Habilitation à Diriger les Recherches

Université de Bordeaux, Ecole Doctorale Mathématiques et Informatique
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« Scientific Visualization to Enhance Understanding of Simulation Data »

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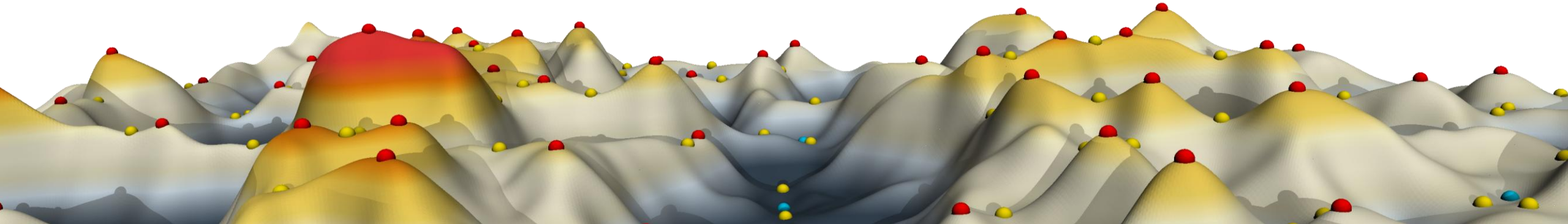
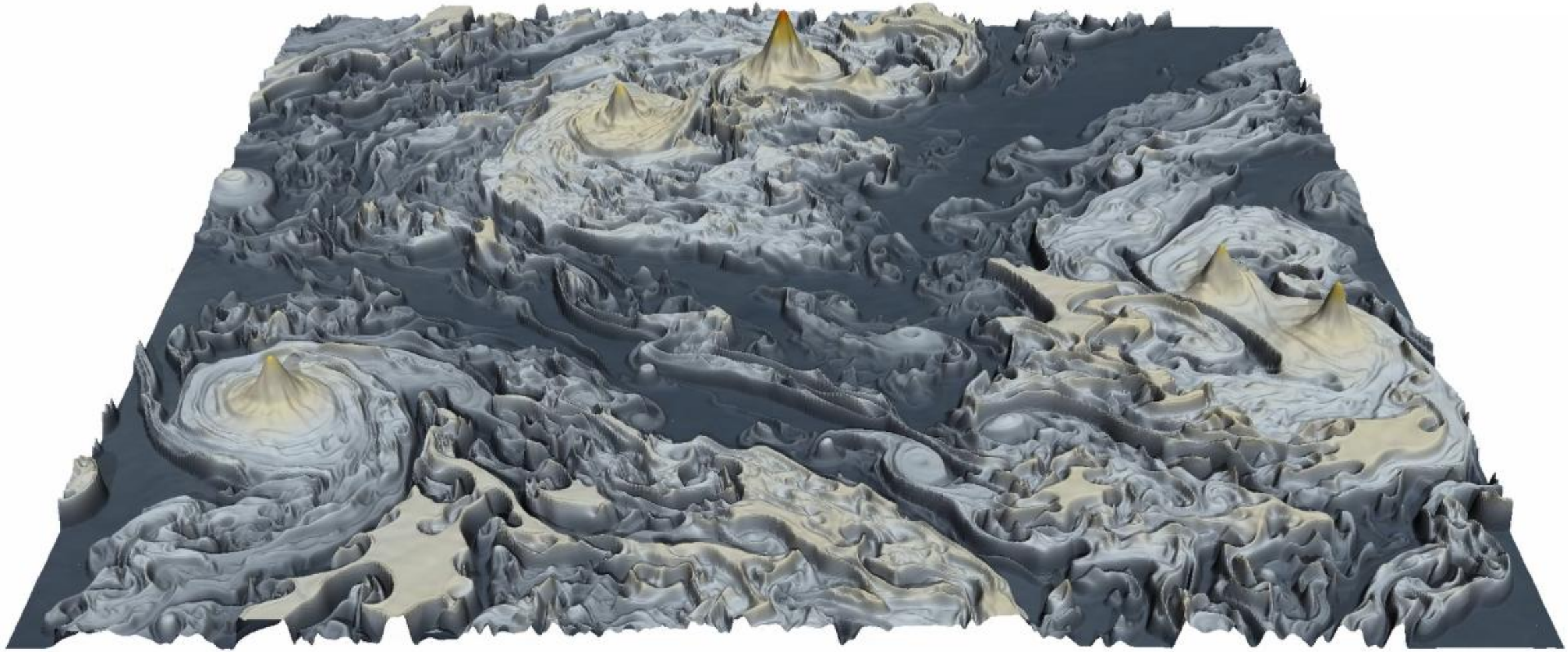
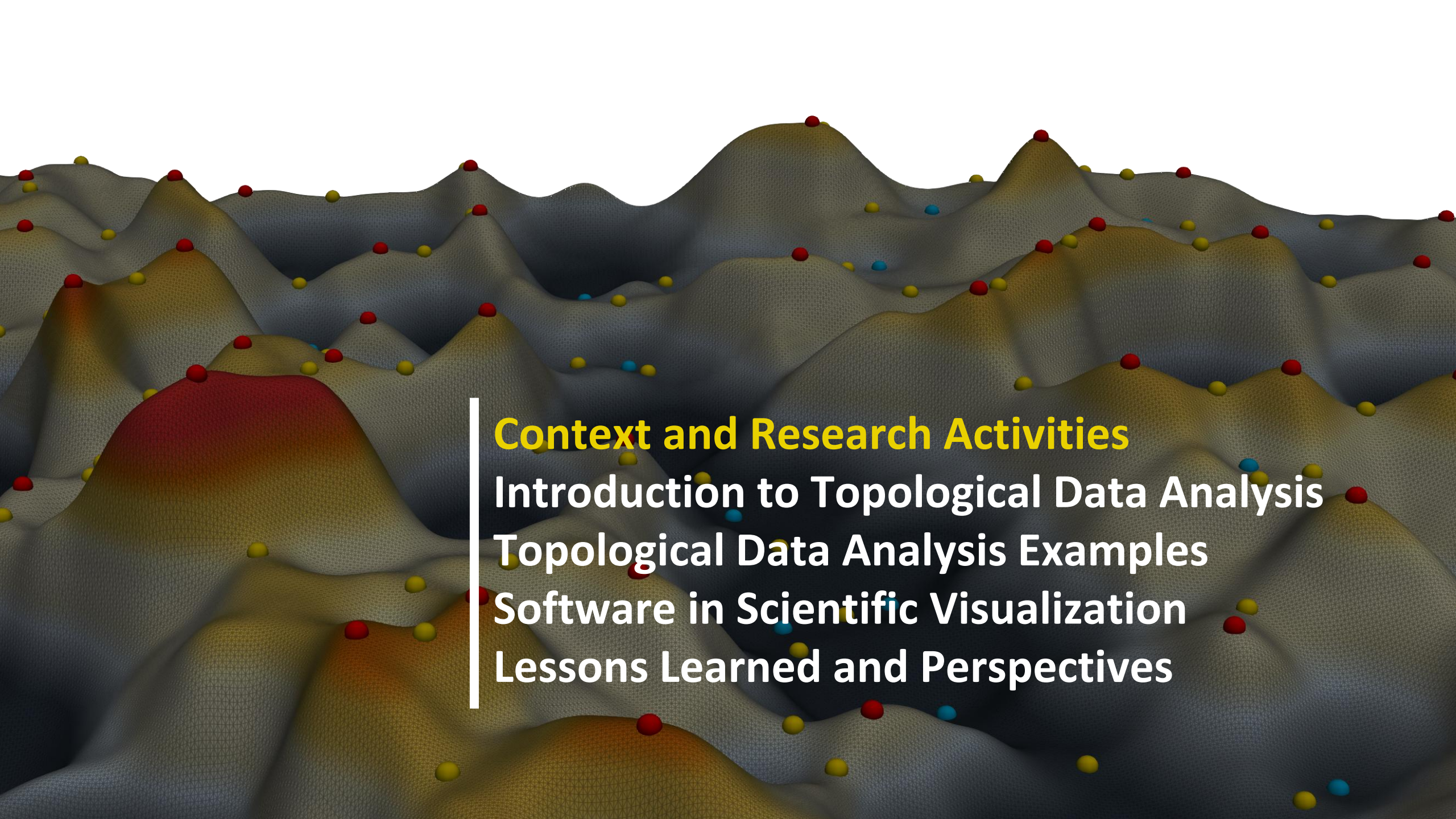




“Exploring, interpreting and communicating simulation data to better understand complex physical phenomena.”



Context and Research Activities

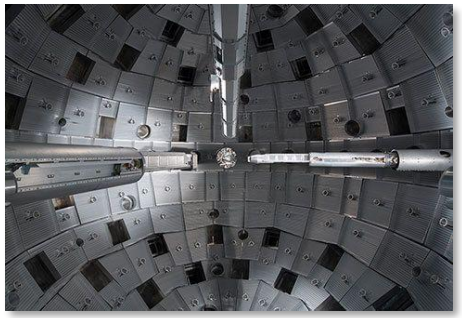
Introduction to Topological Data Analysis

Topological Data Analysis Examples

Software in Scientific Visualization

Lessons Learned and Perspectives

Simulations and Exascale Computing



Deluge of data

- Large Experimental Facilities (NIF, LMJ …)
- High Performance Computing (El Capitan, EXA1-HE …)

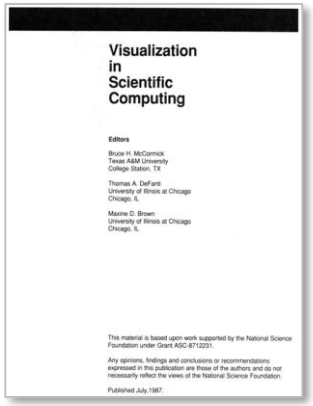
Many domains

- Material sciences, fusion energy, computational biology, turbulent combustion, hypersonic flow …

Many initiatives and investments

- US : Advanced Simulation and Computing Program (ASCR)
- EU : European High Performance Computing Joint Undertaking (EuroHPC)
- FR : CEA Simulation Program

Scientific Visualization of Complex Data


Visualization in Scientific Computing

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Published July 1987.

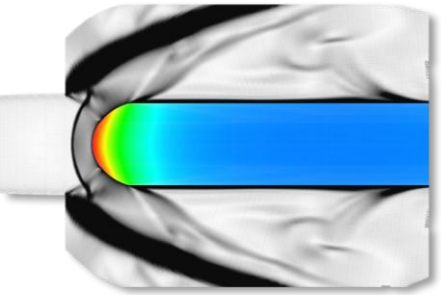
"Visualization in Scientific Computing can bring enormous leverage to bear on scientific productivity and the potential for major scientific breakthroughs, at a level of influence comparable to that of supercomputers themselves." [MD87]

Interdisciplinary field

- Methods for transforming and generating visual representations of complex data
- Many strategies : in-situ, topological and statistical methods, multiresolution …
- Many goals : *discover, understand, compare, debug, communicate, capitalize, train, convince* ...

Unlocking scientific understanding

- Groundbreaking decision-making (robustness, uncertainty, interpretability)
- Powered by new technologies (HPC, AI, XR …)
- Equitable and intuitive ways of communication



[MD87] B.Mc Cormick, T. De Fanti and M.Brown. *Visualization in Scientific Computing* Report of the NSF Advisory Panel on Graphics, Image Processing and Workstations, 1987

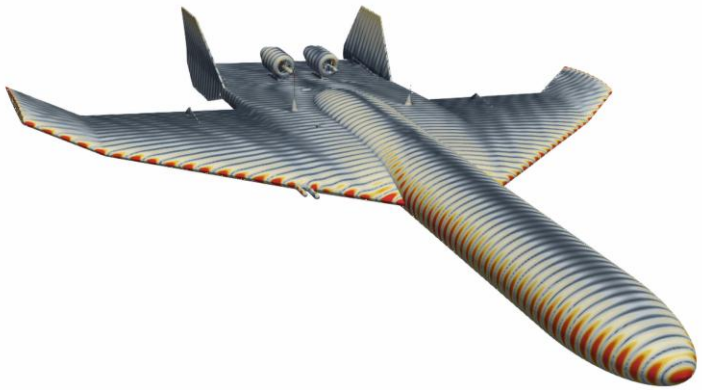
Data Analysis Challenges

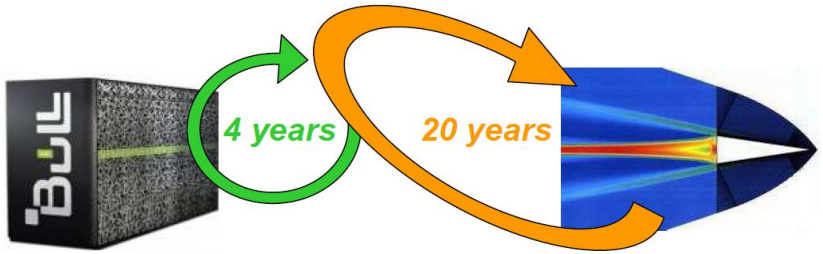
Data complexity

- Noise everywhere
- Origin : multi-physics, multi-scale, multi-user ...
- Dimensions : 1D, 2D, 3D, time-dependent ...
- Number : multivariate, parametric study ...
- Volume : trillions of cells or particles …

Data Environment

- Domain specific I/O requirements
- Remote supercomputers from the production site
- Differing lifecycles for software and hardware





My Research Goals

Better understanding of the physics

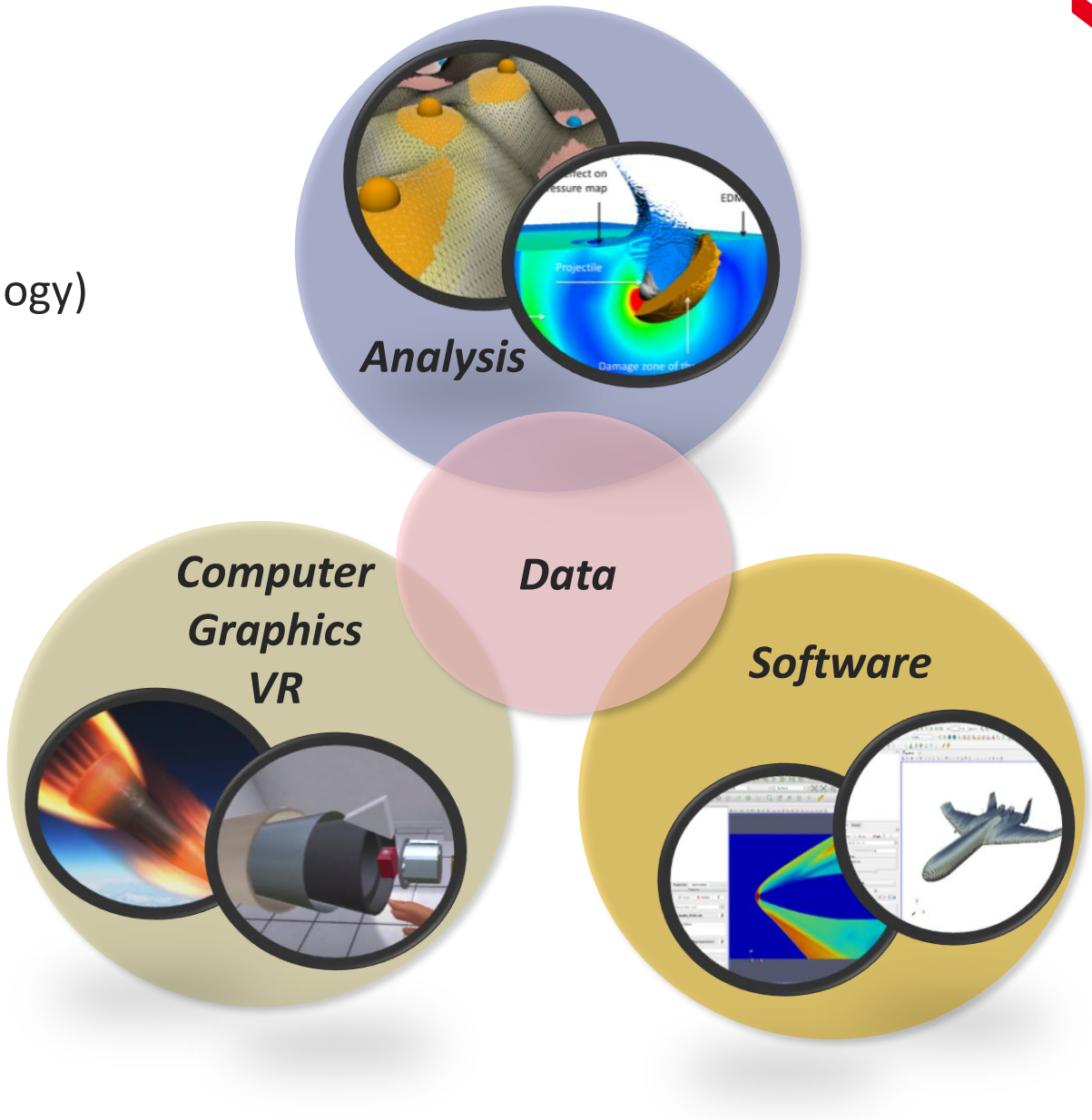
- Domain specific data analysis
- Visual abstractions (multiresolution, topology)
- Provide meanigful visualization

