Visual Exploration of Turbulent Combustion and Laser-Wakefield Accelerator Simulations

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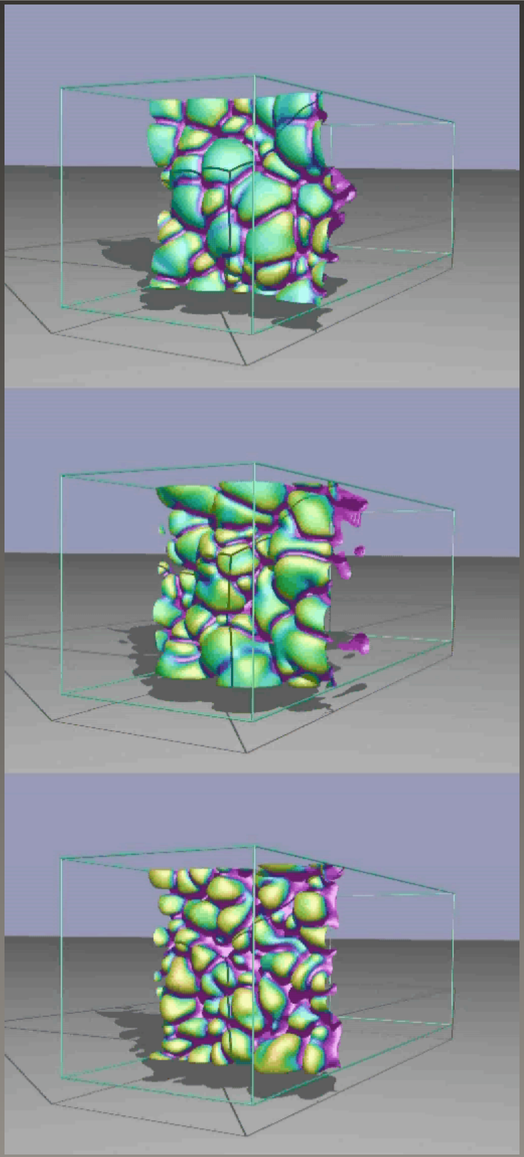
Feature Tracking in Turbulent Combustion Simulations

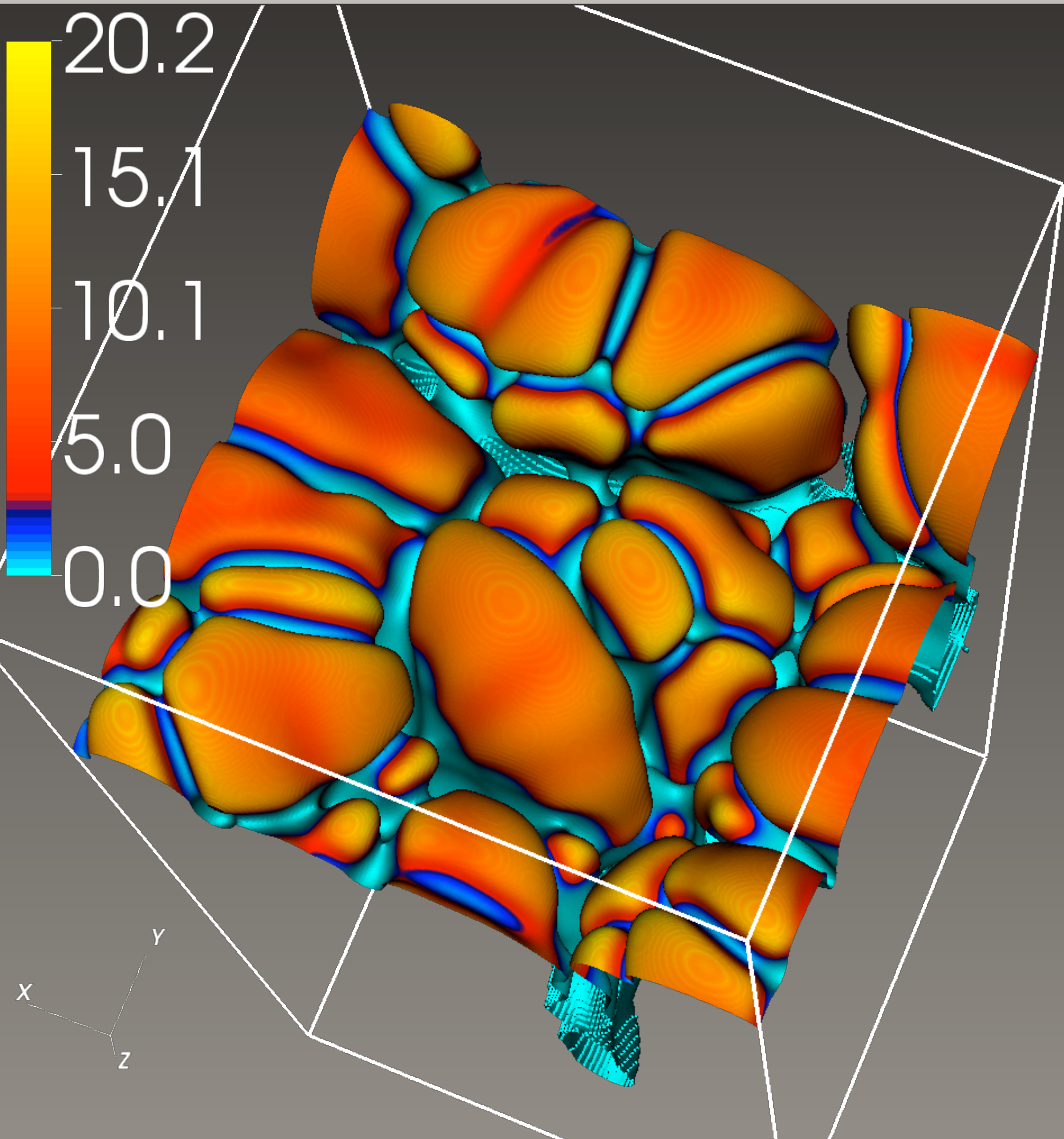
Joint work with
Peer-Timo Bremer (CASC LLNL),
Valerio Pascucci (SCI Institute, University of Utah),
Marcus Day (CCSE LBNL) and
John Bell (CCSE LBNL)

Feature Tracking in Combustion Simulations



- **Application:**
  - Simulation of premixed lean hydrogen flames under different levels of turbulence
  - Lean combustion reduces emissions
  - ➔ Important for engine and power plant design (among other areas)
  - Lean flames burn in cellular mode (non-uniform, time-dependent, difficult to characterize)
- **Scientific Goal:**
  - Understanding the temporal evolution of burning cells
  - Influence of turbulence

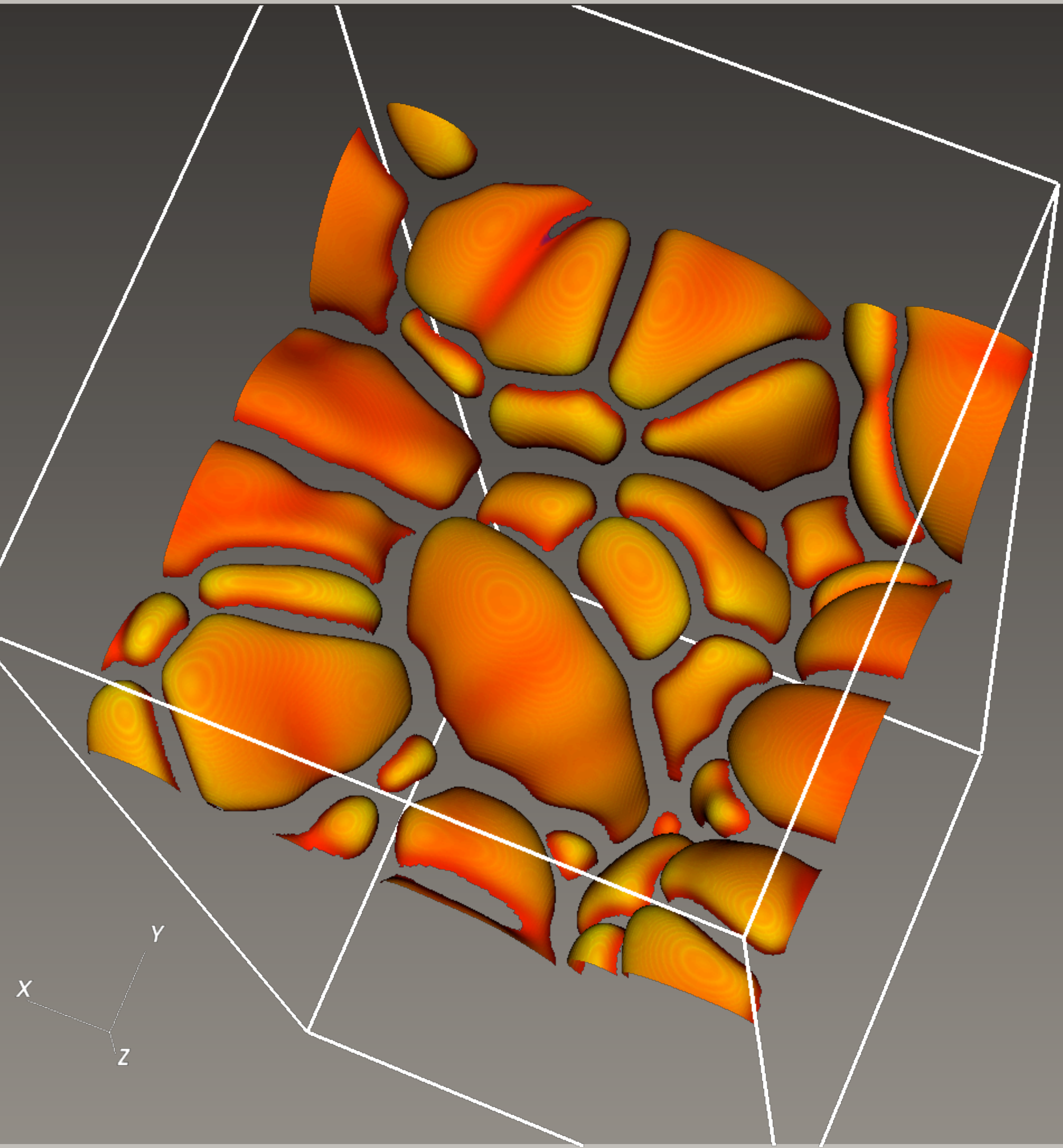
Feature Tracking in Combustion Simulations



- Isotherm represents "flame surface"
- Fuel not evenly consumed: Burning cells separated by extinction regions

- **Interested in evolution of burning cells**

Individual Burning Regions



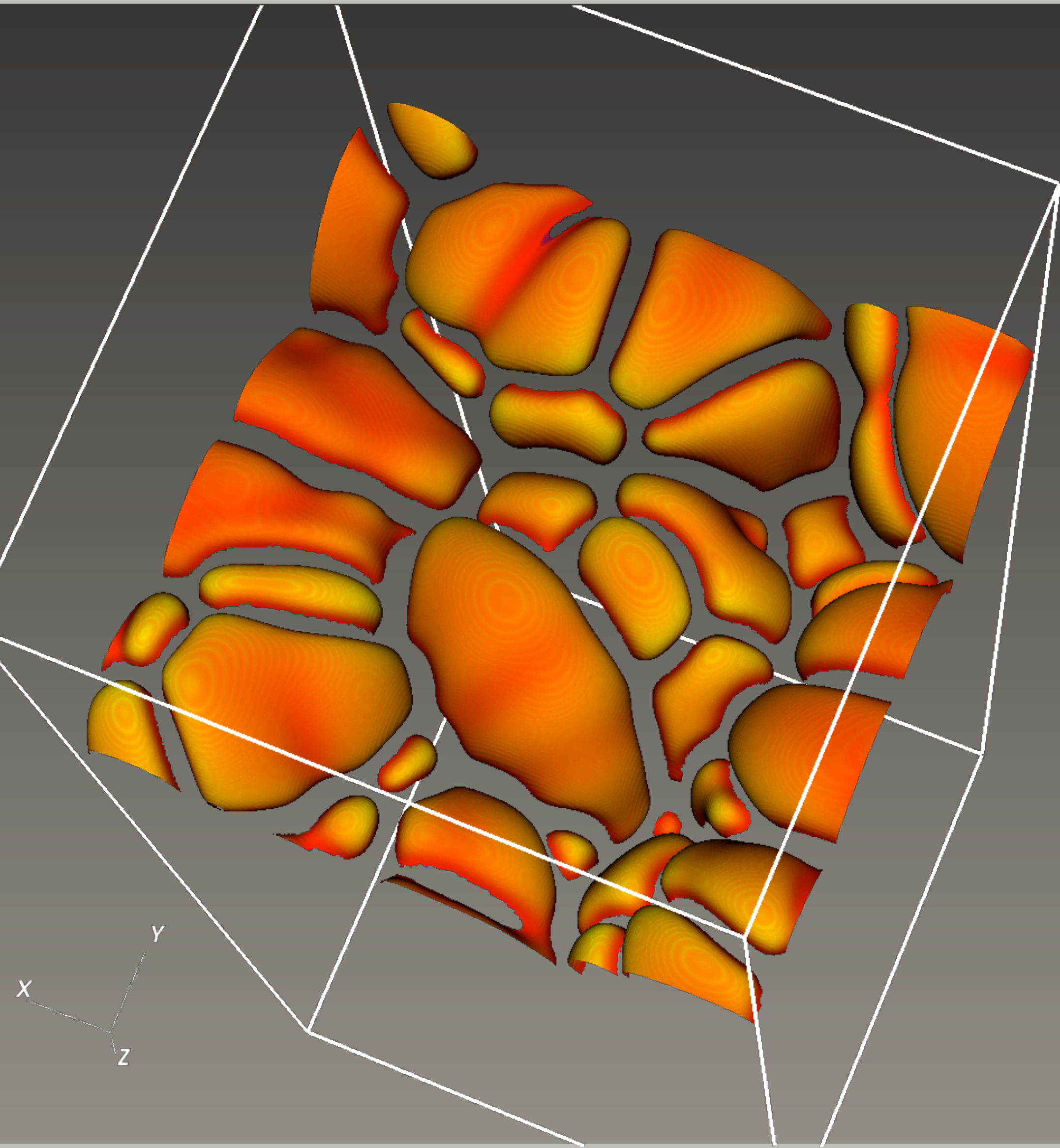
- Threshold isotherm by fuel consumption rate

➔ Burning regions (connected components)

- When do regions emerge, die, split, or merge?

