Scientific Visualization: Grids

CS 6630, Fall 2015
Aaron Knoll

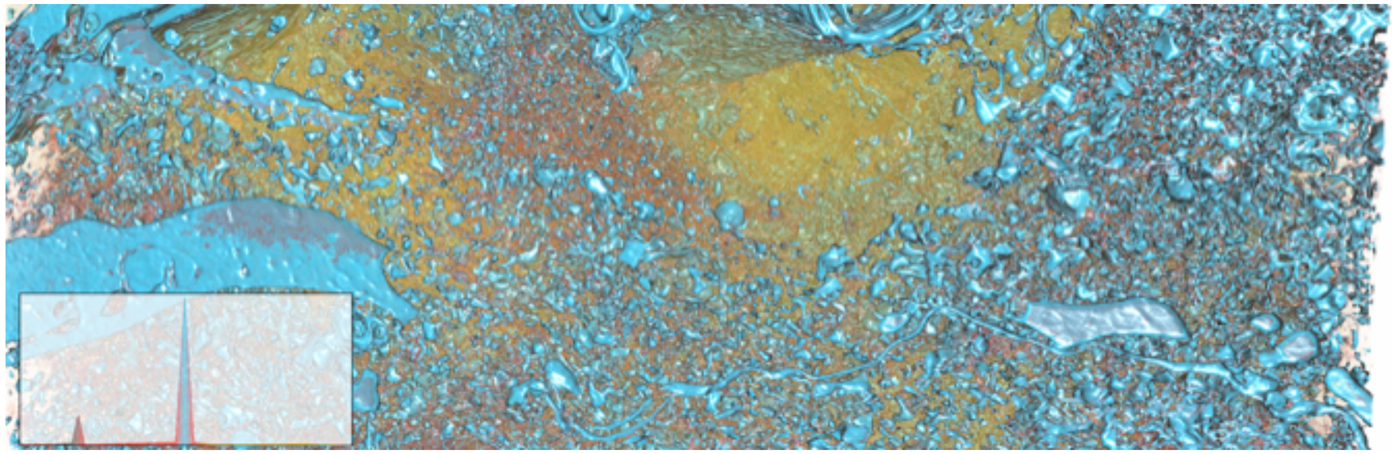
www.sci.utah.edu

Recap from Alex's first lecture: the traditional "branches" of visualization

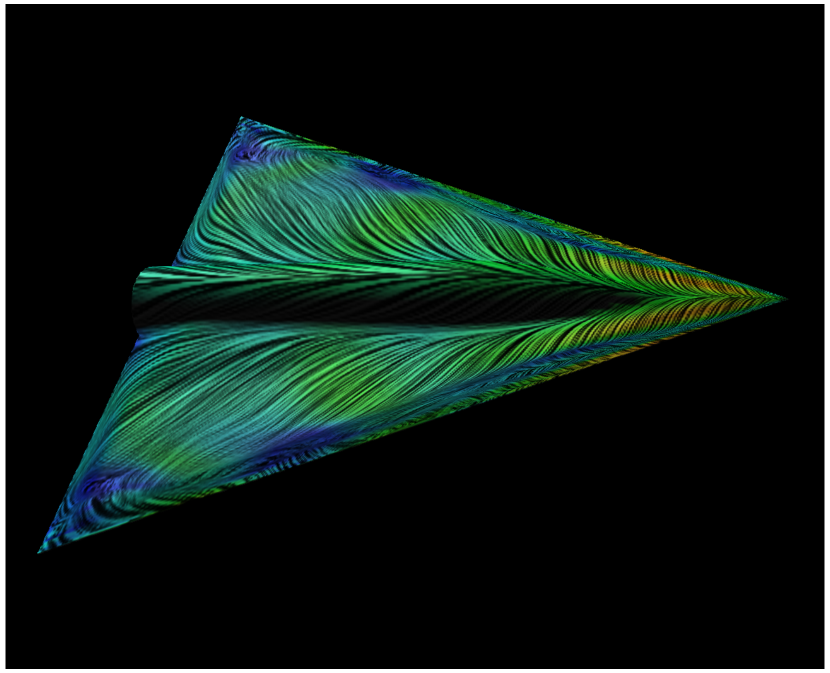
- Scientific Visualization
- Information Visualization
- Visual Analytics

Scientific visualization

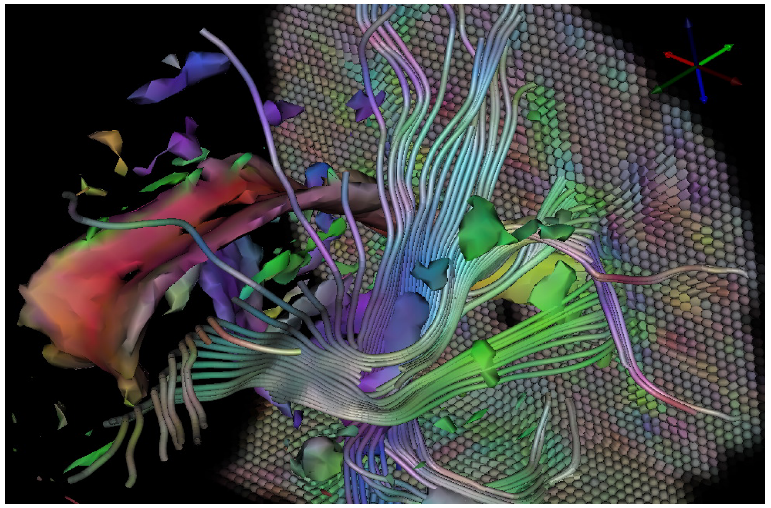
- Data have spatial context (usually from simulation or scan)
- Map spatial quantities to colors or geometry, *f(space, time) -> rgba*
- **2D or 3D graphics for visualization.**



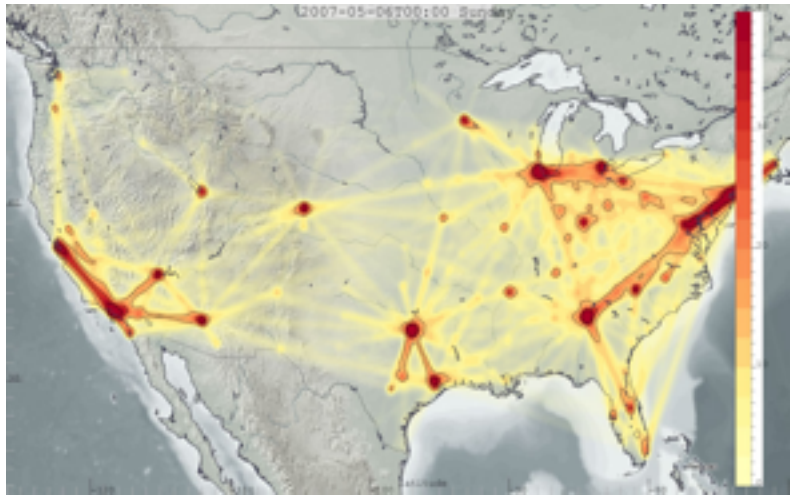
Volume rendering



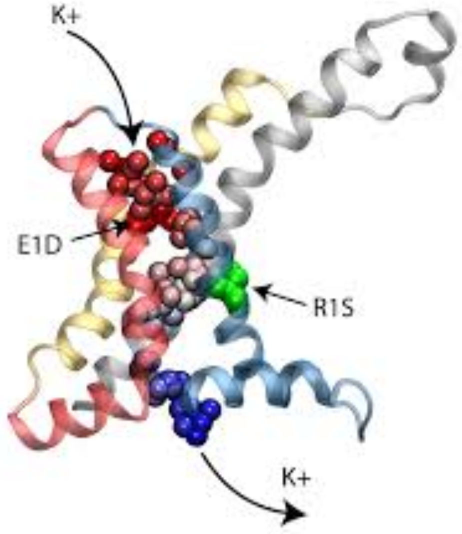
Flow visualization



Tensor field visualization



Map and GIS visualization



Molecular visualization

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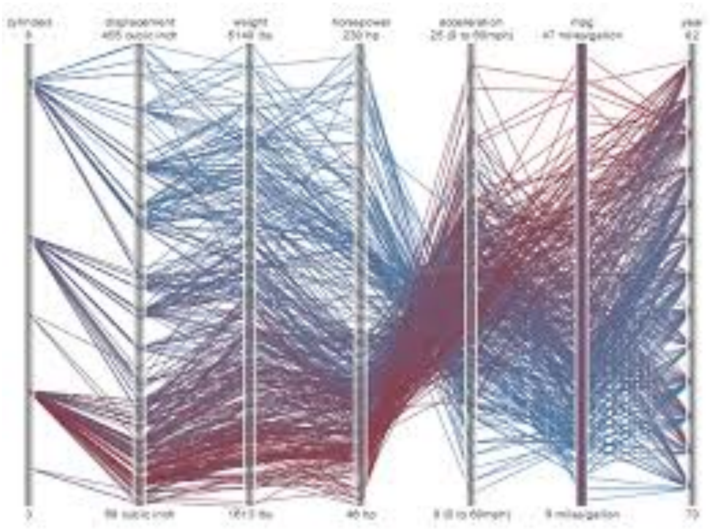
Information visualization

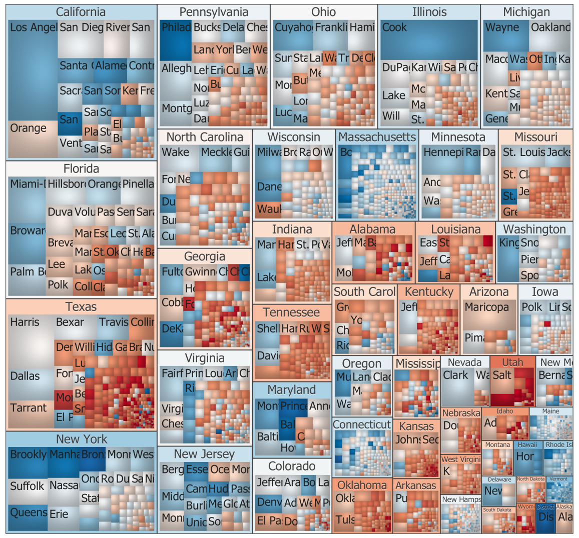
- Spatial position is secondary or non-existent.

- Illustrate relationships between abstract attributes.

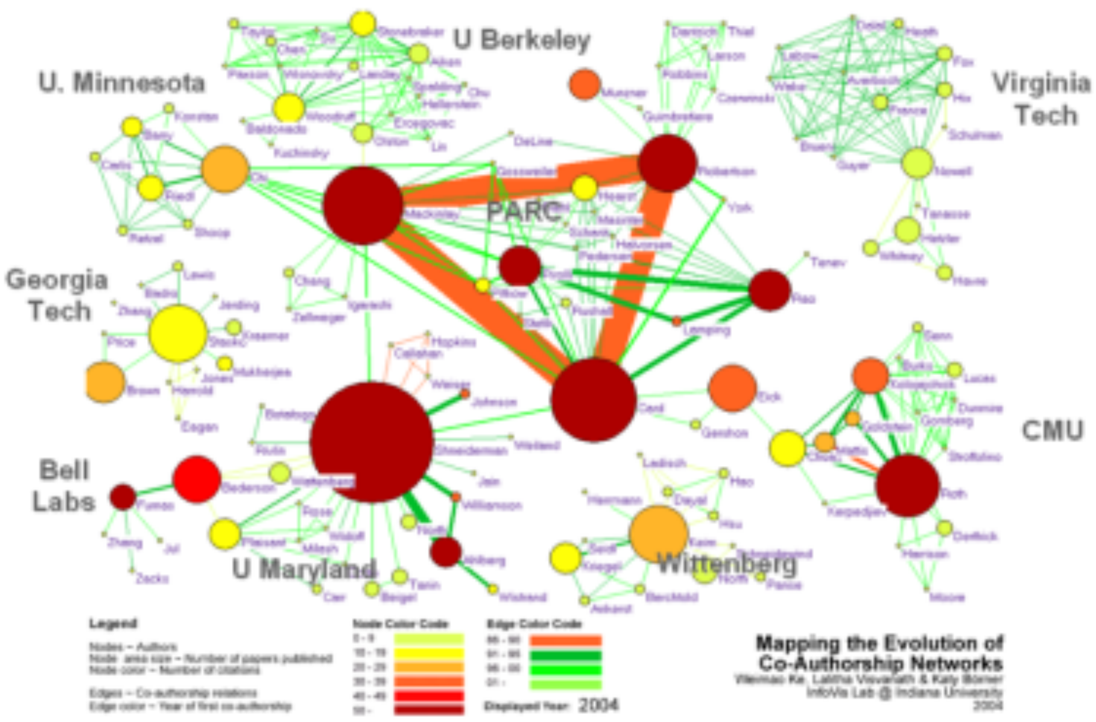
- **Plots, charts, graphs, diagrams.**



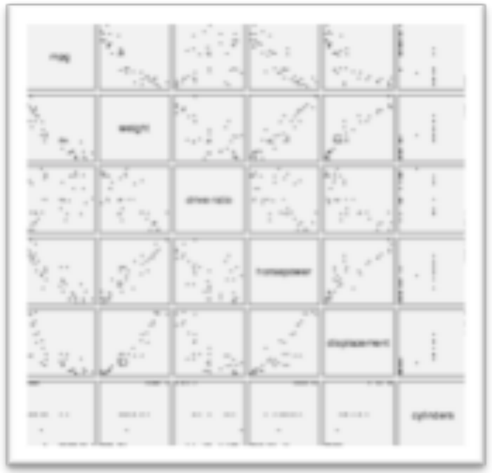
Parallel coordinates



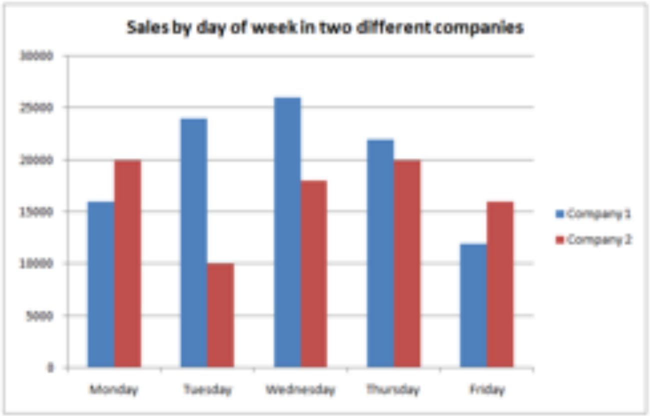
Treemaps



Graph and network visualization



Scatterplots



Charts

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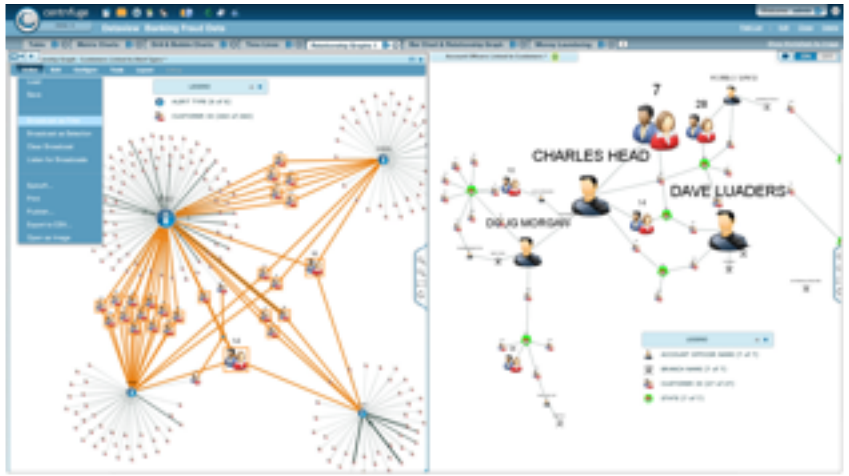
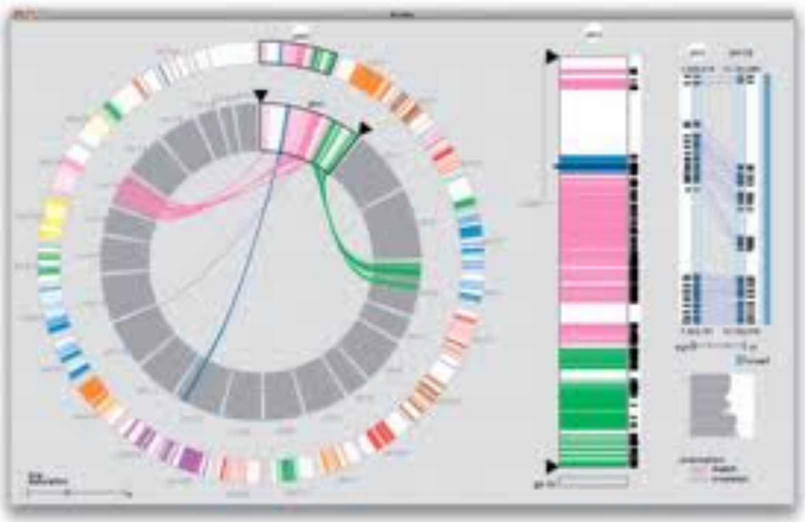
Visual Analytics

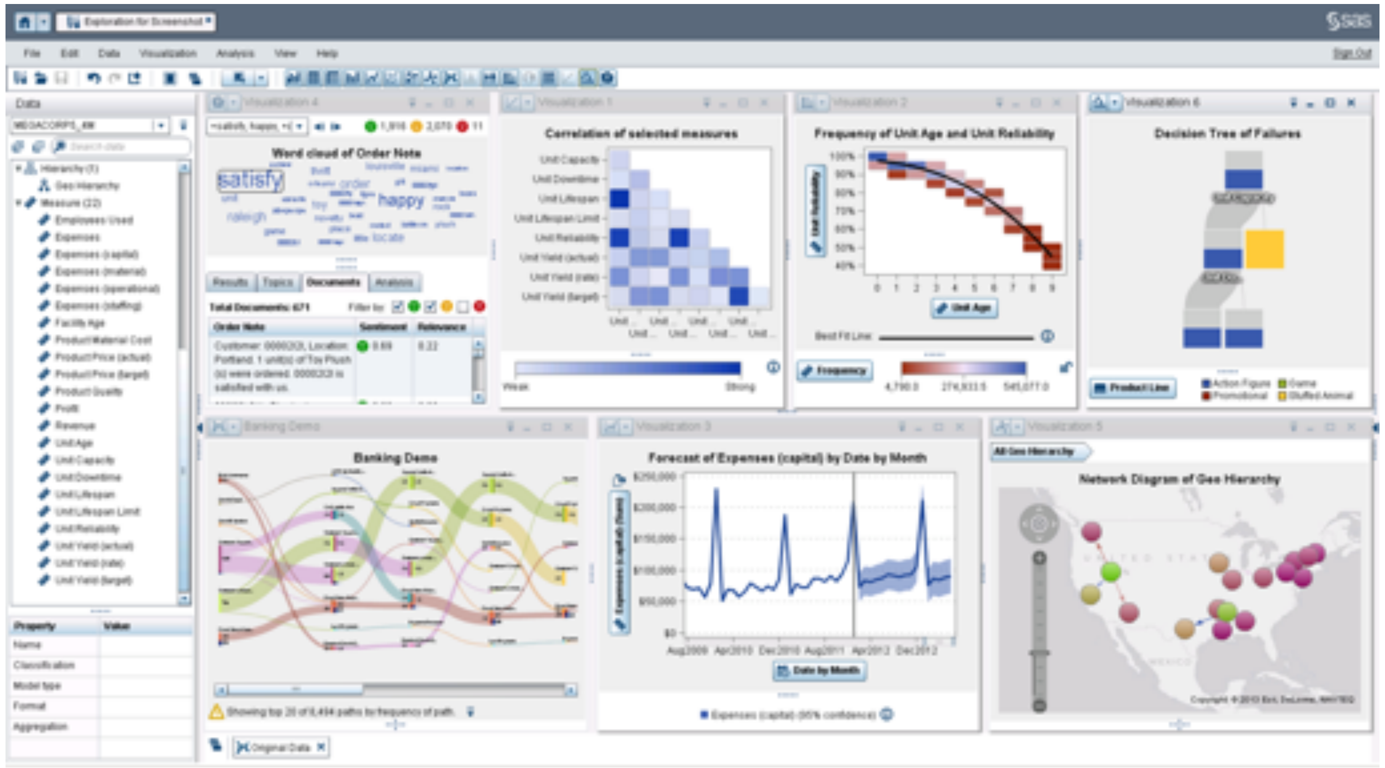
- More about **interactive user interfaces** for data analysis.
- Uses techniques from both scientific visualization and information visualization, as well as statistics, perception, cognition.
- D3+Javascript, R, Matlab
- “Putting it all together”



Security visualization (Centrifuge)



Genomics (Meyer et al. “Mizbee”)


sas
Word cloud of Order Note
Correlation of selected measures
Frequency of Unit Age and Unit Reliability
Decision Tree of Failures
Banking Demo
Forecast of Expenses (capital) by Date by Month
Network Diagram of Geo Hierarchy

Management Information Systems (SAS)

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Scientific Visualization

- **Sci-vis is about interpreting and rendering spatial data.**
- Today:
  - where do spatial data come from?
  - what do they look like?
  - what can we do with them?
  - *HW6 - your very own volume renderer, in a web browser!*
- Thurs, Oct 22: Volumes
  Tues, Nov 10: Isosurfaces
  Thurs, Nov 12: Vector and Tensor Fields