Better communication of the physics

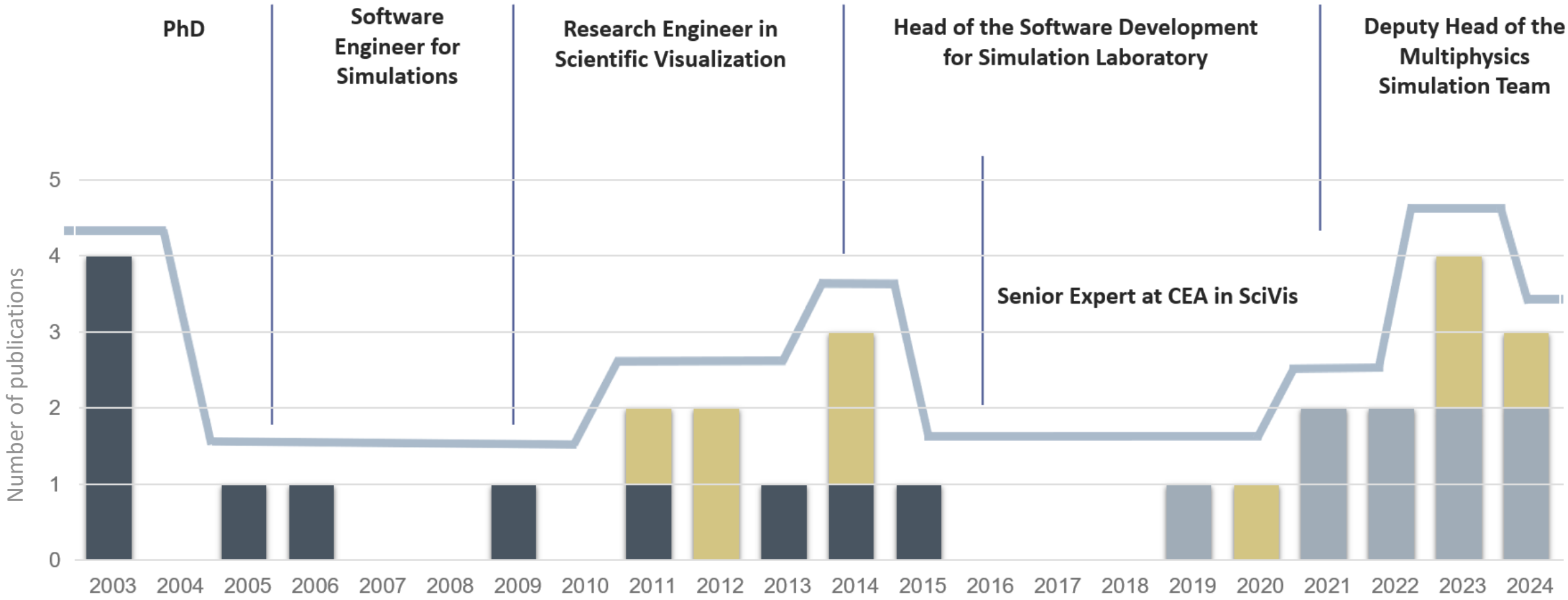
- Storytelling for interdisciplinarity
- Computer graphics and virtual reality (VR)

Optimize research engineering time

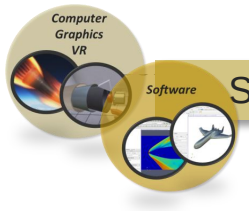
- Provide end-users tools
- Support and teach data analysis



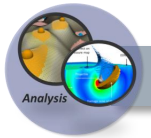
Positions at CEA and Publications



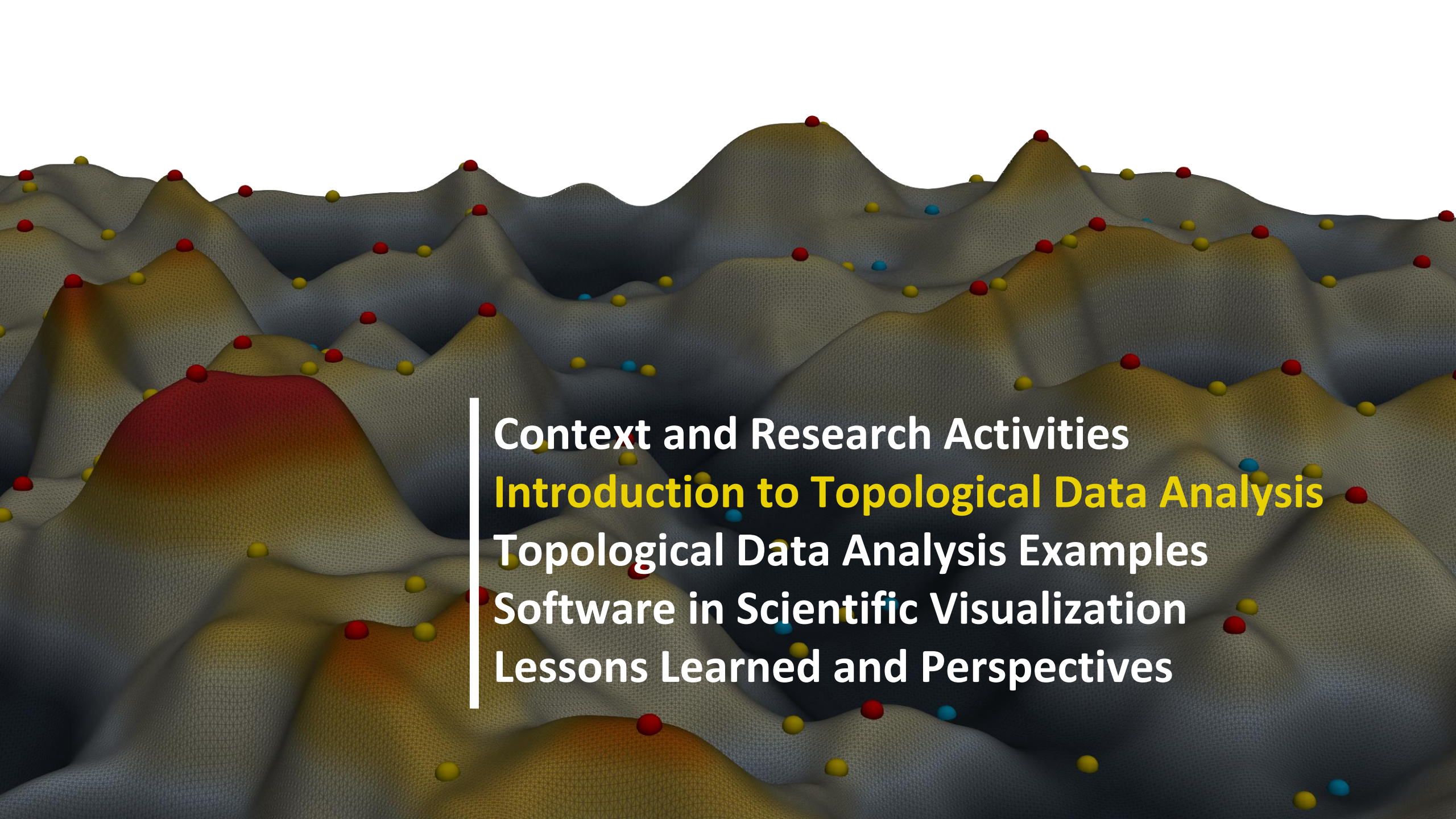
Multiresolution



Software and virtual reality



Topological data analysis



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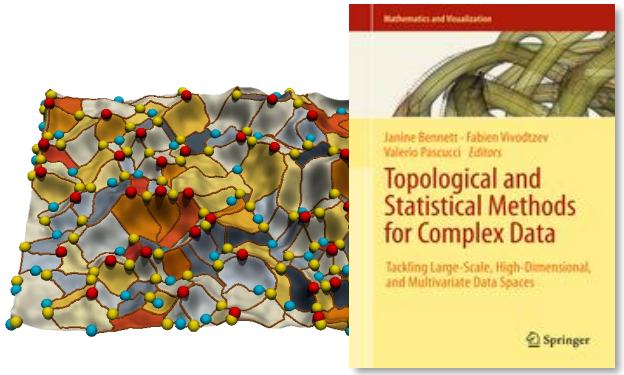
Topological Data Analysis (TDA)

TDA studies the structure of complex data

- Theories and algorithms for multi-scale representations and analysis of structural features
- Measurable topological attributes : connectedness, non-contractable cycles, invariant …

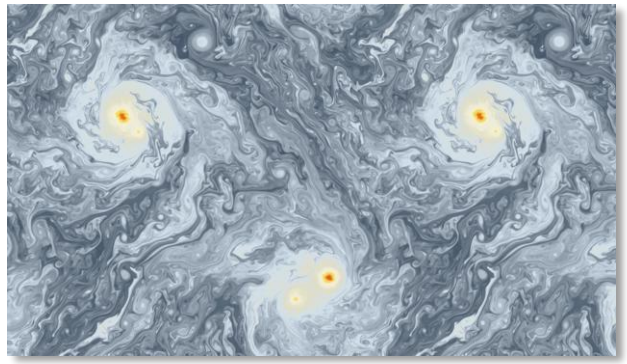
Many fields of application

- Materials science: porosity, deformation …
- Computational Fluid Dynamics : turbulence, vortex tracking …
- …



Why investigating TDA ?

- Independent from the geometrical description
- Stable and robust to noise
- Efficient on a unique dataset (no learning step)

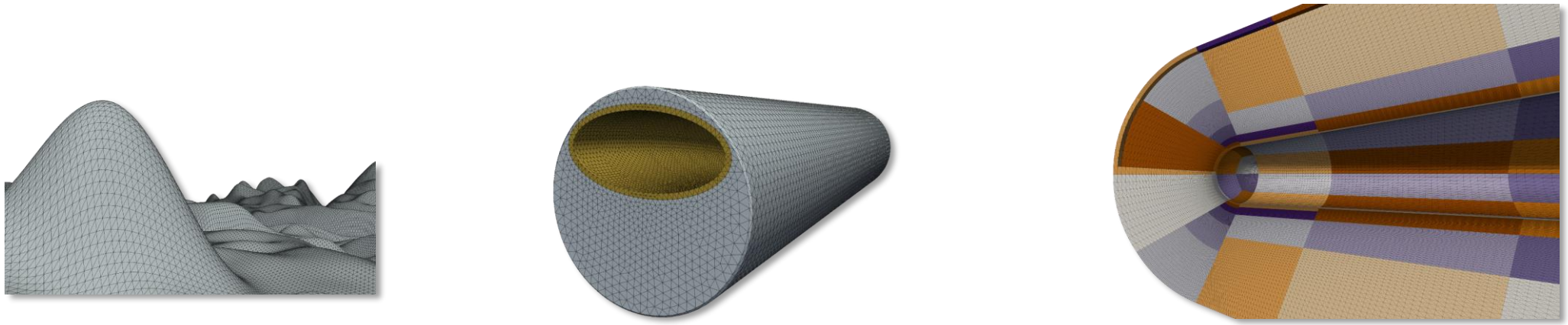


H. Edelsbrunner and J. Harer. *Computational Topology: An Introduction*. AMS, 2009
J.Tierny *Topological Data Analysis for Scientific Visualization*. Springer, 2017

Discrete Domain Representation

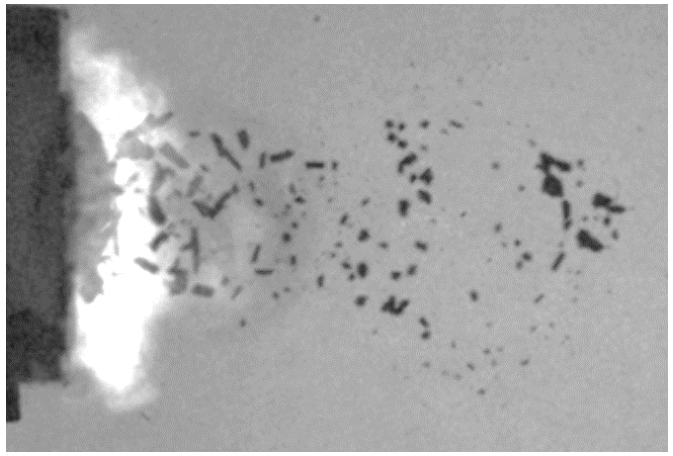
Simplicial complexes, stars *(St)* and links *(Lk)* around a simplex

