Scientific Visualization and Virtual Reality

2a. Recap
2b. Data dimensions
2c. Scientific Visualisation in the Computational Science domain
2d. The Visualisation Pipeline

Robert Belleman, PhD
Visualisation Lab & Computational Science Lab
Universiteit van Amsterdam

To reach me, send email to R.G.Belleman@uva.nl (please add “[SVVR]” to subject)

Note: I do not read conversations on Canvas!

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Bertin's "Levels of organization"

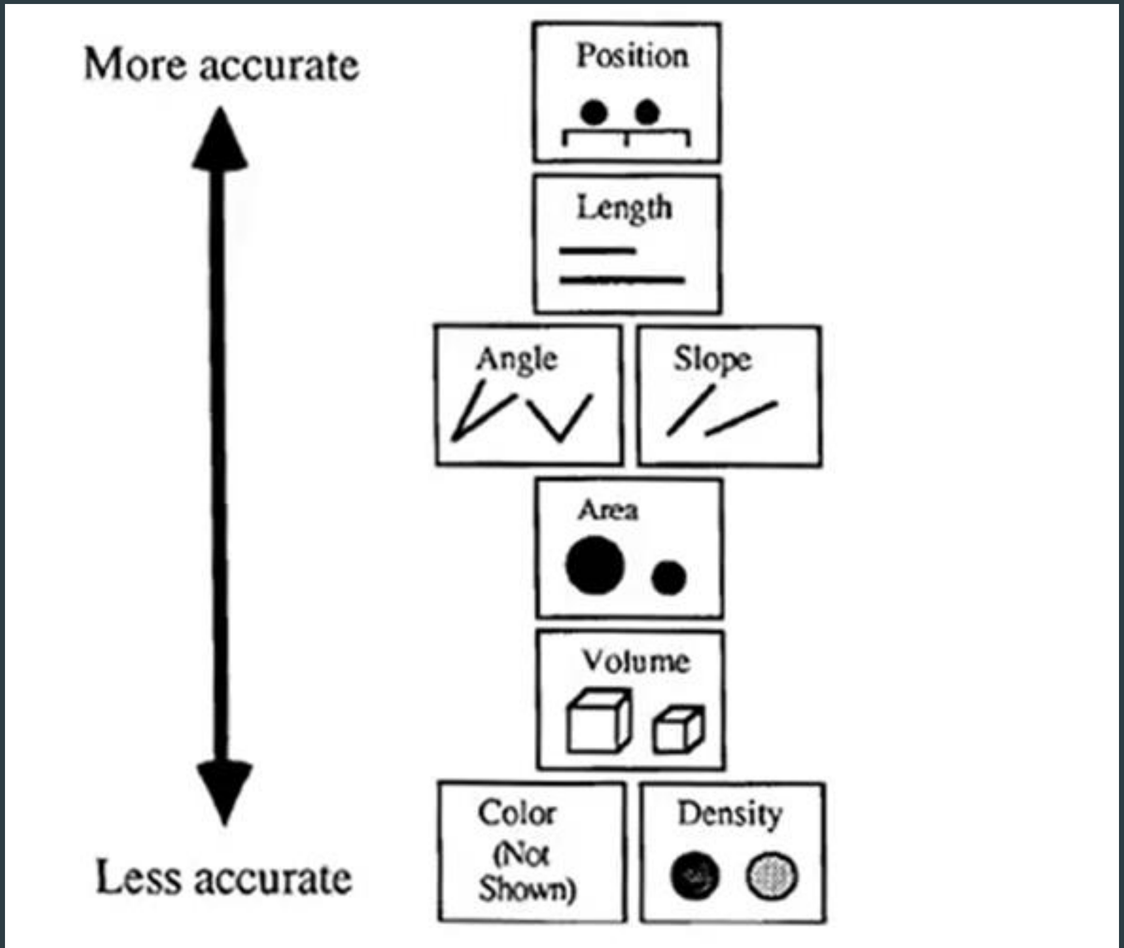
Position	N	O	Q
Size	N	O	Q
Value	N	O	Q
Texture	N	O	
Colour	N		
Orientation	N		
Shape	N		

N Nominal
O Ordered
Q Quantitative

Note that Bertin disregarded:

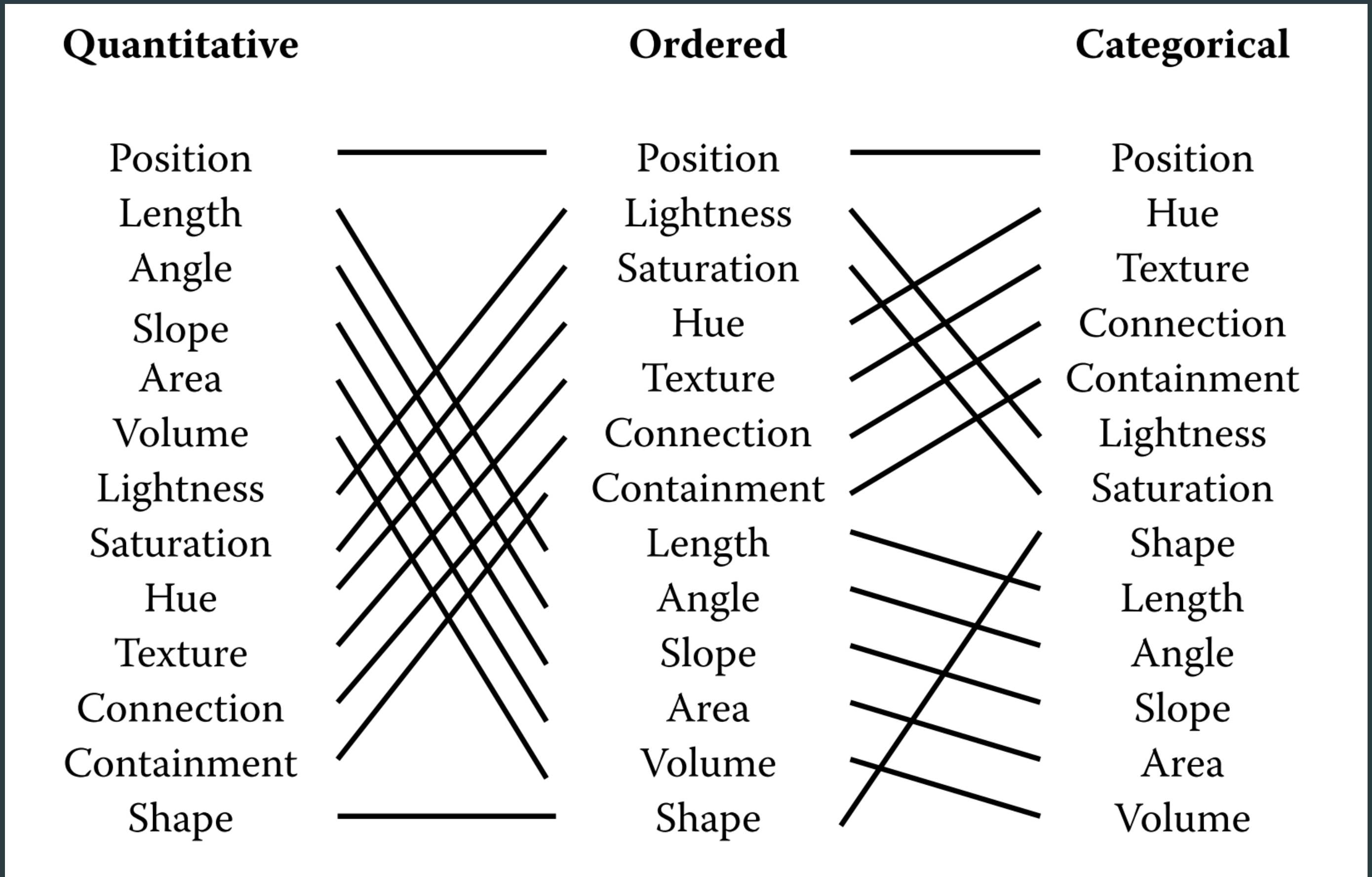
- Position in 3D
- Embedding/containment
- Time (animation)
- Interaction

Mackinlay's "Perceptual properties"



Mackinlay, (APT) A Presentation Tool, 1986.

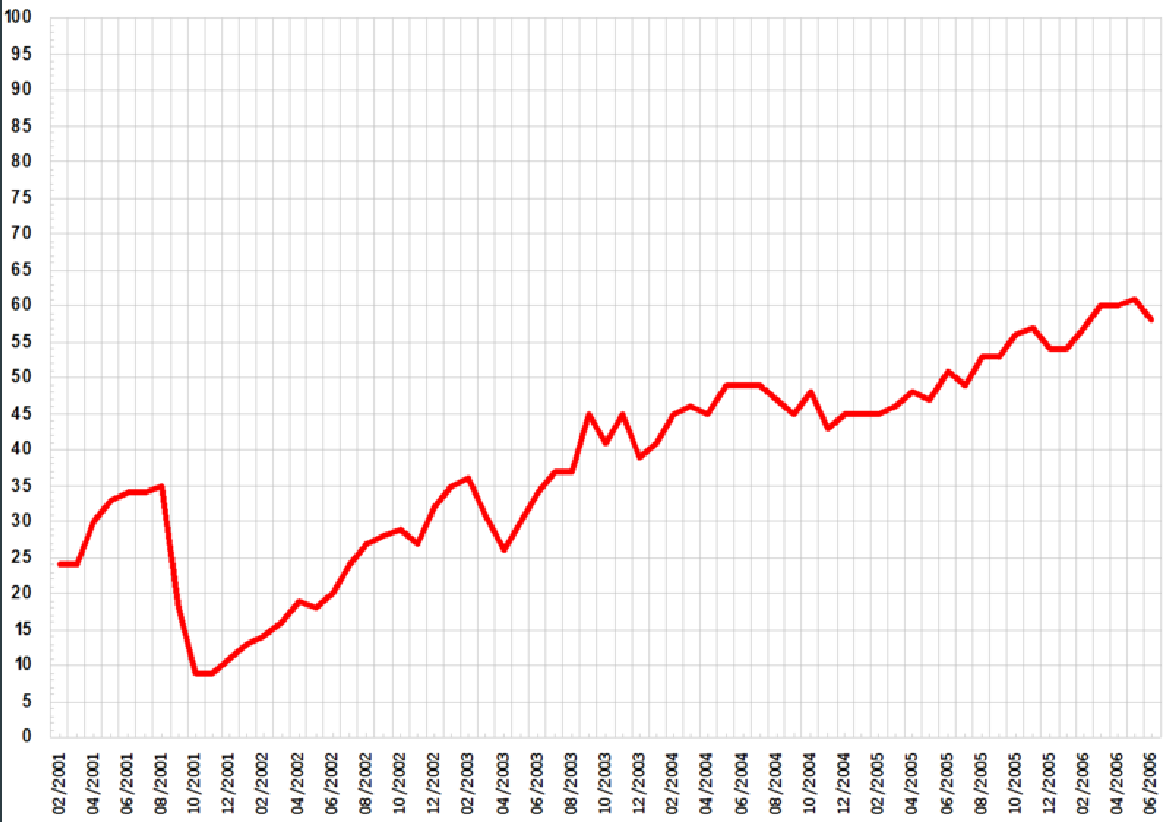
Perceptual properties



Our ability to perceive information encoded by a visual channel depends on the type of data used, from most accurate at the top to least at the bottom. Redrawn and adapted from (Mackinlay, 1986)

Source: Jock Mackinlay. 1986. Automating the design of graphical presentations of relational information. ACM Trans. Graph. 5, 2 (April 1986), 110–141. https://doi.org/10.1145/22949.22950

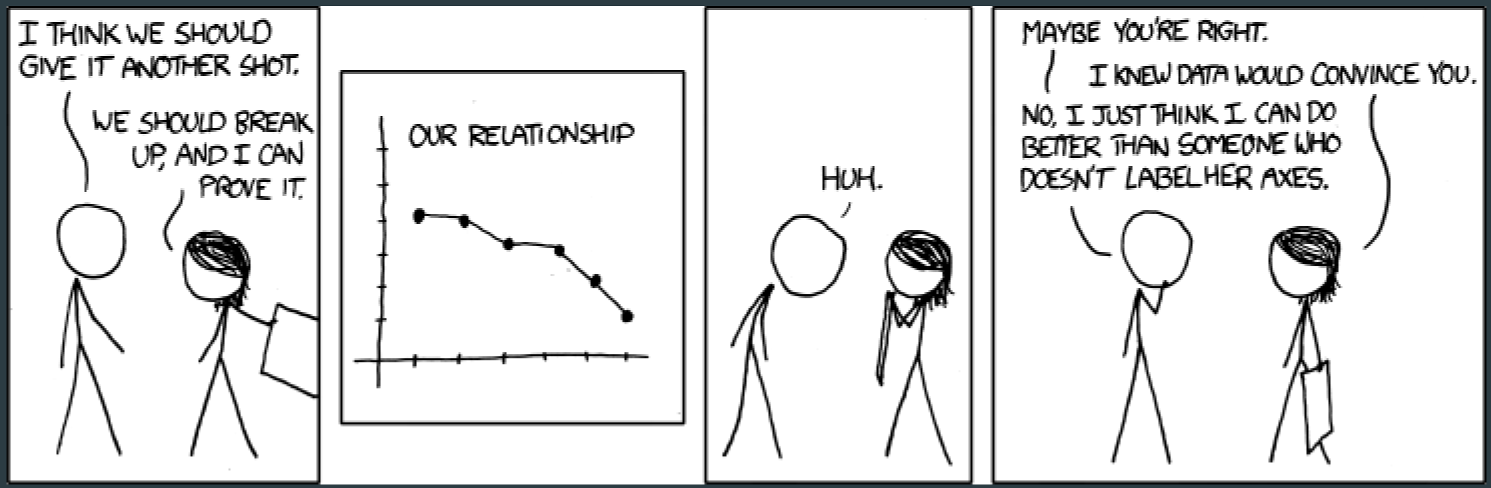
“Bush disapproval ratings”



- X-position: time (Q)
- Y-position: percentage (Q)

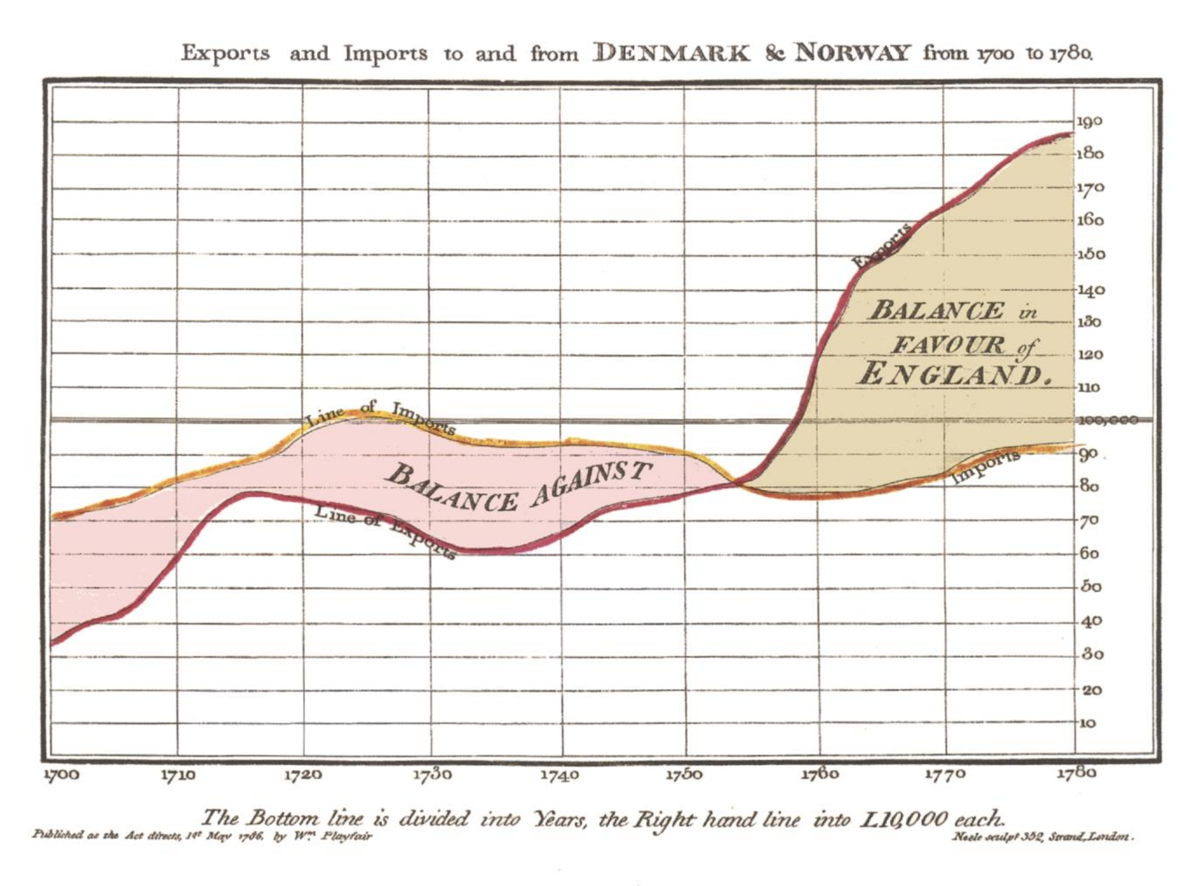
Don’t forget!

- Label axes!
- Add keys, ticks, title!