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Scientific Visualization

- Data sources
- Data representation
  - fields
  - grids
- Data interpretation
  - The scientific visualization pipeline
  - Interpolation

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Data sources

Computational Data

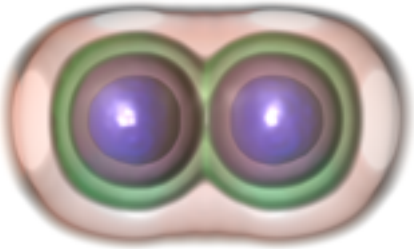
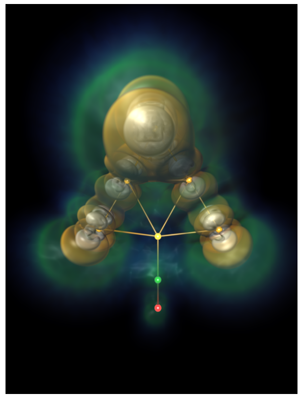
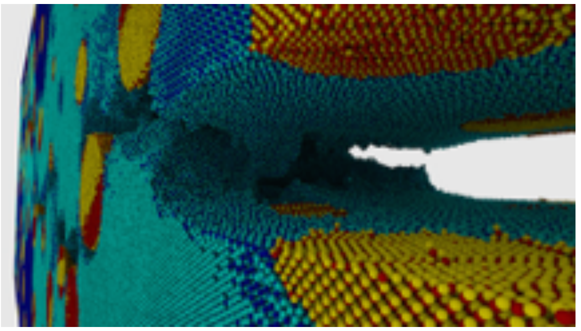
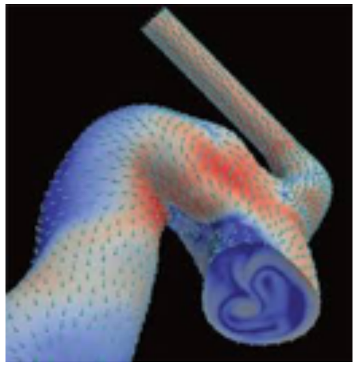
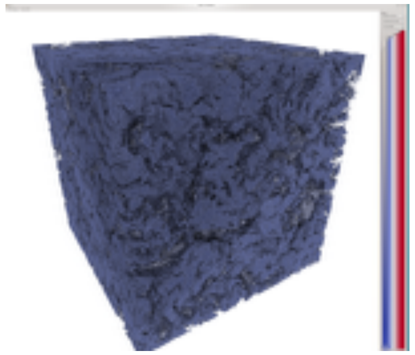
The output of scientific computing:
physics, chemistry, blood flow,
neurophysiology, meteorology,
climatology, astronomy…

- Nuclear physics
- Quantum chemistry
- Molecular dynamics
- Computational fluid dynamics
- Rigid-body and structural mechanics
- Coarse-grained dynamics, agents simulations
- Meteorology
- Astrophysics
- Cosmology

kilobytes

↓

petabytes

Scanned data

The output of instruments in medical imaging, microscopy, telescopy, GIS

- X-ray crystallography
- Synchrotron / radiation light sources
- Transmission electron microscopy
- Confocal microscopy
- Camera imagery
- Ultrasound
- Magnetic resonance imaging
- X-ray tomography
- Satellite
- Telescope

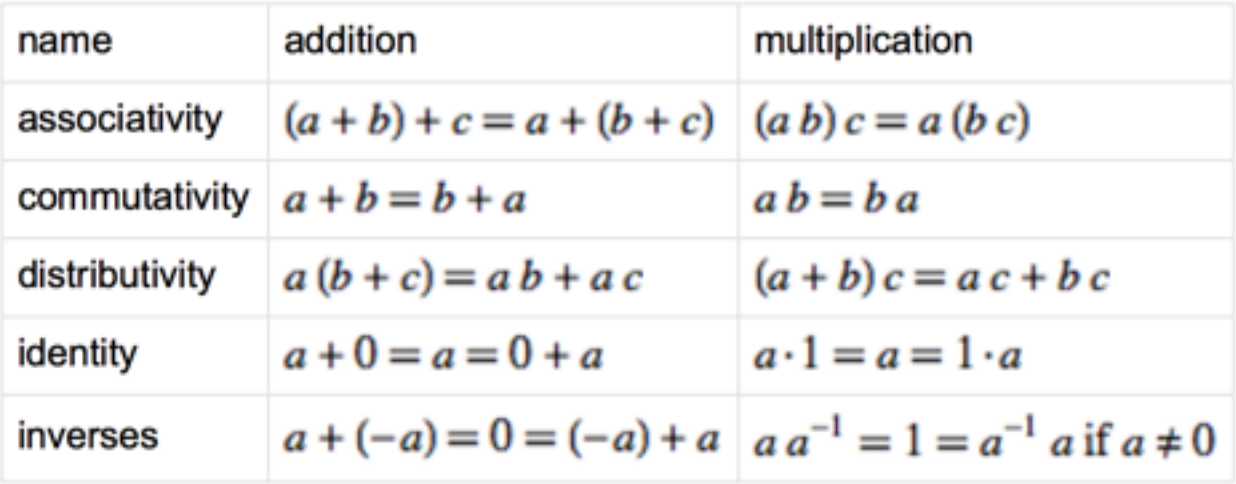
Angstroms

Megaparsecs

Data representation

Fields

- Mathematically, a *field* is a set of elements with addition, multiplication operators that satisfy the field axioms



name	addition	multiplication
associativity	$(a+b)+c=a+(b+c)$	$(a\,b)\,c=a\,(b\,c)$
commutativity	$a+b=b+a$	$a\,b=b\,a$
distributivity	$a\,(b+c)=a\,b+a\,c$	$(a+b)\,c=a\,c+b\,c$
identity	$a+0=a=0+a$	$a\cdot 1=a=1\cdot a$
inverses	$a+(-a)=0=(-a)+a$	$a\,a^{-1}=1=a^{-1}\,a$ if $a\neq 0$

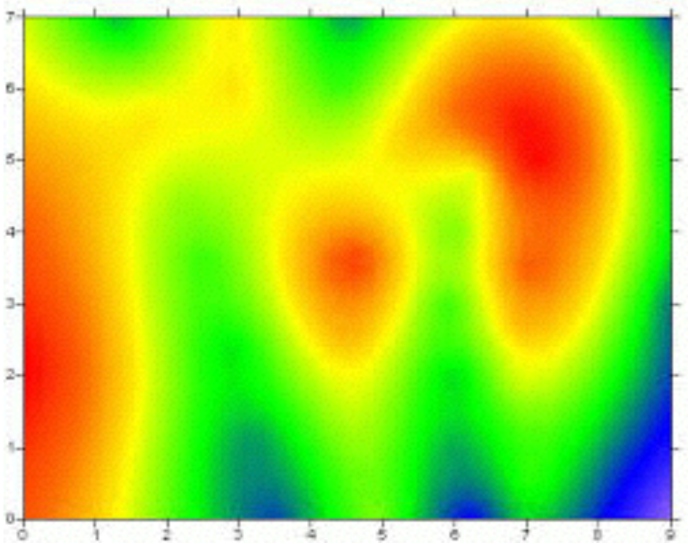
wolfram.com

- Intuitively, a field is a varying quantity defined continuously over space.

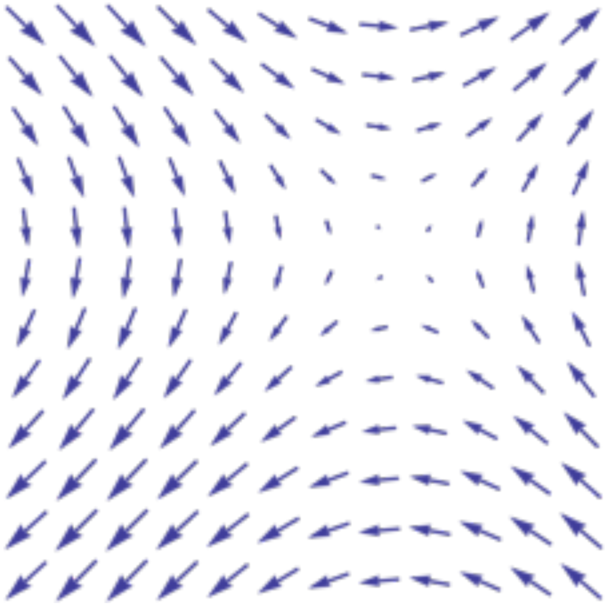
Fields

with a 2D domain

scalar field

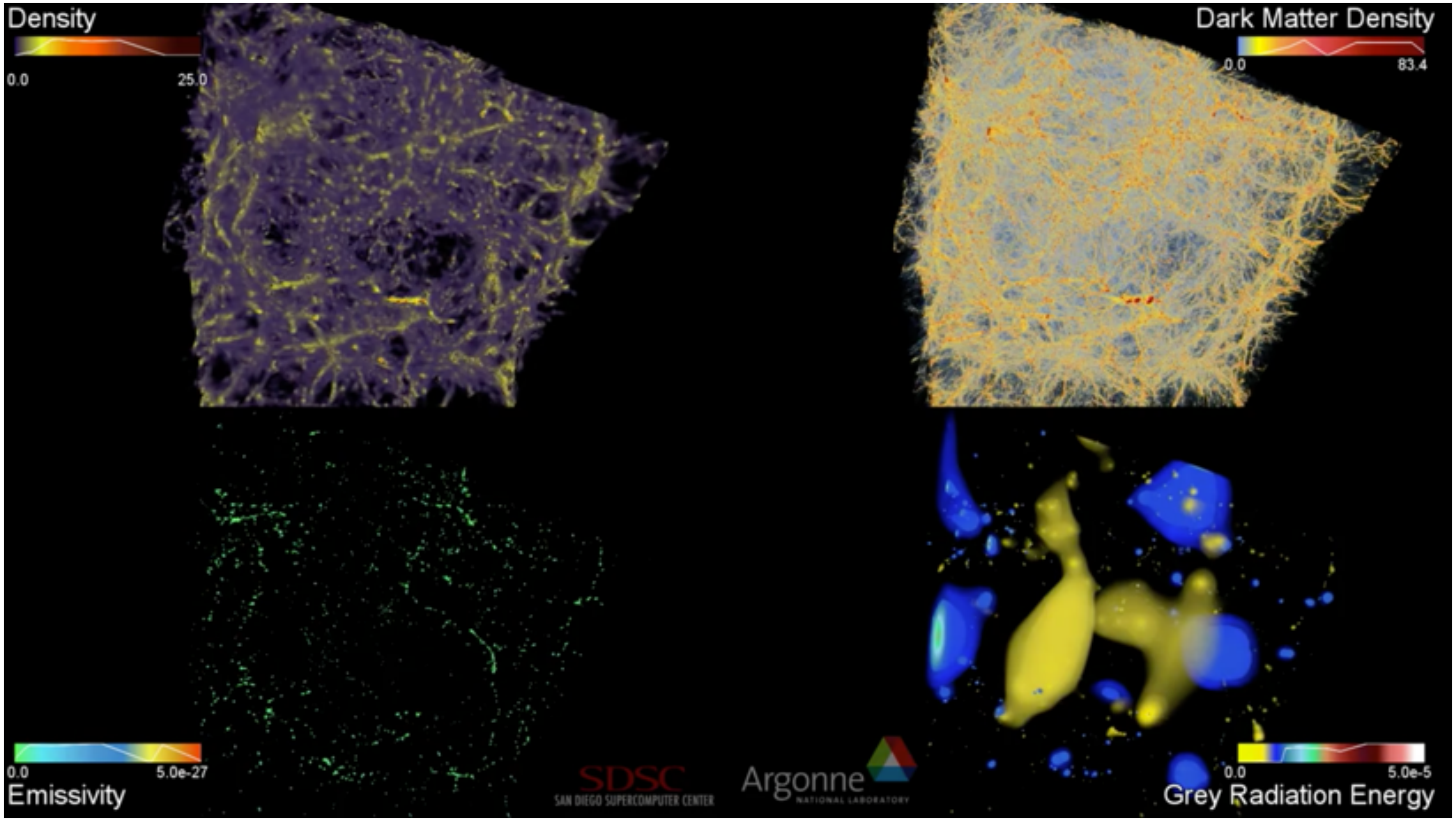


vector field



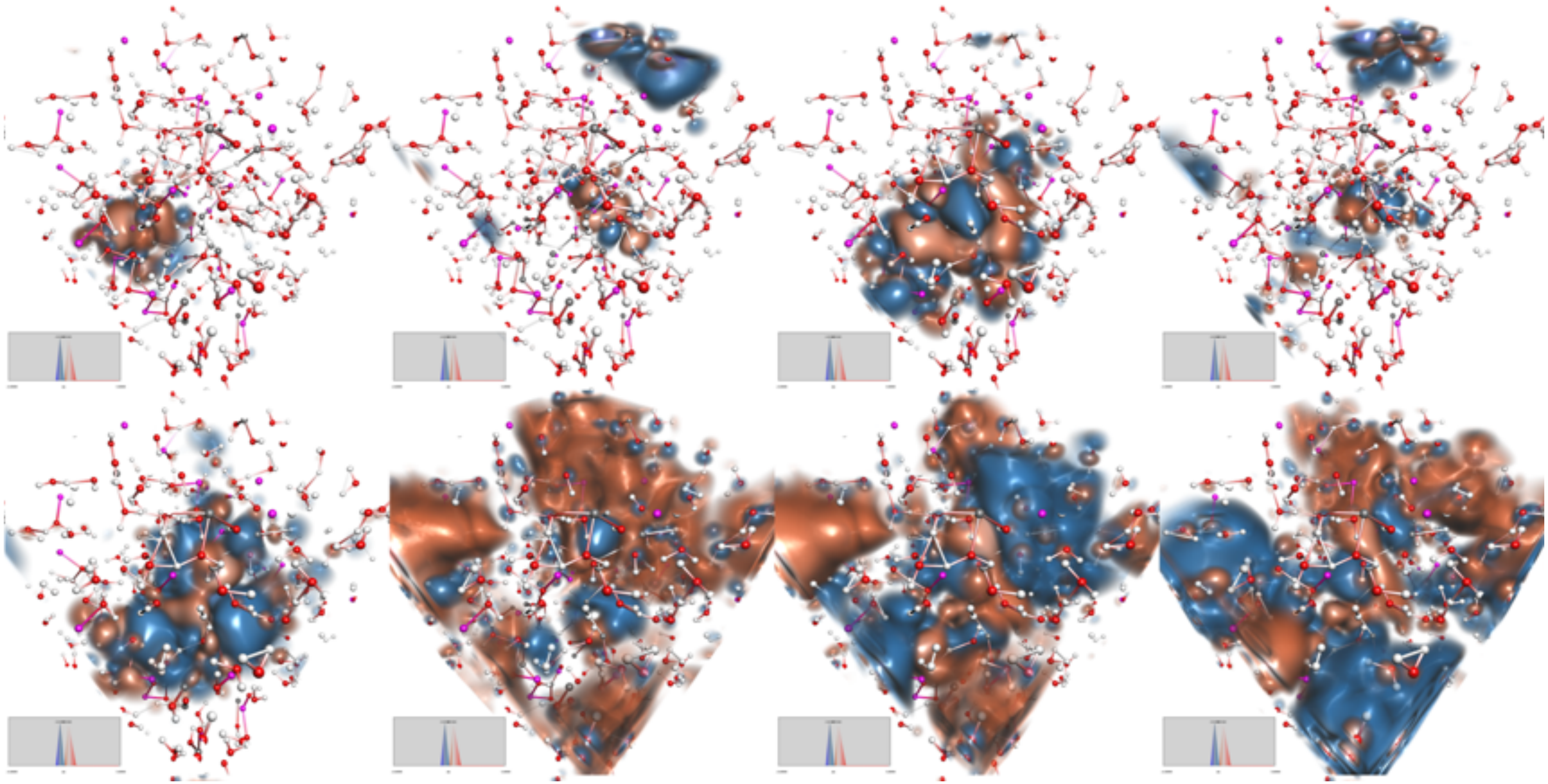
tensor field

Multifields



Radiation hydrodynamics in Enzo: Joe Insley (ANL), Rick Wagner (SDSC)
https://vimeo.com/17771397

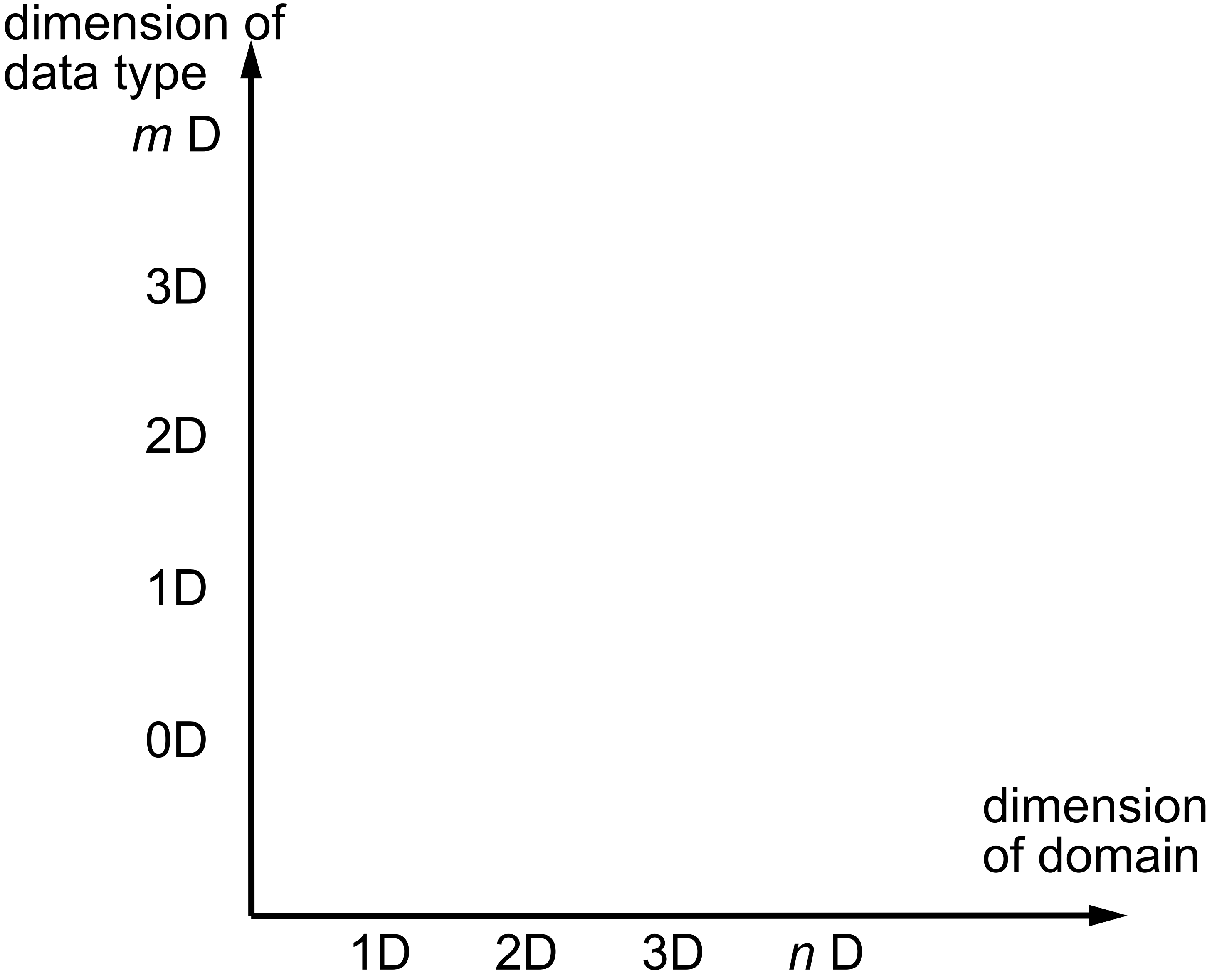
Multifields



8 molecular orbitals of a LiAlH2O DFT simulation, courtesy Aiichiro Nakano, University of Southern California

Types and Classification of Field Data

- dimension of domain (the field)
- dimension of the data to visualize (the geometry)



Examples:

A: gas station along a road
B: map of cholera in London
C: temperature along a rod
D: height field of a continent
E: 2D air flow
F: 3D air flow in the atmosphere
G: stress tensor in a mechanical part
H: ozone concentration in the atmosphere

