

# Visual Analysis of Scientific Data

Dr. Johannes Kehrer

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# Visualization – Major Areas

- Major areas

- Volume Visualization
- Flow Visualization

Scientific Visualization

Inherent spatial reference

3D

- Information Visualization
- Visual Analytics

nD

Usually no spatial reference

# Visualization – Goals

Visualization is good for

– **Visual exploration**

- find unknown/unexpected
- generate new hypotheses

Nothing is known  
about the data

– **Visual analysis (confirmative vis.)**

- verify or reject hypotheses
- information drill-down

There are hypotheses

– **Presentation**

- show/communicate results

“Everything” is known

# Motivation

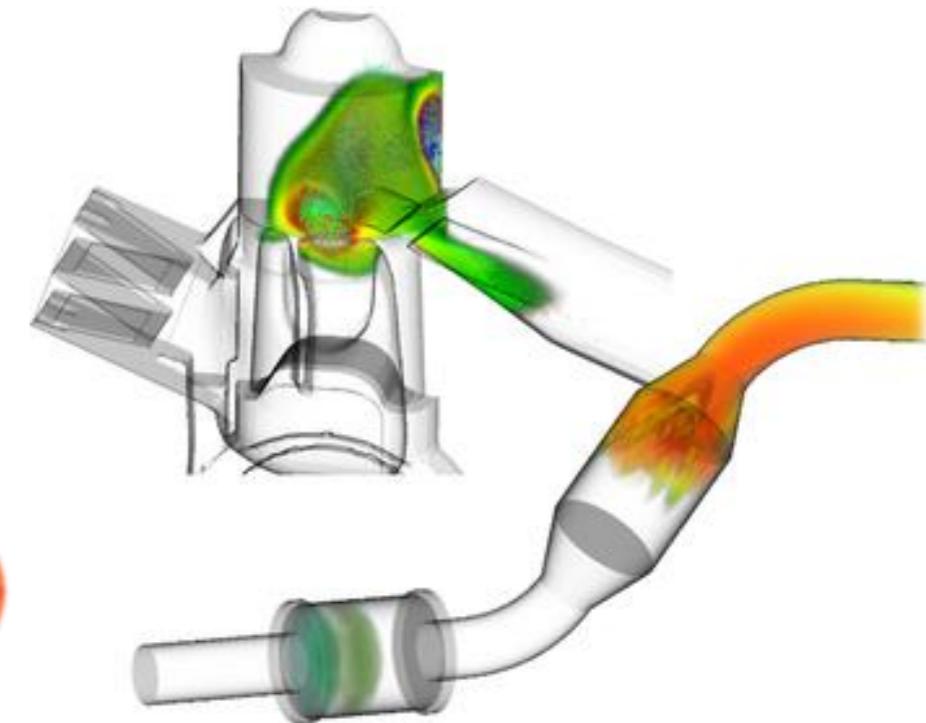
- Large amounts of data are generated everywhere



medical scanners



global climate  
simulations



automotive  
engineering

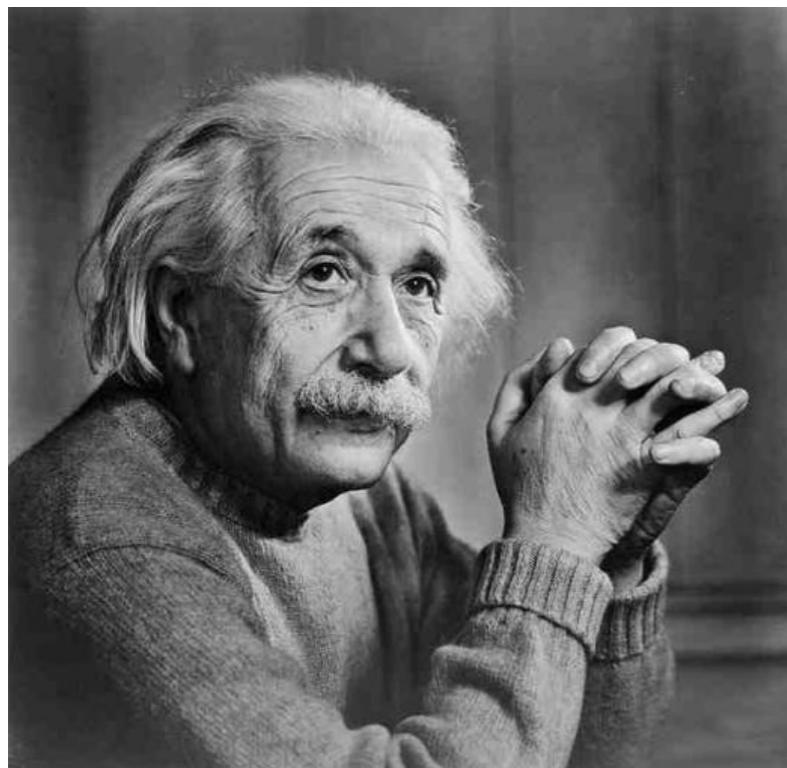
- Data are increasing in complexity & variability

# Problems

- Data size / complexity / variable quality
- Various / heterogeneous data sources
- Data is explicit, but information/insight is often implicit
- Missing involvement of users and their tasks
- Pure visualization methods are not enough for large & complex data
- Pure automatic methods only work for well-defined & clearly specified problems

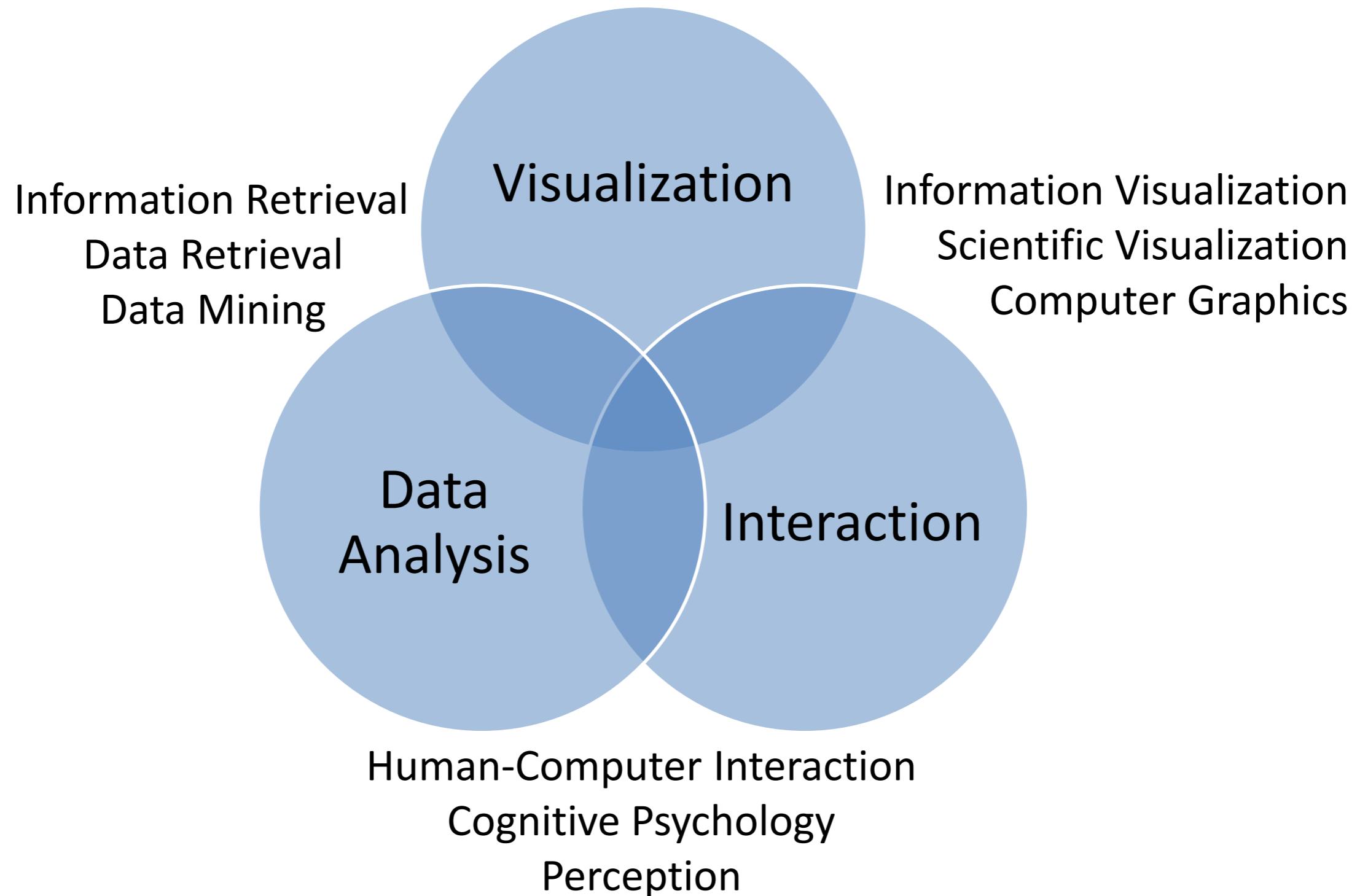
# Humans & Computers

“Computers are incredibly fast, accurate, and stupid;  
humans are incredibly slow, inaccurate, and brilliant;  
together they are powerful beyond imagination.”



Attributed to Albert Einstein

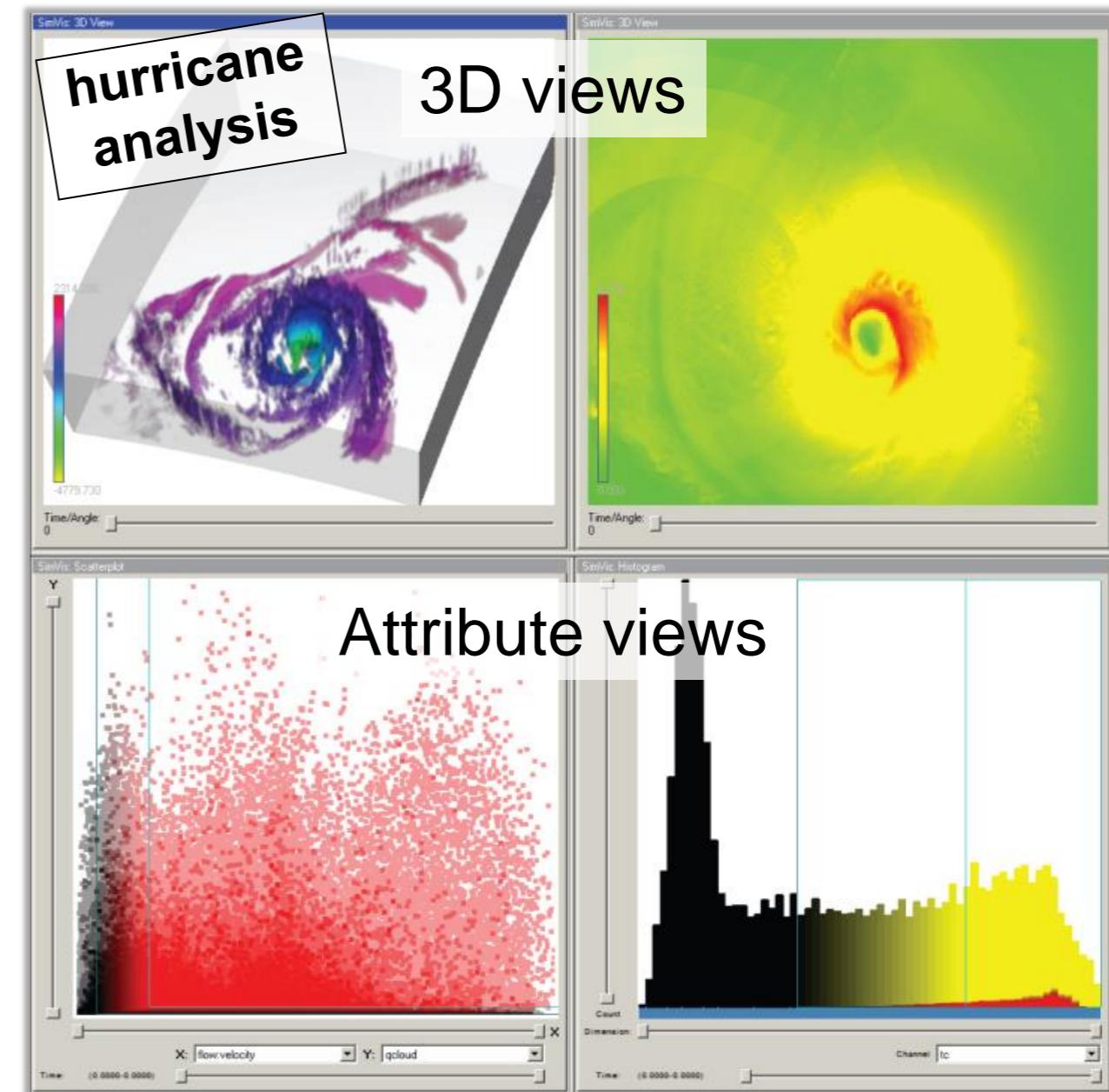
# Visual Analytics / Analysis



# Visual Analysis of Scientific Data

Combines computational & interactive visual methods

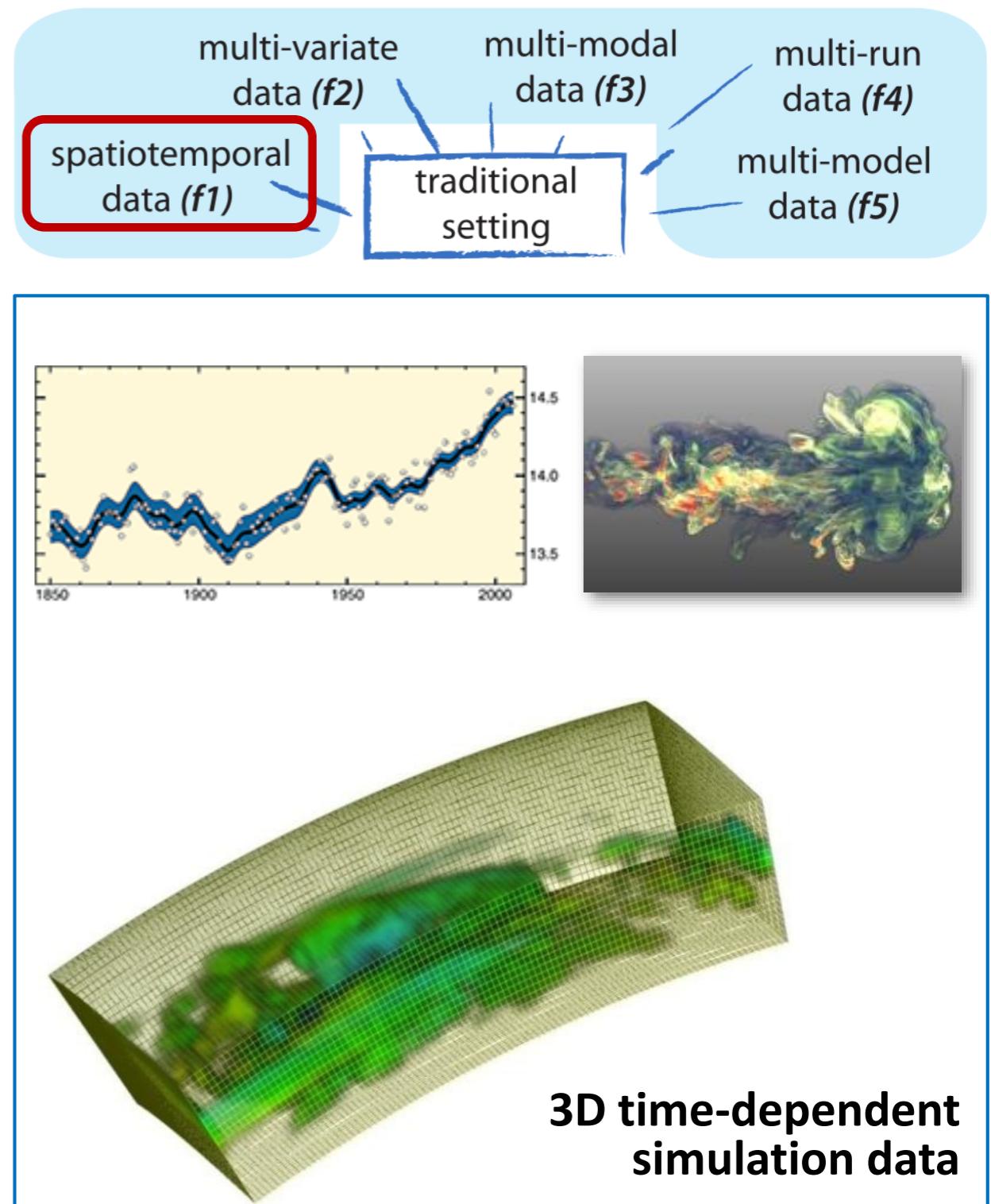
- Multiple linked views
- Interpret large & complex data
- Drill-down into information
- Find relations  
("read between the lines")
- Detect features/patterns that are difficult to describe
- Integrate expert knowledge



SimVis [Doleisch et al. 03]

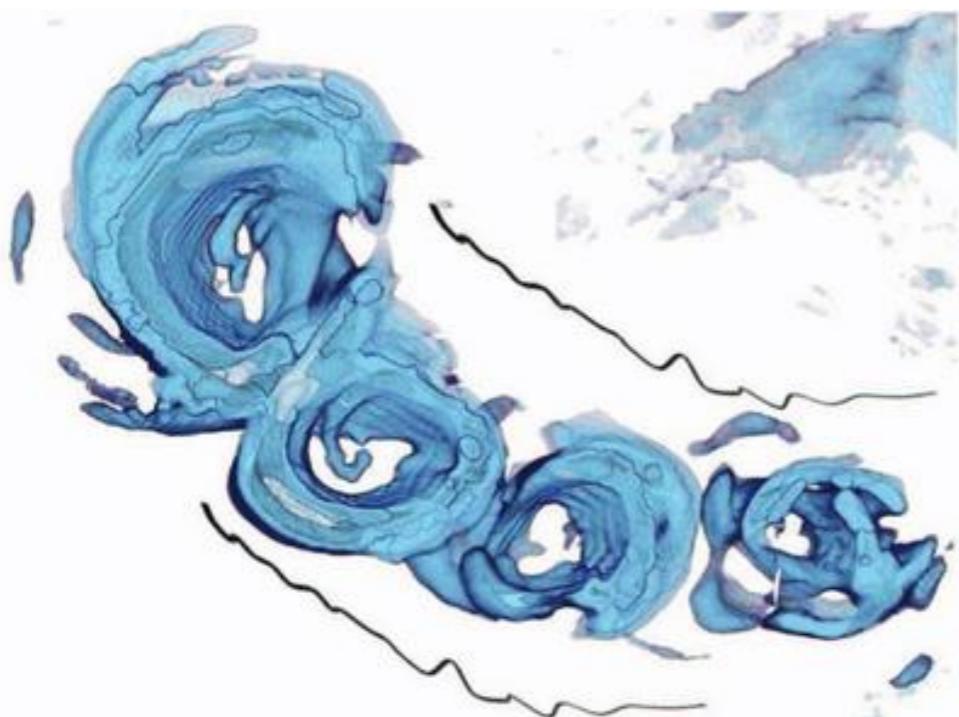
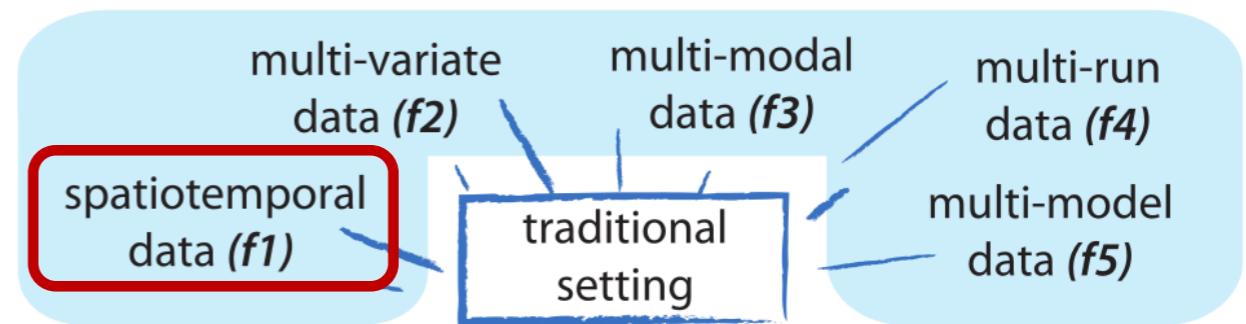
# Multi-faceted Scientific Data

- Spatiotemporal data
- Multi-variate/multi-field data (multiple data attributes, e.g., temperature or pressure)
- Multi-modal data (CT, MRI, large-scale measurements, simulations, etc.)
- Multi-run/ensemble simulations (repeated with varied parameter settings)
- Multi-model scenarios (e.g., coupled climate model)

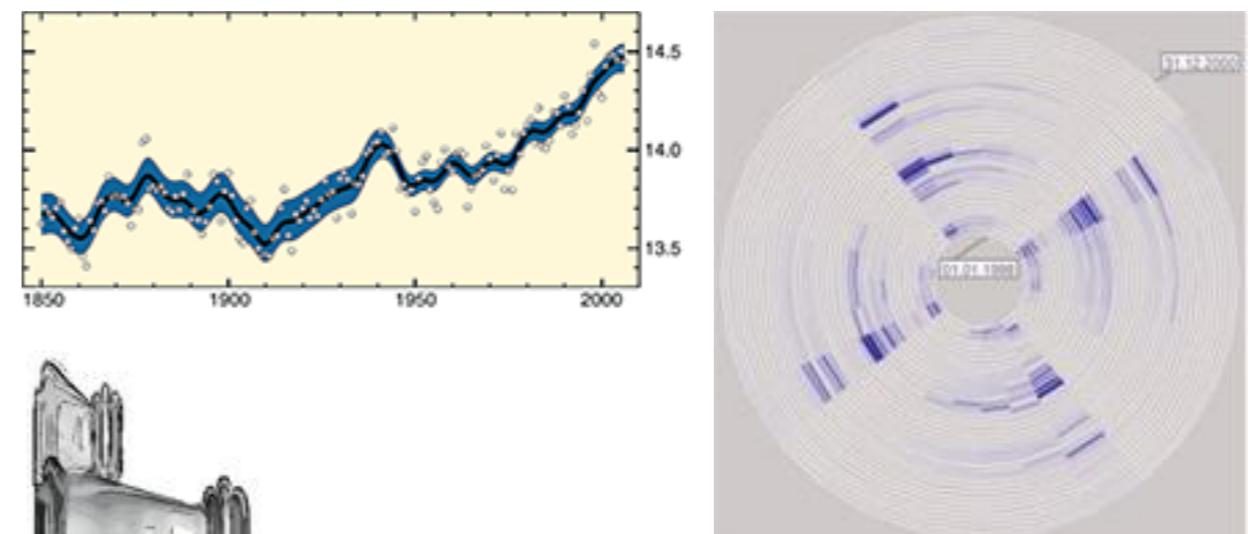


# Multi-faceted Scientific Data

- Spatiotemporal data
  - Cartography, geovis, etc.
  - Linear vs. cyclic time
  - Automatic animations
  - Flow visualization
  - Visualize summary statistics



Illustrative techniques  
[Joshi et al. 09]



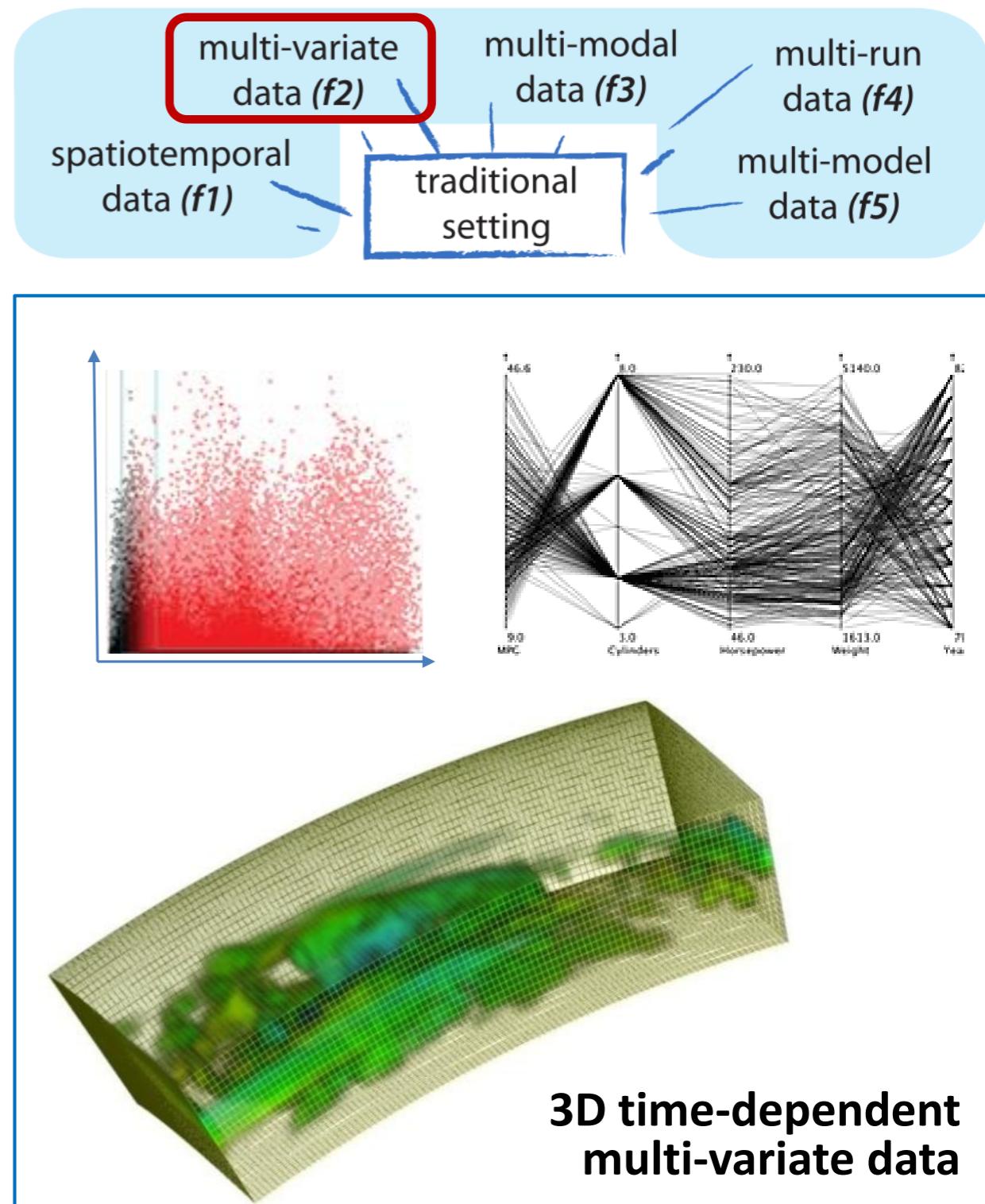
Spiral Graph  
[Weber et al. 01]



[Hsu et al. 10]

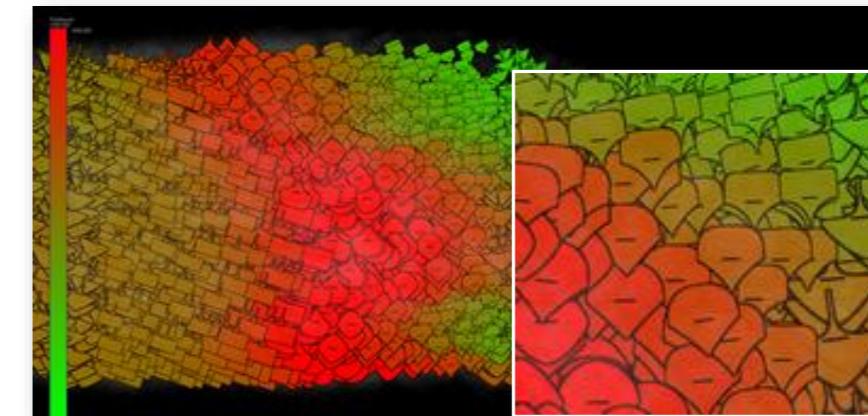
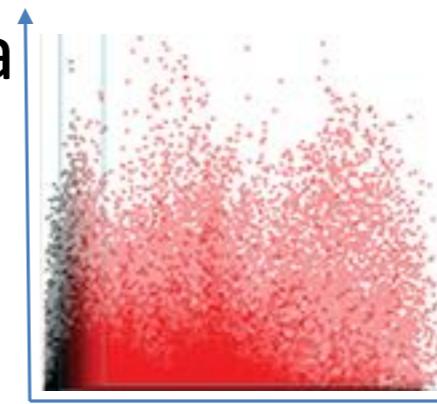
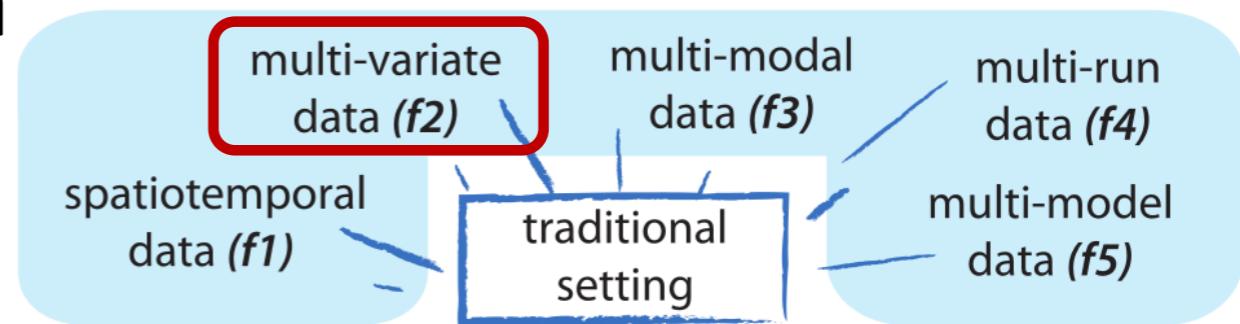
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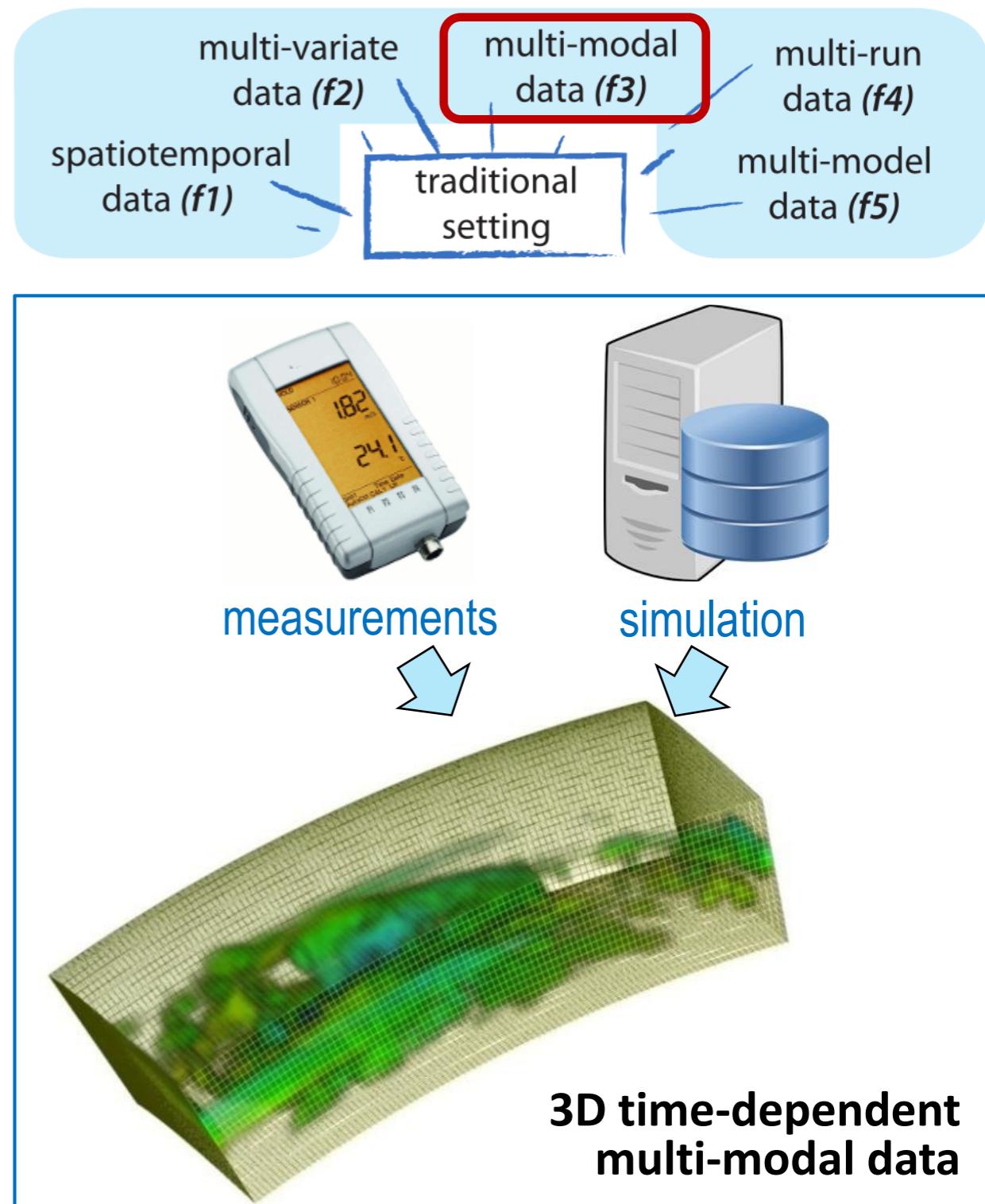
# Multi-faceted Scientific Data

- Multi-variate/multi-field data
  - Attribute views (scatterplots, parallel coordinates, etc.)
    - Find patterns such as correlations or outliers
    - Lack spatial relationships of data
    - Which of the many data variables to show?
  - Volume rendering
    - Difficult to see multi-variate patterns
    - Layering & glyphs
    - Feature-based vis. (brushing, segmentation, ...)
  - Clustering, dimensionality reduction, etc.