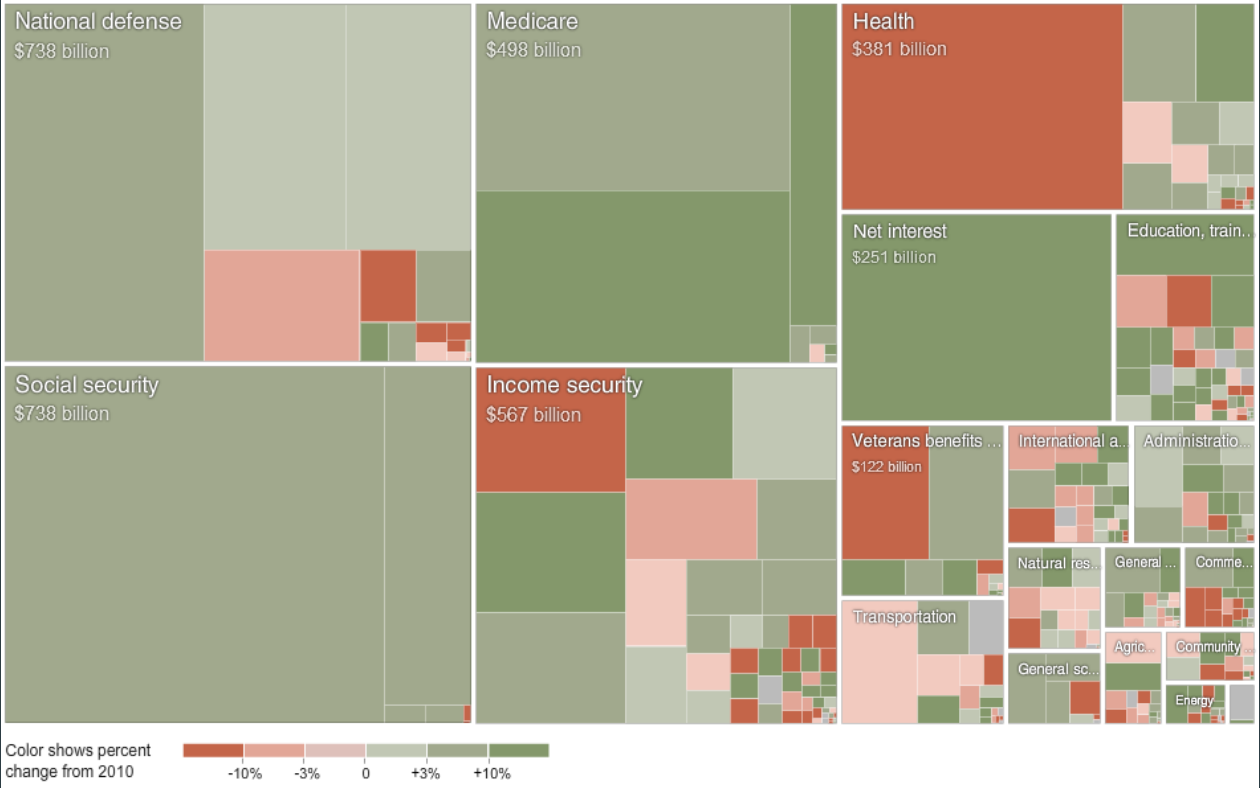
Source: http://xkcd.com/833/

William Playfair (1786)



- X-position: year (Q)
- Y-position: imports/exports currency (Q)
- Colour and area: balance of trade (N, O)

Obama's 2011 budget proposal



- Rectangle position: category (N)
- Rectangle area: amount (Q)
- Color hue: direction of change (N, O)
- Color value: magnitude of change (Q)

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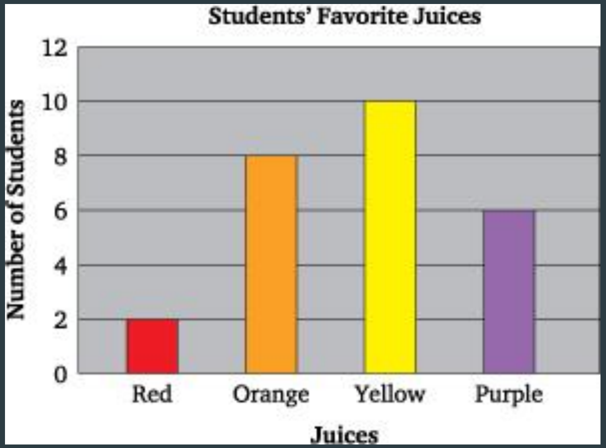
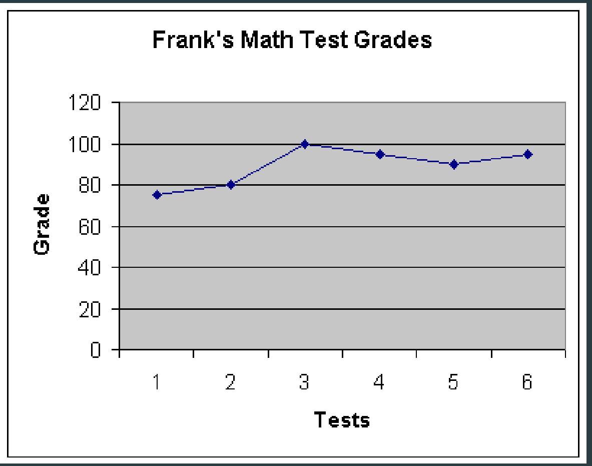
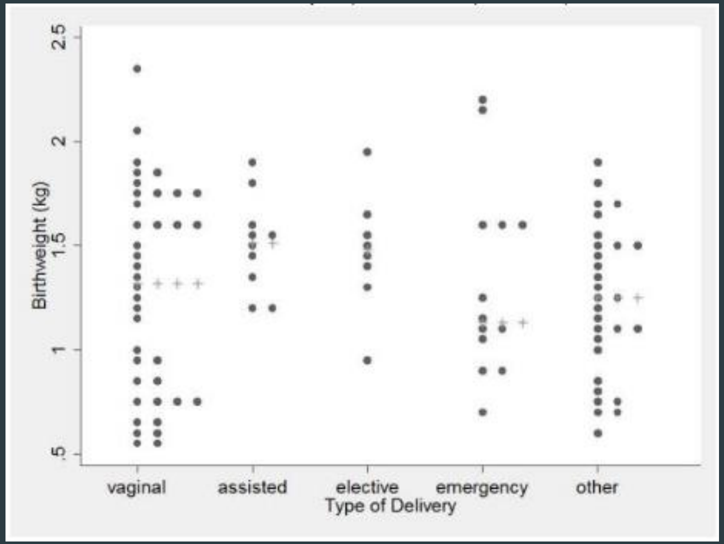
Univariate data

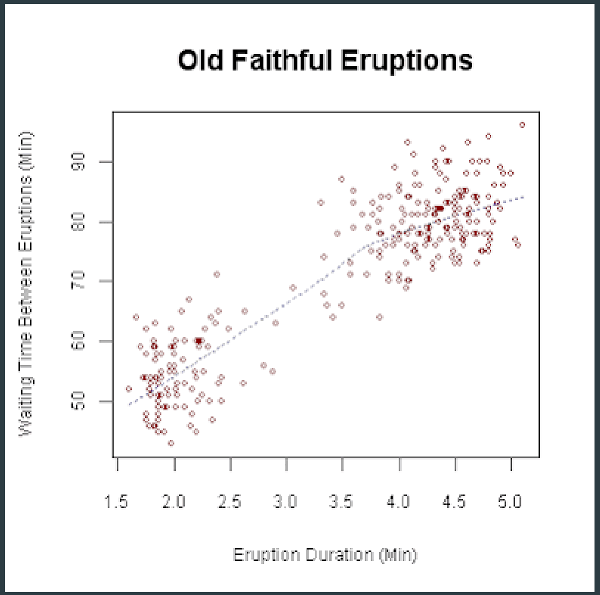


	A
1	
2	
3	
…	





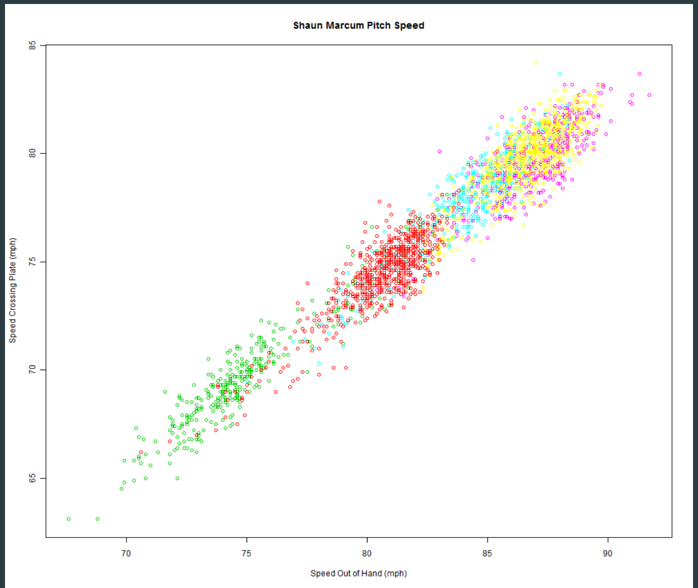
Bivariate data



2D scatter plot (source)

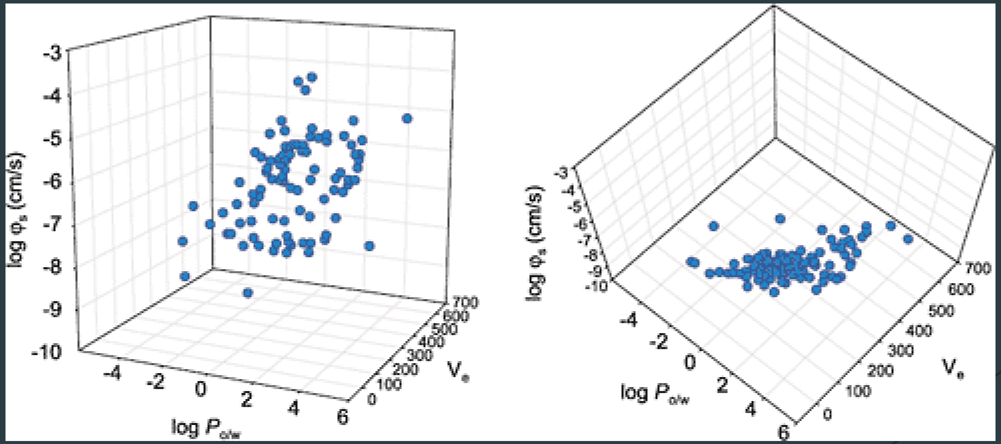
	A	B
1		
2		
3		
…		

Trivariate data



2D scatter plot with third variable mapped to colour

	A	B	C
1			
2			
3			
…			



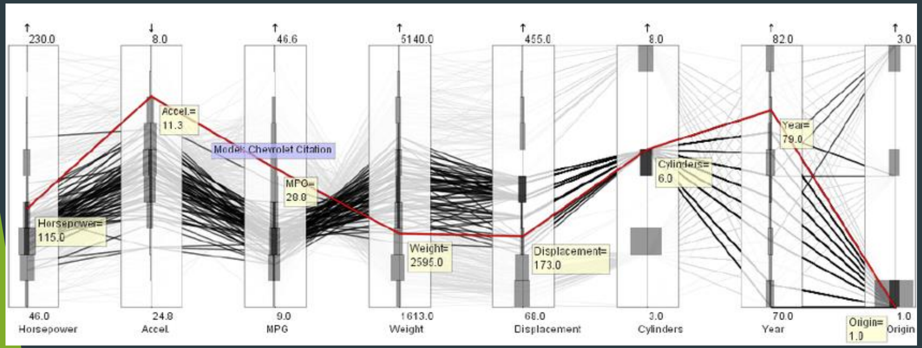
3D scatter plot?

Multidimensional data

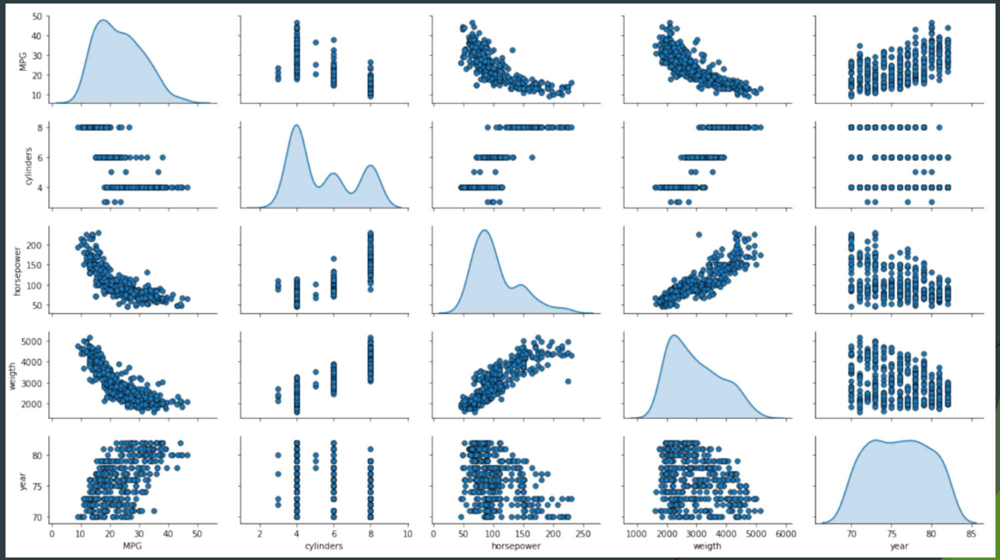
How many variables can be depicted in an image?

"With up to three rows, a data table can be constructed directly as a single image… However, an image has only three dimensions. And this barrier is impassible."
Bertin

	A	B	C	…
1				
2				
3				
…				



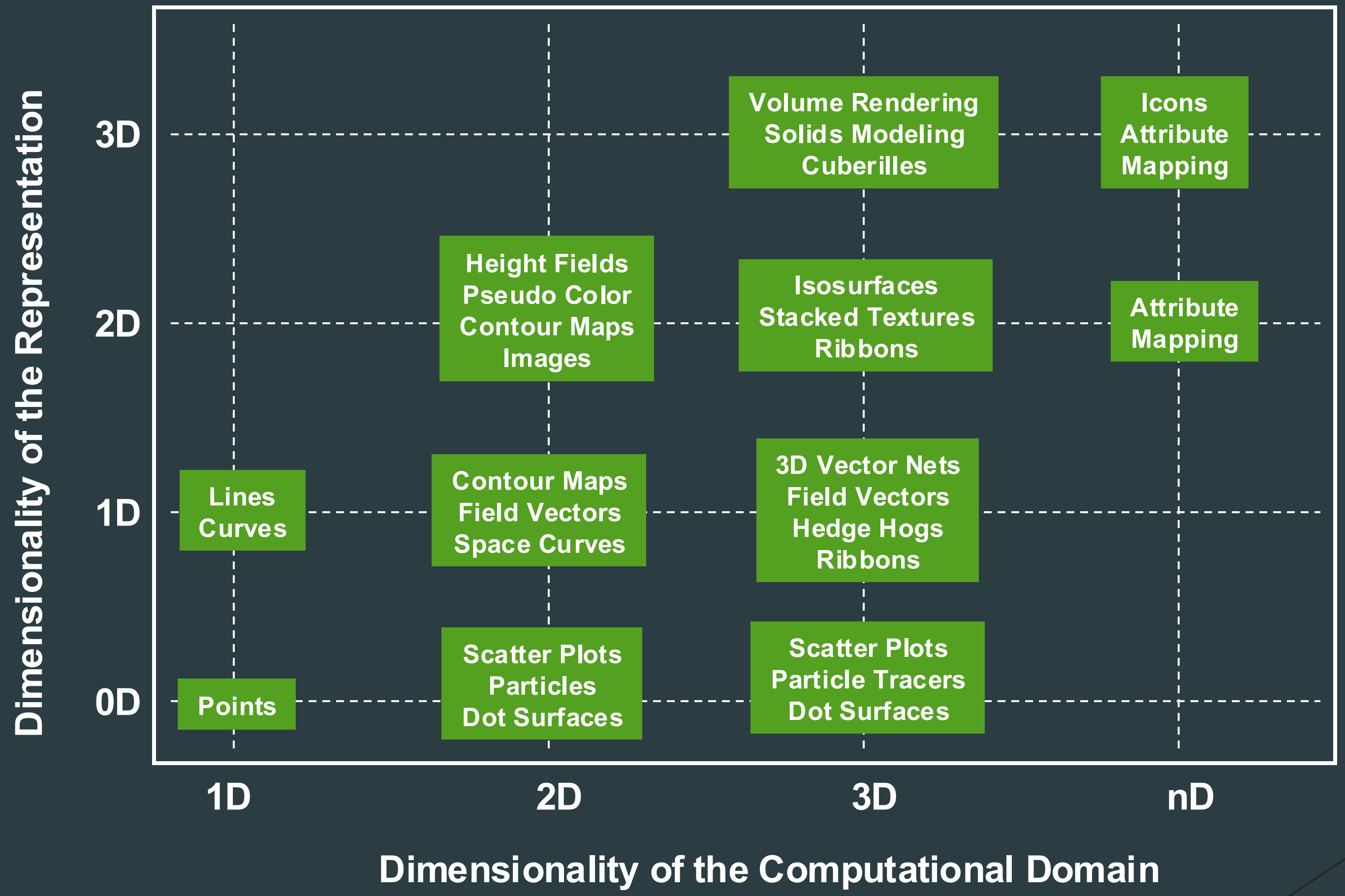
Parallel coordinates



Pair plots / scatterplot matrix / HyperSlice


COVER
stop headtracking
navigation...
view options...
ClipPlane...
File Browser
ModelLoader
PanoView360
Point Model Plugin
Volume
ImagePlugin
CAMERAVis
Floorplan Viewer
PDB Viewer
Protein size
Layout Menu
Show name
Show Topsan Info
Sequence Viewer
Clear Alignment
Delete All

Visualization mapping space



Based on: Craig Upson, *Volumetric Visualization Techniques*, in “State of the Art in Computer Graphics: Visualization and Modeling”, David F. Rogers Rae A. Earnshaw (eds.), Springer-Verlag, 1991, pp. 313-350

Effective visual encoding

Challenge:

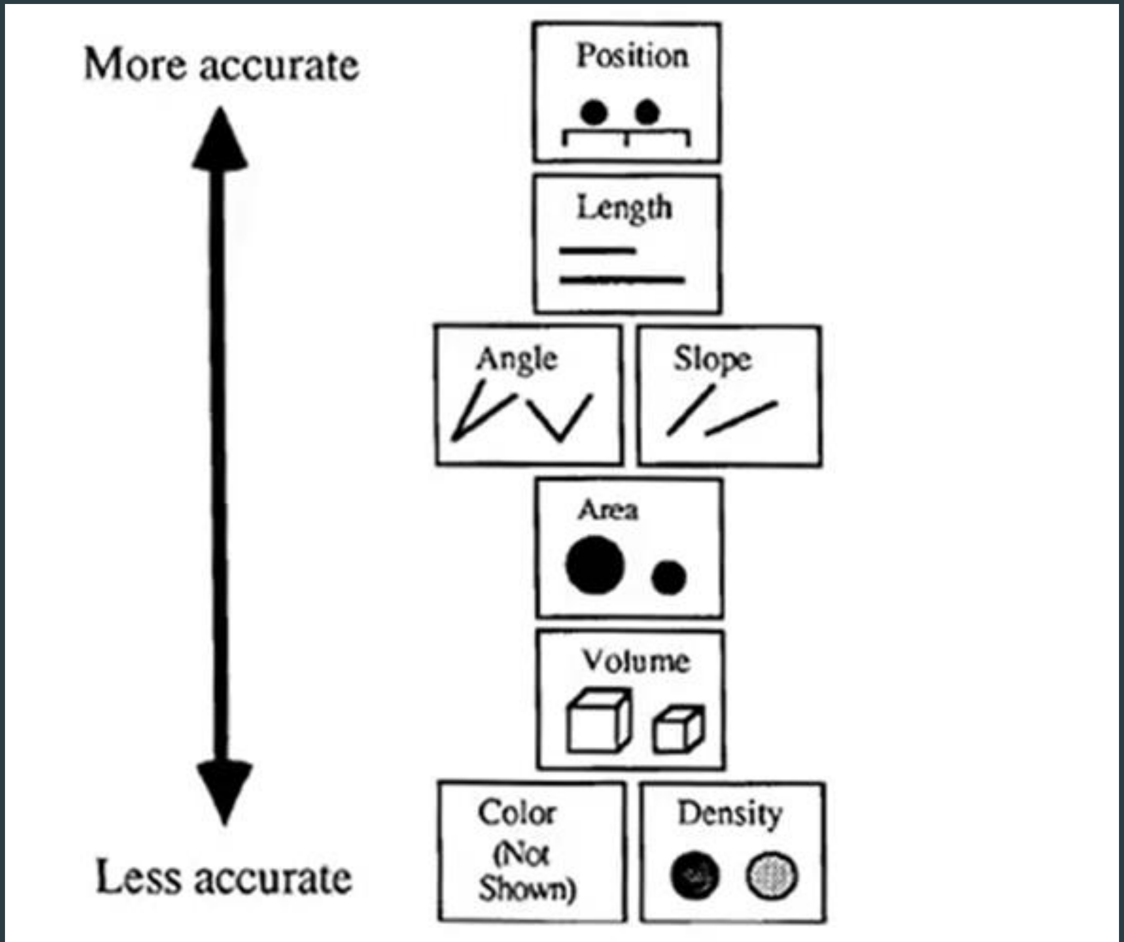
- Choose the best encoding (or mapping) from data to visual attributes

Consider:

1. **Importance ordering**: encode the most important information in the visually most accurate way
2. **Expressiveness**: show all data and *only* the data
3. **Consistency**: the properties of the visual attributes must match the properties of the data

Mackinlay, (APT) A Presentation Tool, 1986.

Importance ordering: perceptual properties

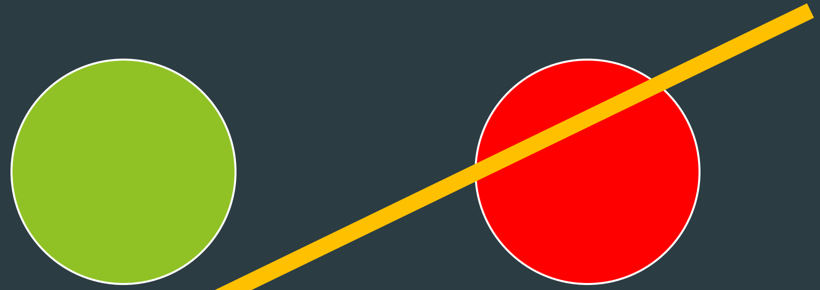


Mackinlay, (APT) A Presentation Tool, 1986.

Expressiveness

Mackinlay:

- “A set of facts is expressible in a visual language if the sentences (i.e. the visualizations) in the language express all the facts in the set of data, and *only* the facts in the data.”



