The Topology ToolKit

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  - video will be posted at `https://westgrid.github.io/trainingMaterials` under one of the top-menu topics
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Today's topic

- Topological data analysis (TDA) can be very useful in analyzing complex multi-dimensional datasets – examples in the next slide
  - filter out features by their persistence value
  - domain segmentation
  - topological simplification
- I have zero background in topology / TDA

⇒ Let's approach this from a non-topologist / research scientist perspective

⇒ Our today's goal is not to learn topology, but to look at an open-source TDA tool that is integrated with VTK and ParaView

Topology-based analysis

This slide is based on Attila Gyulassy's introductory topology tutorial (U. of Utah)

- Measurable topological attributes:
  - measurement of connectedness: pick any two points + find an inside path to connect them
  - count non-contractable cycles: pick a closed loop inside that you can't squeeze down to a point
  - and many others
- Applications in:
  - molecular analysis: e.g. pick up atomic bonds, atoms from the 3D electronic probability density
  - materials analysis: porosity measurement, battery design, defect identification, cavity deformation
  - neural pathways (connectomics)
  - CFD: turbulence and vorticity, buble formation rate, ocean eddies
  - combustion analysis: ignition kernels
  - geological features
  - image segmentation
- Phenomenon of interest in a scalar field in the data $\Rightarrow$ derive its measurable topological equivalent or abstraction

Persistence intervals of a 1D scalar function

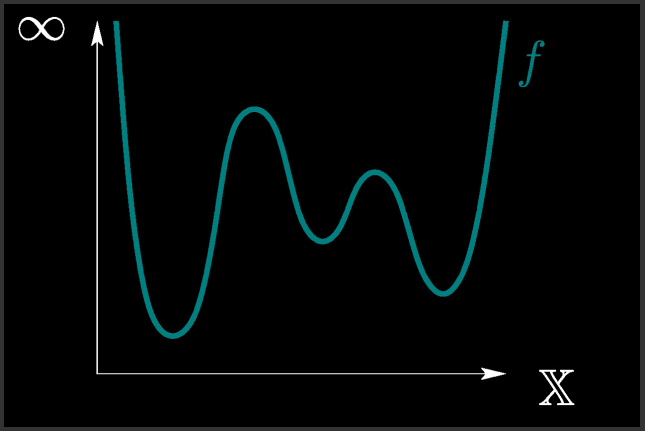

Figure copied from David Cohen-Steiner's slides on Topological Persistence

- Evolution of the topology of connected components during a filtration from $-\infty$ to $+\infty$
- Pair thresholds (critial points) that create components with those that destroy them
- Component persistence = difference in function value between component's birth and death

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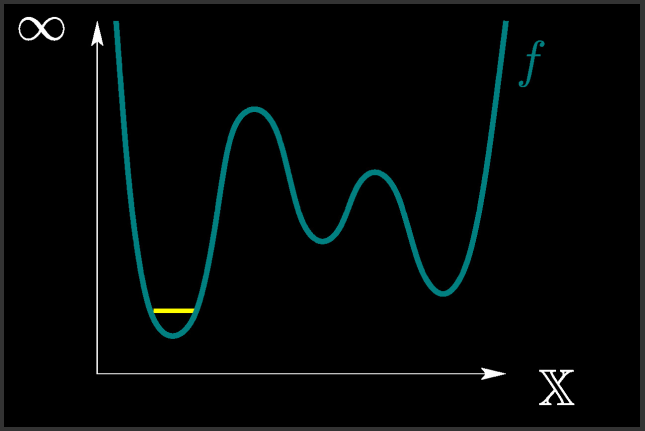

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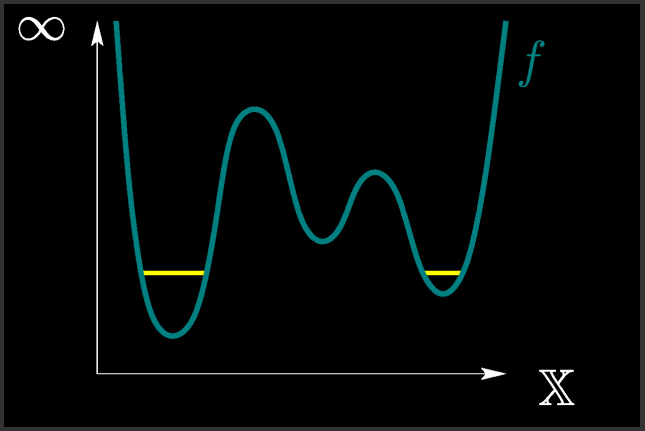

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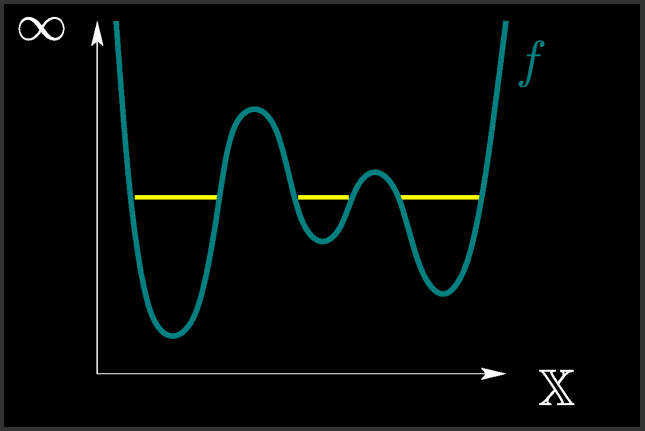