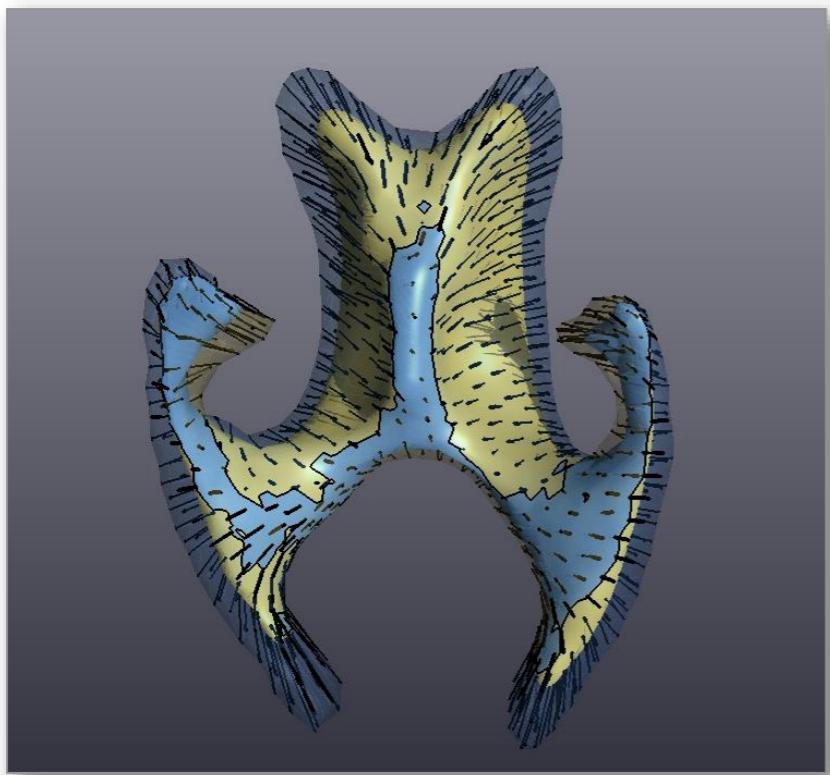
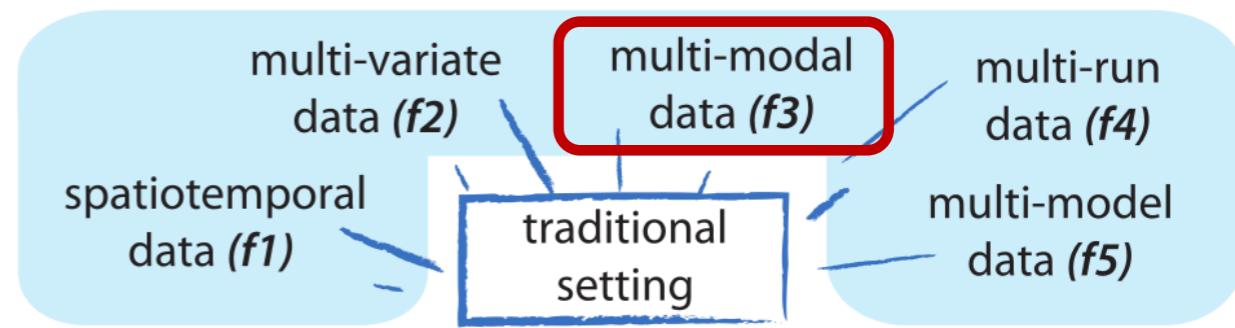
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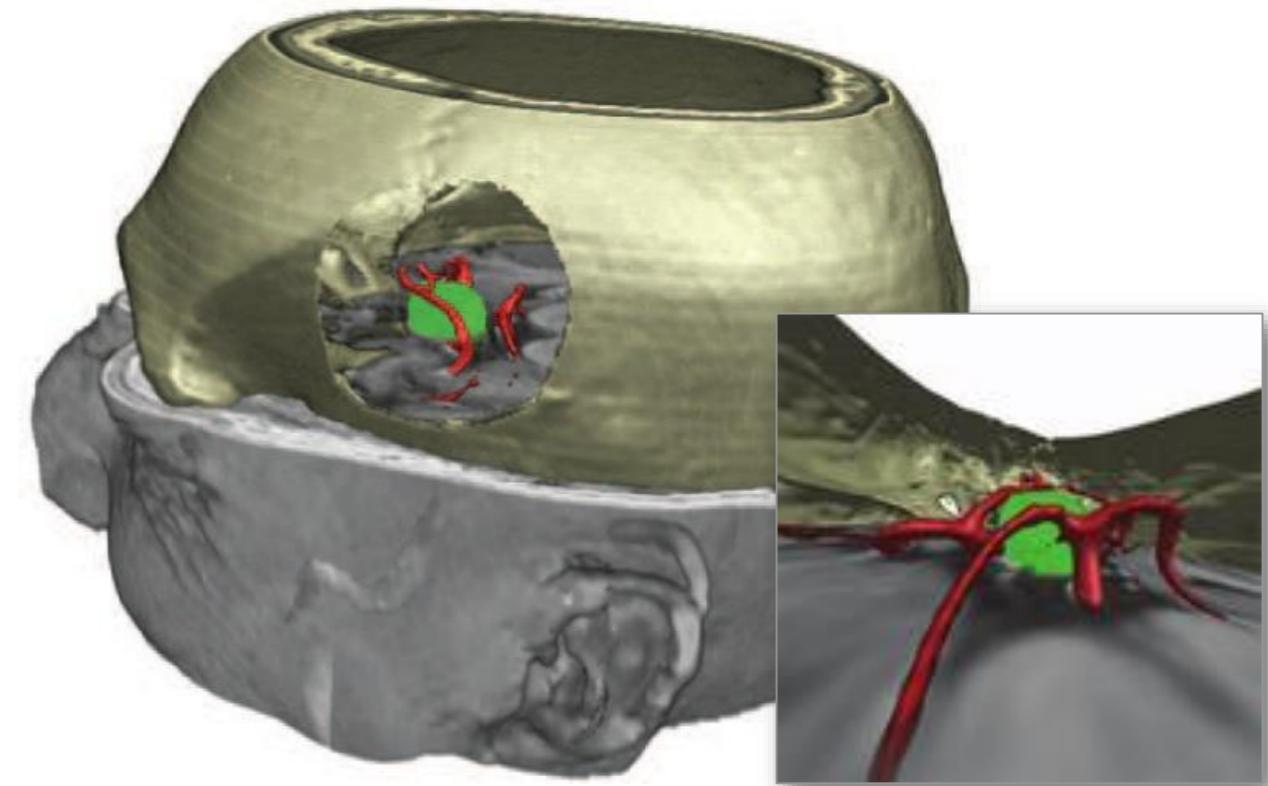


# Multi-faceted Scientific Data

- Multi-modal data
  - Various types of grids with different resolution
  - Coregistration & normalization
  - Multi-volume rendering
  - Visual data fusion
  - Comparative visualization



Nested surfaces  
[Buskin et al. 11]

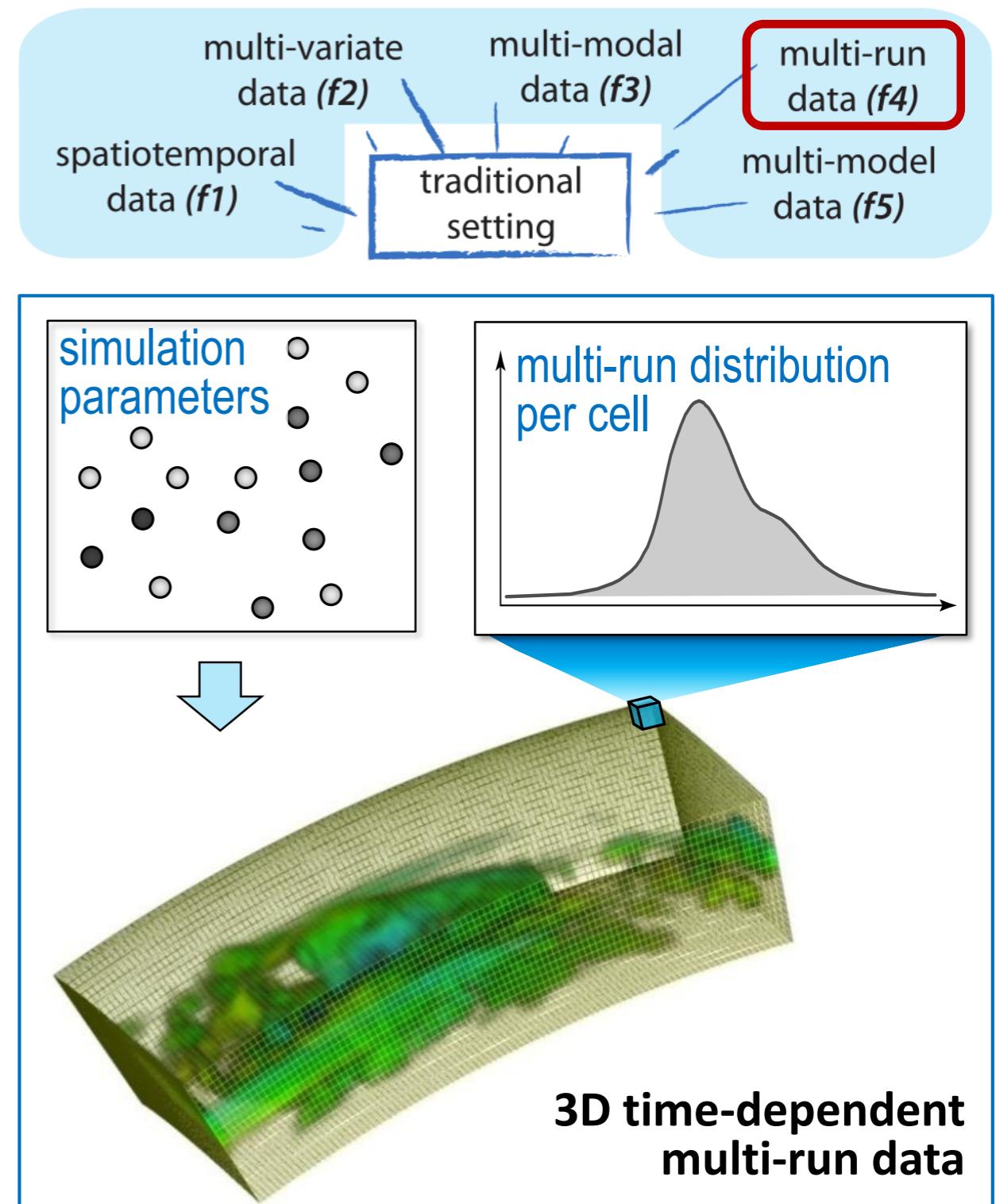


Multi-volume rendering of segmented data  
(green: tumor - MR, red: vessels – MRA,  
brown: skull - CT)

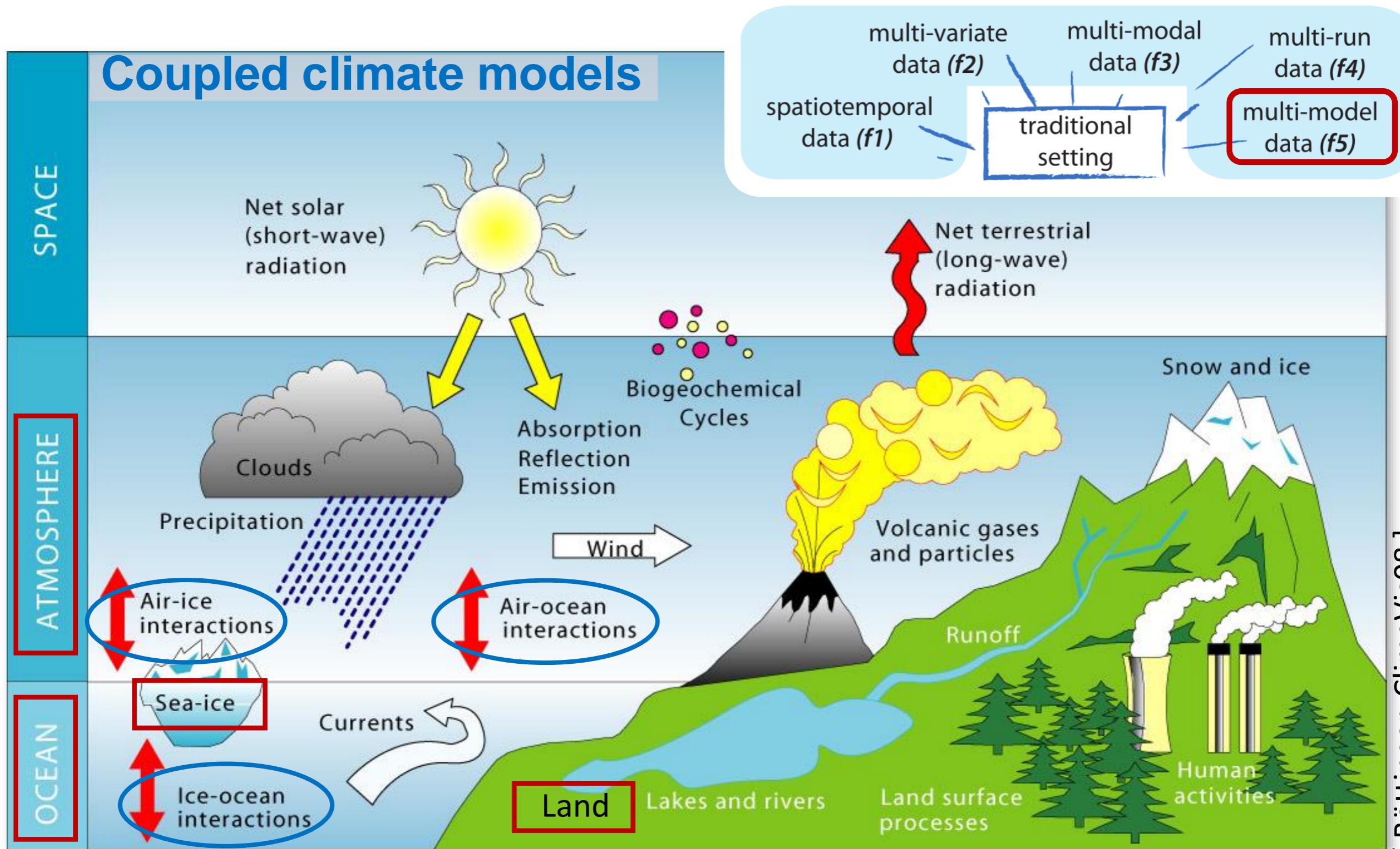
[Beyer et al. 07]

# Multi-faceted Scientific Data

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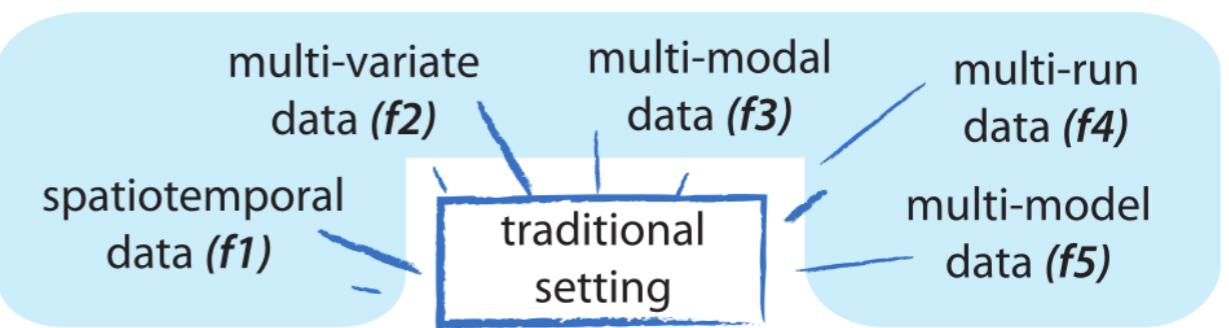


# Multi-faceted Scientific Data

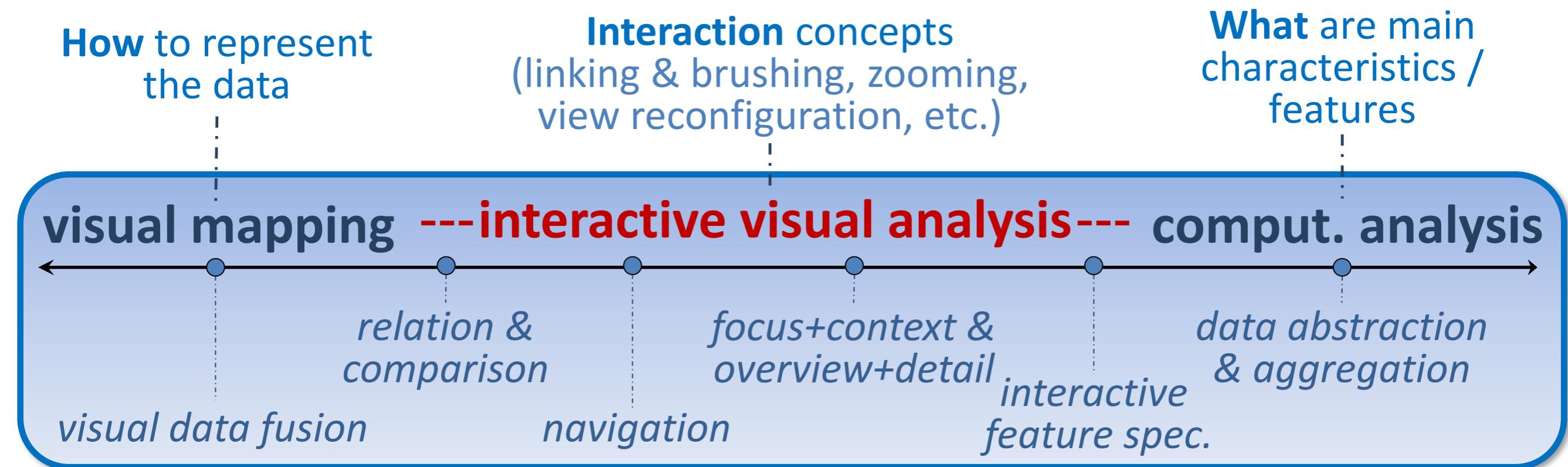


[ Böttinger, Climavis08 ]

# Categorization

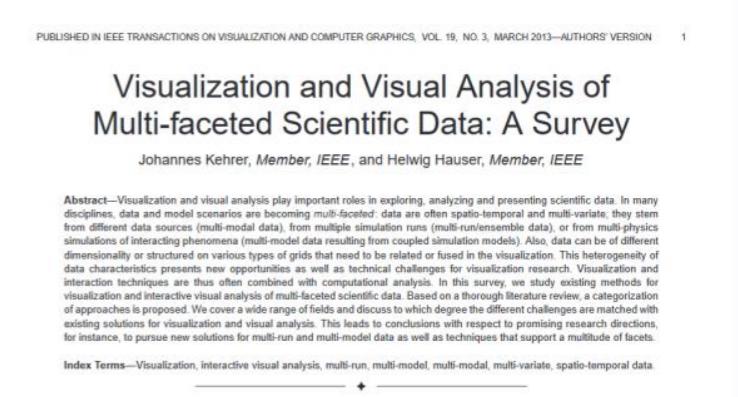


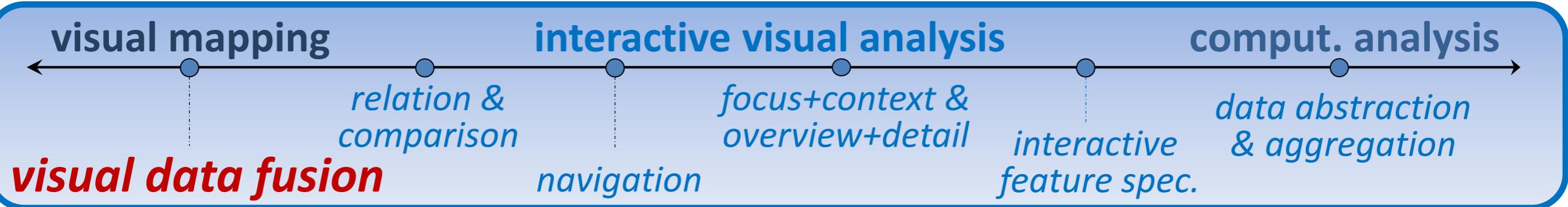
- Literature review of 200+ papers on scientific data
- How are visualization, interaction, & comput. analysis combined?



Compare to Keim et al. 09,  
Bertine & Lalanne 09

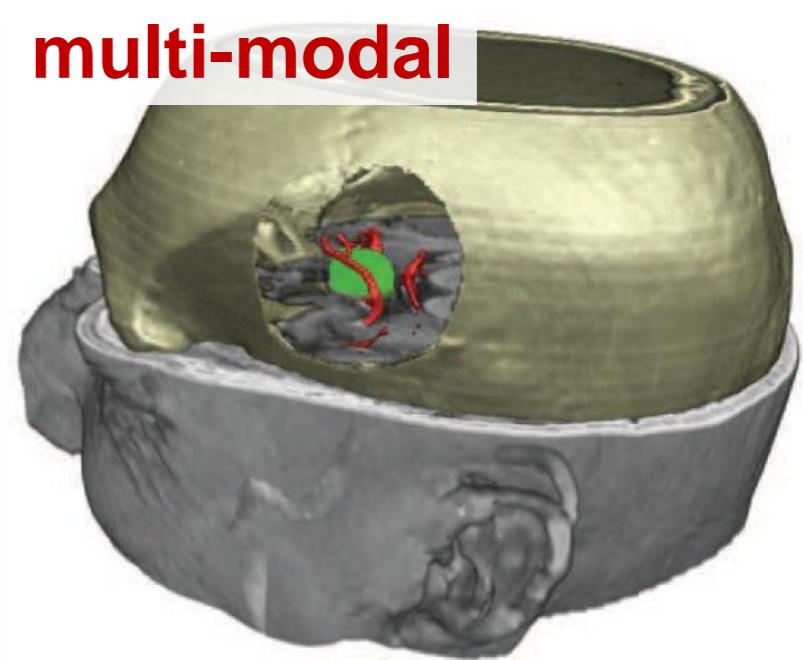
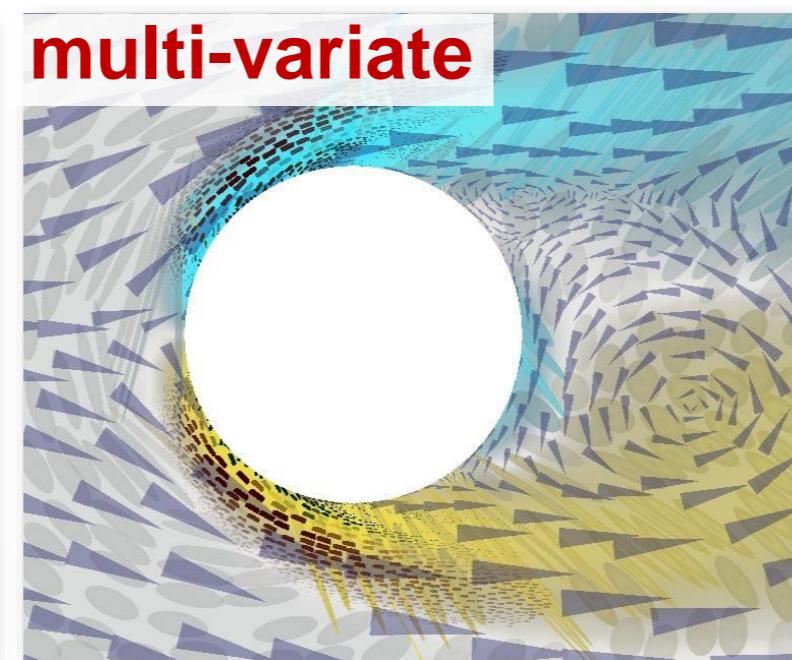
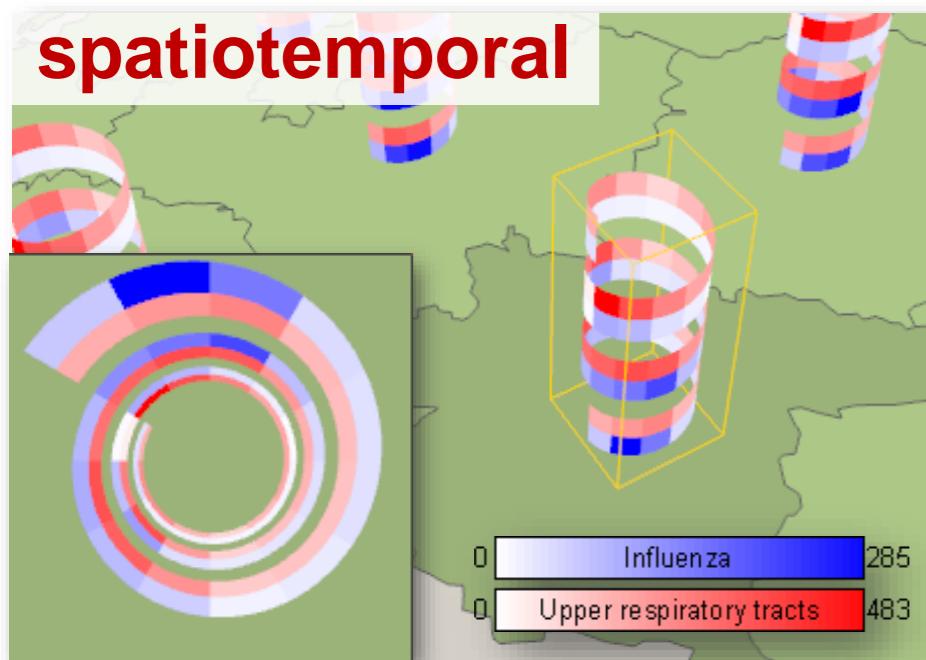
[Kehrer & Hauser 13]





## Fusion within a single visualization

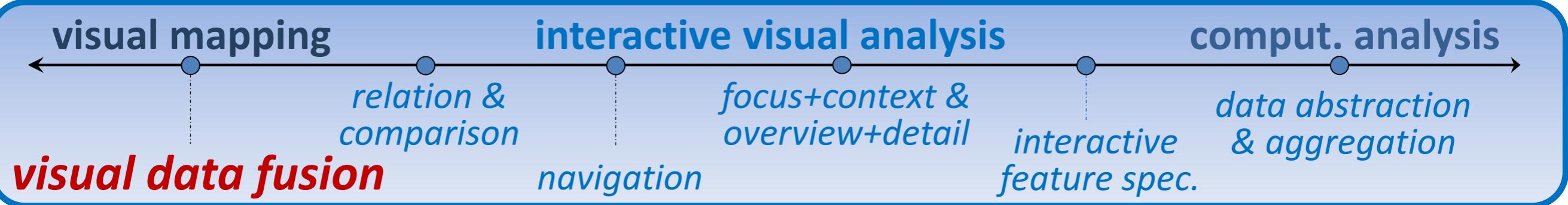
- Use a common frame of reference (e.g., axes)
- Layering techniques (e.g., glyphs, color, transparency)
- Multi-volume rendering (coregistration, segmentation)



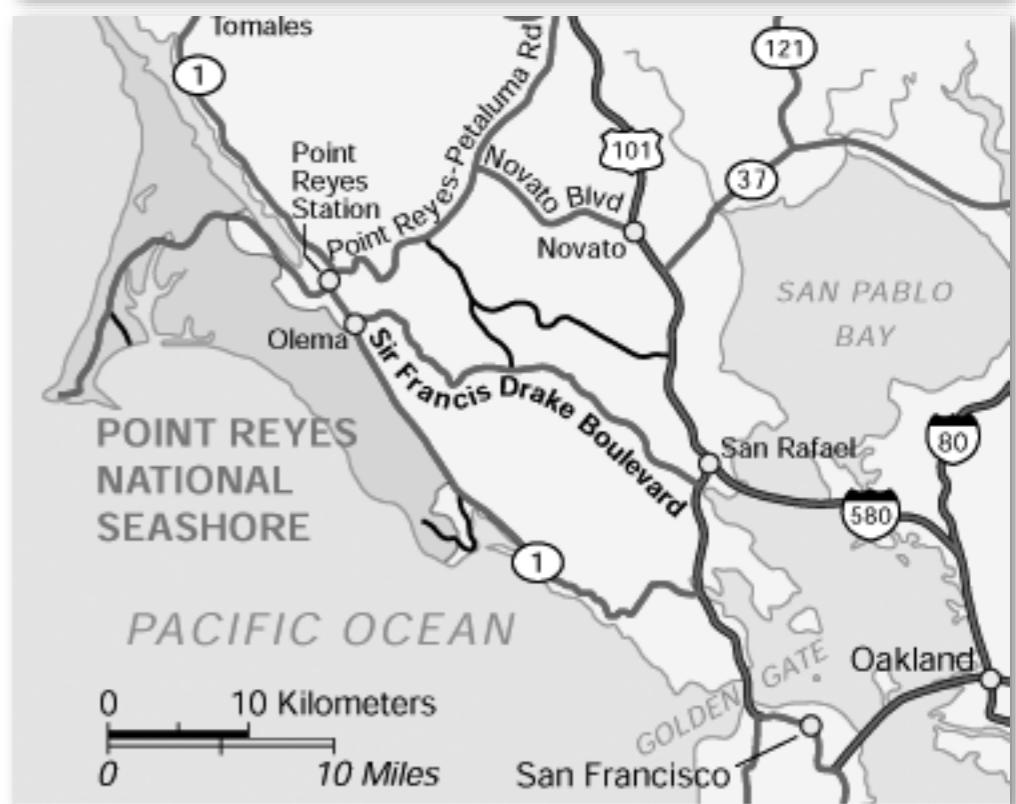
Helix glyphs [Tominski et al. 05]

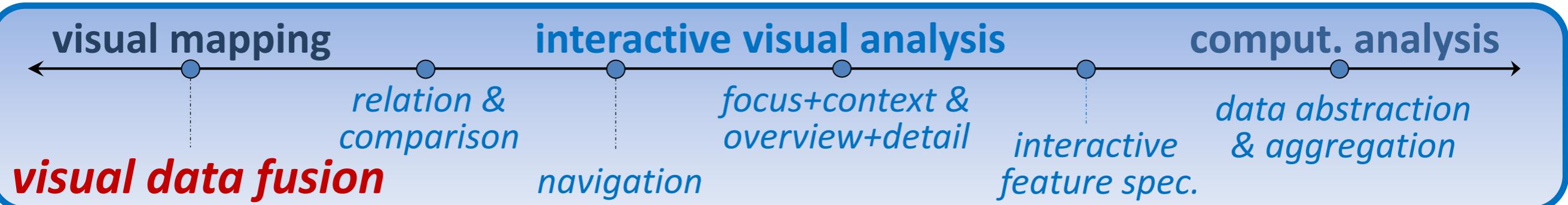
Layering [Kirby et al. 99]

Multi-volume rendering  
[Beyer et al. 07]



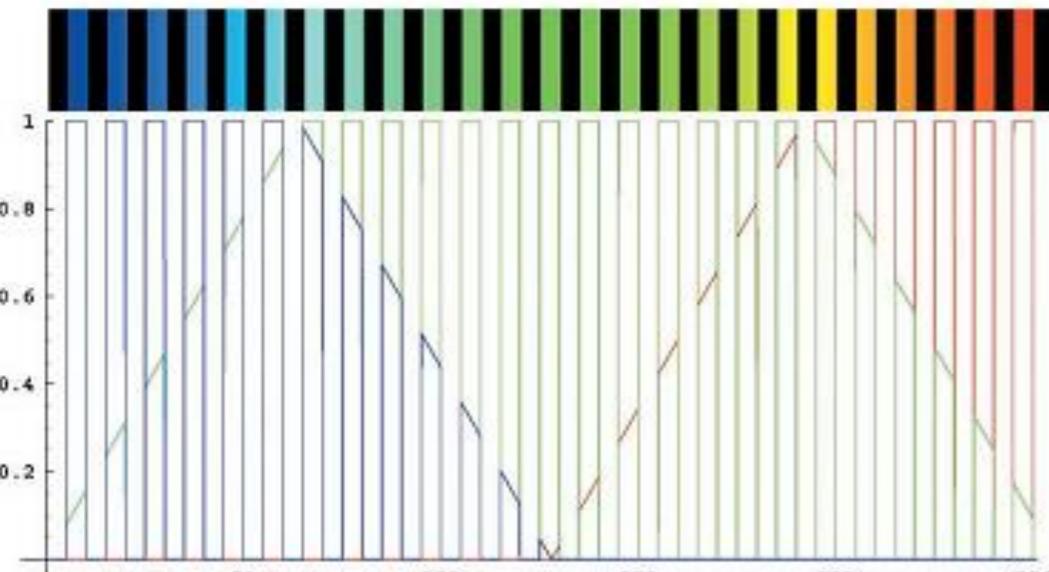
- Layering techniques
  - How many layers?
  - How are layers distinguishable?
- Distinguishable layers
  - Encode with different, nonoverlapping visual channels
  - Foreground layer: roads
    - Hue, size → main from minor
    - Luminance contrast from background
  - Background layer: regions
    - Desaturated colors for water / land