➔ Tracking graph

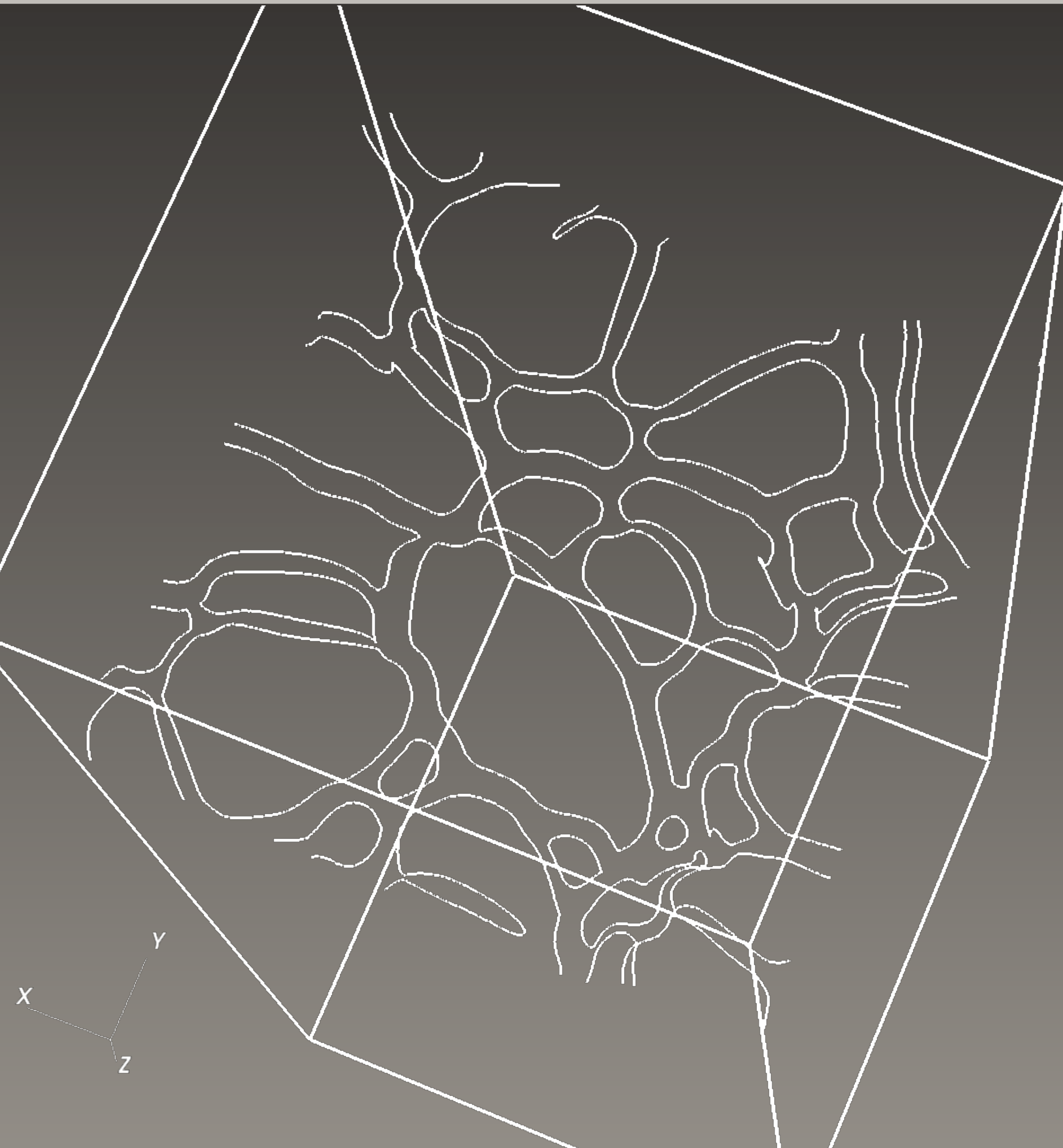
Individual Burning Regions



- Burning cells defined on isotherm
- Isotherm varies over time

➔ Tracking features defined over changing domain

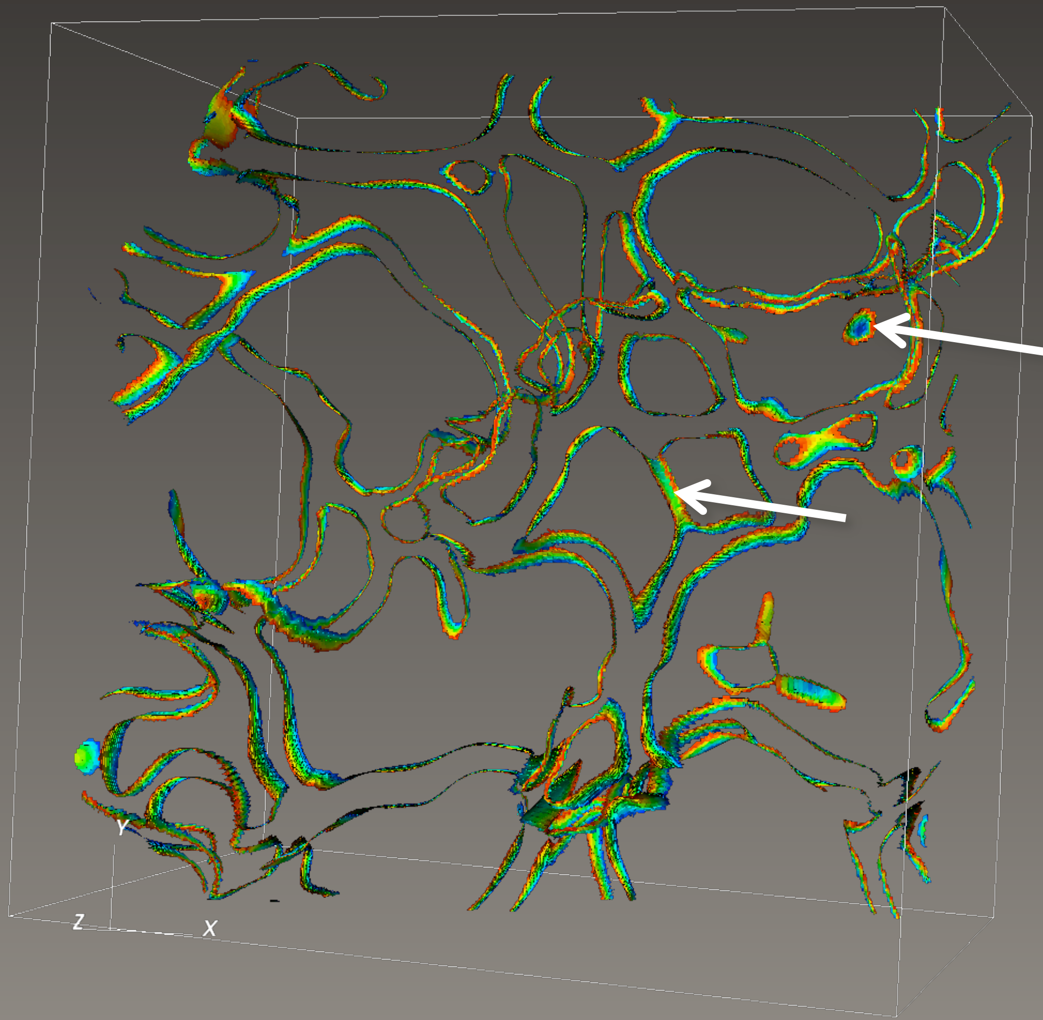
Burning Region Boundaries



- Track burning cells by considering their boundaries
- Obtained by two successive contouring operations

➔ Trace evolution of burning regions by considering contours

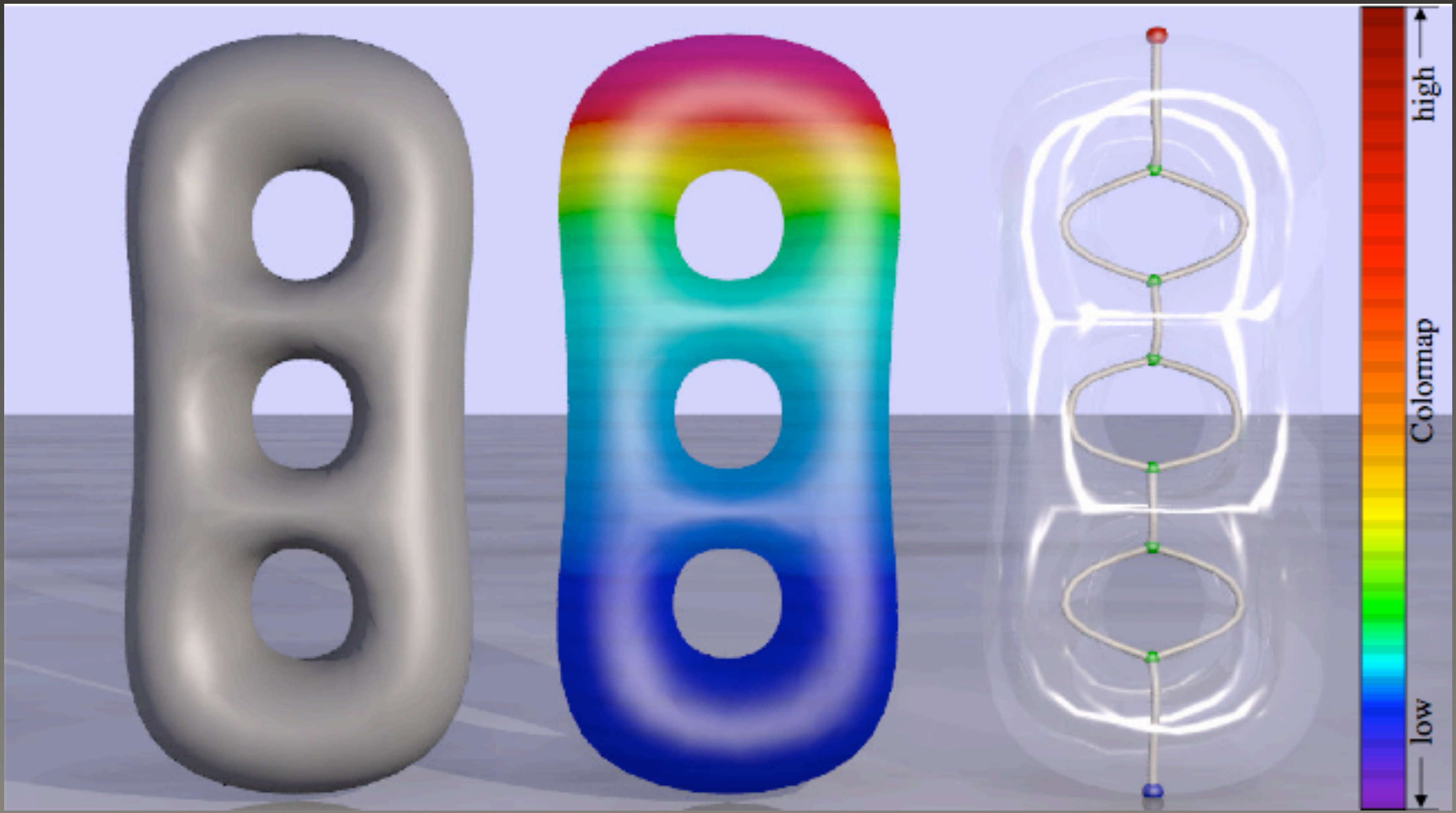
Burning Region Boundaries



- Over time, boundaries create sweep surfaces

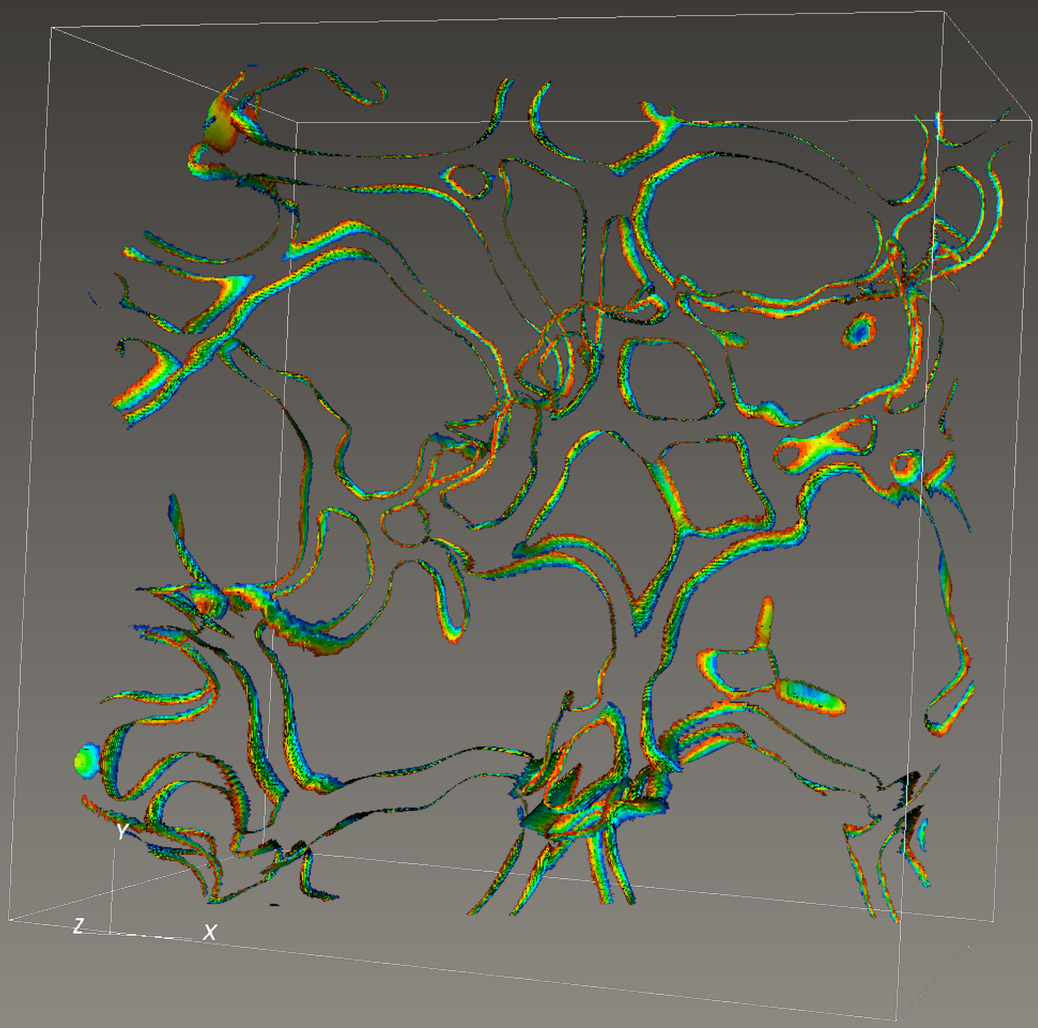
➔ Use Reeb graph (with time as Morse function)

Reeb Graph



[Reeb 1946, Sur les Points Singuliers d'une Forme de Pfaff Complétement Intégrable ou d'une Fonction Numérique]

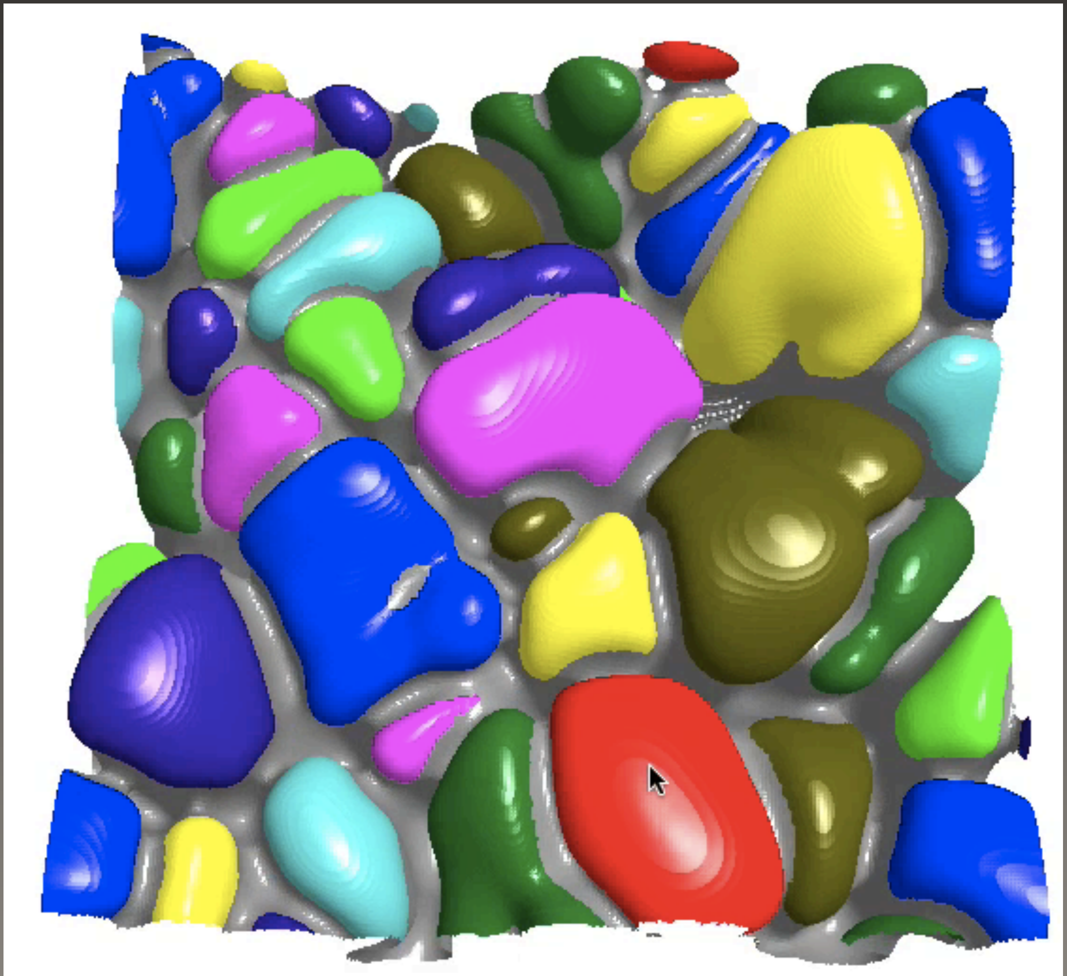
Burning Region Boundaries



- Over time, boundaries create sweep surfaces

➔ Use Reeb graph (with time as Morse function

Classification via Segmentation

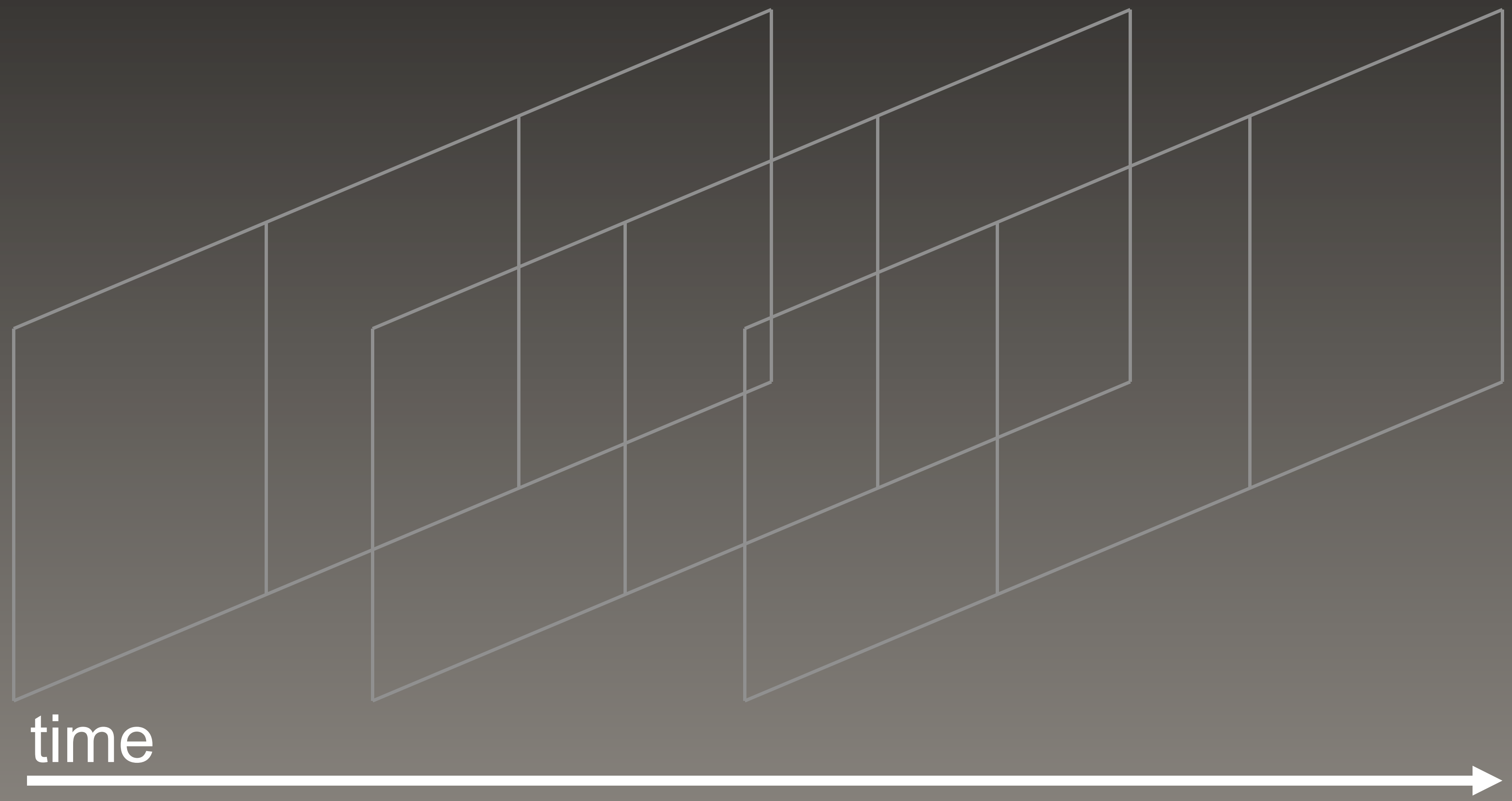


[Bremer et al., to appear in IEEE TVCG, Analyzing and tracking burning structures in lean premixed hydrogen flames]