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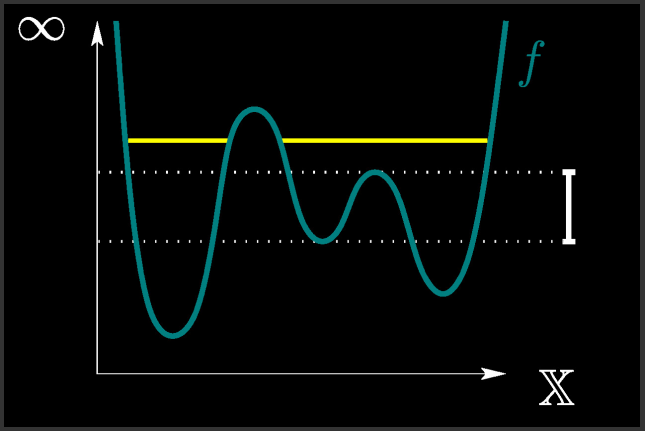

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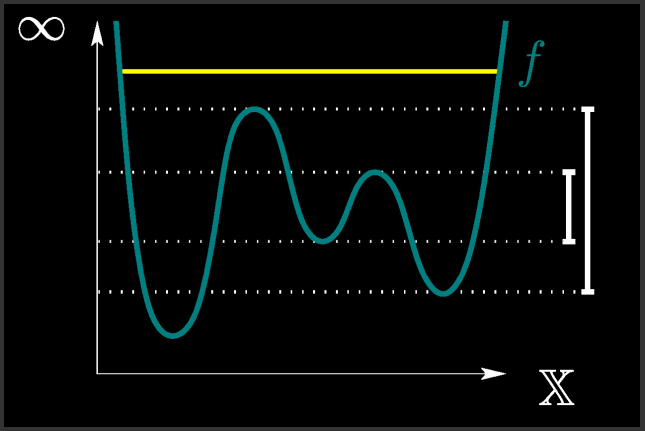

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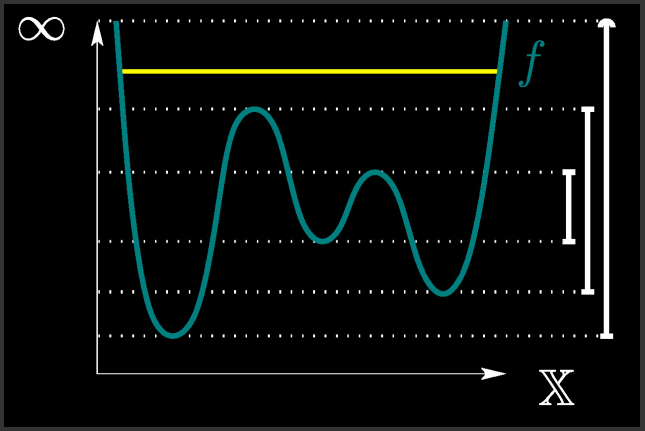

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Persistence diagram

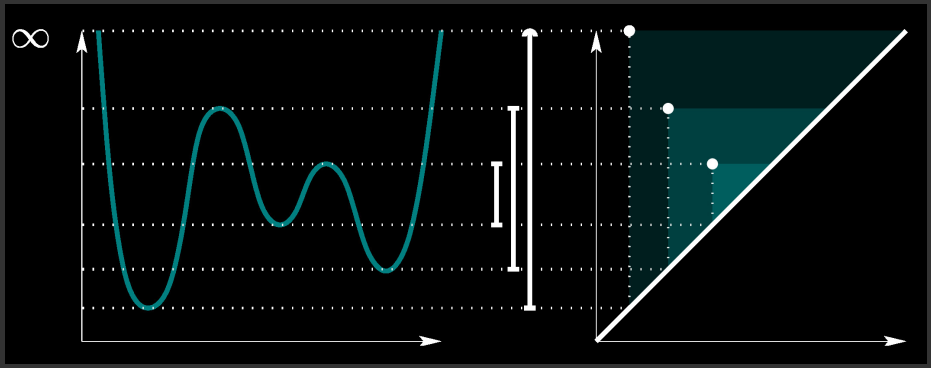
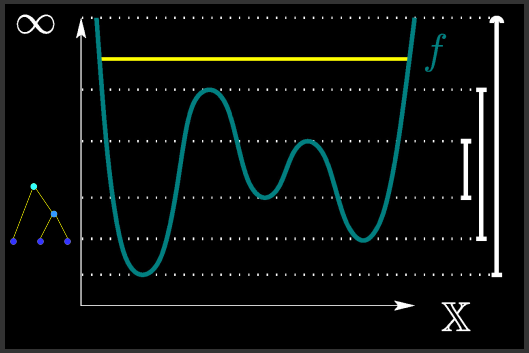
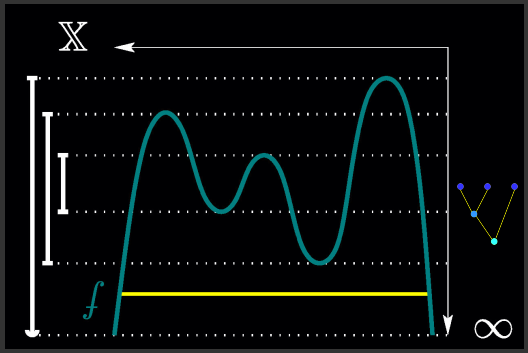