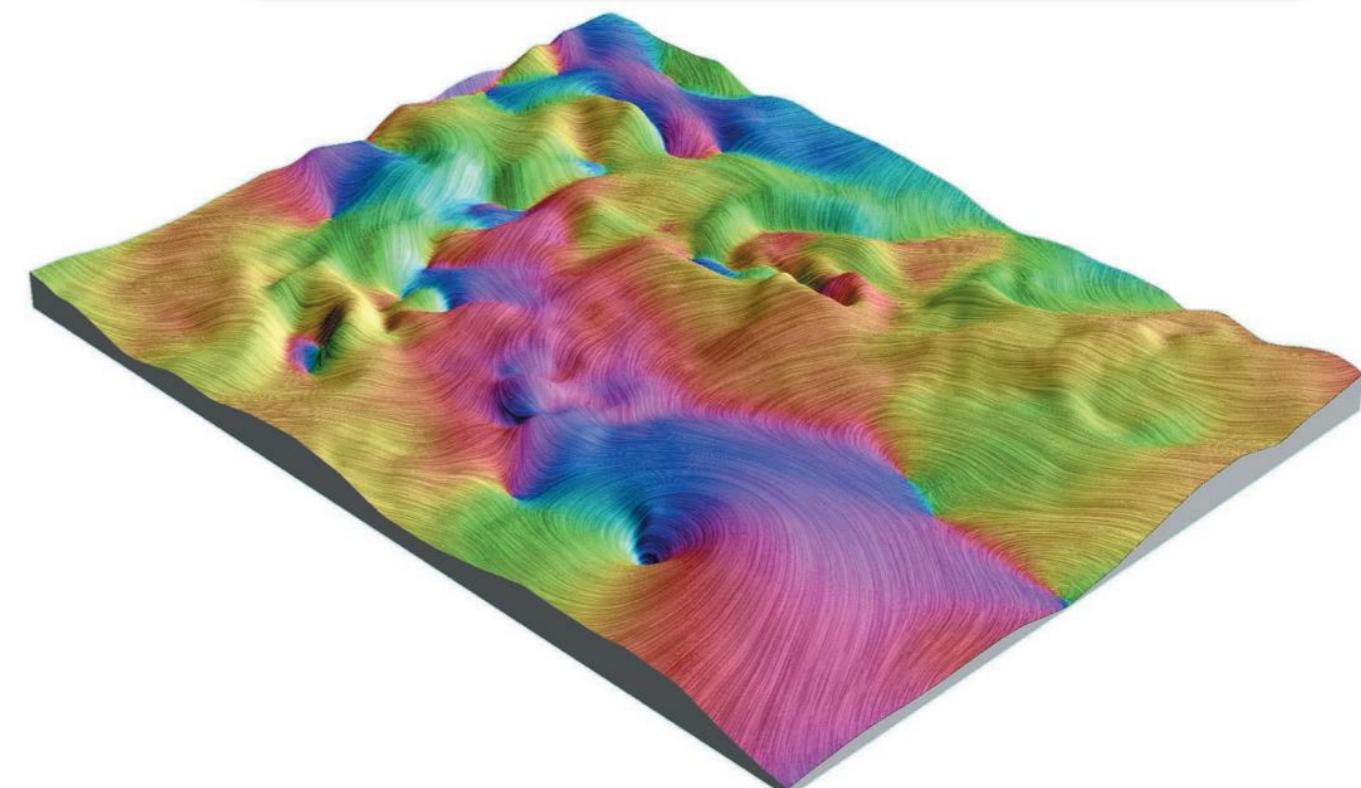
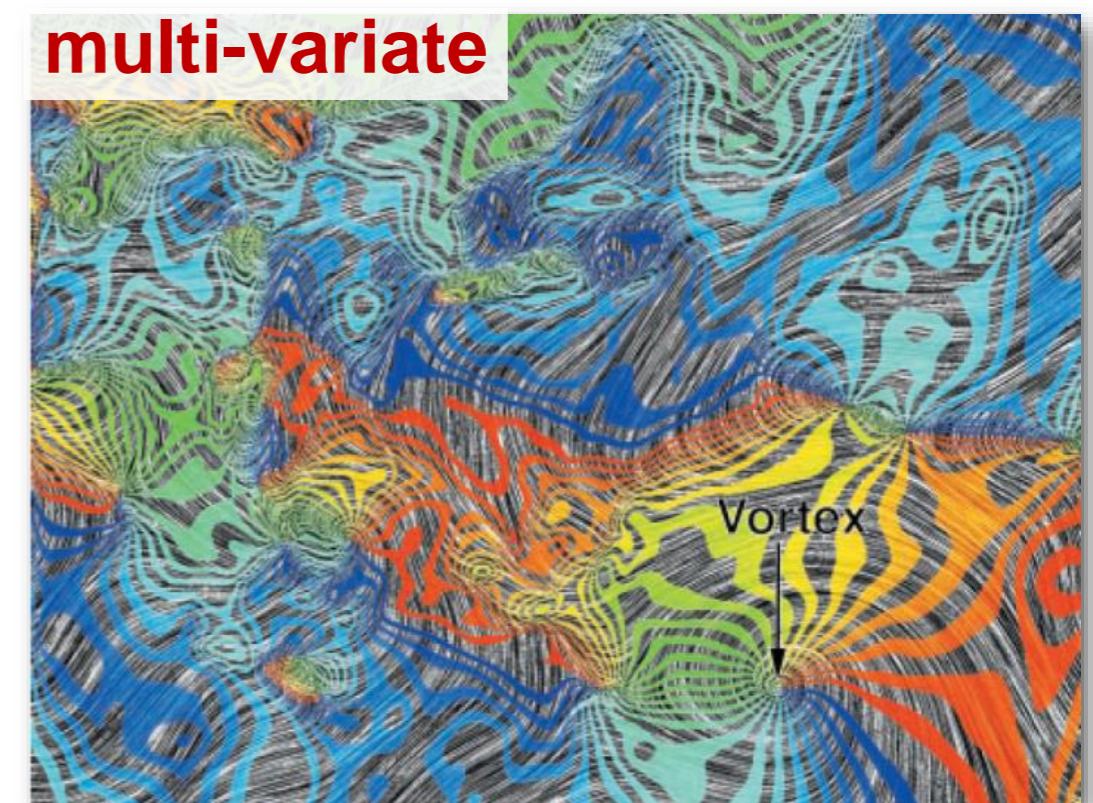


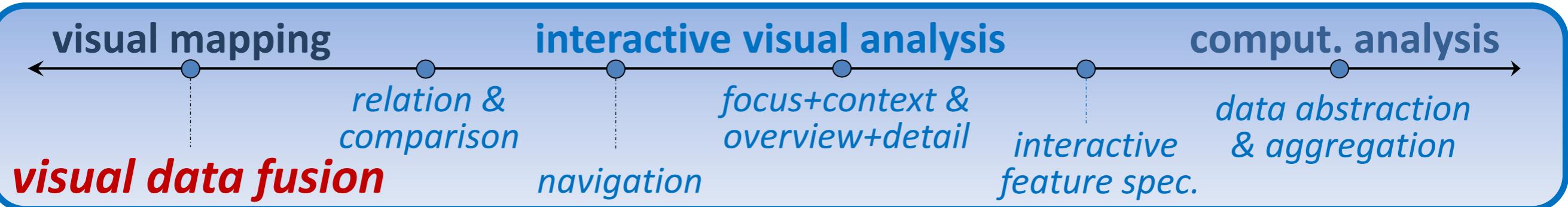
## Layering techniques [Wong 02]

- Opacity modulation
- Filigreed
- Colormap enhancement
- 2D heightmap

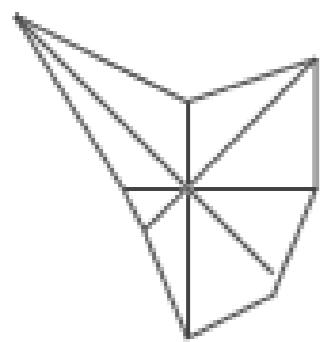


Colormap + square wave modulation





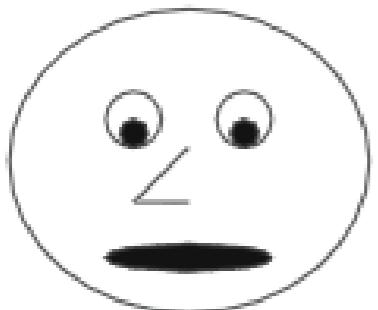
**Glyphs:** Small independent visual objects that depict attributes of a data record



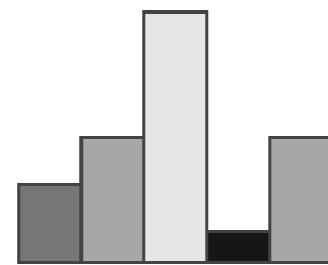
Star glyphs



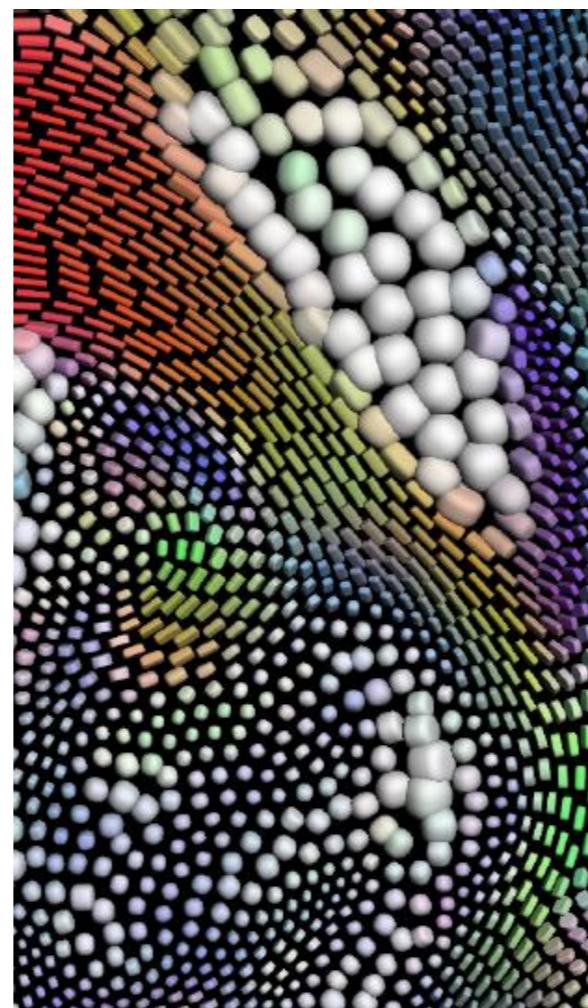
Stick figures



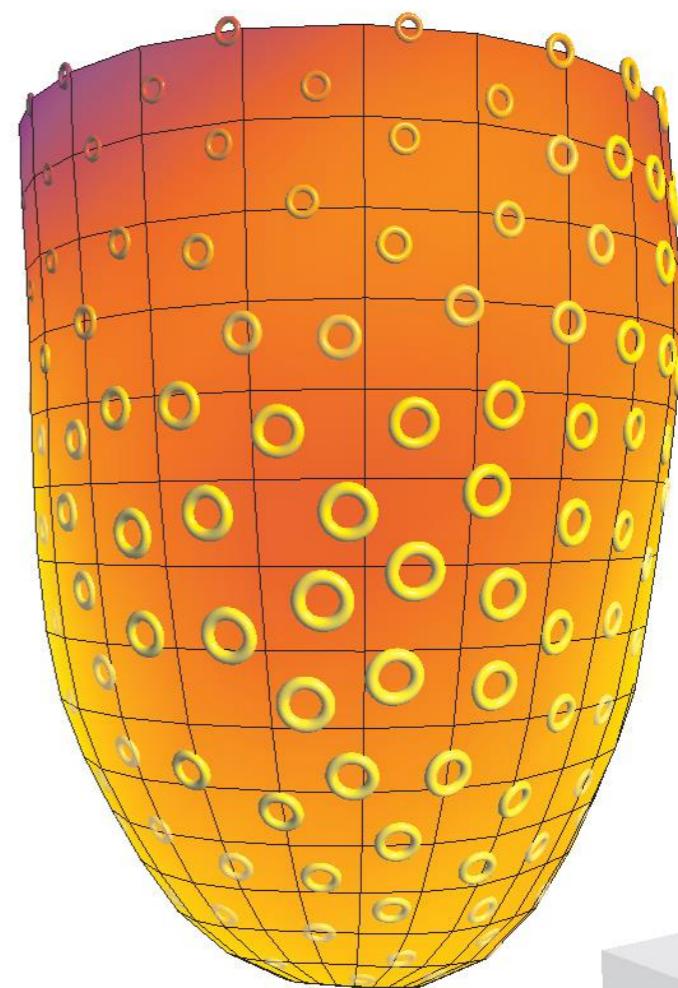
Chernoff  
faces



Profile glyphs

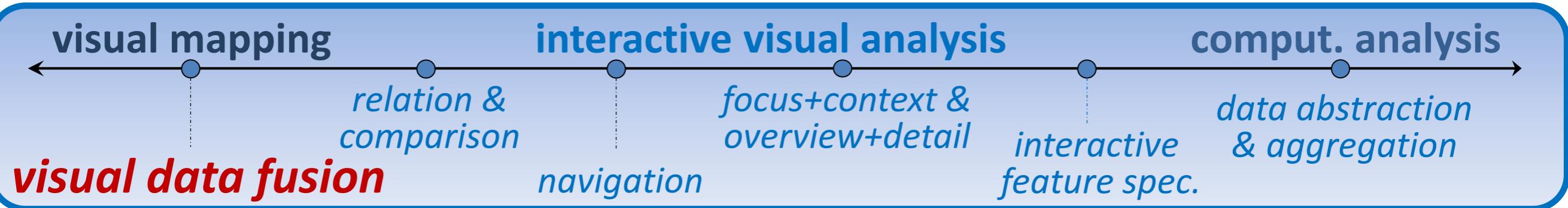


Glyph packing  
[Kindlmann&Westin 06]



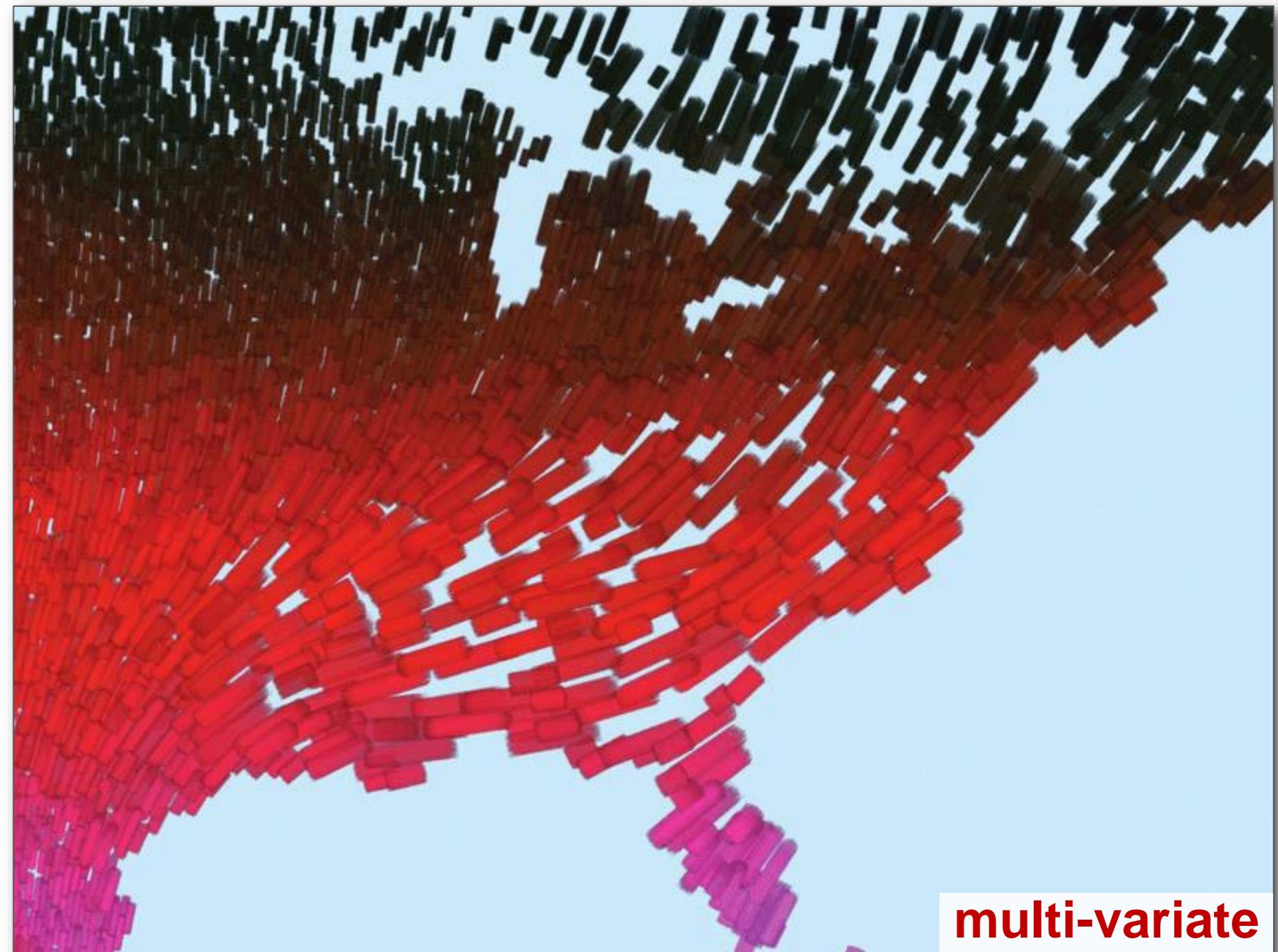
Surface glyphs  
[Meyer-Spradow et al. 08]

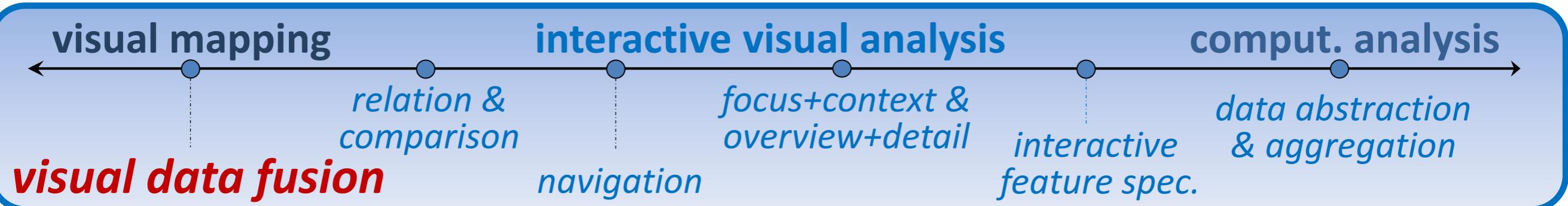




## Textures and Colors [Healey & Enns 02]

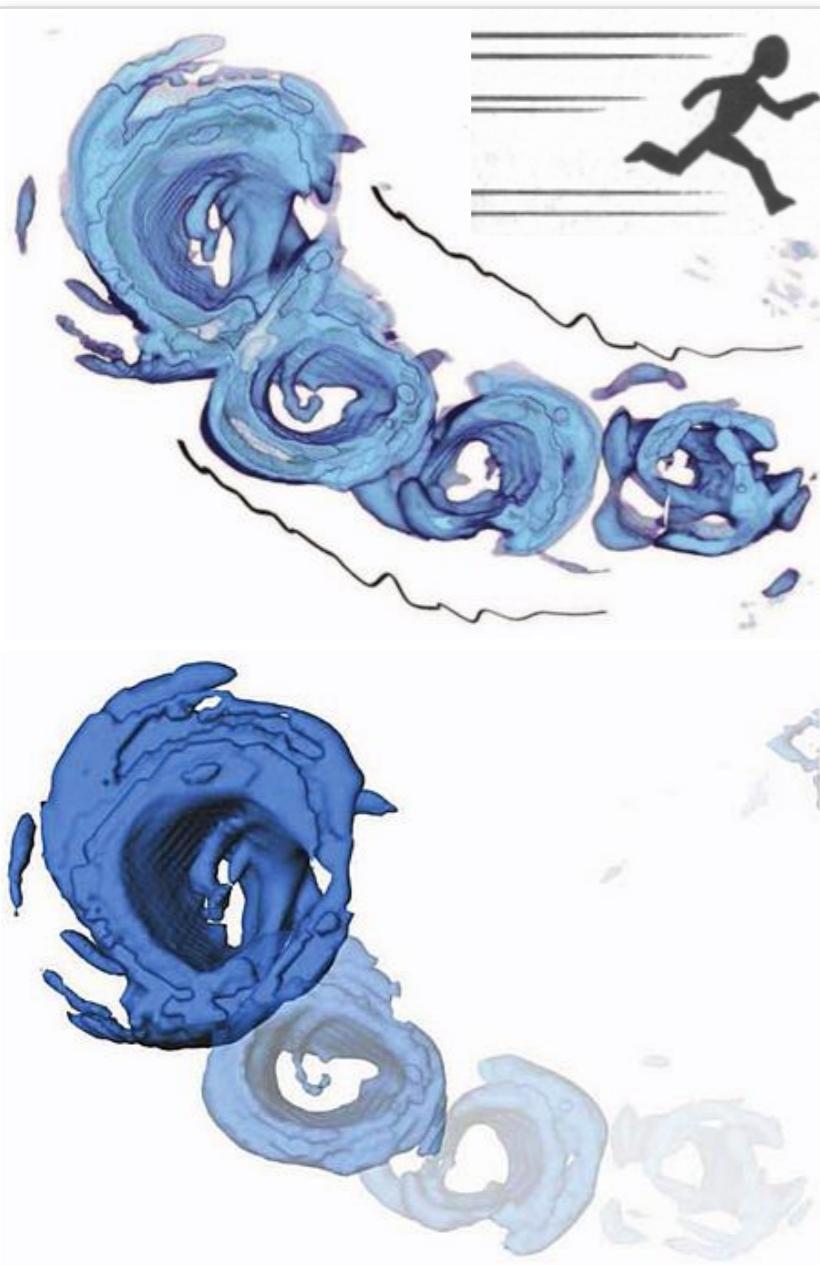
- Temperature  
→ color
- Wind speed  
→ coverage
- Pressure  
→ size
- Precipitation  
→ orientation





## Illustrative visualization techniques

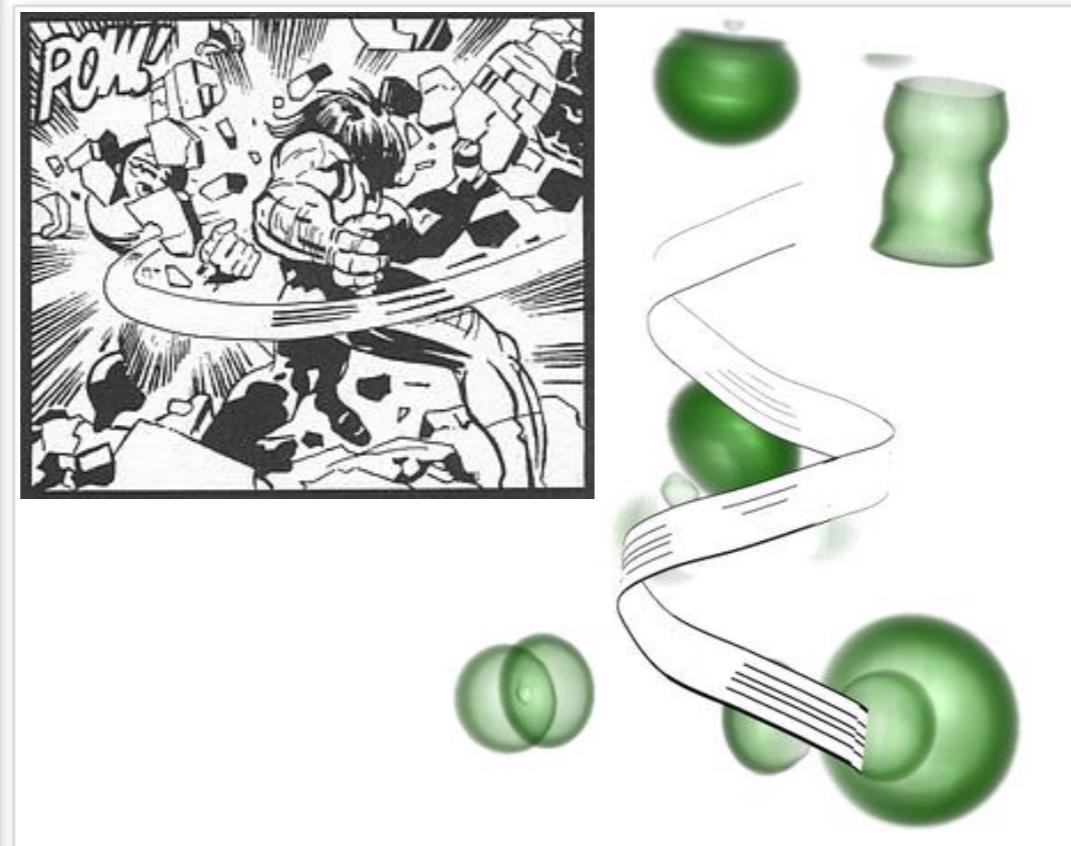
### spatio-temporal



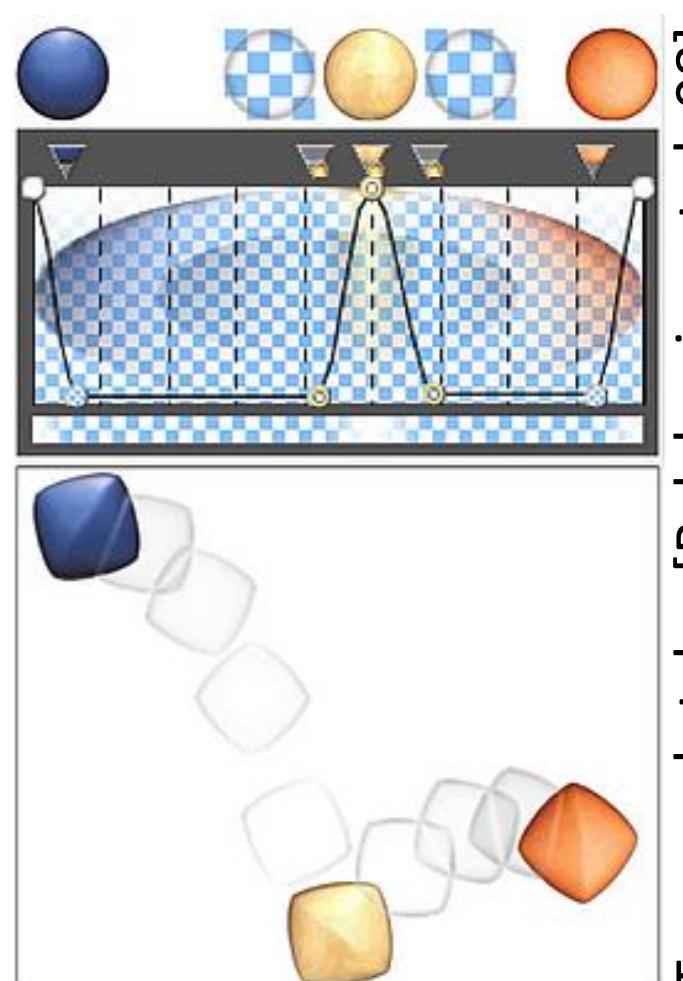
Opacity & speedlines  
[Joshi et al. 09]



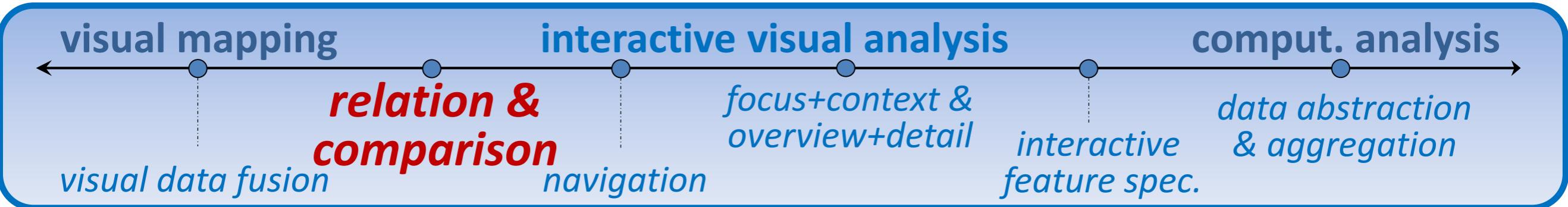
Saturation & silhouettes [Hsu et al. 10]



Flow ribbons  
[Joshi & Rheingans 05]

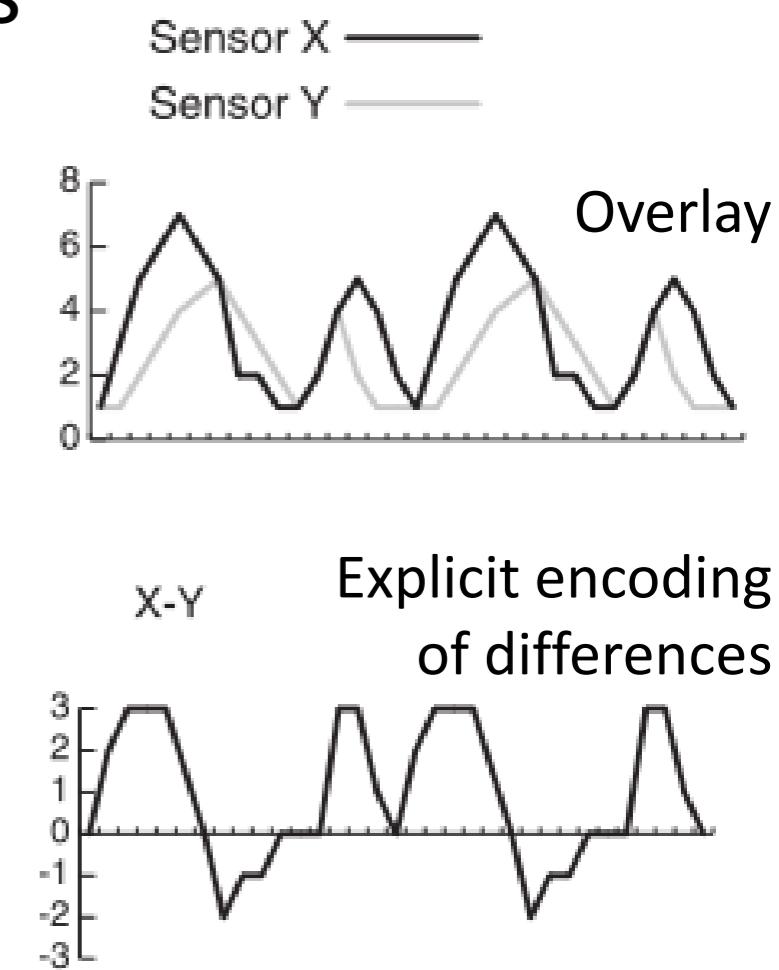
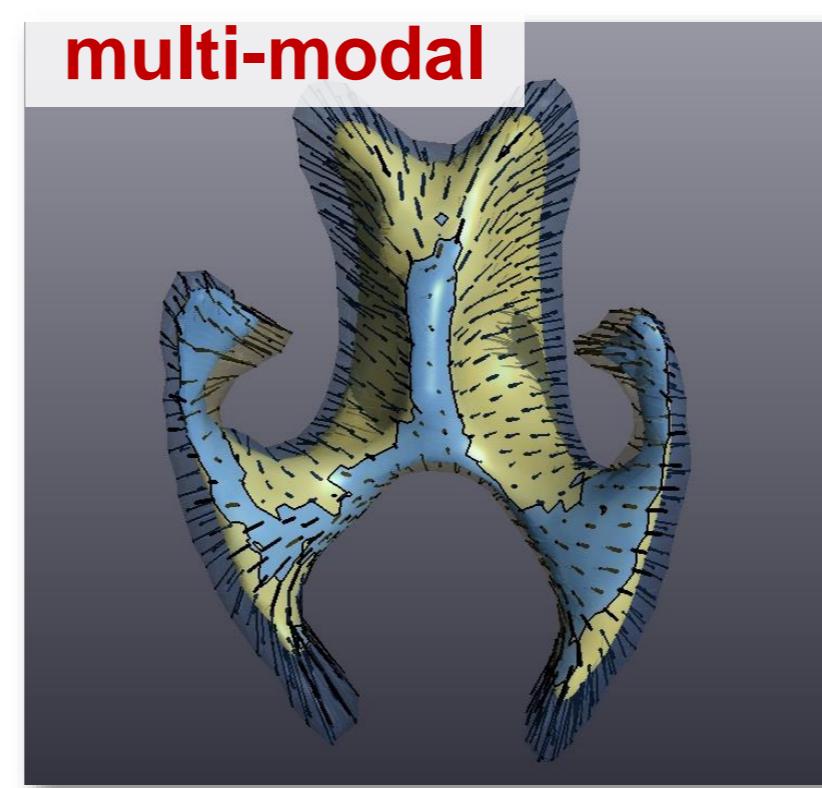
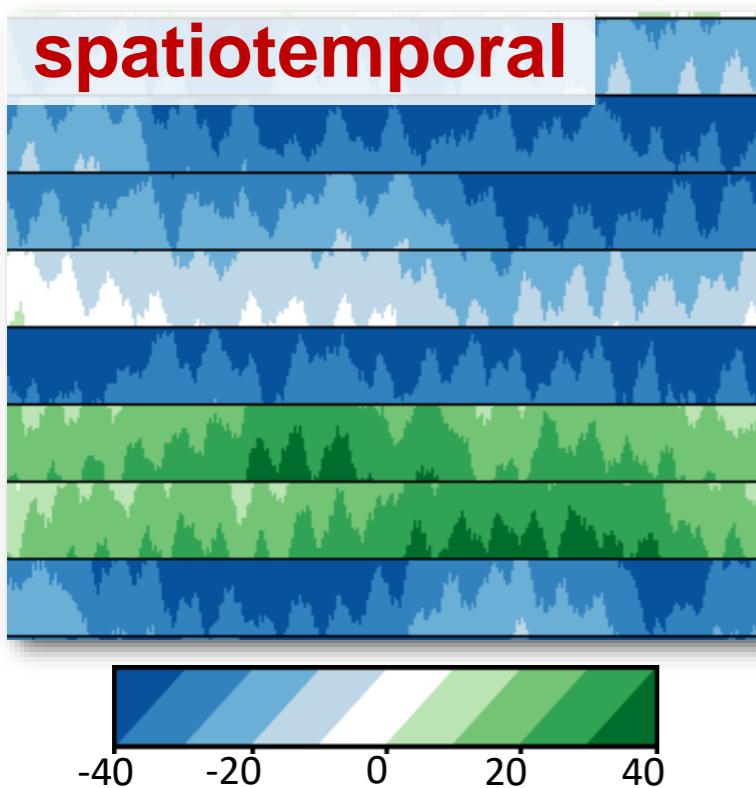


Temporal styles [Balabanian et al. 08]



## Comparative visualization taxonomy [Gleicher et al. 2011]

- Side-by-side comparison (juxtaposition)
- Overlay in same coordinate system (superposition)
- Explicit encoding of differences / correlations



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

**relation &  
comparison**

navigation

focus+context &  
overview+detail

interactive  
feature spec.