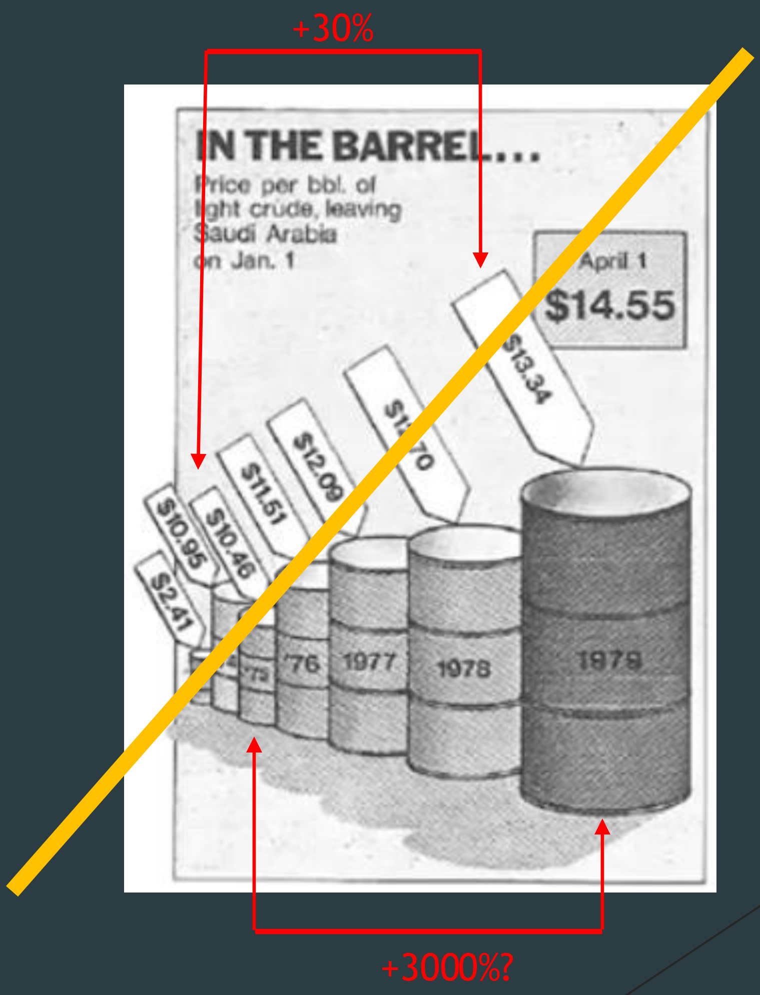
Which of these is greater?

Mackinlay, (APT) A Presentation Tool, 1986.

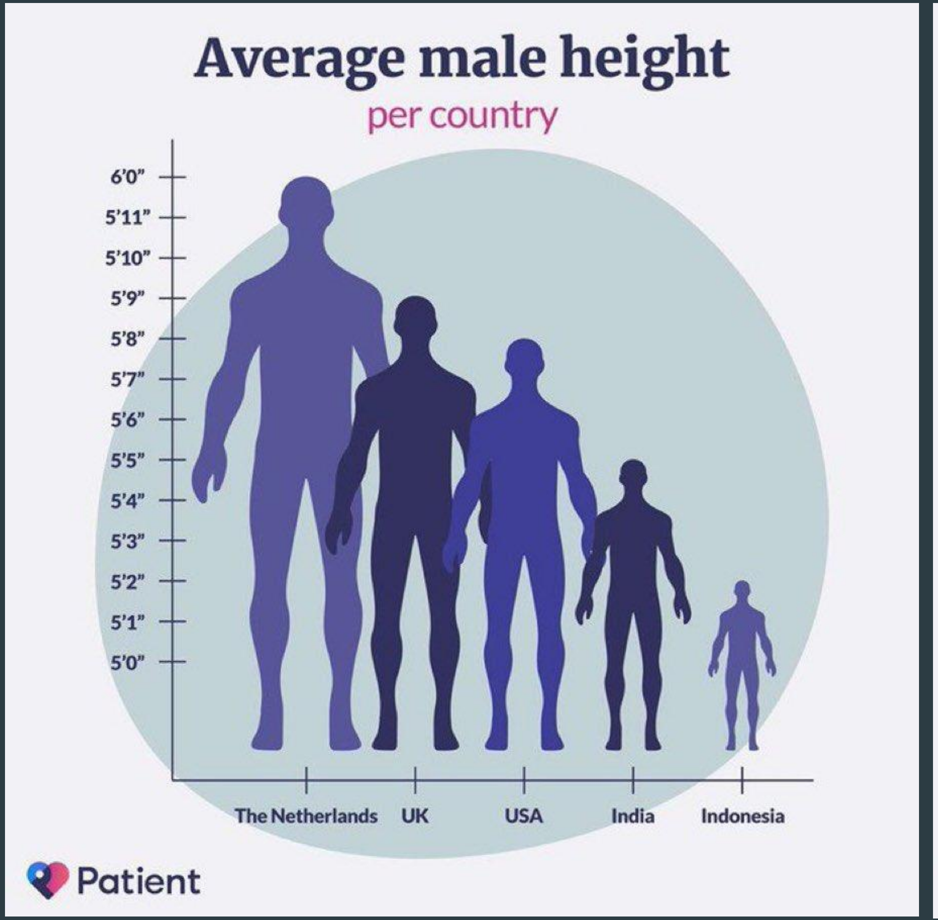
Visual consistency

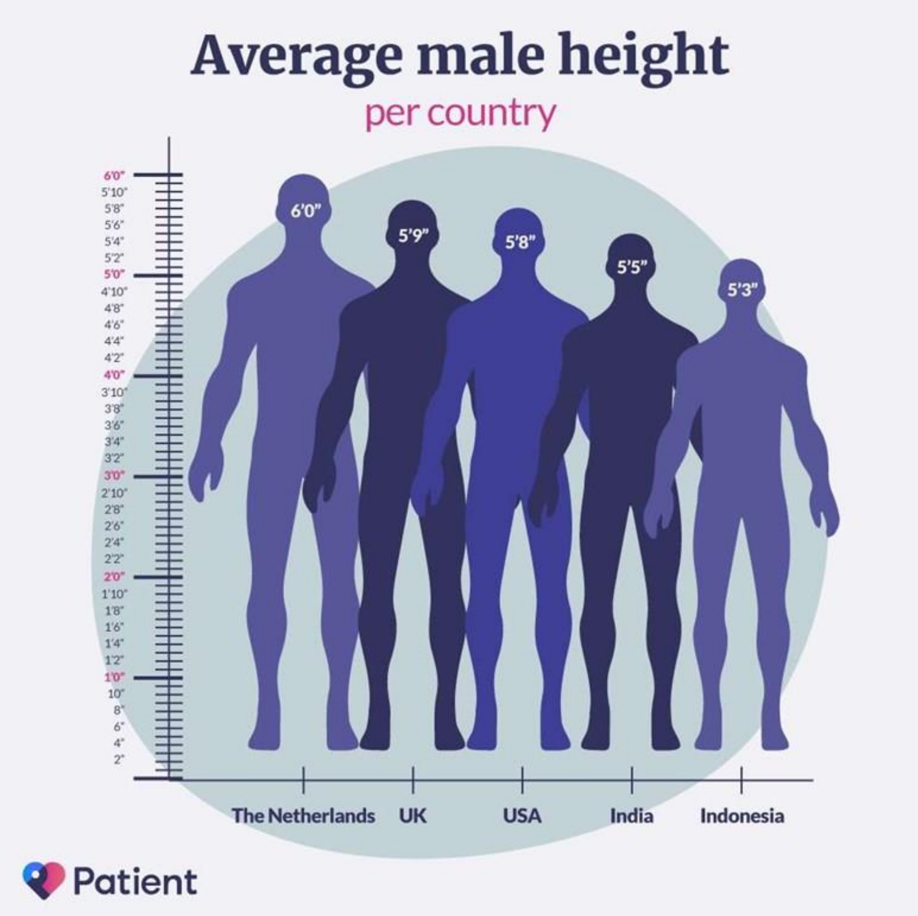
- The properties of the visual attributes must match the properties of the data

E.g. don’t map one-dimensional data to two- or three-dimensional representations!



Visual consistency

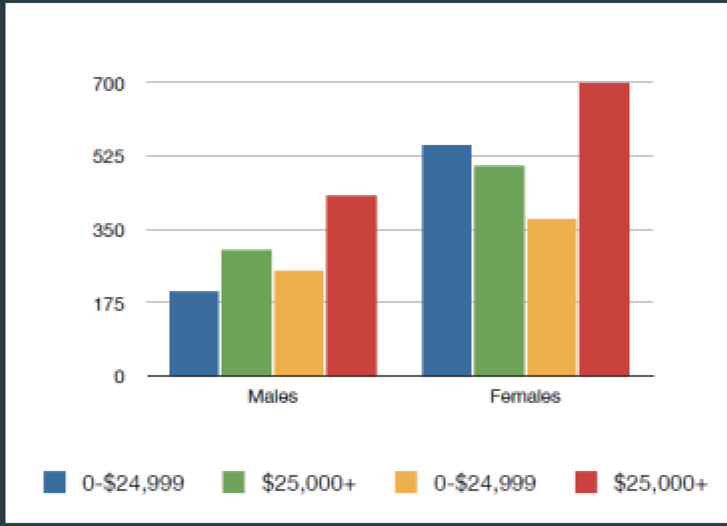




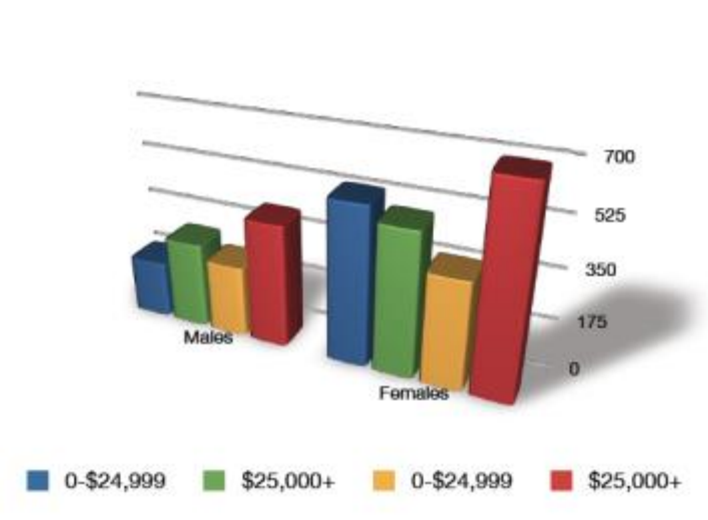
Source

Data-to-ink ratio

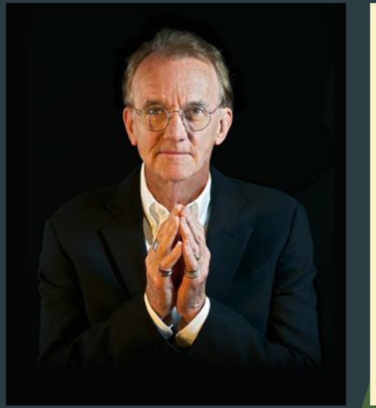
- Maximize Data-to-ink ratio = $\frac{Data\ Ink}{Ink\ used\ in\ graphic}$



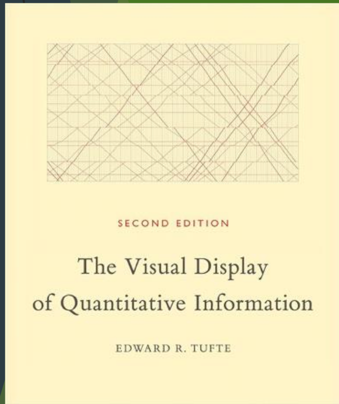
High data-to-ink ratio



Low data-to-ink ratio



Edward Tufte



Esthethics

Photo: Michael Najjar

Remember this

1. All representations of information are subjective interpretations of the information, not the information itself.

2. The challenge in visualization is to find a representation that is both efficient and appropriate.

3. The purpose of visualization is to inform, not to misinform.

4. Any visualization is limited in its interpretation.

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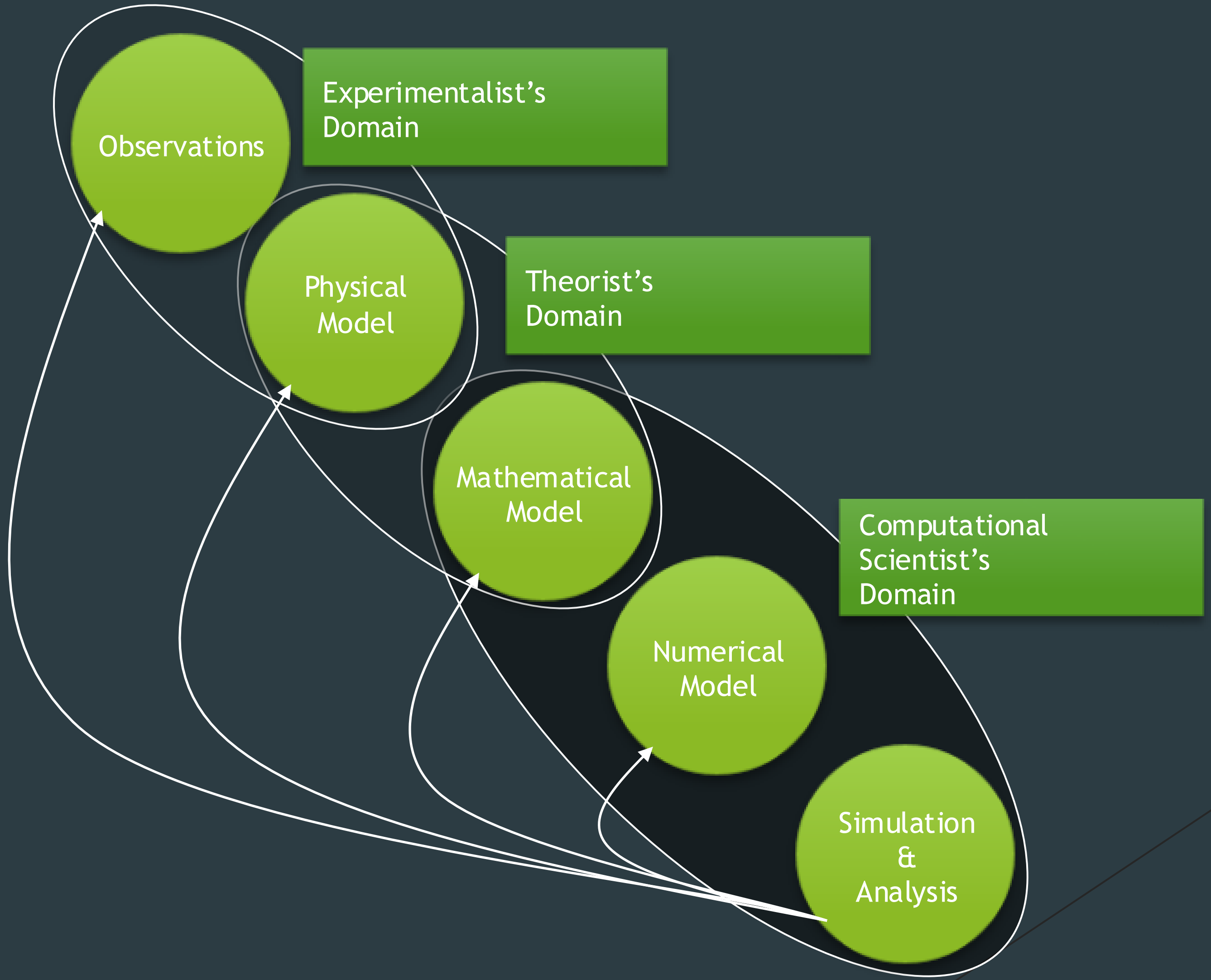
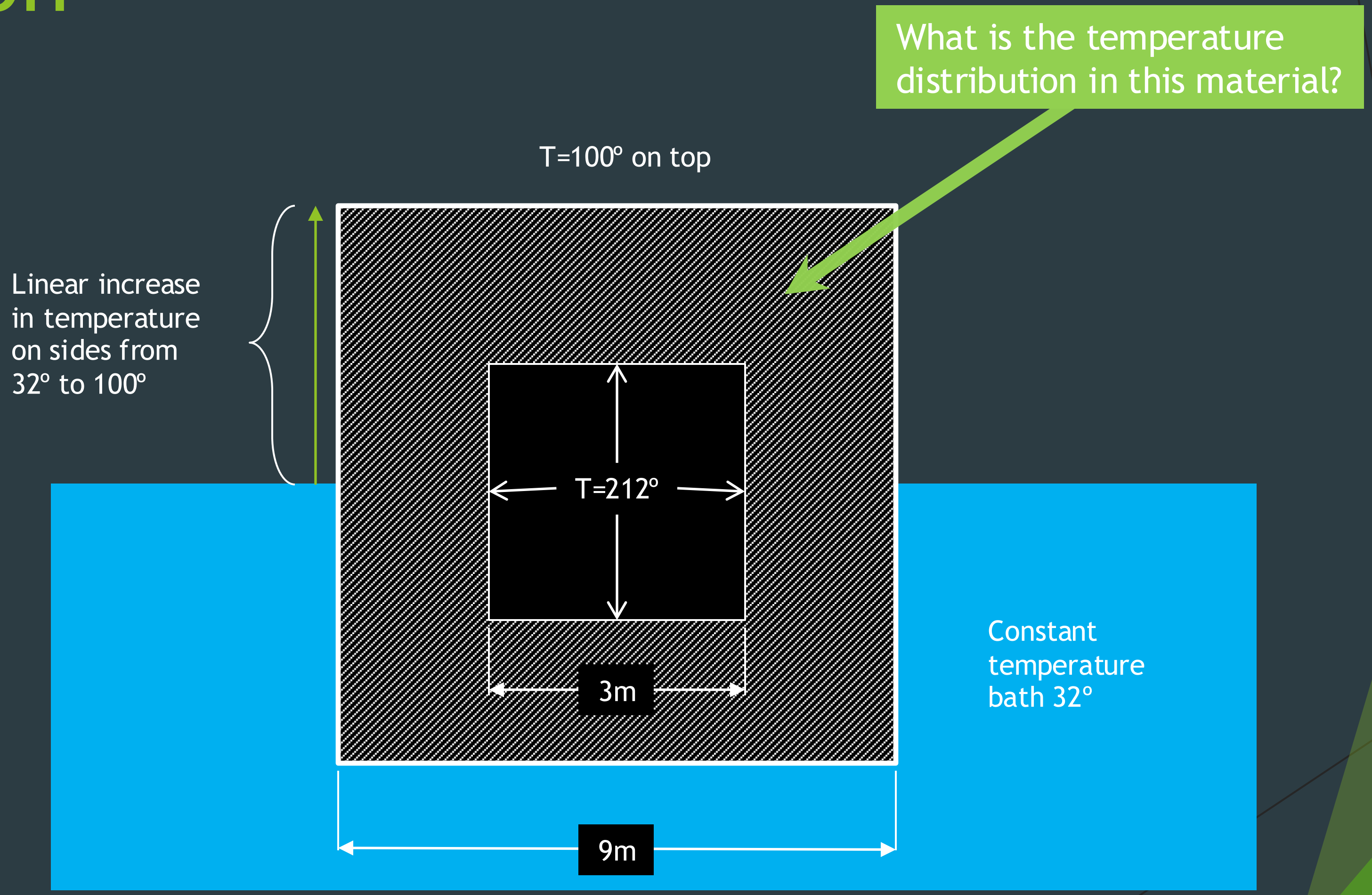
Computational simulation



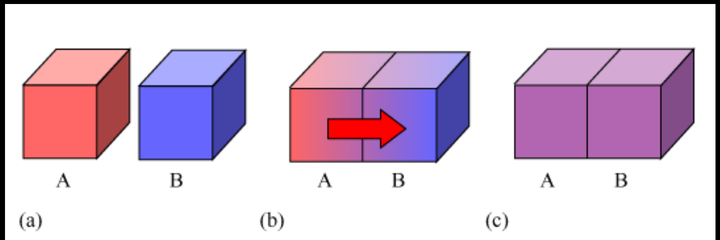
Example physics problem: temperature distribution



Source: Neal Wagner, Univ. of Texas San Antonio
(original source: http://www.cs.utsa.edu/~wagner/CS2073/distill/dsgif.html)

Physical mod

the temperature
ion in this material?