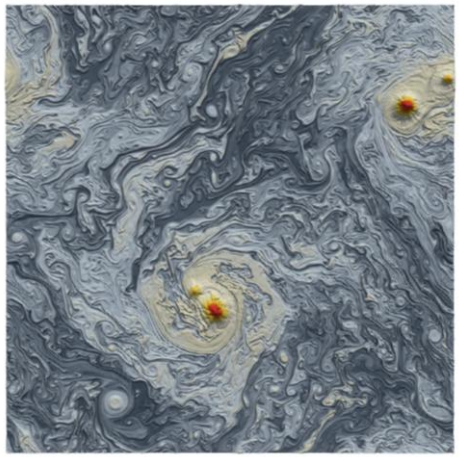
Triangulation and meshes

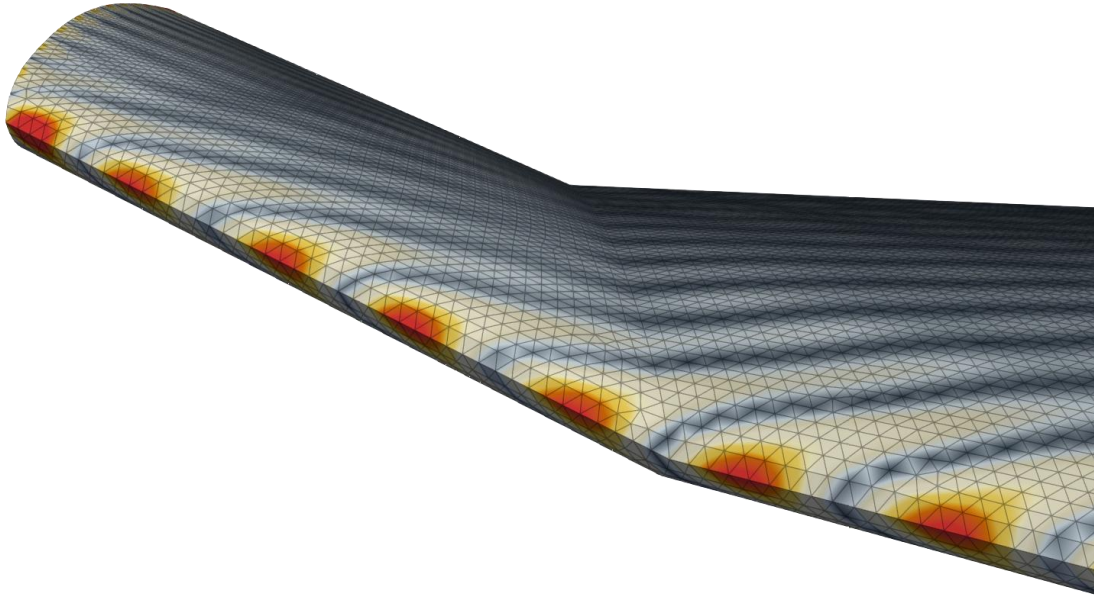


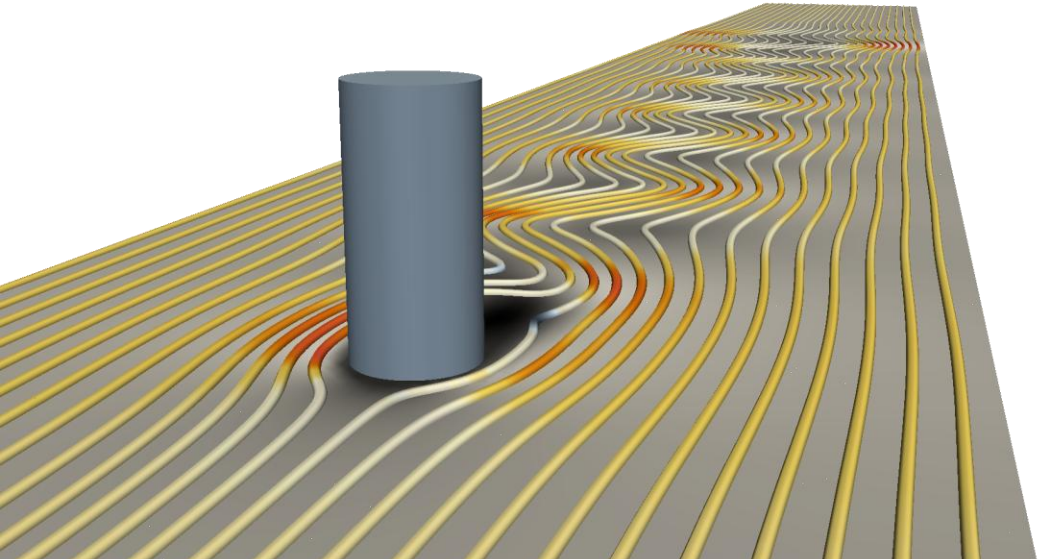
Scalar Field Representation

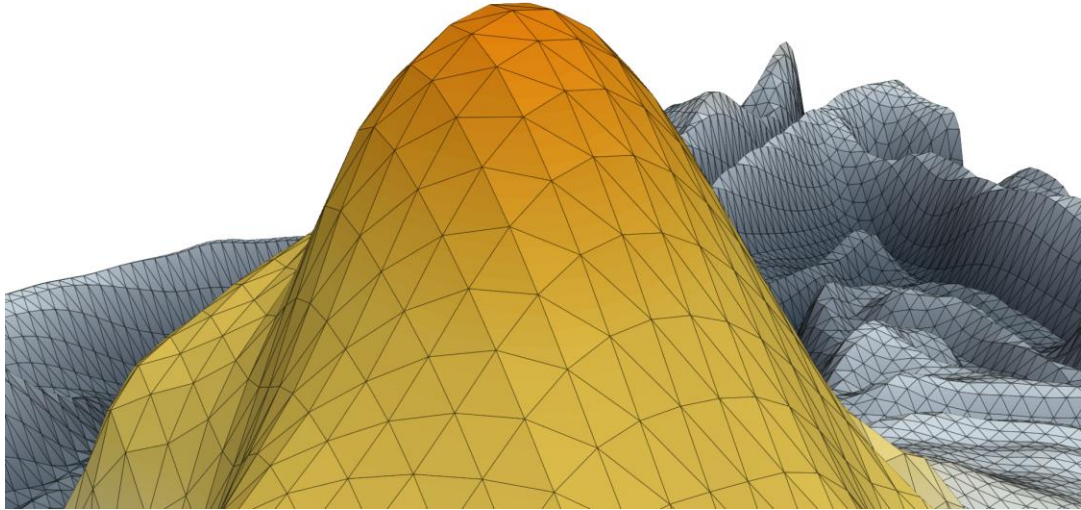
Barycentric coordinates and piecewise linear scalar field











Topological Signature : Simplicial Homology

Notions

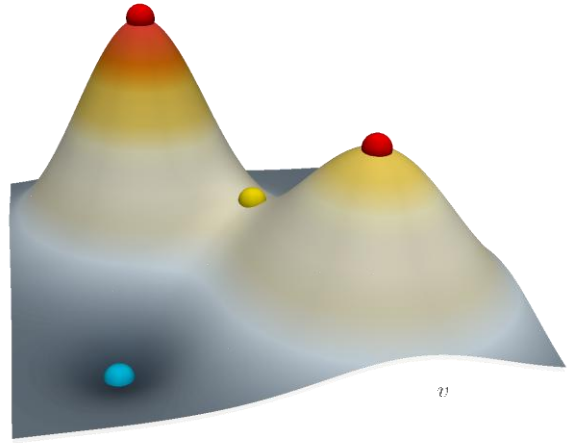
- Homeomorphisms between spaces
- Holes as topological invariants in domains
- Homology group of equivalence of cycles

Betti number in R^3

- β_0 : connected components
- β_1 : handles
- β_2 : 3D voids

H. Edelsbrunner, D.Letscher, A. Zomorodian, *Topological persistence and simplification,* Discrete Computational Geometry, vol. 28, 2002,

Topological Feature : Critical Points

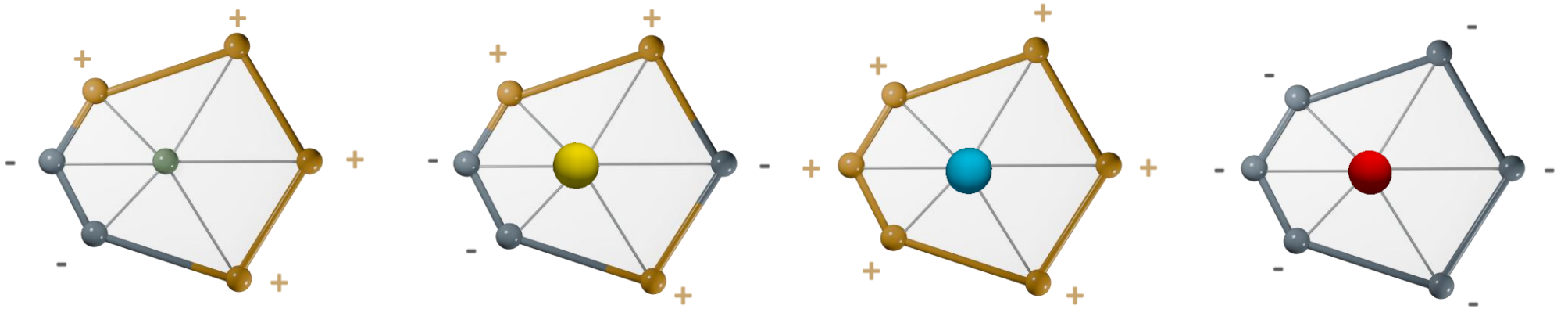


Links

- **Upper link** : $Lk^+(v) = \{\sigma \in Lk(v) \mid \forall v' \in \sigma,\ f(v') > f(v)\}$
- **Lower link** : $Lk^-(v) = \{\sigma \in Lk(v) \mid \forall v' \in \sigma,\ f(v') < f(v)\}$

Construction

- *v* is a regular point if and only if both $Lk^-(v)$ and $Lk^+(v)$ are simply connected
- Otherwise *v* is a critical point of *f*

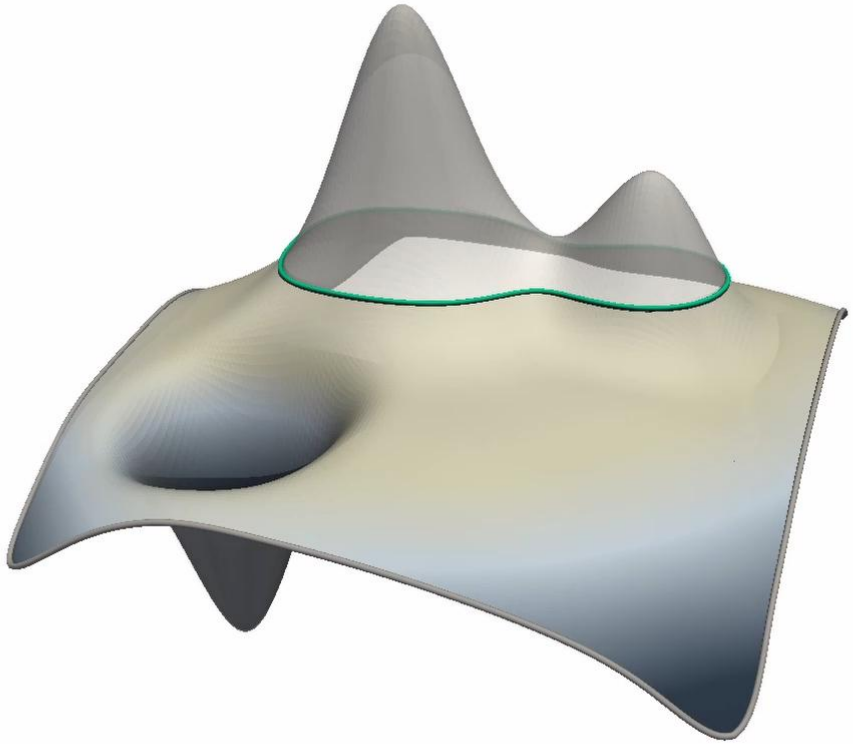


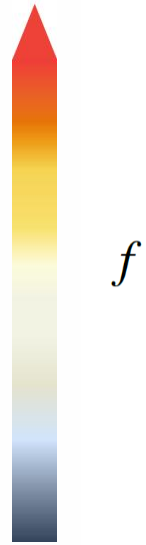
F. Banchoff. *Critical points and curvature for embedded polyhedral surfaces*.
The American Mathematical Monthly, 77(5) : 475–485, 1970.

Topological History : Persistent Homology

Notions

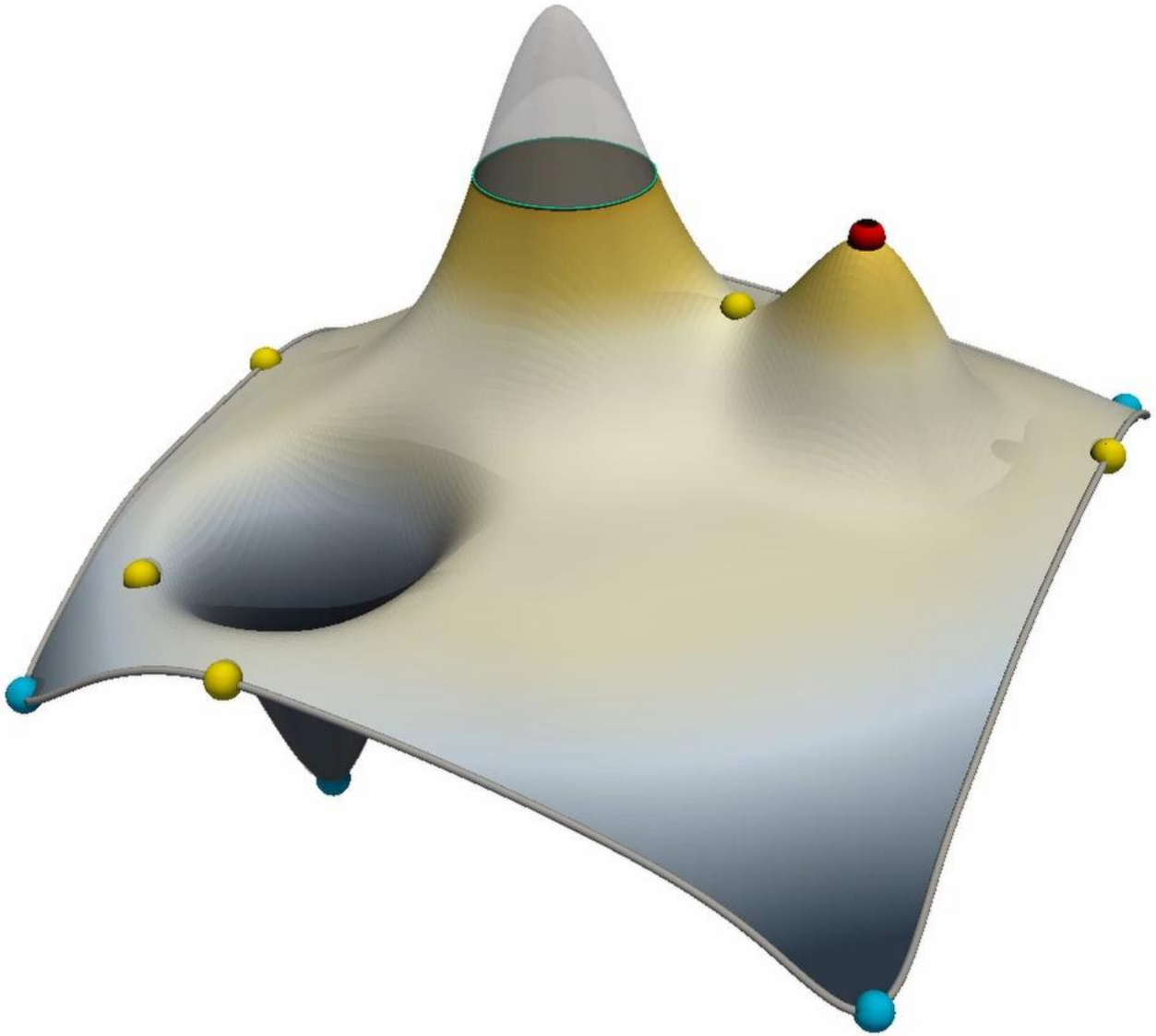
- Filtration used to define sublevel set
- Defined as : $f_{-\infty}^{-1}(w) = \{p \in \mathcal{M} \mid f(p) < w\}$

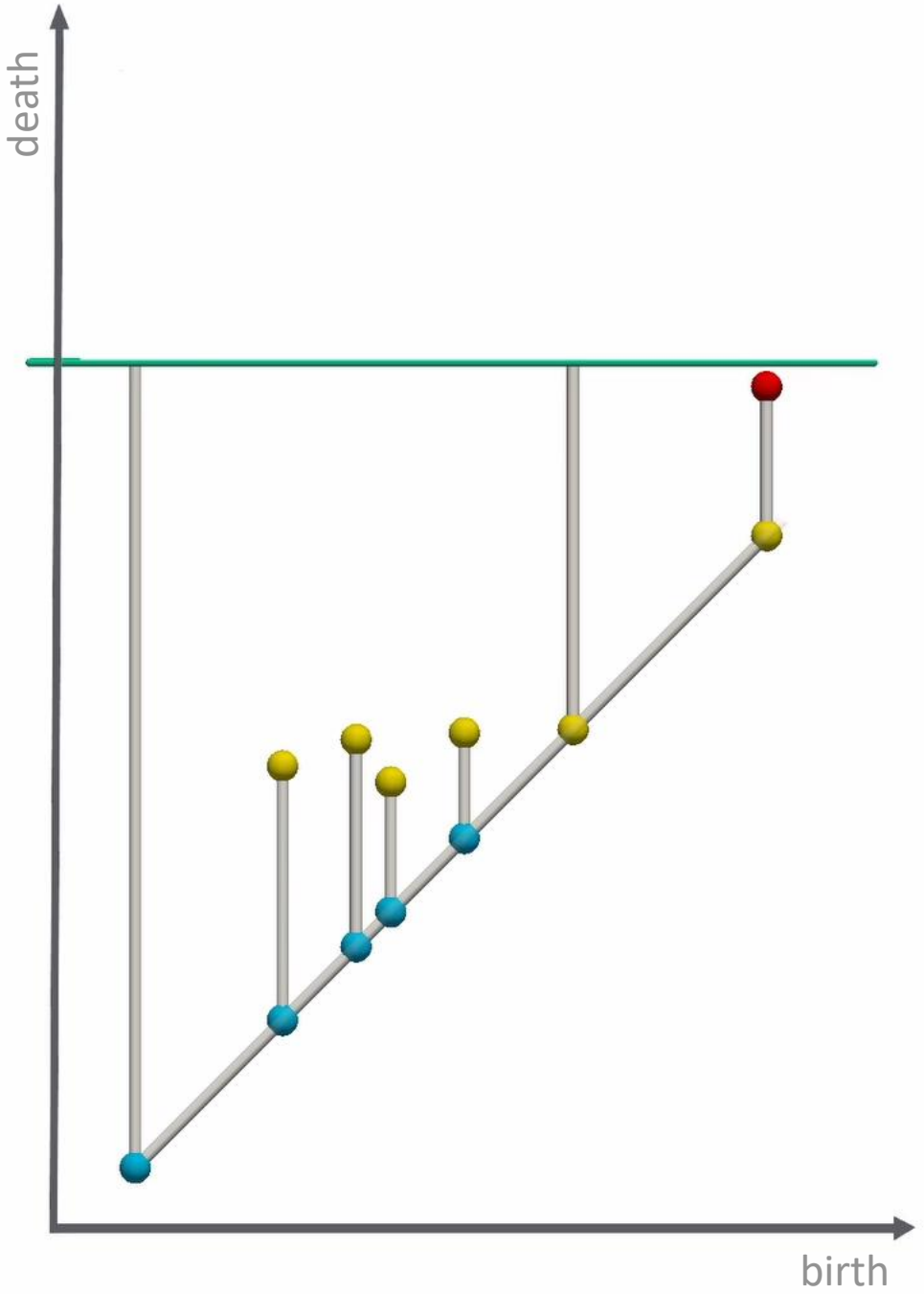




H.Edelsbrunner, J.Harer. *Persistent homology - a survey*. Contemporary Mathematics 453 (2008), 257–282. 8

