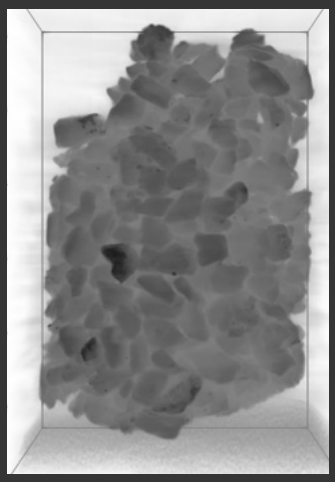
Projections at small increments of rotation are captured on a detector.



X-ray CT experiments

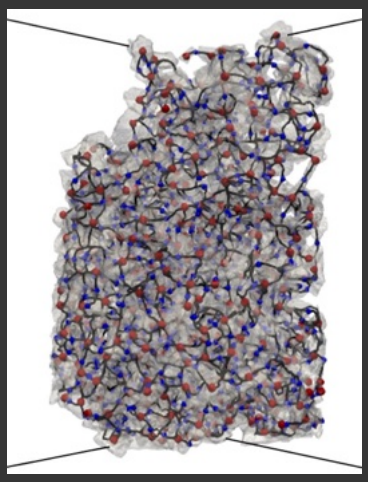


MorseGram: Segmentation and Fabric Quantification of Granular Materials



CT- image

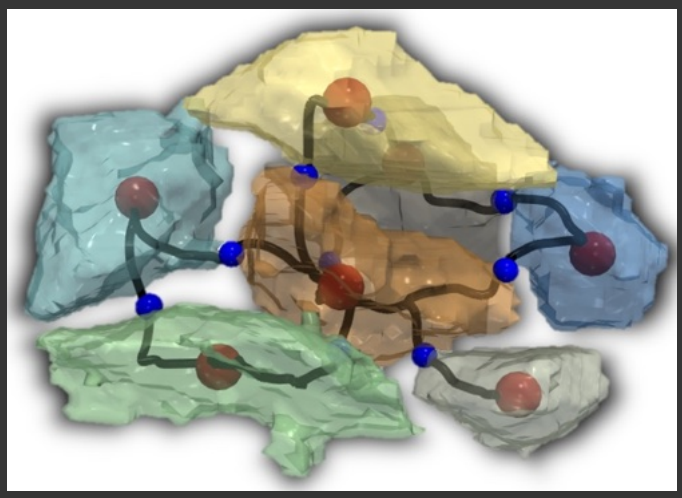
Grain segmentation

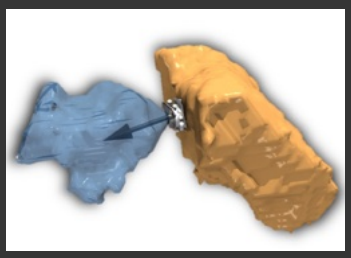


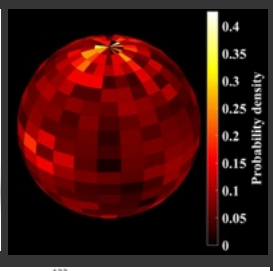
Contact Network

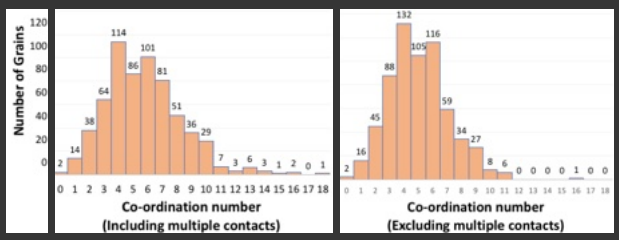
[K Pandey, T BinMasood, S Singh, I Hotz, V Natarajan, TG Murthy. Morse theory-based segmentation and fabric quantification of granular materials. Granular Matter, 24:1–20, 2022.]