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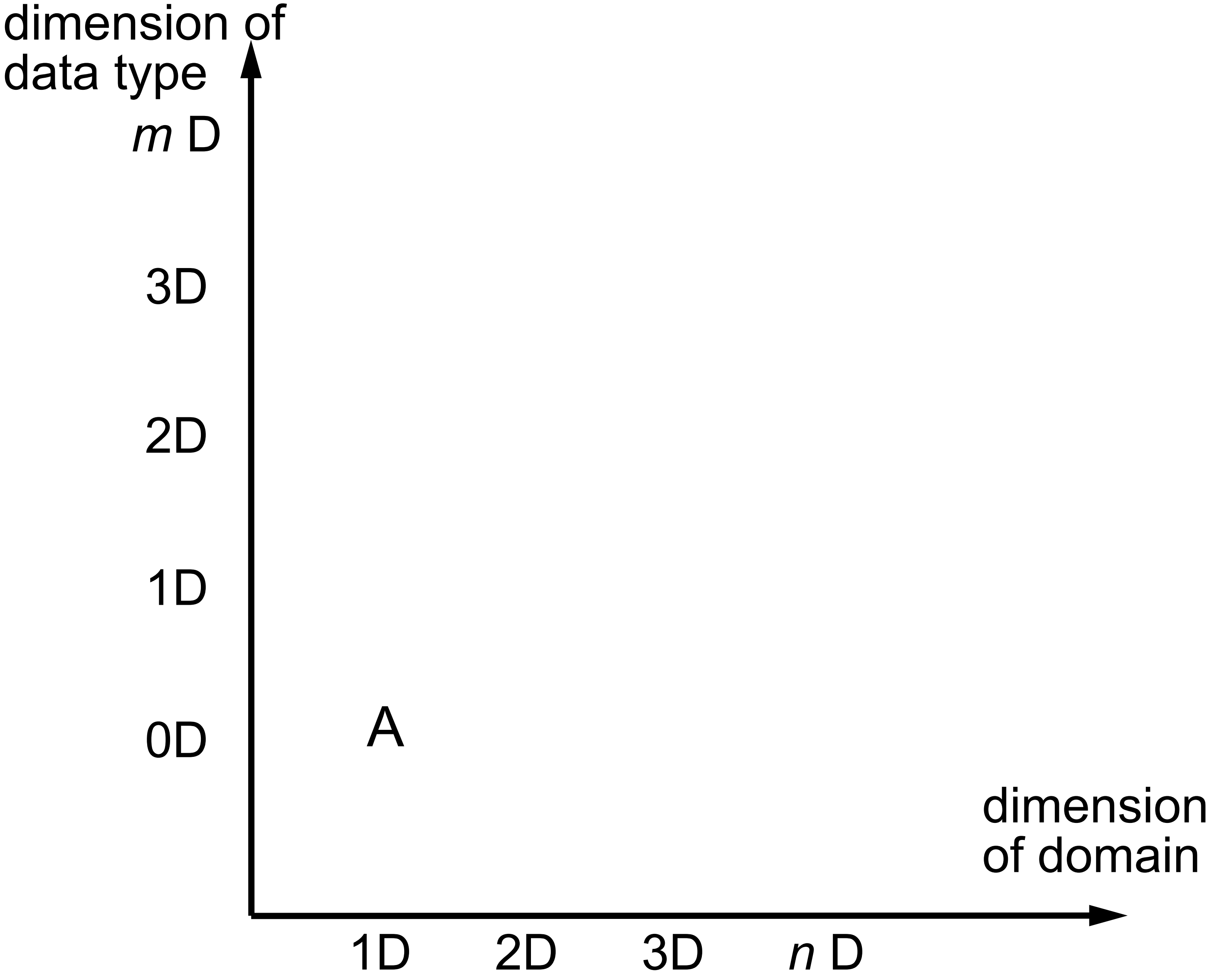

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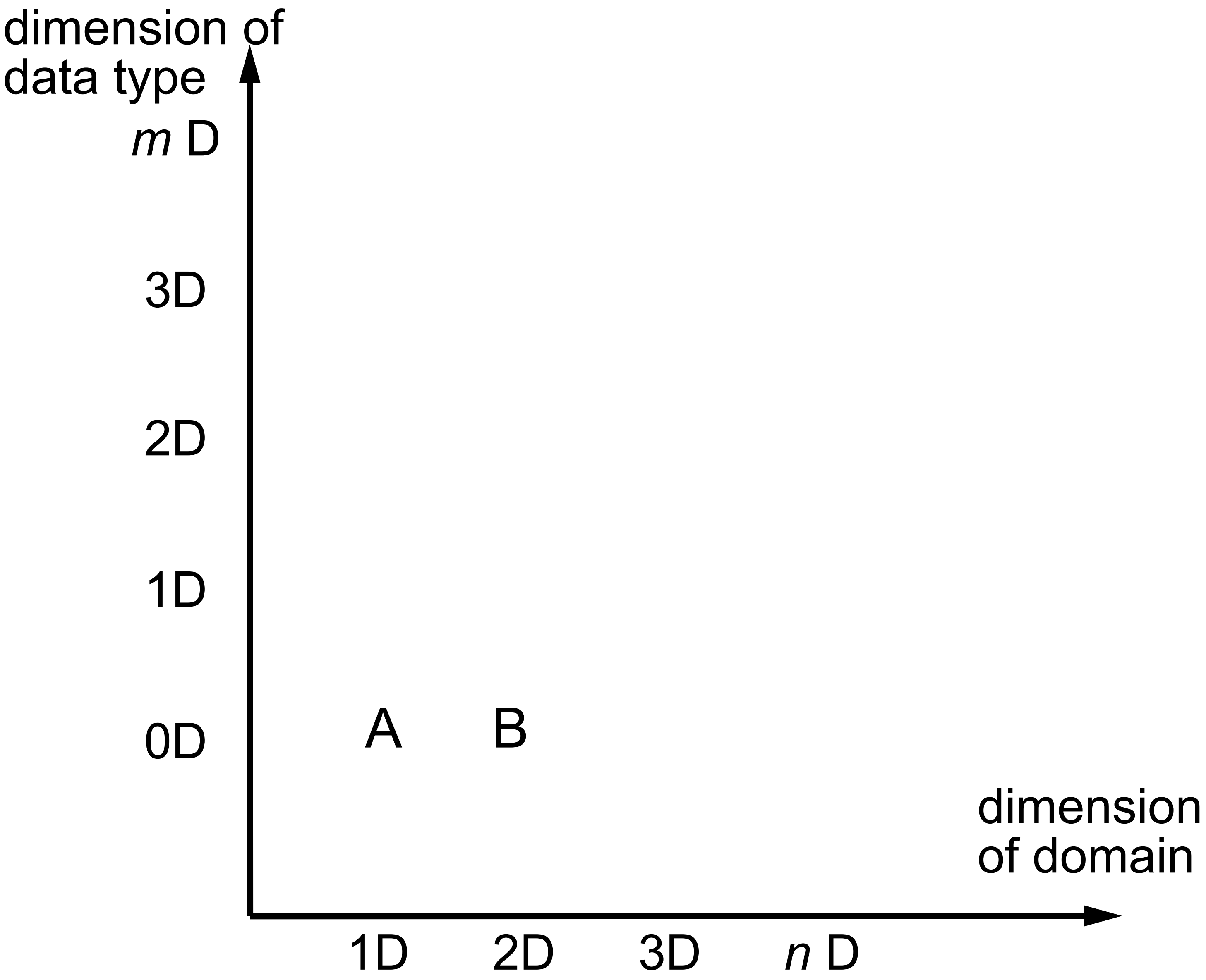

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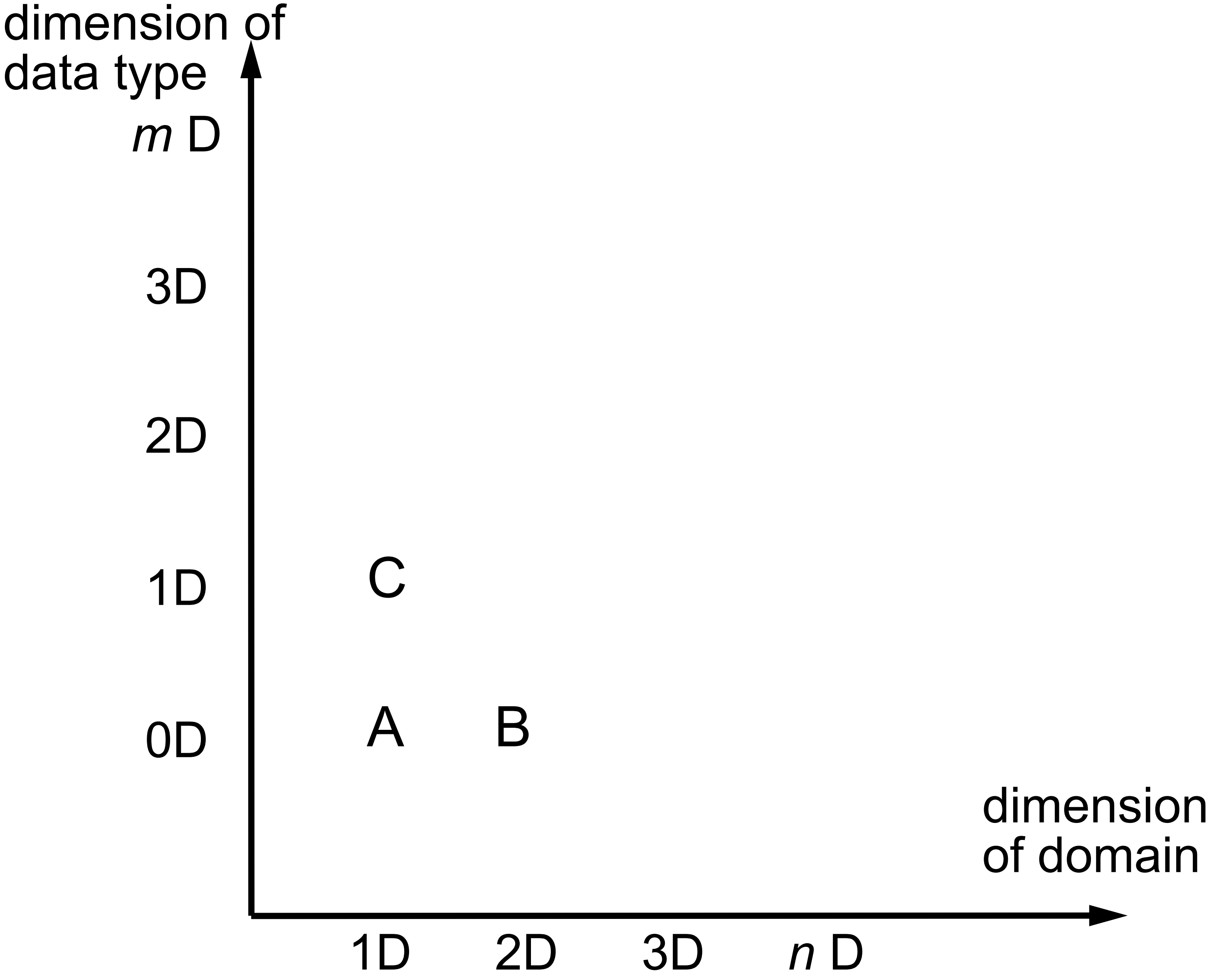

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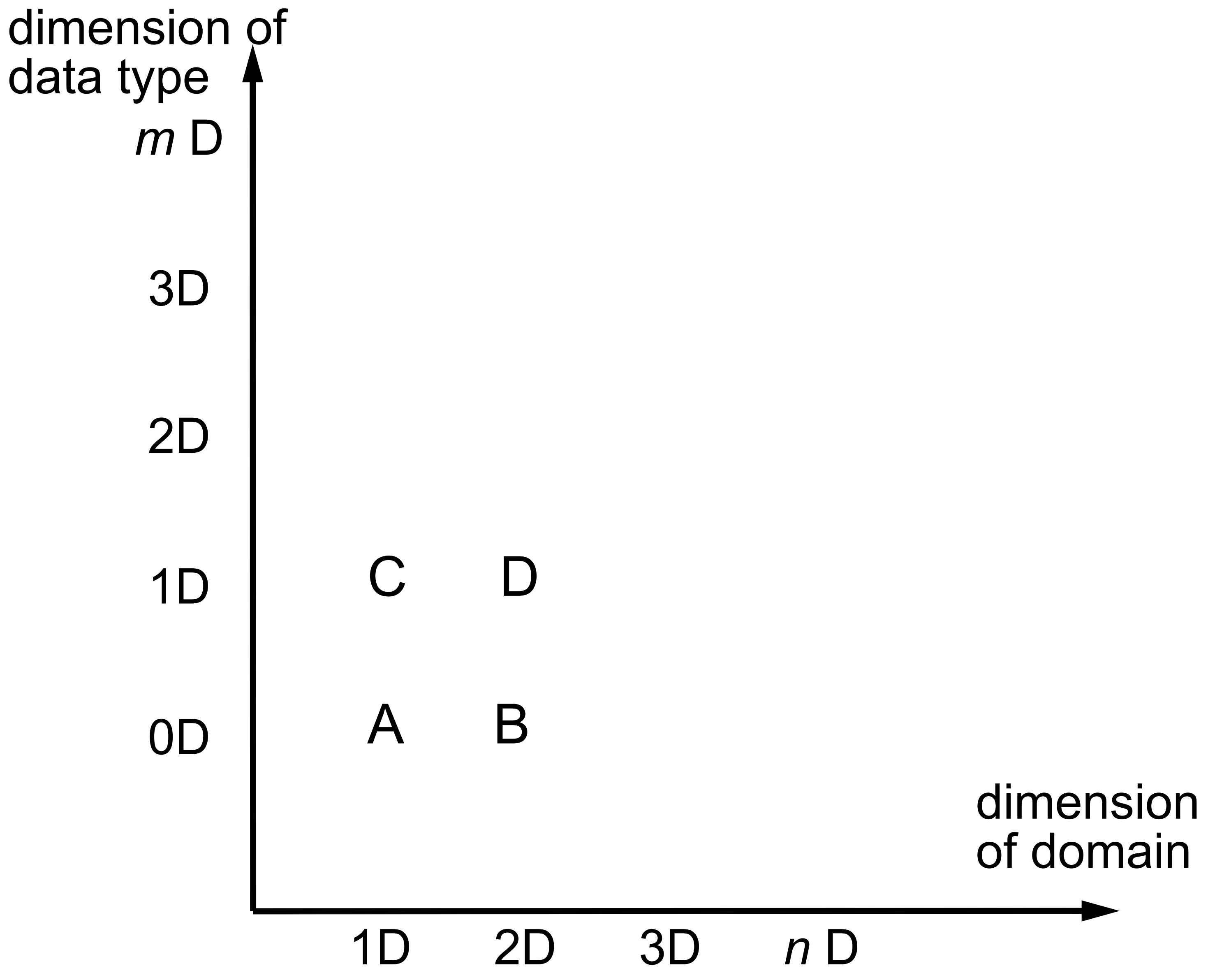

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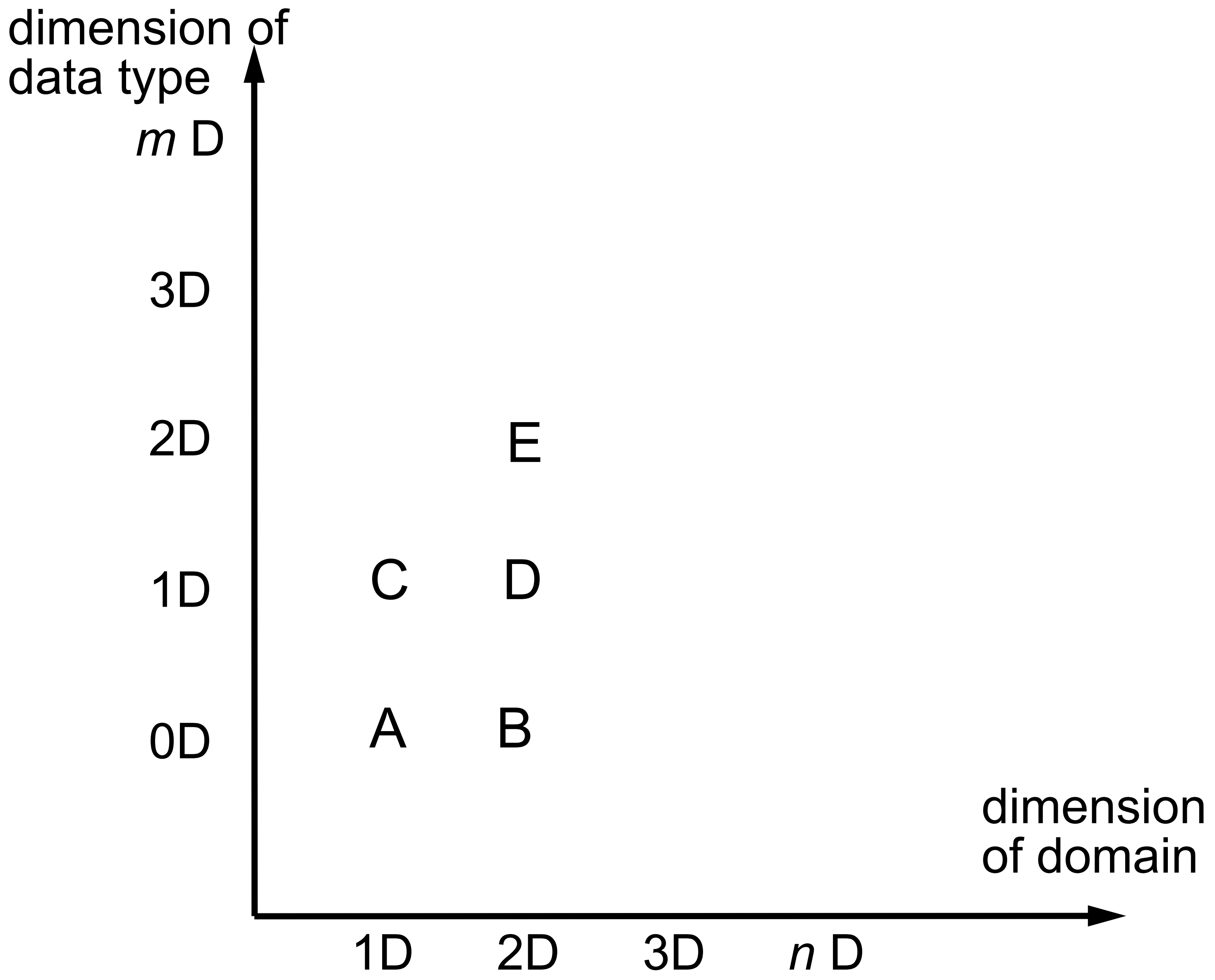

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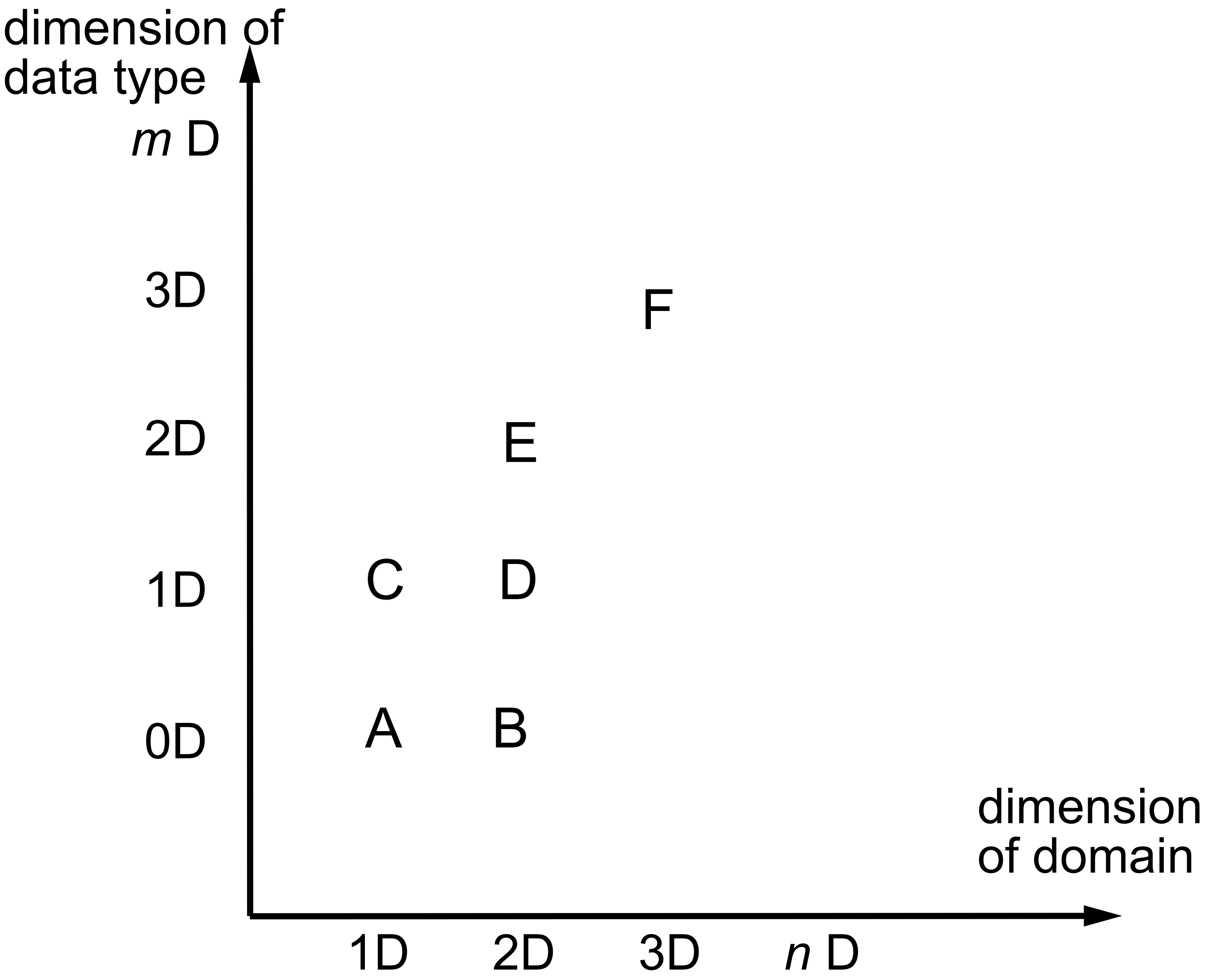