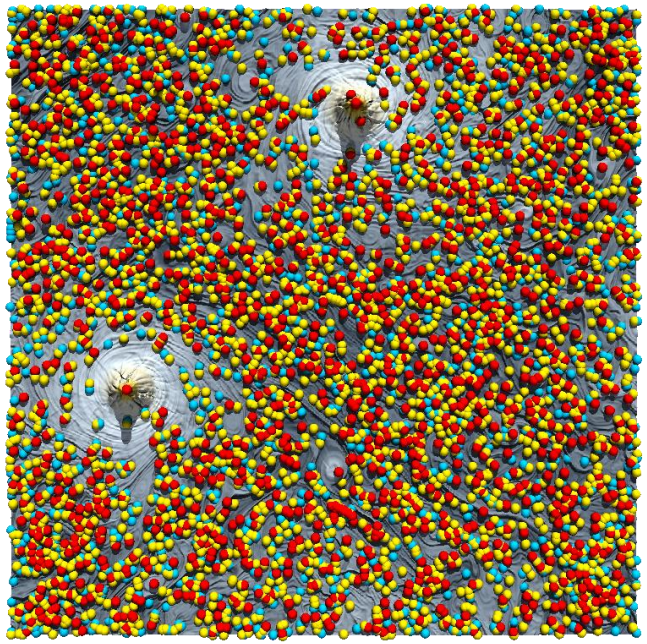
Topological Importance : Persistence

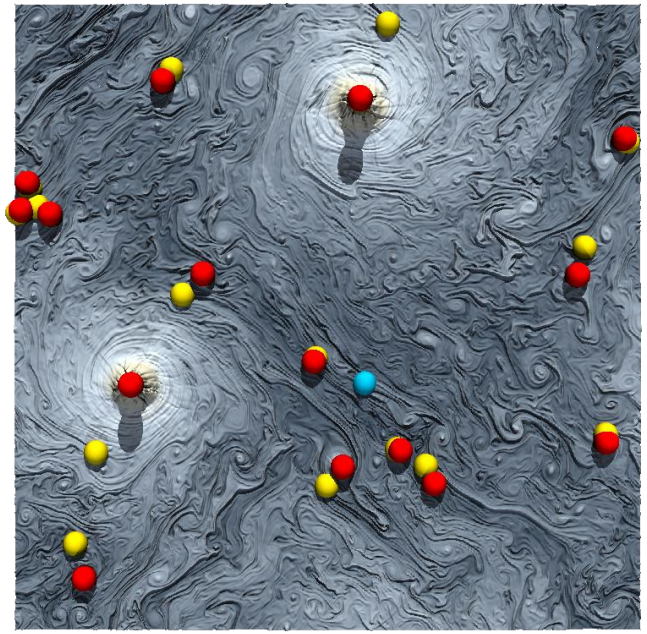


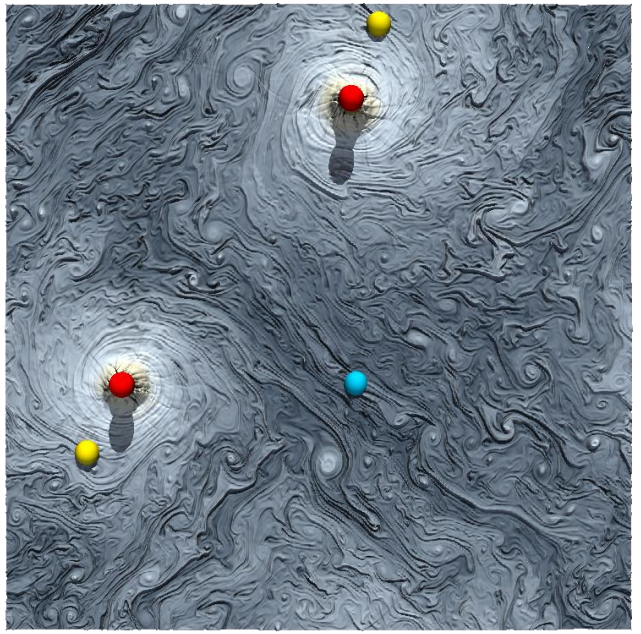


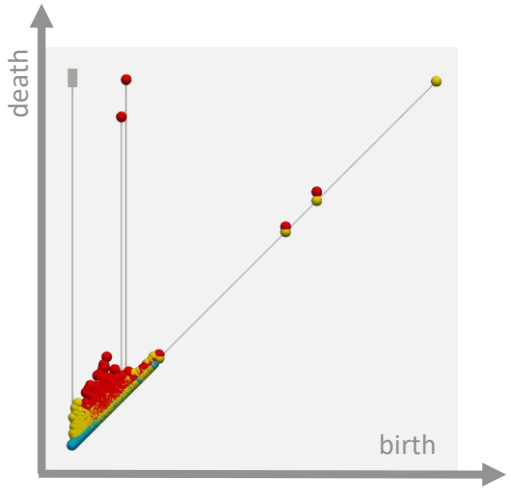
H.Edelsbrunner, J.Harer. *Persistent homology - a survey*. Contemporary Mathematics 453 (2008), 257–282. 8

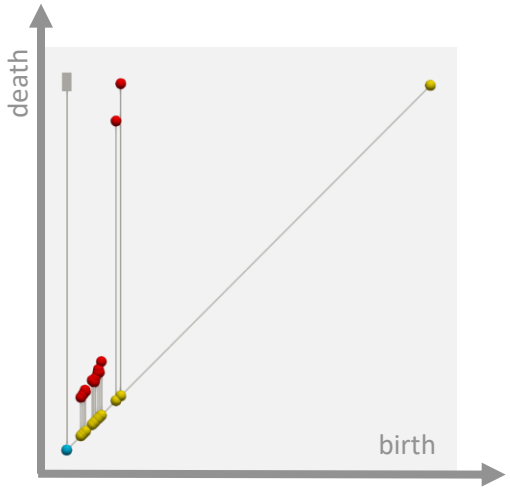
Topological Simplification : Noise Removal

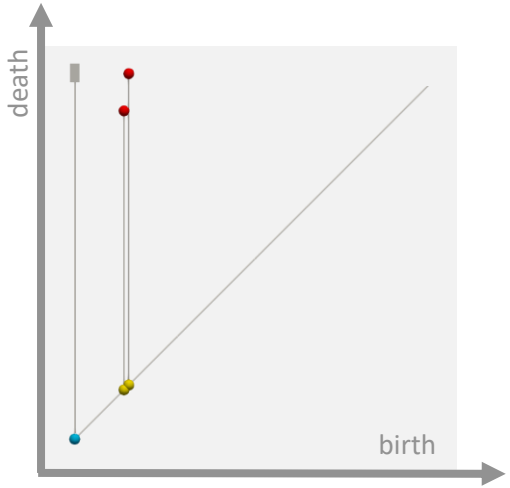






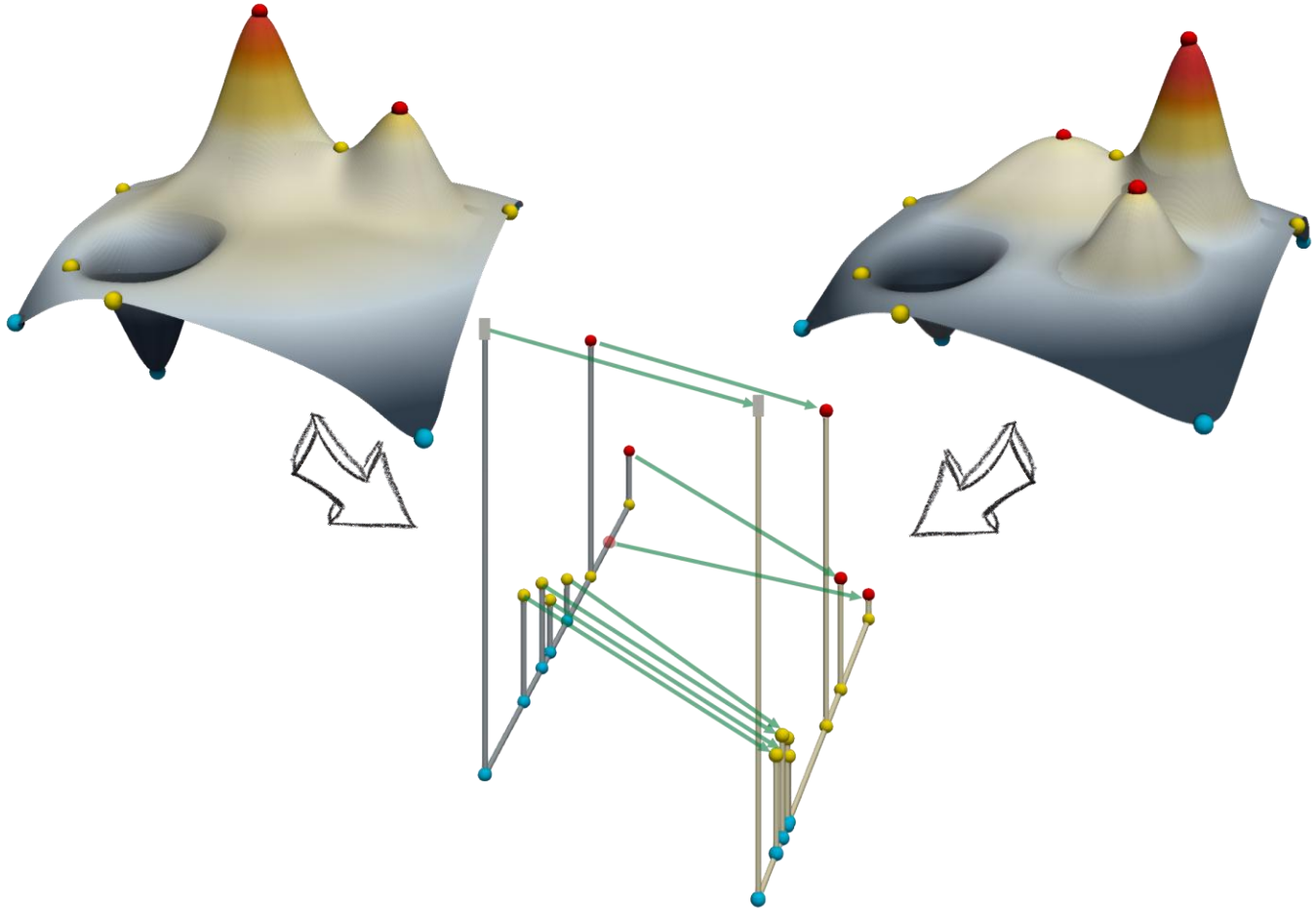


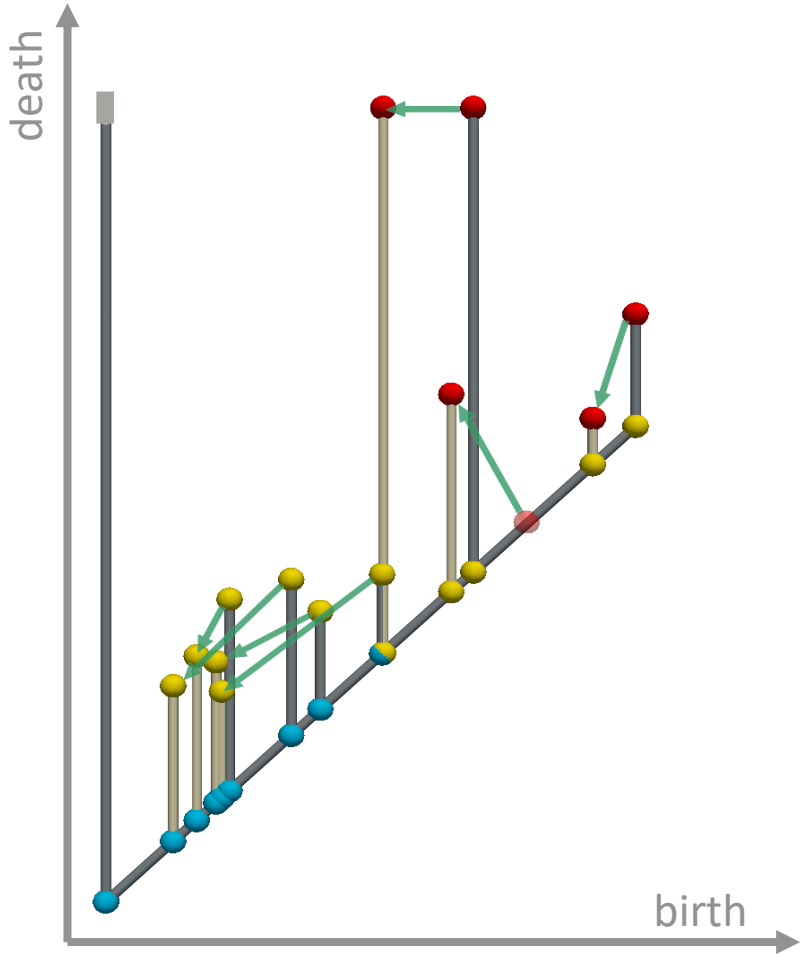




Topological Distance : Persistence Diagram Comparison

- Wasserstein distance between diagrams : $W_q\left(\mathcal{D}(f_i), \mathcal{D}(f_j)\right) = \min_{\phi \in \Phi} \left(\sum_{p_i \in \mathcal{D}(f_i)} d_q\left(p_i, \phi(p_i)\right)^q \right)^{1/q}$



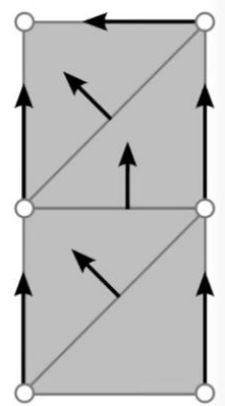


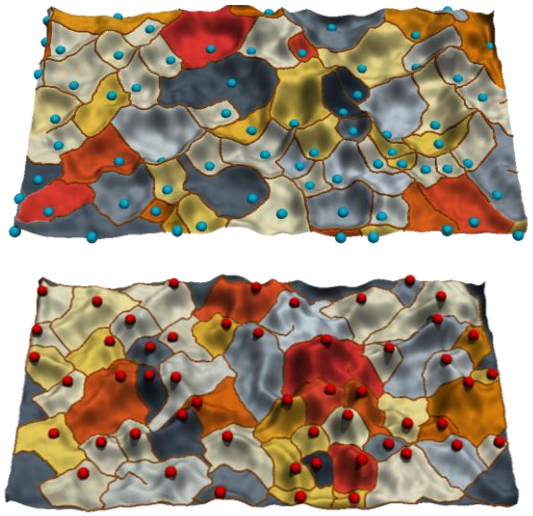
D. Cohen-Steiner, H. Edelsbrunner, J. Harer, *Stability of Persistence Diagrams*
Discrete & Computational Geometry - DCG. 37. 263-271. 10.1007, 2005

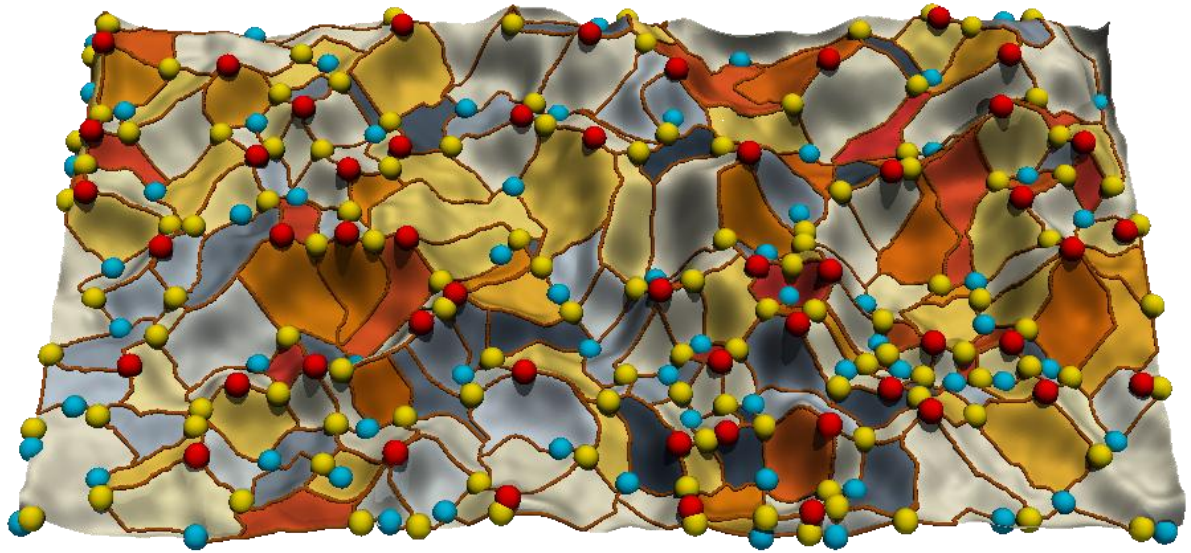
Topological Segmentation : Morse-Smale Complex

Construction

- Build with the discrete gradient field
- Vertices of the MSC correspond to the critical points of the PL scalar field
- Edges are separatrices of monotonic region of the discrete gradient field
- Consider equivalent classes on integral lines sharing the same extremities