(a) Two bodies A and B are of different temperatures, the temperature of A is higher than that of B. (b) When they are in contact, heat is transferred from A to B. (c) Heat transfer will stop when both A and B reach the final temperature

nt
ure

9m

Source: Neal Wagner, Univ. of Texas San Antonio
(original source: http://www.cs.utsa.edu/~wagner/CS2073/distill/dsgif.html)

Mathematical model

- Laplace equation:

$$\nabla^2 c = 0$$

- Two-dimensional Laplace equation:

$$\nabla^2 c = \frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} = 0$$

Mathematical model

Solving the Laplace equation using finite differencing
($c_{i,j}$ is the temperature at lattice site (i, j)):

$$\frac{\partial c}{\partial x} \equiv c_{i+1,j} - c_{i,j}$$

$$\frac{\partial c}{\partial y} \equiv c_{i,j+1} - c_{i,j}$$

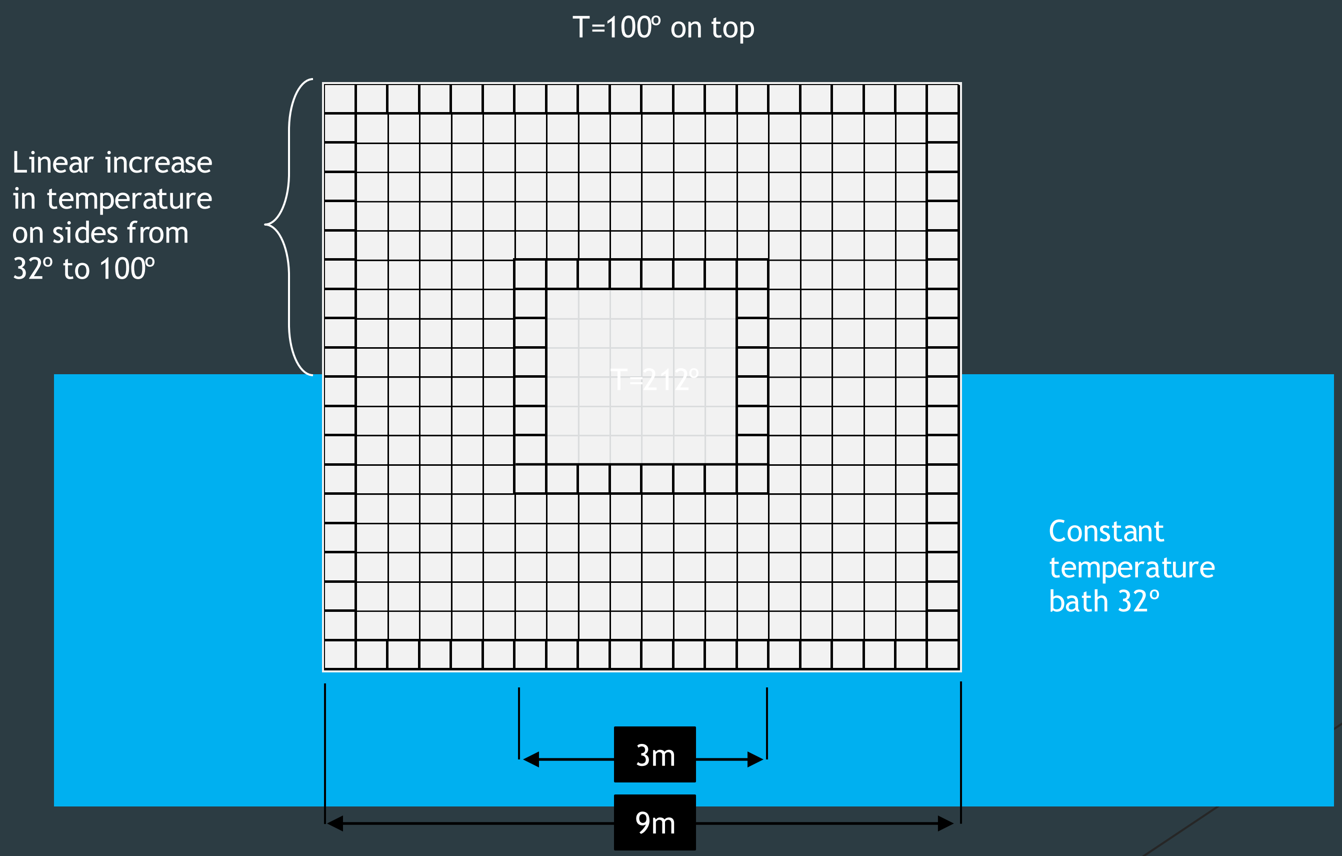
$$\frac{\partial^2 c}{\partial x^2} \equiv \left(c_{i,j} - c_{i-1,j}\right) - \left(c_{i+1,j} - c_{i,j}\right)$$

$$\frac{\partial^2 c}{\partial y^2} \equiv \left(c_{i,j} - c_{i,j-1}\right) - \left(c_{i,j+1} - c_{i,j}\right)$$

$$\frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial y^2} = 0 \equiv 4c_{i,j} - c_{i-1,j} - c_{i,j-1} - c_{i+1,j} - c_{i,j+1} = 0$$

	$c_{i,j-1}$	
$c_{i-1,j}$	$c_{i,j}$	$c_{i+1,j}$
	$c_{i,j+1}$	

Numerical model



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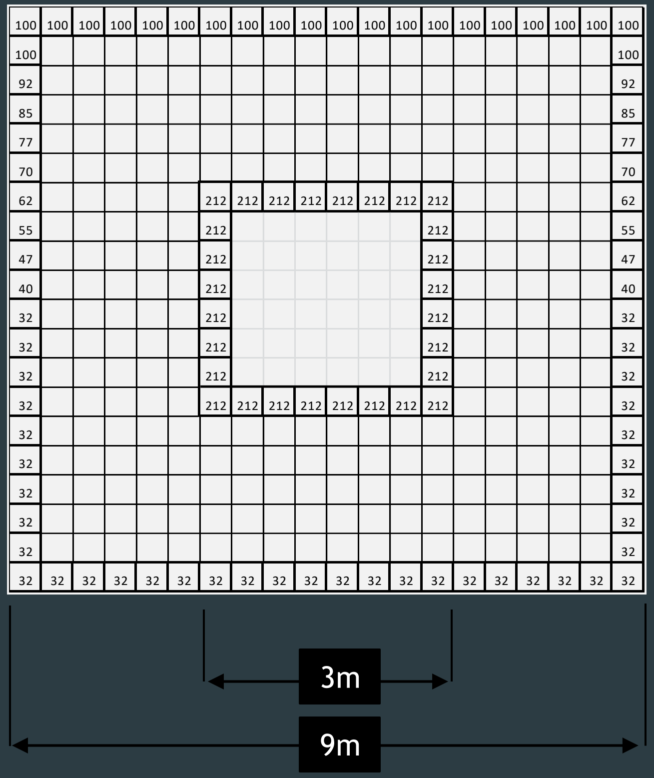
Numerical model



Source: Neal Wagner, Univ. of Texas San Antonio
(original source: http://www.cs.utsa.edu/~wagner/CS2073/distill/dsgif.html)

Numerical model

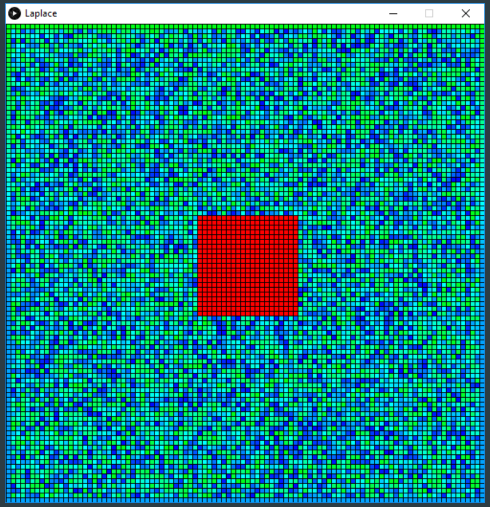
Laplace equation - Jacobi update procedure where $c_{i,j}^{n}$ is the old value, $c_{i,j}^{n+1}$ is the new value:

$$
\begin{aligned}
&\textbf{do}\ \{\\
&\quad c_{i,j}^{n+1} = \frac{1}{4}\left(c_{i-1,j}^{n} + c_{i,j-1}^{n} + c_{i+1,j}^{n} + c_{i,j+1}^{n}\right)\\
&\}\ \textbf{while}\ \left(\left|c_{i,j}^{n} - c_{i,j}^{n+1}\right| > tolerance\right)
\end{aligned}
$$

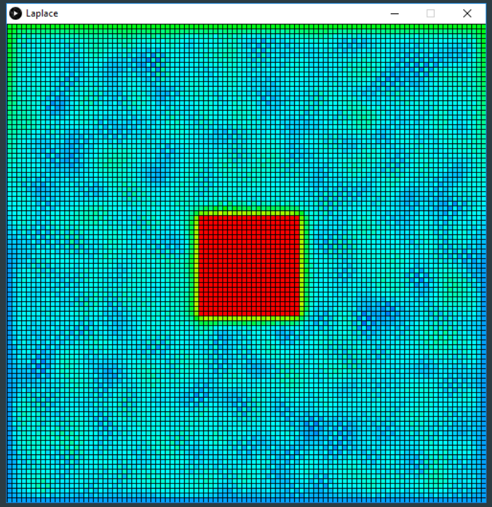
Simulation pseudocode

```
initialize all lattice sites
set boundary conditions
do {
    δ = 0
    for i=1 to IMAX {
        for j=1 to JMAX {
            west_neighbour   = (i==1)    ? c^n_{IMAX,j} : c^n_{i-1,j}
            east_neighbour   = (i==IMAX) ? c^n_{1,j}    : c^n_{i+1,j}
            north_neighbour  = (j==JMAX) ? c^n_{i,1}    : c^n_{i,j+1}
            south_neighbour  = (j==1)    ? c^n_{i,JMAX} : c^n_{i,j-1}
            c^{n+1}_{i,j}=¼(west_neighbour + east_neighbour +
                      north_neighbour + south_neighbour)
            if (c^n_{i,j} - c^{n+1}_{i,j} > tolerance) δ = c^n_{i,j} - c^{n+1}_{i,j}
        }
    }
} while (δ > tolerance)
```

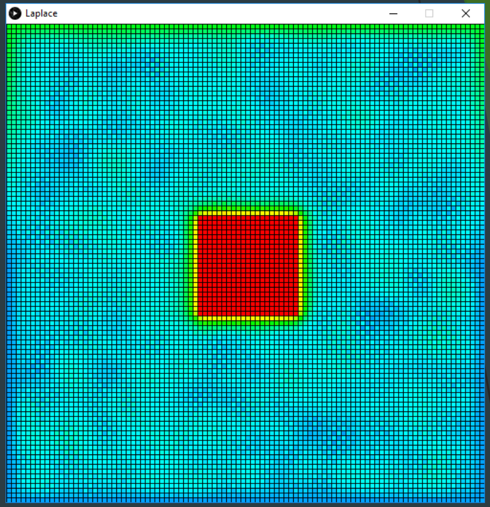
Simulate!



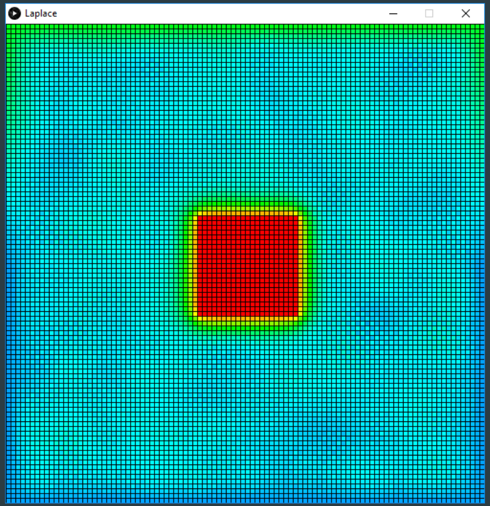
$t=0$ ($\delta \approx 100$)



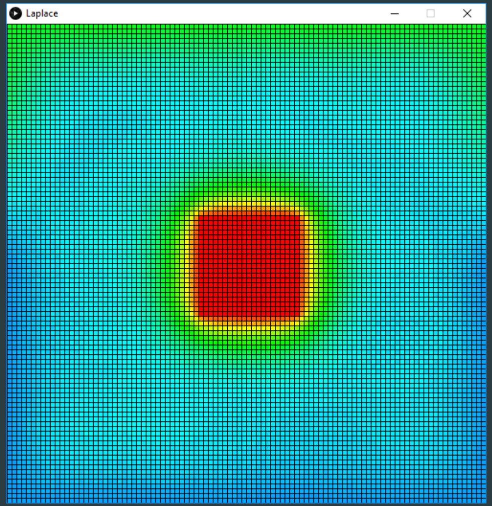
$t=5$ ($\delta \approx 50$)



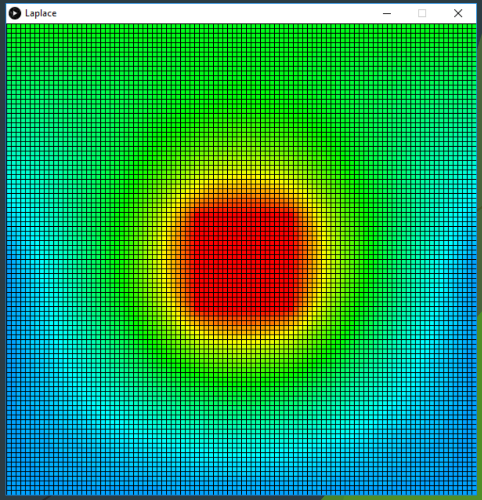
$t=10$ ($\delta \approx 40$)



$t=20$ ($\delta \approx 30$)



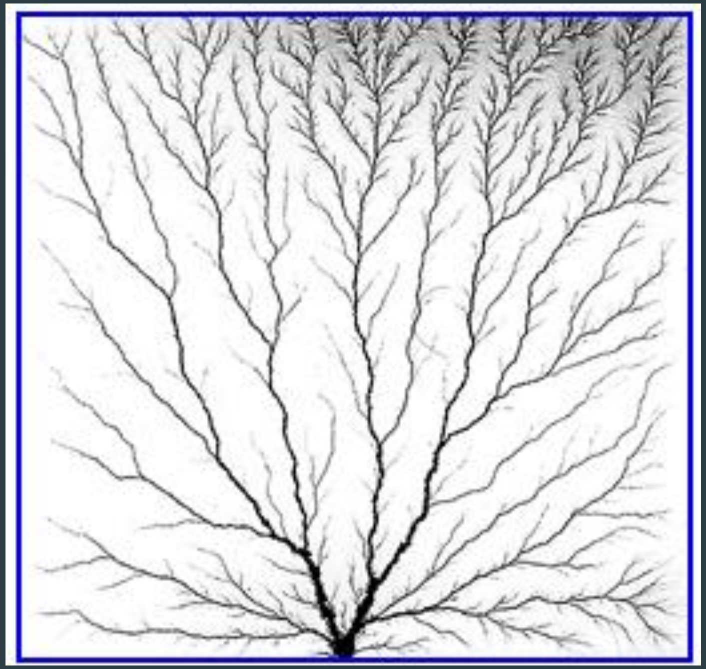
$t=100$ ($\delta \approx 17$)



$t=1000$ ($\delta \approx 9$)

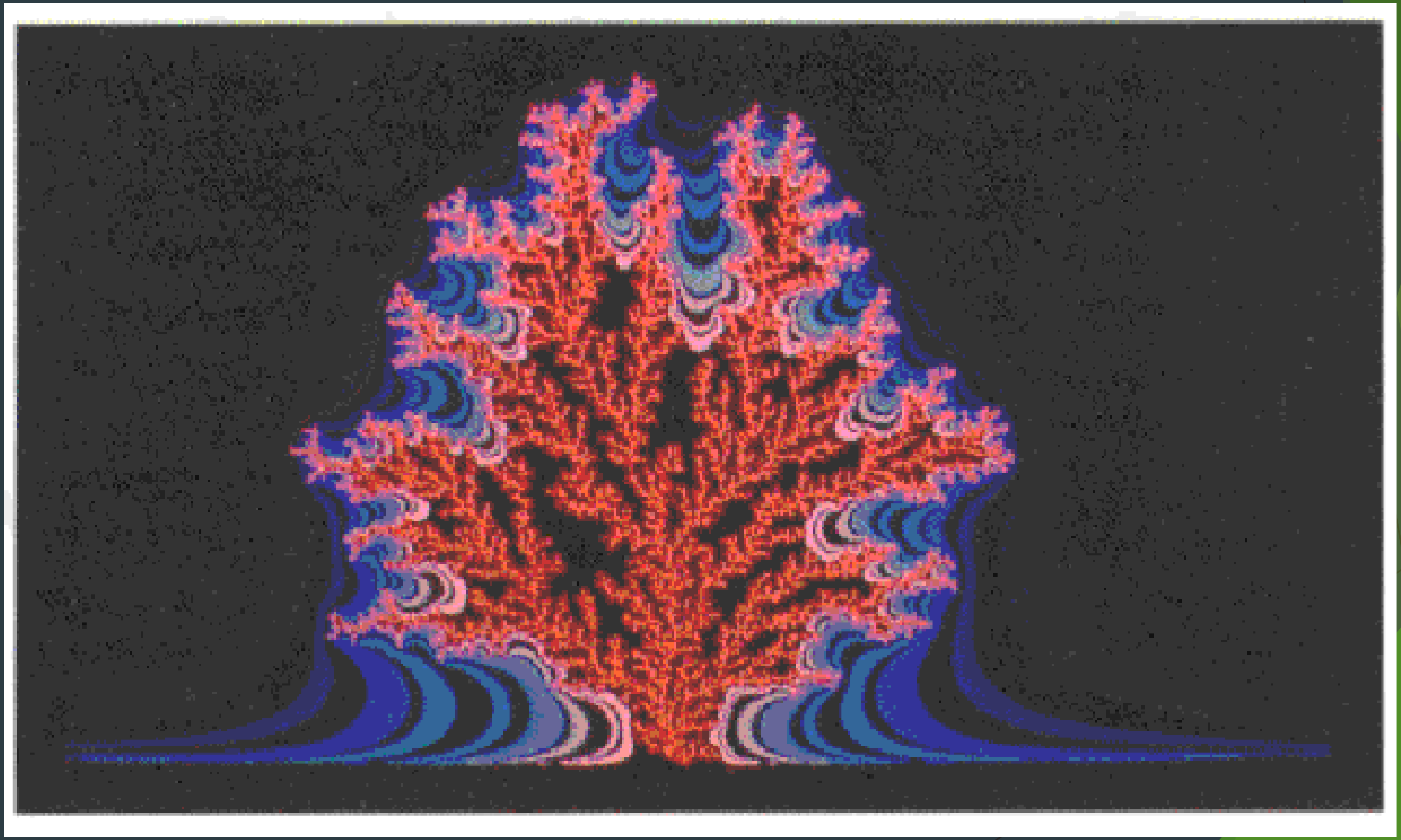
Example: Abiotic growth and form; Lichtenberg patterns