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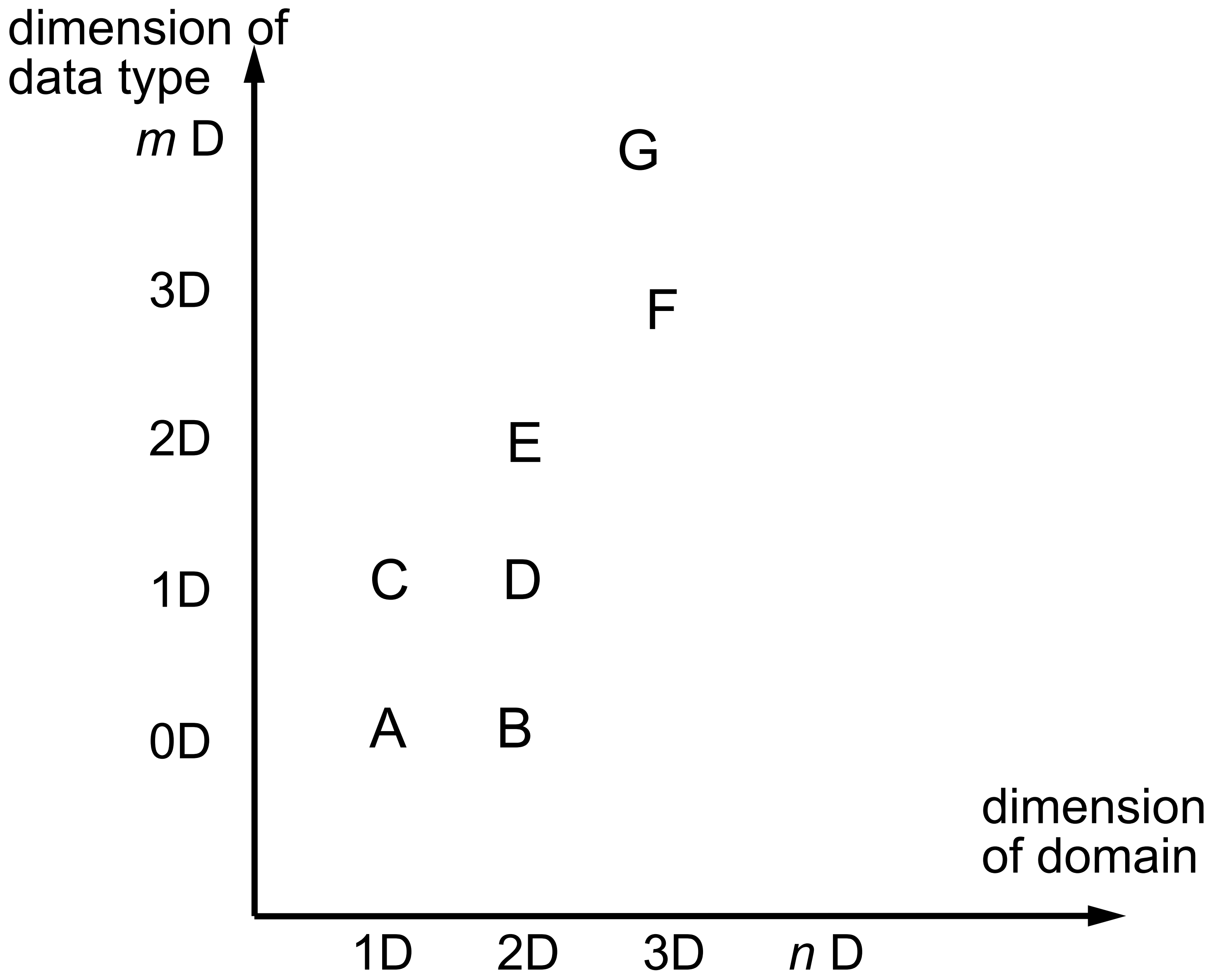

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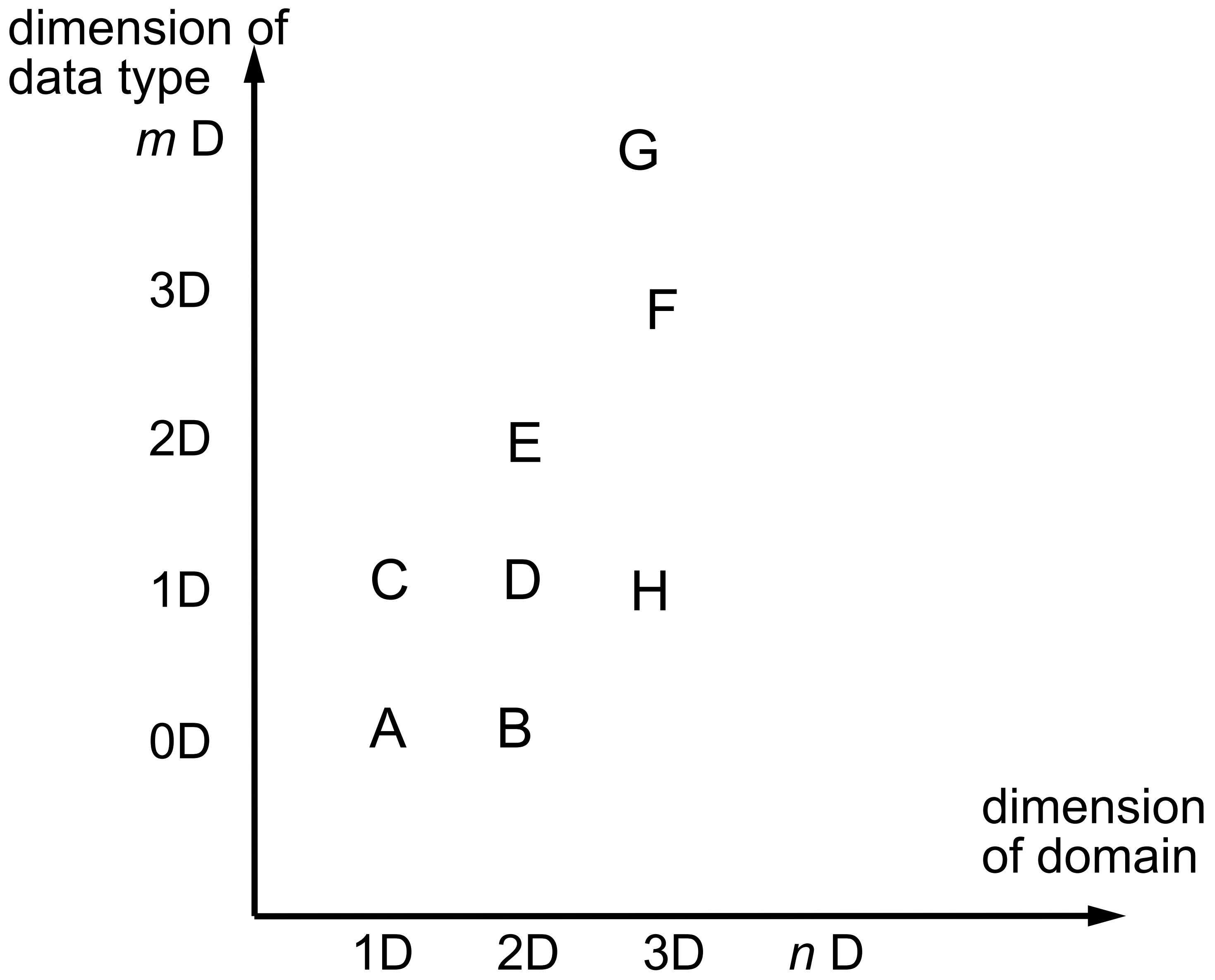

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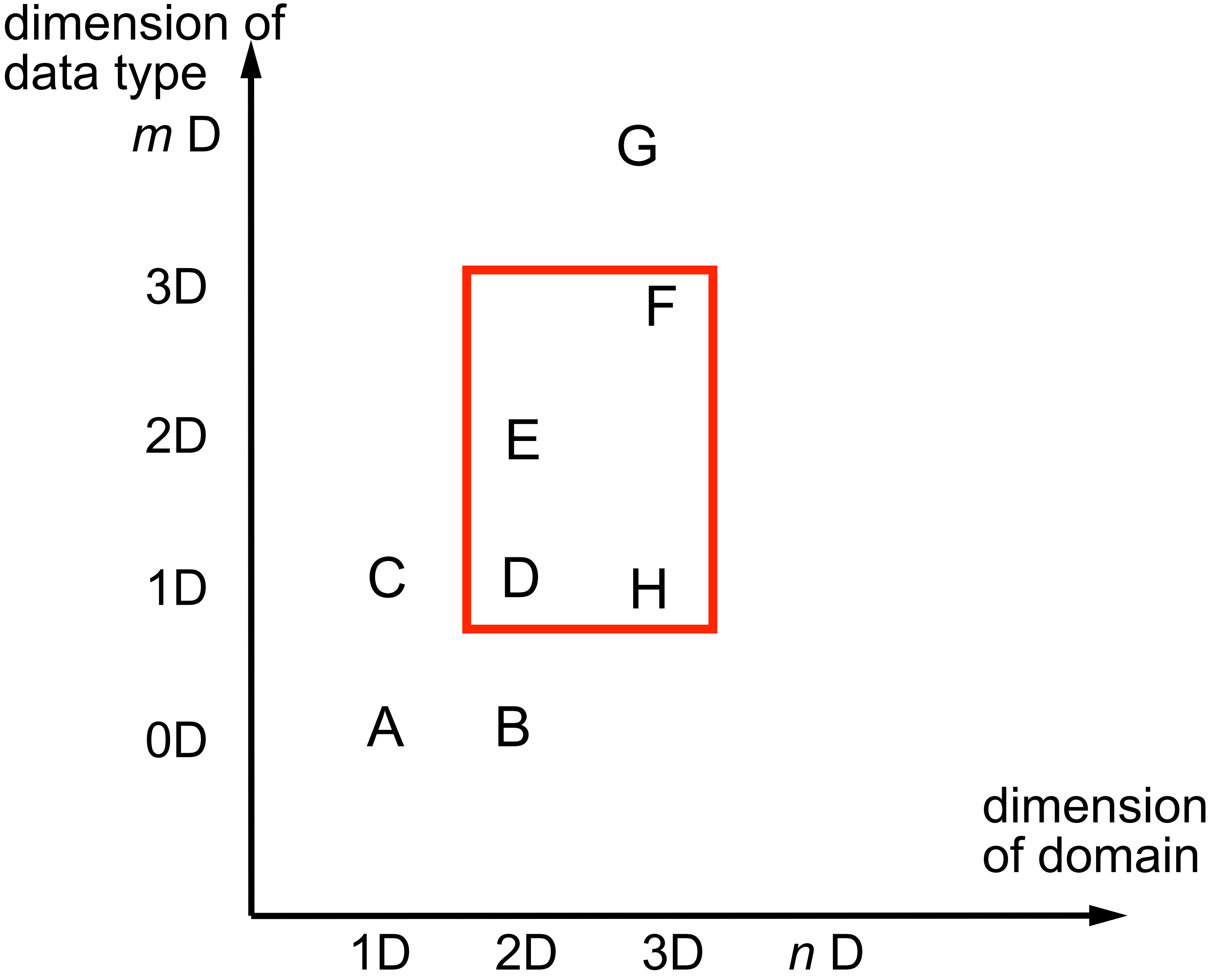

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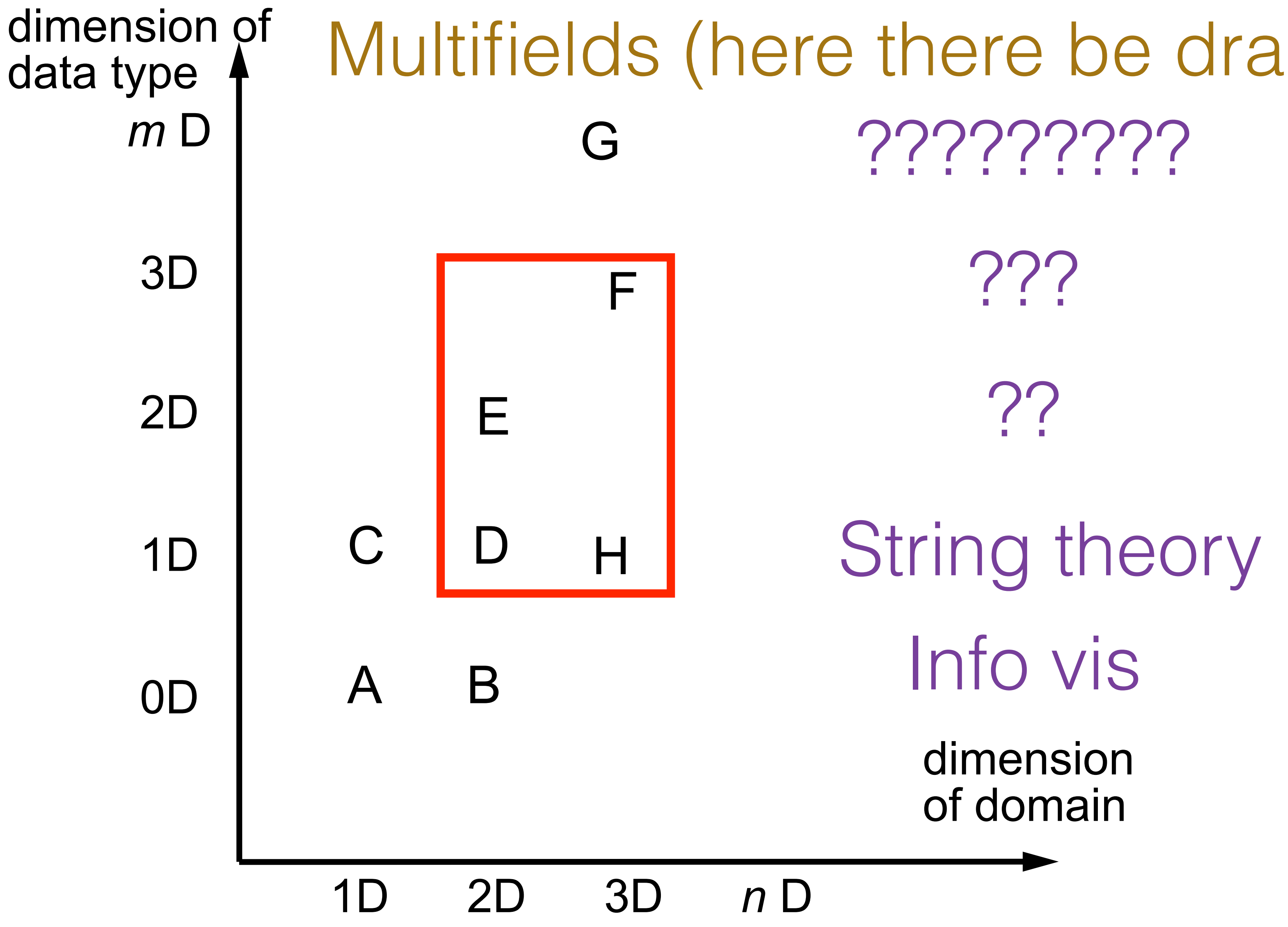

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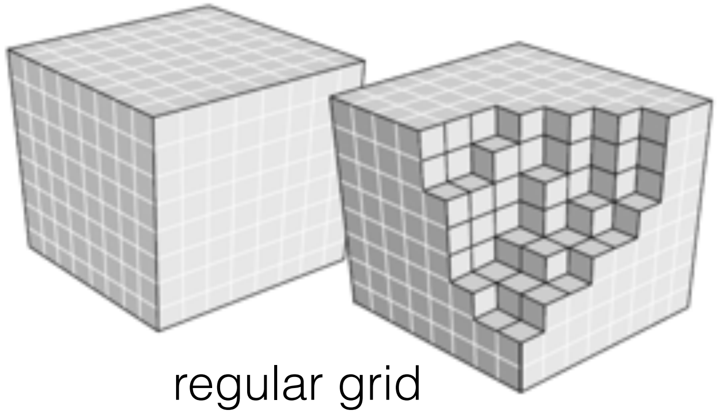
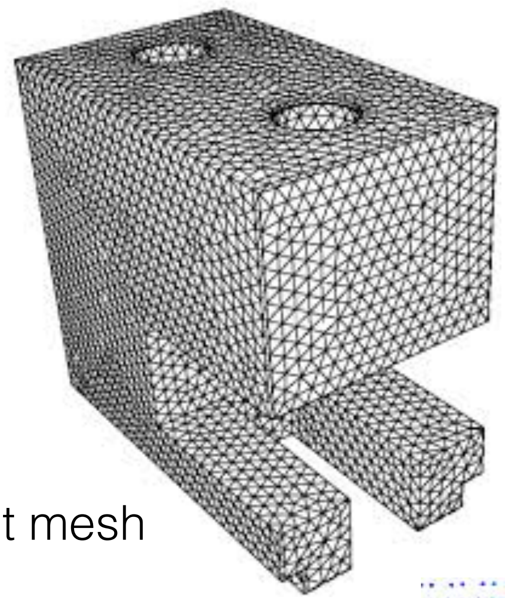
Grids

- Continuous fields are an illusion
- All data are discrete
- Meshes are chosen based on what is computationally efficient for the
- Visualization software must implement data models to handle a wide range of field and non-field data
    - (e.g., VTK)

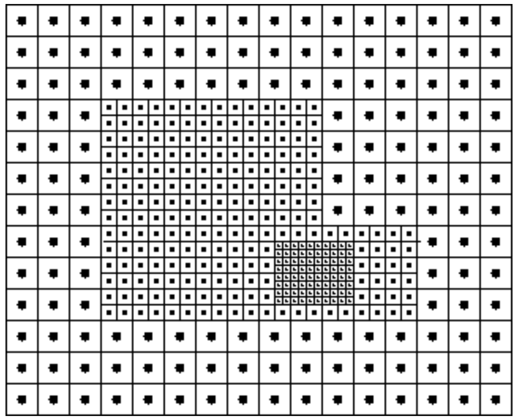


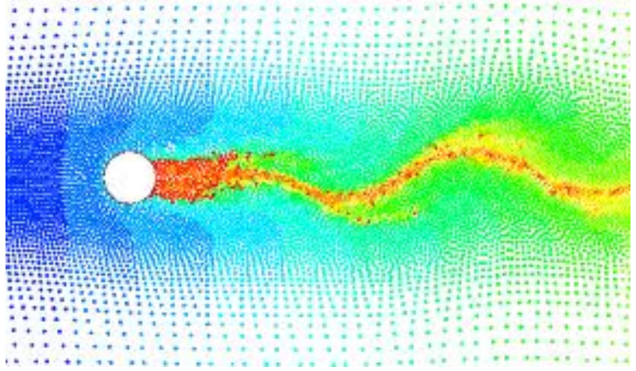
regular grid



tet mesh

AMR





particles

Structured vs Unstructured

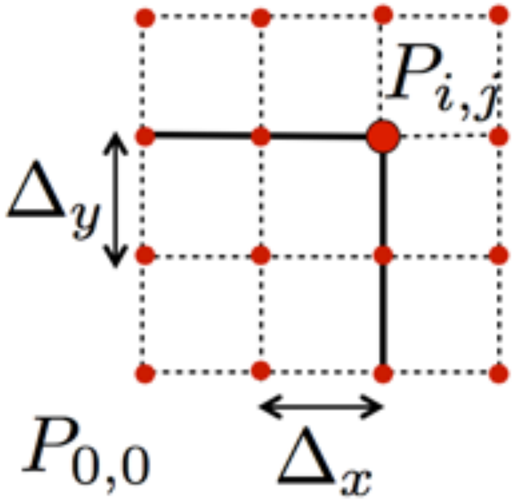
- In general, from the relational database world:
    - **Structured data** are data that are indexed, and can be accessed via a hash, array, or other query.
        - I.e., search time *O(1)* or *O(log N)*.
    - **Unstructured data** are not indexed — you have to brute-force search to find them.
        - I.e. search time *O(N)*
- In information/data visualization:
    - **structured** means data you've already indexed, organized (for example, in D3).
    - **unstructured** is everything else (i.e. text, imagery, video, foo) you have to search through.
- In scientific visualization, this can get a bit confusing…
- First we need to differentiate between geometry and topology.

Geometry vs Topology

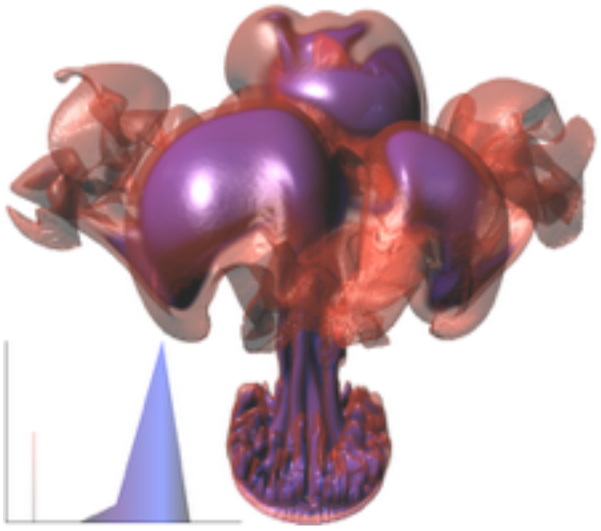
- Geometry
  - Position of vertices in Euclidean space
  - Can be uniform, structured or unstructured.
- Topology
  - Defines the “cells”, or connectivity of the vertices.
  - Can also be structured or unstructured.