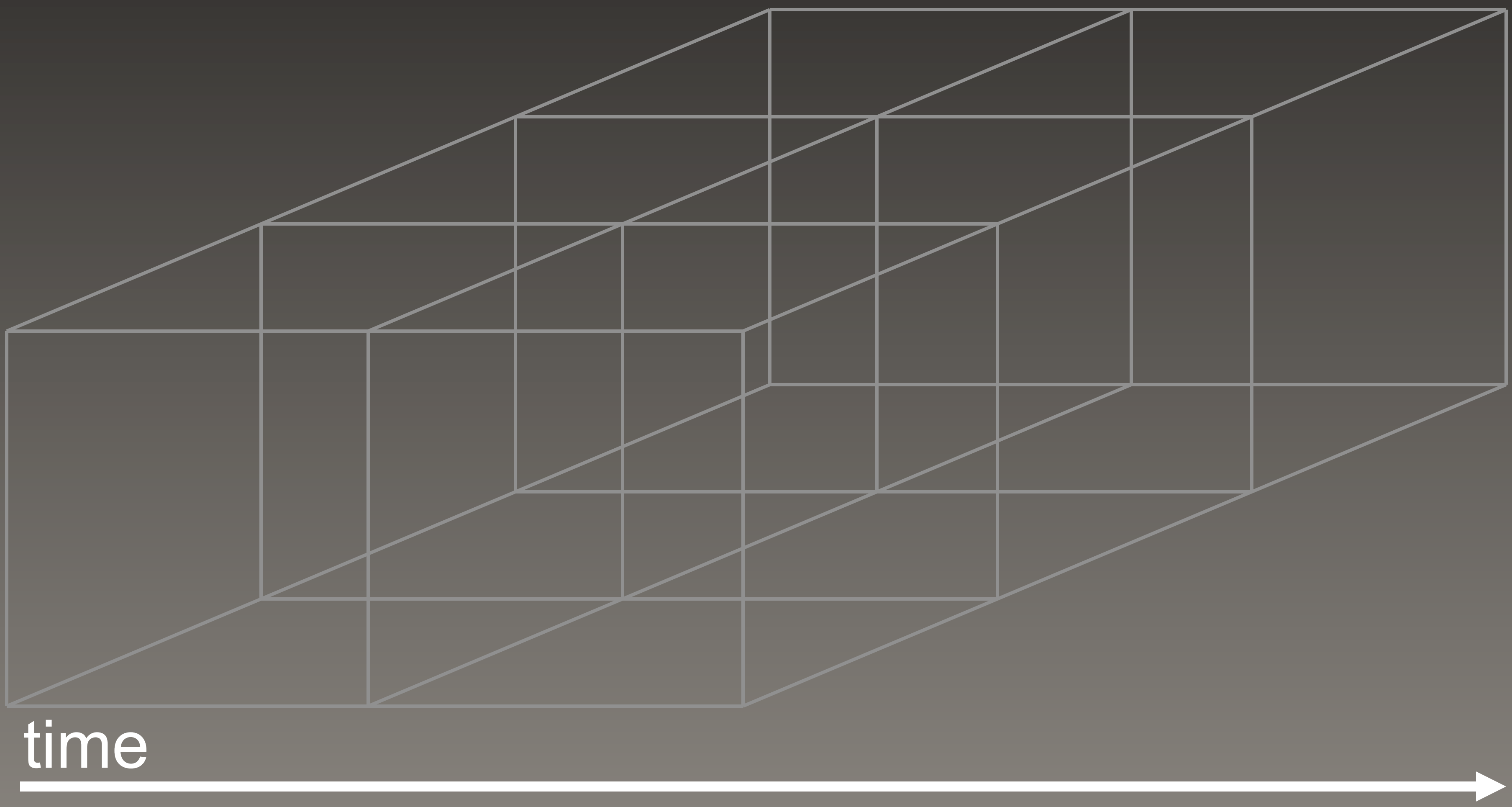
Tracking Graph Extraction Pipeline

1. Concatenate to obtain 4D mesh
2. Extract isotherm in 4D
3. Extract isotherm for original time steps
4. Segment vertices on 3D isosurface
5. Classify 4D isosurface vertices between time steps
6. Construct boundary surface
7. Extract Reeb-graph
8. Simplify Reeb-graph

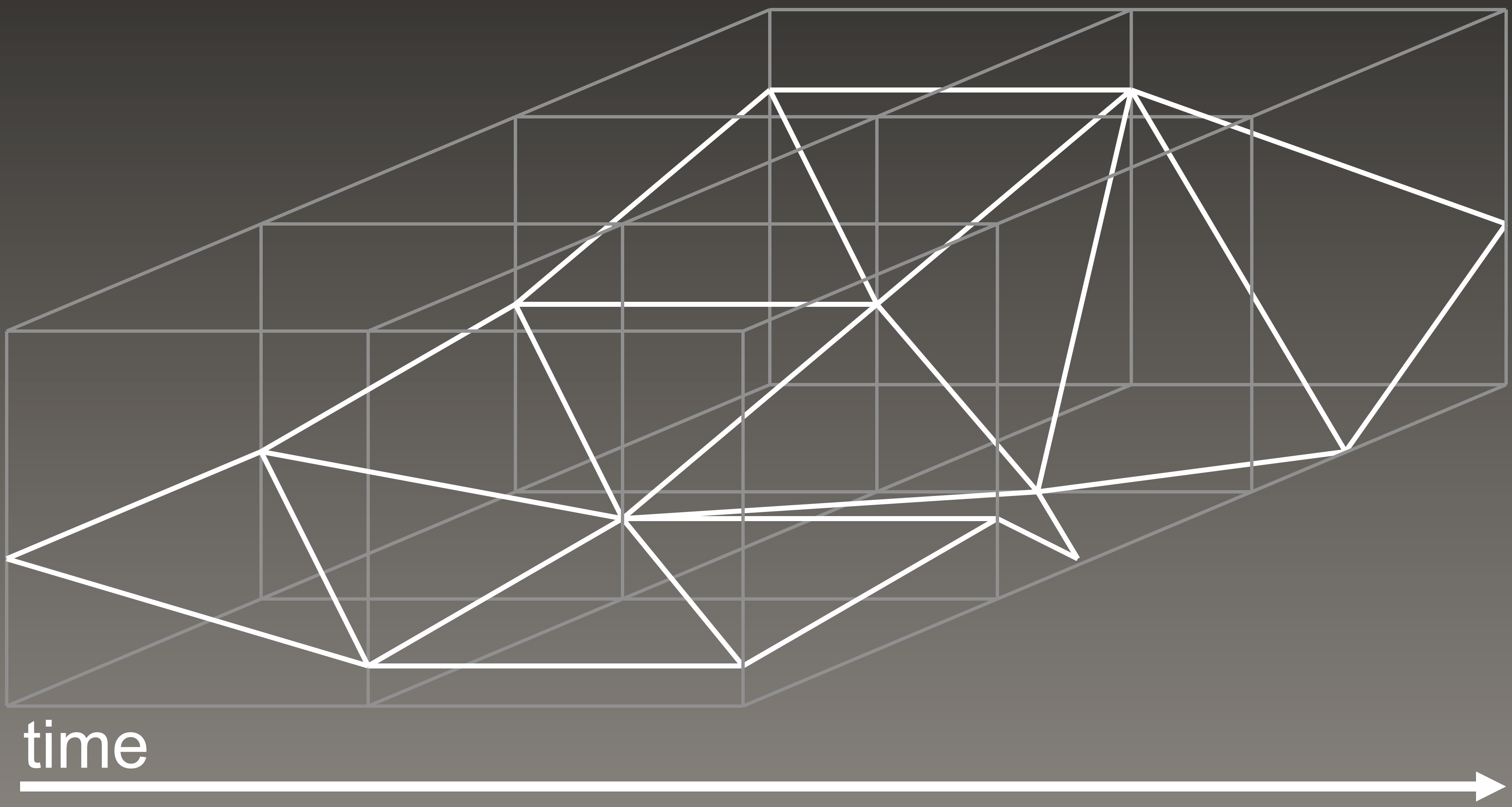
1. Concatenate Time Steps



1. Concatenate Time Steps

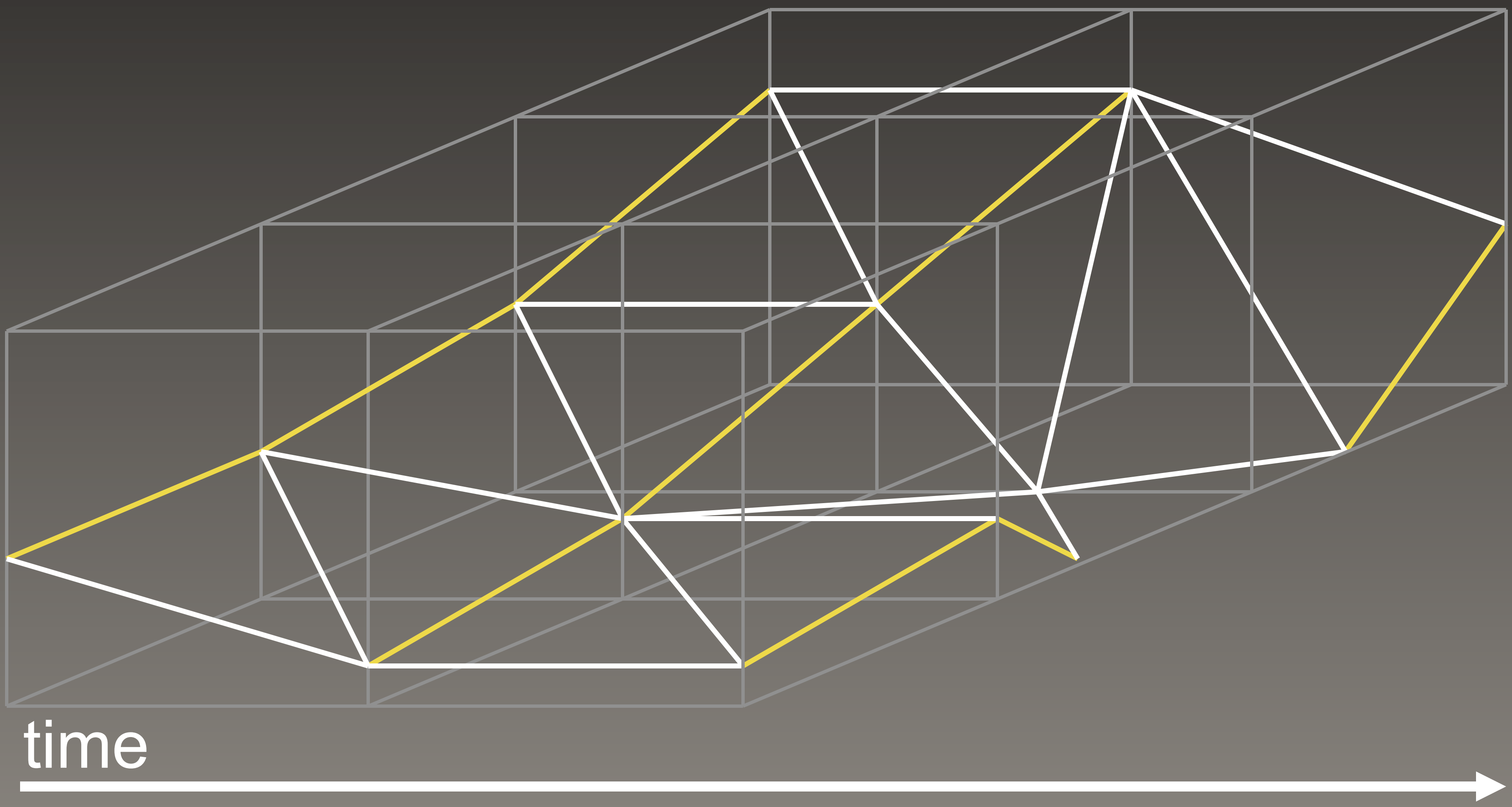


2. Extract Time Surface with Associated Fuel Consumption Values

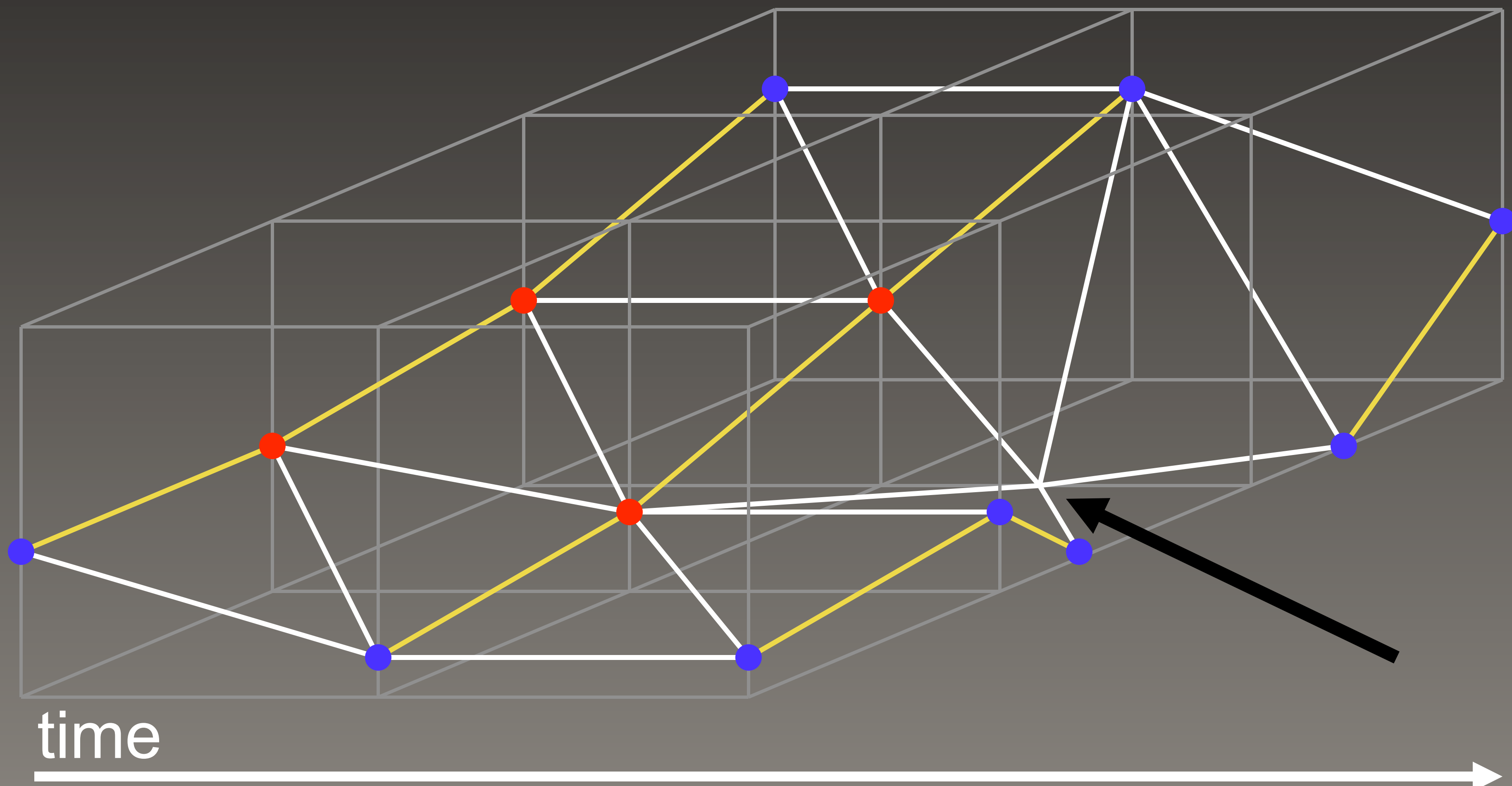


[Bhaniramka et al., IEEE TVCG 2004: Isosurface construction in any dimension using convex hulls]