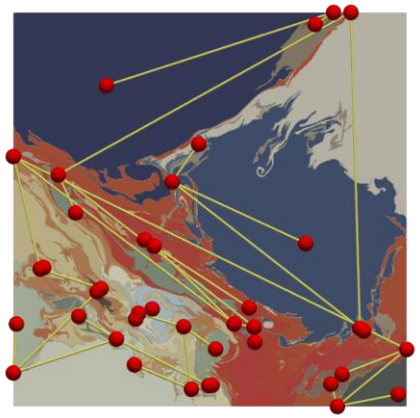


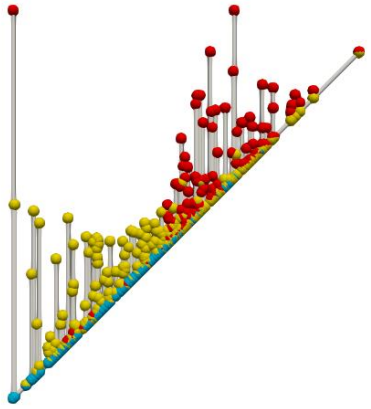
Edelsbrunner, Harer and Zomorodian. *Hierarchical Morse-Smale Complexes for Piecewise Linear 2-Manifolds*. Discrete Comput Geom 30, 87–107, 2003

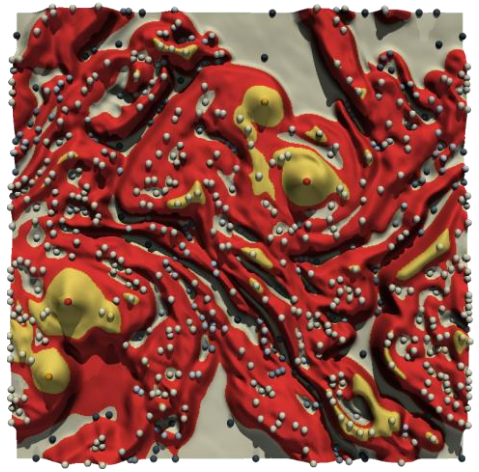
Many other Topological Representations

Find the right abstraction

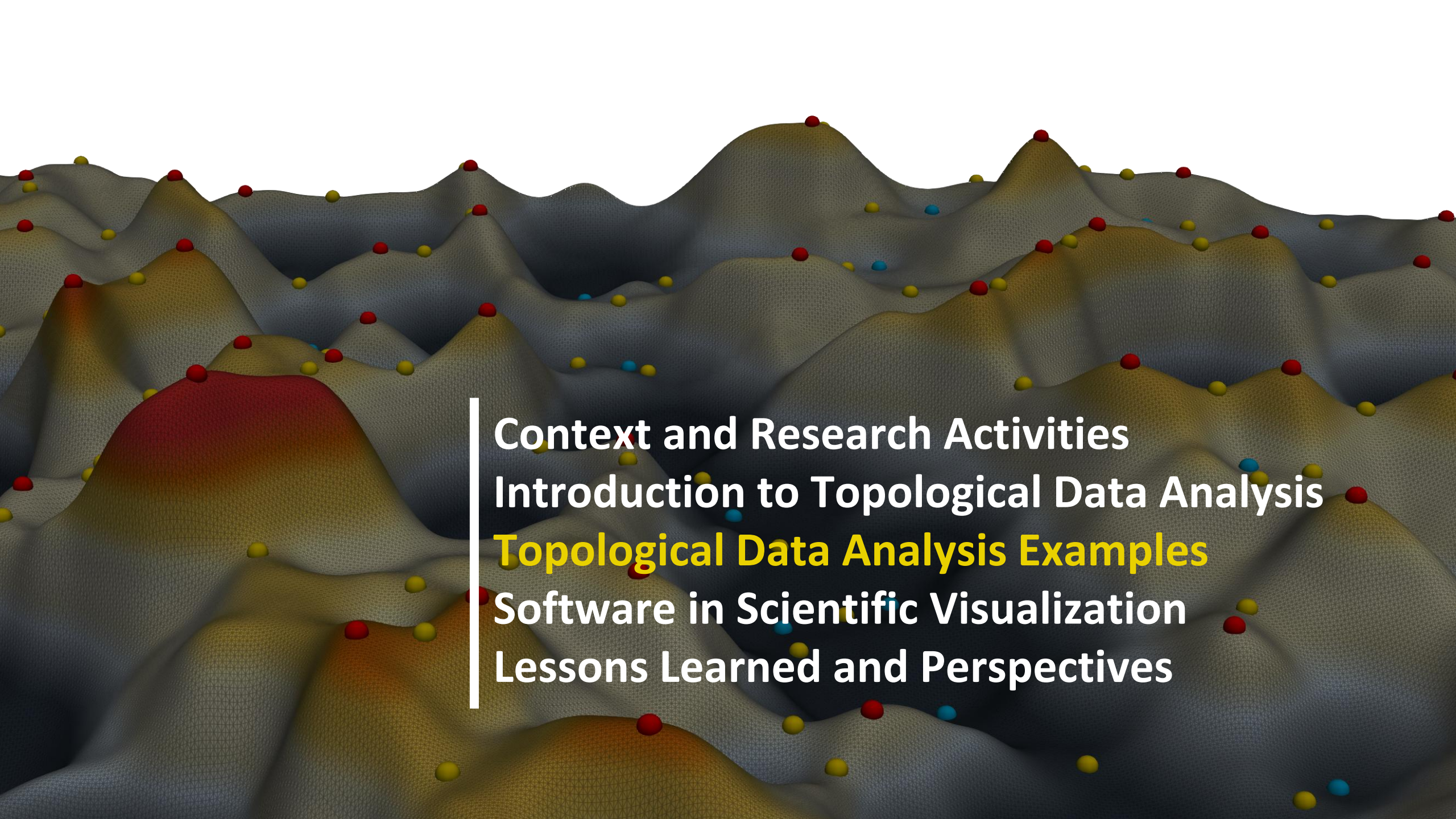
- Identify **points of interest** : Extract **critical points**
- Remove **noise** in chaotic data : **Persistence threshold on the persistence diagram**
- **Compare** features in a field **: Wasserstein distance** between persistence diagrams
- Extrat **filament** structures : **Morse-Smale complex 1-separatrices**
- **Segment** meaningfully areas : Compute **merge trees**







[YB21] L.Yan, T. Bin Masood, R. Sridharamurthy, F. Rasheed, V. Natarajan, I, Hotz, B. Wang,
Scalar Field Comparison with Topological Descriptors: Properties and Applications for Scientific Visualization, Computer Graphics Forum, vol. 40, no. 3, Jun. 2021.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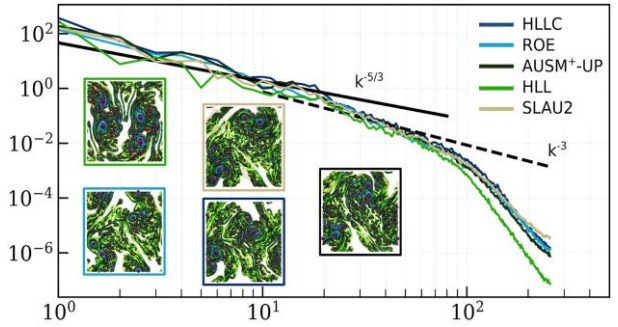
Comparison of Ensembles for Code Development

Context of turbulence

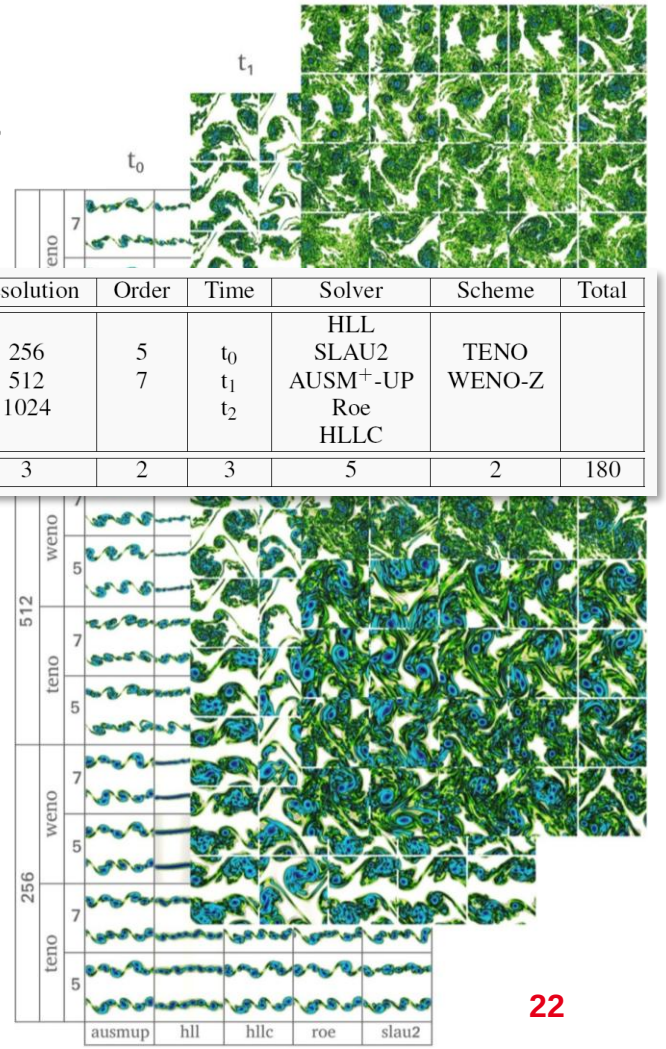
- Compare simulations of inviscid flows with 2D compressible unsteady Euler equations
- Evaluate numerical ingredients and input parameters
- Identify solver configurations realistic simulations with fast computations

?

Averaged kinetic energy power spectrum



Parameter	Resolution	Order	Time	Solver	Scheme	Total
Value	256 512 1024	5 7	t_0 t_1 t_2	HLL SLAU2 AUSM$^+$-UP Roe HLLC	TENO WENO-Z	
Number	3	2	3	5	2	180



CFD hypothesis to validate TDA descriptors

- TENO scheme induces more turbulence than WENO-Z scheme
- HLL solver provides a distinct description for all configurations

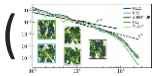
F. Nauleau, F. Vivodtzev, T. Bridel-Bertomeu, H. Beaugendre, J. Tierny, *Topological Analysis of Ensembles of Hydrodynamic Turbulent Flows An Experimental Study,* LDAV 2022, proceedings of 2022 IEEE 12th Symposium on Large Data Analysis and Visualization, Oklaoma City, 2022

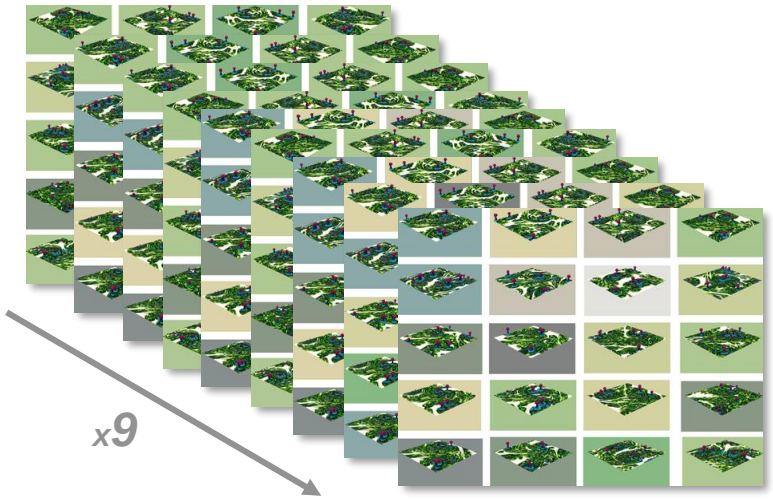
Comparison of Ensembles for Code Development

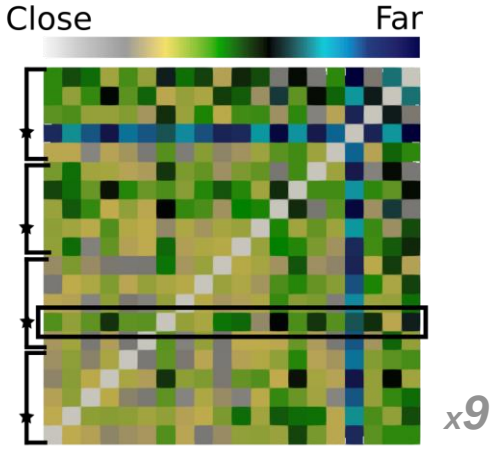
TDA pipeline

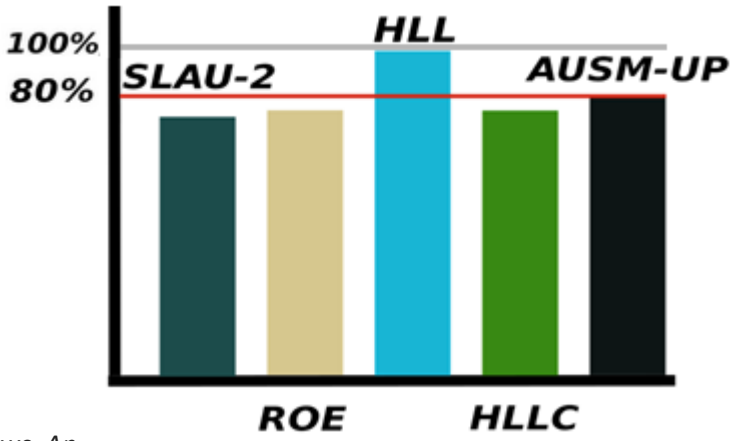
- 20x9 ensemble – Persistence simplification - Distance matrix for the Wasserstein distance - Average

TDA results for hypothesis

- Topology of the vortices captured by the persistence of the critical points
- Wasserstein distance successfully identify HLL solver
- Better discrimination amongst numerical ingredients than traditional approaches ()



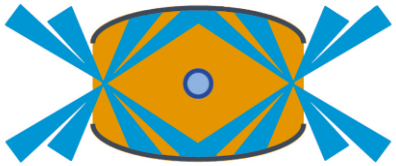




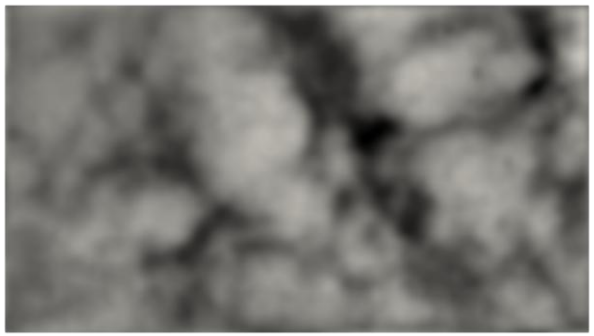
F. Nauleau, F. Vivodtzev, T. Bridel-Bertomeu, H. Beaugendre, J. Tierny, *Topological Analysis of Ensembles of Hydrodynamic Turbulent Flows An Experimental Study,* LDAV 2022, proceedings of 2022 IEEE 12th Symposium on Large Data Analysis and Visualization, Oklaoma City, 2022

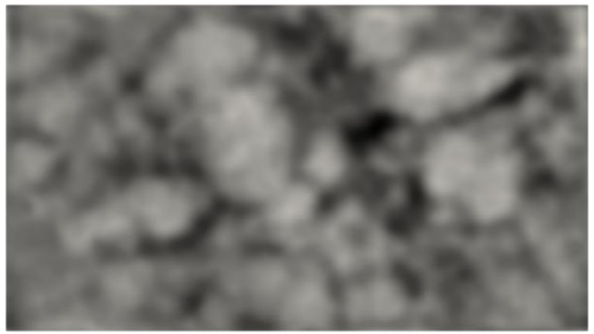
Feature Detection of Hydrodynamics Instabilities

Domain



- Inertial Confinement Fusion in large laser facilities
- Understand hydrodynamics instabilities
- Ablative Rayleigh Taylor instability gives birth to complex 3D patterns
- X-ray obtain during experiments





Goal

- Evaluate topological segmentation to identify bubble structures in the experimental x-ray

F.Vivodtzev, A.Casner, L.Masse, L.Ceurvorst, S.Khan, V.Smalyuk, *Topological Data Analysis of 3D Ablative Rayleigh-Taylor Instability Dataset for Automatic Segmentation*
LDAV poster at 2023 IEEE 13th Symposium on Large Data Analysis and Visualization,Melbourne, Australia, 22-27 October 2023.