data abstraction  
& aggregation

## Comparative visualization taxonomy [Gleicher et al. 2011]

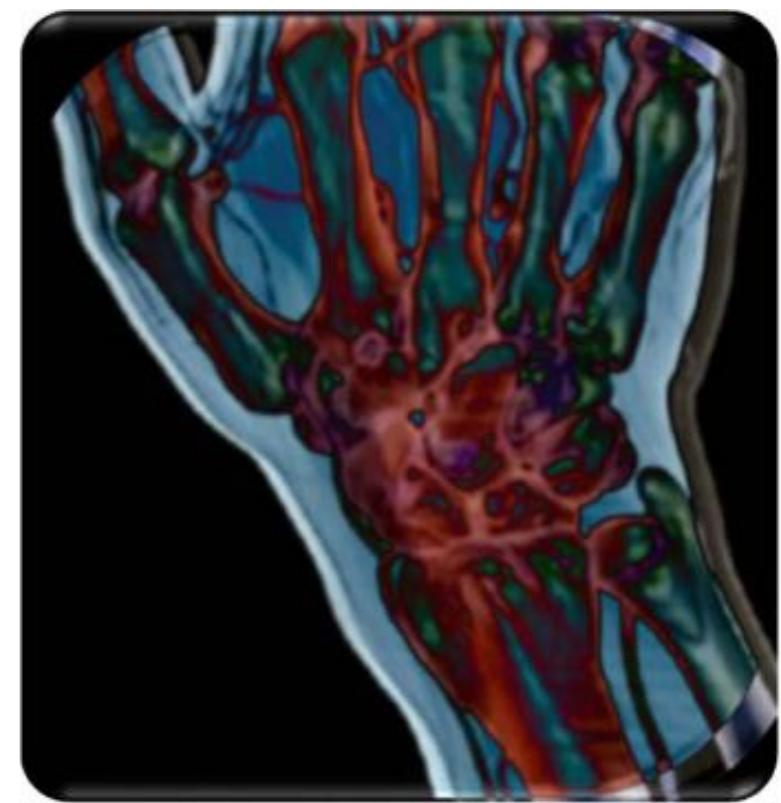
Juxtaposition



Overlay



Explicit encoding



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**relation & comparison**

navigation

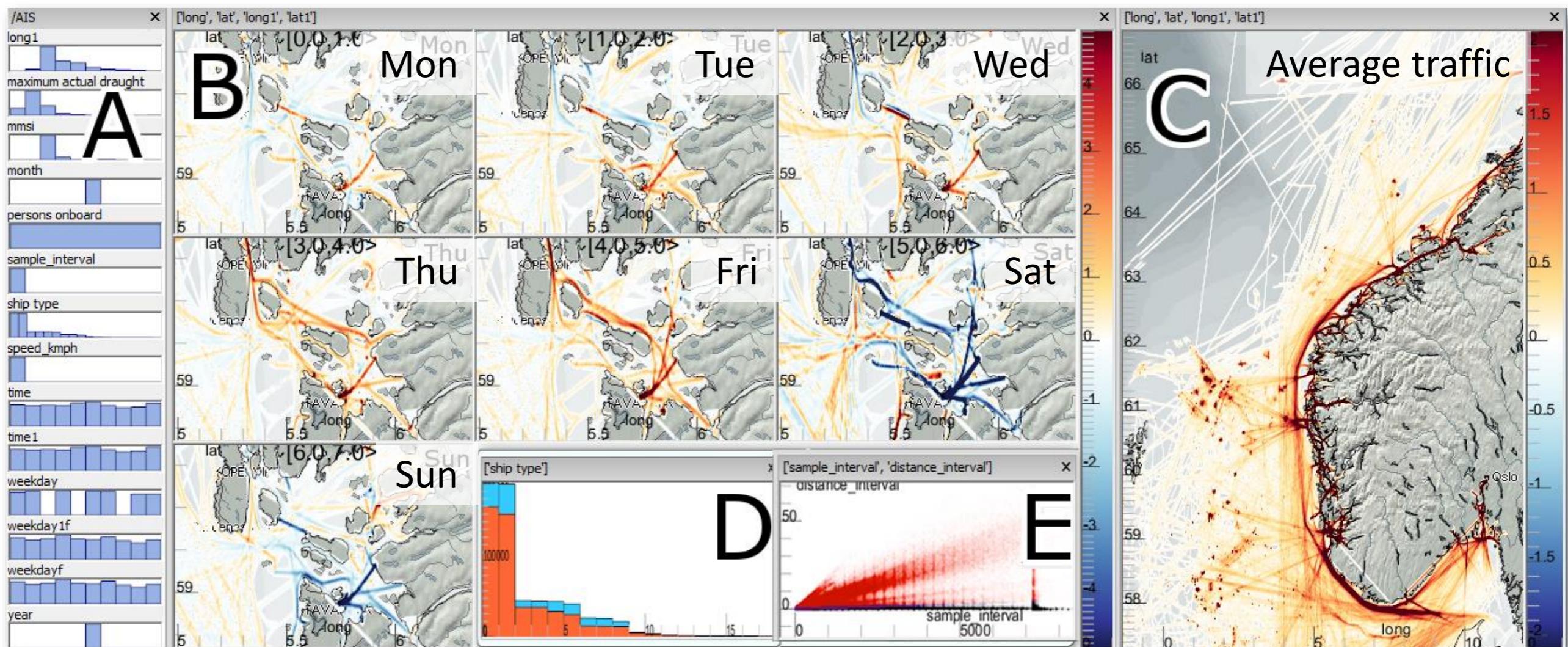
focus+context & overview+detail

interactive feature spec.

data abstraction & aggregation

- Difference Views [Daae Lampe et al. 10, Kehrer et al. 13]
  - Side-by-side comparison + explicit encoding
  - Show difference from average per weekday

**spatiotemporal**



visual mapping

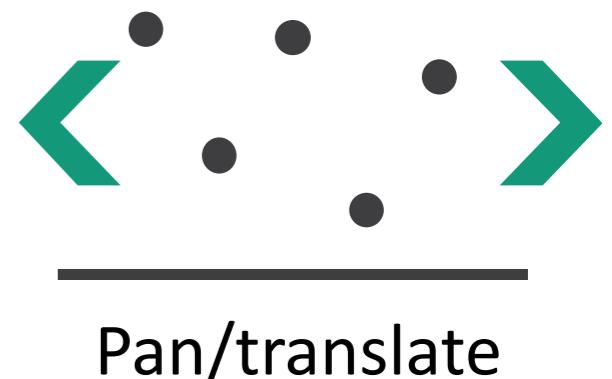
interactive visual analysis

comput. analysis

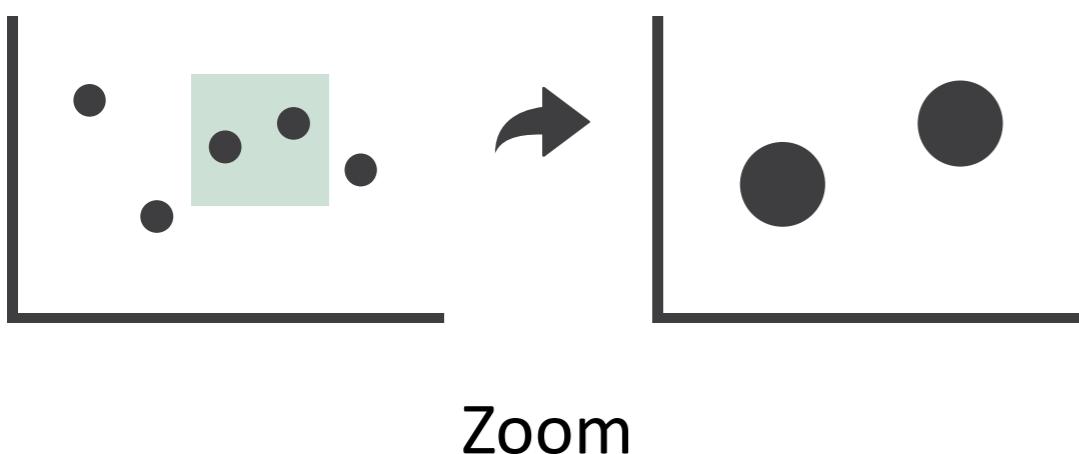


- **Navigation:** Change item visibility

- Change which items are visible
- Camera metaphor
- Zoom, pan, rotate (3D)



Pan/translate

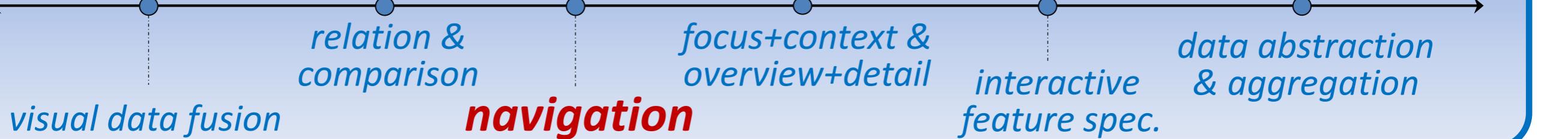


Zoom

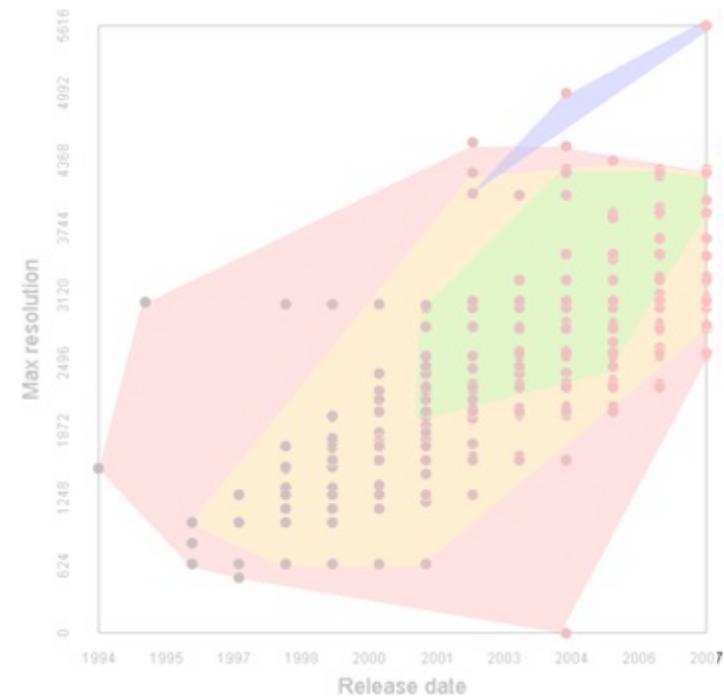
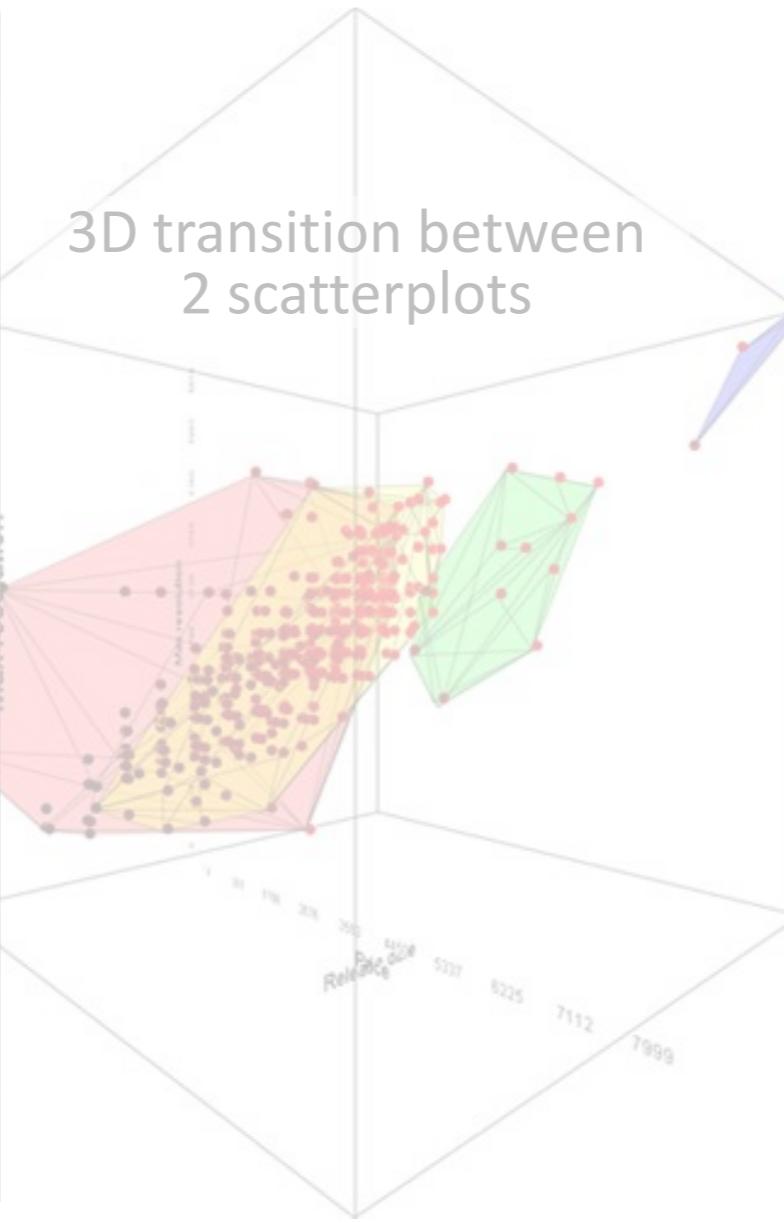
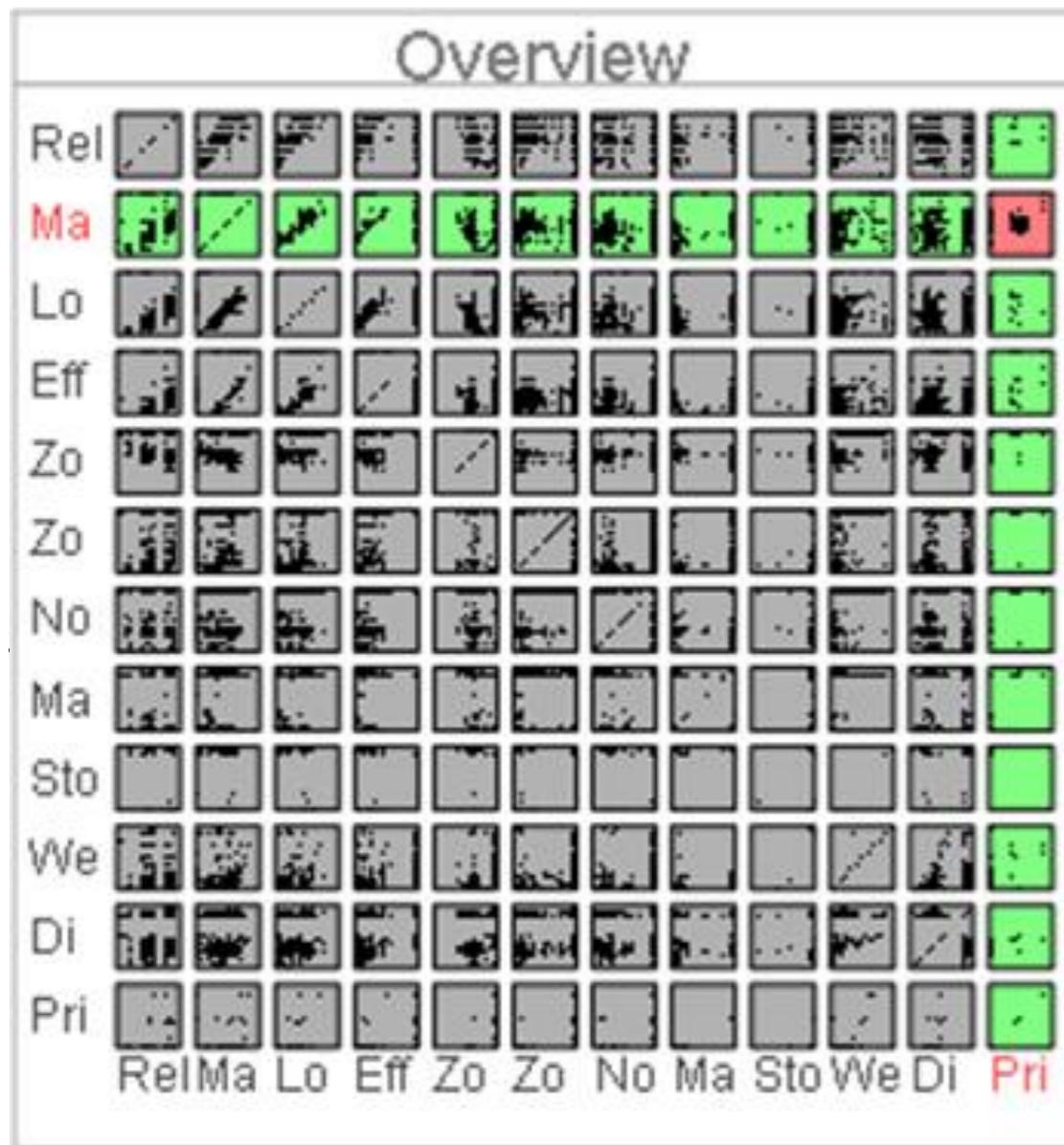
visual mapping

interactive visual analysis

comput. analysis



- Scatterplot Matrix Navigation [Elmqvist et al. 2008]
  - How to navigate a large matrix with scatterplots?



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation & comparison

**navigation**

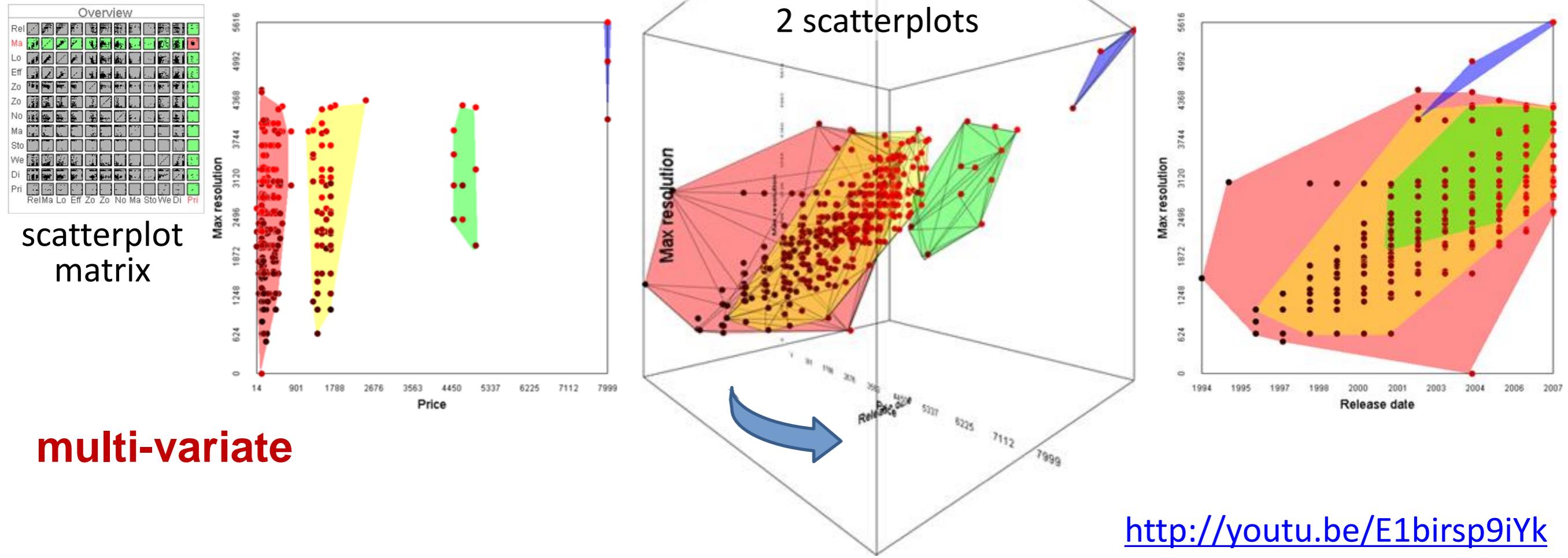
focus+context & overview+detail

interactive feature spec.

data abstraction & aggregation

- Scatterplot Matrix Navigation [Elmqvist et al. 2008]

- How to navigate a large matrix with scatterplots?
- Transitions between scatterplots as animated rotations in 3D space



visual mapping

interactive visual analysis

comput. analysis



*relation & comparison*

*focus+context & overview+detail*

*interactive feature spec.*

*data abstraction & aggregation*

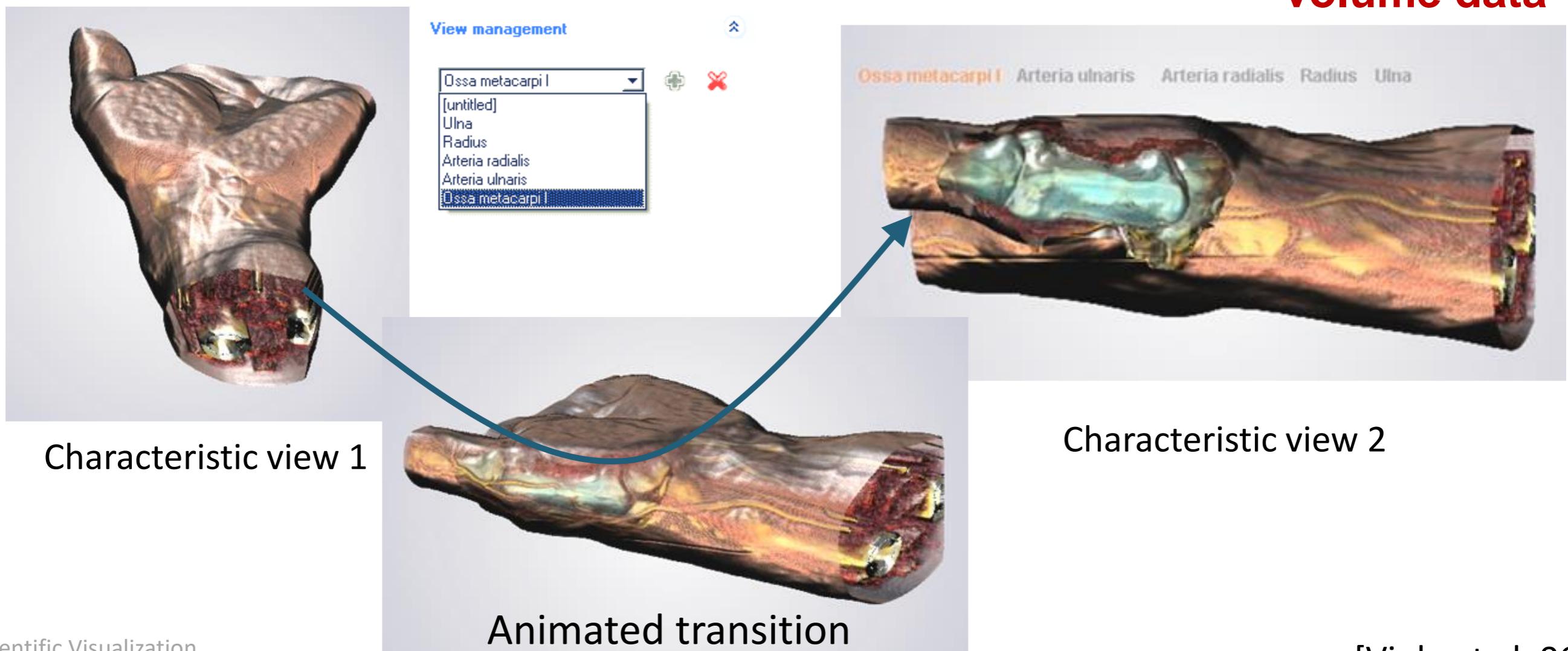
visual data fusion

**navigation**

- Automated viewpoint selection

- Guided navigation between characteristic views
- Based on information-theoretic measures

**segmented volume data**



Characteristic view 1

Characteristic view 2

Animated transition

## visual mapping

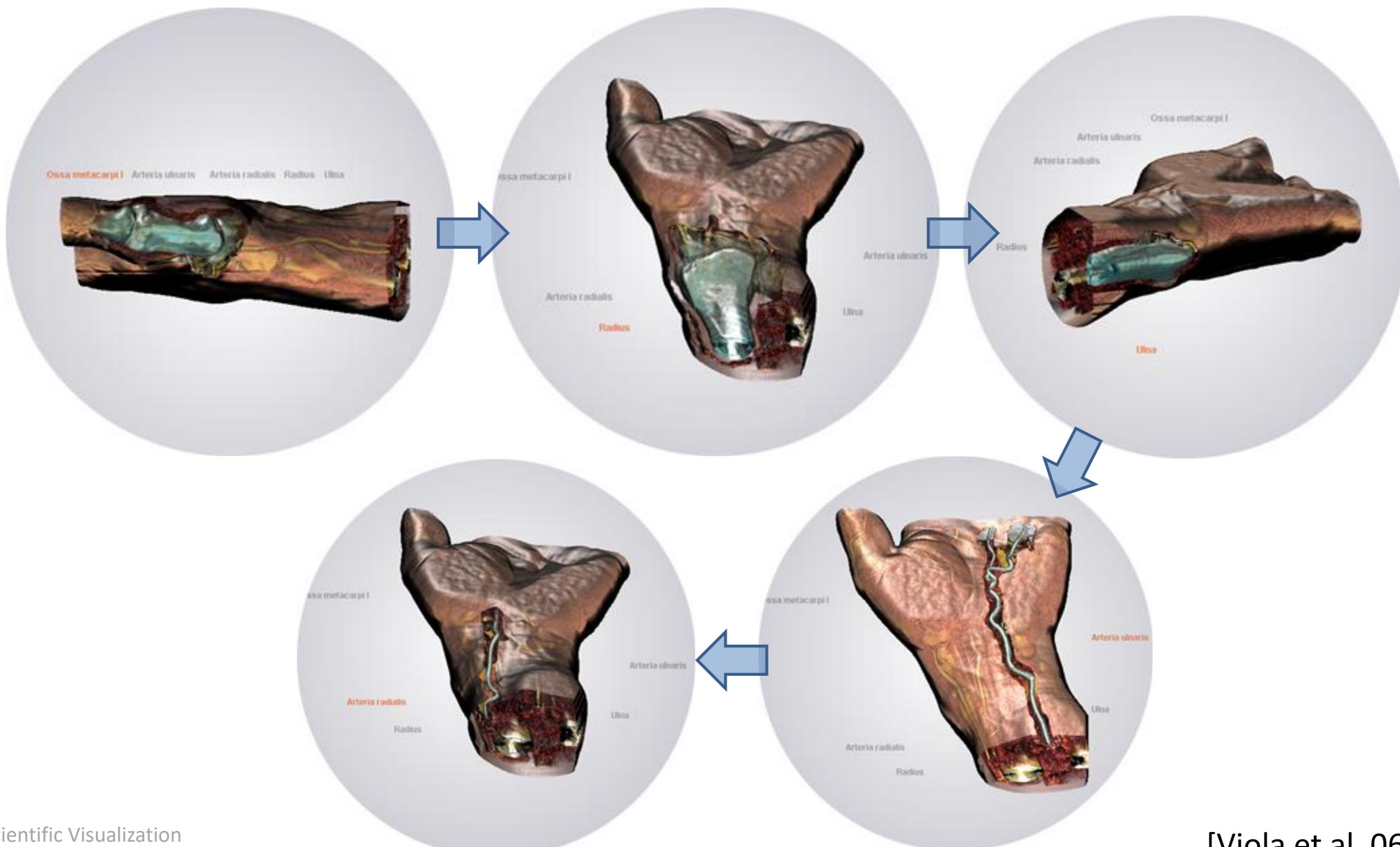
## interactive visual analysis

## comput. analysis

visual data fusion  
*relation & comparison*

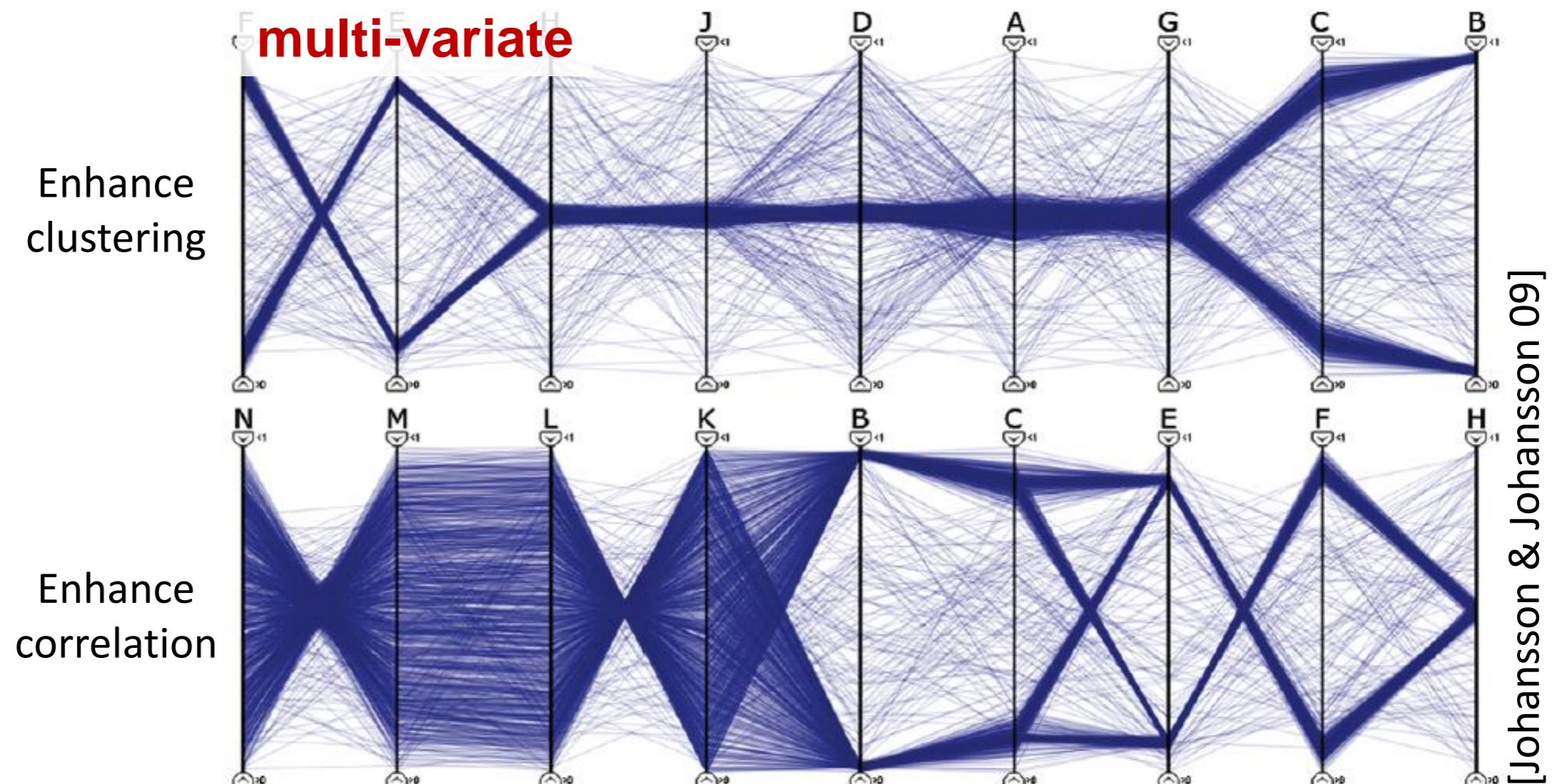
**navigation**

interactive feature spec.  
*data abstraction & aggregation*





- Ranking/quality metrics [Bertini et al. 2011]
  - Automatically order views/axes by quality metrics
  - Enhance clustering, correlations, outliers, image quality, etc.



## visual mapping

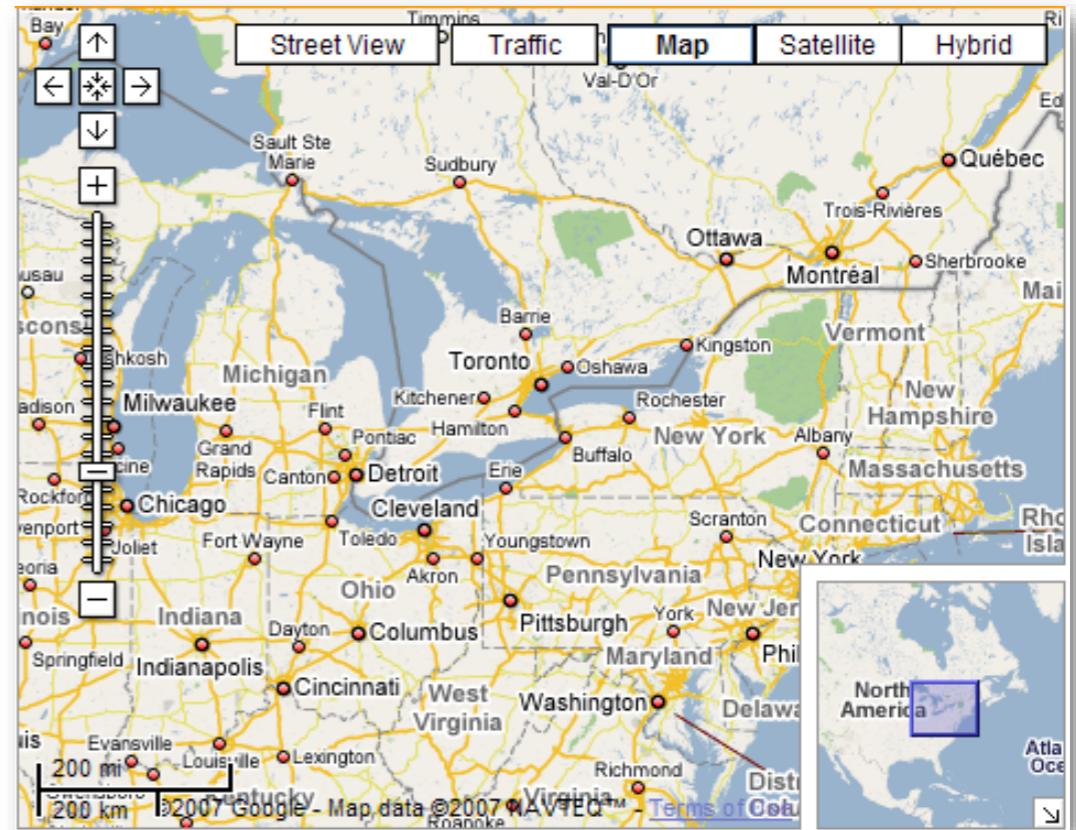
## interactive visual analysis

## comput. analysis



## ■ Problem

- Impossible to show all details of large data set in single image

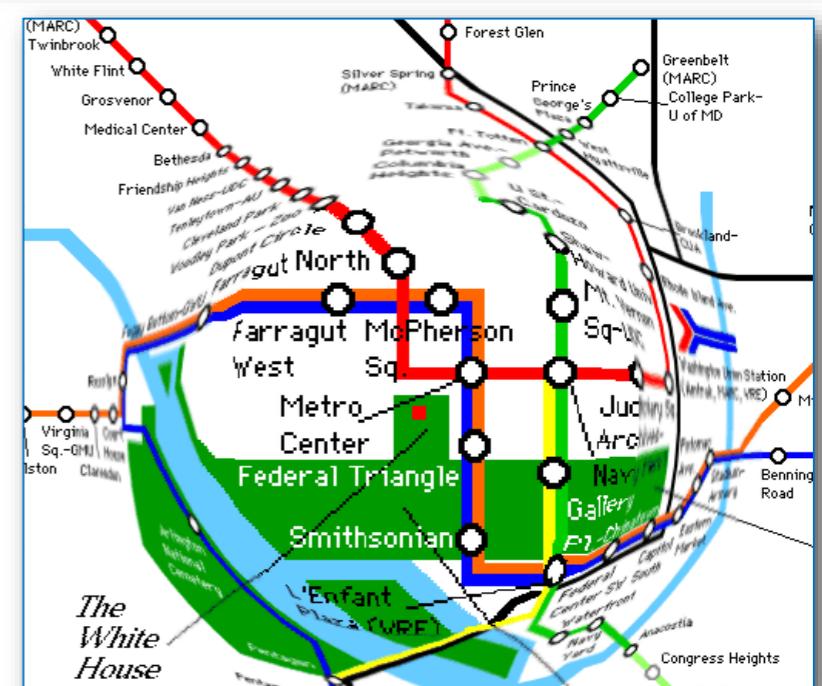


## ■ Overview+detail visualization

- Spatially separate overview / detail (e.g., juxtaposed views)
- User has to switch attention between representations