- “Dielectric breakdown”
- First created by Lichtenberg, 18th century

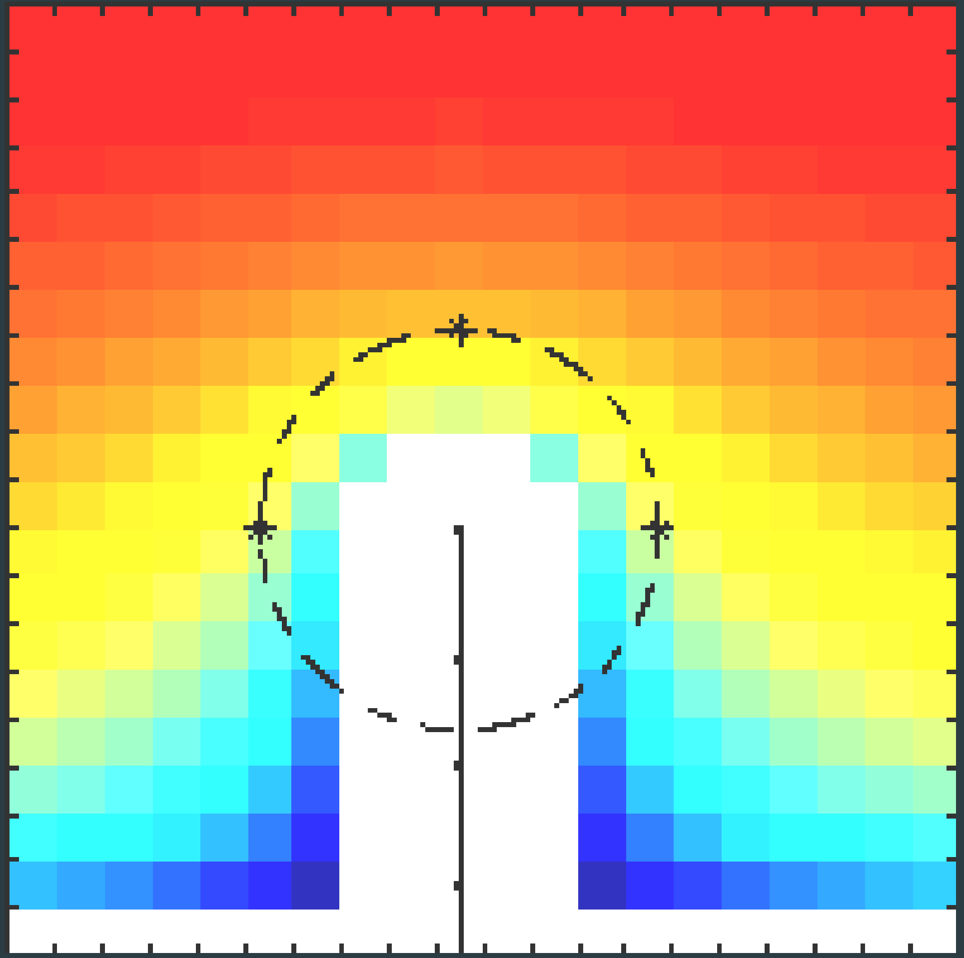


Example: Abiotic growth and form; Lichtenberg patterns

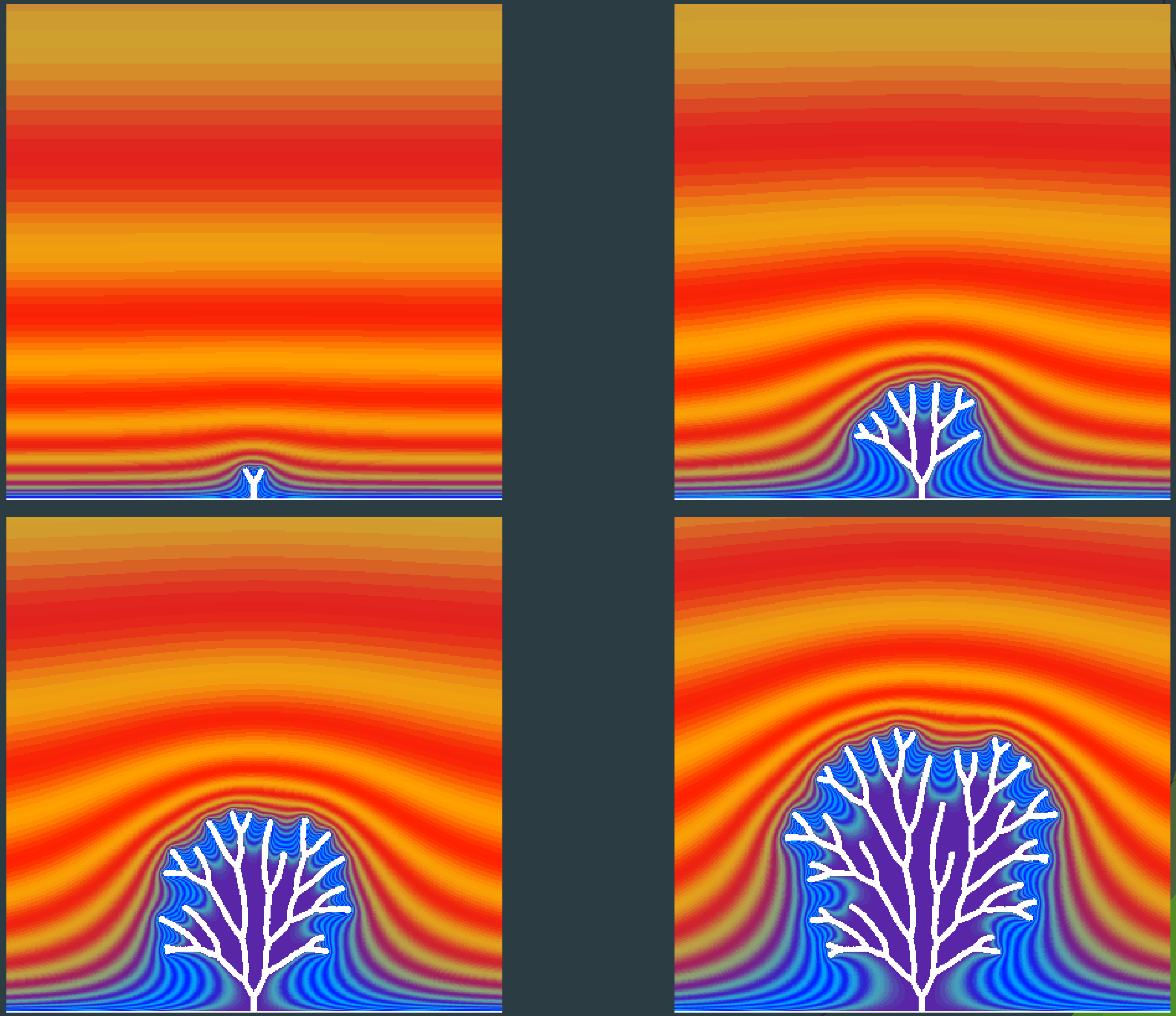
Laplacian growth patterns



Laplacian growth patterns

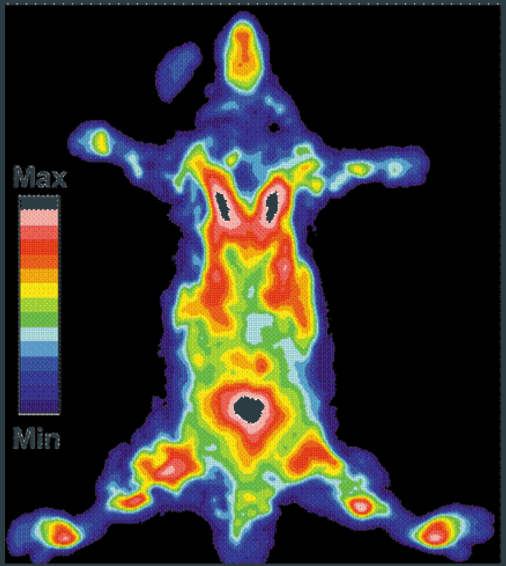


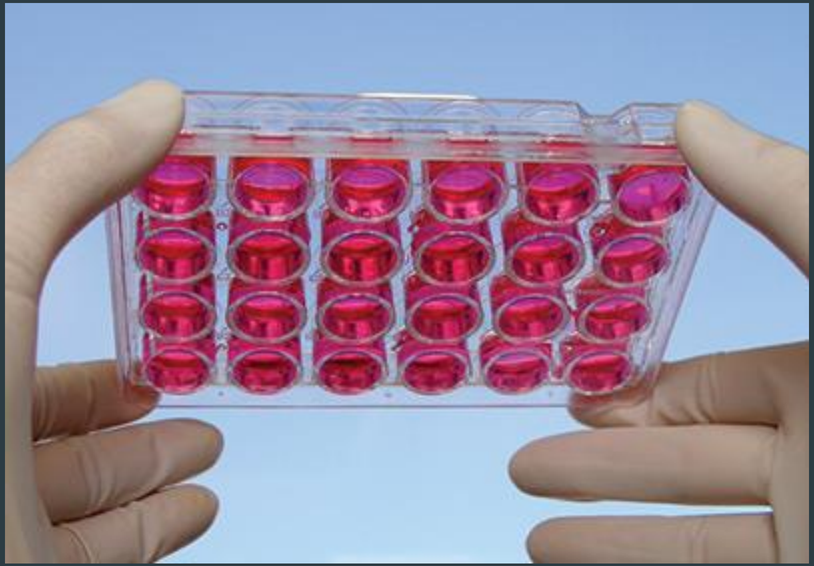
Laplacian growth patterns

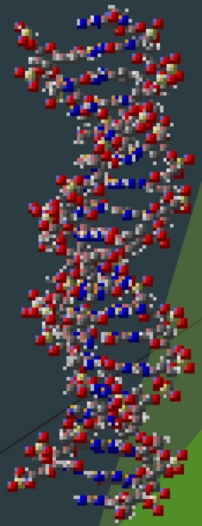


In vivo, in vitro, in silico

- *in vivo*: in the living organism
- *in vitro*: in an artificial environment outside the living organism
- *in silico*: in a computer simulated model







Science in silico

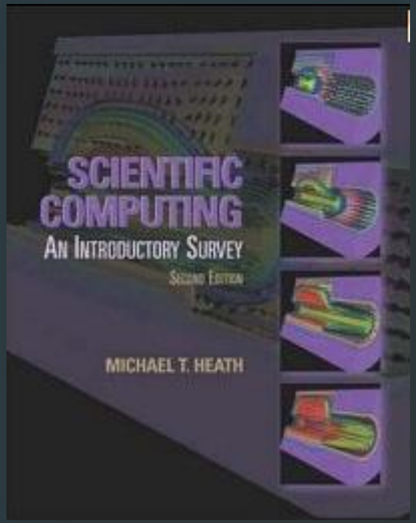
- SEED Magazine, April 19, 2007
  Source: http://seedmagazine.com/content/article/science_in_silico/
- (also available on YouTube)

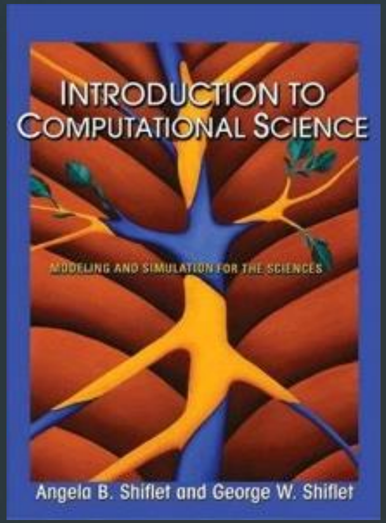
https://www.youtube.com/watch?v=1FvRSJ9W734&t=1s

If you want more

Book suggestions:

- Michael T. Heath, *Scientific Computing, an introduction survey*
- A.B. Shiflet and G.W. Shiflet, *Introduction to Computational Science: Modeling and Simulation for the Sciences*,





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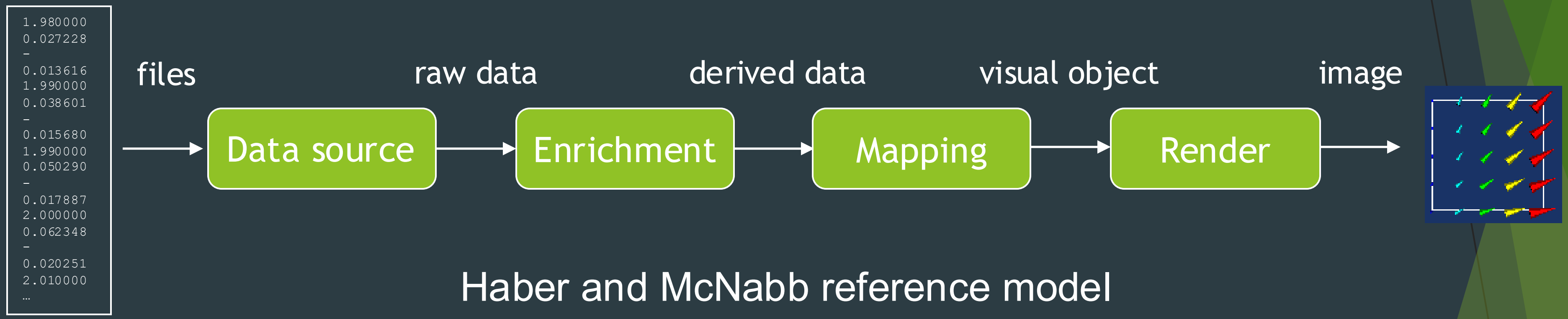
The visualization pipeline

Data enrichment → Mapping → Render

Haber and McNabb reference model

Haber, R.B. and McNabb, D.A. *Visualization idioms: A conceptual model for scientific visualization systems*. In *Visualization in Scientific Computing*, pages 74–93. IEEE Computer Society Press. 1990

The visualization pipeline

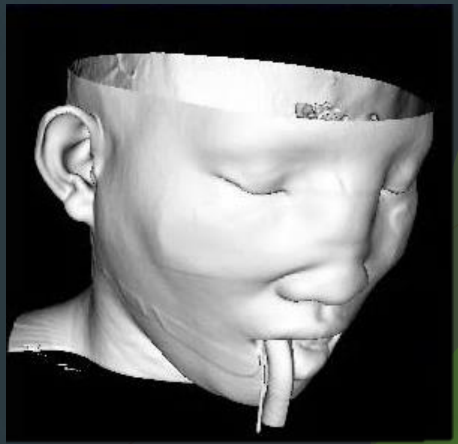


Haber and McNabb reference model

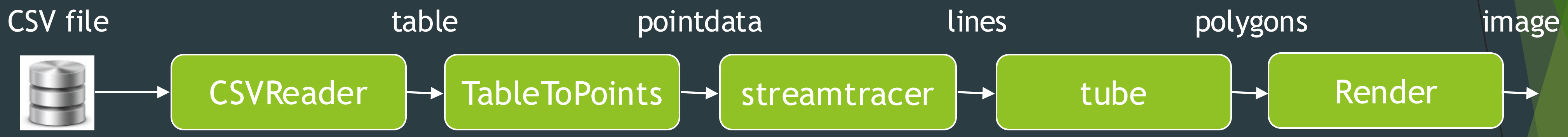
Haber, R.B. and McNabb, D.A. *Visualization idioms: A conceptual model for scientific visualization systems*. In *Visualization in Scientific Computing*, pages 74–93. IEEE Computer Society Press. 1990

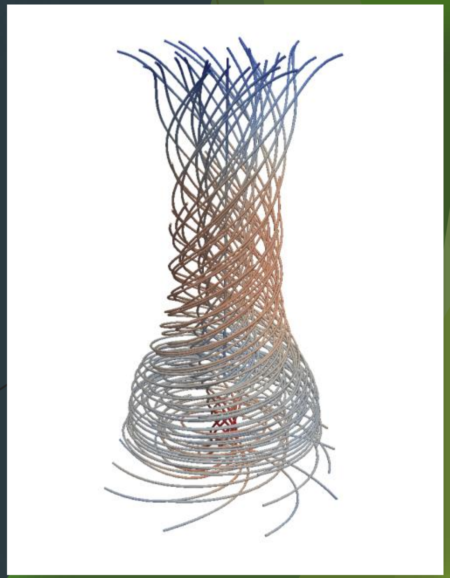
Example:
extracting a contour from medical data

file(s) → DICOMReader → 3D grid → Contour → polygon data → Triangulate → triangles → Render → image

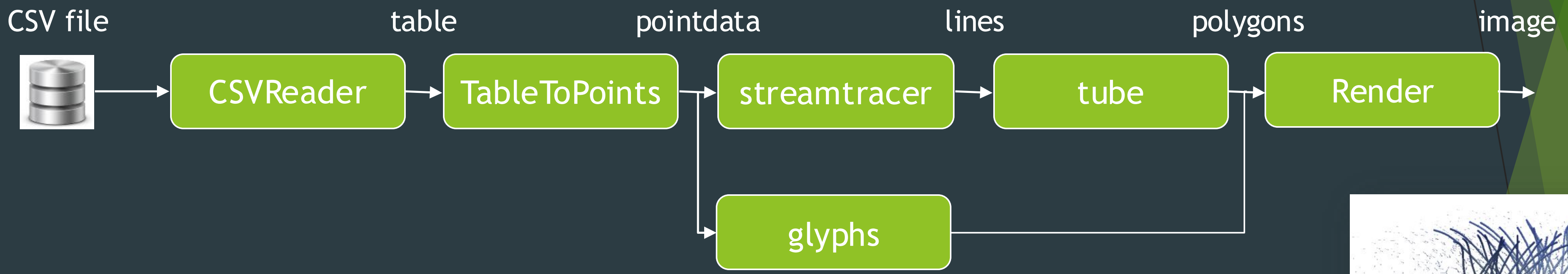


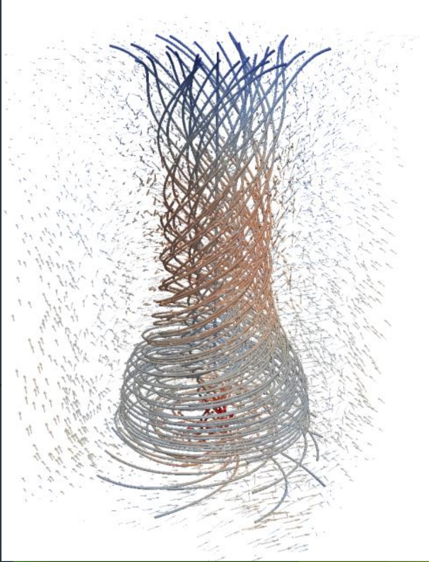
Example:
visualizing flow data with streamlines



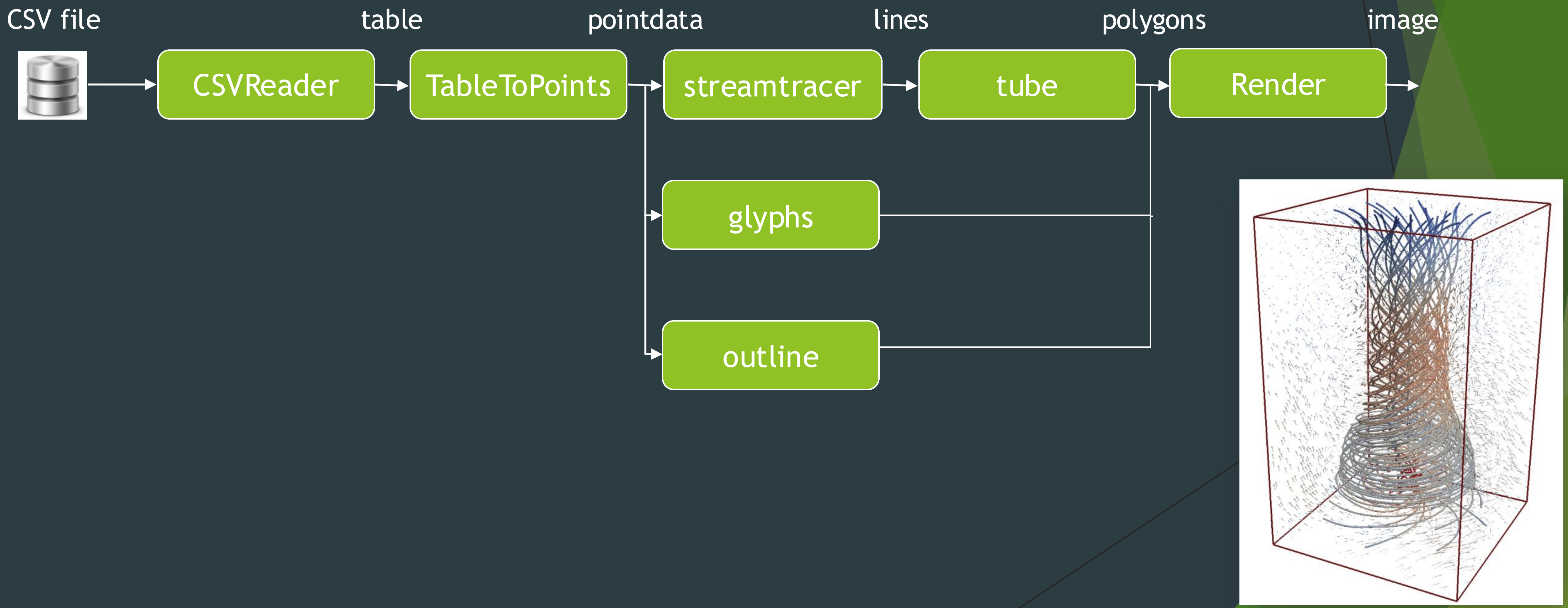


Example:
visualizing flow data with streamlines





Example:
visualizing flow data with streamlines

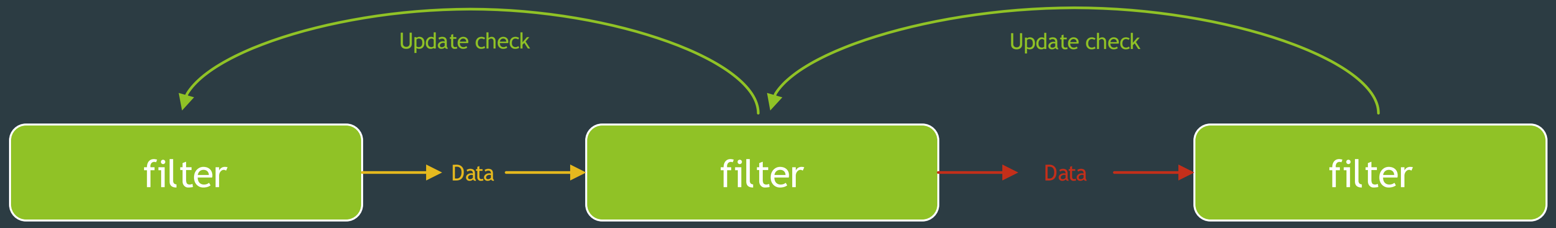


Pipeline creation

- The components in a pipeline are called “filters”
- Filters are connected together to form a “visualization pipeline” or “dataflow network”
- The input port of a filter may only be connected to the output port(s) of (an)other filter(s) if the port types are “similar"