MorseGram: Segmentation and Fabric Quantification of Granular Materials





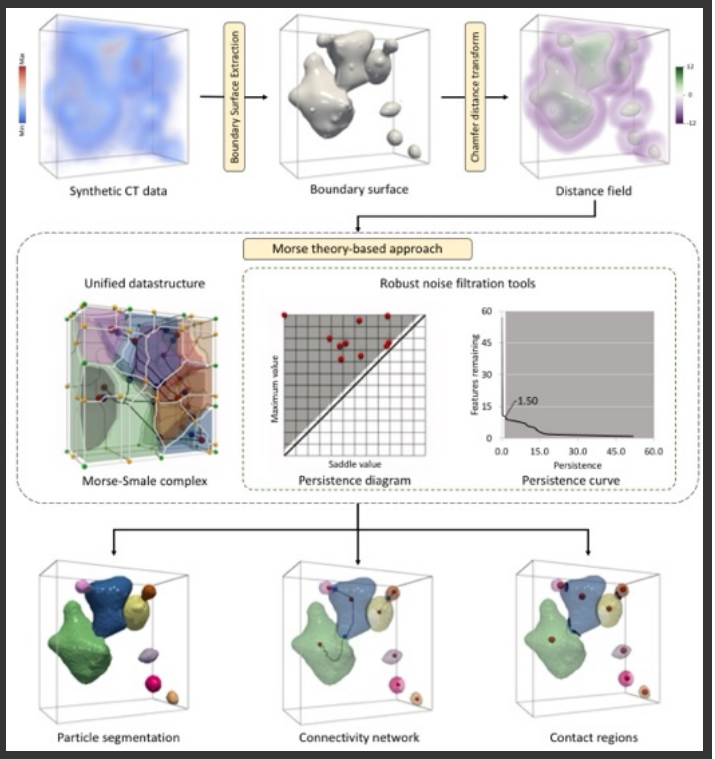




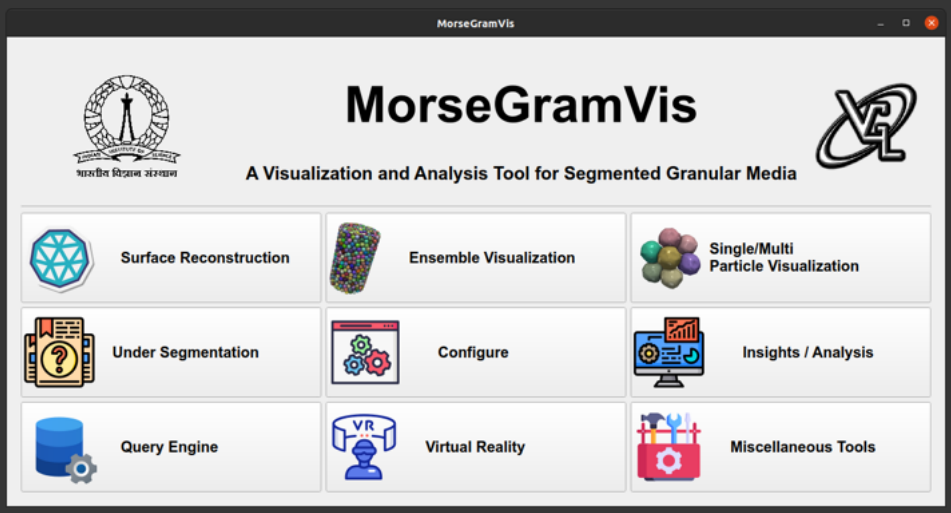
[K Pandey, T BinMasood, S Singh, I Hotz, V Natarajan, TG Murthy. Morse theory-based segmentation and fabric quantification of granular materials. Granular Matter, 24:1–20, 2022.]

MorseGram - pipeline

- Bounding surface computation based on an automatically determined bi-modal threshold and a local active contour-based refinement.
- Signed distance field-computation
- MS complex extraction for distance field (multi-scale).
- Persistence curve used to determine simplification threshold
- Segmentation is computed and reported as the descending manifolds of the maxima in the simplified complex.
- The connectivity network is computed as the collection of ascending 1-manifolds of 2-saddles and the contact region is computed by pruning the descending 2-manifold of the 2-saddles



MorseGramVis – Open-Source Software



[D Rathod. MorseGramVis: A visualization and analysis tool for segmented granular media. Masters thesis, Indian Institute of Science Bangalore, Department of Computer Science and Automation, 2023]