## ■ Focus+context visualization

- Seamlessly integrates focus / context in single visualization



Fisheye views [Furnas 86]

visual mapping

interactive visual analysis

comput. analysis

*relation &  
comparison*

***focus+context &  
overview+detail***

*visual data fusion*

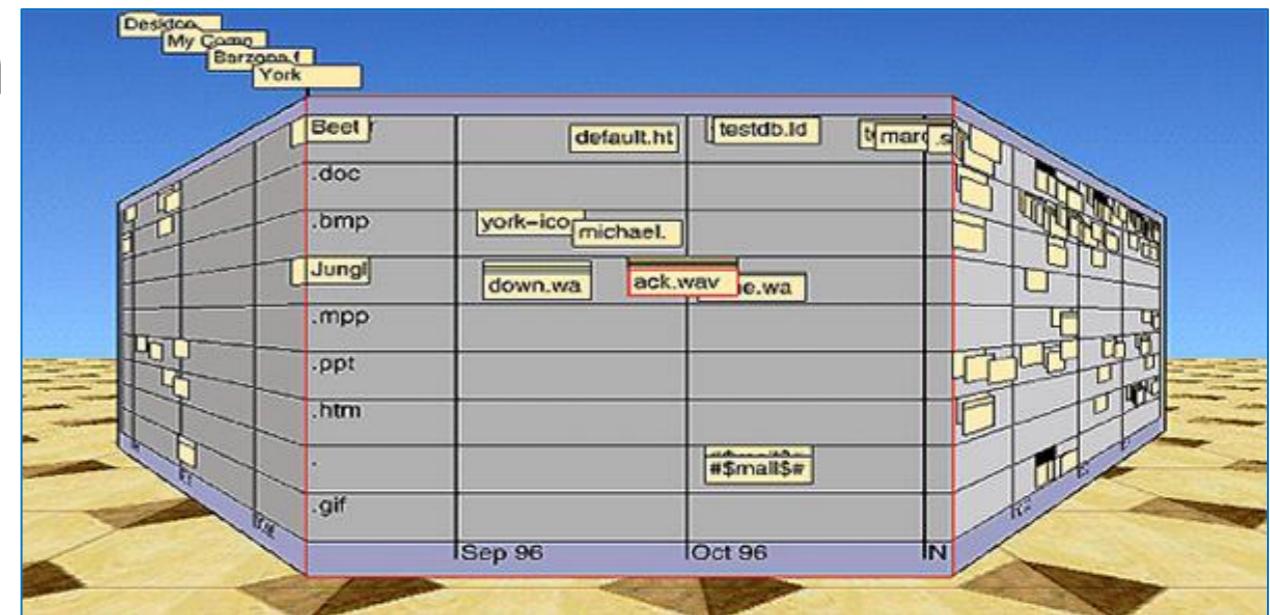
*navigation*

*interactive  
feature spec.*

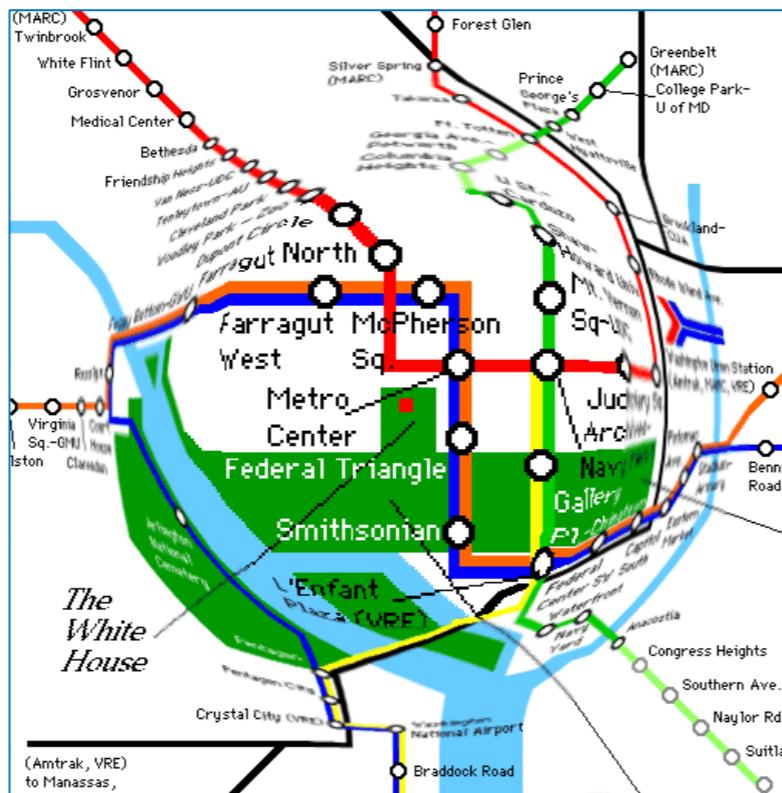
*data abstraction  
& aggregation*

## Focus+context (F+C) visualization

- Originally spaced distortion used
- More space for focus
- Keep context, without cropping away data outside of zoom area



Perspective wall [Mackinlay 91]



Fisheye views [Furnas 86]

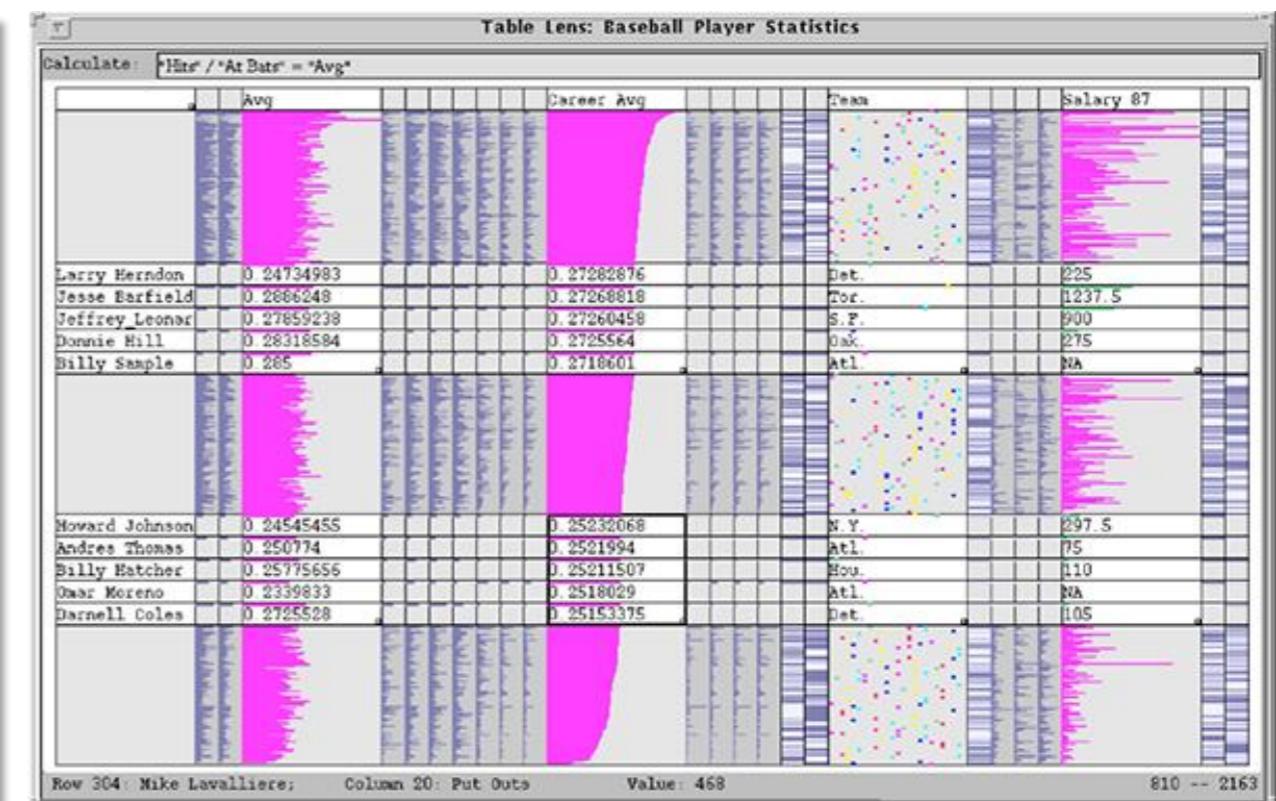
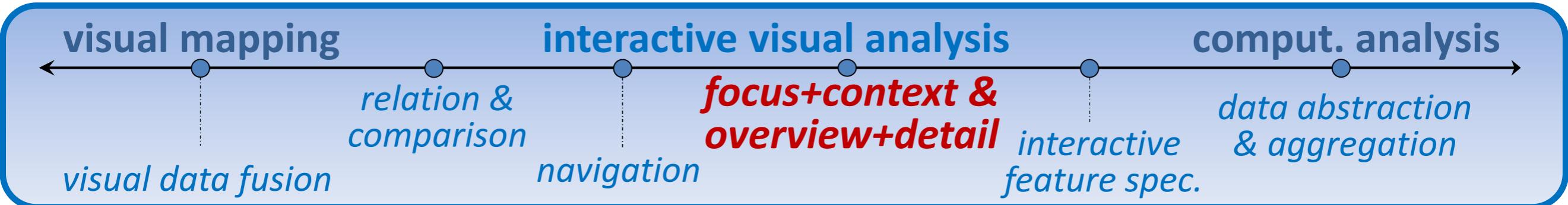


Table lens [Rao/Card 94]



## Generalized F+C visualization [Hauser 05]

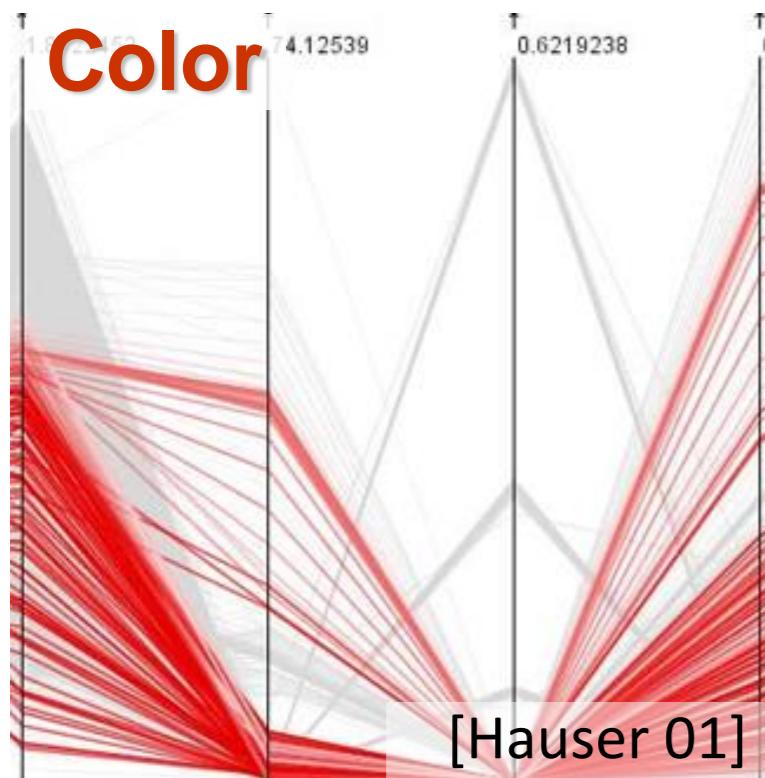
- Emphasize data in focus
- Keep context for orientation/navigation
- Focus specification, e.g., by pointing, brushing or querying

### Opacity/transparency

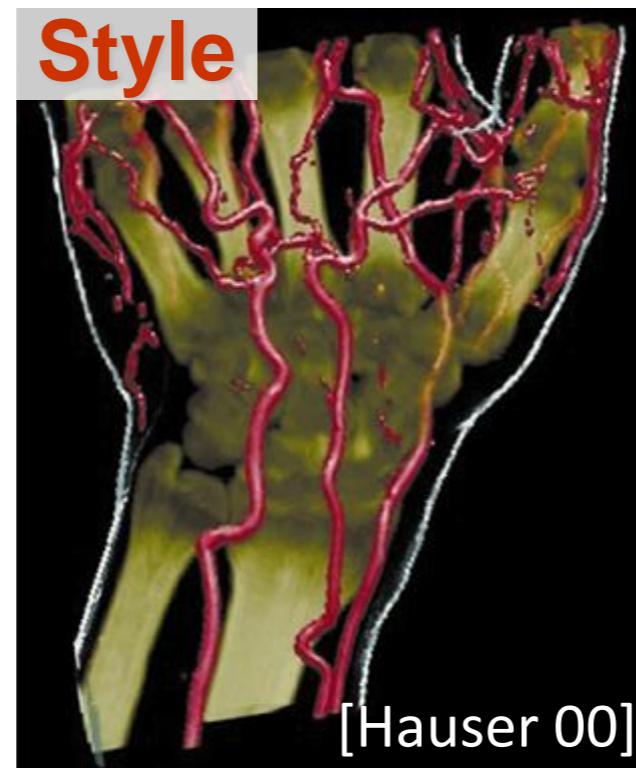


Importance-driven rendering [Viola 04]

### Color



### Style



### Frequency/Blurring



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation &  
comparison

navigation

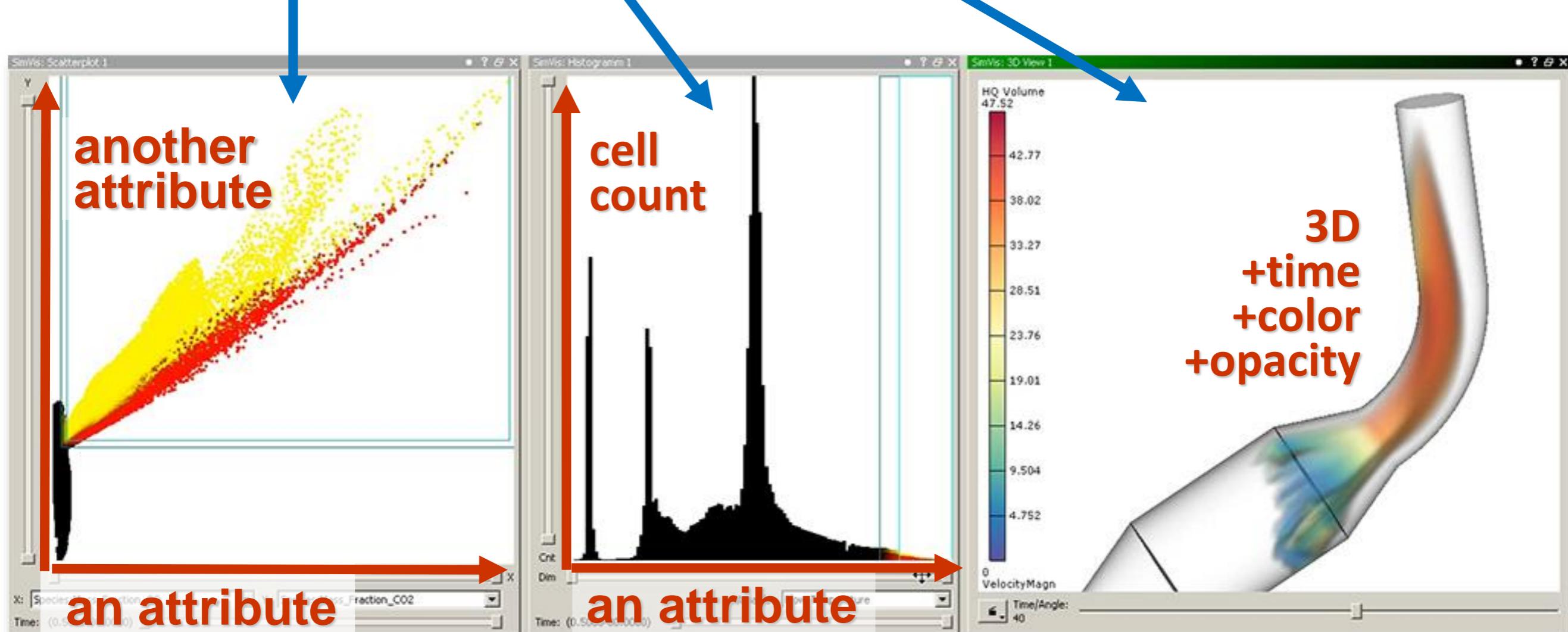
focus+context &  
overview+detail

**interactive  
feature spec.**

data abstraction  
& aggregation

## Brushing in multiple linked views

- One dataset, but multiple views
- Scatterplots, histograms, 3D(4D) views, etc.



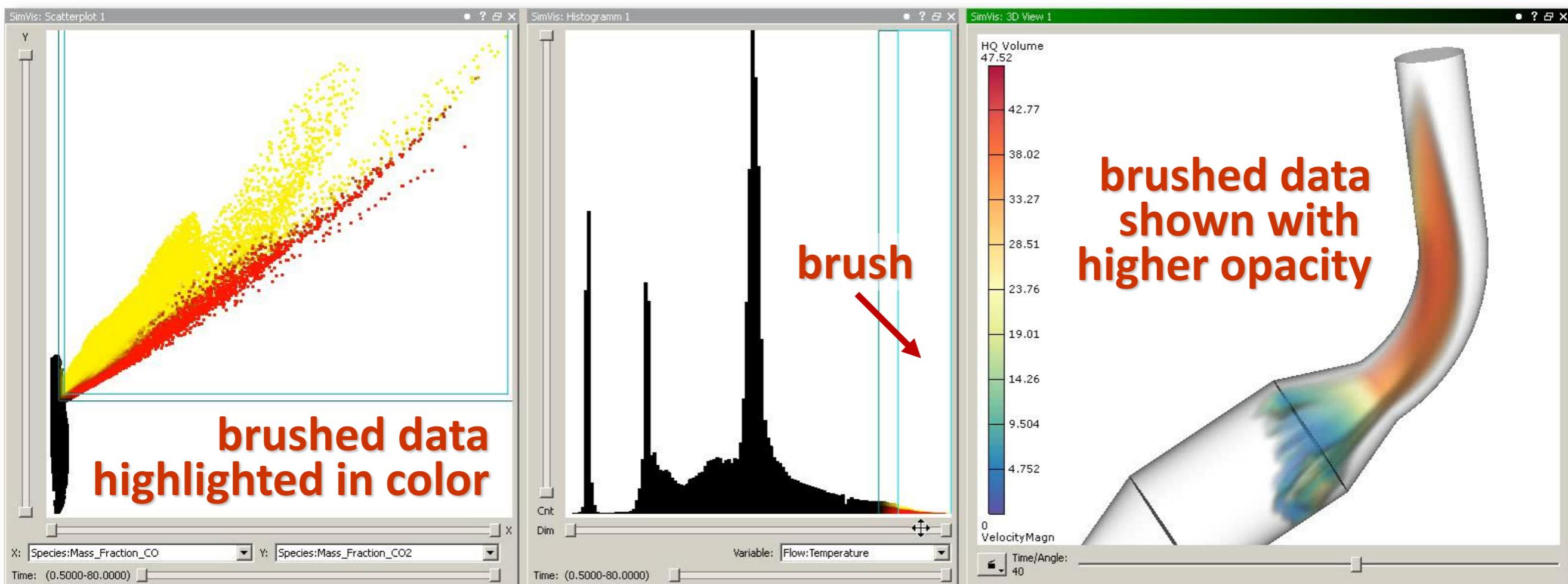
## visual mapping

## interactive visual analysis

## comput. analysis



- **Brushing:** mark interesting data subset
- **Linking:** enhance/highlight brushed data in linked views
- Move/alter/extend brush



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation & comparison

navigation

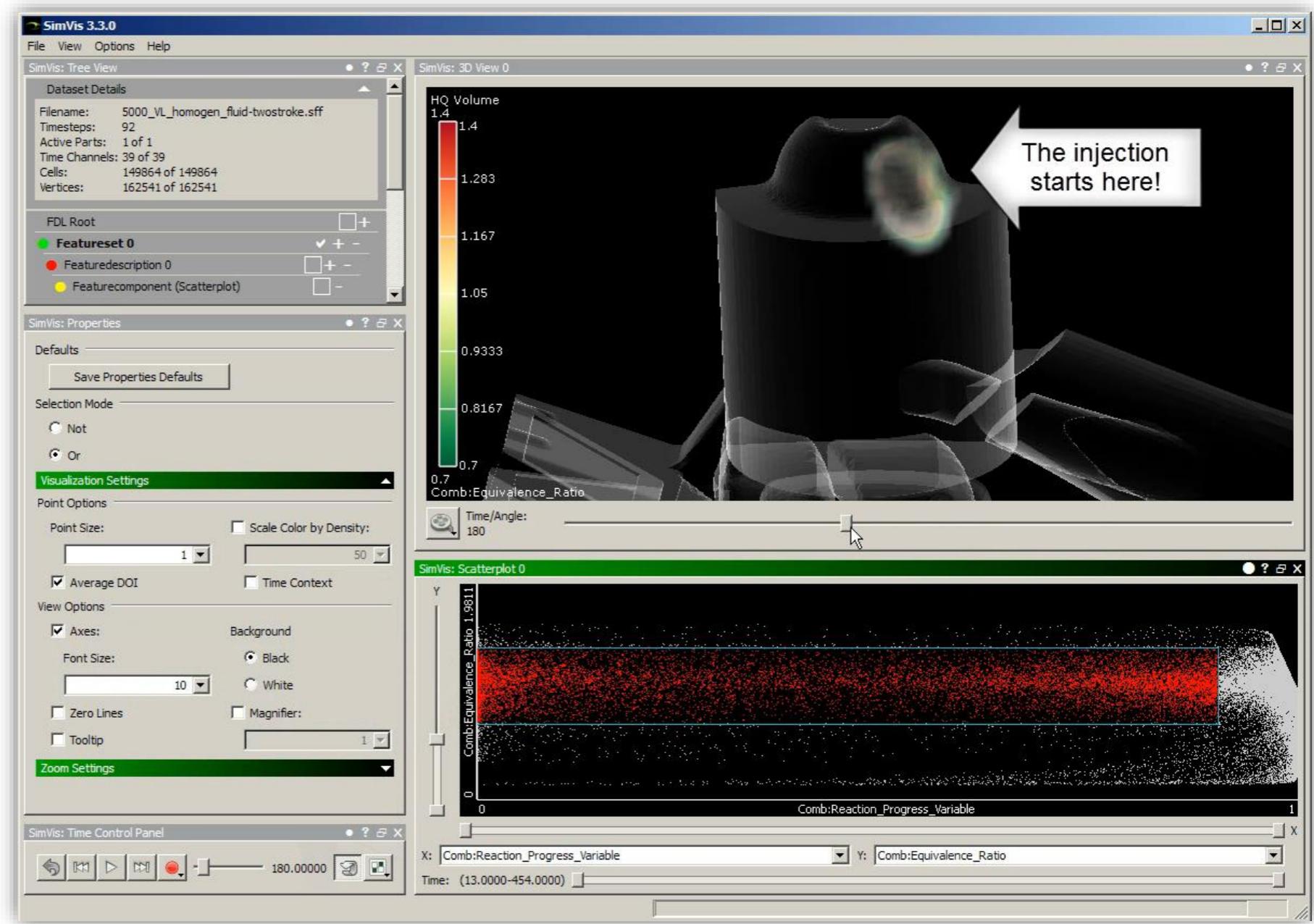
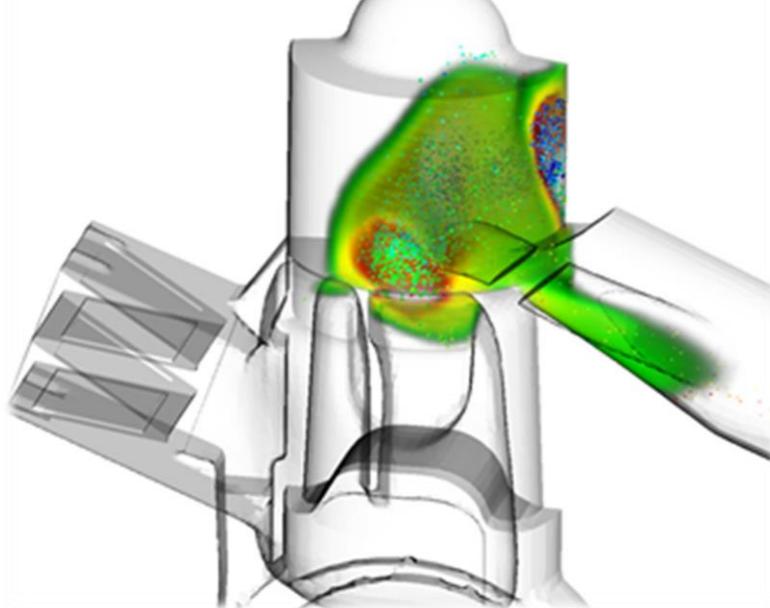
focus+context & overview+detail

**interactive feature spec.**

data abstraction & aggregation

## Brushing in multiple linked views

- Example: Combustion process in a two-stroke engine

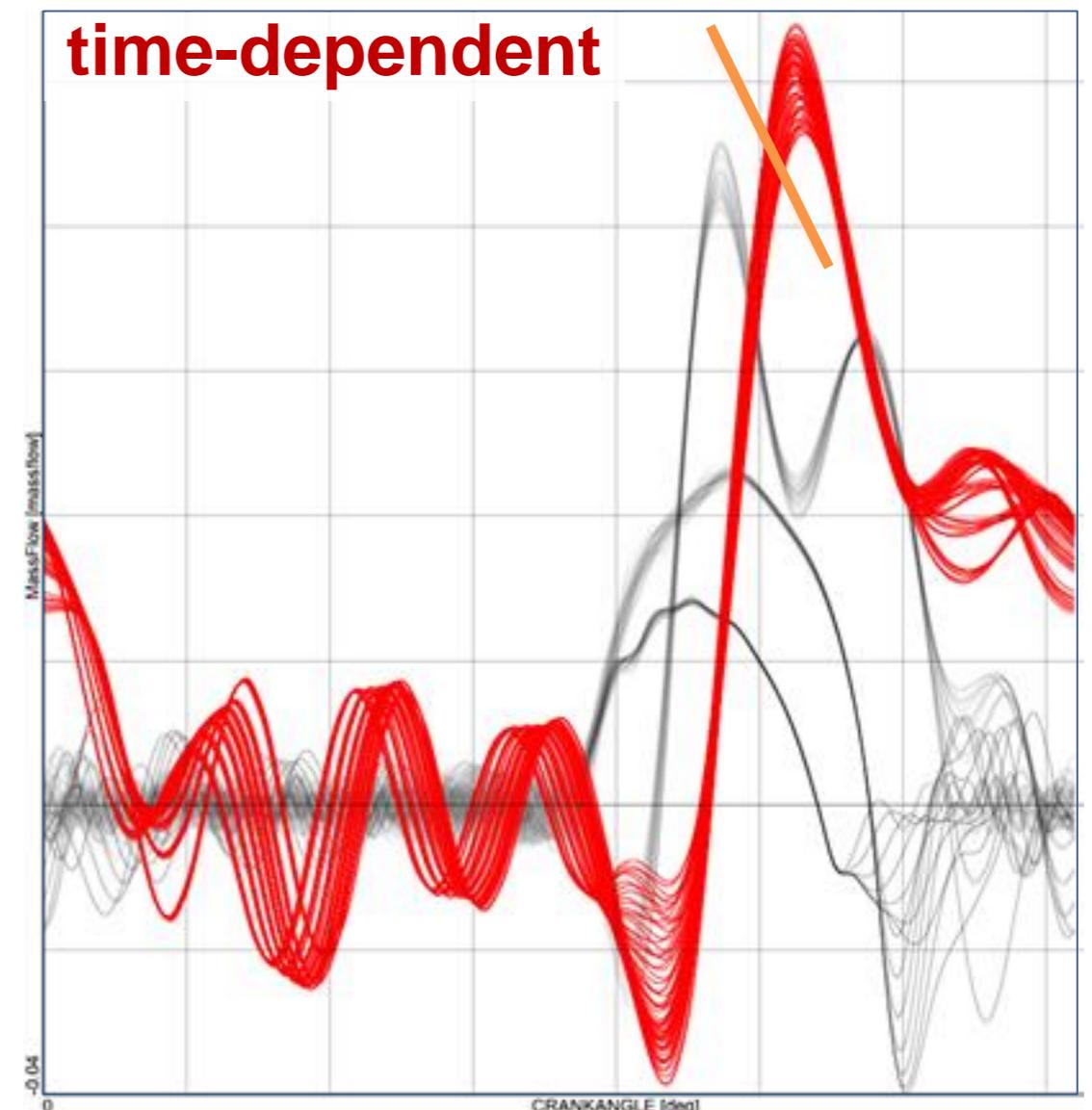


[SimVis GmbH]



## Line brush [Konyha et al. 06]

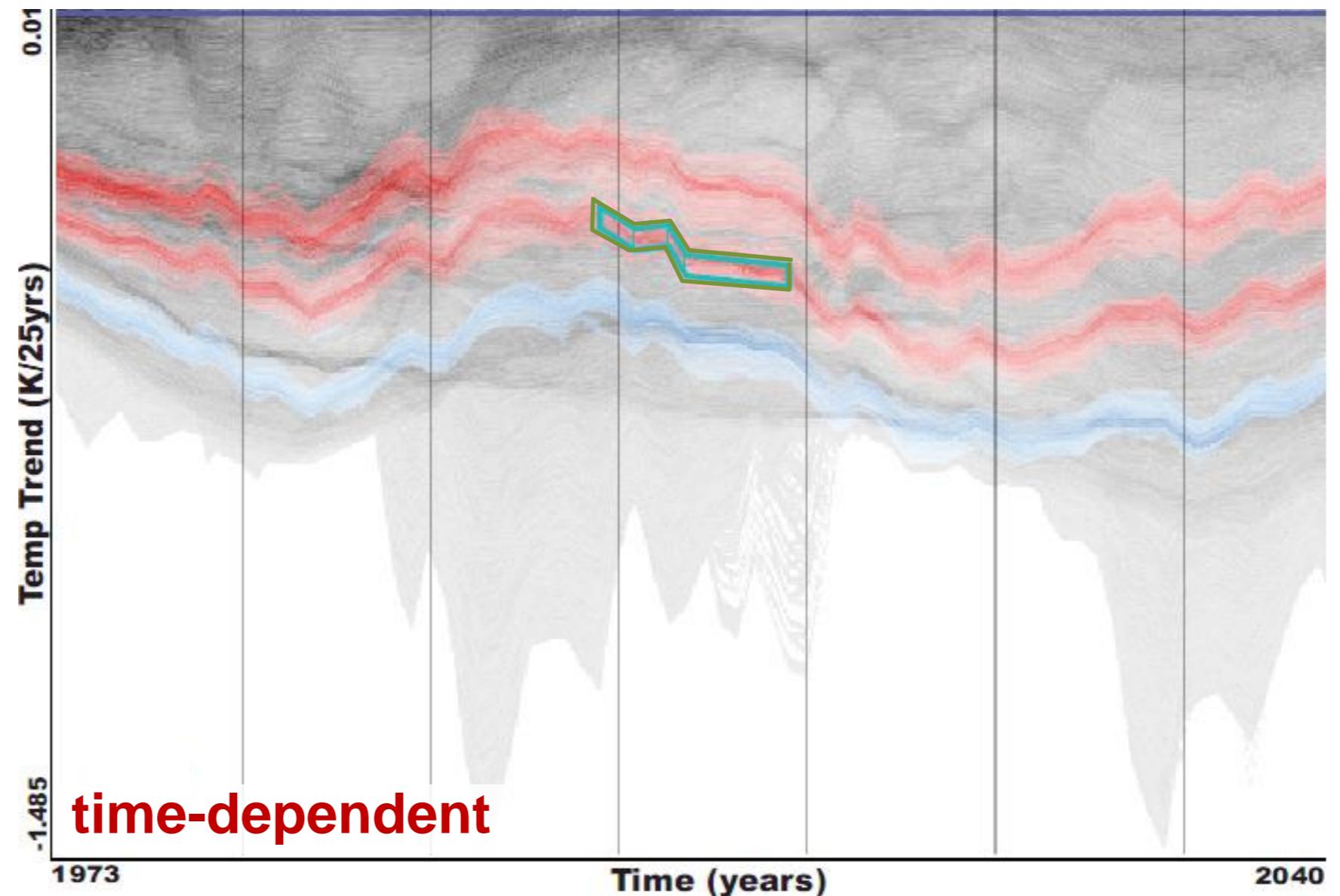
- Select function graphs that intersect with user-specified line





## Similarity-based brushing [Muigg et al. 2008]

- Select function graphs by similarity to user-sketched pattern
- Similarity evaluated based on gradients (1st derivative)



visual mapping

interactive visual analysis

comput. analysis

*relation &  
comparison*

*focus+context &  
overview+detail*

*data abstraction  
& aggregation*

*visual data fusion*

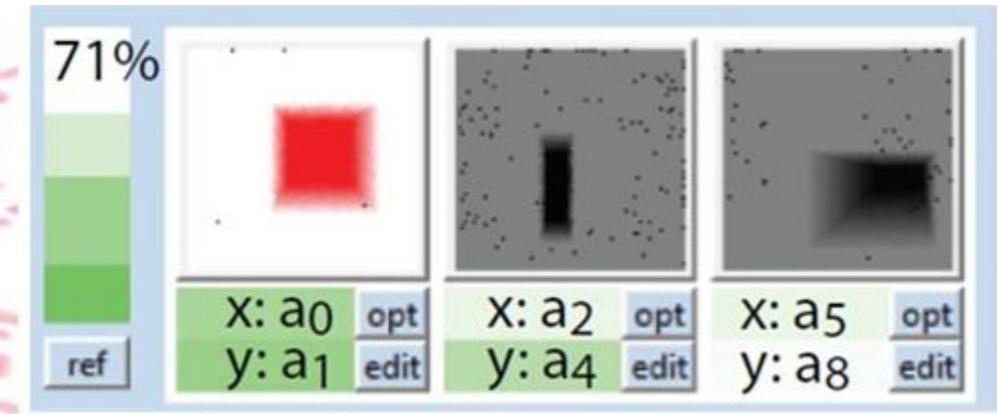
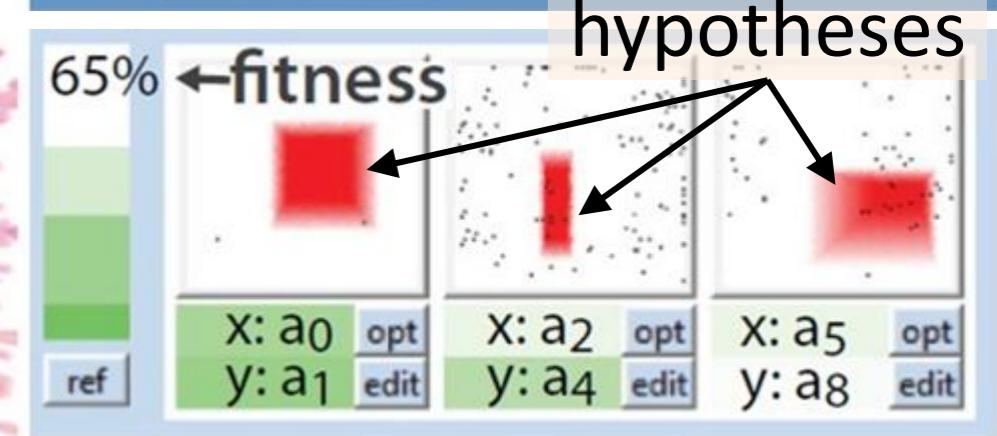
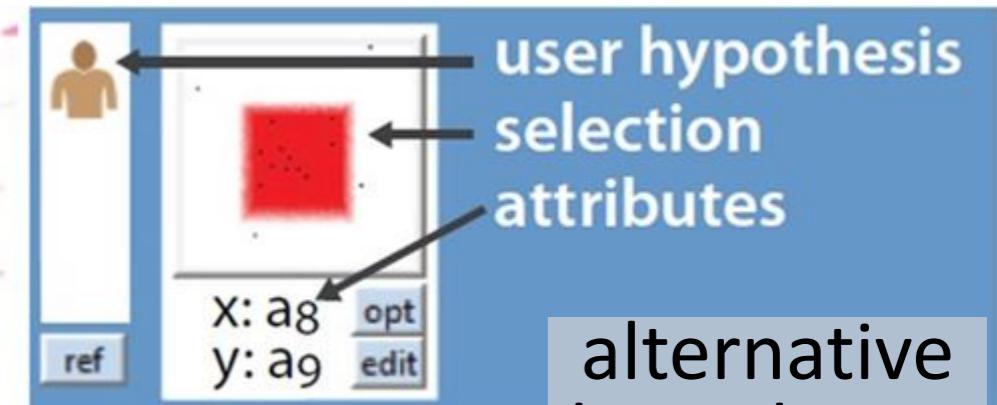
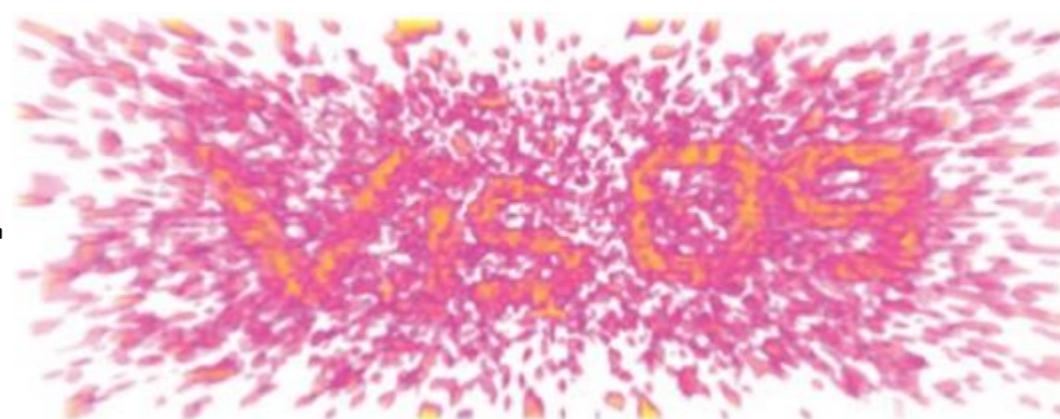
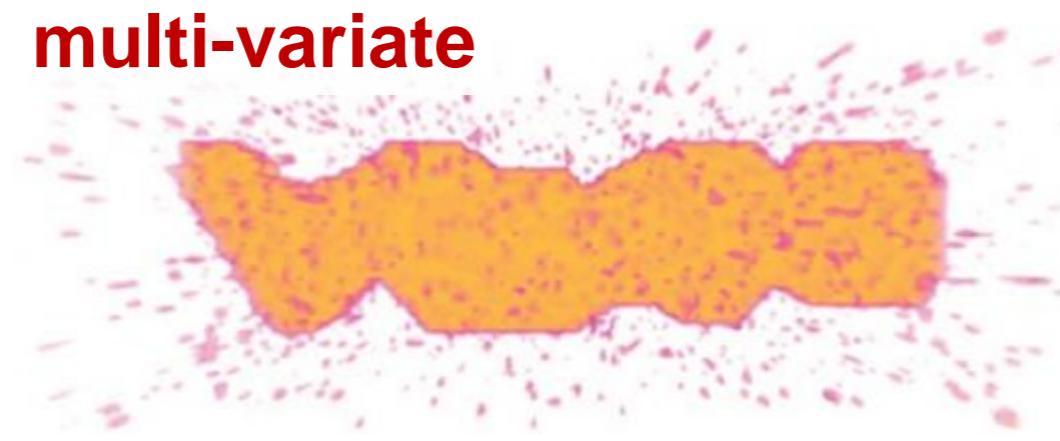
*navigation*

**interactive  
feature spec.**

- Tight integration with supervised machine learning

Visual human+machine  
learning [Fuchs et al. 09]

**multi-variate**



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation & comparison

navigation

focus+context & overview+detail

interactive feature spec.