3. Extract Isosurface in Original Time Steps – Filter Operation

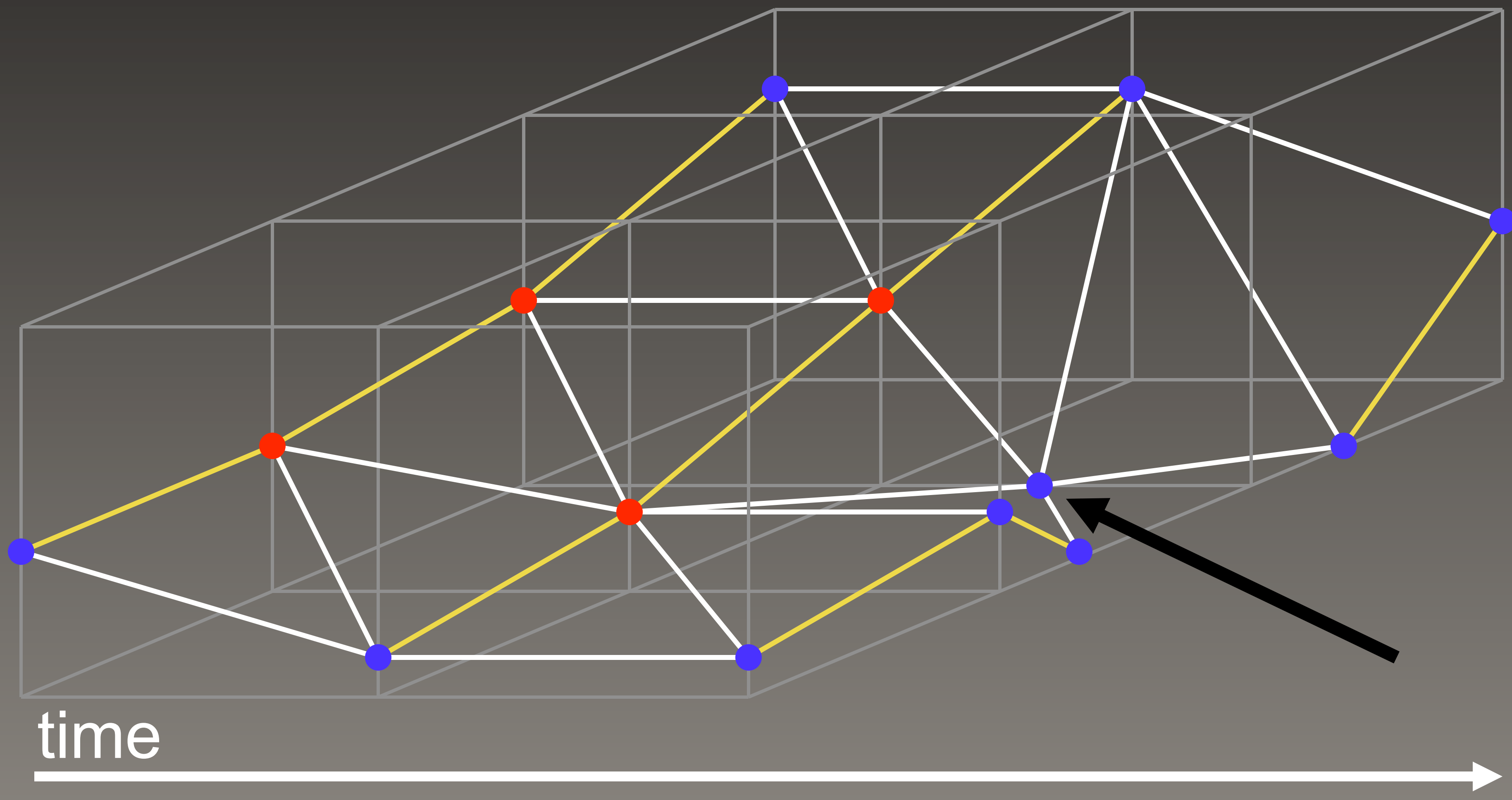


4. Classify 3D Isosurface Vertices – Compute Segmentation within Time Steps

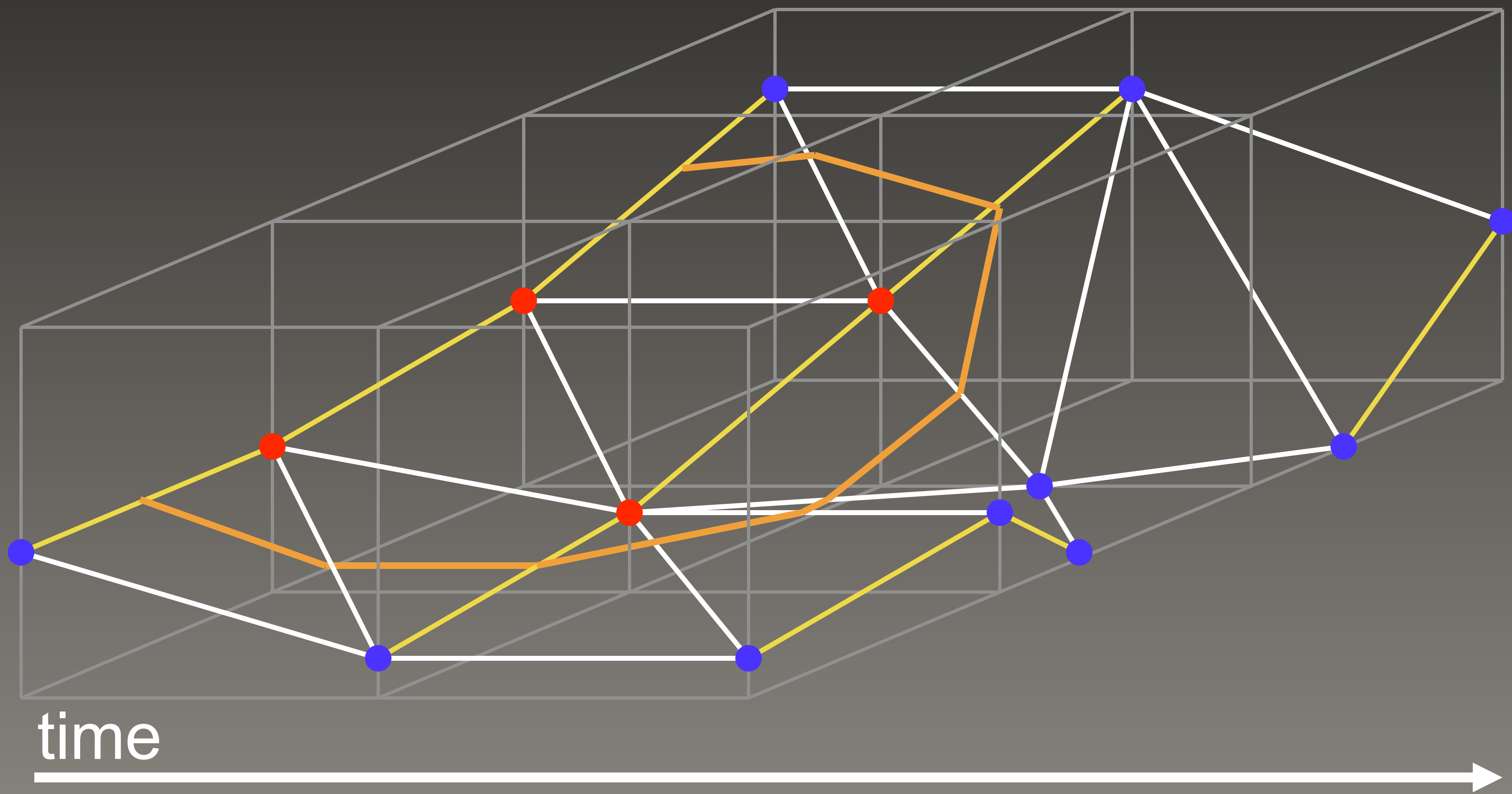


[Bremer et al., submitted to IEEE TVCG, Analyzing and tracking burning structures in lean premixed hydrogen flames]

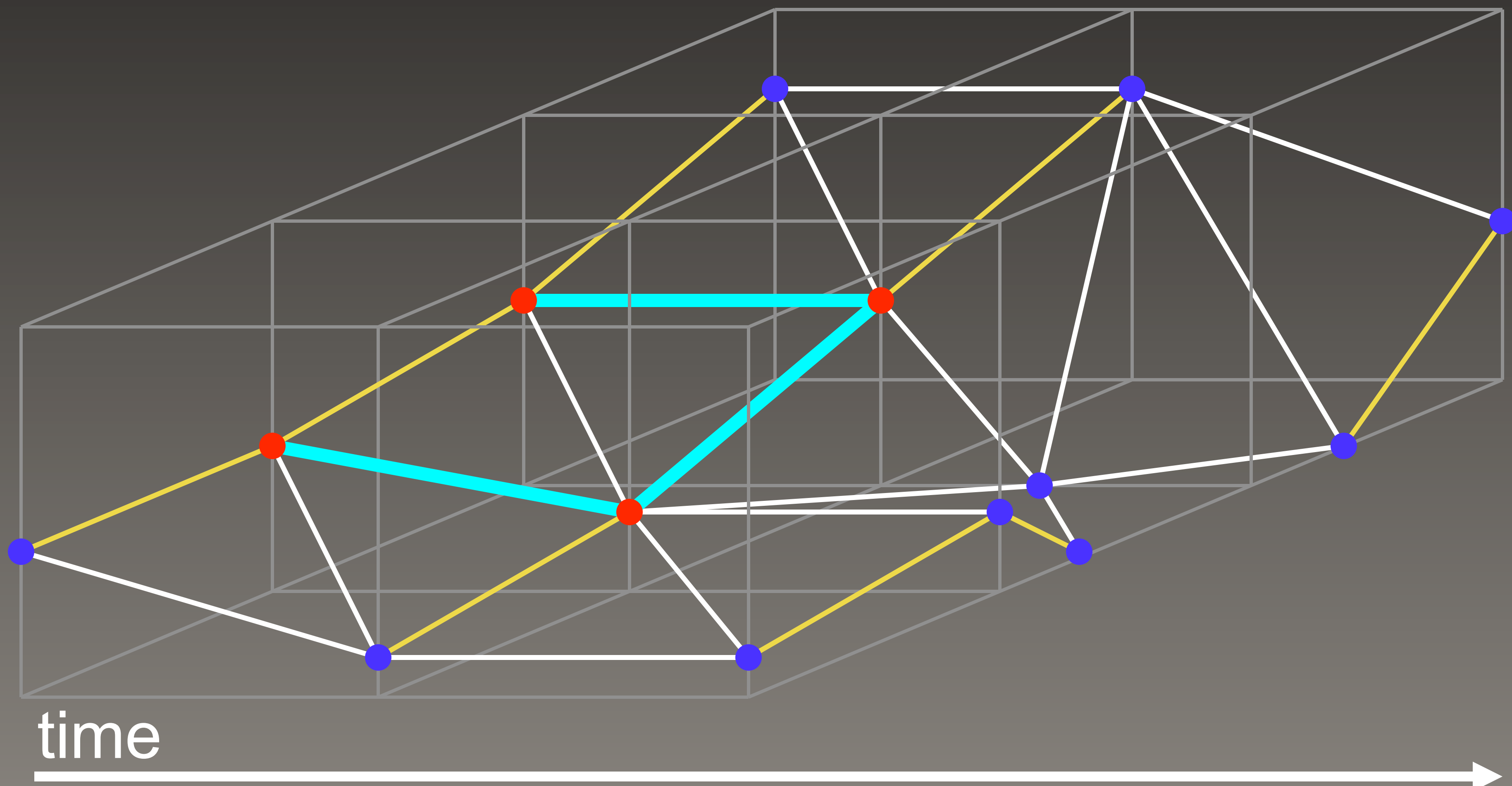
5. Classify 4D Time Surface Vertices Between Time Steps – Simple Thresholding



6. Construct Swept Boundary – "Correct"

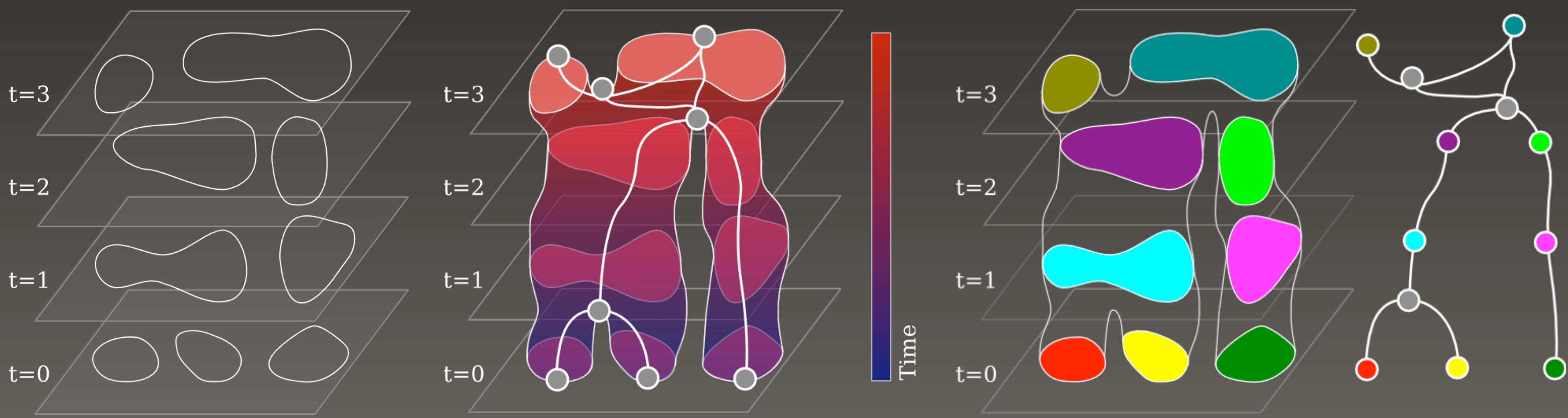


6. Construct Swept Boundary – Snapped to Vertices



- Preserve connectivity
- Simple case table
- Reuse isosurface vertices (intersection points along original grid edges)

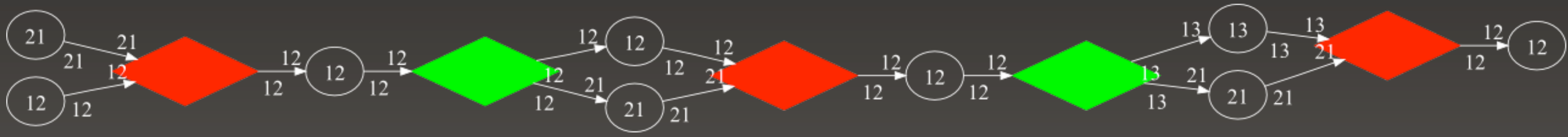
7. Compute Fully Augmented Reeb Graph



- Within each time step unique id per burning region
- Between time steps id not necessarily consistent
- Augment with degree two nodes to preserve correlation between graph and segmentation (and enable genus determination)

[Pascucci et al., ACM SIGGRAPH 2007: Robust On-line Computation of Reeb Graphs: Simplicity and Speed]