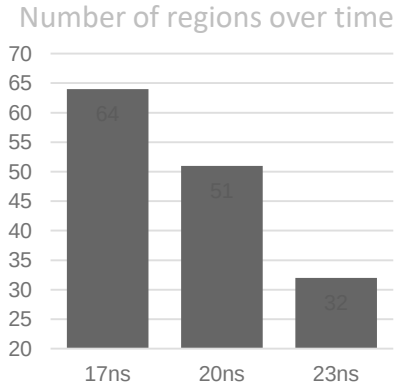
Feature detection of Hydrodynamics Instabilities

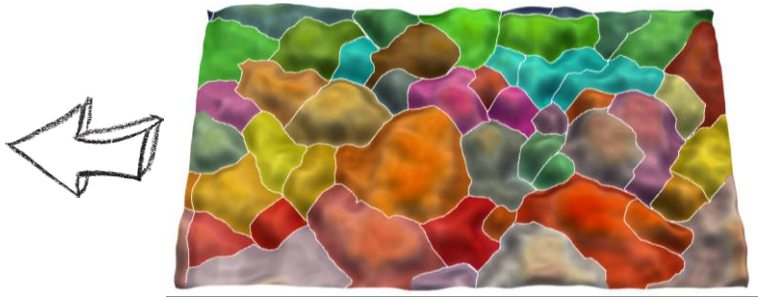
Abstraction

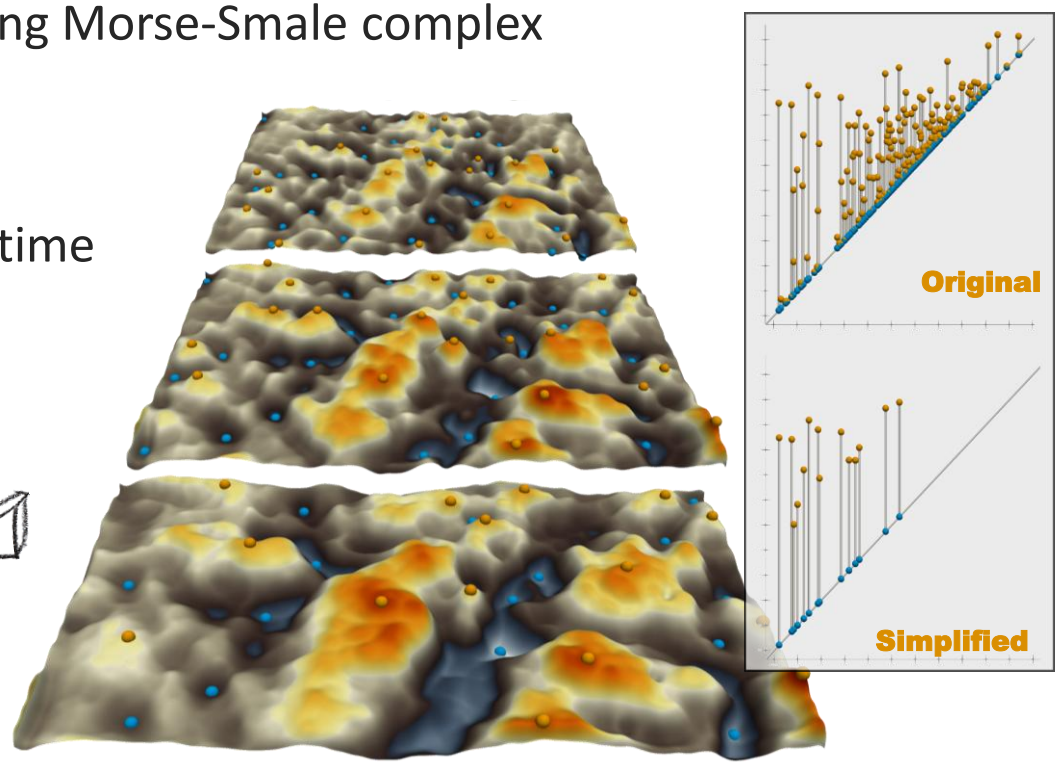
- Correlation between the x-ray pixel intensity and the bubble structure
- Topological simplification using persistence
- Segmentation based on 1-separatrices of the ascending Morse-Smale complex

TDA results for hypothesis

- Decreasing number of bubbles of the instability over time







F.Vivodtzev, A.Casner, L.Masse, L.Ceurvorst, S.Khan, V.Smalyuk, *Topological Data Analysis of 3D Ablative Rayleigh-Taylor Instability Dataset for Automatic Segmentation*
LDAV poster at 2023 IEEE 13th Symposium on Large Data Analysis and Visualization,Melbourne, Australia, 22-27 October 2023.

Segmentation and Tracking for Hyper Velocity Impact

Context

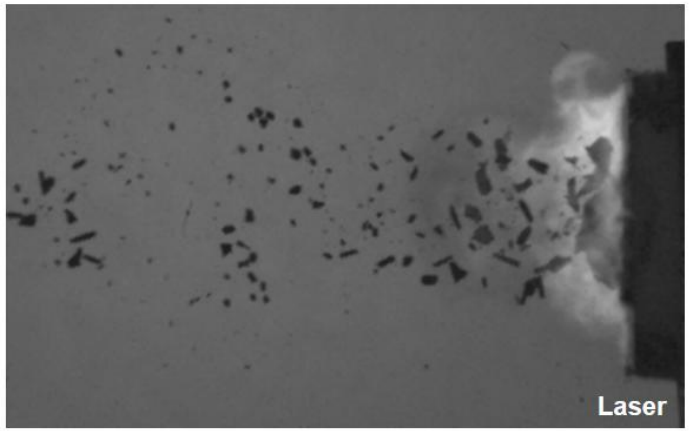
- Improve satellites' sustainability in Low-Earth Orbit
- Avoid threat of hyper velocity impacts (HVI) due to space debris
- Characterize composite shielding materials with carbon components

Hyper Velocity Impact experiments on materials

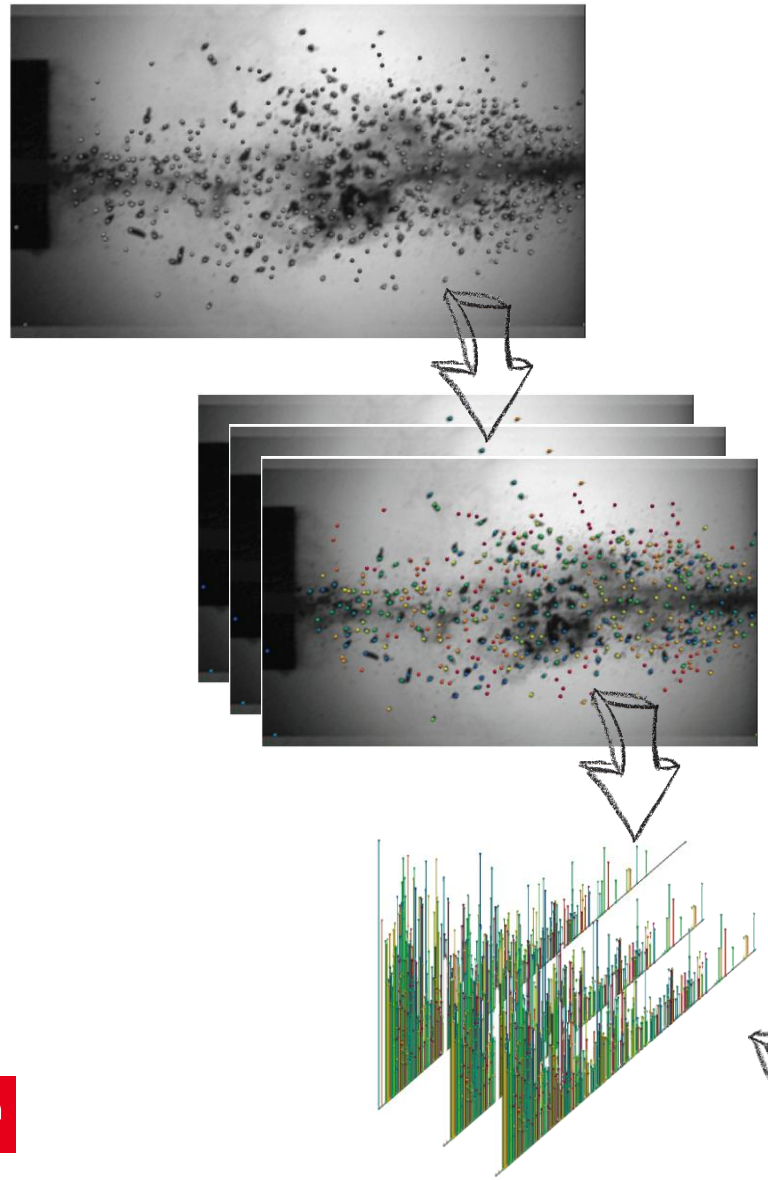
- Materials subjected to extreme loading via projectile or laser impacts
- Events captured with ultra-high-speed imaging (sub-microsecond)

Statistical characterization of impact-generated debris

- Goal : quantify debris populations to assess material resistance
- How : time-resolved imaging and particle-tracking/segmentation
- Why : crater formation and ejecta distribution

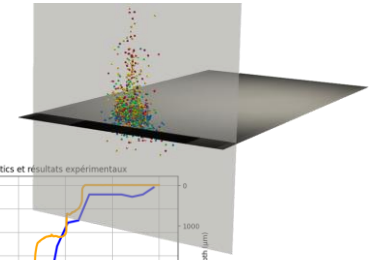


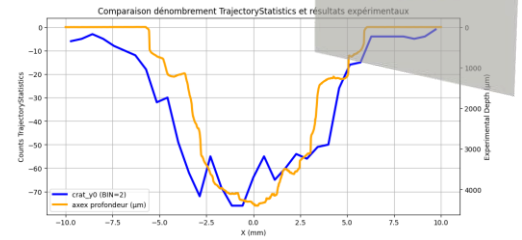
Topological and Statistical HVI pipeline

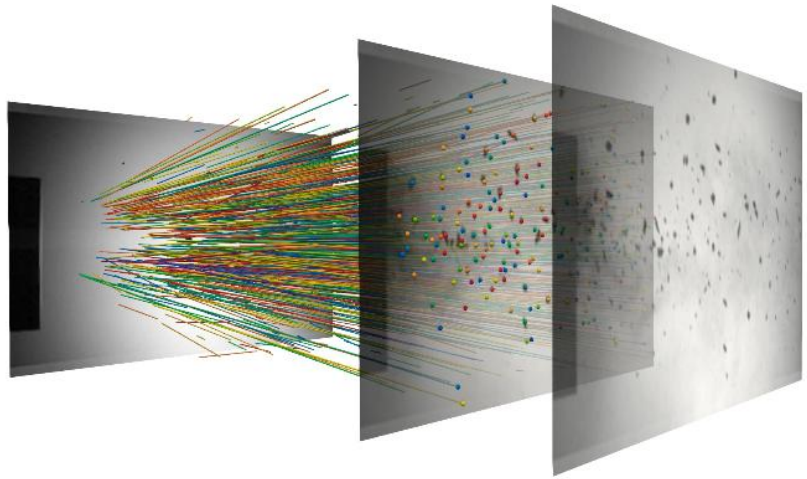


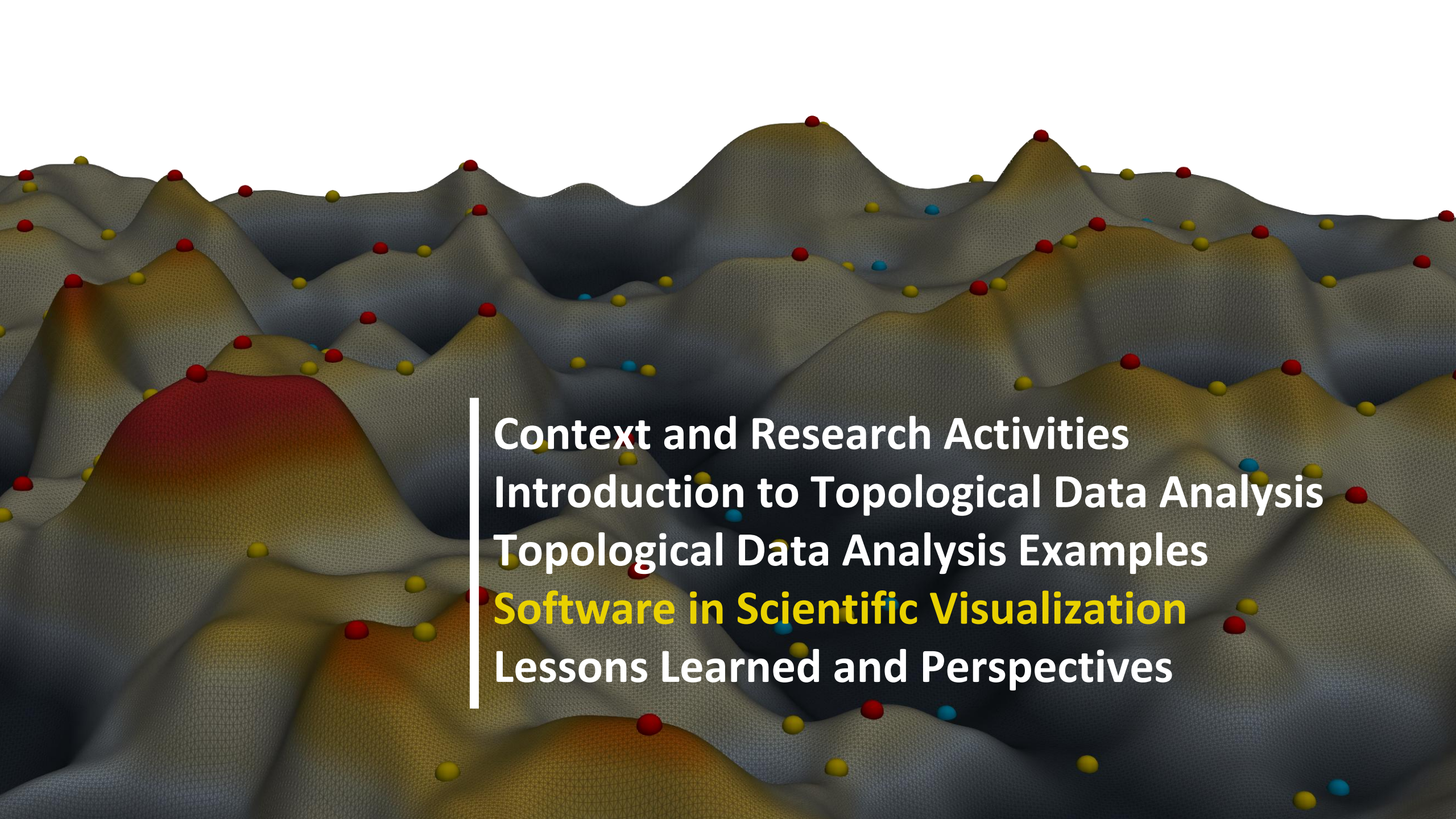
Analysis pipeline

- 2D images to 3D dataset with intensity as scalar field
- Tracking from Wasserstein distance between persitence diagrams
- Debris trajectories generation and improvements
- Fast topological HVI statistical analysis







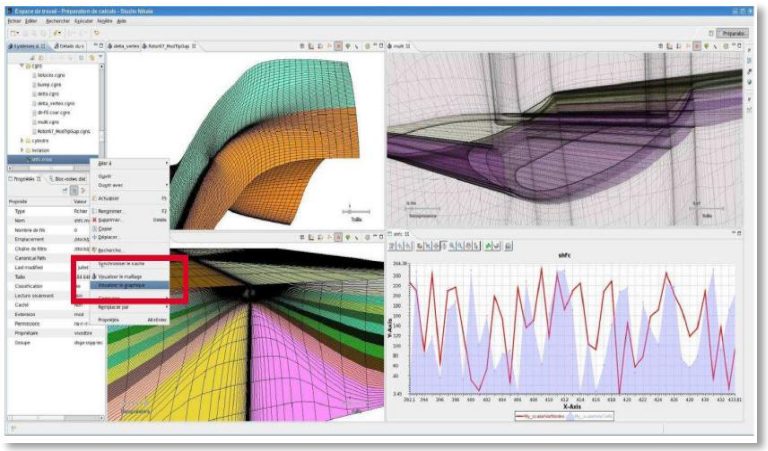

Context and Research Activities
Introduction to Topological Data Analysis
Topological Data Analysis Examples
Software in Scientific Visualization
Lessons Learned and Perspectives