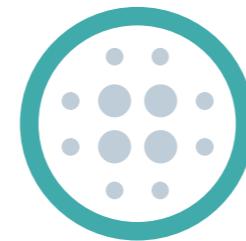
**data abstraction & aggregation**

## Machine Learning Approaches



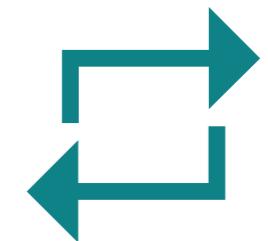
### Supervised Learning

Learning with a **labeled training set**



### Unsupervised Learning

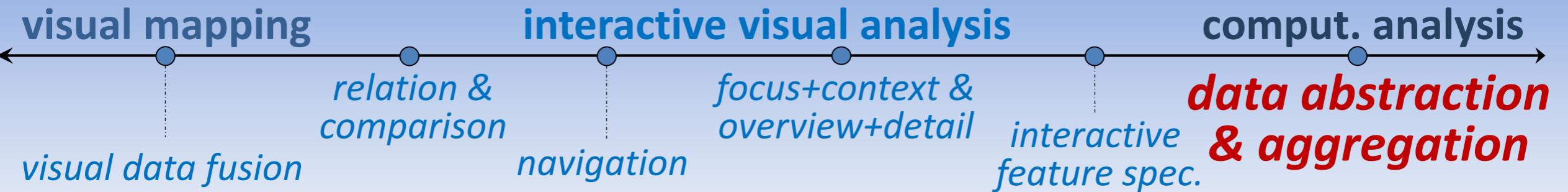
Discovering patterns in unlabeled data



### Reinforcement Learning

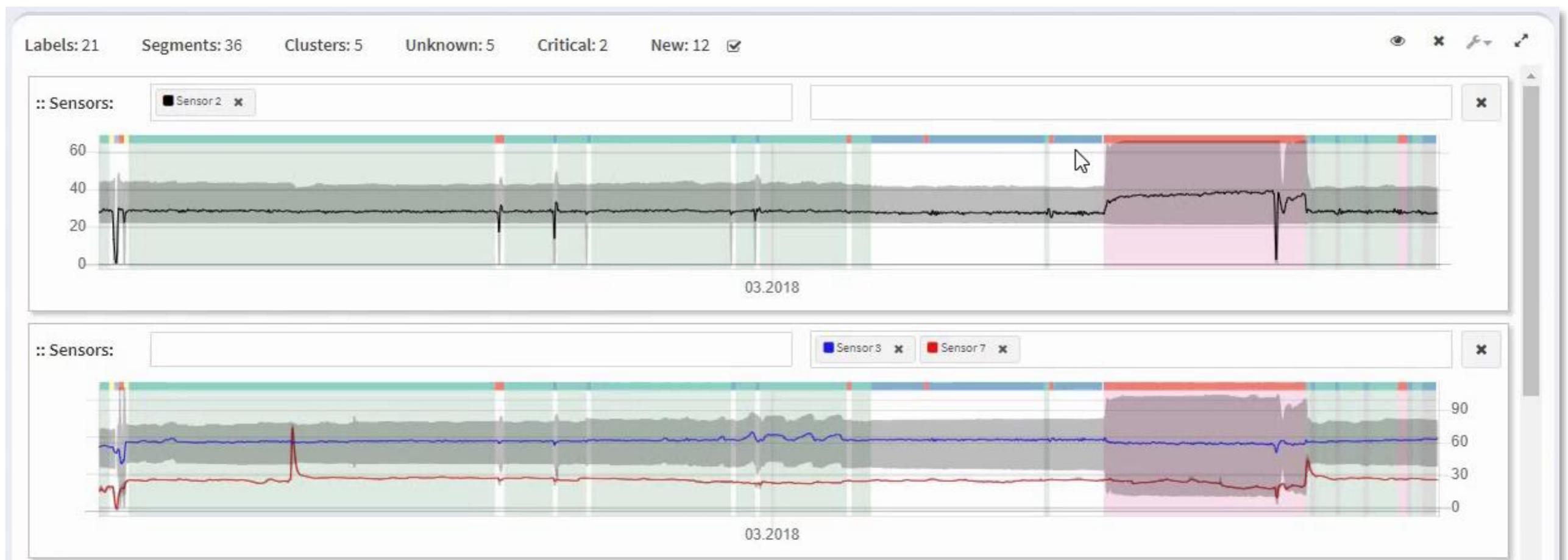
Learning based on **feedback or reward**





## Example: Semi-Automatic Labeling Tool (SALT)

- Labeling of large time series data by domain experts
- Integrates supervised & unsupervised segmentation methods
- User can iteratively improve labeling



visual mapping

interactive visual analysis

comput. analysis

←  
visual data fusion

relation &  
comparison

navigation

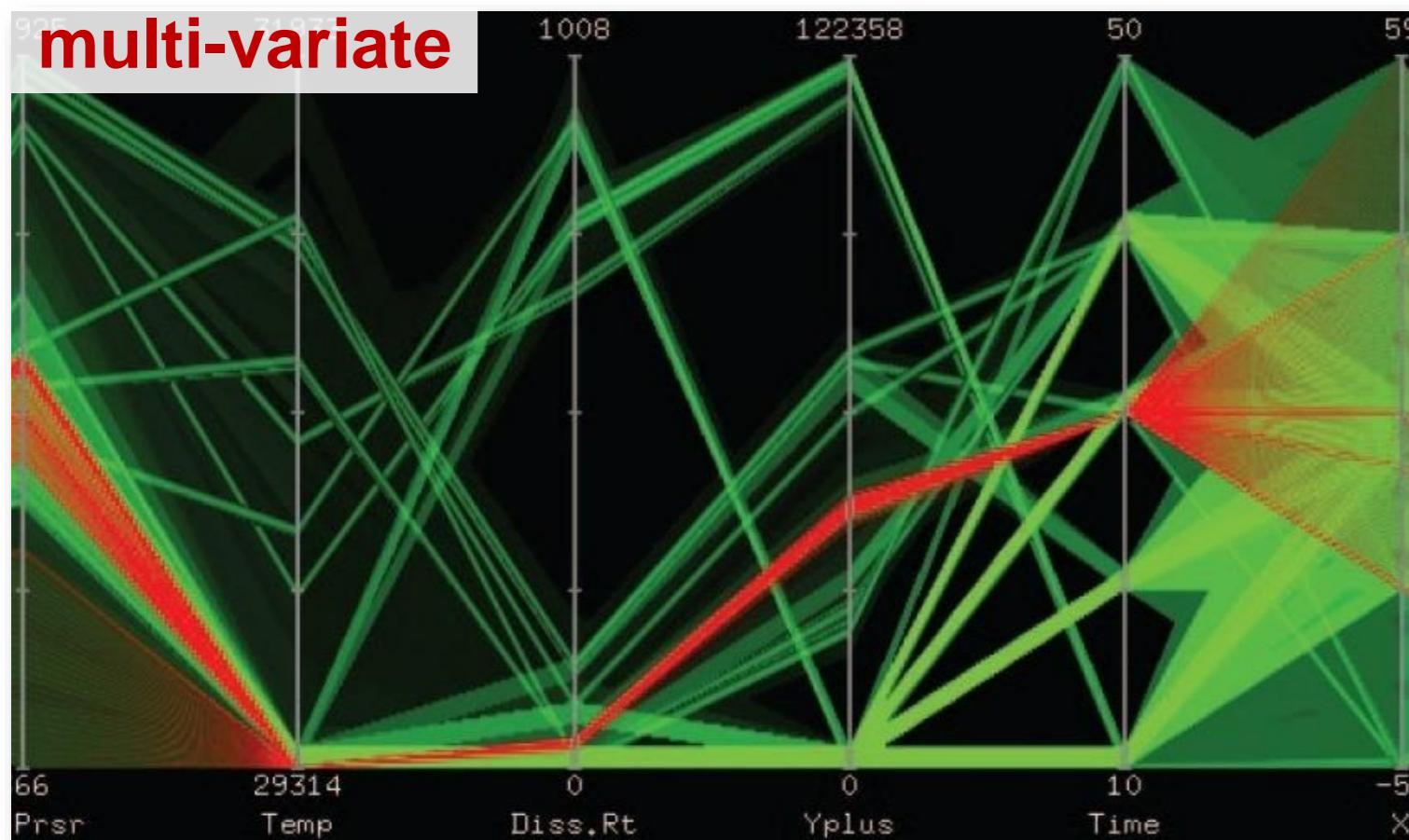
focus+context &  
overview+detail

interactive  
feature spec.

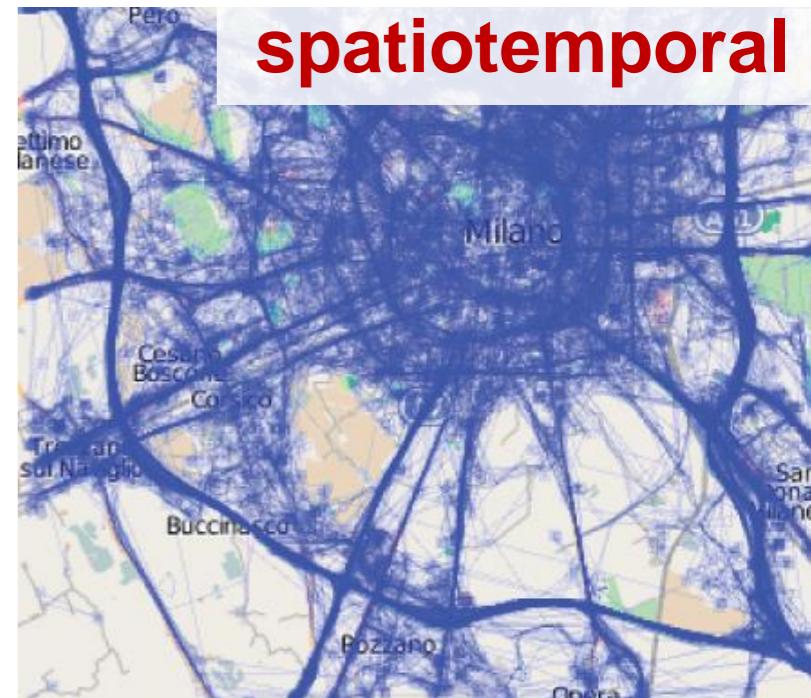
**data abstraction  
& aggregation**

## Algorithmic extraction of values & patterns

- Dimensionality reduction
- Aggregation, summary statistics
- Clustering, classification, outliers, etc.



Clustering+outlier preservation  
[Novotný & Hauser 06]



[Andrienko & Andrienko 11]

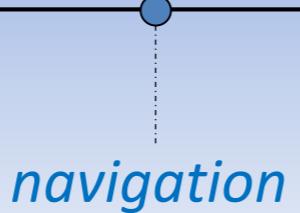
visual mapping

interactive visual analysis

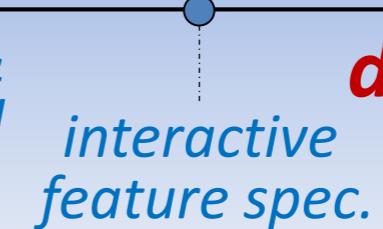
comput. analysis



relation & comparison

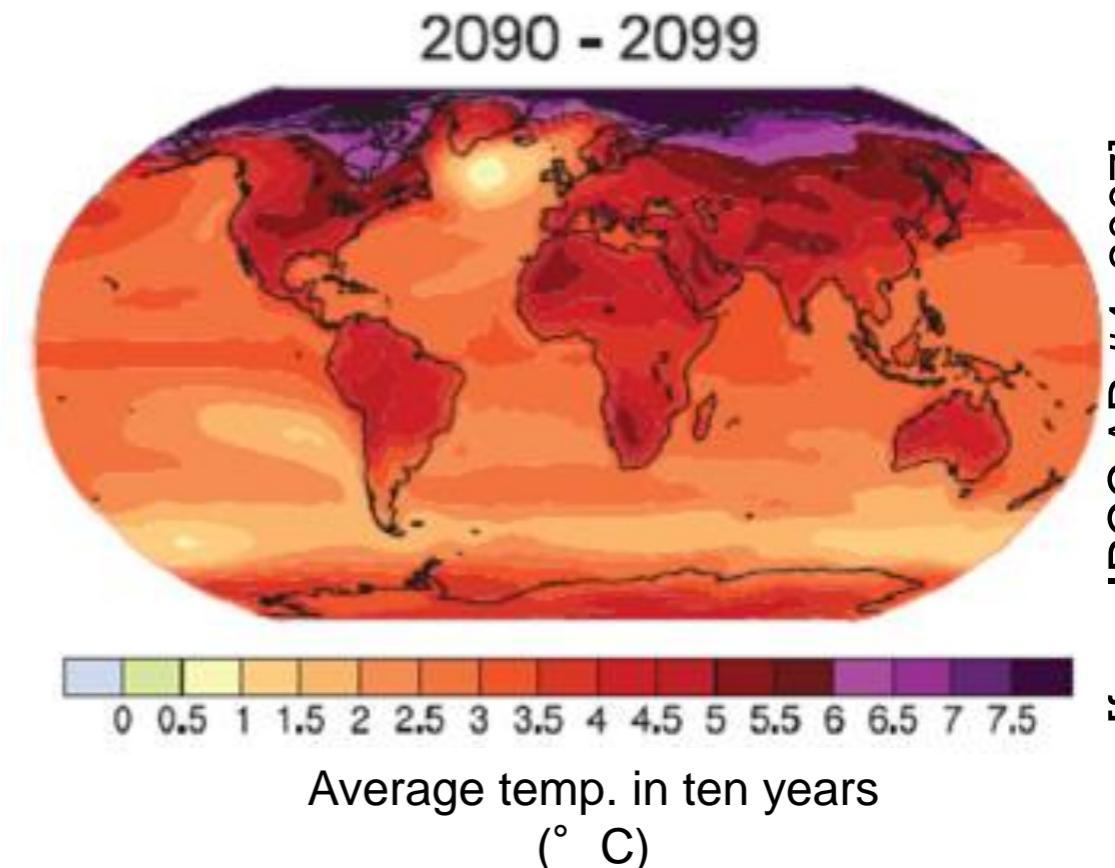


focus+context & overview+detail



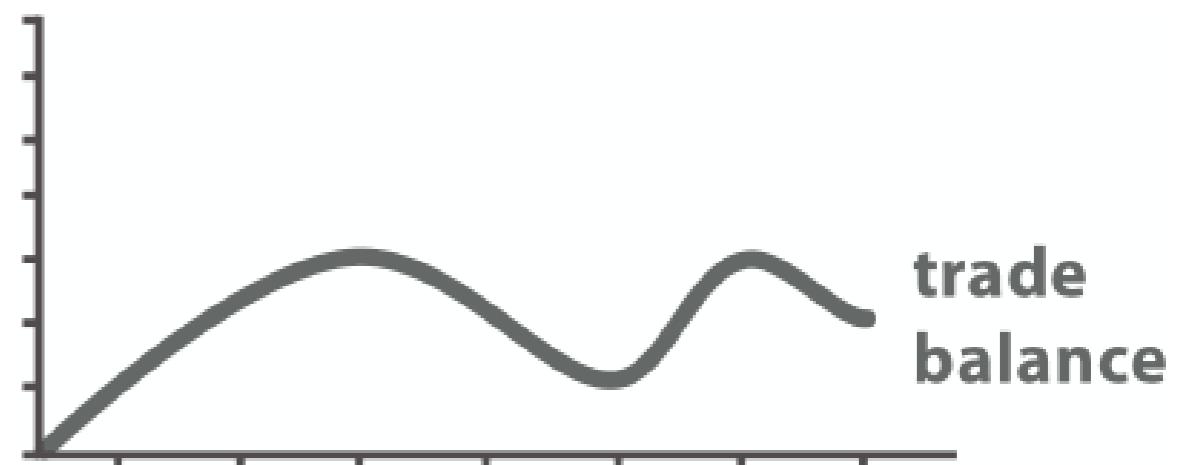
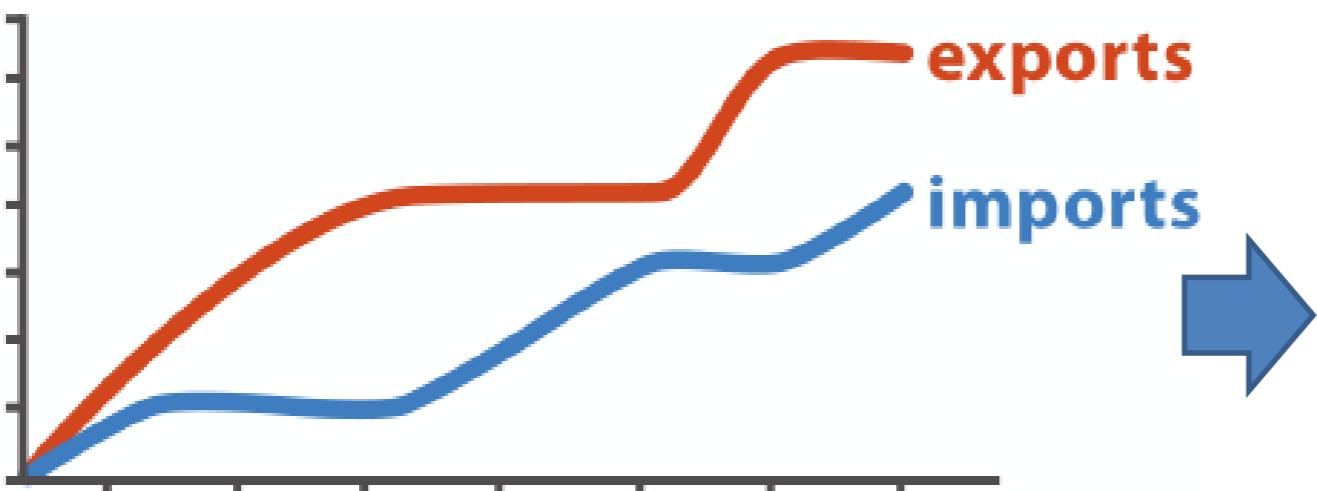
**data abstraction & aggregation**

- Summary statistics
  - Mean, variance, etc.

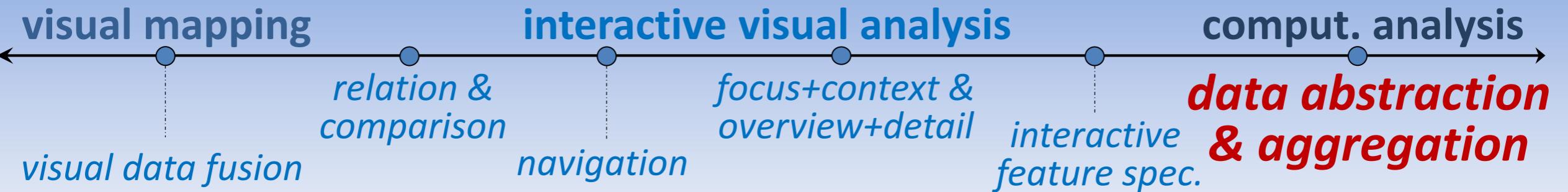


[from IPCC AR #4, 2007]

- Derive new data attributes
  - What do you want to see?

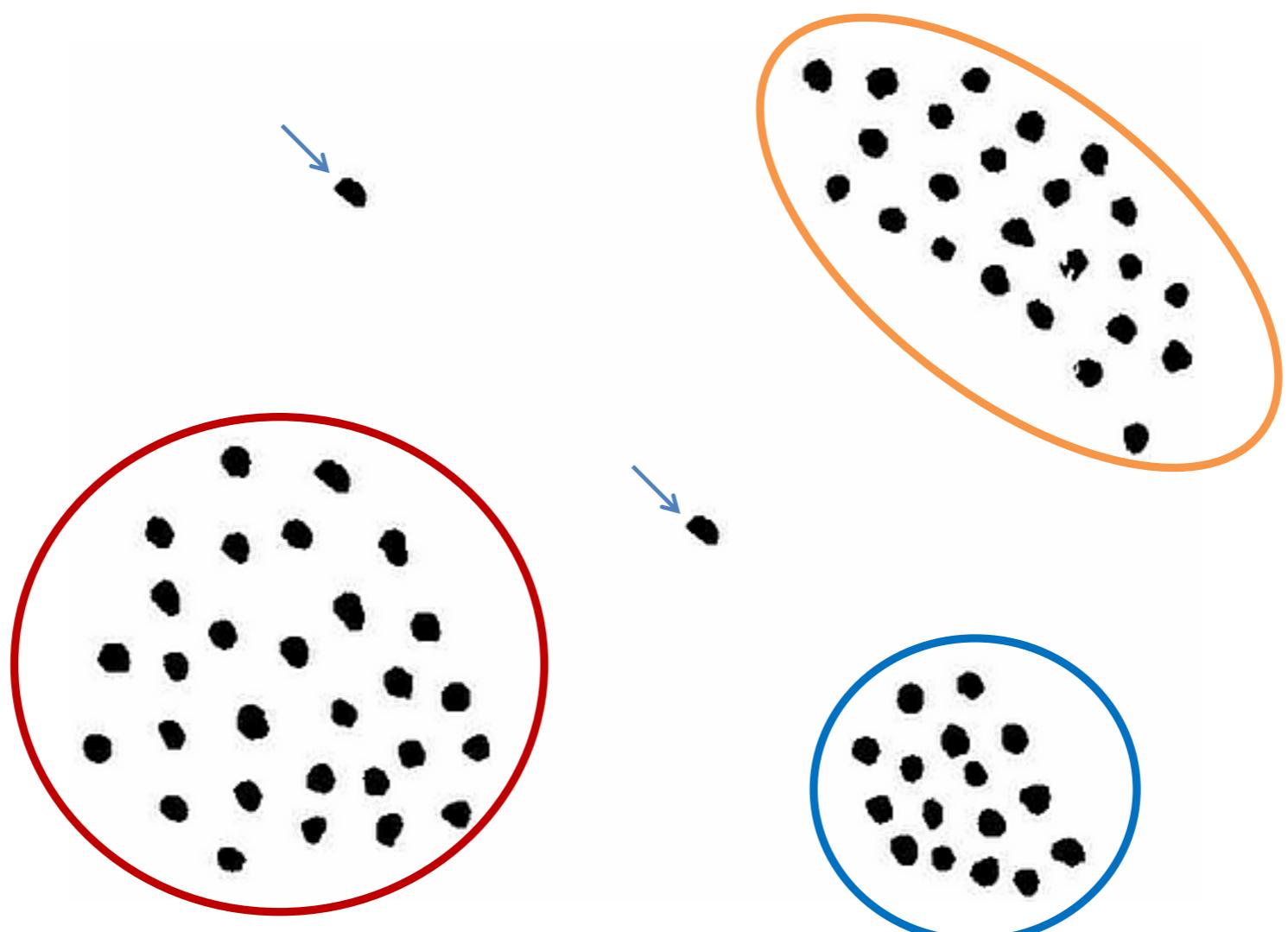


$$\text{trade balance} = \text{exports} - \text{imports}$$



## Clustering

- Given some data points, we'd like to understand their structure



visual mapping

interactive visual analysis

comput. analysis



visual data fusion

*relation &  
comparison*



*focus+context &  
overview+detail*

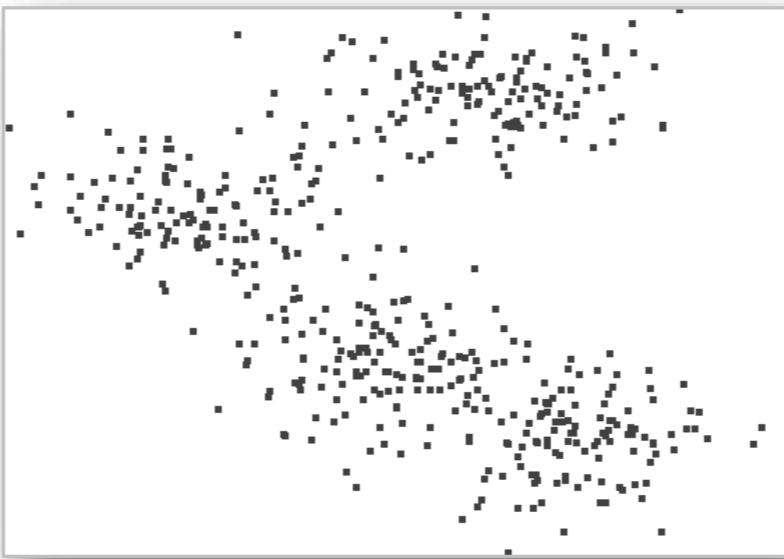
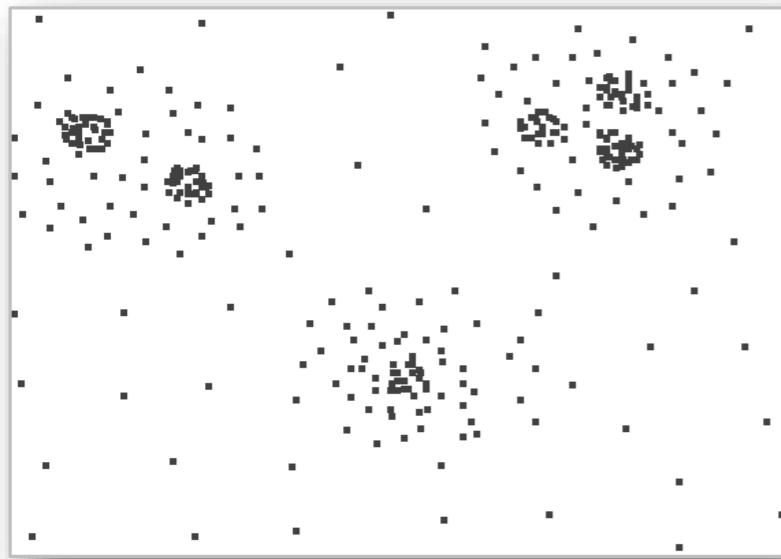
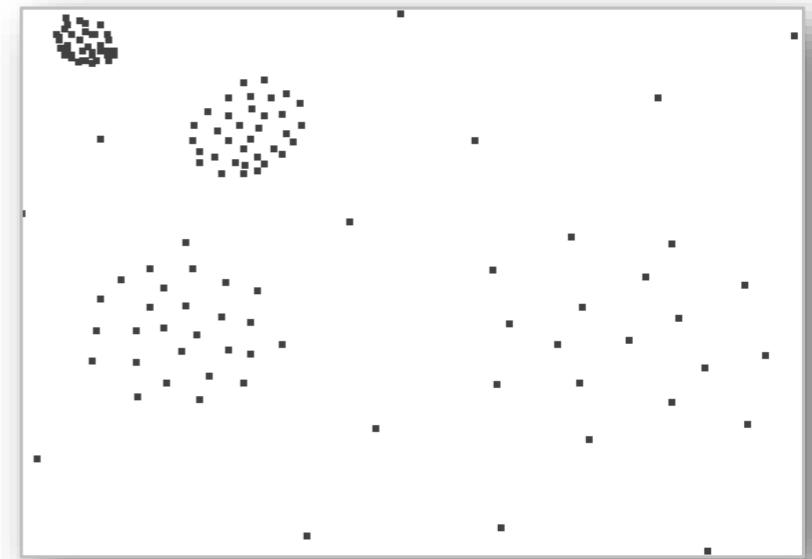
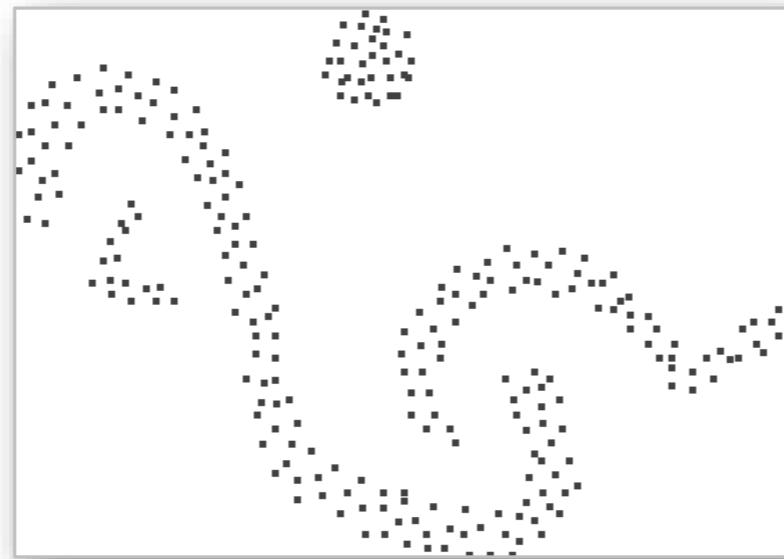
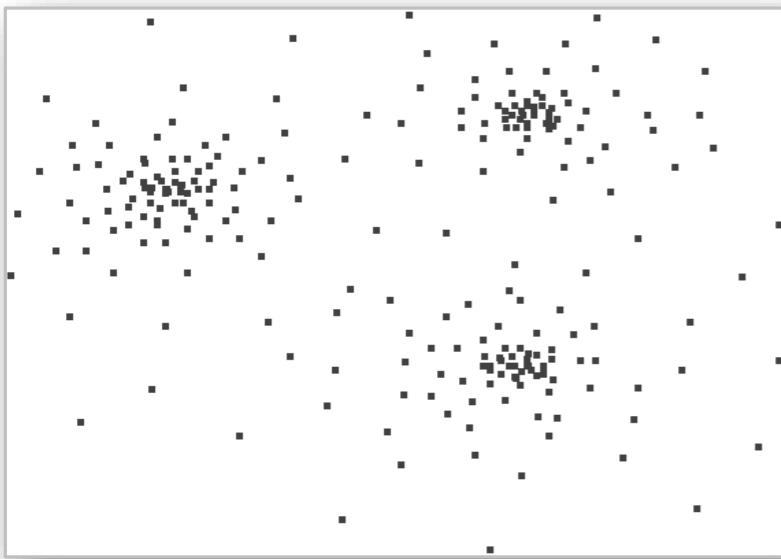
*navigation*