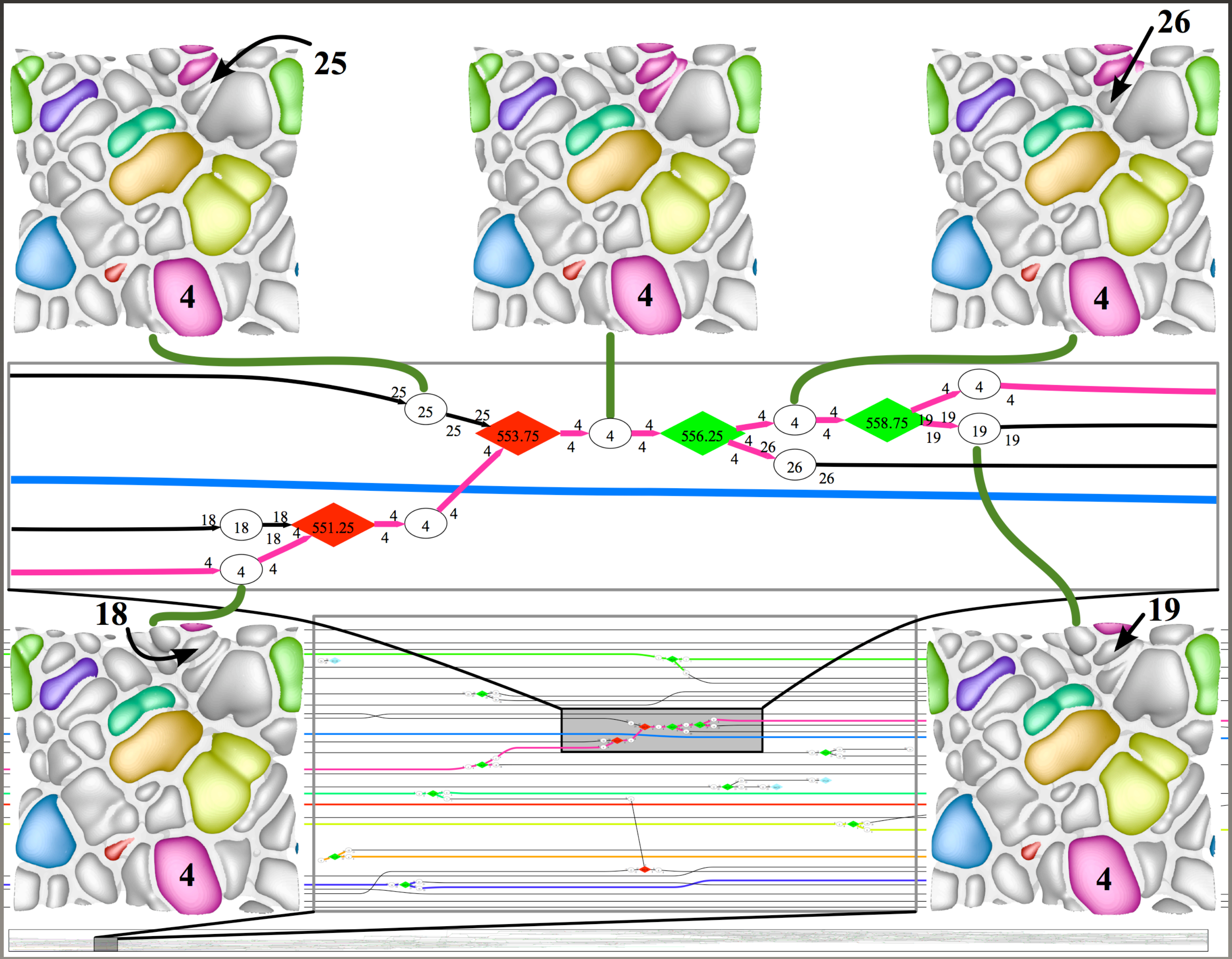
8. Simplify Reeb Graph



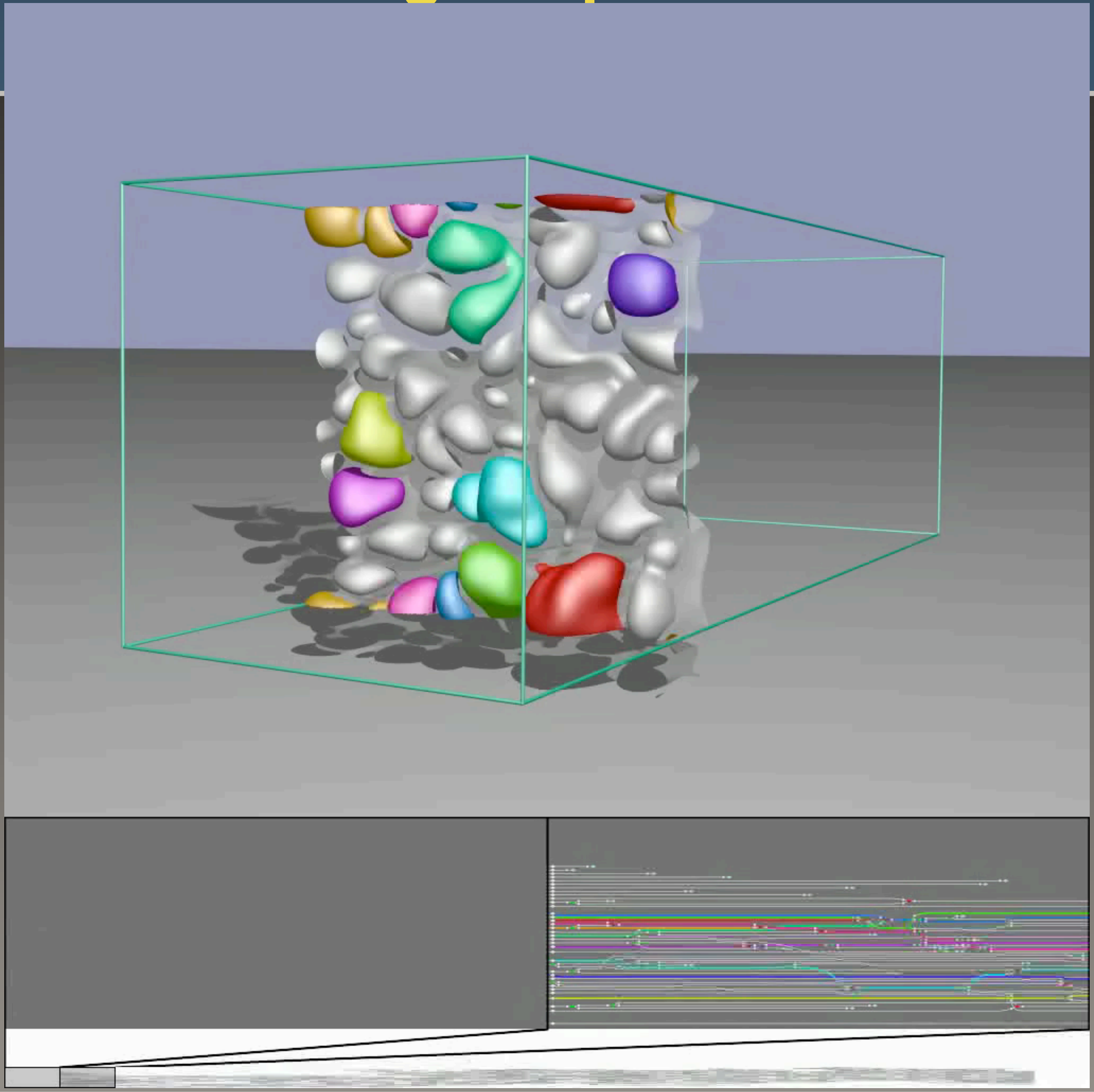
- Simplify loops that span less than one full time step
- Remove all loops spanning exactly one full time step
- Remove features with life span less than two time steps
- Construct simplified graph and layout using GraphViz

- Still "extended" merge/split events
  – Several split/merge events before "full" split/merge

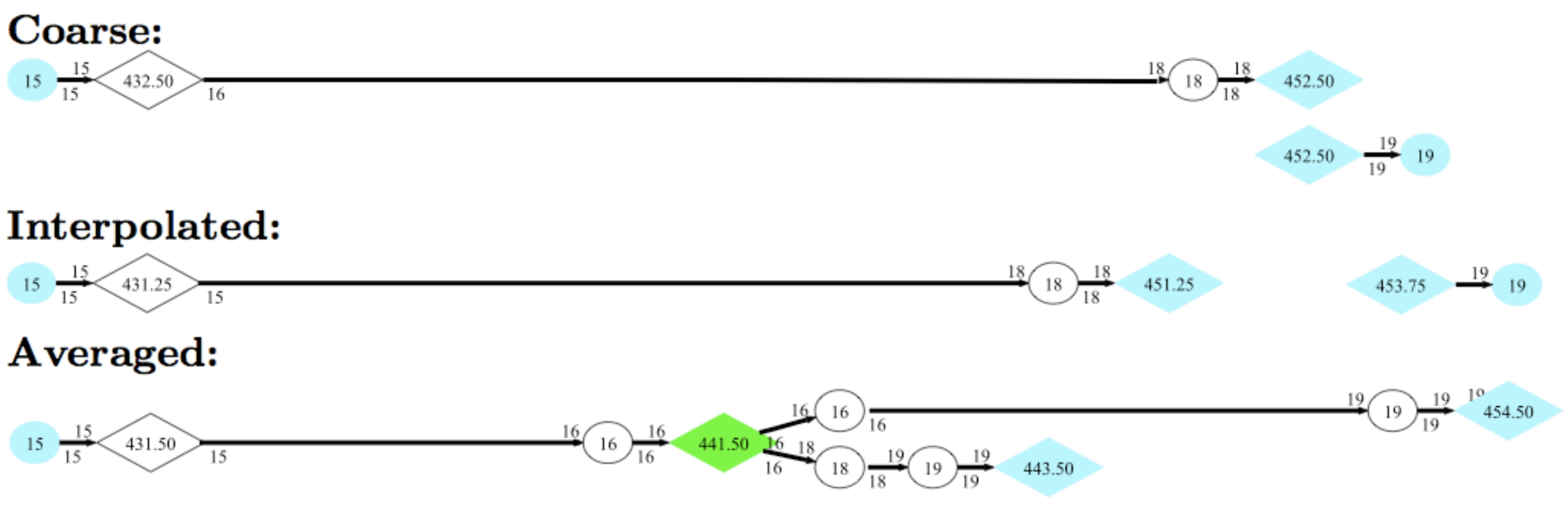
Tracking Graph Example



Tracking Graph – Movie

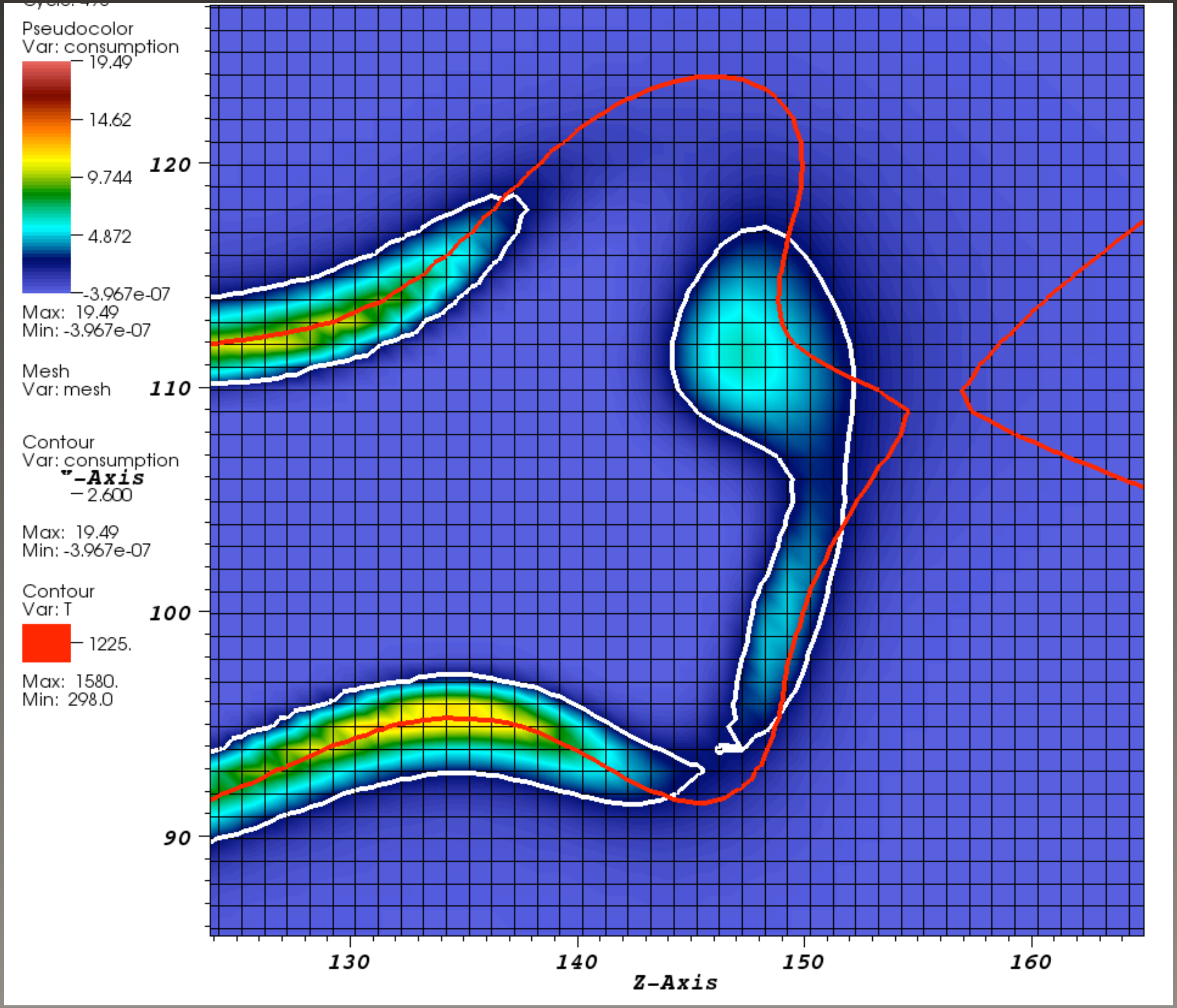


Tracking Graph Comparison – Example

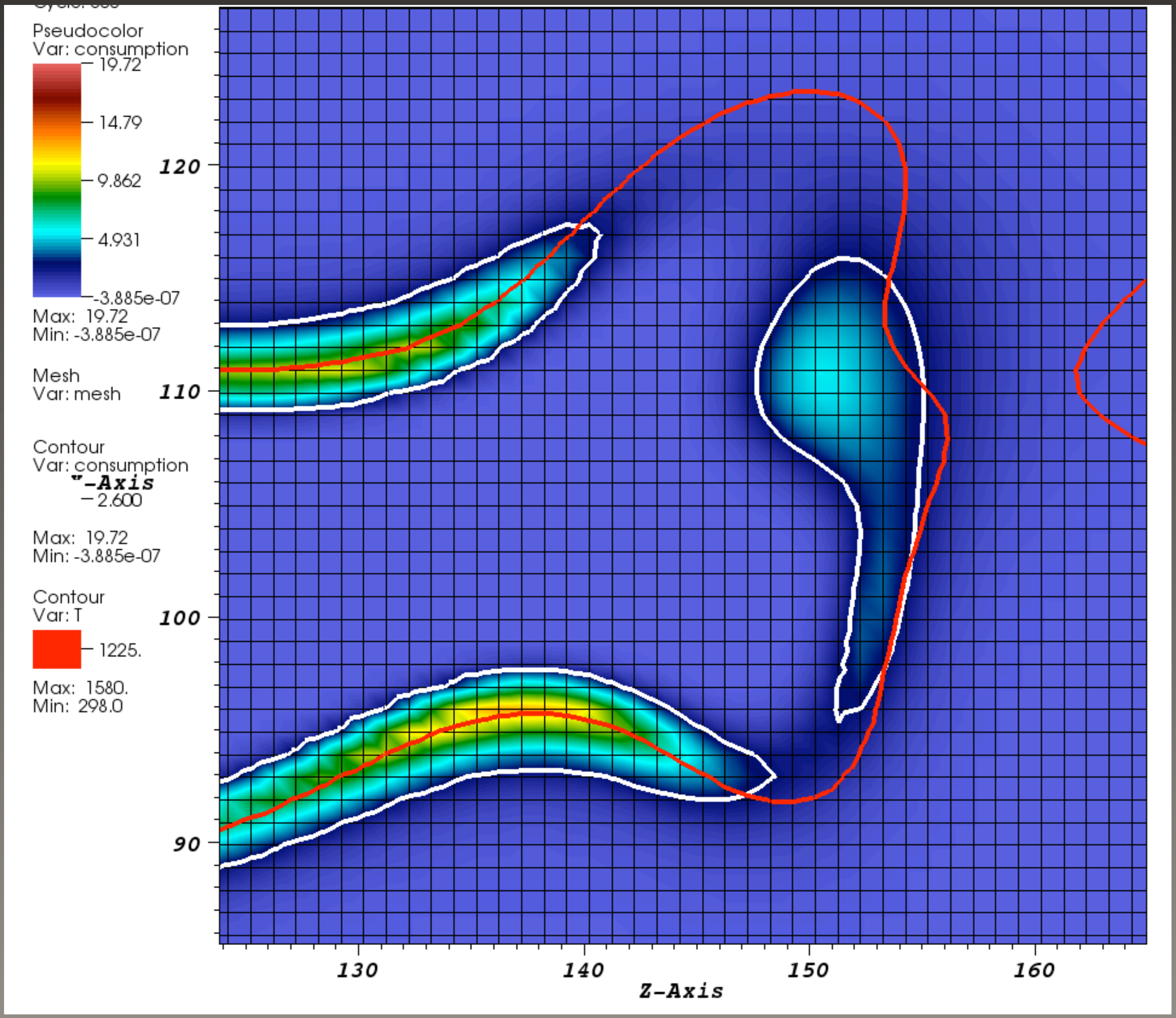


- Coarse: Use original data set
- Interpolated: Create intermediate time steps using linear interpolation
- Averaged = “Ground Truth”: Use finer simulation with more time steps and downsample