Figure copied from David Cohen-Steiner's slides on Topological Persistence

- Persistence diagram: x = function value at feature's birth, y = function value at feature's death
- Small features are mapped closer to the diagonal
- Critical points in 1D: minima and maxima
- Domain segmentation (monotone regions) between critical points, based on the gradient sign
- Mountains = monotone pieces around maxima, basins = monotone pieces around minima





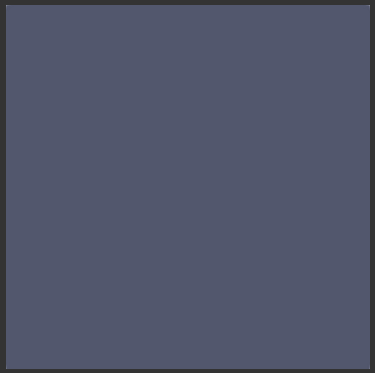
- Join tree of connected components
- Leaves correspond to minima

- Split tree of connected components
- Leaves correspond to maxima

In TTK you can easily:

1. compute persistence diagrams and persistence curves
2. apply a filter to build a tree; areas attached to the leaves have RegionType = 1
3. perform topological segmentation: subdivide domain into (e.g.) monotone regions
4. perform topological simplification: delete some leaves, typically below some threshold persistence

Scalar function in 2D



- Sweep in function value from $-\infty$ to $+\infty$
- Coloured regions shows the subdomain with function value lower than the sweep value
- This time single component with multiple holes that
  - split at the saddles
  - disappear at the maxima
- Critical points in 2D: minima, maxima, and saddle points
- Domain segmentation (monotone regions) between integral lines (orthogonal to the contours), based on the gradient sign
- Same definition for mountains and basins, but there are also ridge lines and valley lines

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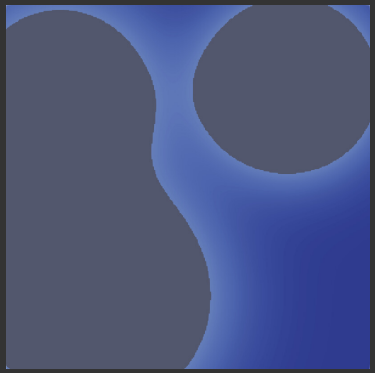

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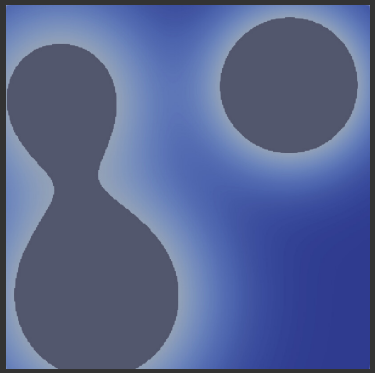

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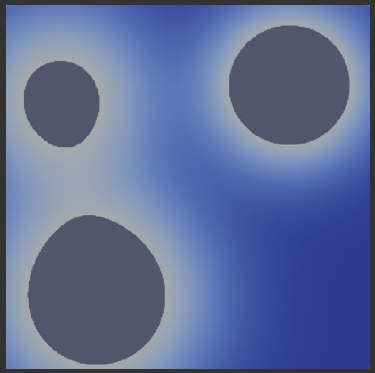

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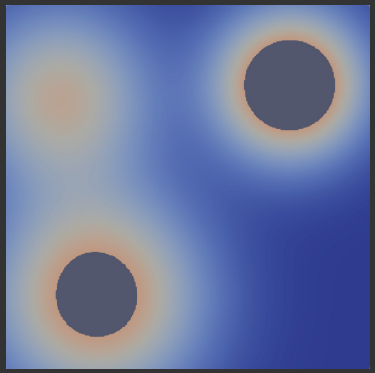

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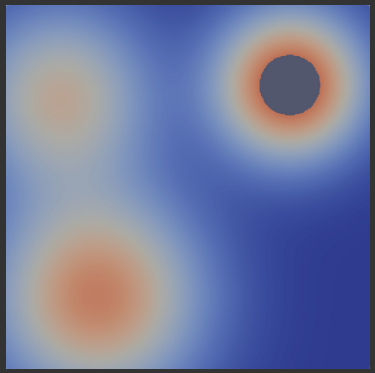

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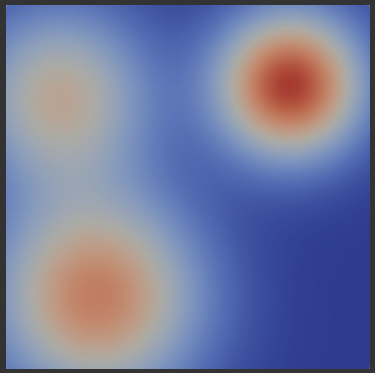