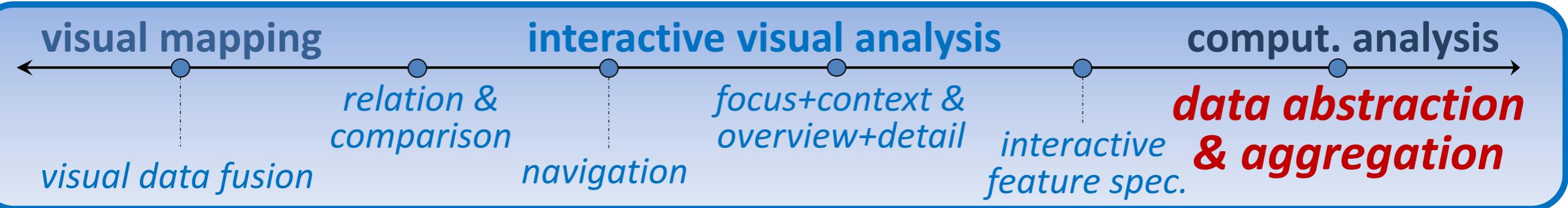


*interactive  
feature spec.*

***data abstraction  
& aggregation***

# How many clusters do you see?



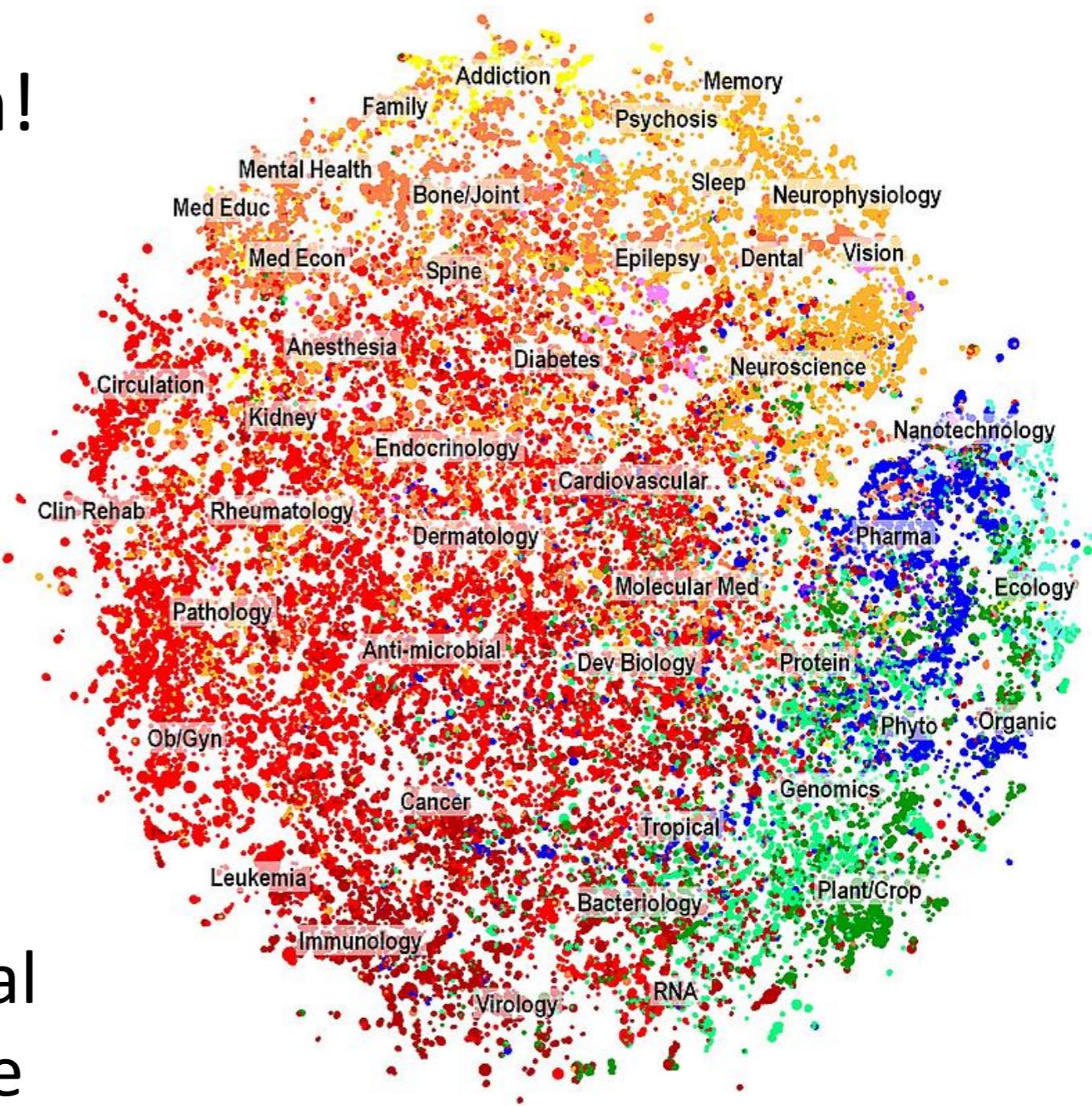


# Clustering is a hard problem!

- Clustering in 2D looks easy
  - Clustering small amounts of data looks easy

**However,**

- many applications involve 10 or 10,000 dimensions
  - distances in high-dimensional spaces are at similar distance

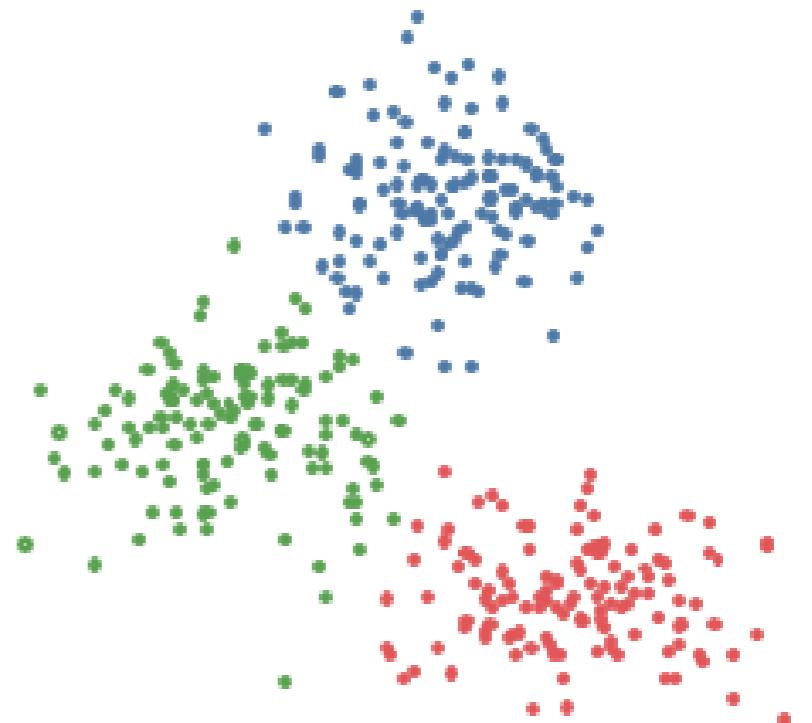


Clustering more than 2 mill. biomedical publications  
Boyack et al., [PLoS ONE](#), 2011.



## Clustering

- Given a **set of points** with some **notion of distance** between points, **group** them into **clusters** such that
  - Members of a cluster are close/similar to each other
  - Members of different clusters are dissimilar
- Usually
  - Points are in high-dimensional space
  - Similarity defined by distance measure (e.g. Euclidean)



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation & comparison

navigation

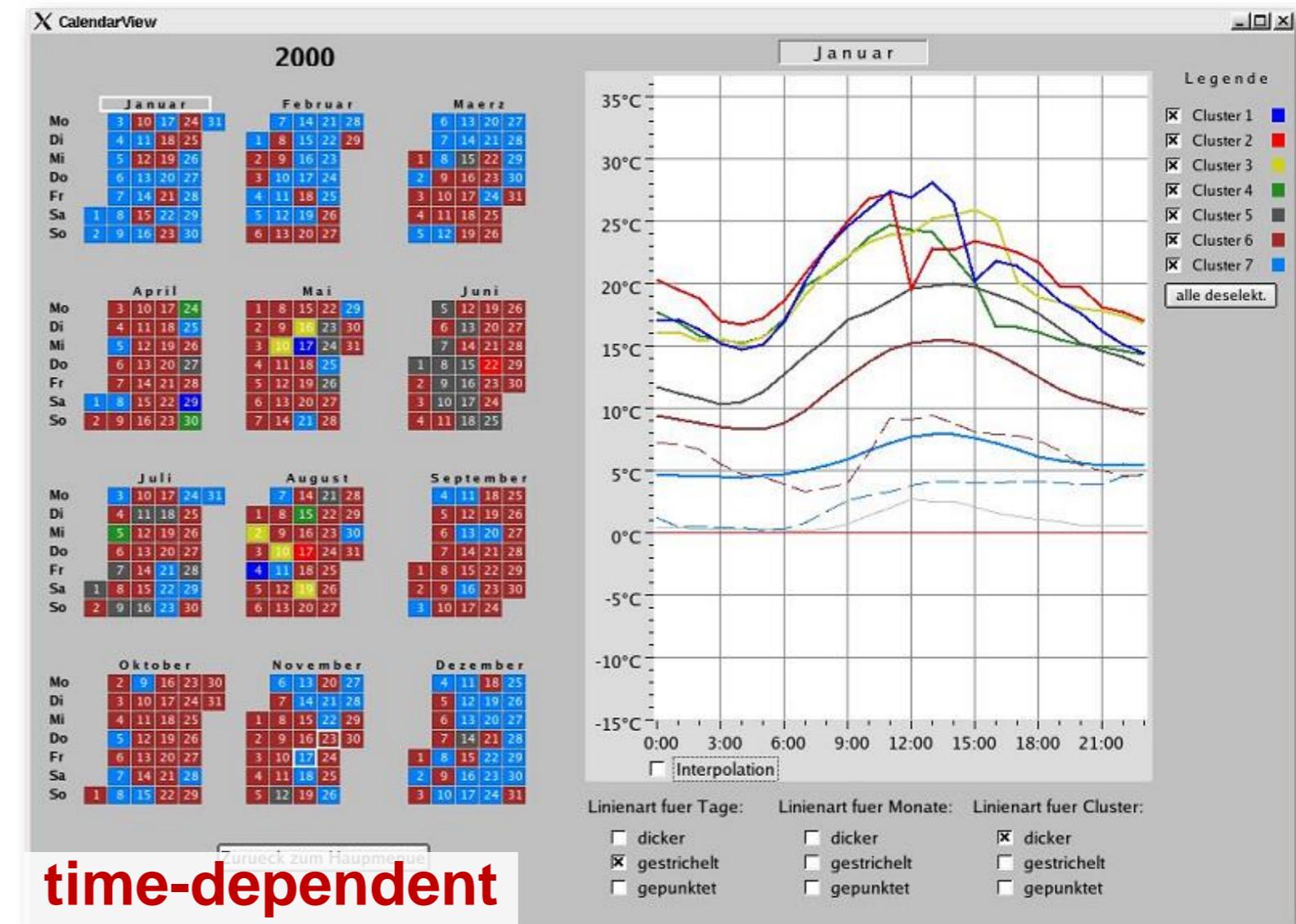
focus+context & overview+detail

interactive feature spec.

**data abstraction & aggregation**

## Cluster Calendar View [vanWijk & van Selow '99]

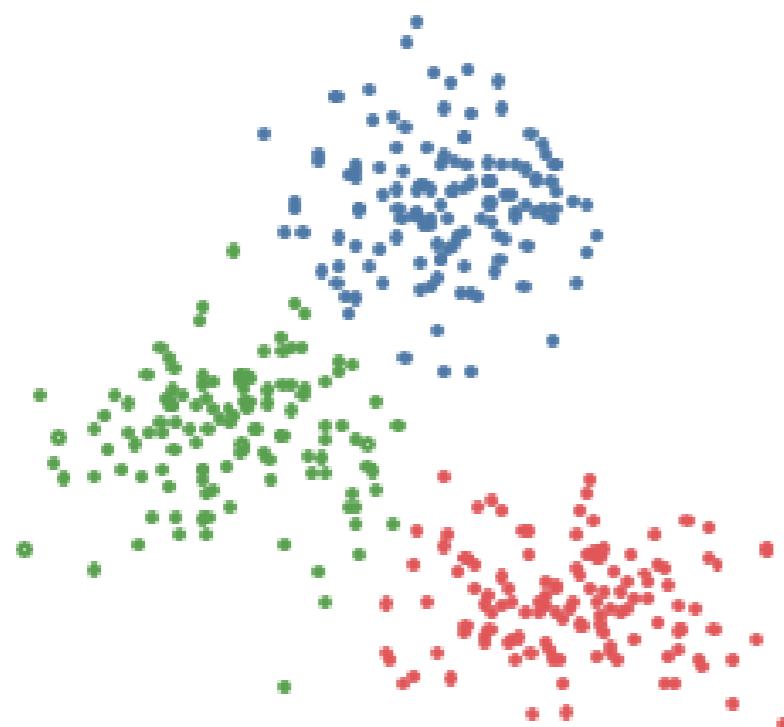
- Time series clustered by similarity (K-means)
- Cluster affiliation of daily pattern shown in calendar





## Density-based Clustering (DBSCAN)

- Identify dense regions in data
- Clusters can be arbitrarily shaped
- Difficult to find good parameter settings

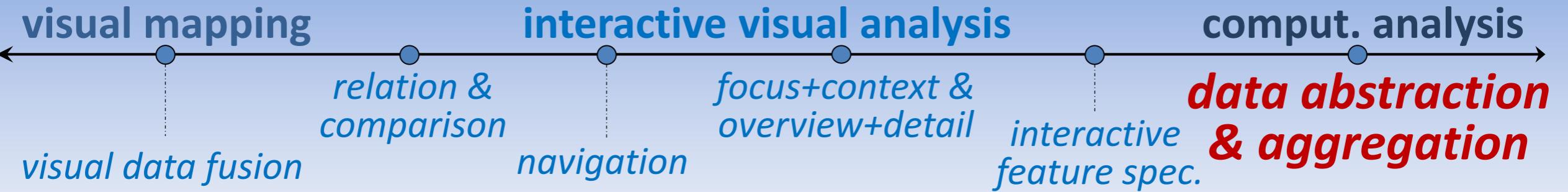


*k*-means



DBSCAN

***data abstraction & aggregation***



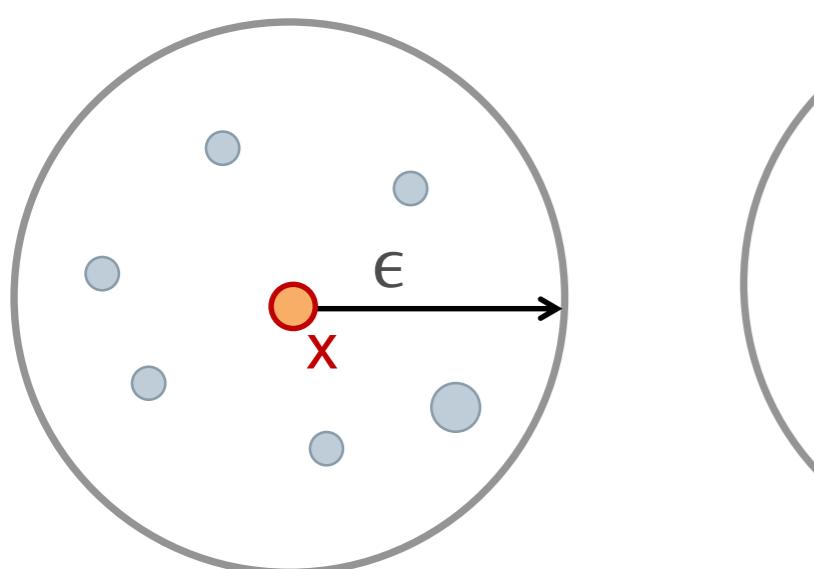
## DBSCAN: 2 parameters

- Radius  $\epsilon$
- Number of MinPts

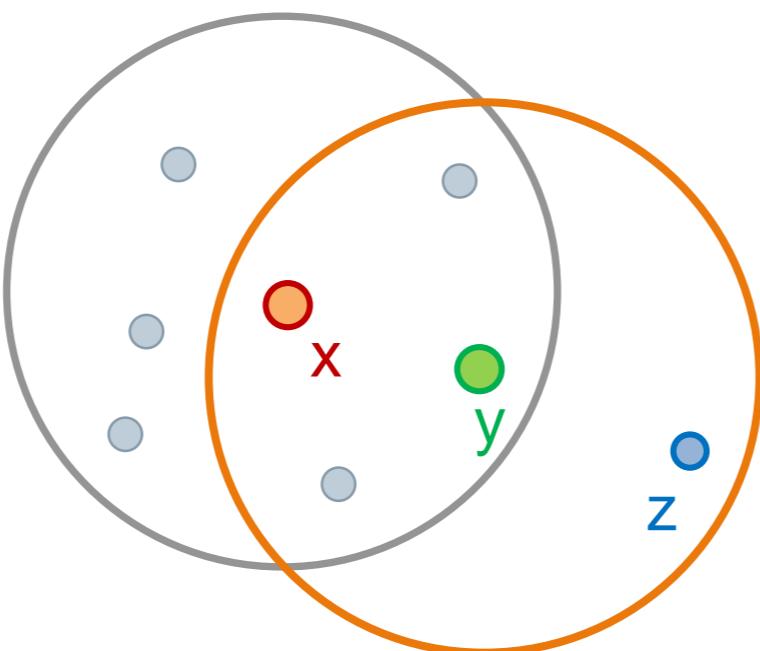
**core point** ( $\epsilon$ -neighborhood contains at least minimum number (*MinPts*) of points)

**border point** (in the  $\epsilon$ -neighborhood of core point)

**noise** (neither a core object nor a border object)



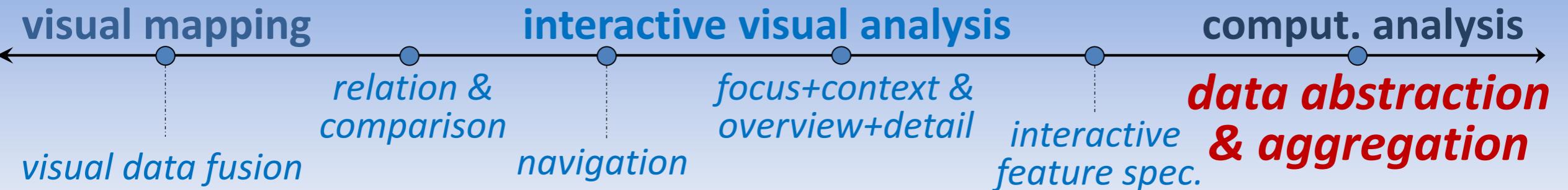
MinPts = 6



x ... core point

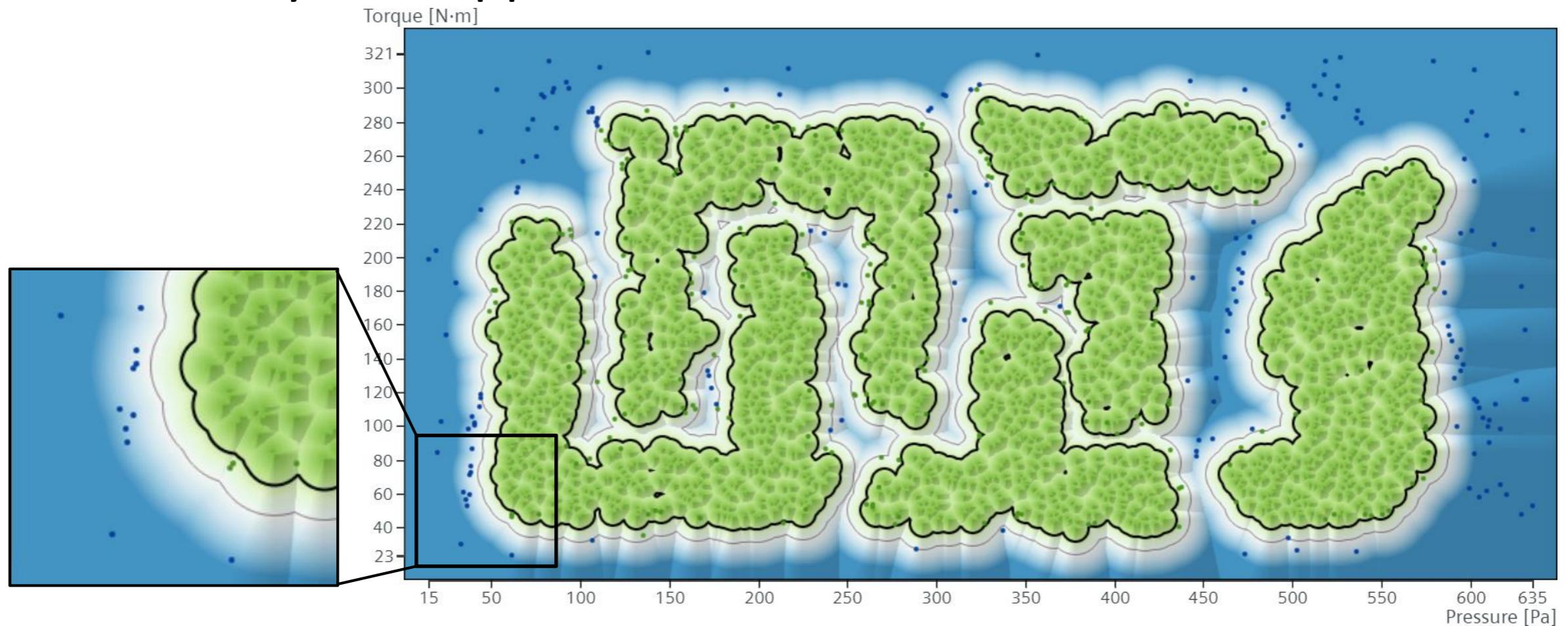
y ... border point

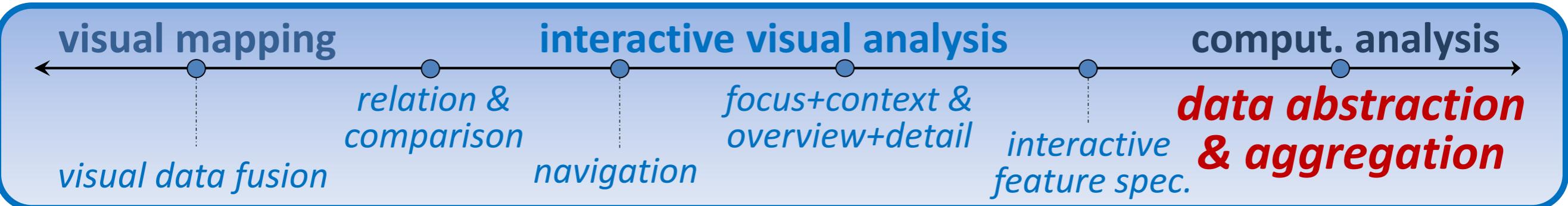
z ... noise



## Interactive parameter tuning

- Real-time approximation of DBSCAN result
- User changes parameter values
- Immediately sees approximation of result



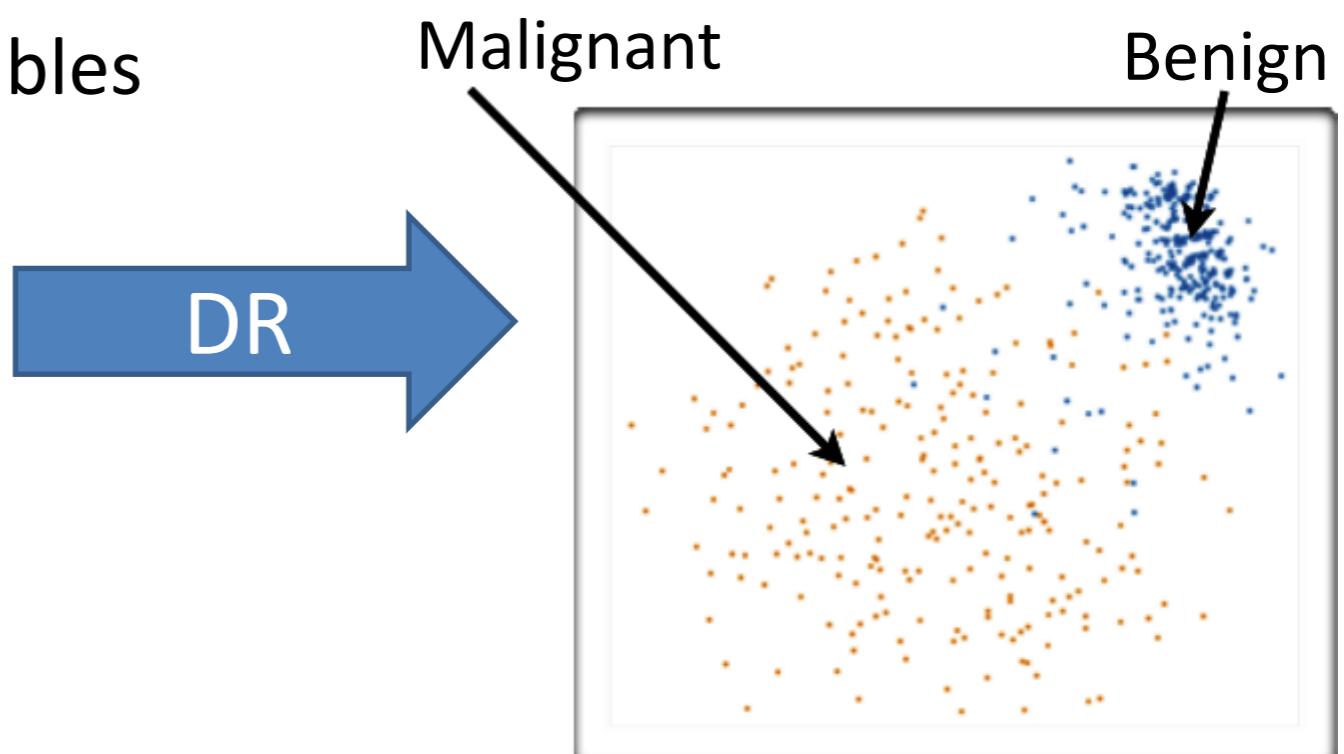


## Dimensionality reduction

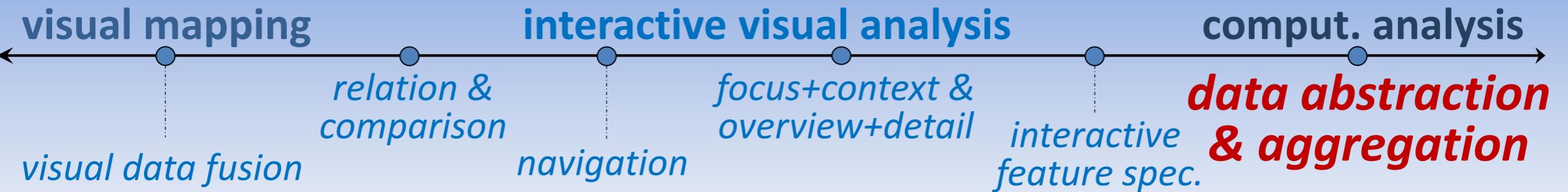
- Derive low-dimensional target space from high-dimensional measured space
- Use when you can't directly measure what you care about
  - True dimensionality of dataset assumed to be smaller than dimensionality of measurements
  - Latent factors, hidden variables

Tumor  
Measurement data

Data: 9D measured space

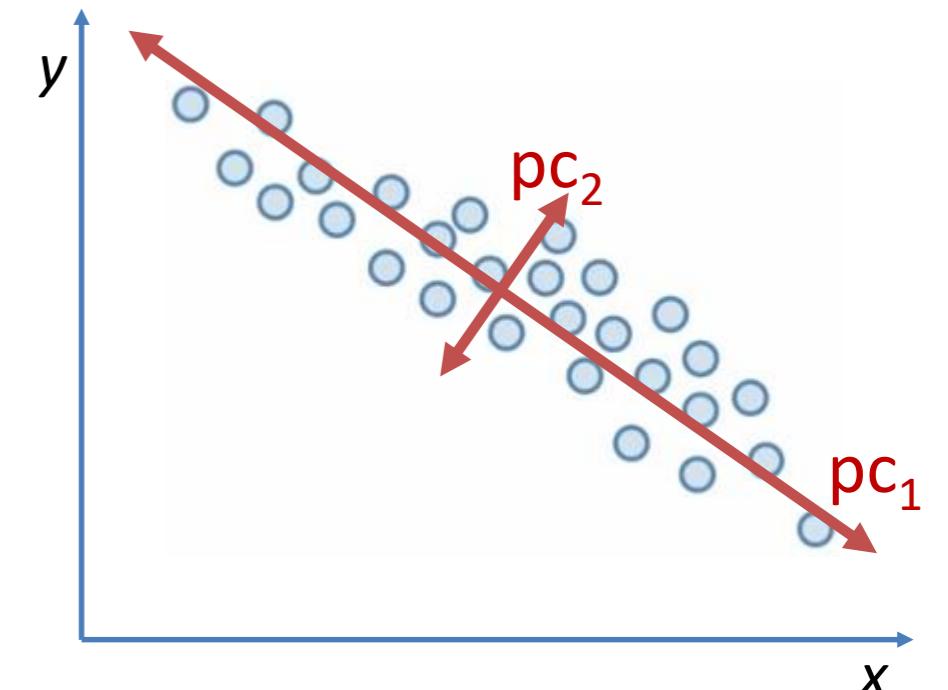


[Munzner]

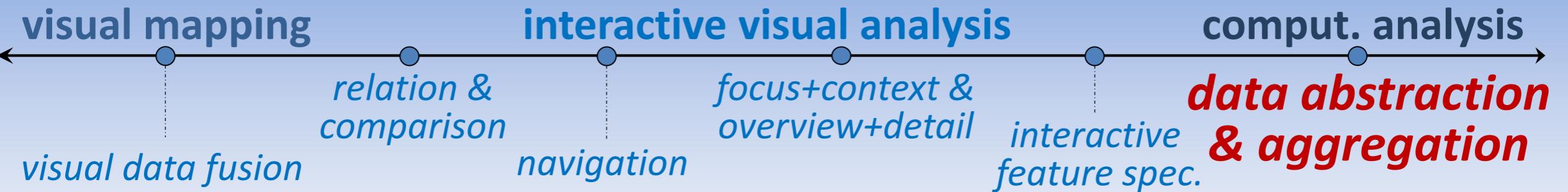


## Principal Component Analysis (PCA)

- Find directions of largest variance
- Neglect directions of small variance (not descriptive)
- Coordinate system transformation (rigid rotation)

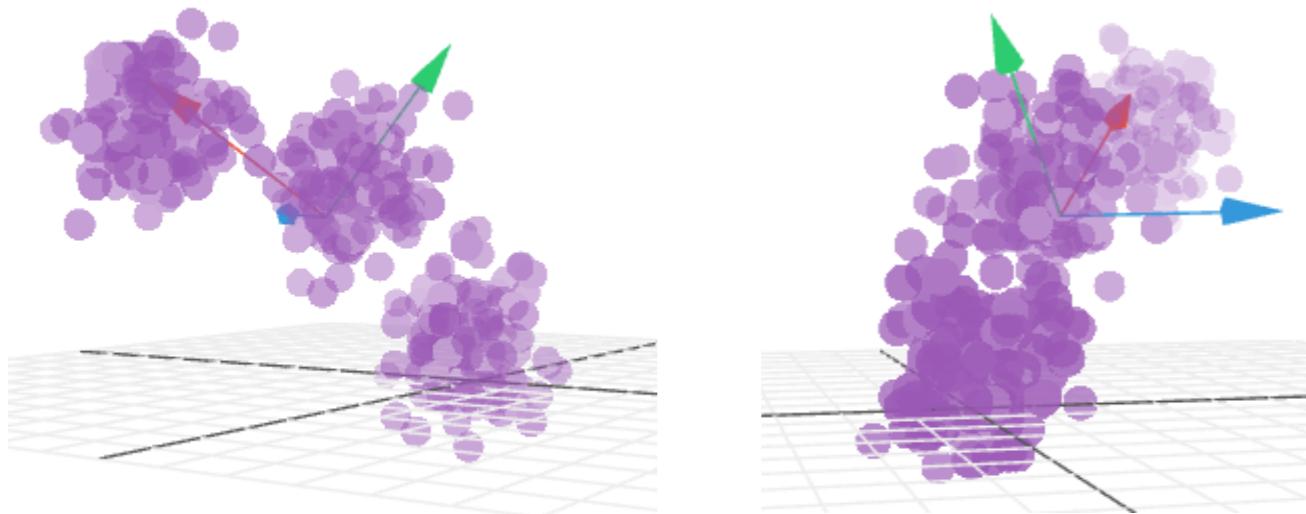


- Result
  - New axes (eigenvectors) & explained variances (eigenvalues)
  - New axes usually don't mean anything physical