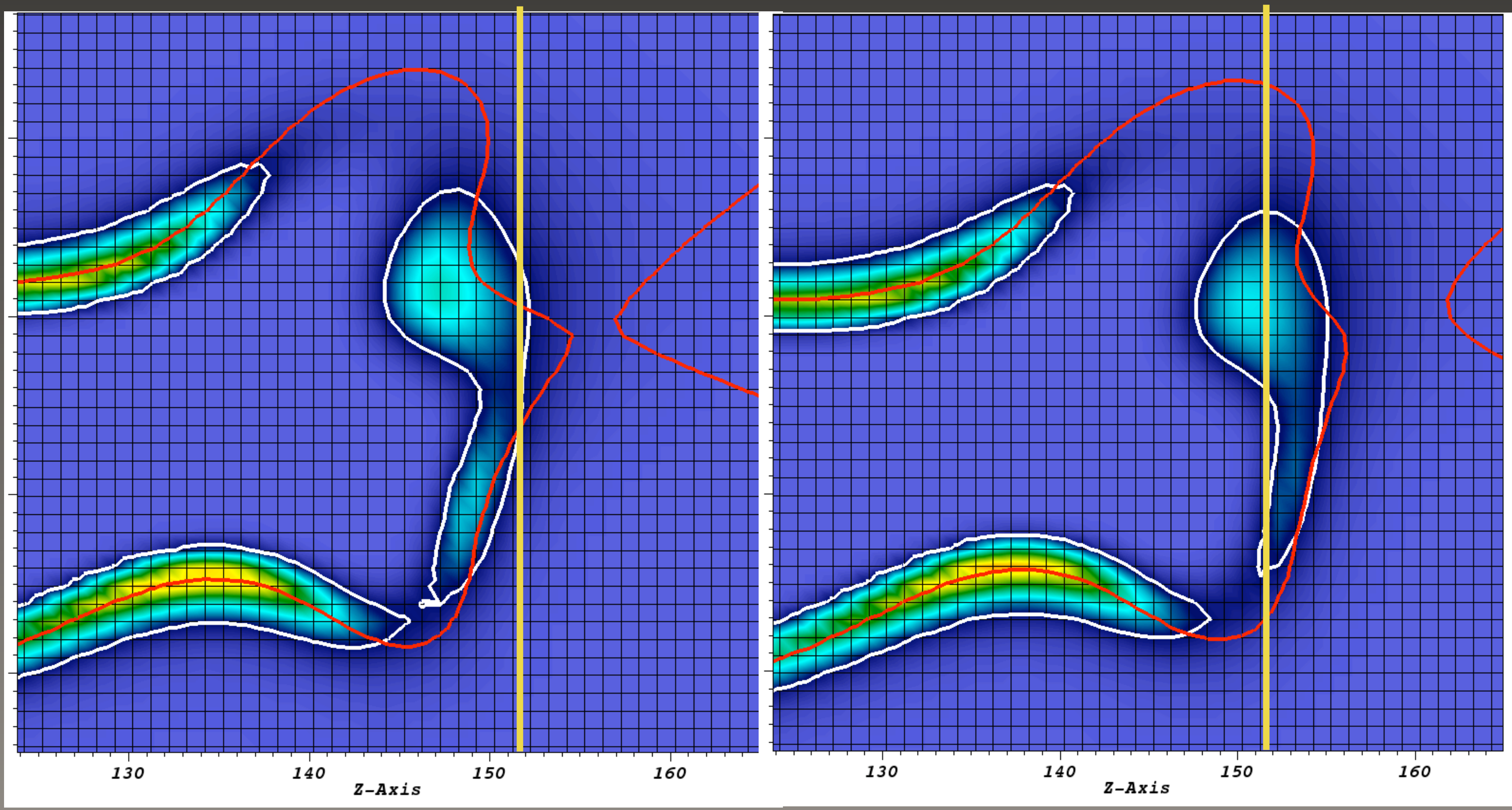
Lost Tracking Explained



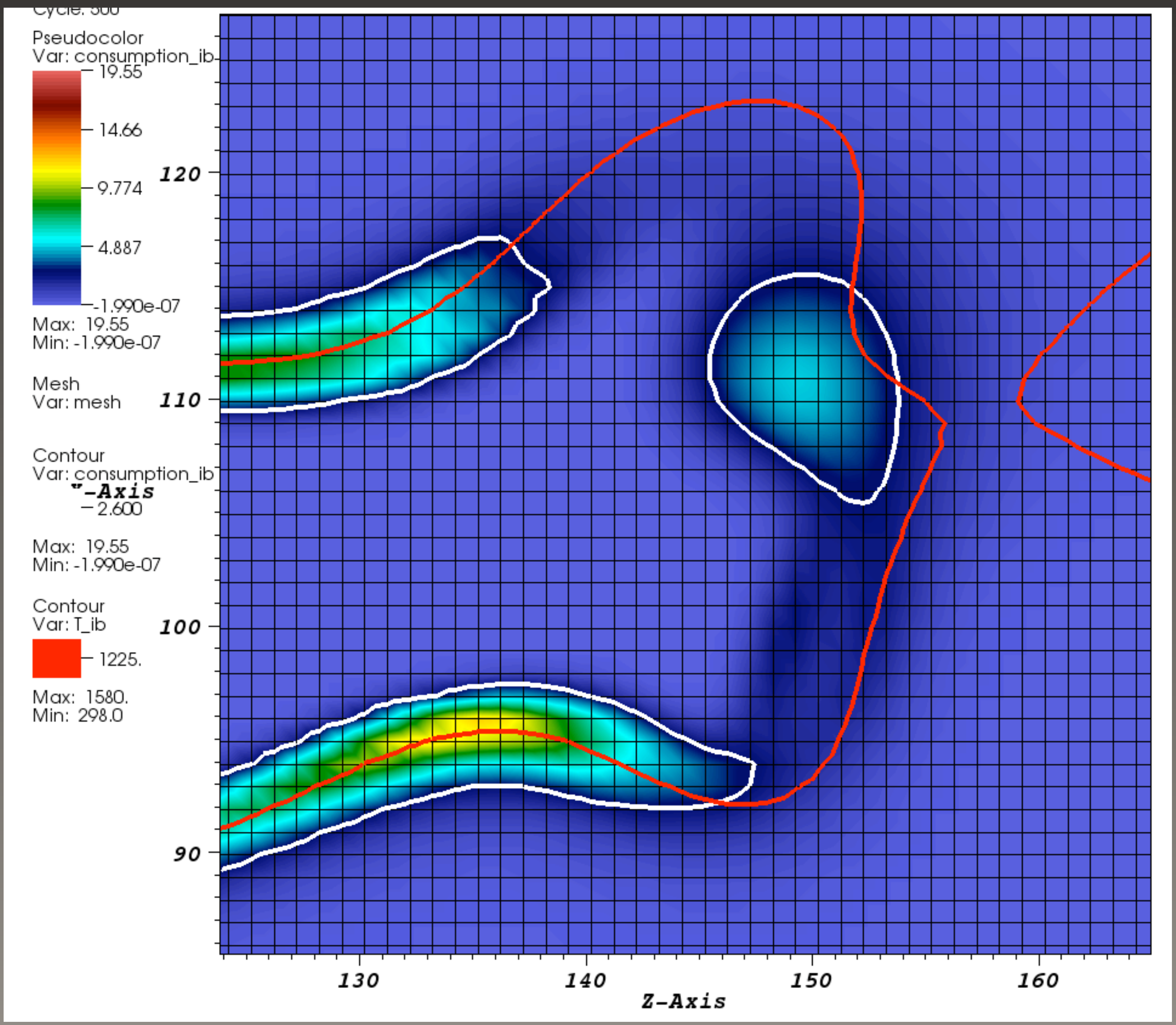
Lost Tracking Explained



Lost Tracking Explained



Lost Tracking Explained



Tracking Graph Comparison – Summary

- During period where fine data available approximately 29 burning regions existed in the domain
- Tracking graphs for 16 of these 29 regions differed between various analysis approaches
  - 3 differences due to data differences between coarse and fine simulation
  - 2 differences due to merging and splitting between coarse time steps
  - 1 difference: region splitting of and dying between coarse time steps
- Discounting those: correct tracking for 19 out of 29 regions
- Other problems mainly due to lack of temporal resolution

Related Work in Feature Tracking

- [Mascarenhas & Snoeyink, 2008] Comprehensive overview of isosurface tracking
- [Samtaney et al., 1994] track thresholded regions with image processing techniques
- [Silver & Wang, 1997 & 1998] use volume for correspondence
- [Laney et al., 2006] use similar approach for tracking in turbulent mixing
- [Reinders et al., 2001] use motion prediction to improve tracking
- [Ji et al., 2003 & 2004] extract time surface and use its connected components to track features

Related Work in Feature Tracking

- [Edelsbrunner et al., 2004] compute time-varying Reeb graphs using Jacobi [Edelsbrunner et al., 2002] sets to correlate critical points
- [Szymczak, 2005] presents related techniques for contour trees
- [Sohn and Bajaj, 2006] use a hybrid approach also defining correspondences between contour trees using volume matching similar to Silver & Wang.
- Also related work in tracking critical points in vector field analysis [Tricoche et al, 2000; Theisel et al., 2003; Garth et al., 2004 ; Weinkauf et al., 2005]

Turbulent Combustion Simulations – Conclusions and Future Work

- **Conclusions**
  - Tracking works if temporal resolution sufficient
  - Artifacts due to insufficient temporal resolution easy to recognize
  - Analysis on isotherm aggravates tracking problems somewhat, but fast moving burning zones would also cause problem to full 3D analysis

- **Future Work**
  - Presentation
    - Layout of tracking graphs
    - Link graphs and physical segmentation views
  - Analysis
    - Integrate with simulation (access to more time steps)
    - Use graphs to compute derived quantities
    - Operate directly on Adaptive Mesh Refinement data
    - Full 3D analysis eliminating need to restrict to isotherm (fewer varying parameter choices)

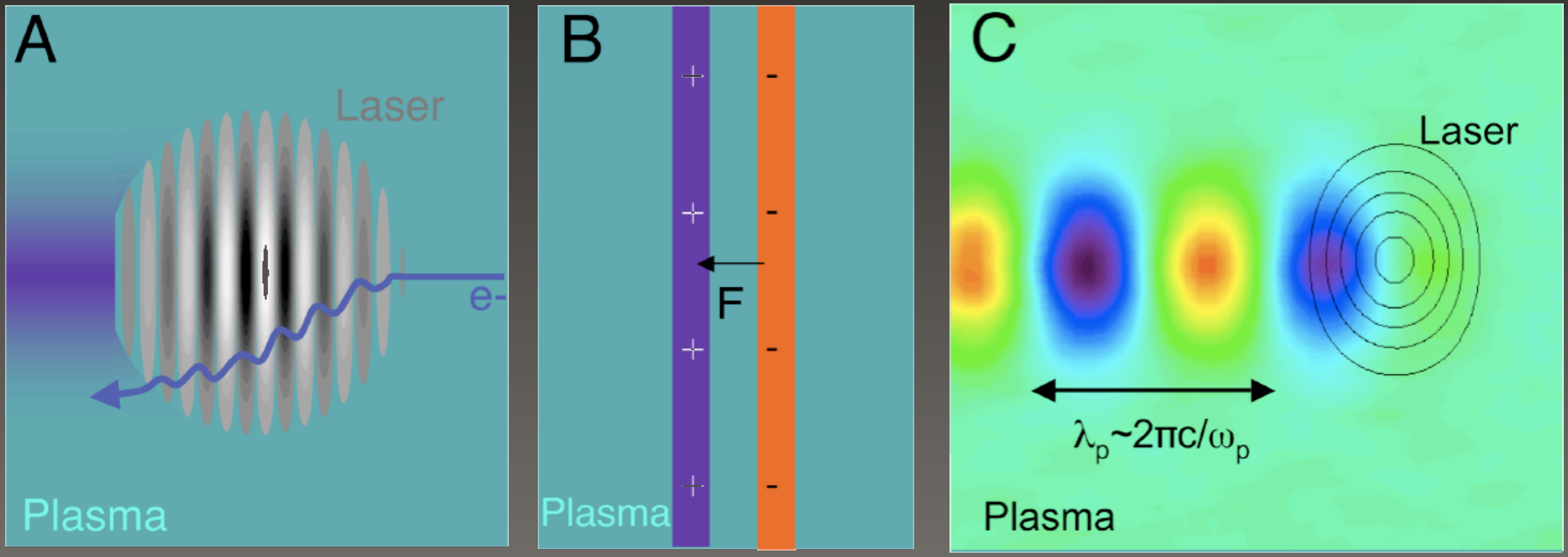
Analysis of Large-Scale Laser Wakefield Particle Acceleration Simulation

Joint work with

Oliver Rübel[1,2,3], Prabhat[1], Kesheng Wu[1], Hank Childs[1], Jeremy Meredith[4], Cameron G. R. Geddes[5], Estelle Cormier-Michel[5], Sean Ahern[4],Peter Messmer[6], Hans Hagen[2], Bernd Hamann[3,2,1] and E. Wes Bethel[1,3]

1. Computational Research Division, Lawrence Berkeley National Laboratory (LBNL)
2. International Research Training Group 1131, University of Kaiserslautern, Germany
3. Institute for Data Analysis and Visualization, University of California, Davis
4. Oak Ridge National Laboratory (ORNL)
5. LOASIS program of Lawrence Berkeley National Laboratory
6. Tech-X Corporation

Laser Wakefield Particle Acceleration (1/2)



Reference:
C.G.R. Geddes, C. Toth, J. van Tilborg, E. Esarey, C. Schroeder, D. Bruhwiler, C. Nieter, J. Cary, and W. Leemans, “High-Quality Electron Beams from a Laser Wakefield Accelerator using Plasma-Channel Guiding,” *Nature,* vol. 438, pp. 538-541, 2004

Laser Wakefield Particle Acceleration (2/2)

[Image courtesy of http://worldwakesurfingchampionships.com]

- **Advantages:**
  Can achieve electric fields thousands of times stronger than in conventional accelerators

➔ Can achieve high acceleration over very short distance.

Laser Wakefield Particle Acceleration

Simulation

- Performed over 2D and 3D domains using the VORPAL code
- Simulations restricted to window covering only a plasma subset in x direction in beam vicinity
- Simulation window moves along local x axis
- Produces particle and field data (at typically 40-100 timesteps)

Particle data

- Scattered data with particle location, momentum and identifier

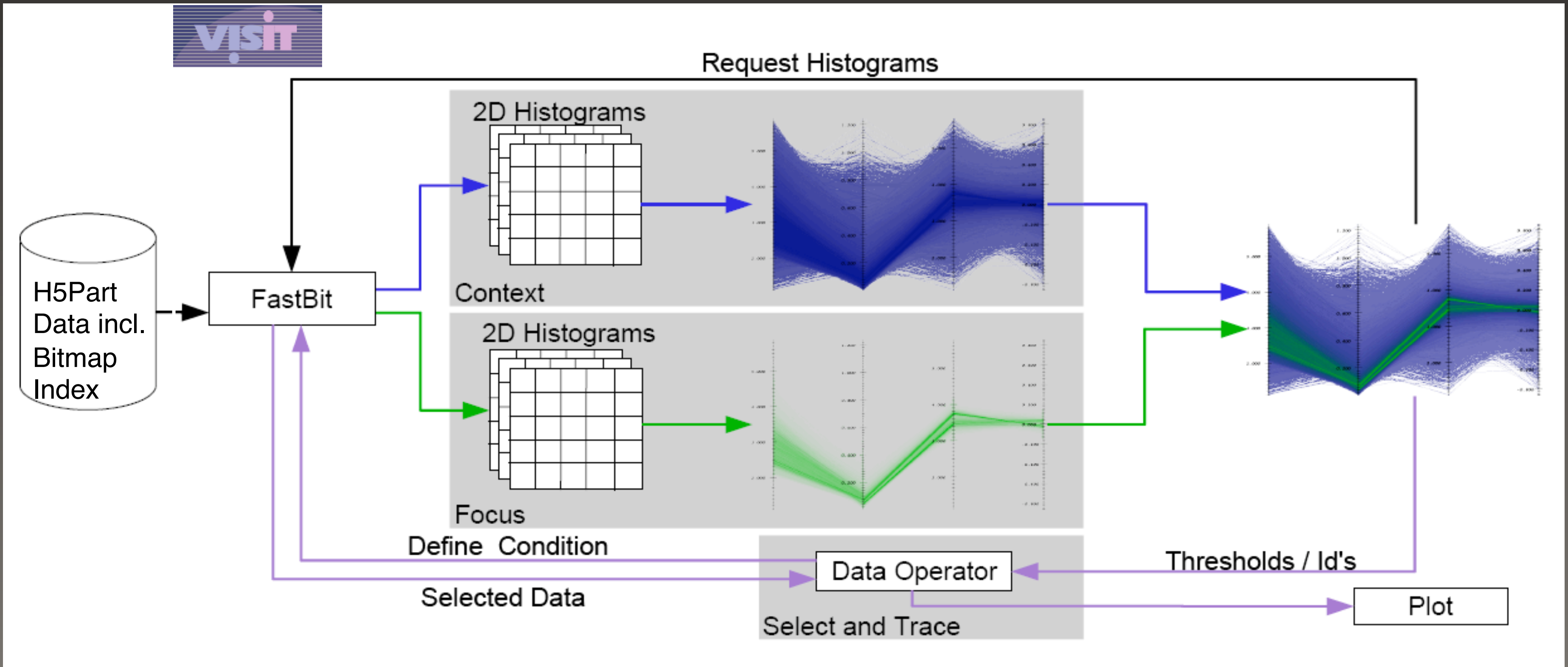
  ~ $0.4*10^6$ – $30*10^6$ (in 2D) and ~$80*10^6$ – **$200*10^6$** (in 3D) per time step

  ➔ Total size: ~1.5GB – >30GB (in 2D) and ~100GB – **>1TB** (in 3D)

Field data

- Electric field, magnetic field, and RhoJ (regular grid)
  - Resolution: Typically ~0.02-0.03μm longitudinally, and ~ 0.1-0.2μm transversely
  - Total size: ~3.5GB - >70GB (in 2D) and ~200GB - >2TB (in 3D)

System Design



References:

- VisIt is available from https://wci.llnl.gov/codes/visit/
- FastBit is available from https://codeforge.lbl.gov/projects/fastbit
- H5Part is available from http://h5part.web.psi.ch/ or http://vis.lbl.gov/Research/AcceleratorSAPP/

Data Selection via FastBit

Value	b_0	b_1	b_2	b_3	b_4	b_5
0	**1**	0	0	0	0	0
1	0	**1**	0	0	0	0
5	0	0	0	0	0	**1**
3	0	0	0	**1**	0	0
1	0	**1**	0	0	0	0
2	0	0	**1**	0	0	0
4	0	0	0	0	1	0
…						
	=0	**=1**	**=2**	**=3**	**=4**	**=5**

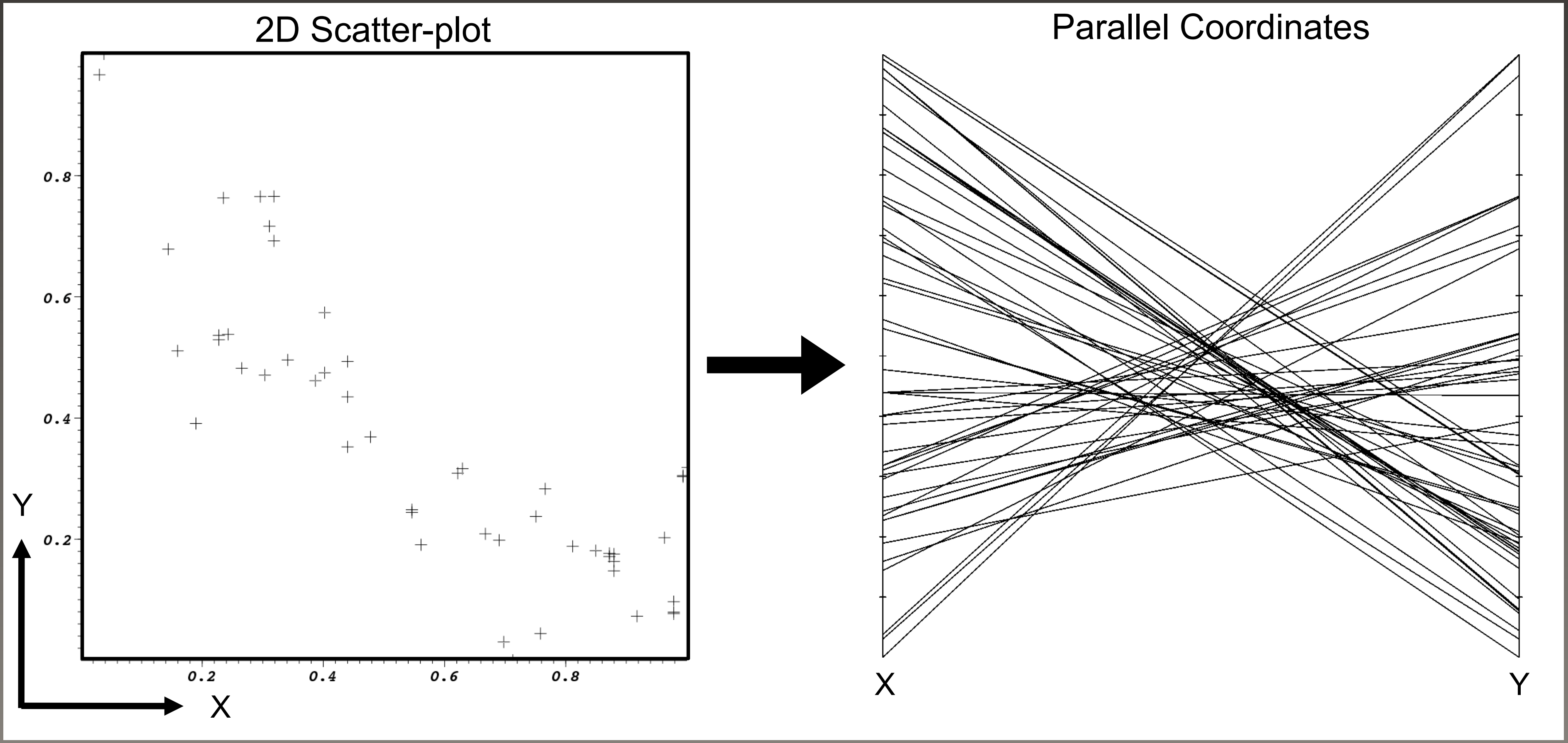
- Use FastBit to accelerate:
  - Computation of conditional histograms for parallel coordinate rendering
  - Multi-dimensional threshold queries for particle of interest identification
  - ID-queries for tracing of particles over time:

Reference: K. Wu, E. Otoo, and A. Shoshani, "Compressing bitmap indexes for faster search operations", ACM Transactions on Database Systems, vol 31, pp. 1-38, 2006

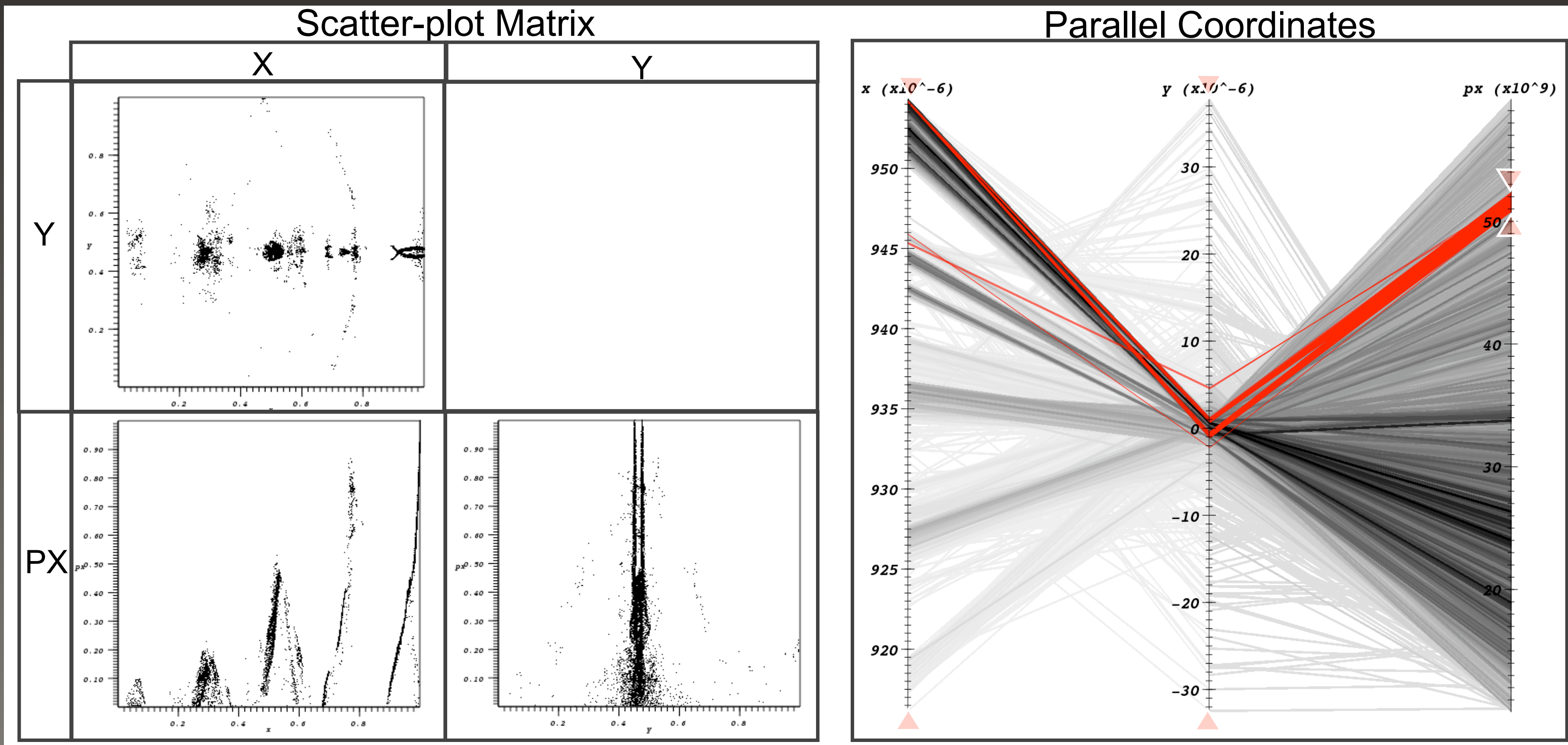
Data Storage in H5Part

- Developed in collaboration between Paul Scherer Institut and Lawrence Berkeley National Laboratory
- Based on HDF5 file format
- Supports particle and field data
- High-level API for particle and field data
- FastBit integration via HDF_FQ (available from LBNL)

Introduction to Parallel Coordinates



Introduction to Parallel Coordinates, cont.



Advantages:

Parallel display of many data dimensions

Easy interface for data thresholding

Immediate feedback during data selection

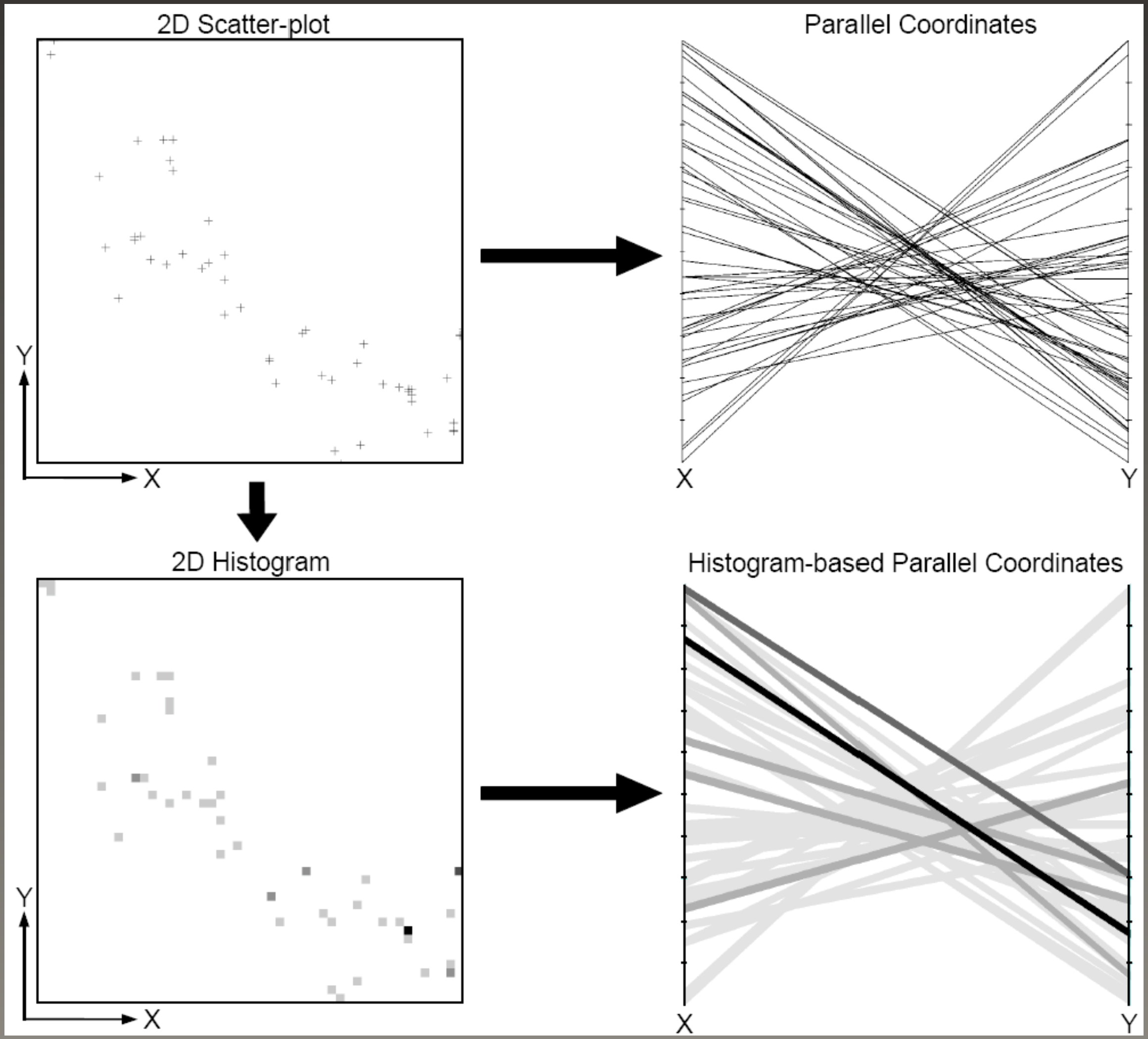
Disadvantages:

Order dependent visualization

Clutter, Occlusion

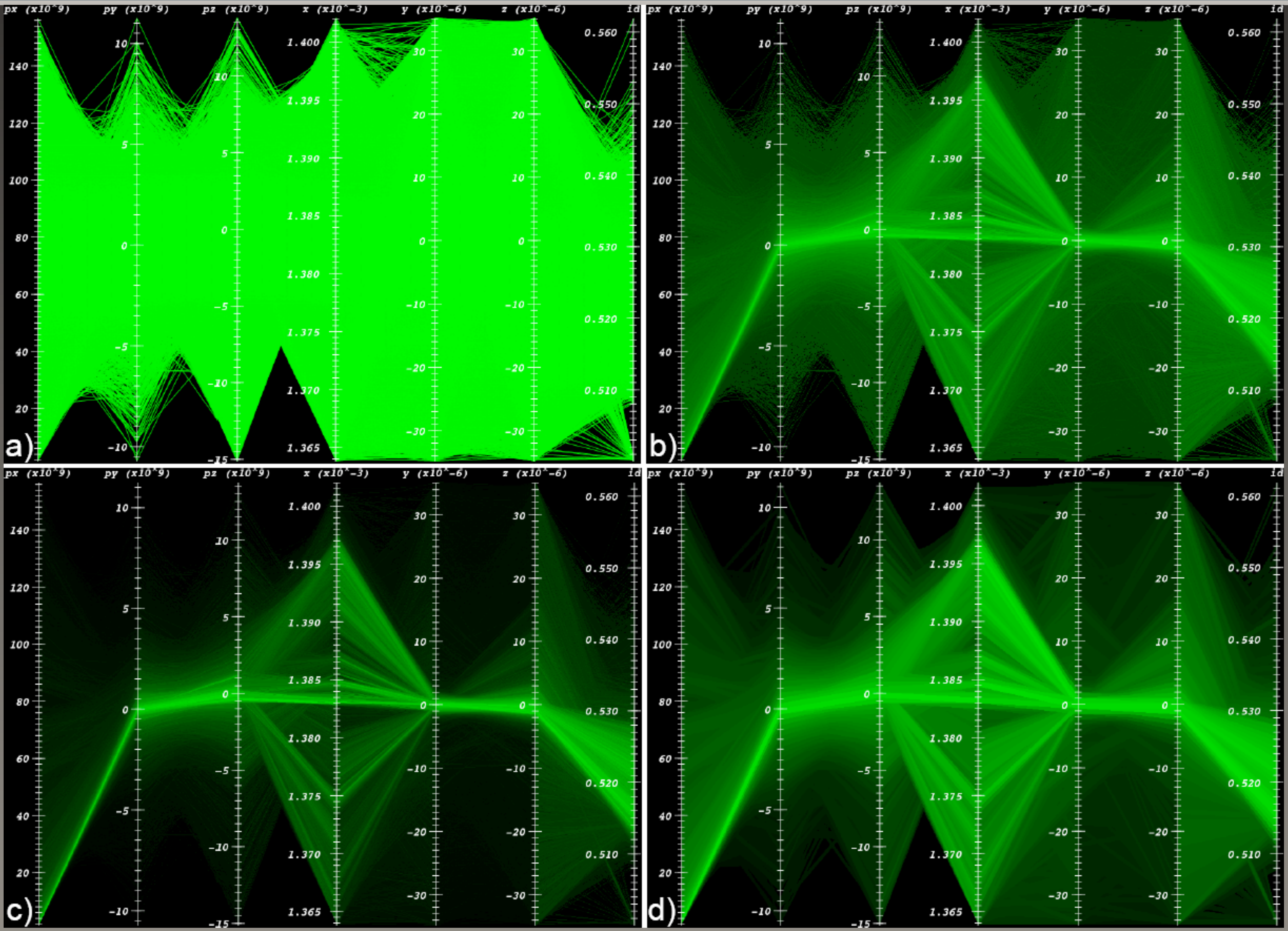
Comp. complexity proportional to data size

Histogram-based Parallel Coordinates



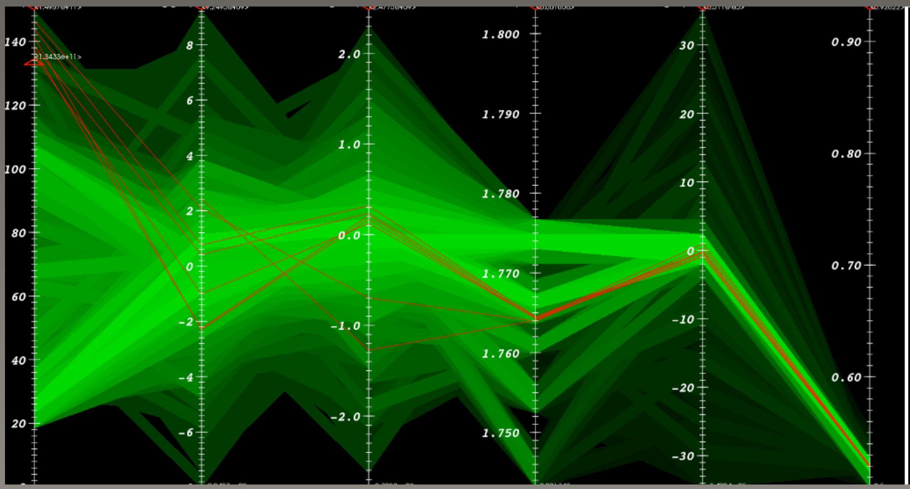
Reference: M. Novotny and H. Hauser, "Outlier-preserving focus+context visualization in parallel coordinates," *IEEE Transactions on Visualization and Computer Graphics,* vol. 12, no. 5, pp. 893-900. 2006.

Histogram-based Parallel Coordinates cont.

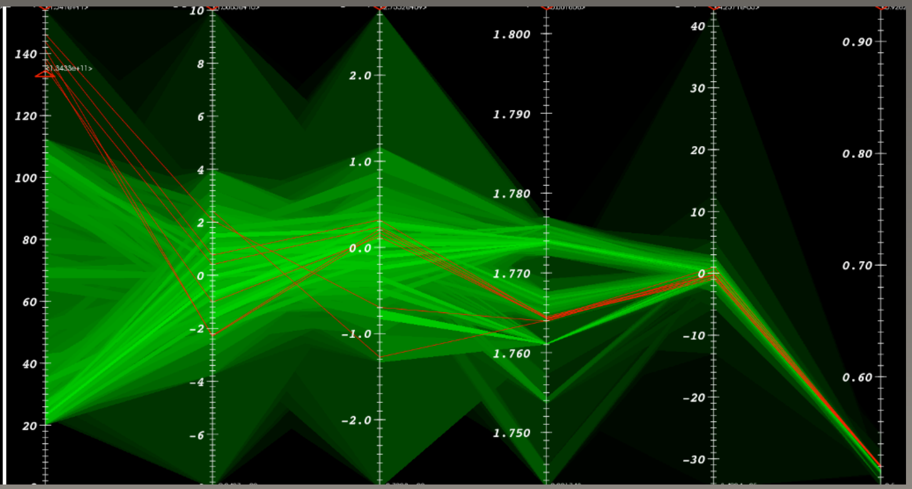


Histogram-based Parallel Coordinates, cont.