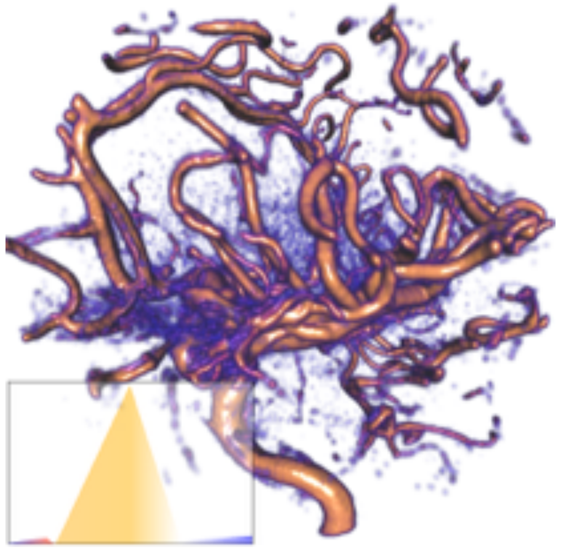
Uniform grid geometry

- Uniform spacing along the axes, also known as “raster data”.
- Most volume data look like this; structured data usually means this.
- You still need metadata to know the size of the axes!

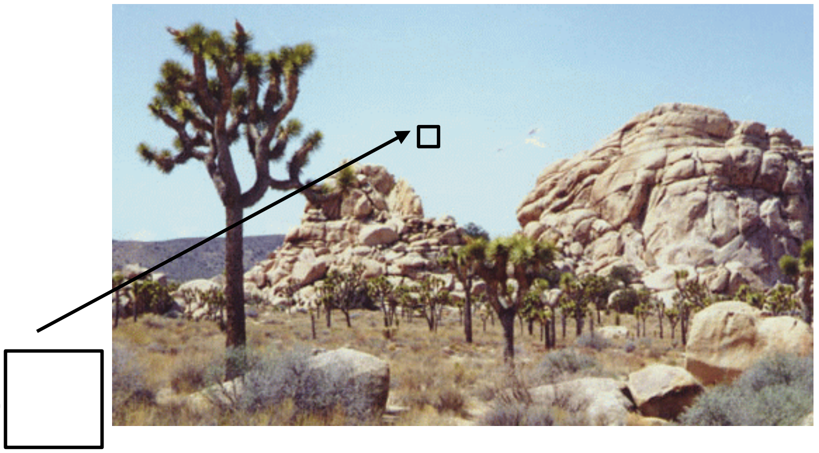


$$P_{i,j,k} = P_{0,0} + i\Delta_x\vec{e}_x + j\Delta_y\vec{e}_y$$

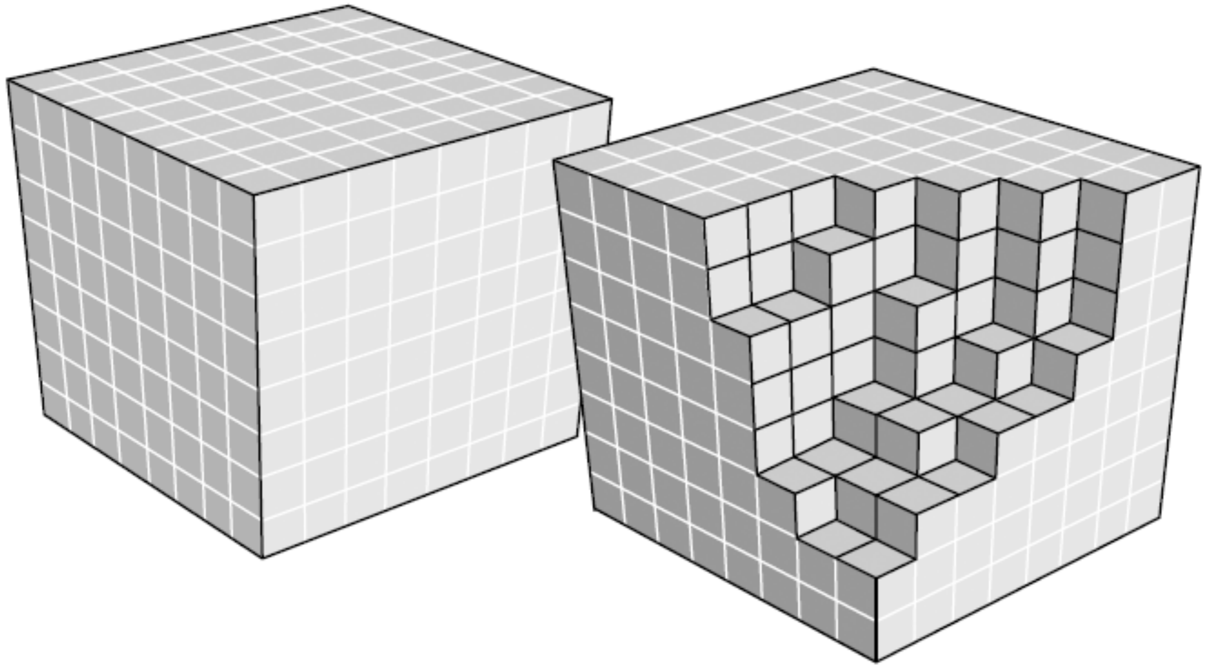




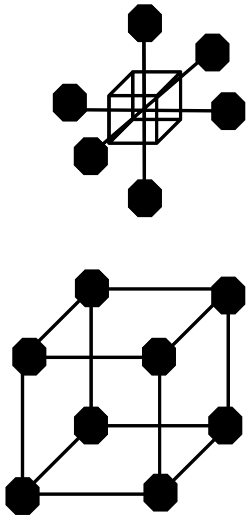
- Representation of scalar 3D data set $\Omega \in R^3 \rightarrow R$
- Analogy: pixel (picture element)



- Voxel (volume element), with two interpretations:
  - Values between grid points are resampled by interpolation



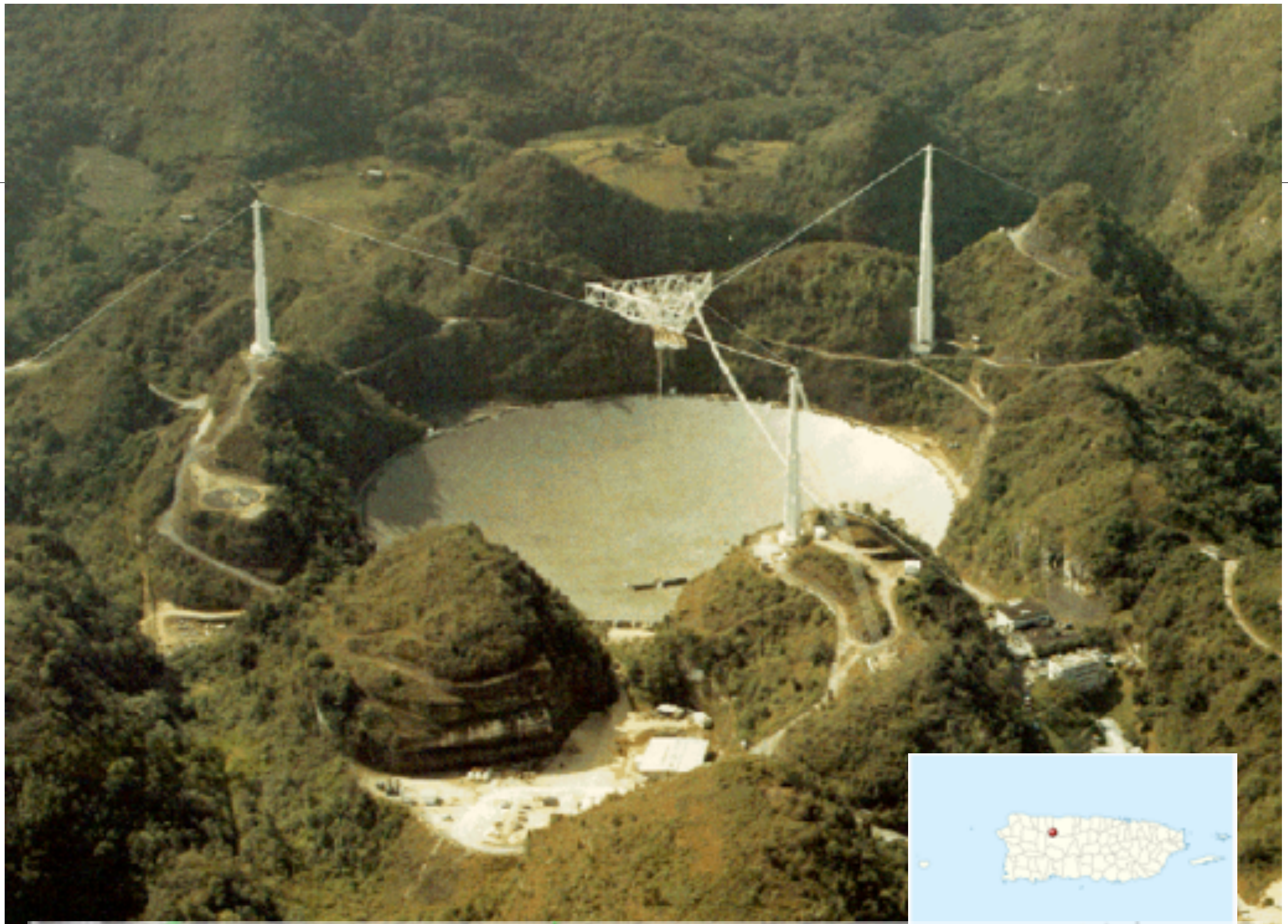
- Collection of voxels
- Uniform grid

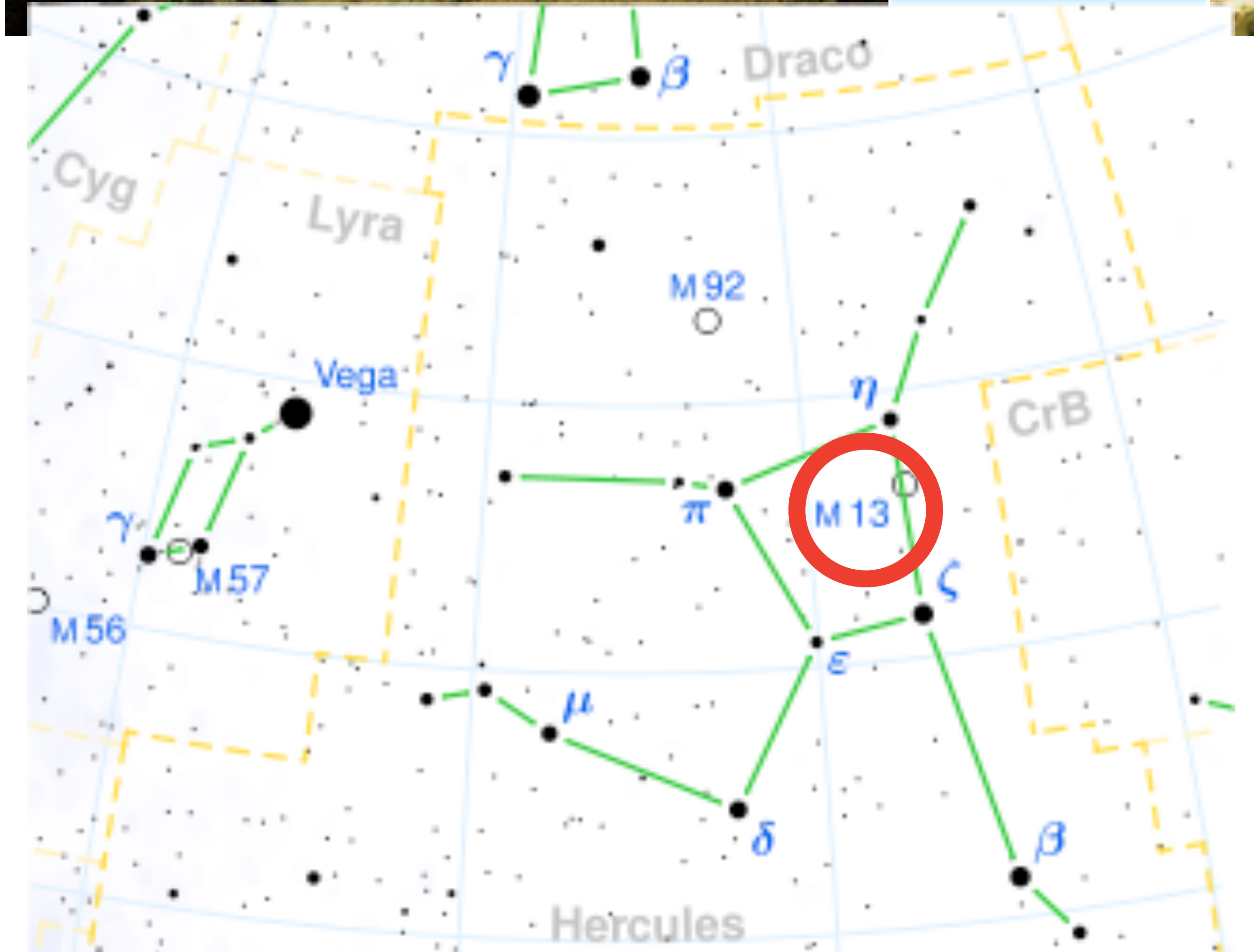


Arecibo Message

http://en.wikipedia.org/wiki/Arecibo_message

- Way of understanding mechanics of raster image representation
- Radio telecope in Puerto Rico
- built in 1964, renovated in 1974
- To celebrate: Frank Drake and Carl Sagan (Cornell University) sent message to M13 in Hercules (25,000 light years away)
- 1679 bits, frequency modulate 2380 MHz





The Message

http://www.physics.utah.edu/~cassiday/p1080/lec06.html

1679 bits were encoded as 2380MHz plus and minus some frequency

```
0 0 0 0 0 0 1 0 1 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 1 0 1 0 0 0 0 0 0 0 1 0 0 1 0 0 0 1 0 0 0 1 0 0 0 1 0 0 1 0 1 1 0 0 1 0 1 0 1
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1 1 1 0 0 0 0 1 1 1 0 0 0 0 0 1 1 0 1 1 1 0 0 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 1 1 1 0 1 1 0 0 1 0 0 0 0 0 0 1 0 1 0 0 0 0 0 1 1 1 1 1 1 0 0 1 0 0
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0 1 1 1 1 1 0 0 1 1 1 1 1 0 1 0 0 1 1 1 1 0 0
```

This is a **1-D** sequence of bits in time

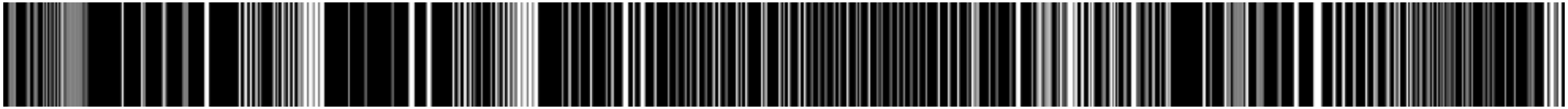
How will an alien understand this list of bits?

(will have different symbols than “0” “1”)

No meta-information!

Understanding the message

- Perhaps some “visual” representation of bits



  - (what is black vs white?)

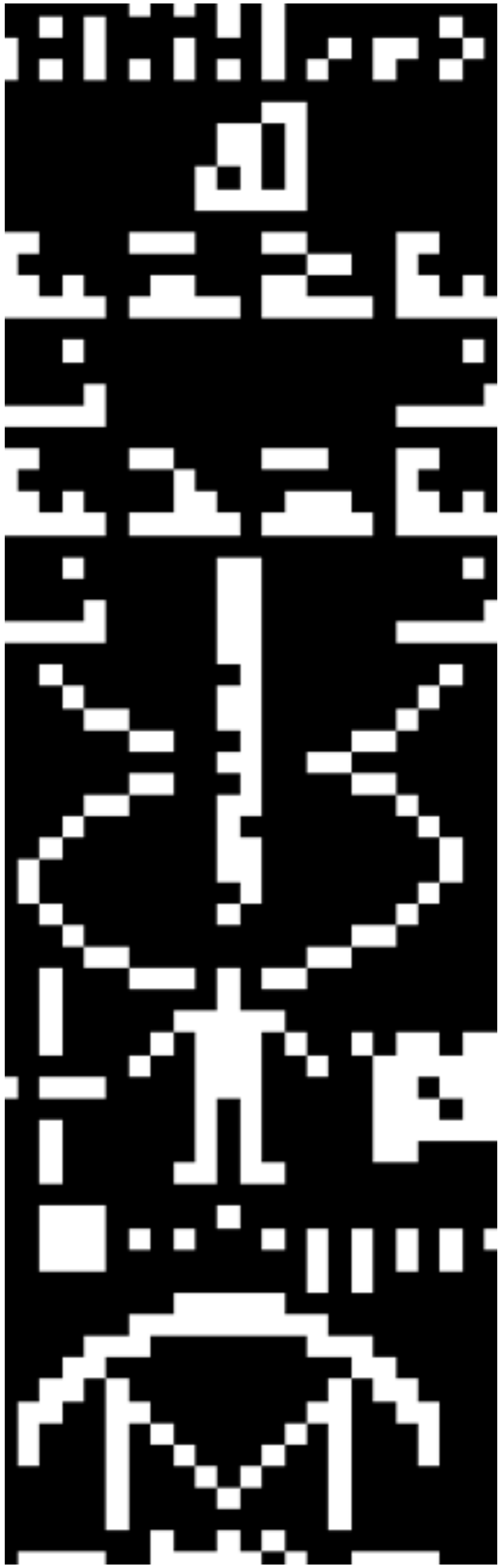
- Aliens notice 1679 = 23 x 73 (product of two primes)

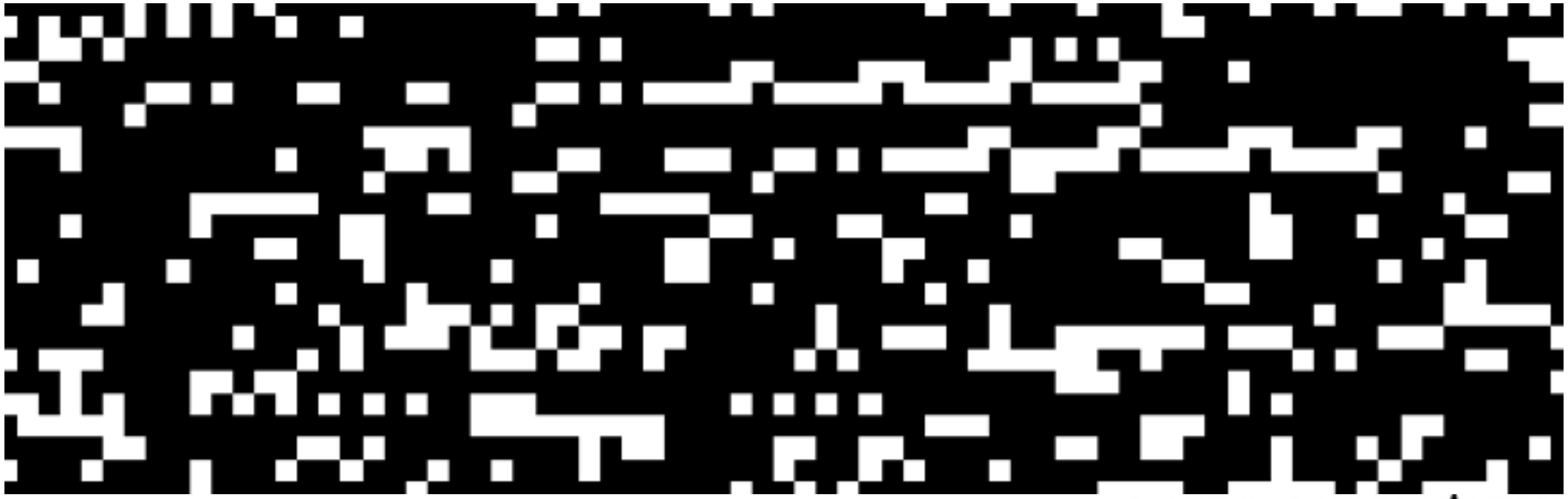
- Perhaps its not a linear sequence: 2-D array

- Two ways of sequencing values in 2D array

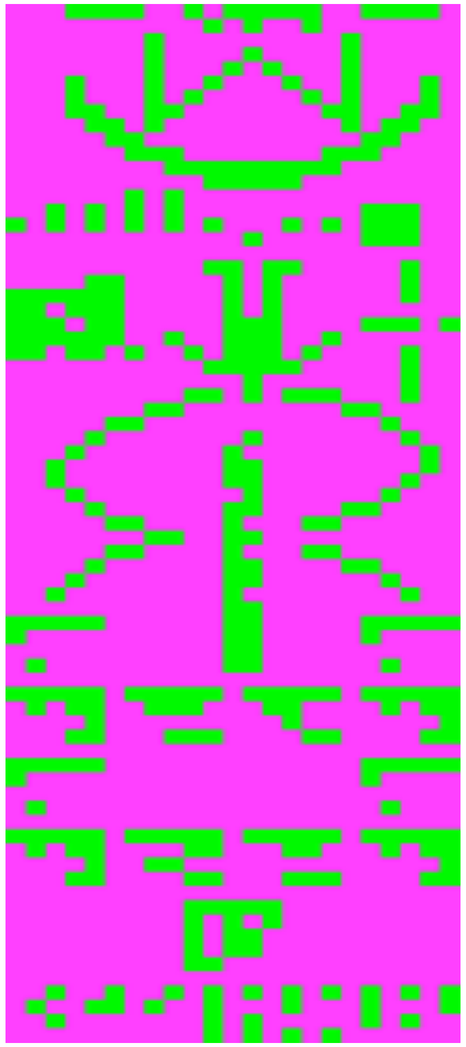
- Various ways of laying them out in 2D space

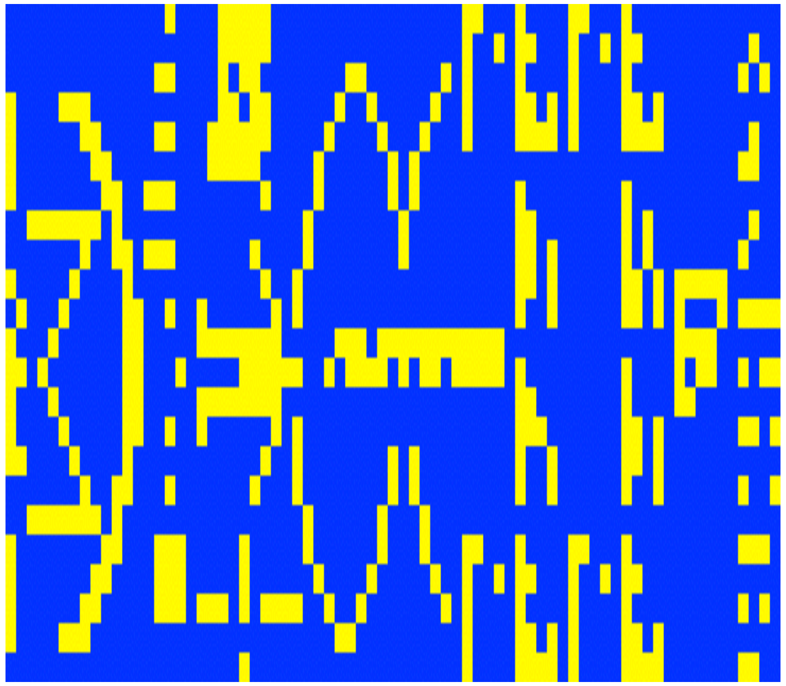
- Then: have to decipher it!