Improve Scientific Visualization Tools

Optimize research engineering time

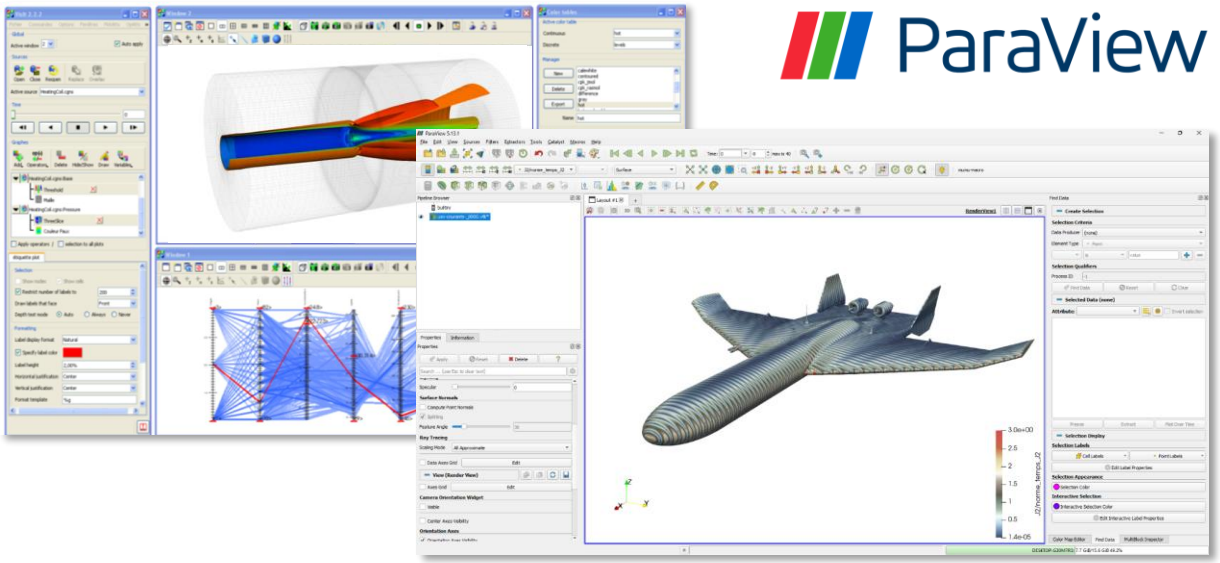
- Remote and integrated visualizations into simulation platforms
- Adapting the visualization capabilities of VisIt and ParaView for HPC

eclipse VTK



Java

VisIt

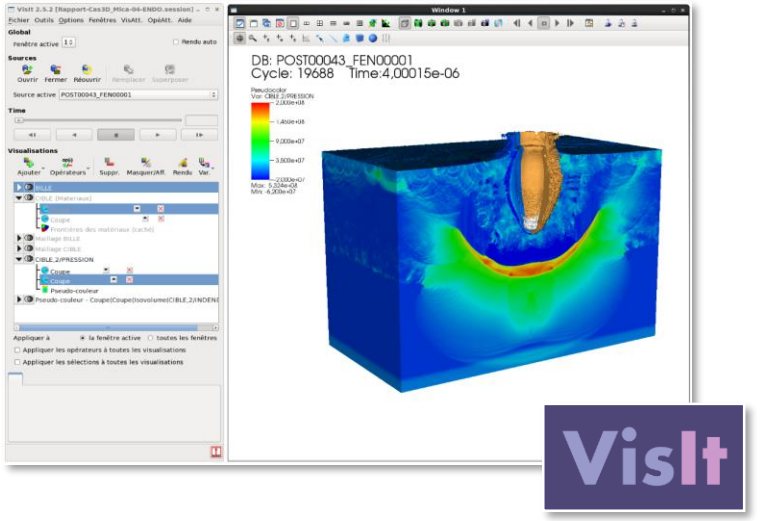


ParaView

D.Nassiet, F.Vivodtzev, *User experience feedback: how to make remote visualization issues compatible in a highly secure environment*, Forum TeraTec 2012.

F. Vivodtzev, T. Carrard, *Open source Software to Visualize Complex Data on Remote CEA's Supercomputing Facilities*, Workshop on Open Source in Visualization at EUROVIS 2014, Swansea, Wales, 2014.

Address Large Scale Data Visualization

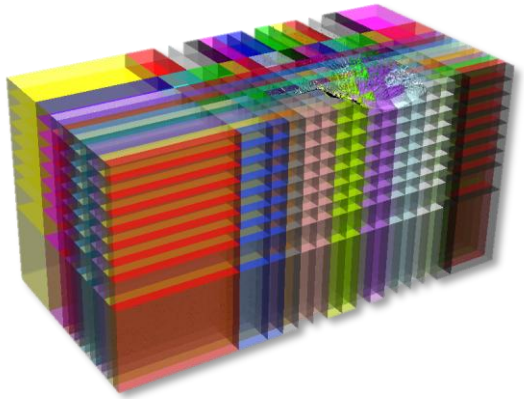


Several strategies for VisIt

- I/O evolution of the simulation code data model (HDF5, SILO …)
- Development of conversion tools (VTK)
- Development of specific database readers

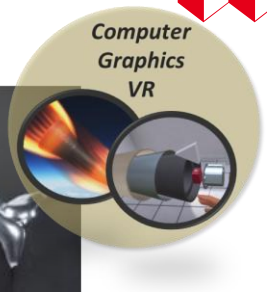
HPC setup

- Remote: Client/Server architecture between a local workstation and a supercomputer
- Parallel: Parallel I/O and visualization computations



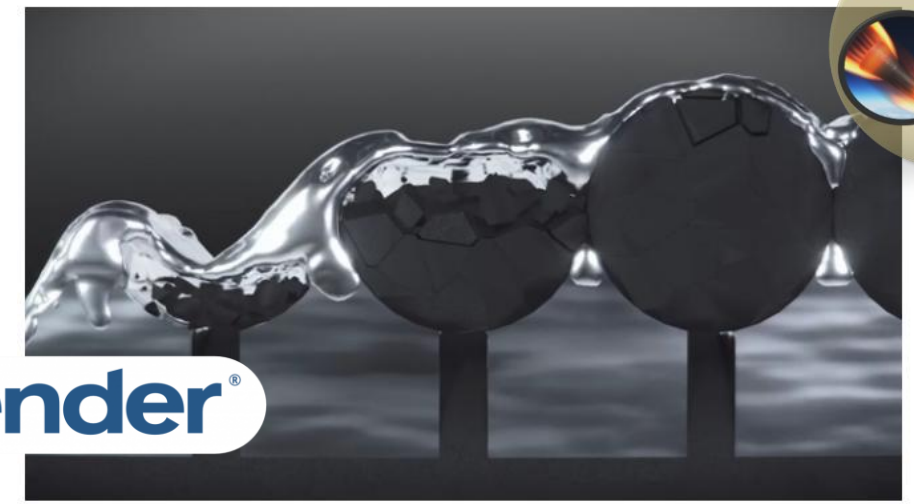
F. Vivodtzev and I. Bertron, *Remote Visualization of Large Scale Fast Dynamic Simulations in a HPC Context,* Proceedings of 2014 IEEE Symposium on Large Data Analysis and Visualization, Paris, November 2014

Computer Graphics for Scientific Representations



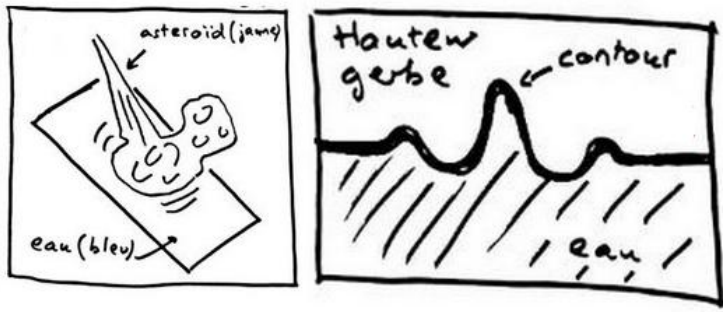
Better communication of the physics

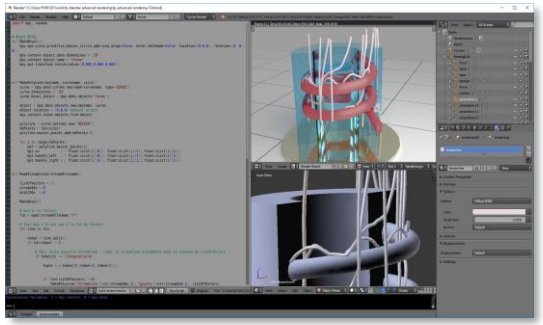
- Storytelling for interdisciplinarity
- Computer graphics



Many steps / many people

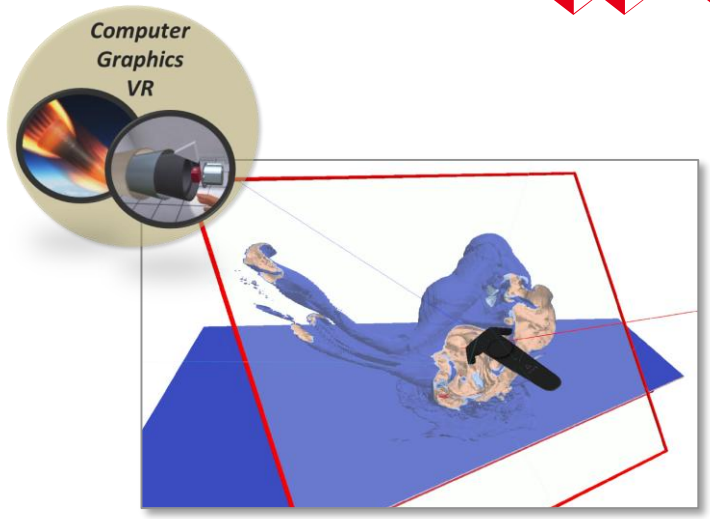
- Pre-poduction : idea, storyboard, animatic, design, data acquisition
- Production : modeling, texturing, rigging, animation, lighting, rendering
- Post-production : compositing, motion graphics, color correction, validation





A. Gomez, F. Vivodtzev, *short clips from scientific movies in the context of PhD projects.*

Immersive Data Exploration



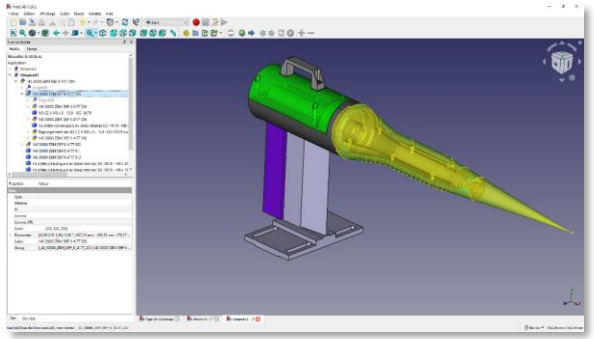
Many hardware and software extended reality solutions

- SciViz pipeline : SteamVR, XRInterface Paraview, Omniverse …
- Game engine approach : Unity, Unreal, Godot …

VR technologies driven by the entertainment companies

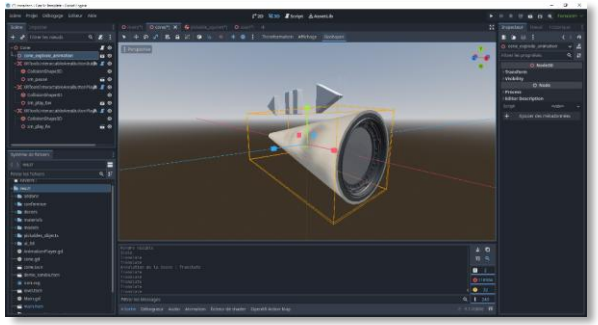
- Need solutions under Linux with no internet access

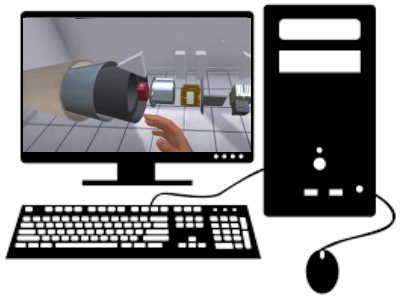
FreeCAD



glTF

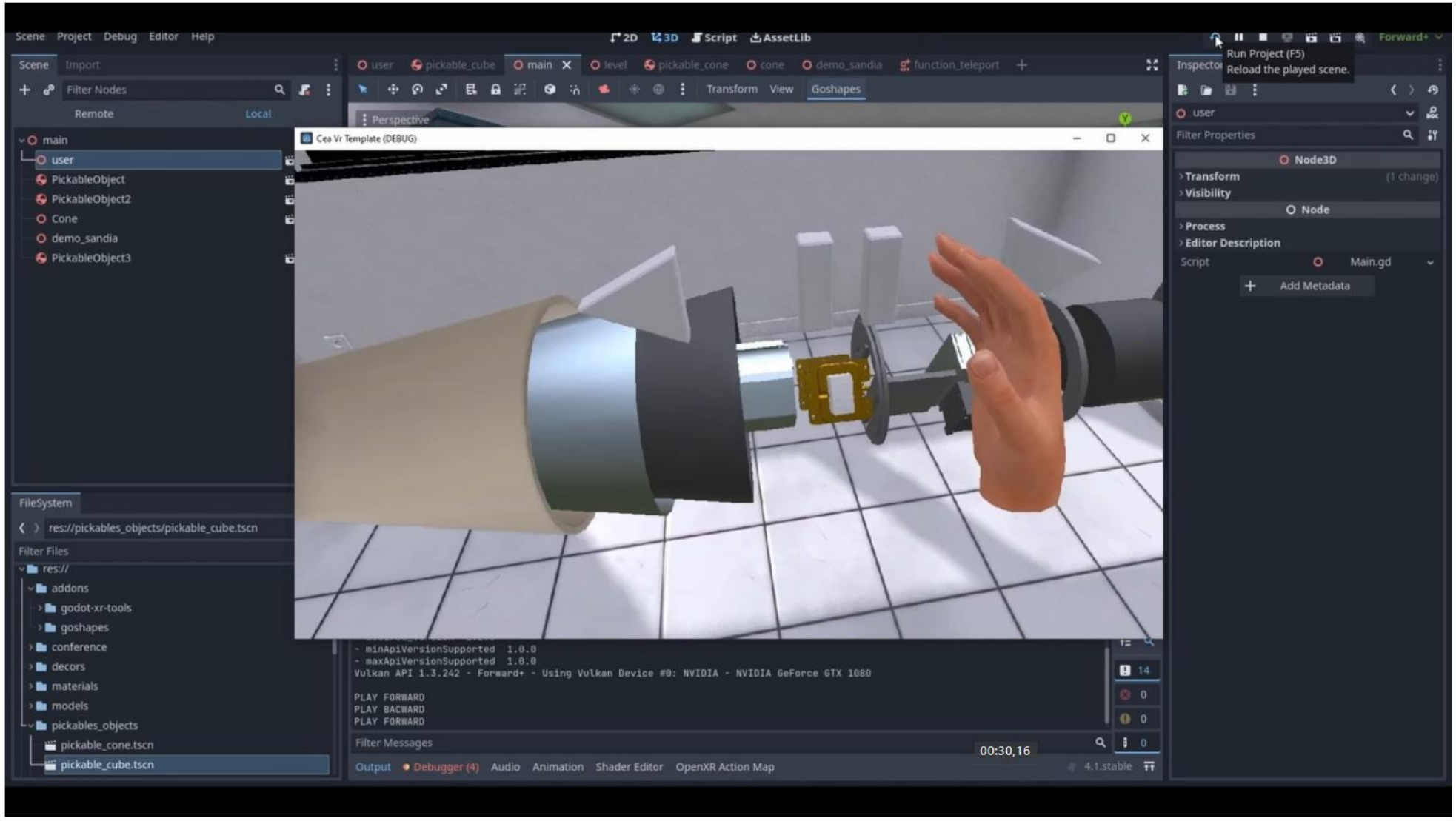
GODOT
Game engine

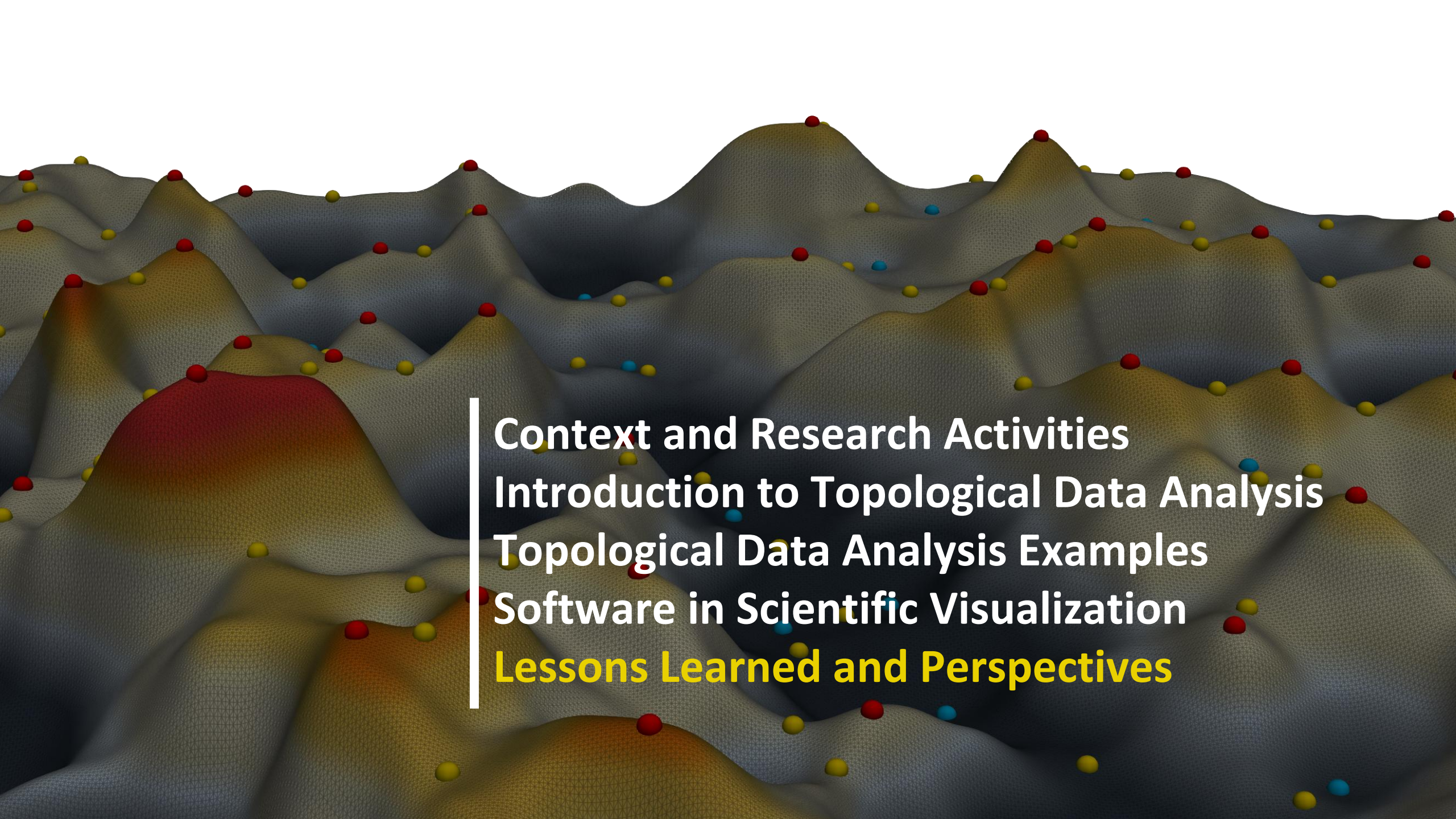




F. Vivodtzev, A. Gomez, *On the road to build an open-source VR workflow in a Linux restricted network environment,* Sandia 5th Annual XR conference, Sandia National Laboratories, August 1-4 2023.