- Histograms computed on request:
  - Rendering of data subsets using histograms
  - Close zoom-ins and smooth drill-downs into the data
  - Rendering with arbitrary number of bins
- Support adaptively binned histograms:
  - More accurate representation in lower-level-of-detail views



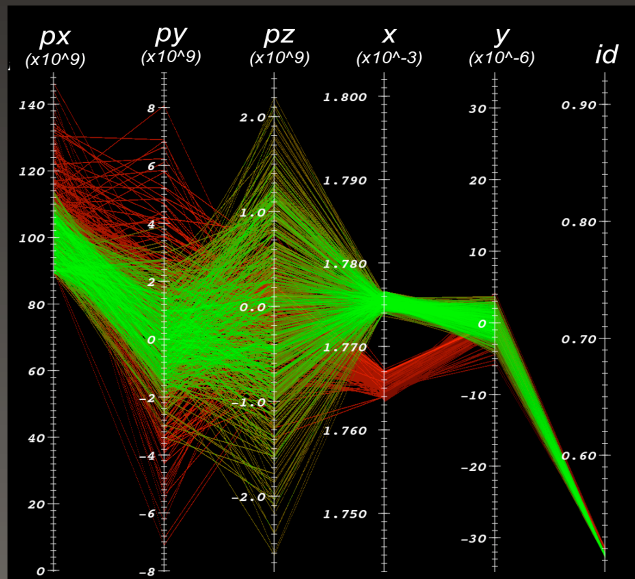
32x32 uniform binning

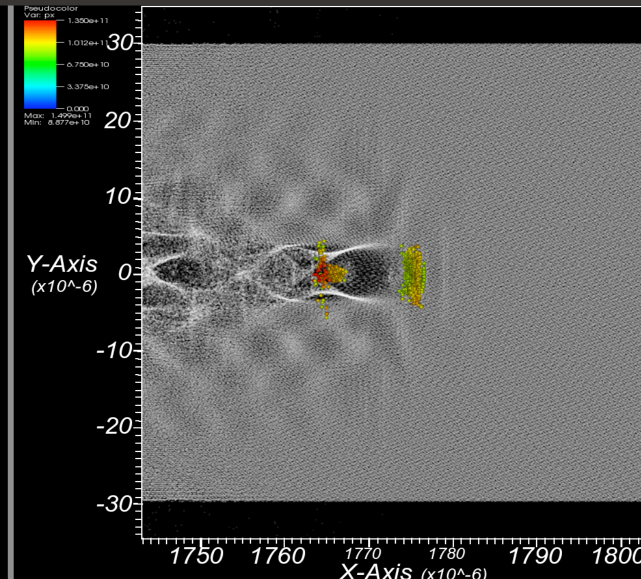


32x32 adaptive binning

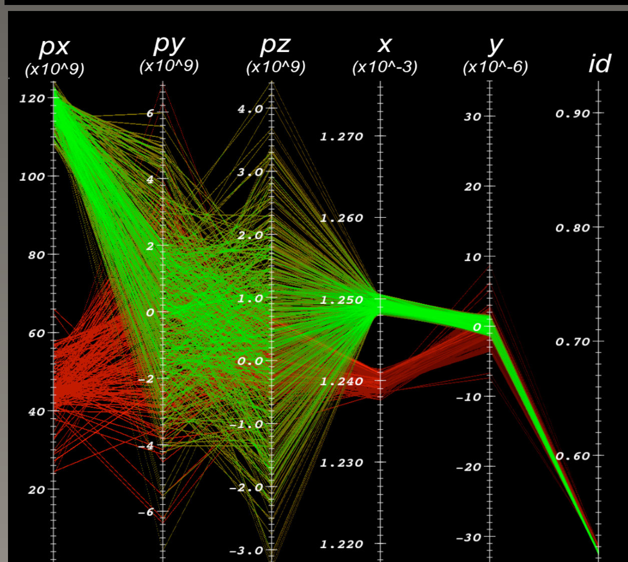
Beam Selection and Assessment

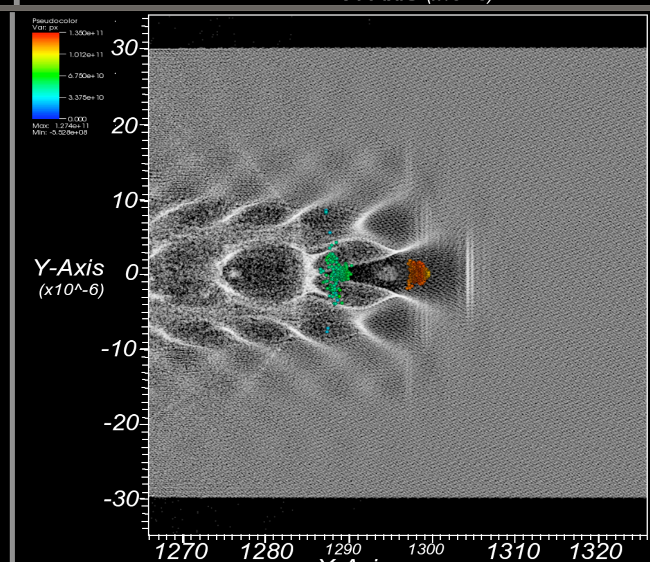
t=37



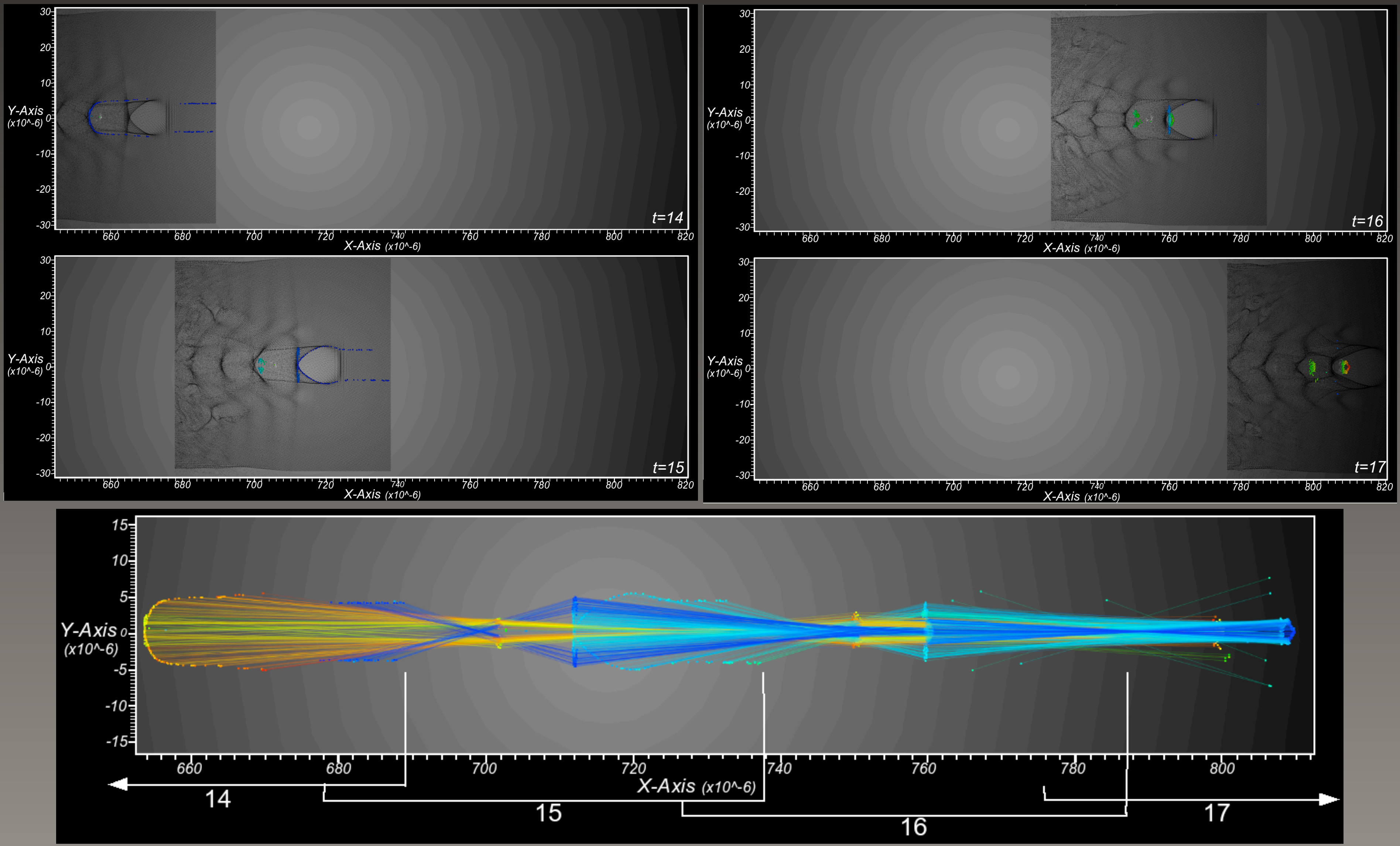


t=27

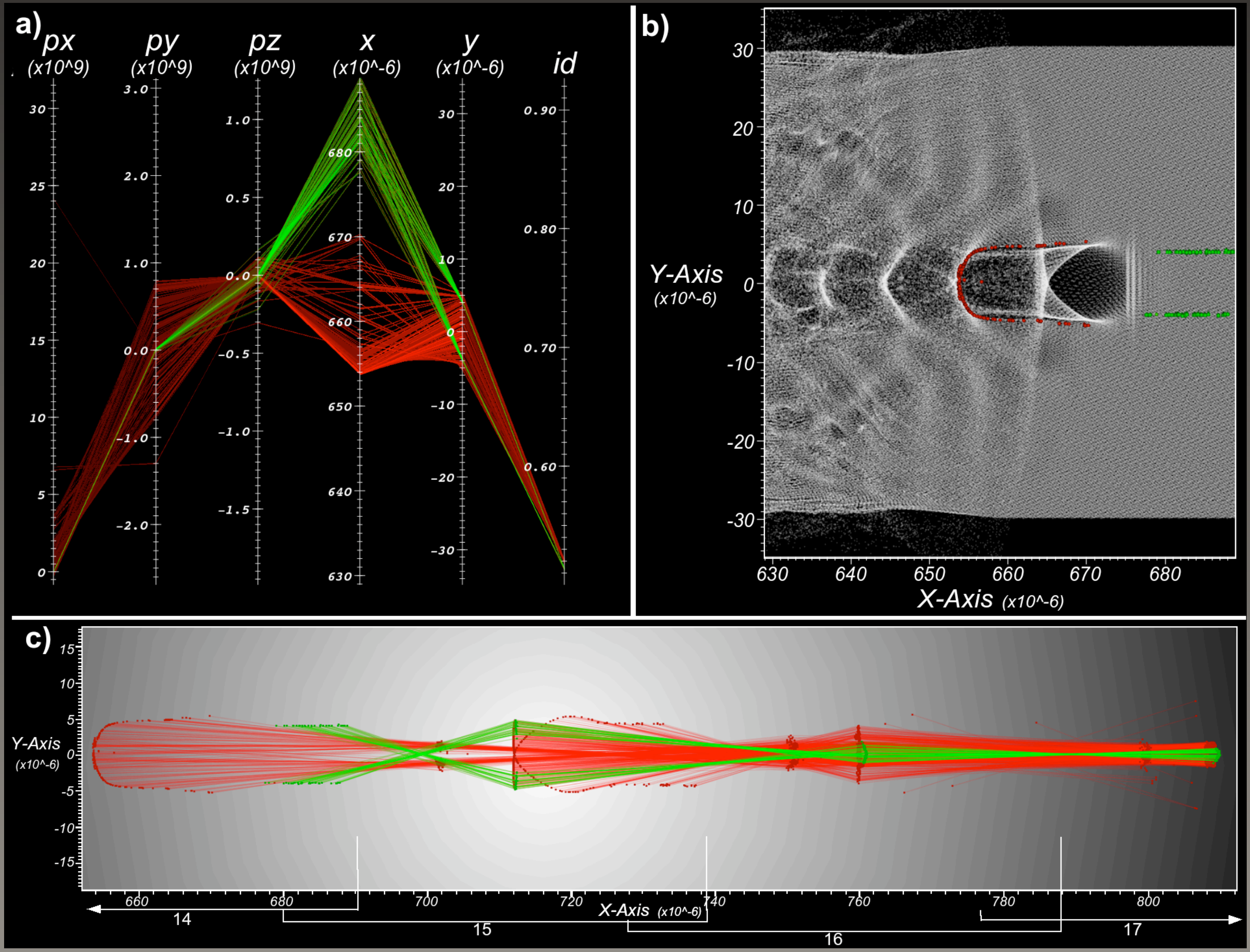




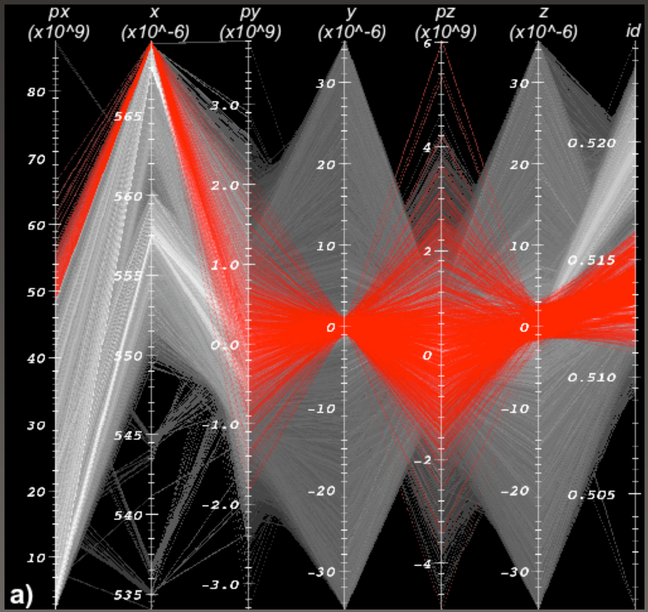
Beam Formation

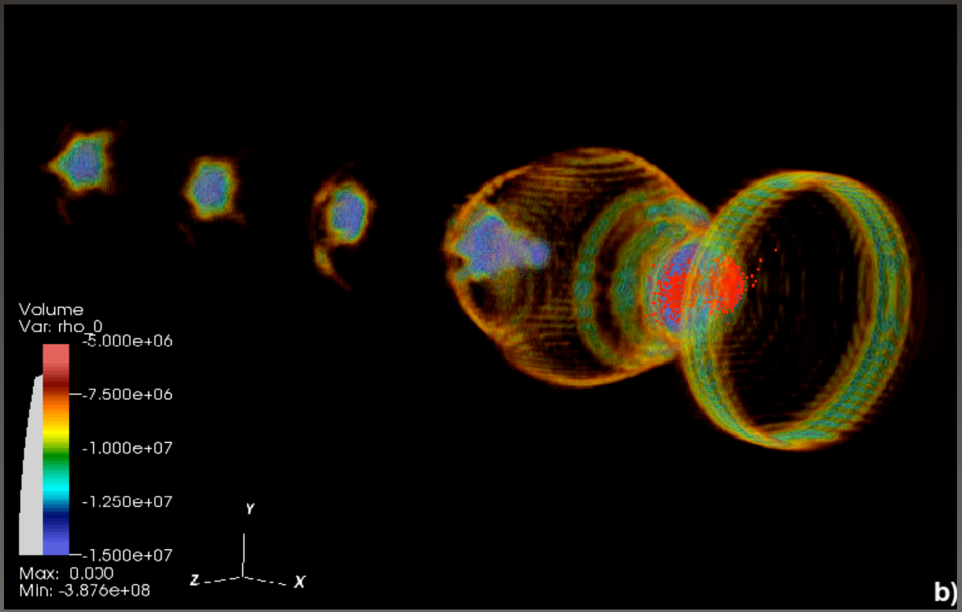


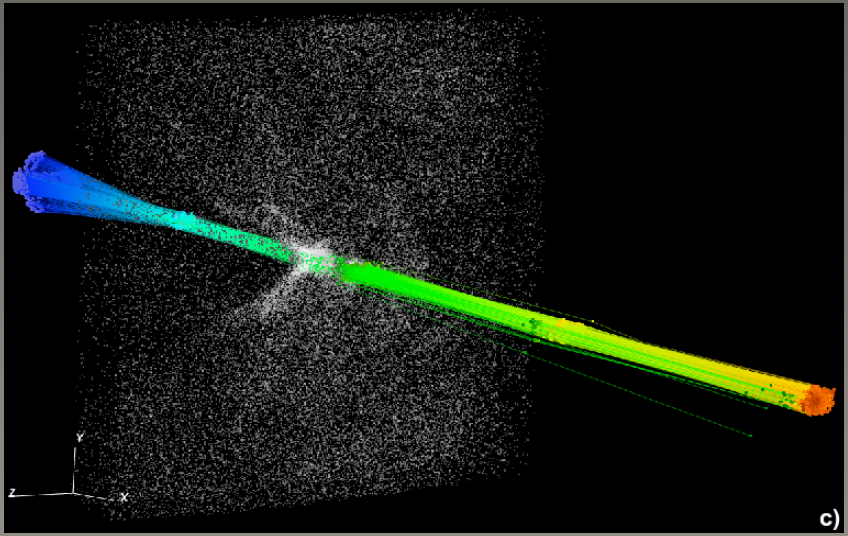
Beam Refinement



3D Analysis Example







Laser Wakefield Acceleration Simulations – Conclusions and Future Work

- **Conclusions**
  - Rapid knowledge discovery from large, complex, multivariate, time-varying data
  - New approach for quickly generating histogram-based parallel coordinates
  - Case study on how system can be used to analyze laser wakefield particle acceleration data effectively

- **Future Work**
  - Distribute in public VisIt version
  - Explore parallelizing the most expensive system parts
  - Improve integration of field and particle data
  - Couple with other traditional data analysis methods, e.g., clustering

Acknowledgements

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  - Director, Office of Advanced Scientific Computing Research, Office of Science, U.S. Department of Energy under Contract No. DE-AC02-05CH11231 through the Scientific Discovery through Advanced Computing (SciDAC) program's Visualization and Analytics Center for Enabling Technologies (VACET).
  - U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.
  - National Energy Research Scientific Computing Center, supported by Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.
- **We would like to thank**
  - Members of the VisIt team
  - Members of VACET
  - Members of LBNL Vis Group
  - Members of LBNL Center for Computational Sciences and Engineering
  - Terry Ligocki, LBNL Applied Numerical Algorithms Group

Questions?