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Scalar function in 3D

- The topology becomes more complex
- 4 types of critical points: minima, maxima, and two kinds of saddles
  - 1-saddles are located between 2 minima, 2-saddles are located between 2 maxima
- Domain segmentation (monotone regions) between integral surfaces, based on the gradient sign
- Monotone regions combined into mountains and basins, with ridge lines and valley lines and saddle connector lines, ridge surfaces (separating the mountains) and valley surfaces (separating the basins)

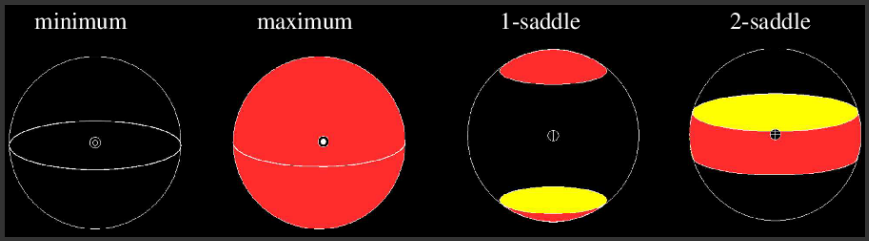


Figure copied from Guoning Chen's slides on Morse-Smale Complex

TTK = the Topology ToolKit

- Toplogical analysis of multi-dimensional scalar functions
- `https://topology-tool-kit.github.io`
  - great documentation, many tutorials and step-by-step videos
- Open source, development since 2014, first public release in 2017
- Lead author Julien Tierny + active development community
- Some workflows in this presentation were taken from the excellent half-day TTK tutorial at IEEE VIS 2020
- Interfaces:
  - pure C++
  - VTK/C++ (∼3X shorter code)
  - ParaView Python (∼5X shorter code) and ParaView plugin

Installing TTK

Compilation instructions `https://topology-tool-kit.github.io/installation.html`

Here is what I did on my Macbook:

1. Create Python 3.7 (older than my default!) environment and install scikit-learn and vtk==8.2.0
2. Install latest Qt with Homebrew into `/usr/local`
3. Download/copy Intel's Threading Building Blocks library to `/opt/local/{lib,include}`
4. Download ParaView 5.6.1 and TTK 0.9.8
5. Apply TTK patch to ParaView's source code (only available up to 5.6)
6. Compile ParaView with TBB and Qt5
   - ParaView compile scripts were selecting the default system's Qt $\Rightarrow$ ParaView was hanging on startup
   - had to specify `-DQt5_DIR=/usr/local/Cellar/qt/5.15.1/lib/cmake/Qt5`
7. `export PV_PLUGIN_PATH=/usr/local/lib/plugins`
8. Compile TTK (showing the difficult flags only)

```
-DParaView_DIR=~/ttk/ParaView-v5.6.1/build
-DTTK_INSTALL_PLUGIN_DIR=/usr/local/lib/plugins
-DPYTHON_NUMPY_INCLUDE_DIR=~/miniconda/envs/p37/lib/python3.7/site-packages/numpy/core/include
-DPYTHON_INCLUDE_DIR=/Users/razoumov/miniconda/envs/p37/include/python3.7m
-DPYTHON_LIBRARY=/Users/razoumov/miniconda/envs/p37/lib/libpython3.7m.dylib
-DTTK_ENABLE_SCIKIT_LEARN=ON
-DQt5_DIR=/usr/local/Cellar/qt/5.15.1/lib/cmake/Qt5
```

Running TTK in Docker: alternative, painless solution

An easy way to use TTK without manual compilation of TTK, ParaView, and their dependencies

1. Install Docker Desktop (Linux, Mac, Windows) and run a pre-built Docker image with `pvserver` + TTK on local port 11111

```
docker run -it --rm -p 11111:11111 -v "$HOME:/home/`whoami`/" --user $UID \
       topologytoolkit/ttk:5.6.1-stable

docker run -it --rm -p 11111:11111 -v "$HOME:/home/`whoami`/" --user $UID
       topologytoolkit/ttk:5.8.1-dev
```

2. Launch a ParaView client (same major version!) on your laptop and connect to port `localhost:11111`
   - all your server-side TTK plugins will be available on the client!

Later in this webinar I will demo running client-server ParaView + TTK from a Singularity container on Cedar

Scalar function in 2D

Toy data similar to `https://topology-tool-kit.github.io/persistentHomologyDummies.html`
On presenter's notebook `~/ttk/mydata/multiGaussianAnalysis.pvsm`

Let's create some toy data: three 2D Gaussians $f(\vec{r}) = e^{-\frac{|\vec{r}-\vec{r}_0|^2}{2\sigma^2}}, \quad \vec{r} \in \mathbb{R}^2$

1. Apply Sources | **Plane** at 100^2 resolution, turn on the Axes Grid
2. Apply three successive **Python Calculator**s with three Gaussians

```
p1 = exp(-((inputs[0].Points[:,0]-0.28)**2+(inputs[0].Points[:,1]-0.28)**2)/(2*0.02))
p2 = 0.8*exp(-((inputs[0].Points[:,0]+0.25)**2+(inputs[0].Points[:,1]+0.3)**2)/(2*0.04))
p3 = 0.6*exp(-((inputs[0].Points[:,0]+0.35)**2+(inputs[0].Points[:,1]-0.25)**2)/(2*0.03))
```