Pipeline behaviour

- Filters in a pipeline only execute when necessary
  - When data at the input has changed, or a parameter
- Data flows downstream, update checks go upstream

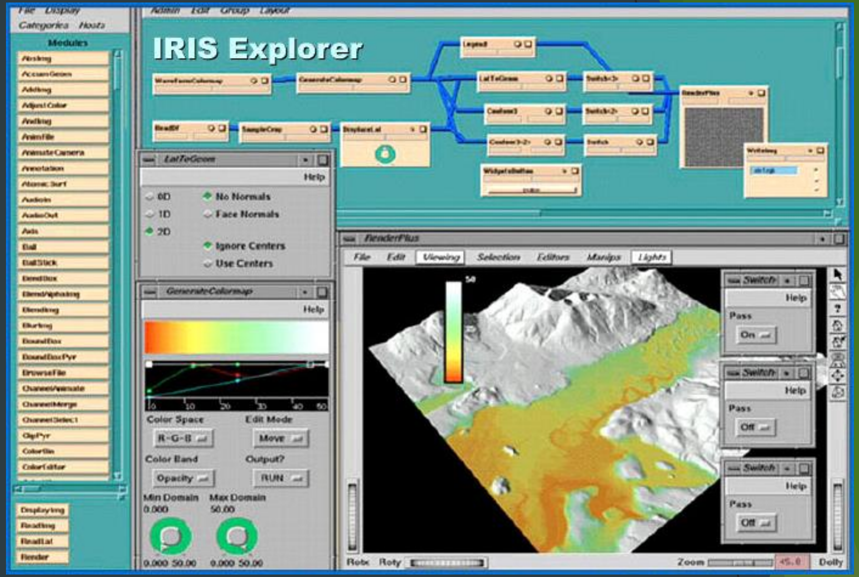


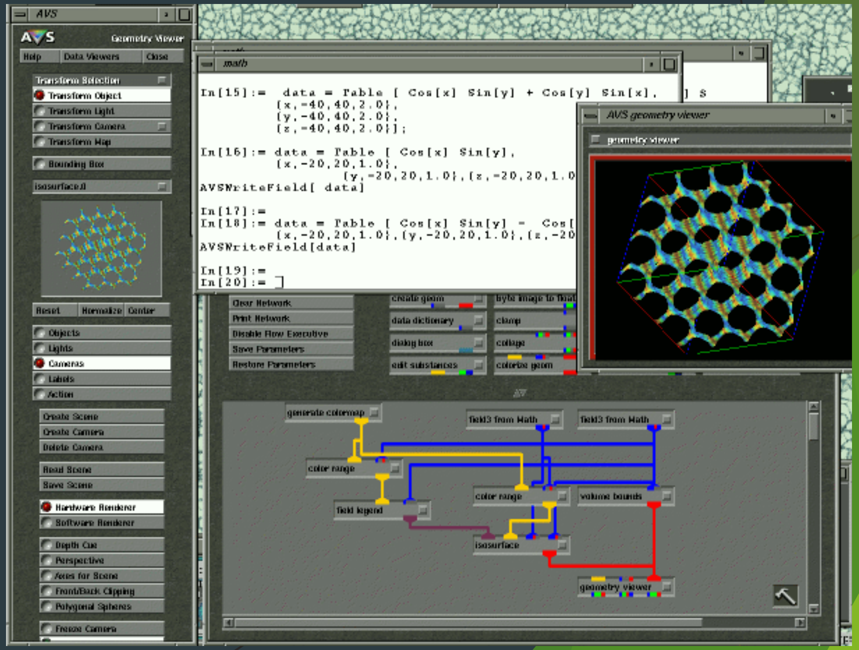
Software

- Often domain-specific
- Almost all based on visualization pipeline / dataflow concept

Commercial:

- AVS (Advanced Visual Systems)
- OpenDX (now open source?)
- IRIS Explorer (?)
- Amira
- Matlab, Mathematica, IDL
- Spotfire, Tableau
- …





Software

- Often domain-specific
- Almost all based on visualization pipeline / dataflow concept

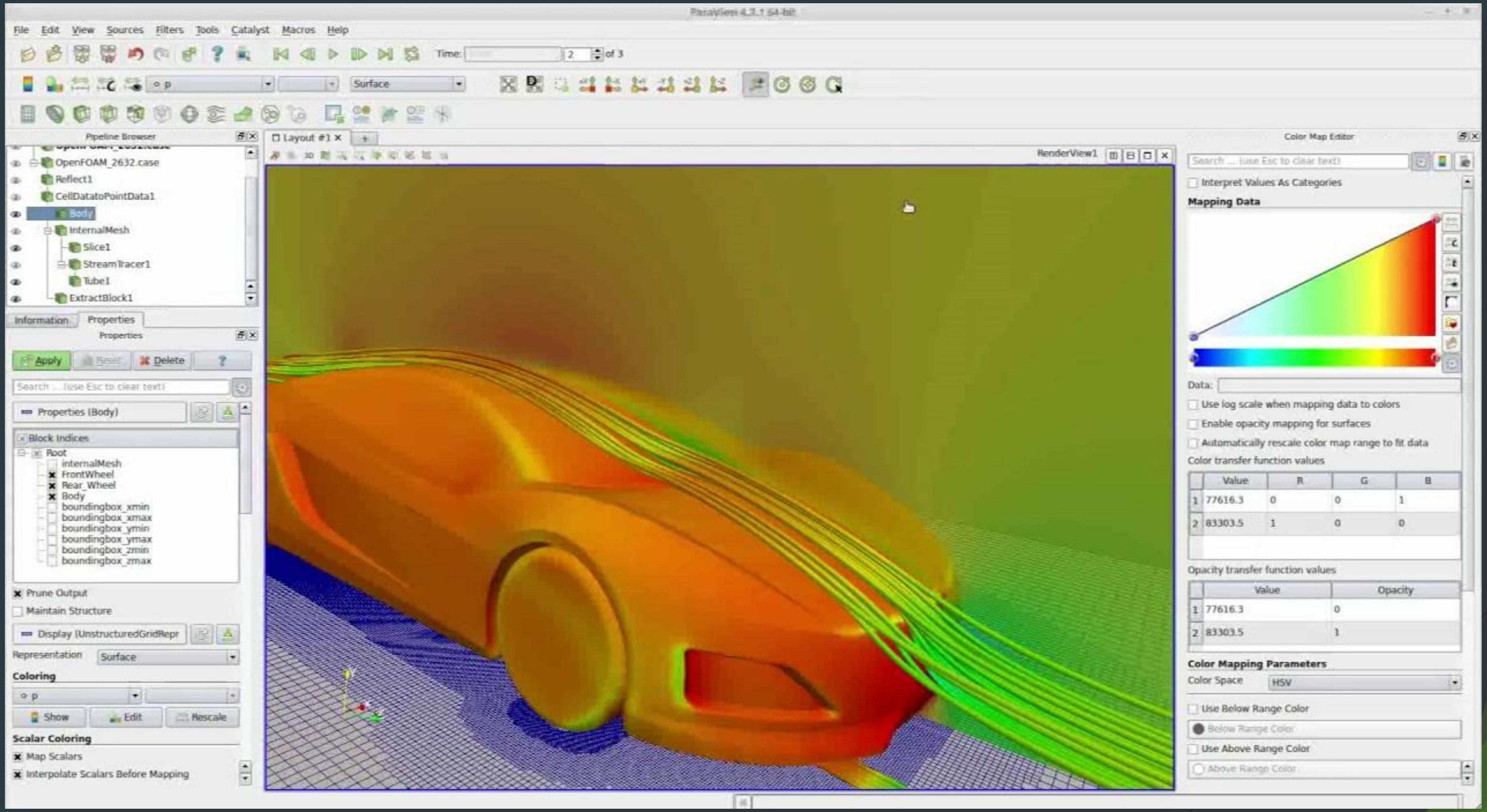
Public domain:

- ParaView
- Visualization toolkit (VTK)
- 3D Slicer
- VolView
- MayaVI, VisIt, DeVIDE, MeVisLab, SCIRun, Gephi, Cytoscape, R, …

Kitware

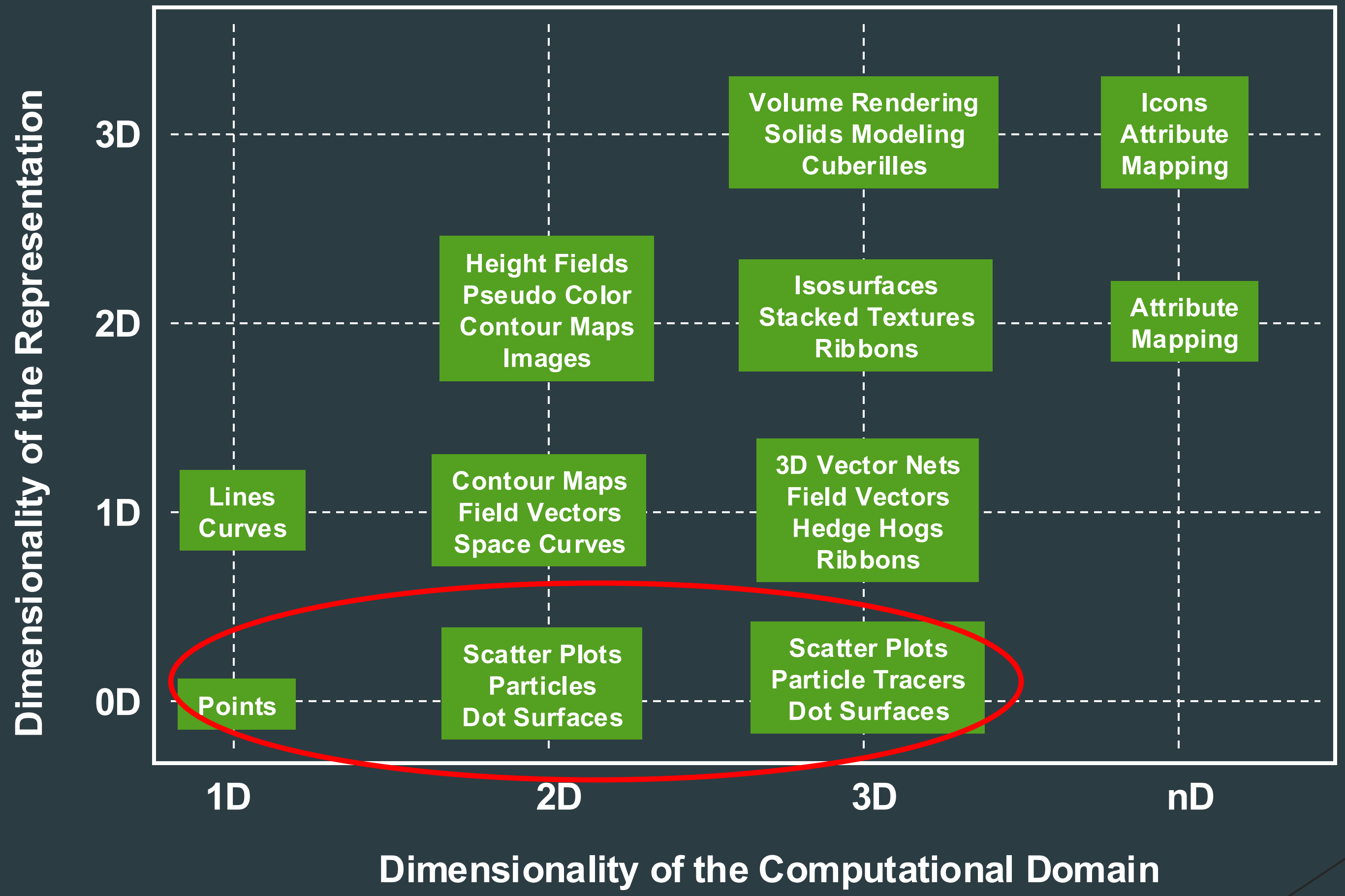
ParaView: install v5.13 before next Wednesday!

Go to https://www.paraview.org/download/



Scientific Visualisation I

Visualization mapping space

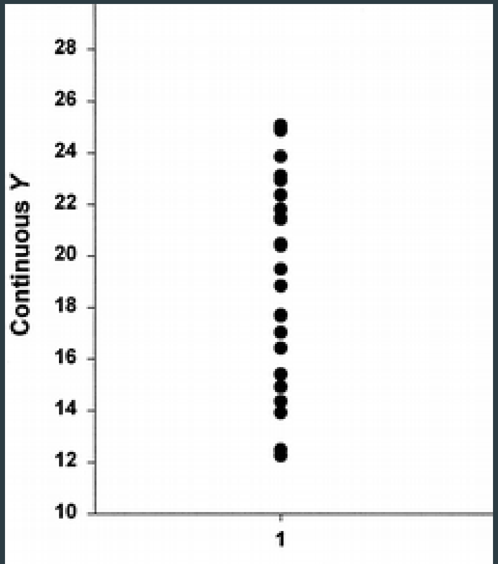


Based on: Craig Upson, *Volumetric Visualization Techniques*, in “State of the Art in Computer Graphics: Visualization and Modeling”, David F. Rogers Rae A. Earnshaw (eds.), Springer-Verlag, 1991, pp. 313-350