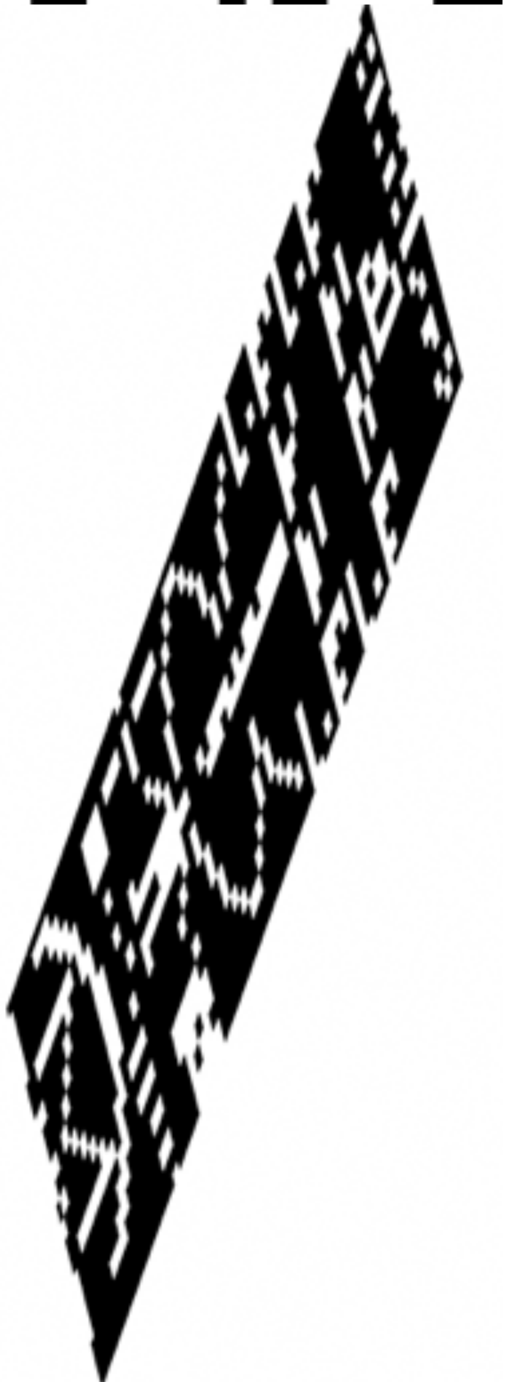


73 x 23





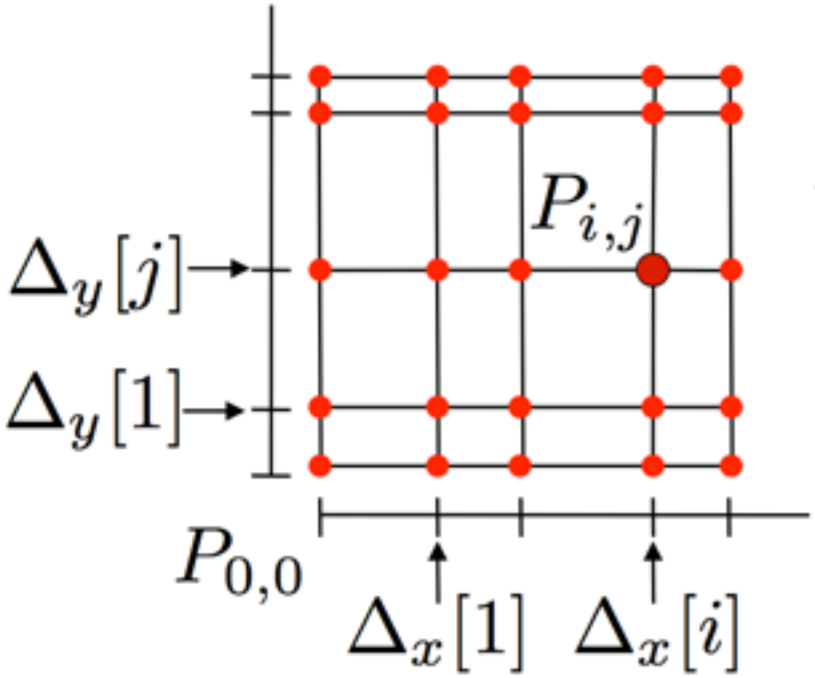
compare to:
http://en.wikipedia.org/wiki/Arecibo_message



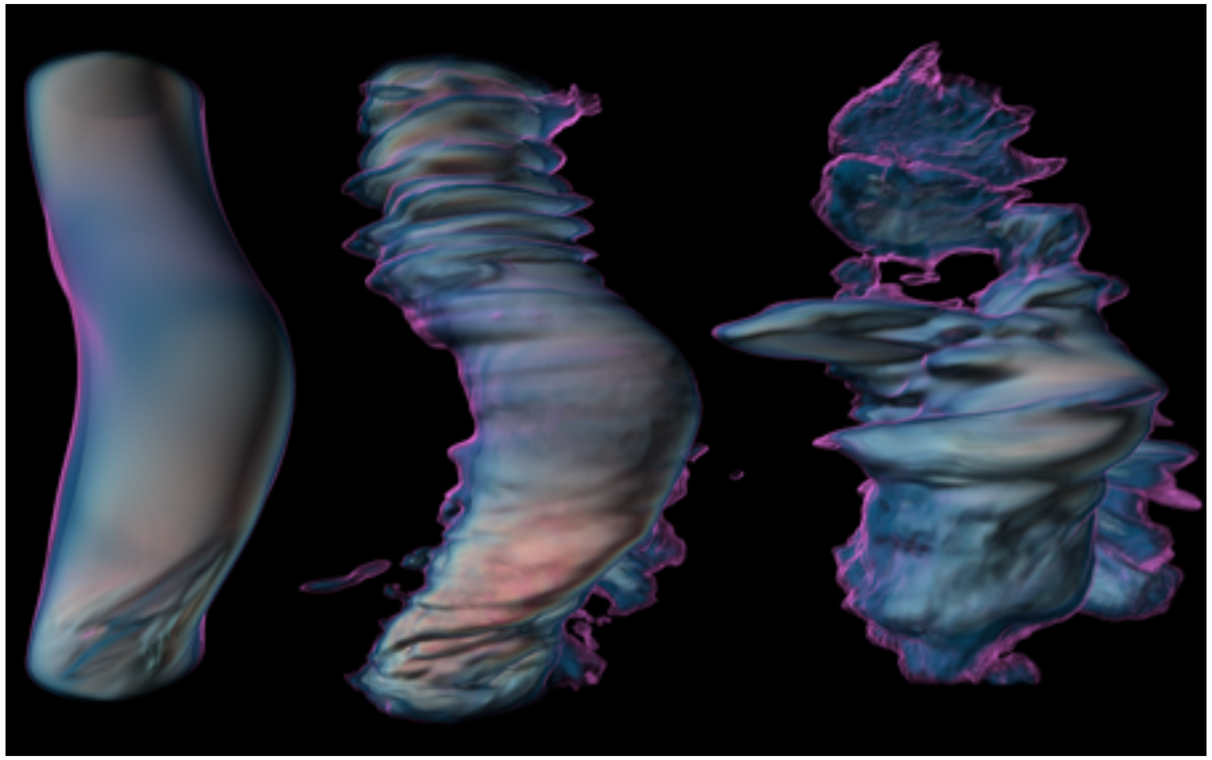
23 x 73: what was different?

Structured (rectilinear) grid geometry

- Still structured, but with non-uniform spacing along the axes.
- Positions can still be computed procedurally
- Some meteorology, climate CFD data like this.



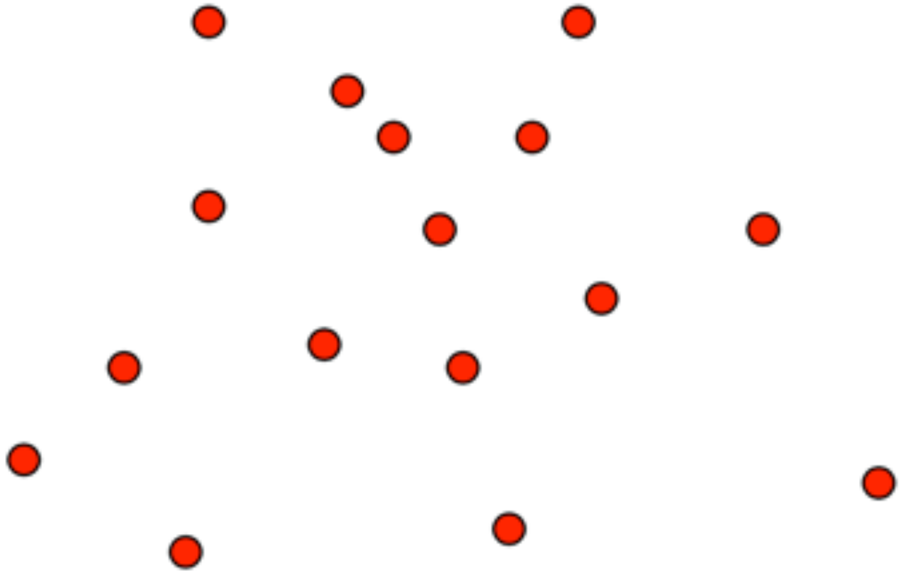
$$P_{i,j,k} = P_{0,0} + \Delta_x[i]\vec{e}_x + \Delta_y[j]\vec{e}_y$$

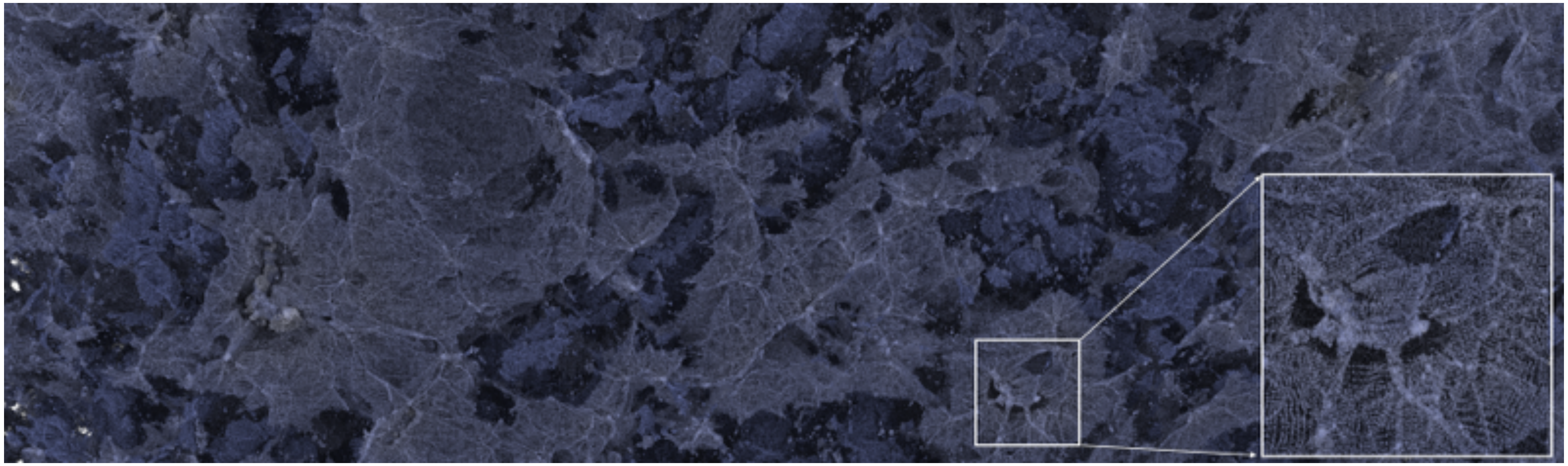


Turbulence in the Ionosphere - Greg Foss, TACC

Unstructured geometry

- Raw, unstructured point data.
- You actually need to store the x,y,z positions of vertices.
- Some of the largest computational and scanned data
  - LiDAR, RGB-D point clouds, range scans
  - n-body codes — molecular dynamics, cosmology
- Note: this is unstructured topology, too!

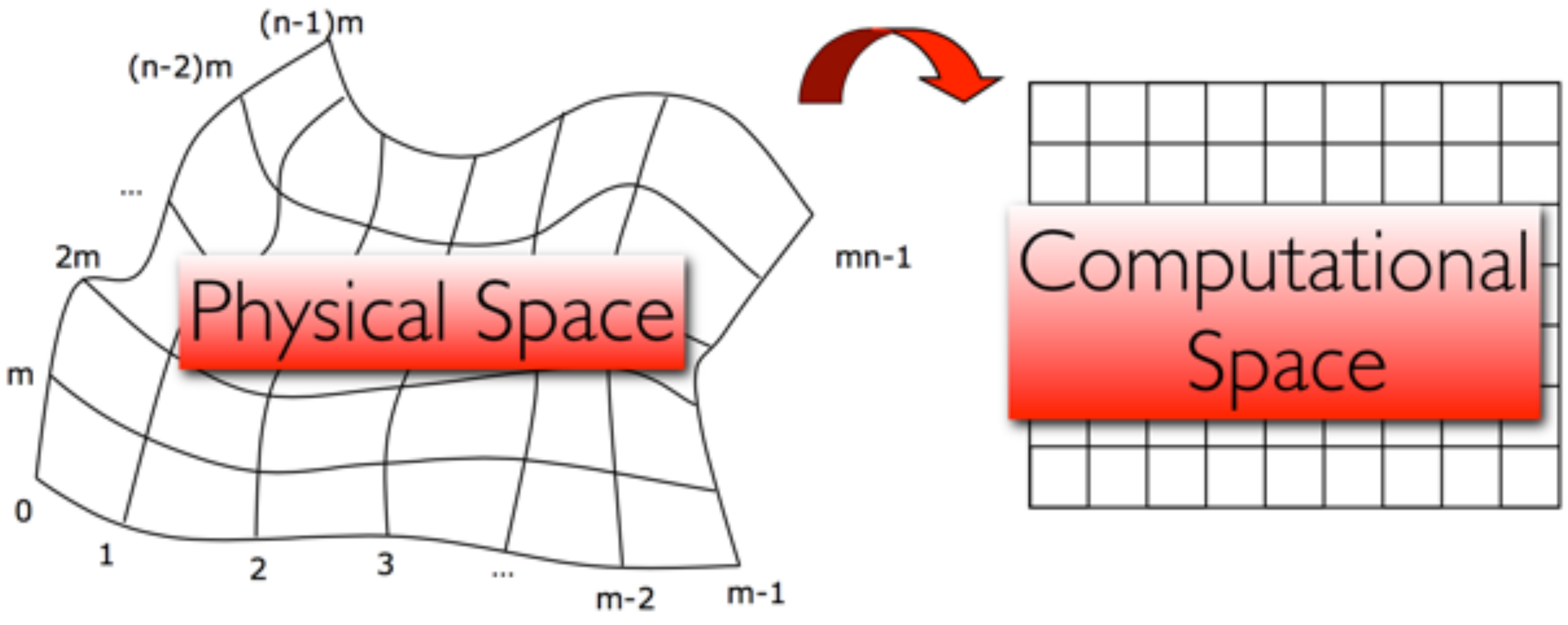


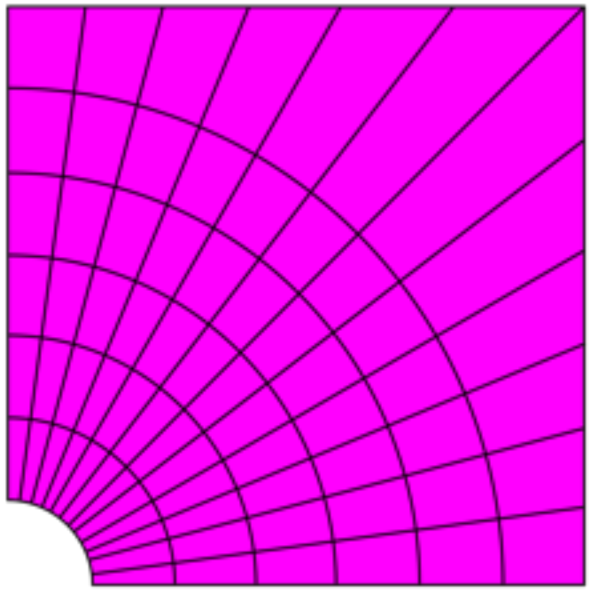


30-billion particle “Cosmic Web” data — Paul Shapiro, University of Texas at Austin
I Wald, A Knoll, G.P. Johnson, W. Usher, V. Pasccci & M.E. Papka: “CPU Ray Tracing Large Particle Data
with P-k-d Trees” IEEE Visualization 2015 (to appear)

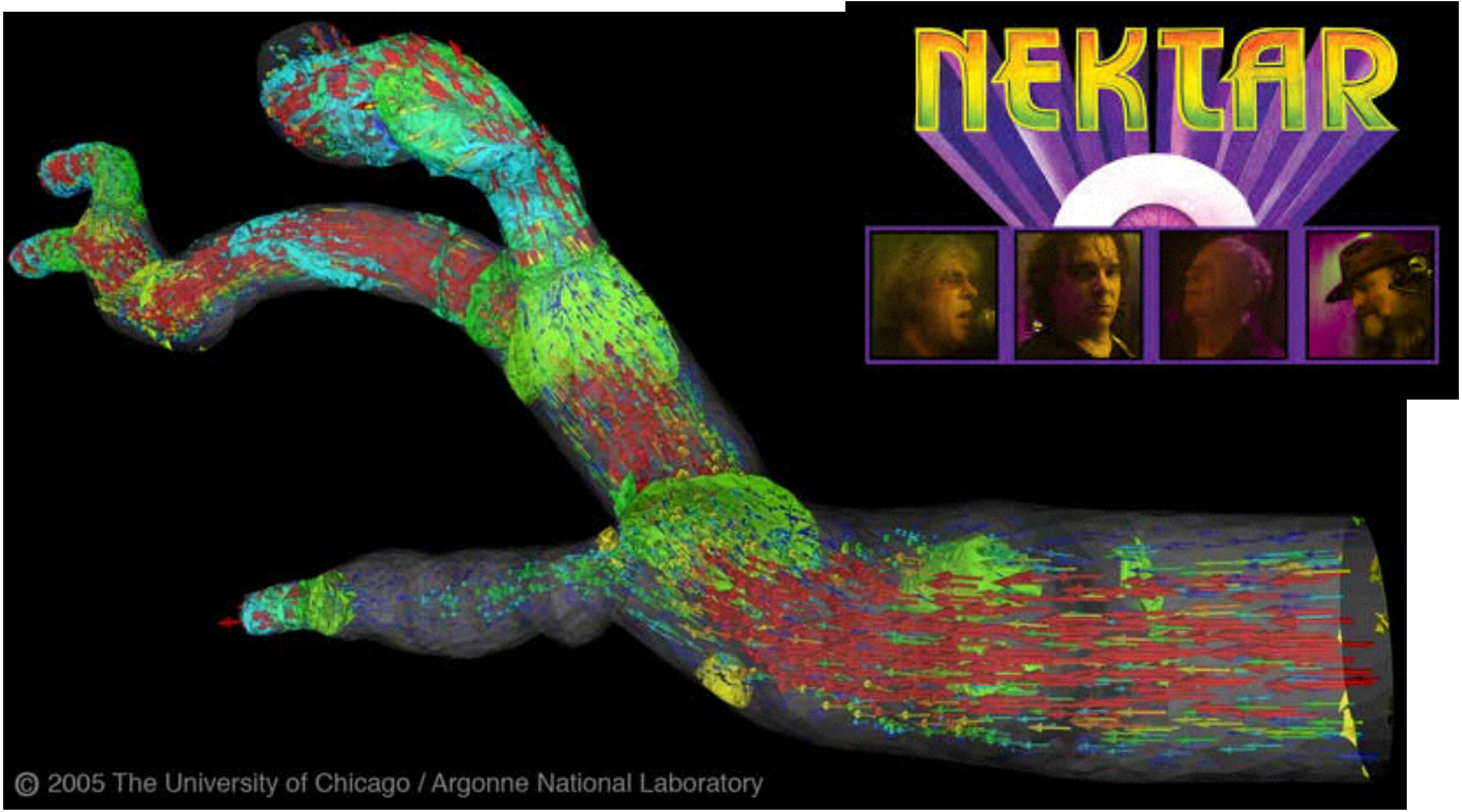
Structured grid topology

- You can have unstructured geometry but structured topology
  - Implicit definition of cells
  - Implicit connectivity between vertices
- More exotic options with structured grid topology:
  - Finite elements, finite differences on curvilinear grids
  - spectral F/E, some spline-based finite elements simulations
  - Good for precision-critical flow computations (blood flow, CFD)