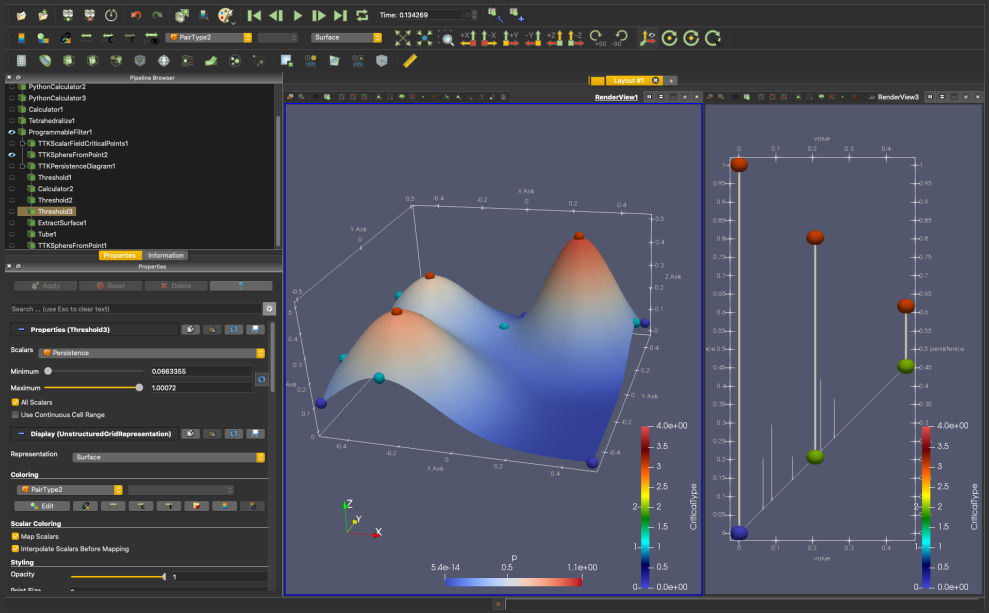
3. Apply non-Python Calculator `p=p1+p2+p3`
4. Apply **Tetrahedralize** to triangulate the plane (we'll use these triangles to generate the 3D terrain)
   - WarpByScalar is fast but produces inaccurate results for topological analysis
5. Apply **ProgrammableFilter** with

```
output.Points[:,2] = 0.5*inputs[0].PointData["p"]          # set the output's z-axis
output.PointData.append(inputs[0].PointData["p"], "p")     # add the data array 'p' to our output
```

6. To ProgrammableFilter apply **TTKScalarFieldCriticalPoints**
7. Apply **TTKSphereFromPoint**, set Radius, colour by CriticalType

Scalar function in 2D (cont.)

8. Create a new render view
9. Apply **PersistenceDiagram**, check Axes Grid, edit X Title = value, Y Title = persistence
   - we'll use its output variables PairIdentifier, PairType, and Persistence
10. Apply **Threshold** on PairIdentifier, keep only non-negative
11. Apply **Calculator** on CellData with PairType2 = abs(PairType)
    - we want to get rid of the "spurious" pairs created by boundary points, i.e. keep PairType=$\pm$1
    - PairType=-1 is the largest persistence pair, PairType=0 are spurious/edge pairs (want to exclude these), PairType=1 are the real internal pairs
12. Apply **Threshold** on PairType2, keep only PairType2=1
13. Apply **Threshold** on Persistence, keep all values for now
14. Show the diagonal
15. Apply **ExtractSurface** and then **Tube**
16. To last Threshold apply **TTKSphereFromPoint**, set Radius, colour by CriticalType



Now apply **Threshold** to ProgrammableFilter, vary its *min* value, and check for connected components

Topological simplification on 2D scalar function

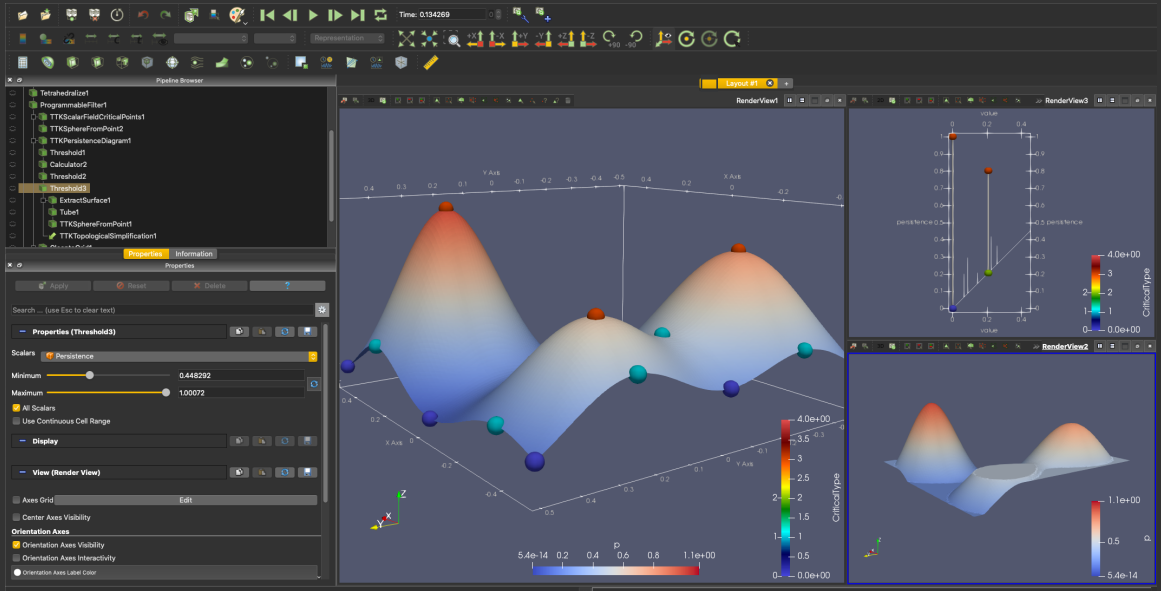
On presenter's notebook `~/ttk/mydata/multiGaussianSimplification.pvsm`