Immersive Data Exploration





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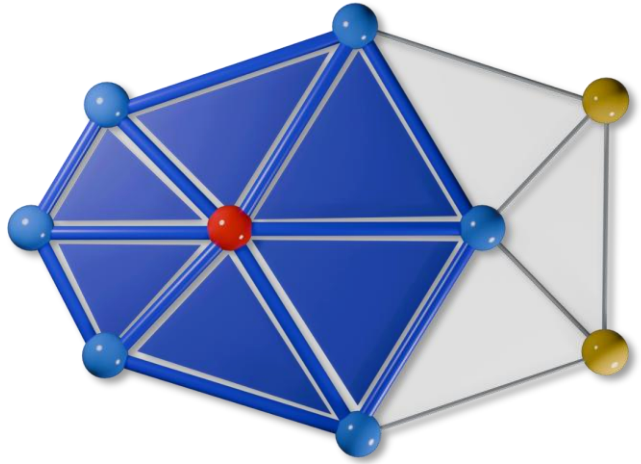
Lessons Learned for Future Work



Scientific visualization of simulation data improved with

- Combinatorial approachs
- Data management first
- Interdisciplinary approaches and hybrid rendering
- Supervision, teaching and collaborations

kitware

SCIENCES SORBONNE UNIVERSITÉ

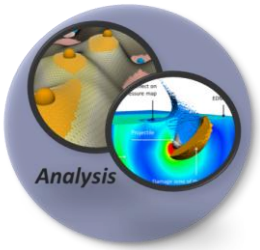
Los Alamos NATIONAL LABORATORY

Sandia National Laboratories

Inria

NNSA National Nuclear Security Administration

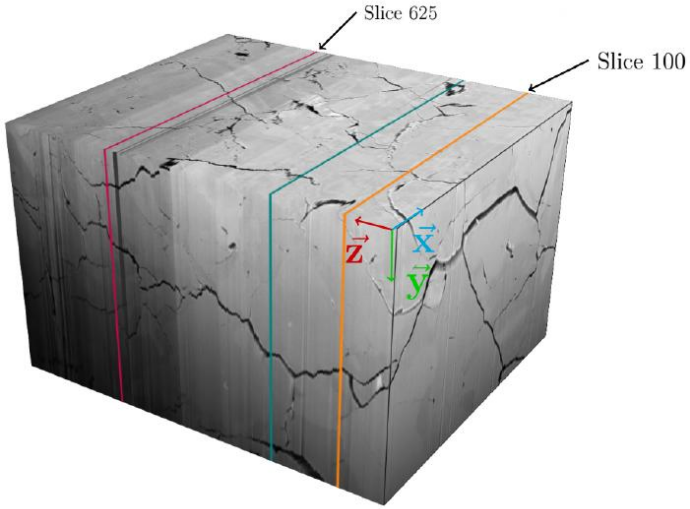
cnrs



Perspectives : Domain Specific Exploration

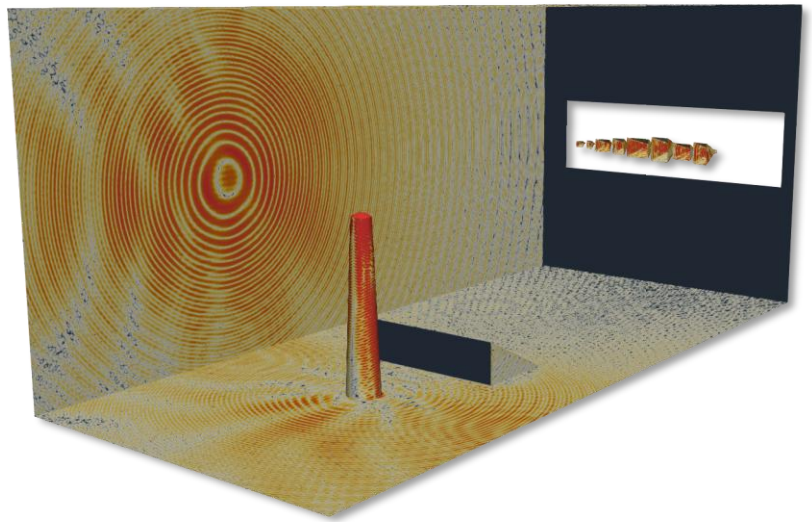
TDA for material design

- Tracking of over time for experimental data
- Experimental feature segmentation for numerical modeling



Investigate abstraction for other physics with *noisy/chaotic data*

- Pyrolysis phenomena
- Electromagnetic vulnerability simulations
- Neural network optimizers



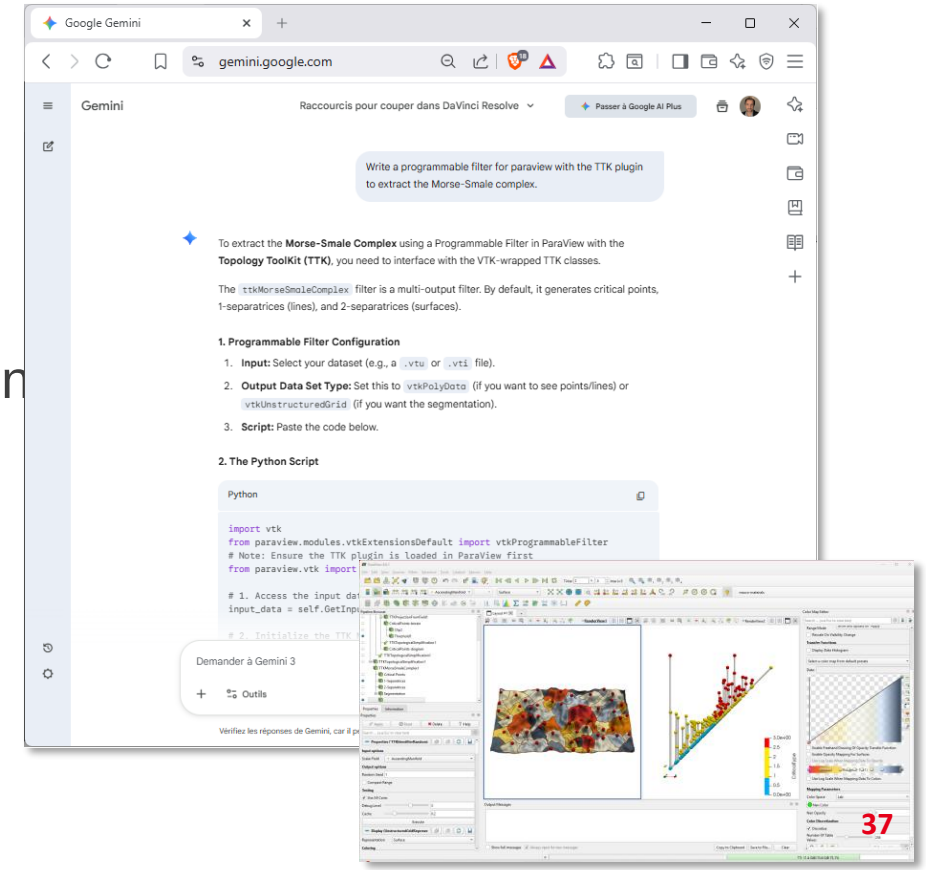
Perspectives : Data and Software

Data preparation

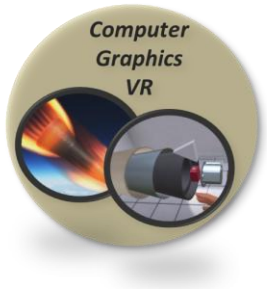
- Management of data between the simulation code and the visualization pipeline
- Work on parallel I/O (HDF5, VTK …)
- Investigate in-situ technologies : Catalyst, Conduit …

AI visualization paradigm

- On site LLM with Retrieval-Augmented Generation
- Model Context Protocol for connecting AI application
- Multimodal large language models (MLLM)



S. Liu, H. Miao, and P.-T. Bremer. *Paraview-MCP: Autonomous visualization agents with direct tool use*. In Proc. IEEE VIS 2025 Short Papers, page 00. IEEE, 2025.



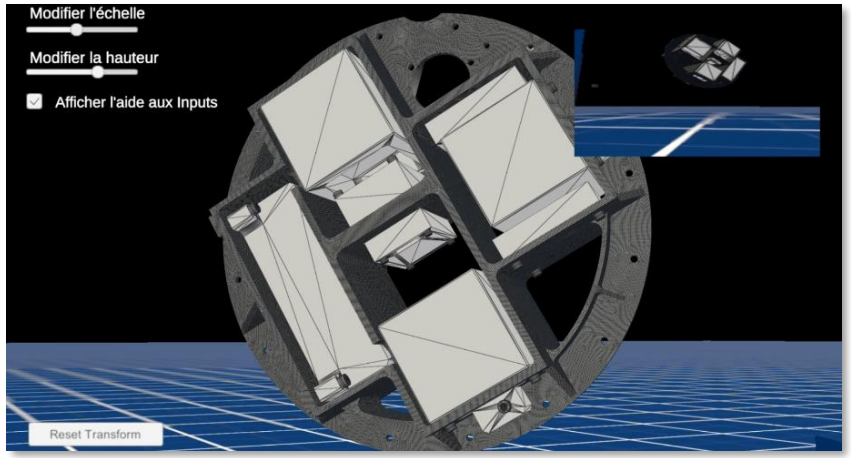
Perspectives : Display

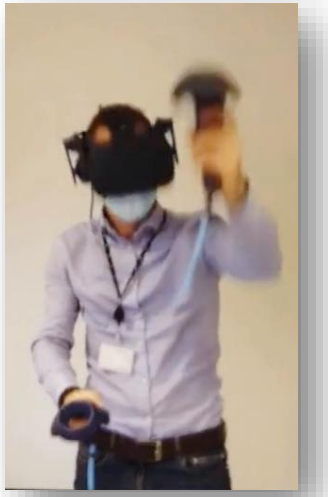
Fill the gap between design space and computer graphics

- CAD models and meshes preparation
- 3D scene from CAD (formats such as USD, glTF …)

Continuously adapt displays to science

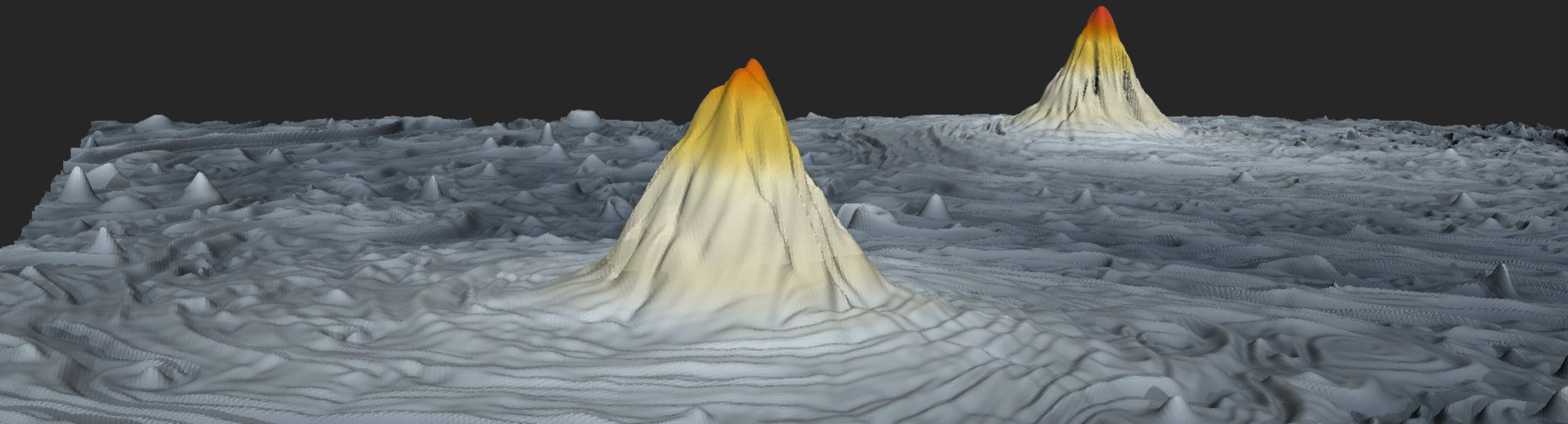
- Follow fast entertainment technologies
- Build collaborative and immersive environments





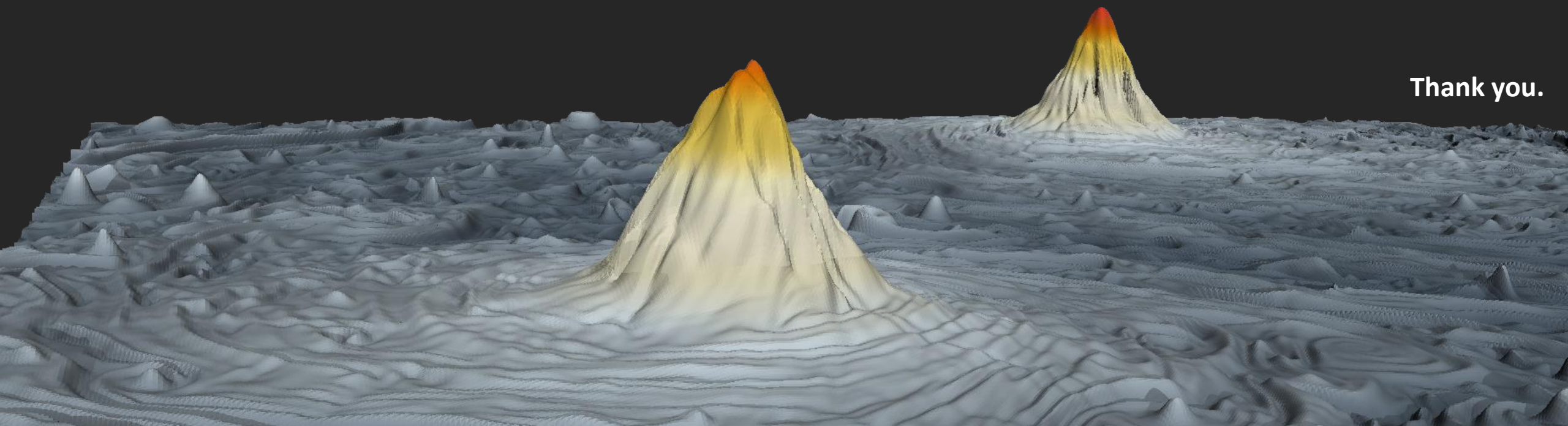
“Intelligence is not the ability to store information, but to know where to find it”

[A.Einstein 1921]



“Have fun with VIS”

[K.Joy 2001]



Thank you.