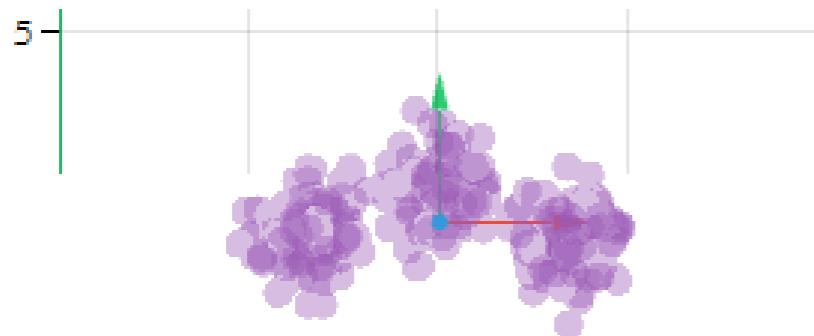


## Principal Component Analysis (PCA)

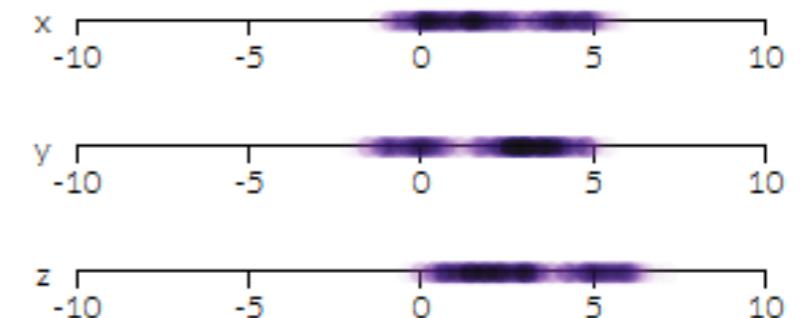
– 3D example



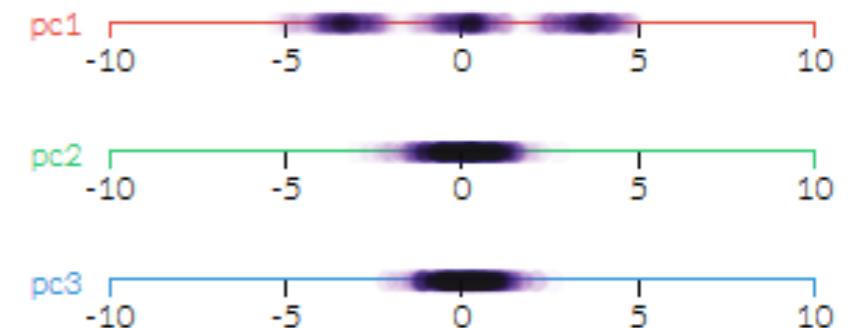
– Axes aligned with highest variation



Variation along x, y, z



Variation along principal components



Using pc1, we can see 3 clusters

visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation & comparison

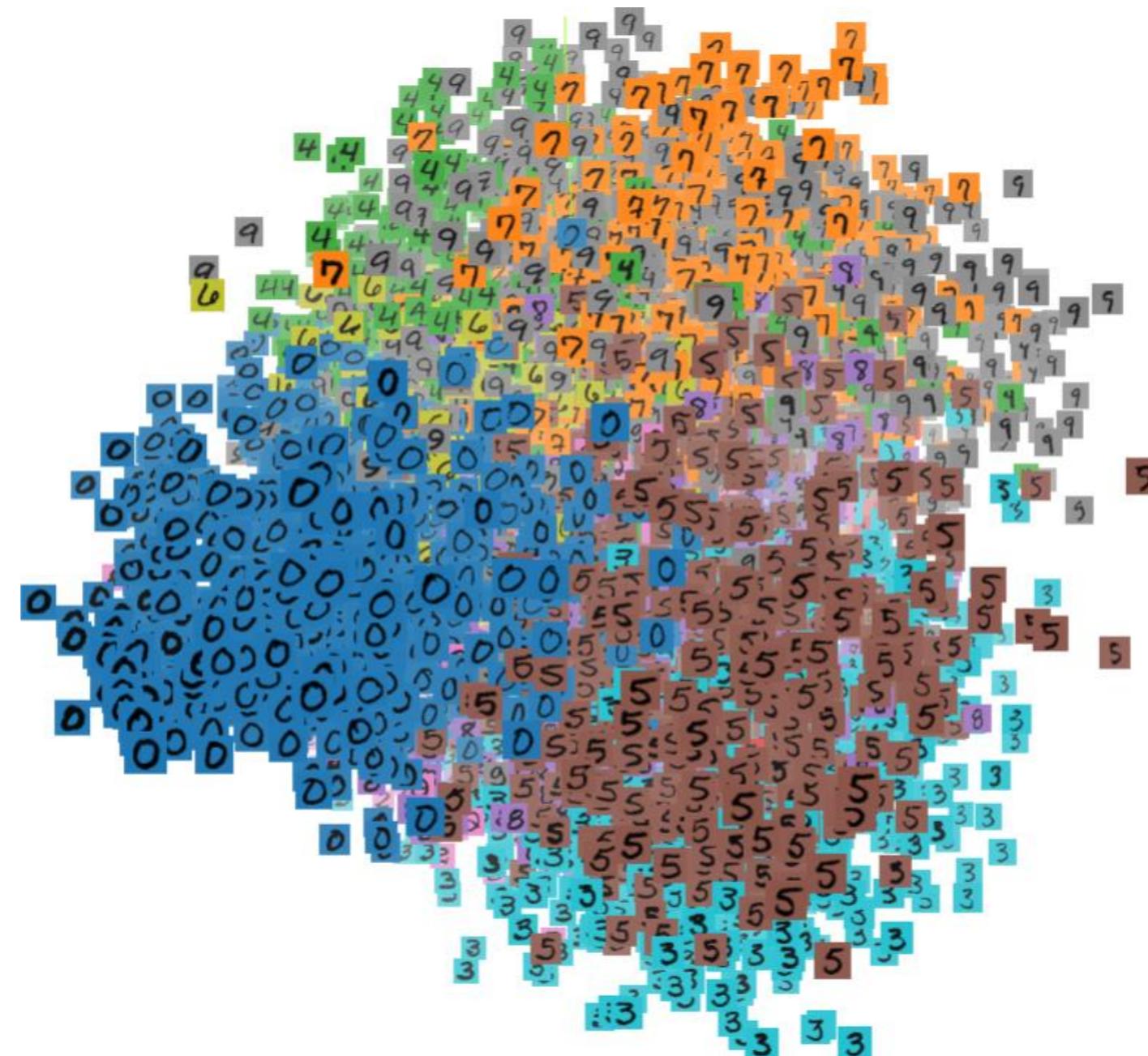
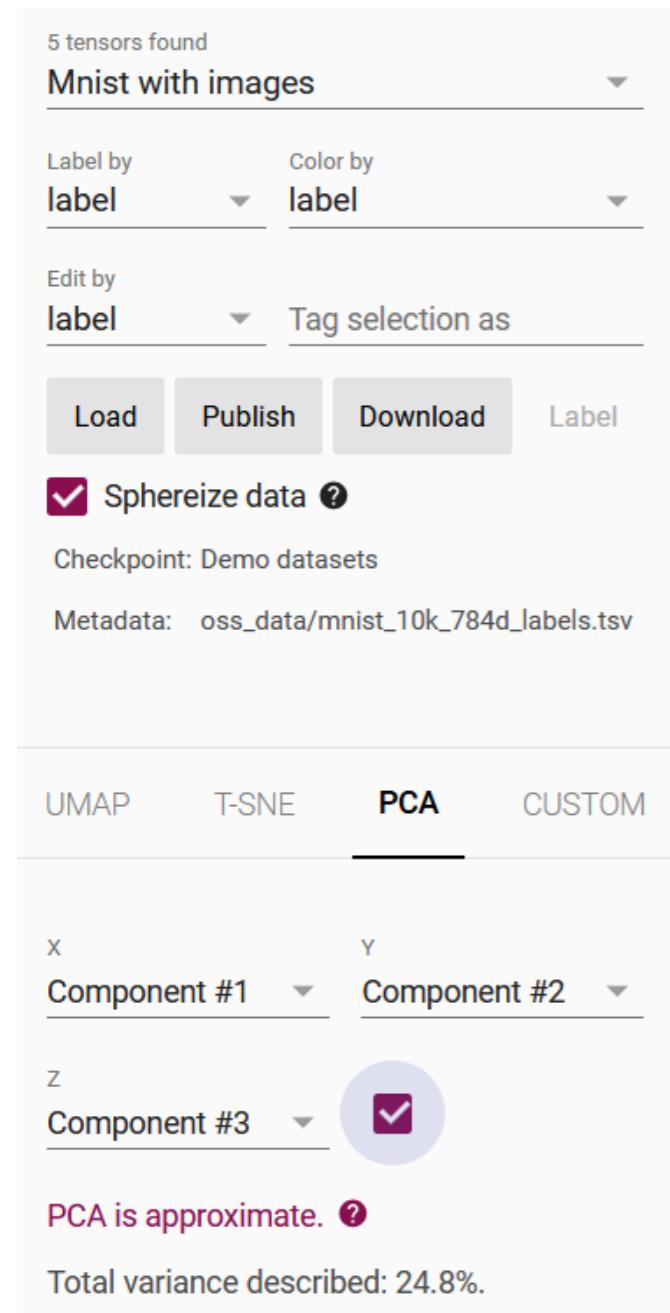
navigation

focus+context & overview+detail

interactive feature spec.

**data abstraction & aggregation**

## Embedding Projector: Inspect results of dimensionality reduction



visual mapping

interactive visual analysis

comput. analysis

visual data fusion

relation & comparison

navigation

focus+context & overview+detail

interactive feature spec.

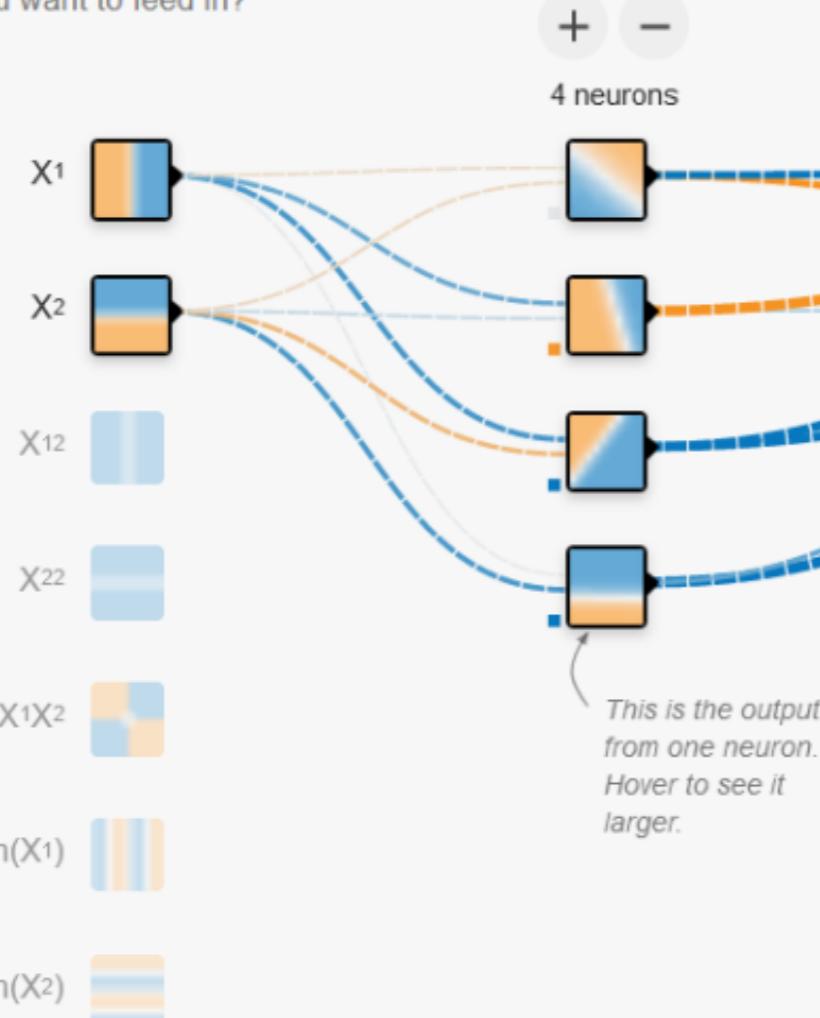
**data abstraction & aggregation**

## Explainable AI (XAI) allows to open the black box

FEATURES

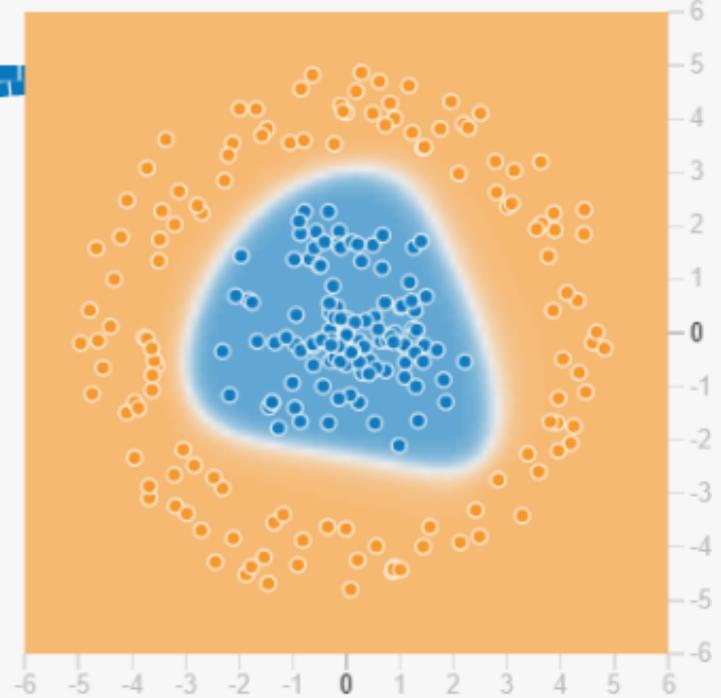
Which properties do you want to feed in?

+ - 2 HIDDEN LAYERS

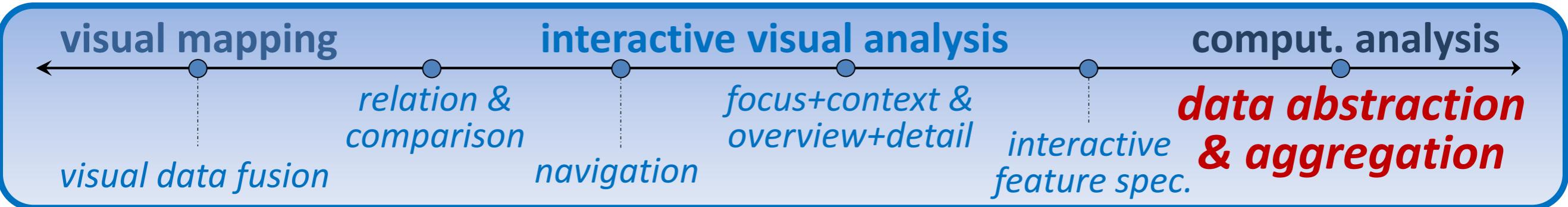


OUTPUT

Test loss 0.008  
Training loss 0.001



Tensor Flow Playground  
[playground.tensorflow.org](http://playground.tensorflow.org)



- Summary: Data abstraction & aggregation
  - Extract meaningful values/patterns (e.g., clustering)
  - Preserve main data characteristics (e.g., mean, variance, outliers) while suppressing irrelevant details
- Combine best of two worlds [Keim et al.]
  - data exploration/analysis by the user, based on interactive visualization
  - and data analysis by the computer, based on statistics, machine learning, etc.

visual mapping		interactive visual analysis			comput. analysis	
spatio-temporal multi-variate multi-modal multi-run model	relation & comparison	navigation	focus+context & overview+detail	interactive feature spec.	data abstraction & aggregation	
	maps [13], [14], [92]; Helix glyphs [93]; flow maps [105]; function graphs [70], [71], [72]; Time Histograms [94], [110], [111]; chrono volumes [98]; illustrative techniques [99]; texture-based flow vis. [100]	2-tone coloring [20]; Helix glyphs [93]; juxtaposed views [19], [110]; difference views [107]	search, zooming and panning [40], [54]	2-tone coloring [20]; multi-level focus+context [71]; pixel-based multi-resolution techn. [104]	brushing [21], [70], [71], [95], [113]; transfer functions [110], [111]	aggregation [15], [103], [105]; trends [21]; flow features [82]; clustering [83], [84], [110]; PCA [17], [78], [85]; SOM [89], [90]; KDE [106], [107]; information theory [108]; wavelet analysis [109], [110]
	attribute views [22], [50], [67]; color & texture [119]; layering [115], [124], [126]; 2-level volume rendering [127], [128]; glyphs [120], [121], [122], [123], [124], [125]	correlation fields [133]; operators [134]; multiple linked views [9], [26], [29], [73], [74], [76]	grand tour [47]; ScatterDice [46]; ranking & quality metrics [48], [130], [131], [132]	illustrative vis. [115], [116]; oulier-preserving methods [69]; smooth brushing [80]	brushing [9], [50], [74], [75], [112]; multi-dim. transfer func. [114], [115]; machine learning [91], [135], [136]	clustering [68], [130]; data binning [69]; PCA [78]; MDS [86], [87]; SOM [88], [89]; projections [47], [48], [130], [132]; point clouds [129]
	resampling [138]; data model [142]; illumination model [143]; multi-volume rendering [128], [139], [143], [144], [145], [146]	difference views [107]; multi-image view [153]; nested surfaces [31], [154], [156]; features [44], [155]	viewpoint selection [49]	cutaway views [147], [139], [49]	transfer functions [143], [144]	registration [27]; mutual information [28]; comparison metrics [148], [151], [152], [133]
	glyphs & box plots [37], [43], [162], [163], [164]; shape descriptors [164]; families of surfaces [41]; spaghetti plots [35], [42], [165]	aggregated & multi-run data [36], [37], [41], [174]; HyperMoVal [51], [52]	aggregated & multi-run data [36], [37], [41]; parameter space nav. [51], [52]	aggregated & multi-run data [36], [37], [41]; simulation process vis. [173], [174]	trends & outliers [36], [37], [41]; visual steering [172]	overview statistics [31], [35], [36]; projections [41], [51], [170], [171]; operators [33]; PCA [169]; clustering [167], [168], [169]
	feature fusion across multiple data parts [37]	feature relation across data parts [37]	x	x	feature spec. across data parts [37]	x

# MultiVis.net

Data facet



Technique



Main goal

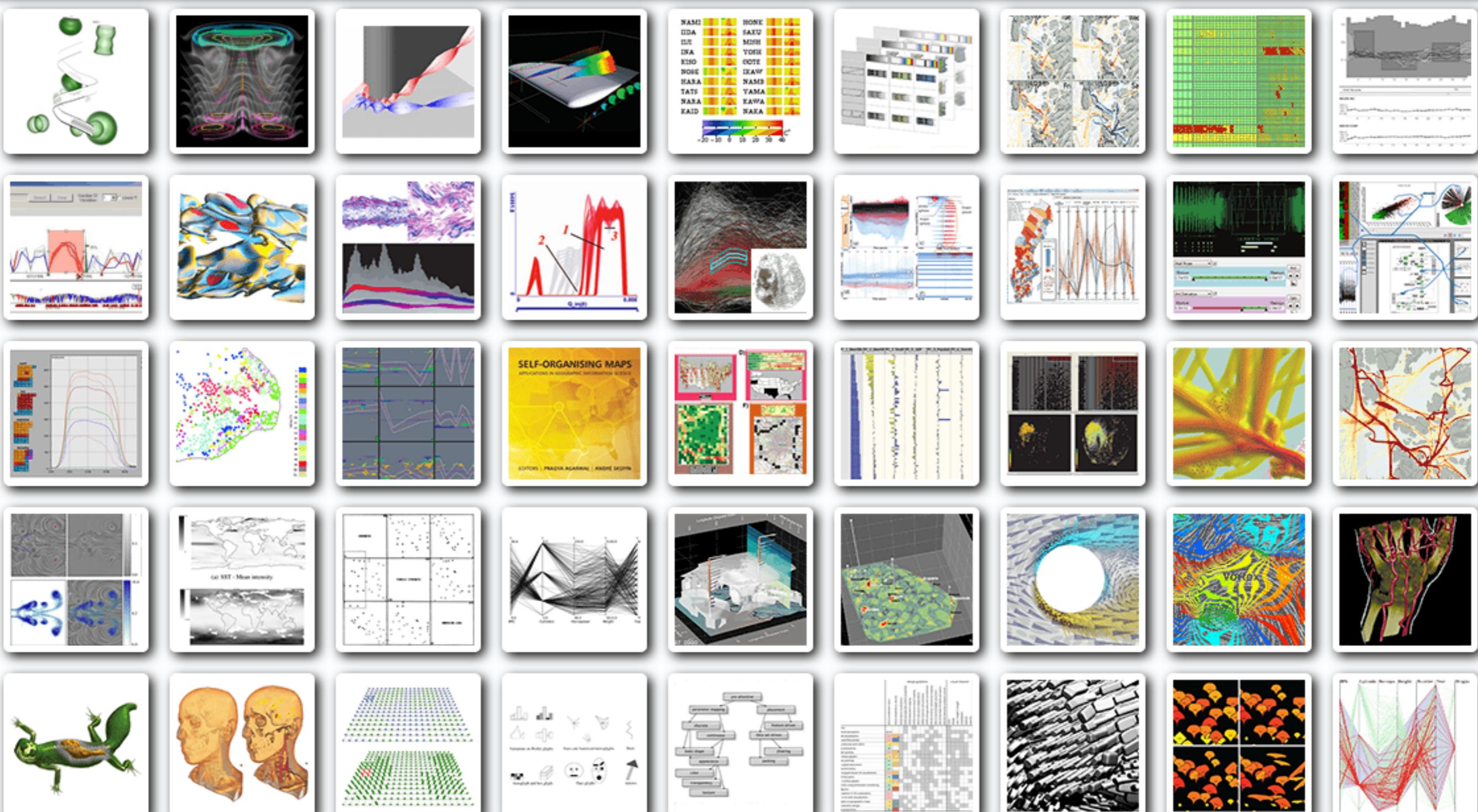


Fulltext Search

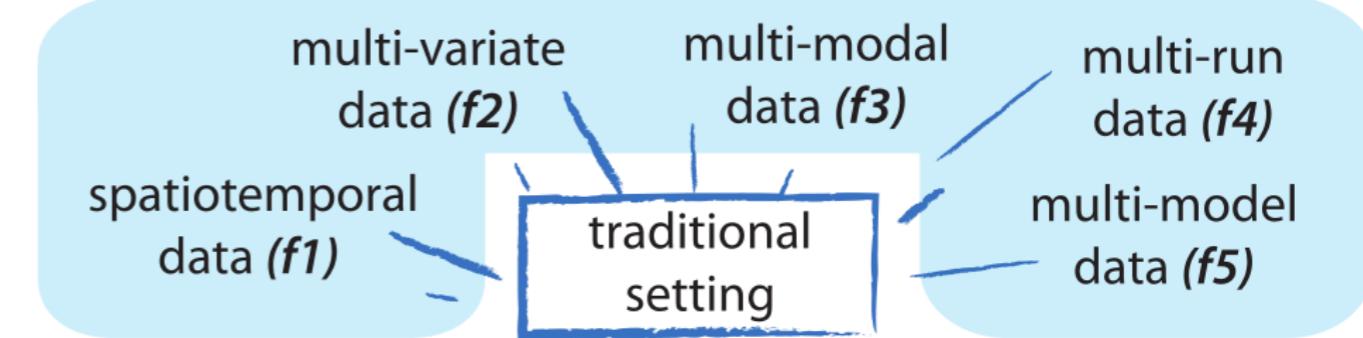
 x

# Publications

162

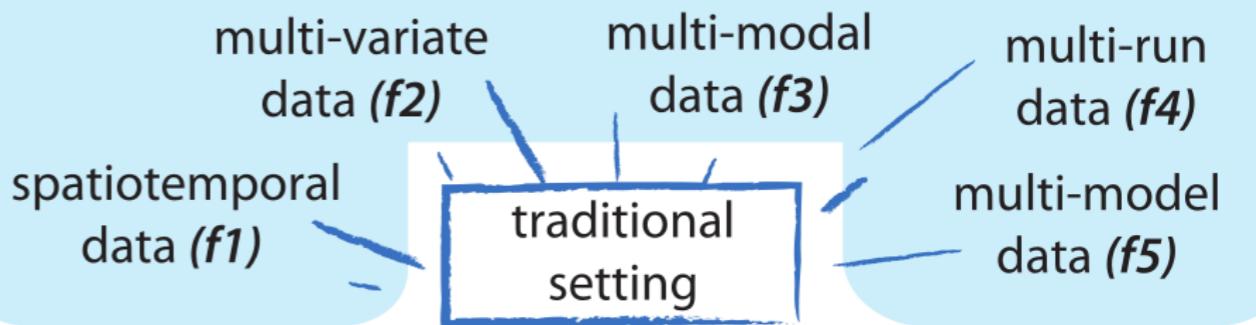


# Open Issues

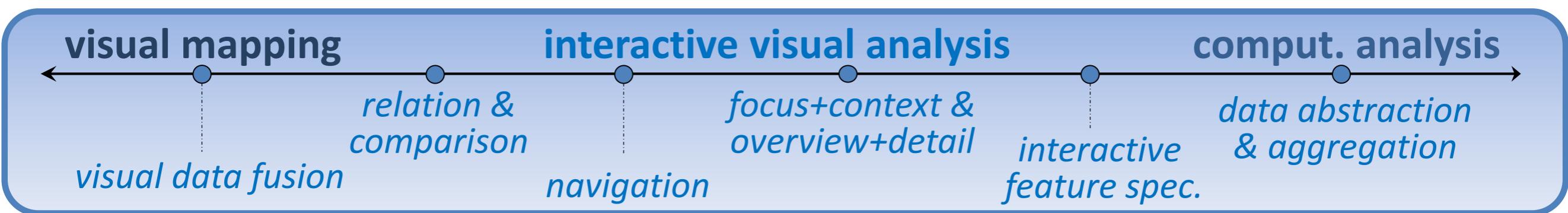


- How to deal with data heterogeneity?
  - Most approaches only address one or two data facets
  - Coordinated multiple views with linking & brushing
  - Investigation of features across views, data facets, levels of abstraction, and data sets
  - Fusion of heterogeneous data at feature/semantic level
- Combination of vis., interaction, and comput. analysis
  - Analytical methods can control steps in visualization pipeline (e.g., visualization mapping or quality metrics)
  - Interactive feature specification + machine learning

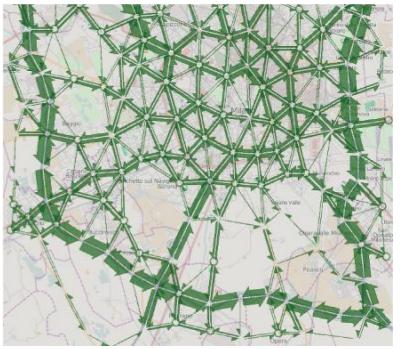
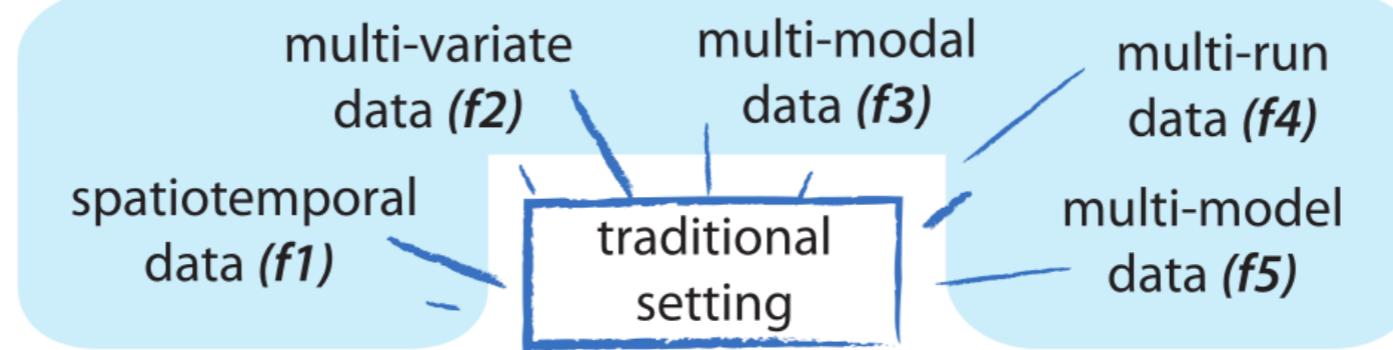
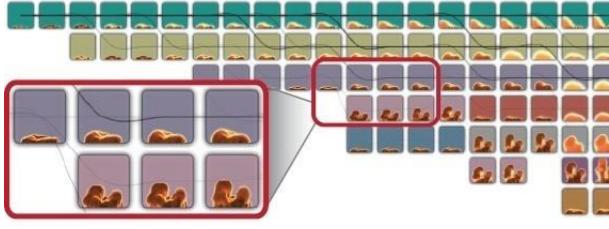
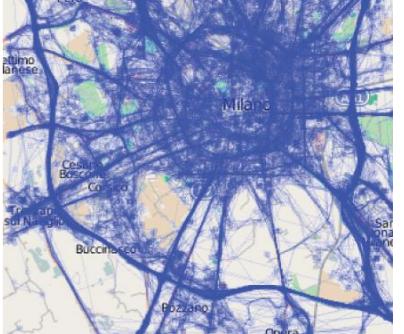
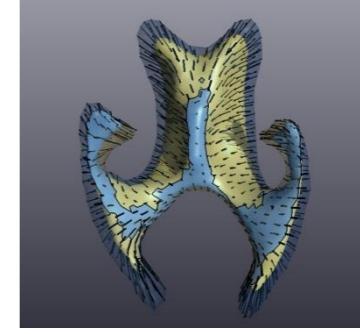
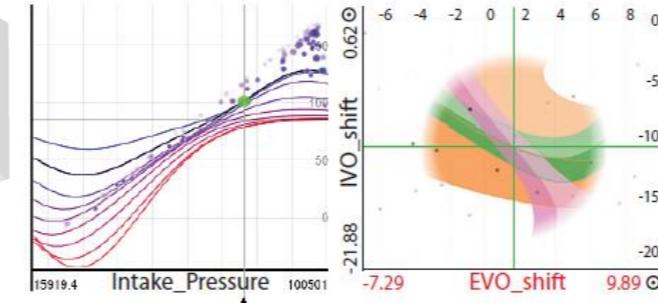
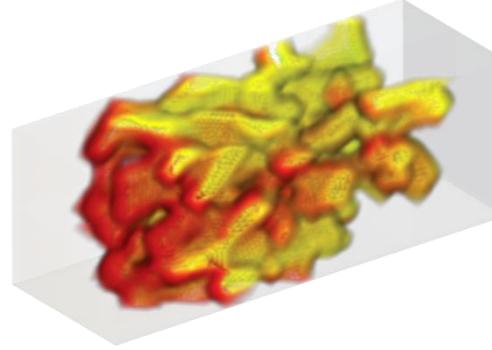
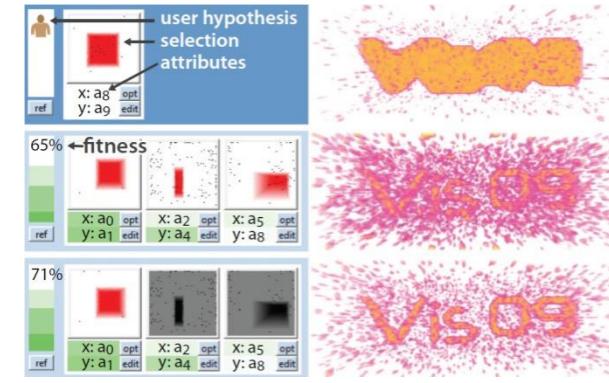
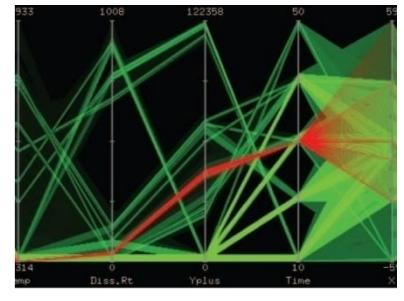
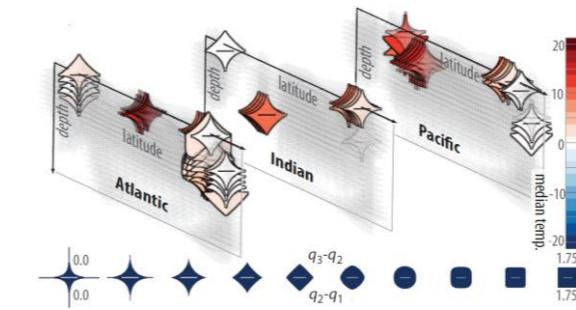
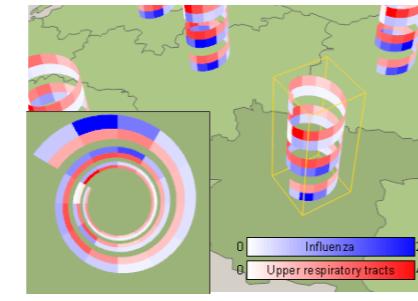
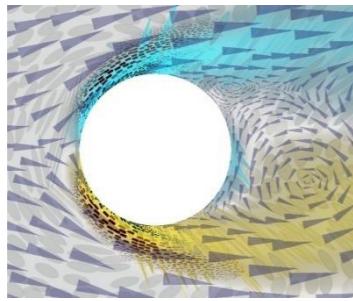
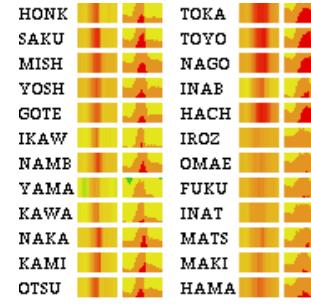
# Conclusions



- Scientific data are becoming multi-faceted
- Categorization based on common visualization, interaction, and comput. analysis methods



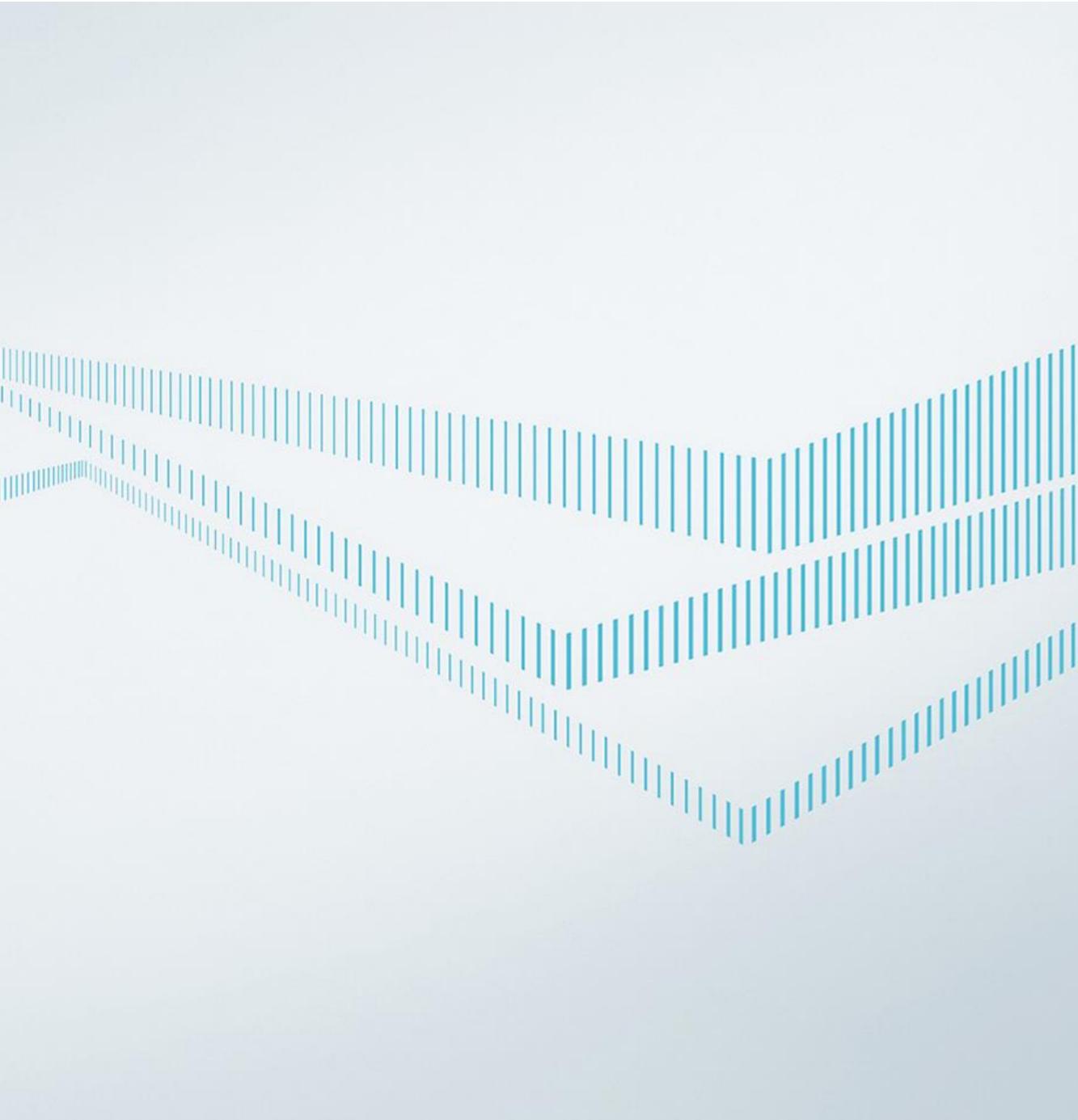
- Promising data facets, e.g., multi-run & multi-model data



# Acknowledgements

H. Hauser, H. Schumann, M. Chen, T. Nocke,  
 H. Piringer, M. Streit, M.E. Gröller,  
 VisGroup in Vienna/Bergen

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