1. Start with the last pipeline `~/ttk/mydata/multiGaussianAnalysis.pvsm`
2. Open a new render window
3. To ProgrammableFilter apply **CleanToGrid**
4. Apply **TTKTopologicalSimplification** with 2 inputs: Domain = CleanToGrid, Constraints = the last Threshold, scalar field = `p`, check Numerical Perturbation
5. Apply **ProgrammableFilter** (WarpByScalar does not work here)

```
output.Points[:,2] = 0.5*inputs[0].PointData["p"]
output.PointData.append(inputs[0].PointData["p"], "p")
```

6. Colour by `p`
7. Modify persistence range (set min=0.45) in the last Threshold

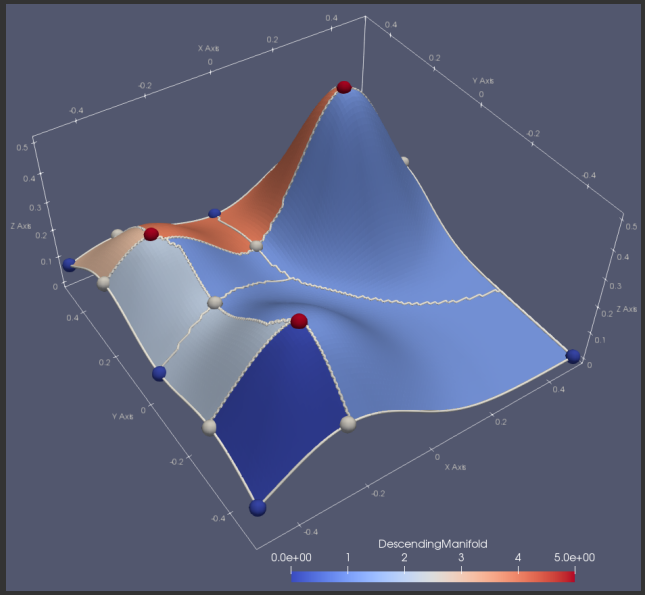
Topological simplification on 2D scalar function (cont.)



Extracting the TTK Morse Smale Complex from a dataset

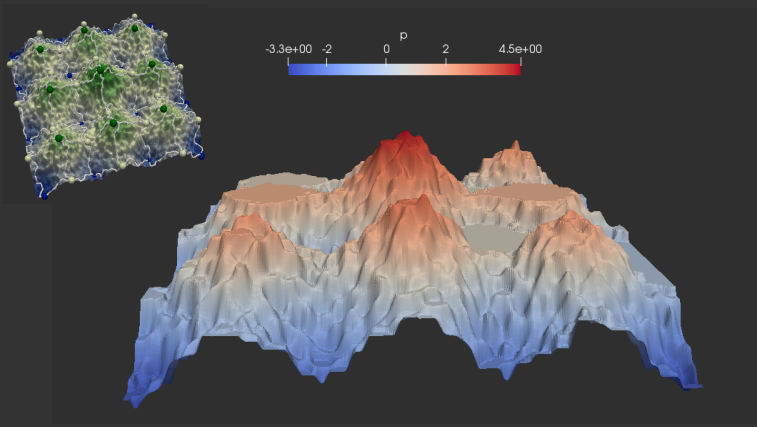
TTKMorseSmaleComplex filter provides information about critical points and separatrices that link these points $\Rightarrow$ segmentation of the dataset

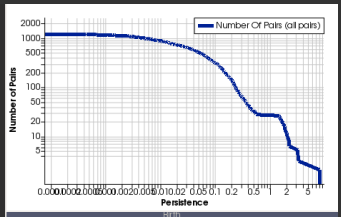
1. Load just the 2D function `multiGaussianOnly.pvsm`
2. To ProgrammableFilter apply **TTKMorseSmaleComplex**
3. To Critical Points apply **TTKSphereFromPoint**, colour by CellDimension
4. To 1-Separatrices apply **ExtractSurface** and then **Tube**
5. Colour Segmentation by AscendingManifold or DescendingManifold