Spectral/hp finite elements



© 2005 The University of Chicago / Argonne National Laboratory

Data: George Karniadakis, Brown University. Visualization: Joe Insley, ANL

Curvilinear grids

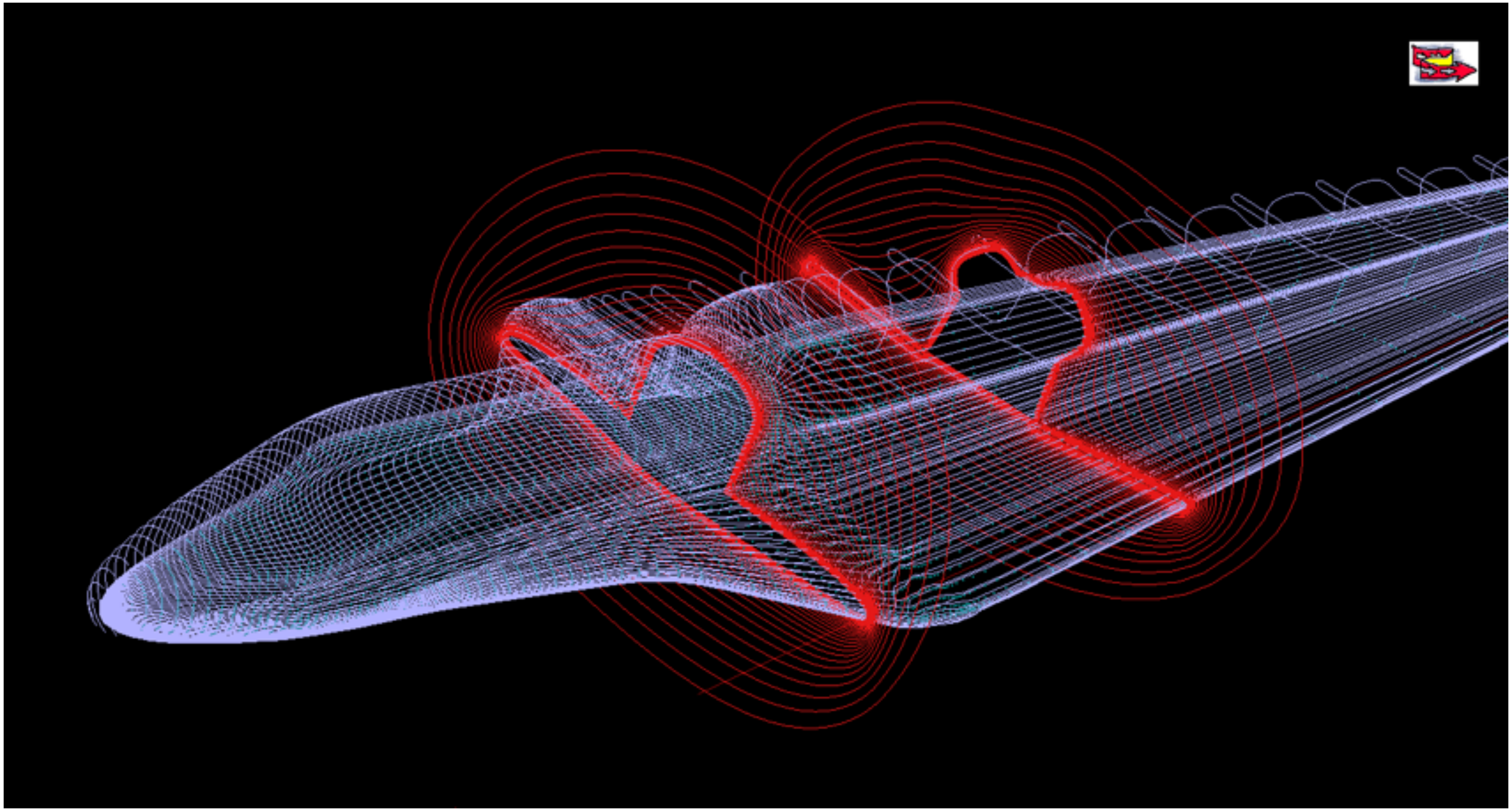
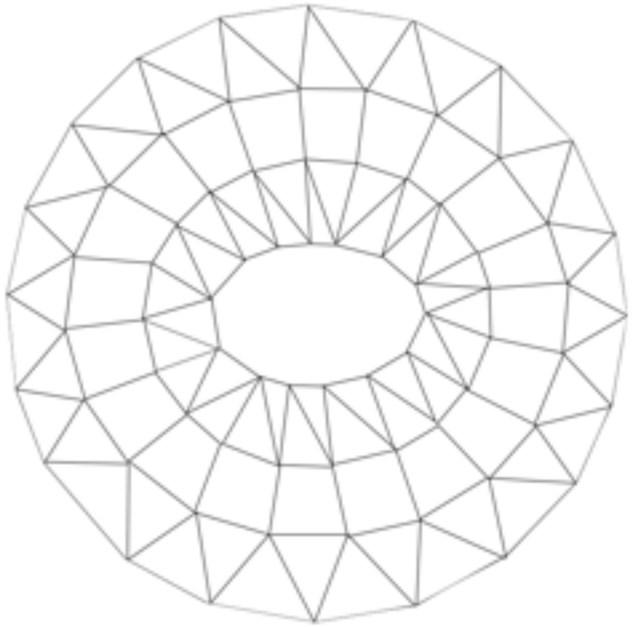
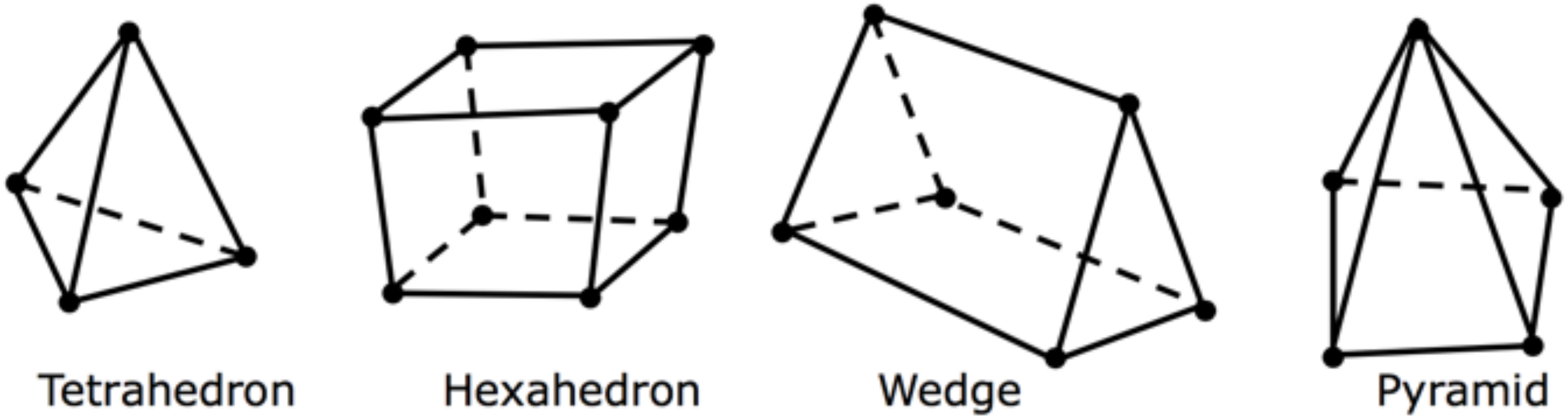


Image:T.U. Graz

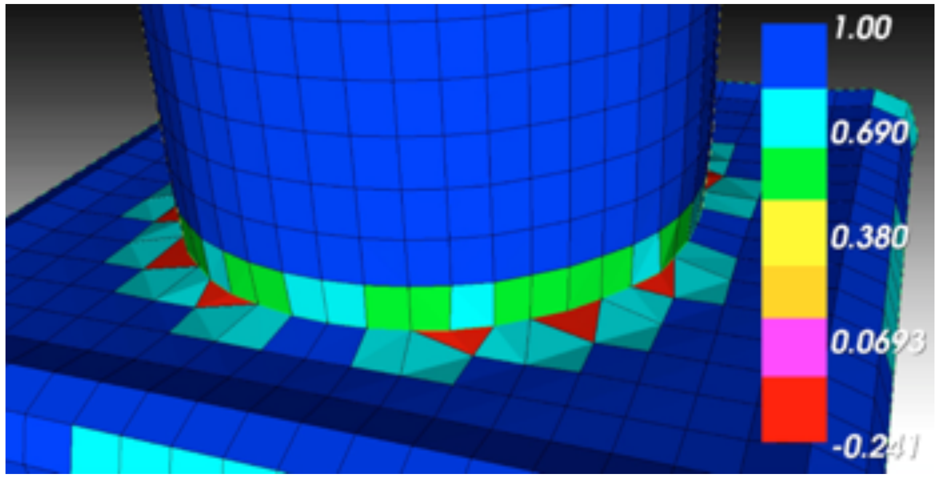
Unstructured grid topology

- Both uniform elements and “mixed elements” (allowing any cell type)
- Need to store vertices and indices separately
  - mixed elements: vertices, indices and count
- Many, many finite elements codes.
  - solid mechanics, CAD
  - bioelectric modeling

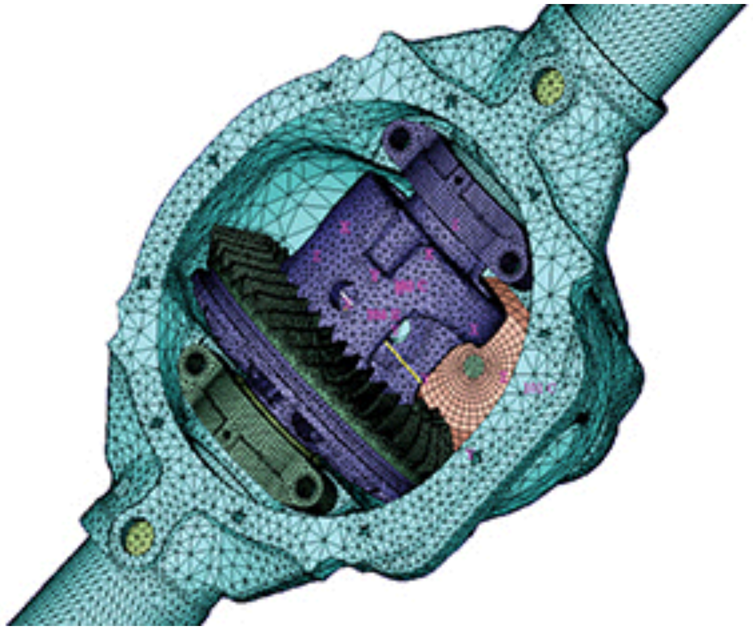


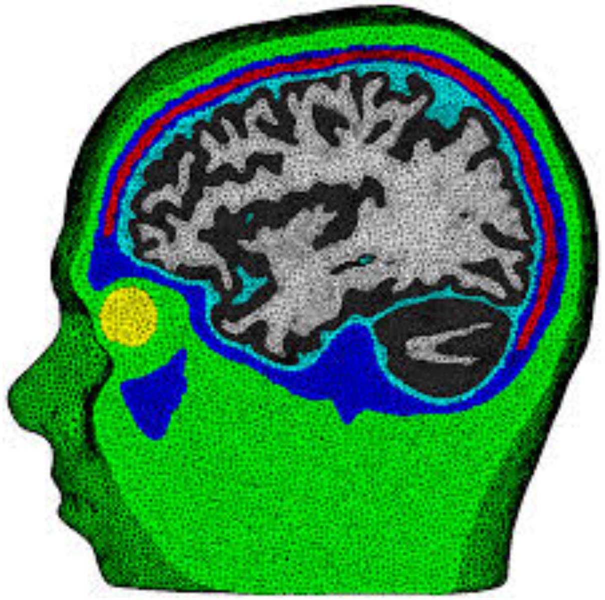


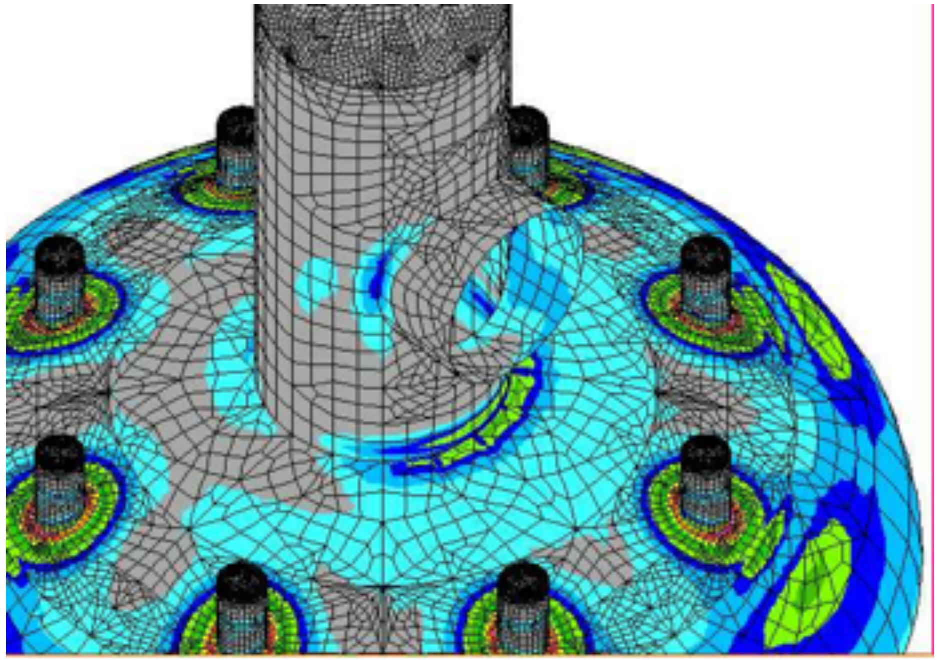
Finite elements

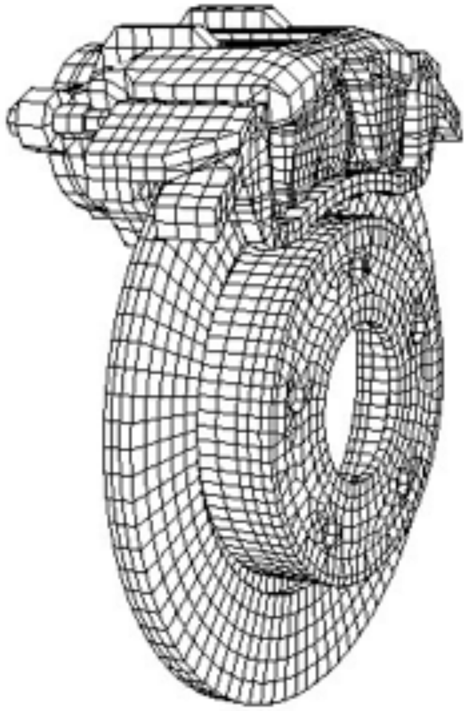


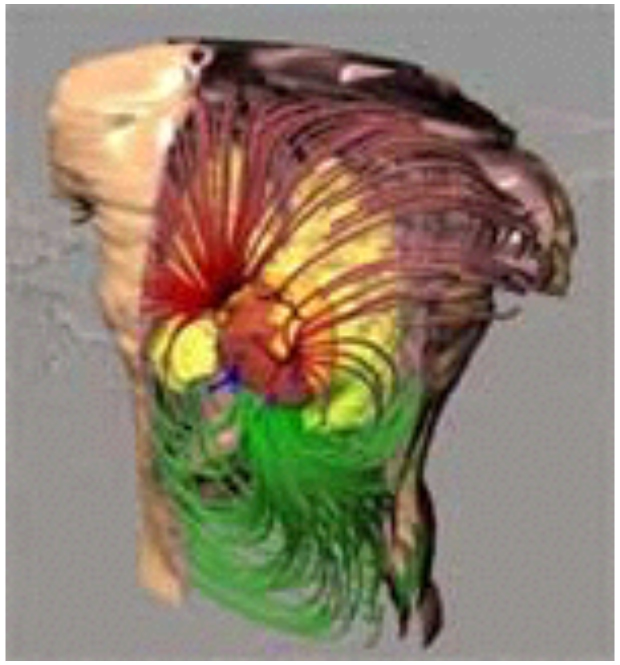
Visualization: Steve Owen, using Cubit











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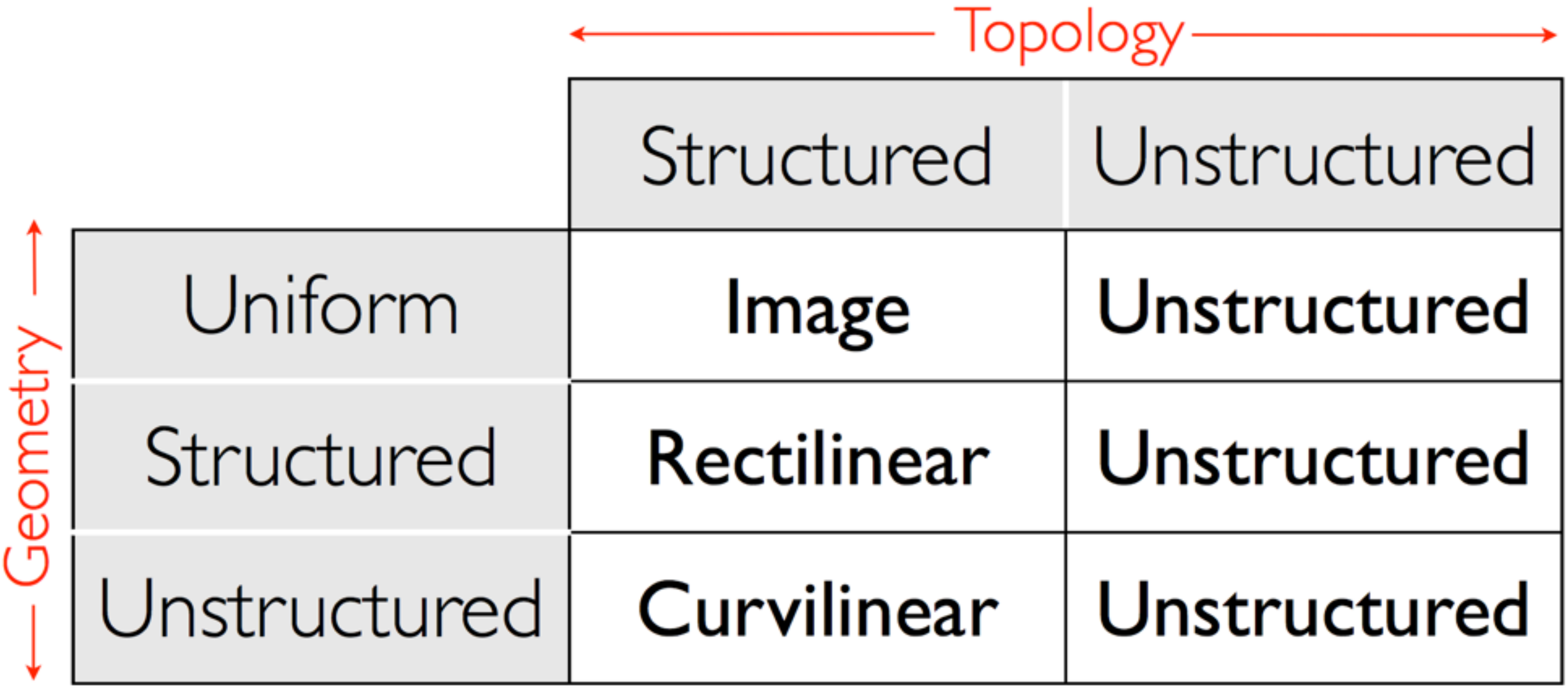
To summarize…