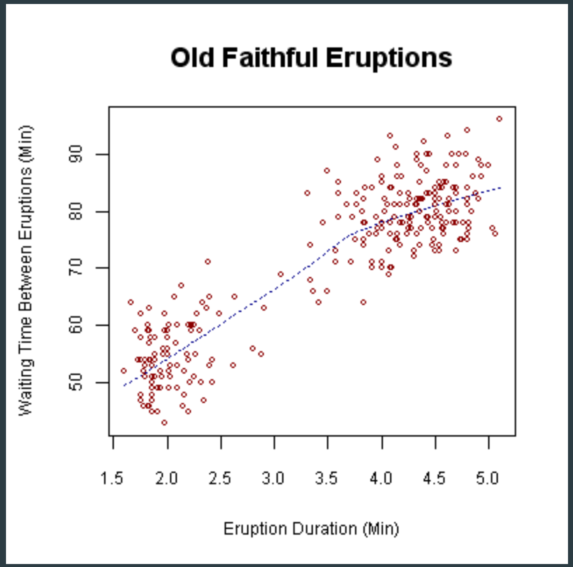
Zero-dimensional primitives

- Dots
- Points
- Markers
- (Tracked) particles

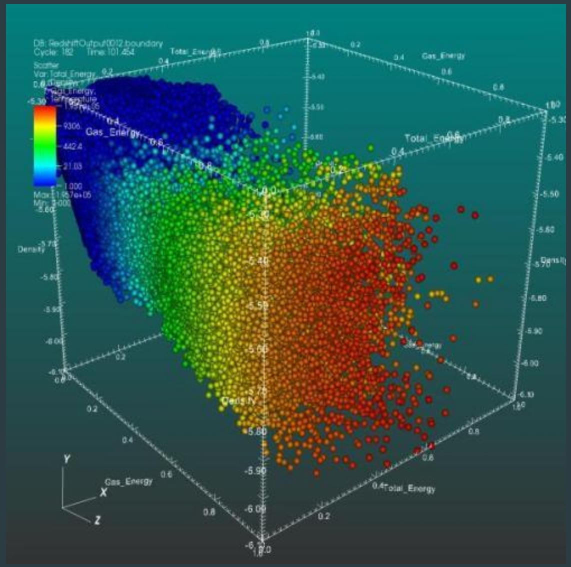
Scatterplot



1D computational domain

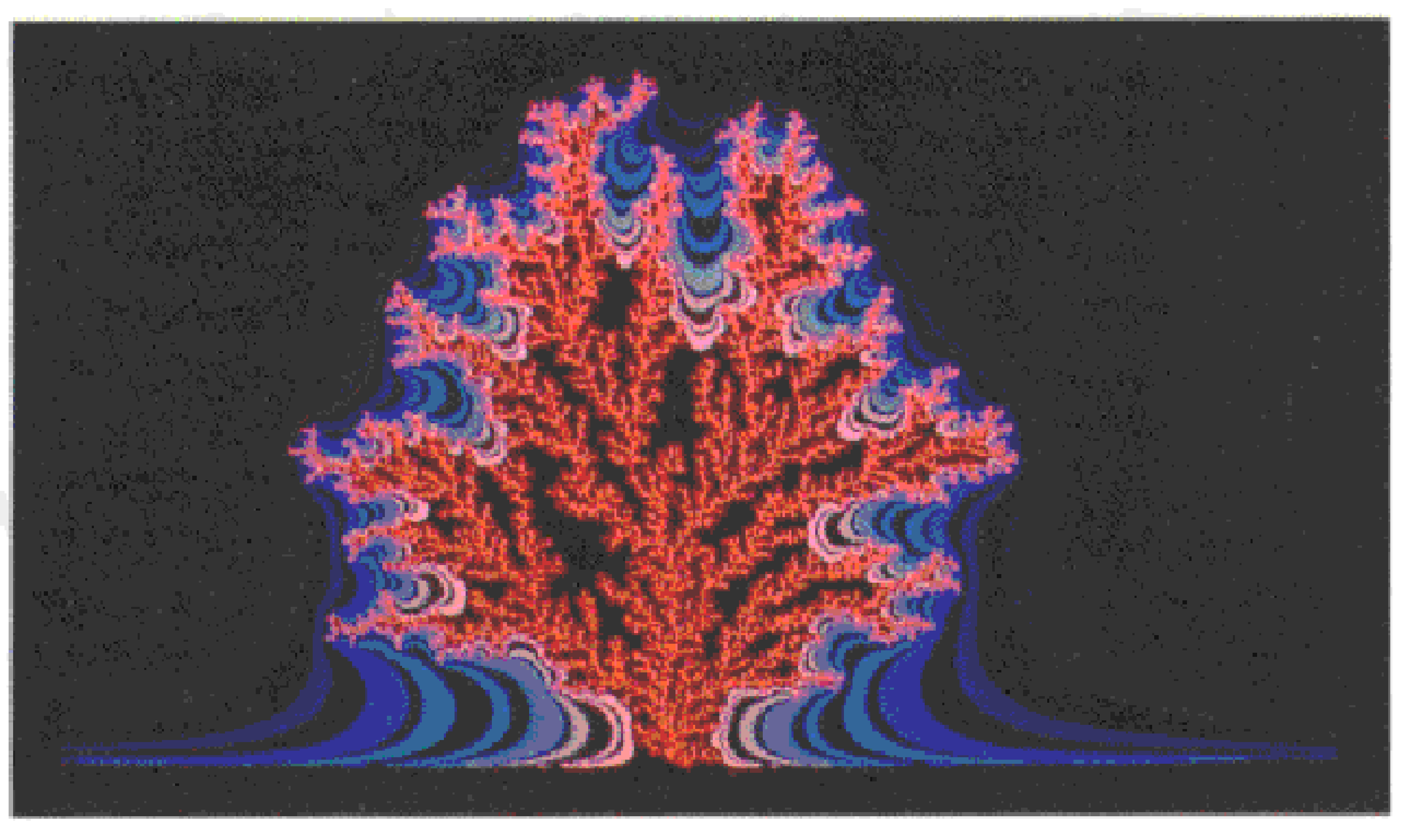


2D computational domain

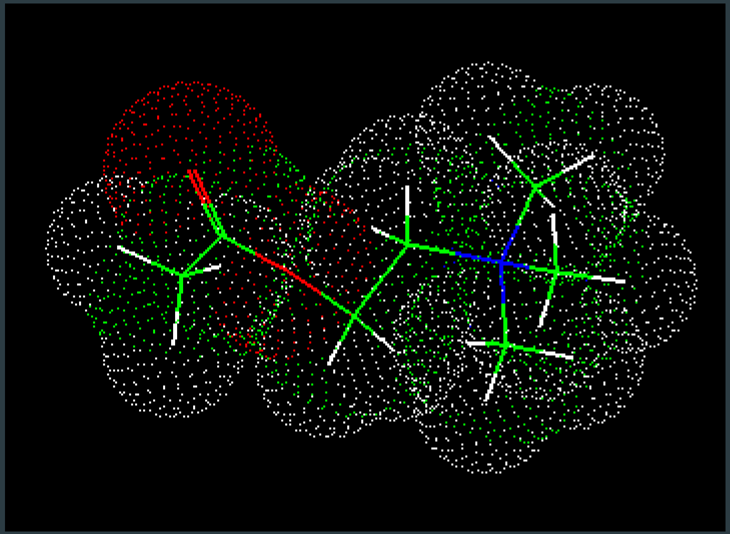


3D computational domain

Dot surface representation of Laplacian growth pattern

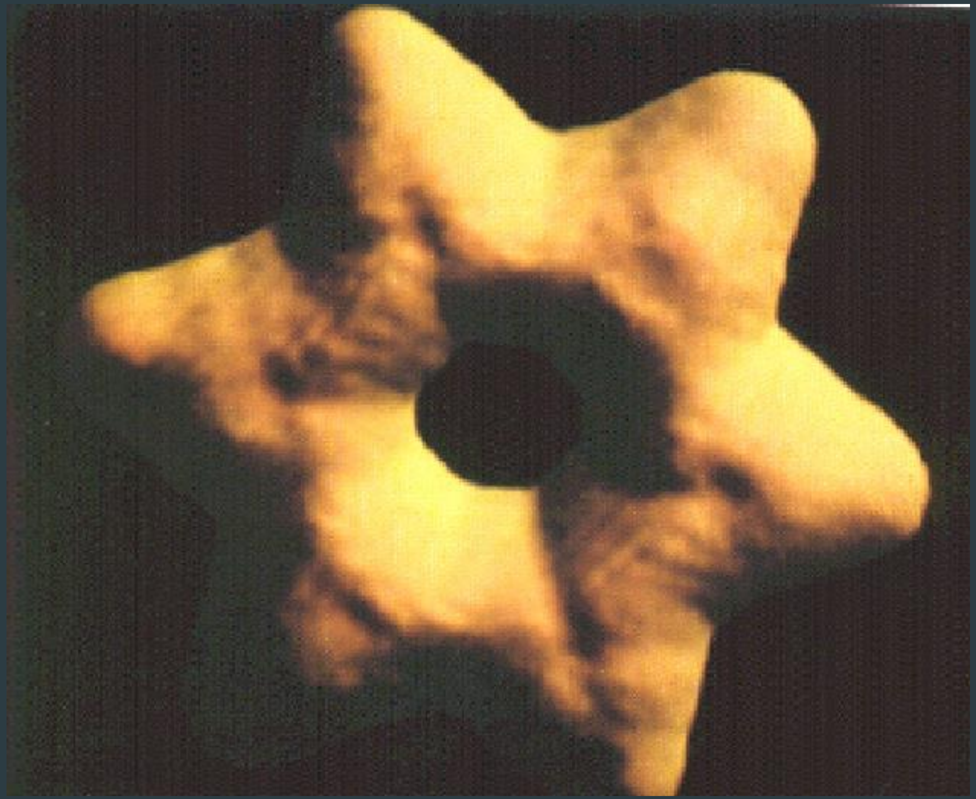


Dot surface representation of a molecule



Physical boundaries of a molecule: Van der Waals surface representation of acetylcholine

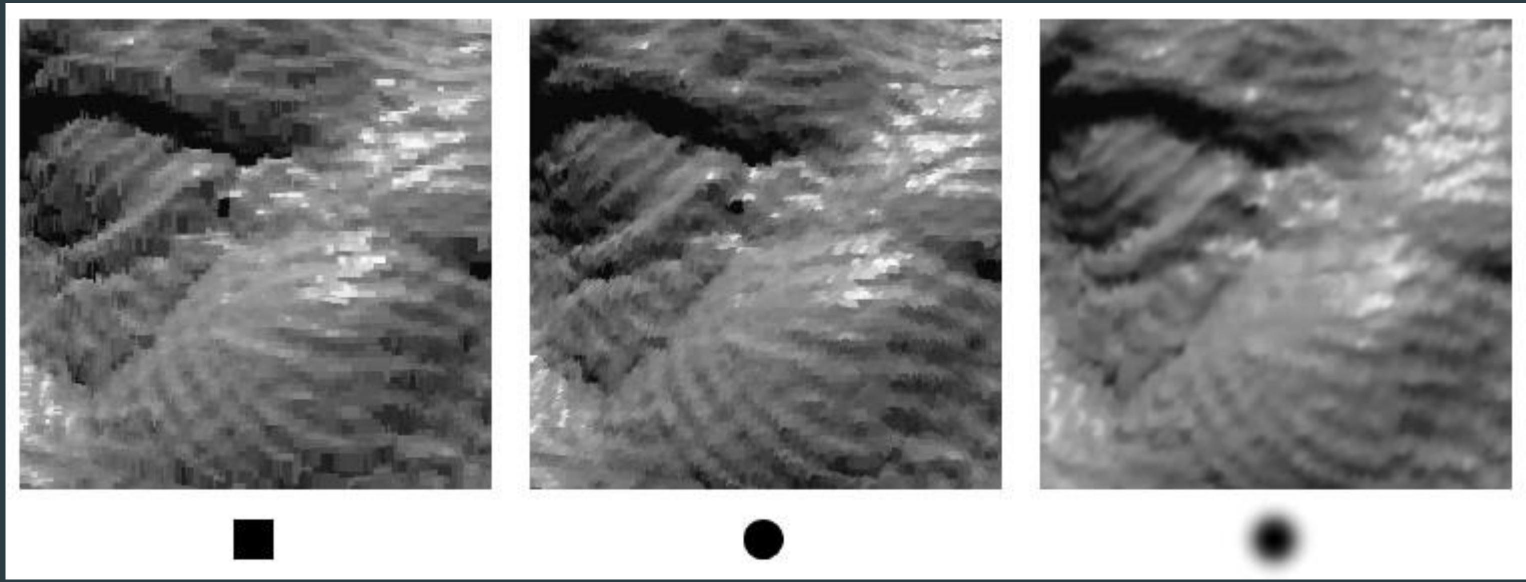
Dot surface representation benzene's electron density function



Craig Upson, *Volumetric Visualization Techniques*, in "State of the Art in Computer Graphics: Visualization and Modeling", David F. Rogers Rae A. Earnshaw (eds.), Springer-Verlag, 1991, pp. 313-350

Point rendering

- Splatting



Szymon Rusinkiewicz, Marc Levoy, QSplat: A Multiresolution Point Rendering System for Large Meshes, SIGGRAPH 2000, pp 343 - 352

Point cloud rendering

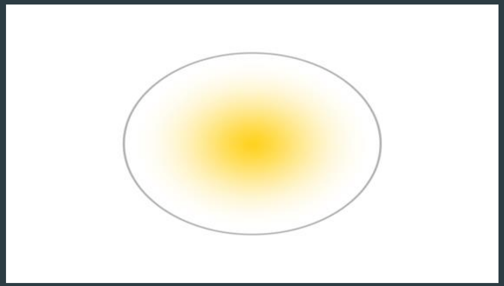
Source: Valentin Kraft, Univ. Bremen (YouTube)

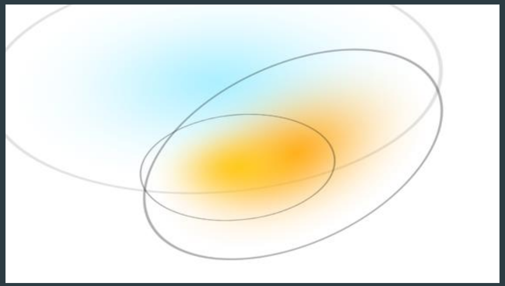
A. Kalaiah and A. Varshney, Statistical Point Geometry, Symposium on Geometry Processing 2003, pp 107 - 115

Gaussian splatting

- “A method using 3D Gaussians for scene representation and optimized rendering allows high-quality, real-time novel-view synthesis at 1080p resolution”

- **Position**: where it's located (XYZ)
- **Covariance**: how it's stretched/scaled (3x3 matrix)
- **Color**: what color it is (RGB)
- **Alpha**: how transparent it is (α)





Source: Kerbl et al. 3D Gaussian Splatting for Real-Time Radiance Field Rendering.

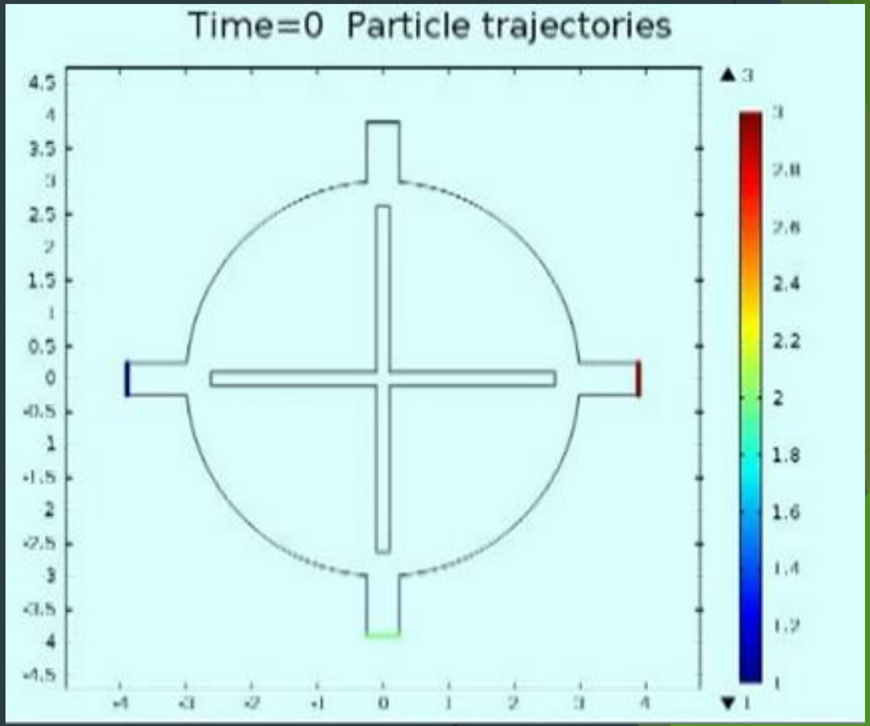
See also: “What is 3D Gaussian splatting?” on YouTube.

Gaussian splat using 7 million gaussians, with opacity

Gaussian splat using 7 million gaussians, without opacity

Particle tracers: advection

- Data domain: unsteady rectilinear grid of vectors
- Associated with each particle:
  - Location (x,y,z)
  - Colour triplet (R,G,B)
  - Transparency
  - Size
  - Lifespan



Y. Yang, Particle tracing in a Micromixer
Source: https://www.youtube.com/watch?v=GPyHT-r0XpI

Particle advection

- Solve equation of motion:

  $V = dP/dt$

  where:

  V is the vector velocity (u, v, w)
  P is the particle location (x, y, z)

- Euler approximation:

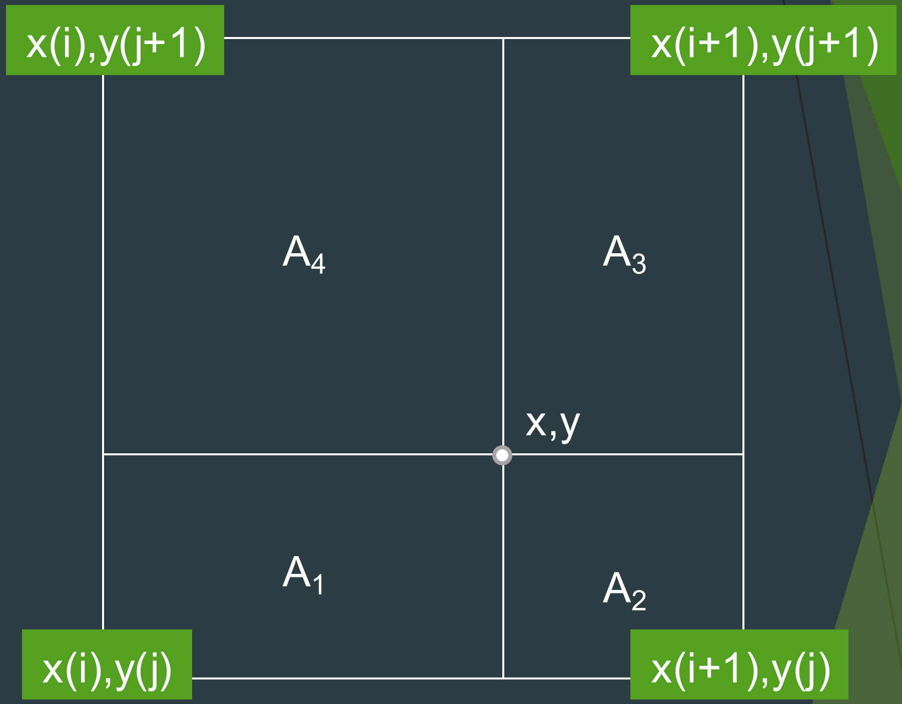
$$x(t + dt) = x(t) + u(x(t), y(t), z(t))\ dt$$
$$y(t + dt) = y(t) + v(x(t), y(t), z(t))\ dt$$
$$z(t + dt) = z(t) + w(x(t), y(t), z(t))\ dt$$

Interpolation in a cell

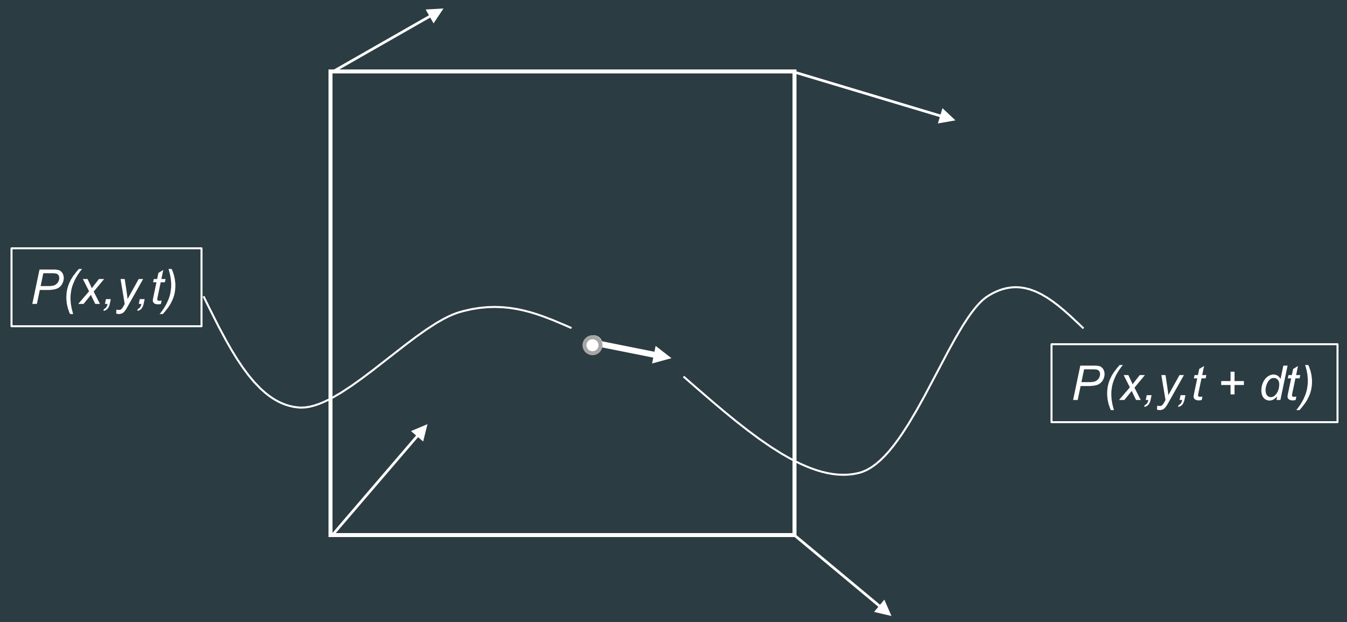
$A_1 = (x - x(i))\ (y - y(j))$
$A_2 = (x(i+1) - x)\ (y - y(j))$
$A_3 = (x(i+1) - x)\ (y(j+1) - y)$
$A_4 = (x - x(i))\ (y(j+1) - y)$

Interpolated velocity:

$$\begin{aligned} u(x,y) = \ & A_1\, u(x(i+1),y(j+1)) + \\ & A_2\, u(x(i),y(j+1)) + \\ & A_3\, u(x(i),y(j)) + \\ & A_4\, u(x(i+1),y(j)) \end{aligned}$$