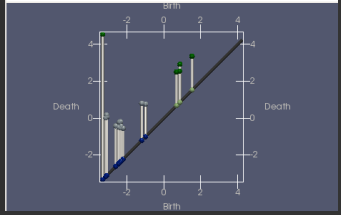


Noisy 2D terrain

- TTK cover visualization: example from TTK tutorials
  `ppp --state=ttk/ttk-data-0.9.8/states/morsePersistence.pvsm`
- Flat plateau on the persistence curve separating noise from the data
- To show the result of topological simplification with the 3D surface, apply **ProgrammableFilter** to the output of TTKTopologicalSimplification making sure to pass `Blend` variable

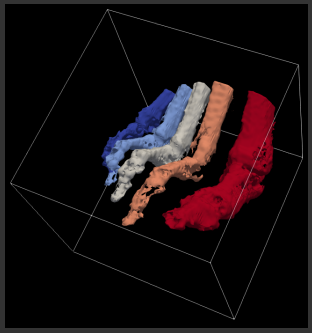






3D scalar field segmentation

This slide is based on Charles Gueunet's "3D foot segmentation" tutorial (Kitware)



1. Load the 3D scan of a human foot `ttk_tutorial_data/foot.vti`
   - load only Scalars field, switch to volumetric rendering
2. Locate 5 largest persistence pairs
   - apply **TTKPersistenceCurve**, close all panes but one
   - show only saddle-maximum pairs
   - uncheck Use Index For XAxis, X Array Name = Persistence (x-axis)
   - Series Parameters = Number Of Pairs (y-axis)
   - check Left Axis Log Scale
   - if want to keep 5 pairs $\Rightarrow$ need to use persistence = 187
3. Use topological simplification on the persistence diagram to extract only 5 maxima
   - open a new render view
   - apply **TTKPersistenceDiagram** to the original data
   - apply **Threshold** on Persistence, click reset, remove all the pairs below 187
4. Remove the diagonal in the persistence diagram
   - apply **Threshold** on PairIdentifier, click reset, remove all negative pairs (min=0)

   $\Rightarrow$ 5 vertical lines

3D scalar field segmentation (cont.)

5. Optionally beautify our persistence diagram
   - add the axes, apply **ExtractSurface** and then **Tube**
6. Perform Topological simplification on the 3D scalar field
   - apply **TTKTopologicalSimplification** with 2 inputs: Domain = foot.vti, Constraints = the first Threshold

   $\Rightarrow$ now we have a new version of the foot: no visual difference, but the small noise has been removed

   $\Rightarrow$ we want to extract bones, identify toes $\Rightarrow$ need to show areas attached to maxima $\Rightarrow$ use a merge tree
7. Compute the split tree of the maxima
   - click on TTKTopologicalSimplification
   - apply **TTKMergeandContourTreeFTM** (FTM = Fibonacci Task-based Merge tree), in Output Options set Tree Type = Split Tree

   $\Rightarrow$ we get 5 leaves = toes
8. Attach 3D regions to the leaves
   - click on Segmentation output of the tree in the browser
   - apply **Threshold** on Region Type keeping only the value of 1 (regions attached to the leaves)
9. Beautify the segmented regions
   - apply **ExtractSurface** and then **TTKGeometrySmoother**
   - optionally apply **GenerateSurfaceNormals** to provide smooth shading of the dataset

More complex version of this pipeline:

```
cd ~/ttk/ttk_tutorial_data && ppp --state=tutoSegmentation.pvsm
```

3D scalar field segmentation: same algorithm, simpler dataset

On presenter's notebook `~/ttk/mydata/stvol.pvsm`

Discretized 3D Styblinski-Tang function inside a unit cube ($x_i \in [0, 1]$)

$$f(x_1, x_2, x_3) = \frac{1}{2} \sum_{i=1}^{3} (\xi_i^4 - 16\xi_i^2 + 5\xi_i), \text{ where } \xi_i \equiv 8(x_i - 0.5)$$