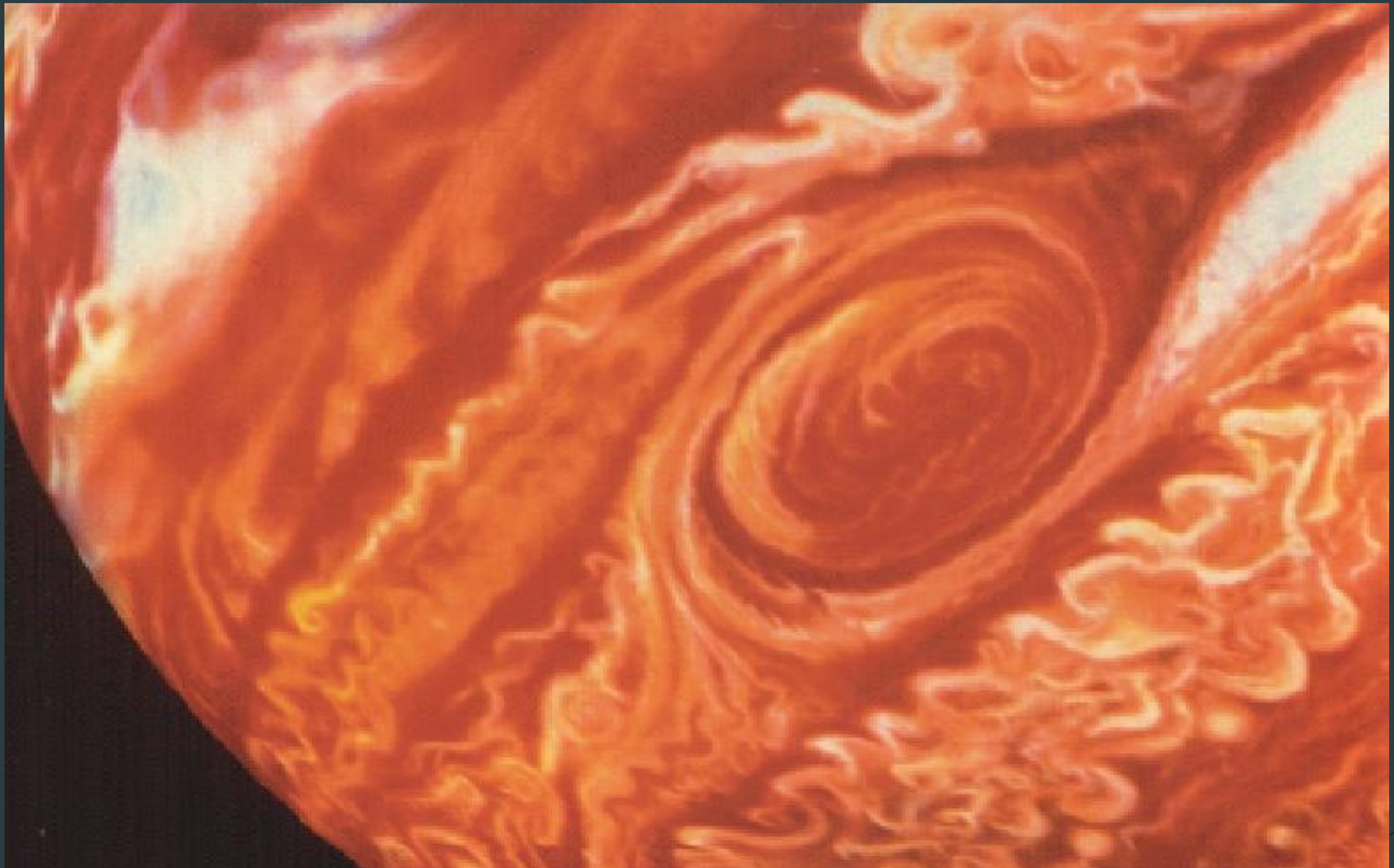
Particle motion



Large scale structure in a turbulent shear layer

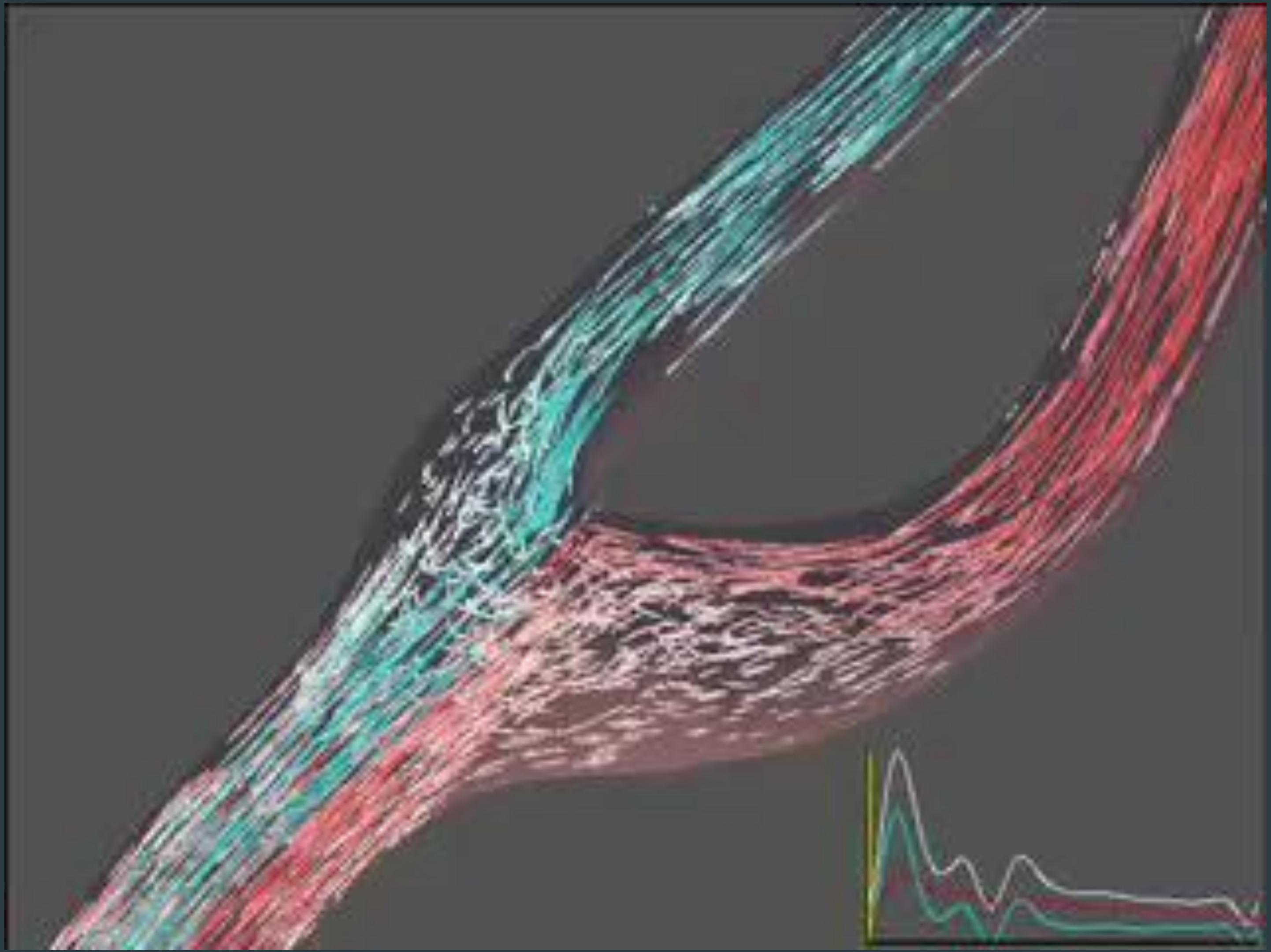
Craig Upson, *Volumetric Visualization Techniques*, in “State of the Art in Computer Graphics: Visualization and Modeling”, David F. Rogers Rae A. Earnshaw (eds.), Springer-Verlag, 1991, pp. 313-250

Flow visualization of Jupiter



Craig Upson, *Volumetric Visualization Techniques*, in “State of the Art in Computer Graphics: Visualization and Modeling”, David F. Rogers
Rae A. Earnshaw (eds.), Springer-Verlag, 1991, pp. 313-250

Particle animation

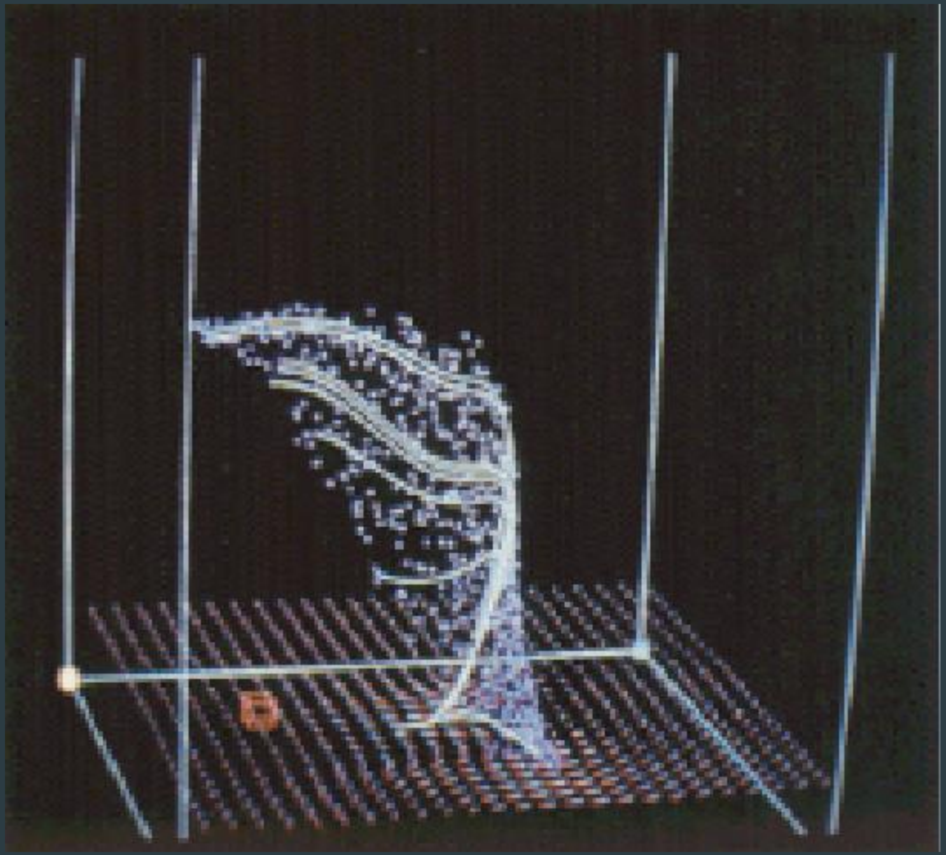


Steinman DA. Simulated pathline visualization of computed periodic blood flow patterns. J Biomech. 2000 May;33(5):623-8. doi: 10.1016/s0021-9290(99)00205-5. PMID: 10708784.

Particle animation

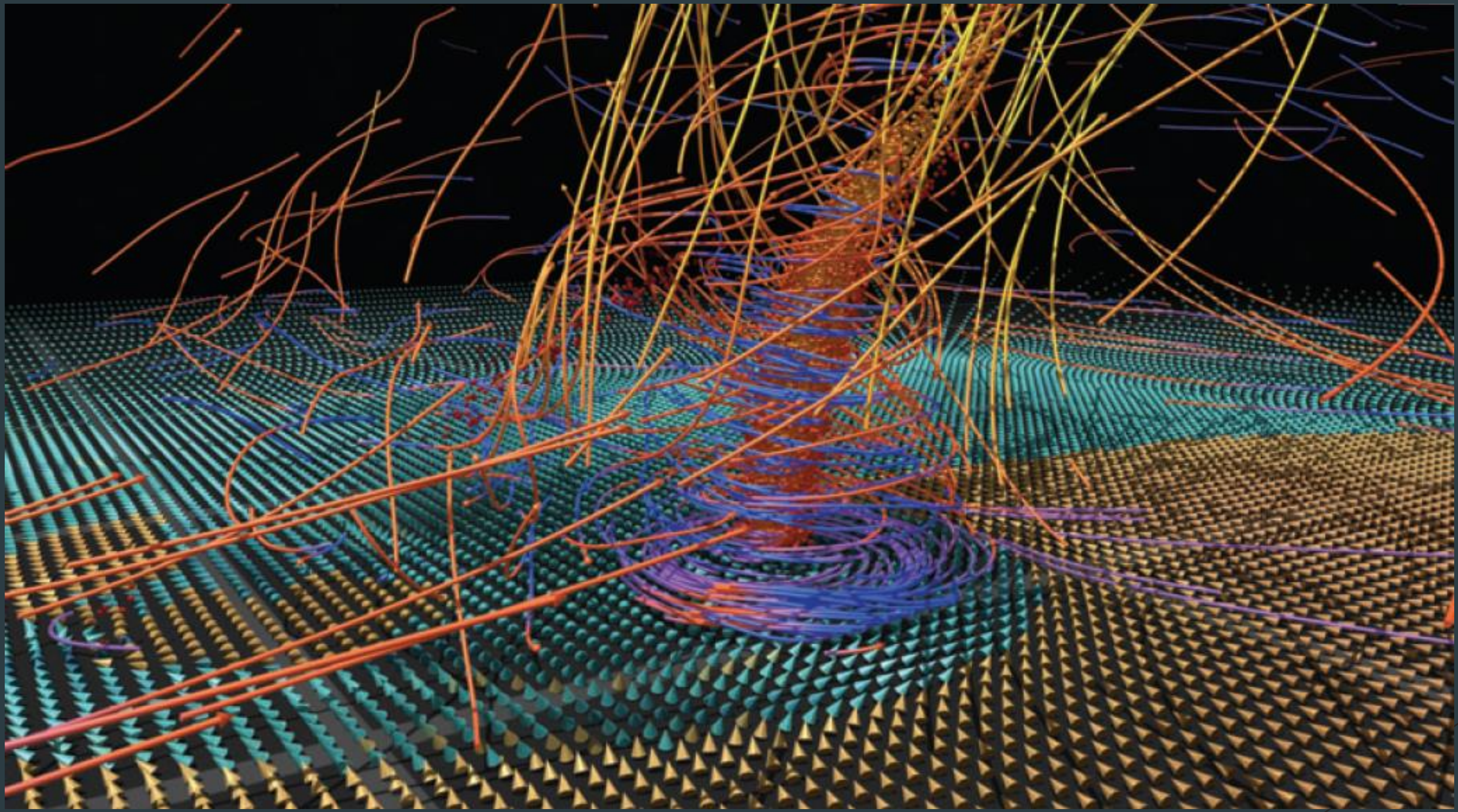
Source: Computational Visualization of 4D Cardiac Flow (YouTube, 2010)

Particle traces from a numerical simulation of a thunderstorm



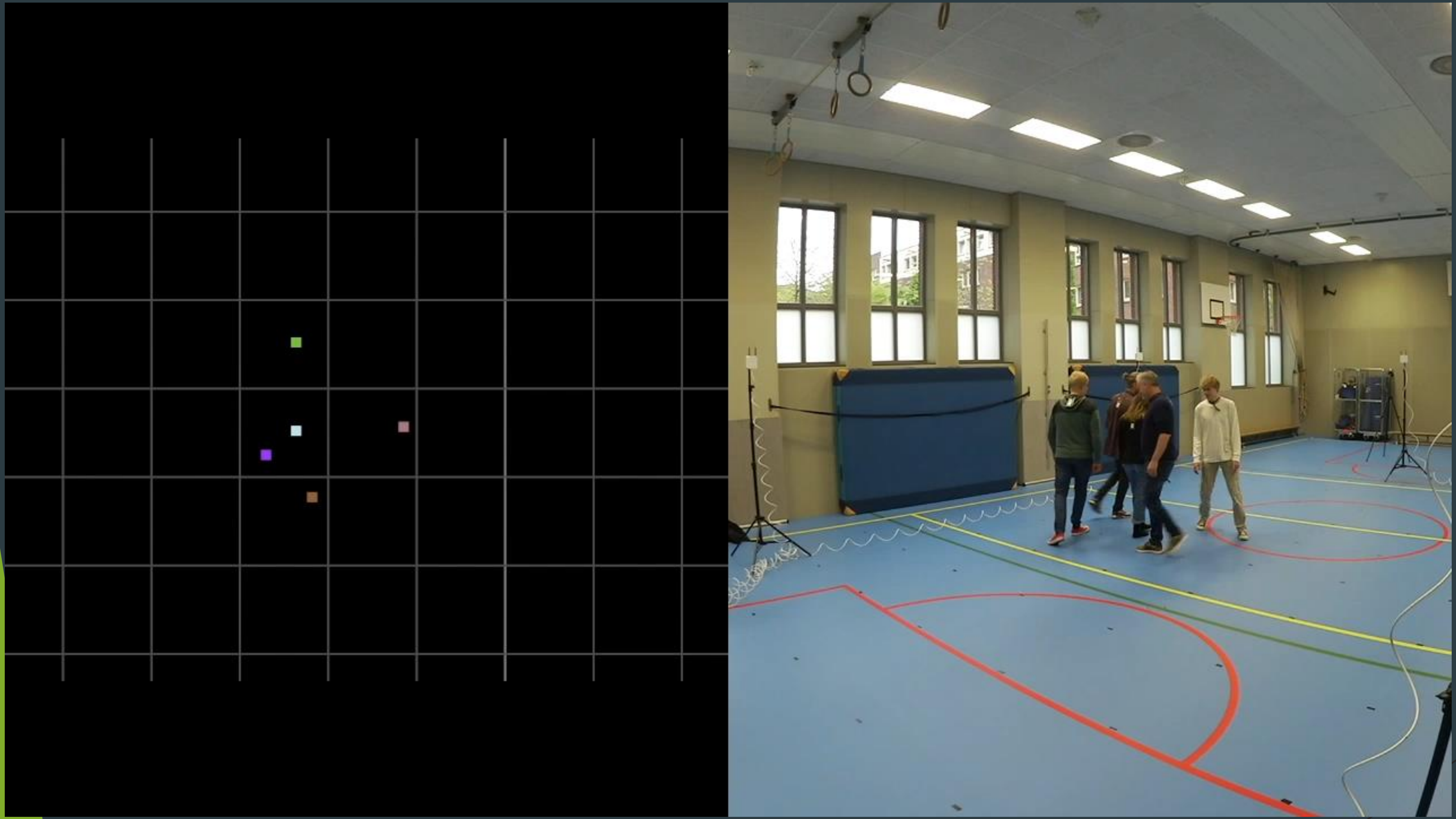
Craig Upson, *Volumetric Visualization Techniques*, in “State of the Art in Computer Graphics: Visualization and Modeling”, David F. Rogers Rae A. Earnshaw (eds.), Springer-Verlag, 1991, pp. 313-250

NCSA Visualization of an F3 Tornado



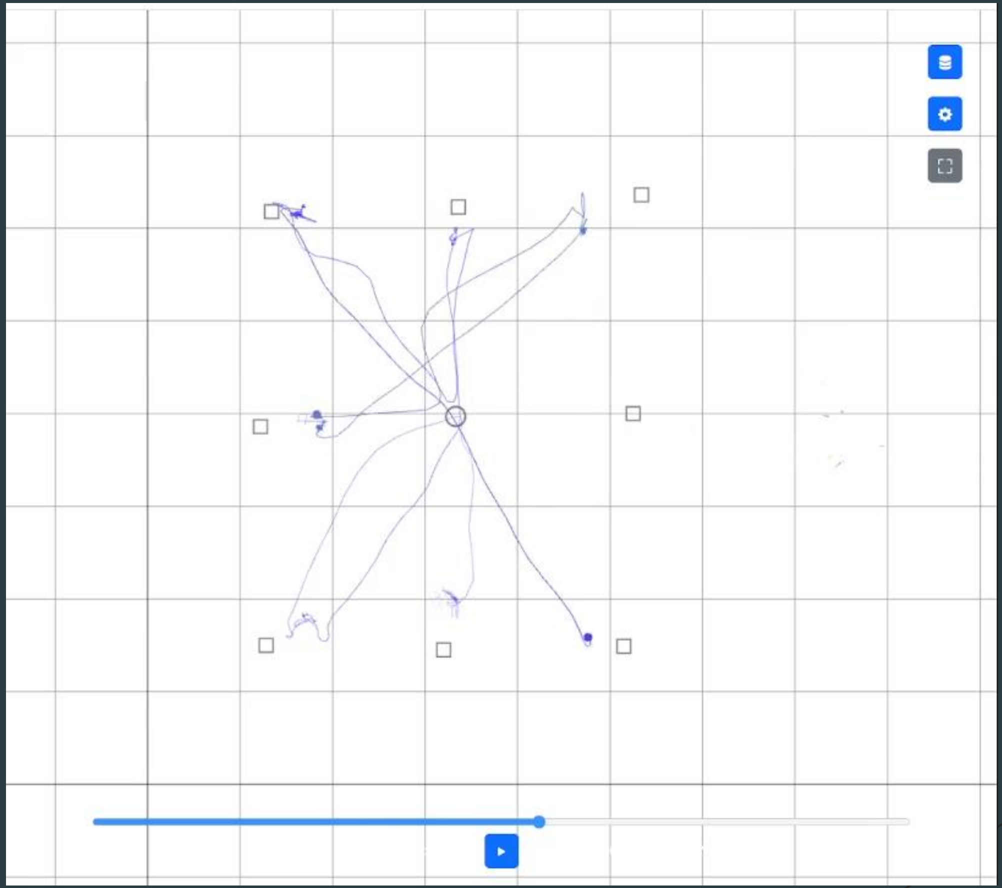
YouTube link. Source: Advanced Visualization Lab, National Center for Supercomputing, University of Illinois

POLDER/NEMO experiment
October 15-28, 2022

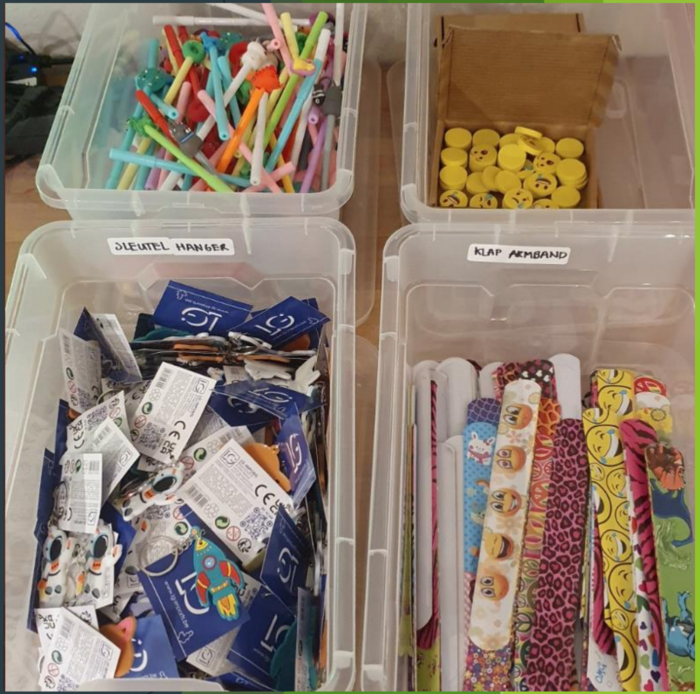


POLDER/NEMO experiment
October 15-28, 2022

Setup at NEMO Science Center



Visualisation by Mark Wijzenbroek, Computational Science Lab, UvA



Choice of presents for participants