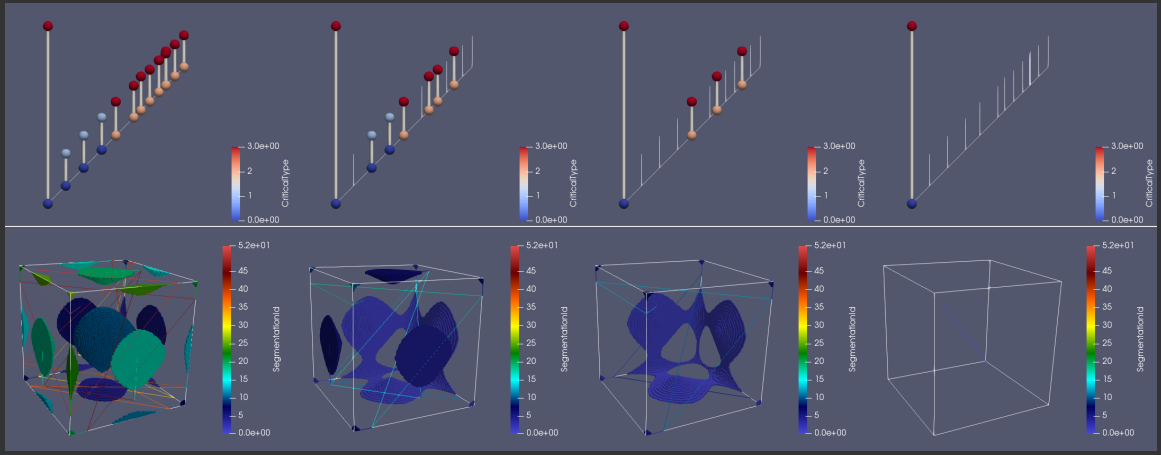
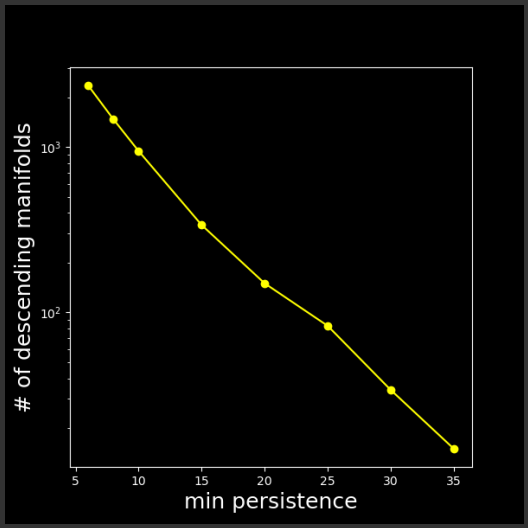


Image segmentation using topological persistence

- Area of active research
- Use TTK as a computational tool to test your ideas
- TTK sample datasets include one example
- I modified the workflow: simplied, added a persistence curve – let's take a look at the algorithm




```
cd ~/ttk/mydata
ppp --state=imageProcessingModified.pvsm
```

Image segmentation using topological persistence (cont.)

Let's apply the same technique to another image

1. Copy `imageProcessingModified.pvsm` into a new state file
2. Edit it, replacing (2X) `naturalImage.png` with your new image's name
   - here we'll use a scaled-down aurora image from `https://en.wikipedia.org/wiki/Image_segmentation`
3. Load your new state file into ParaView
4. Modify (1) the persistence min/max thresholds and (2) the colour range in the segmented image

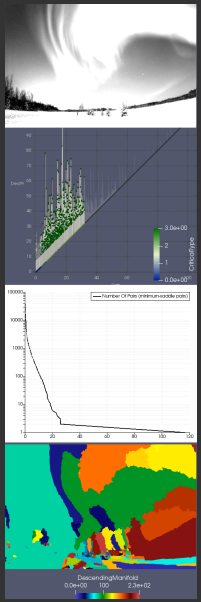


Image segmentation using topological persistence (cont.)

- In the previous two examples the key was to use the PNG image's (which filter?) gradient as the scalar function
- This *won't work* for all images, so it is your task as a researcher to find a better scalar function, to be used for topological image segmentation
- Active research area

Image segmentation using topological persistence (cont.)

- In the previous two examples the key was to use the PNG image's (which filter?) gradient as the scalar function
- This *won't work* for all images, so it is your task as a researcher to find a better scalar function, to be used for topological image segmentation
- Active research area

- More complex example from TTK tutorials: cell enumeration in confocal microscopy, based on the example from Herbert Edelsbrunner's and John Harer's book "Computational Topology: An Introduction", AMS (2009)

```
cd ~/ttk/ttk-data-0.9.8 && ppp --state=states/tribute.pvsm
```

  - very noisy input image
  - different scalar function

Running client-server ParaView + TTK via Singularity on Cedar

1. Build ParaView 5.6.2 + TTK Docker in Ubuntu 20.04 image on Cedar
   `https://docs.computecanada.ca/wiki/Singularity`

```
$ cd ~/scratch
$ wget https://raw.githubusercontent.com/moby/moby/\
    master/contrib/download-frozen-image-v2.sh
$ sh download-frozen-image-v2.sh build \
    topologytoolkit/ttk:5.6.2-stable   # download an image from Docker Hub into build/
$ cd build && tar cvf ../topologytoolkit.tar * && cd ..
$ salloc --mem-per-cpu=3600 --cpus-per-task=2 --time=0:15:0 --account=...
$ module load singularity
$ singularity build topologytoolkit562.sif \
    docker-archive://topologytoolkit.tar   # build the Singularity image
$ /bin/rm -rf build topologytoolkit.tar
```

- TTK source code includes scripts for building Docker and Singularity images from scratch
- alternatively can use topologytoolkit/ttk:5.8.1-dev to build topologytoolkit581.sif
  (it did not work for me ...)

Running client-server ParaView + TTK via Singularity on Cedar (cont.)

2. Start ParaView server on a compute node

```
$ cd ~/scratch
$ salloc --mem-per-cpu=3600 --time=0:30:0 --account=...
$ module load singularity
$ singularity run -B /home -B /scratch topologytoolkit562.sif pvserver
```

3. Connect from the ParaView client on your computer

```
$ ssh cedar.computecanada.ca -L 11111:cdr768:11111
start ParaView 5.6.x on your computer and connect to localhost:11111
File | Load State - local ~/ttk/ttk-data-0.9.8/states/dragon.pvsm
Choose File Names - remote cedar:/scratch/razoumov/dragon.vtu
```

Questions?