Topology

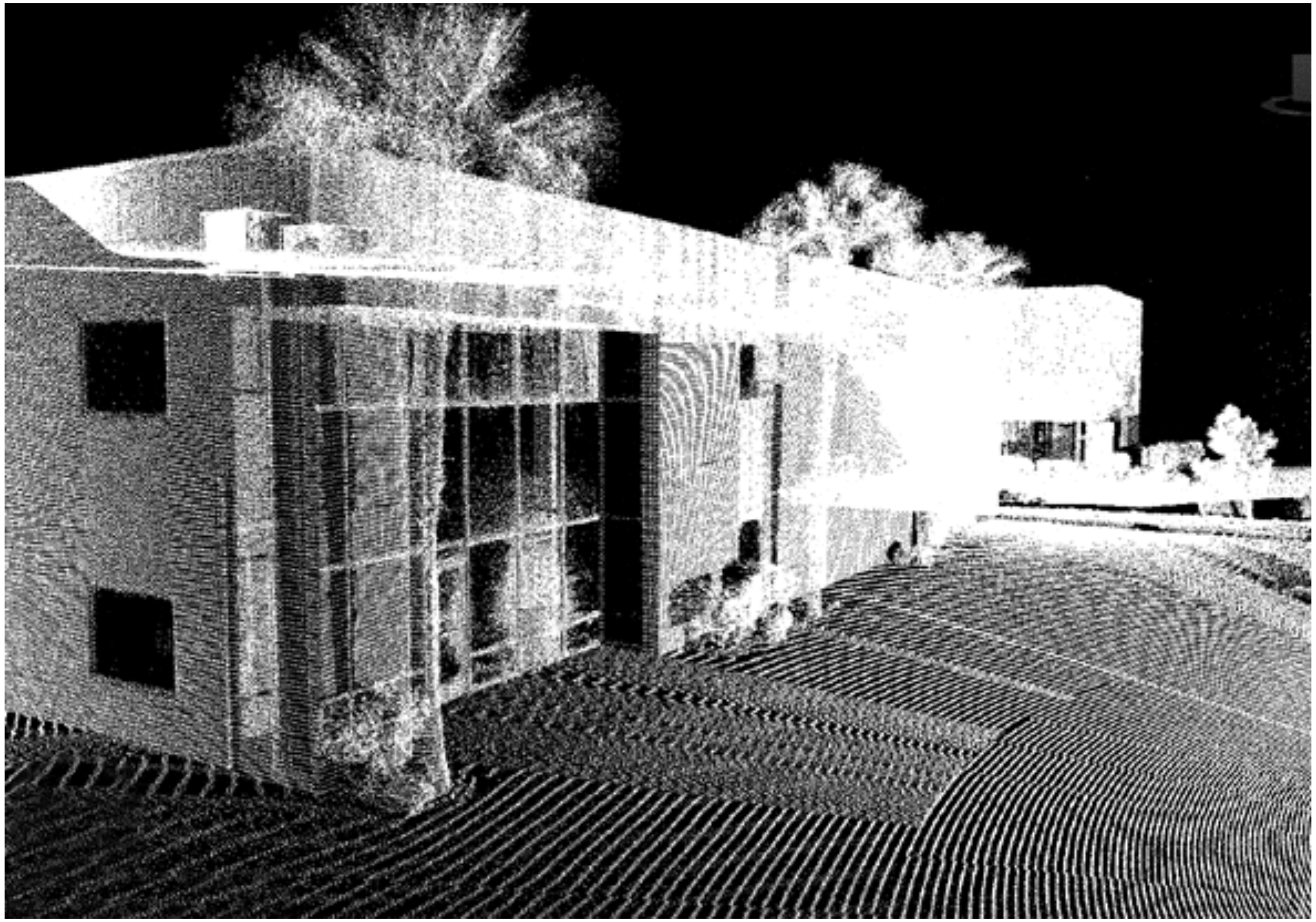
Geometry

	Structured	Unstructured
Uniform	**Image**	**Unstructured**
Structured	**Rectilinear**	**Unstructured**
Unstructured	**Curvilinear**	**Unstructured**

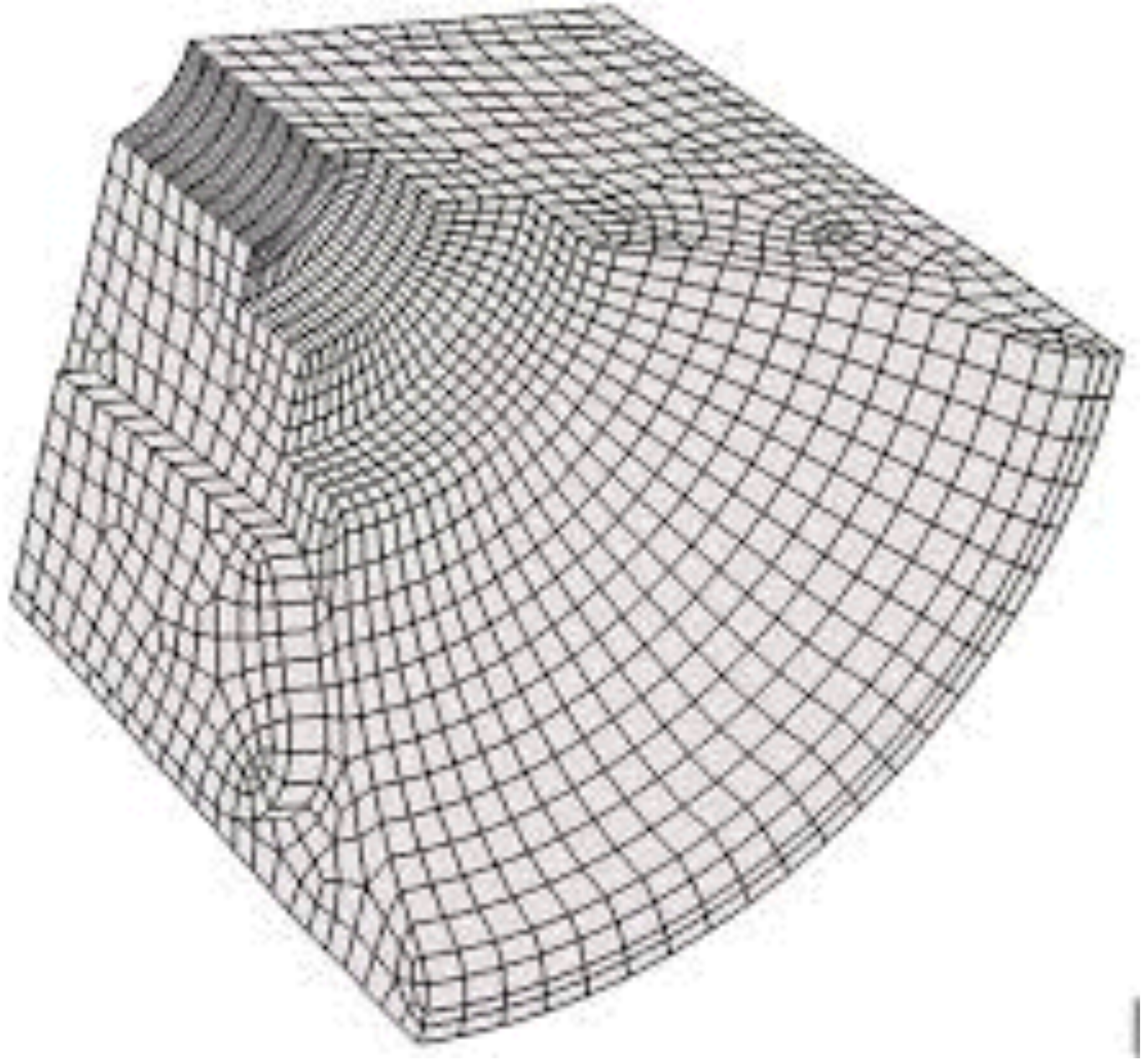
Colloquially

- In sci-vis we usually talk about geometry, thus:
  - **structured** means rectilinear grid (not *necessarily* uniform… but almost always).
  - **unstructured** means everything else (curvilinear grids, tetrahedra, hexahedra, points, etc.)

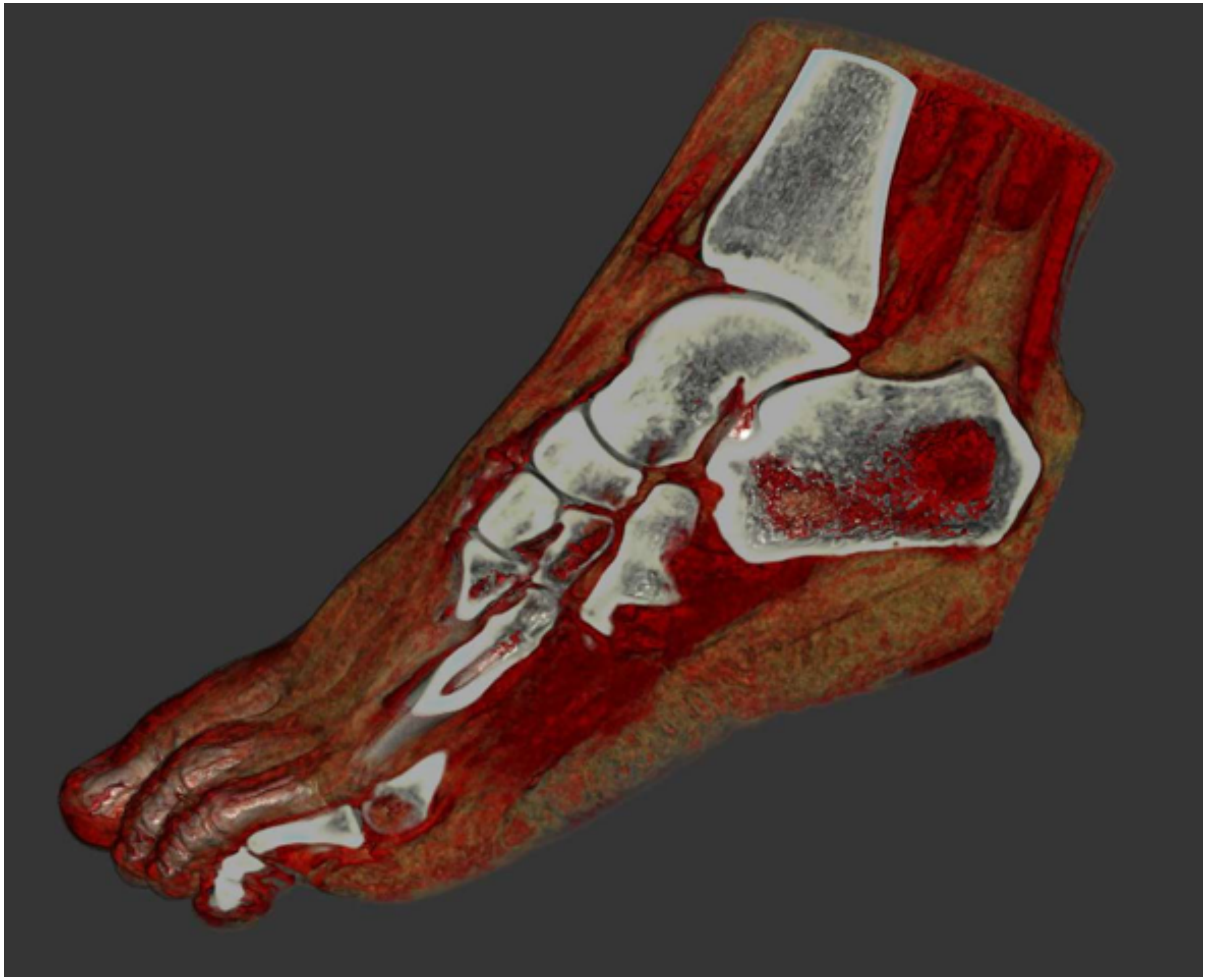
Is it (geometrically) structured or unstructured?



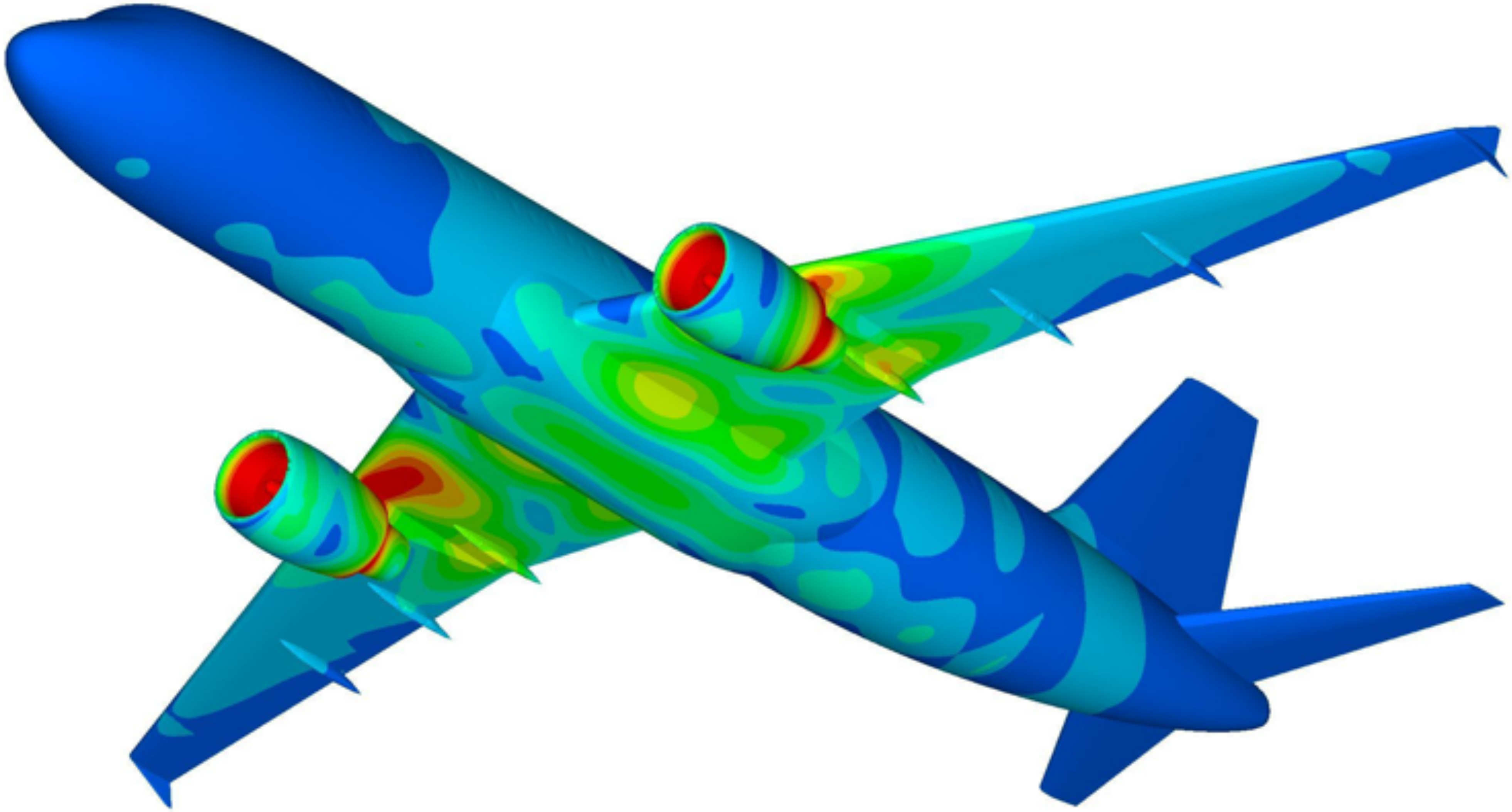
Is it (geometrically) structured or unstructured?



Is it (geometrically) structured or unstructured?



Is it (geometrically) structured or unstructured?



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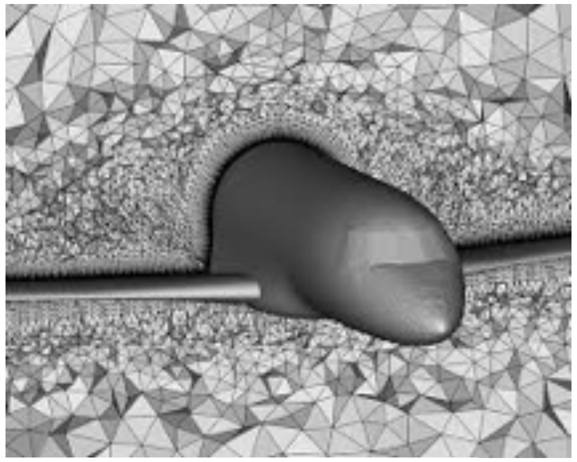
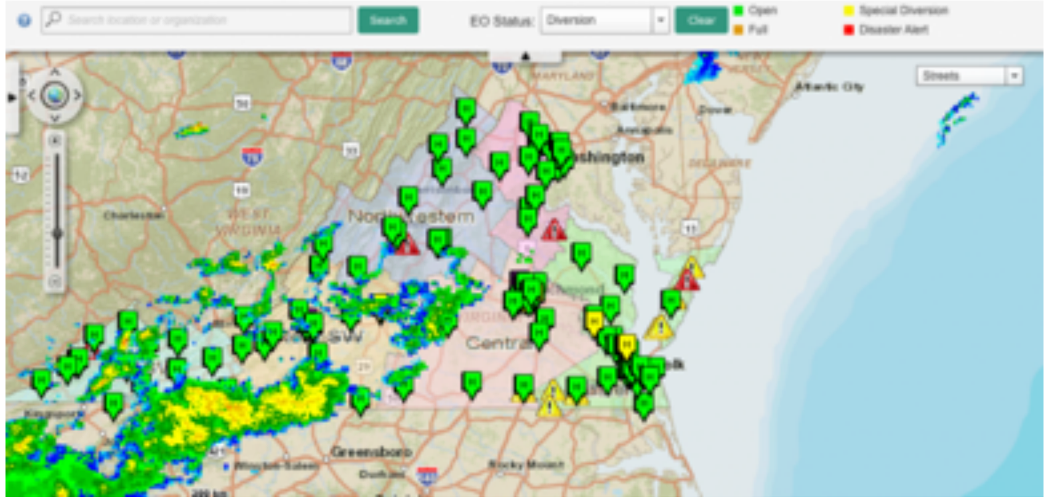
Non-field and other data

- In addition to structured/unstructured field data, you can have non-field geometry.
  - Boundary surface meshes
  - Atom positions, bonds, ribbons
- Non-geometric annotations
  - Especially in GIS.
- Visualization data models are complex!





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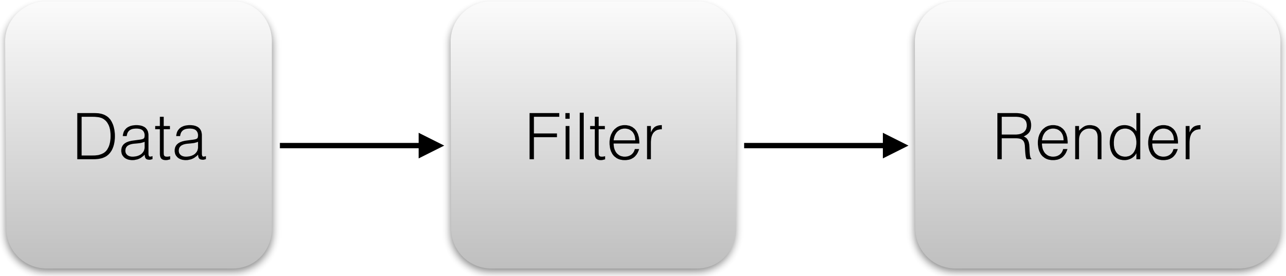
What do we do with these data?

- In computer graphics, life is “easy”
  - Have a triangle mesh, render it!
- Visualization is more than just rendering.
- Two approaches:
  - direct visualization:
    i.e. render from a (usually 3D) field directly
  - indirect visualization:
    i.e. convert the field to triangles and render those (usually with GPU rasterization)

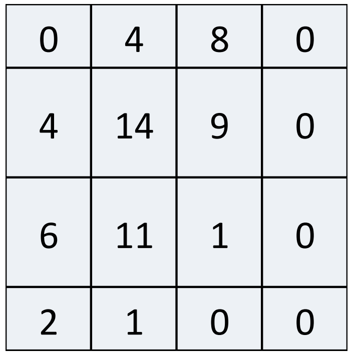
Indirect visualization



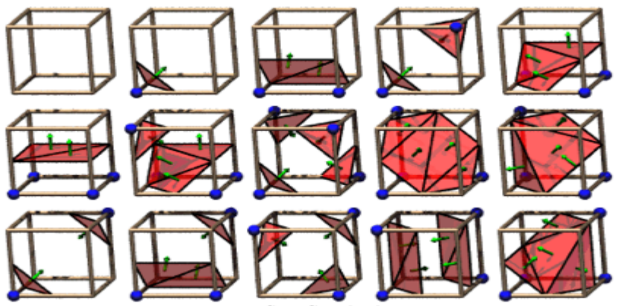
Data

Filter

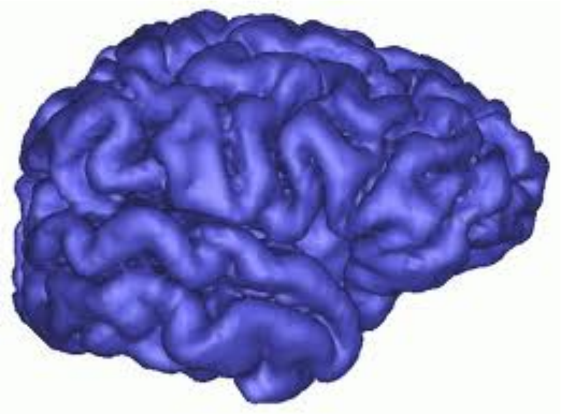
Render



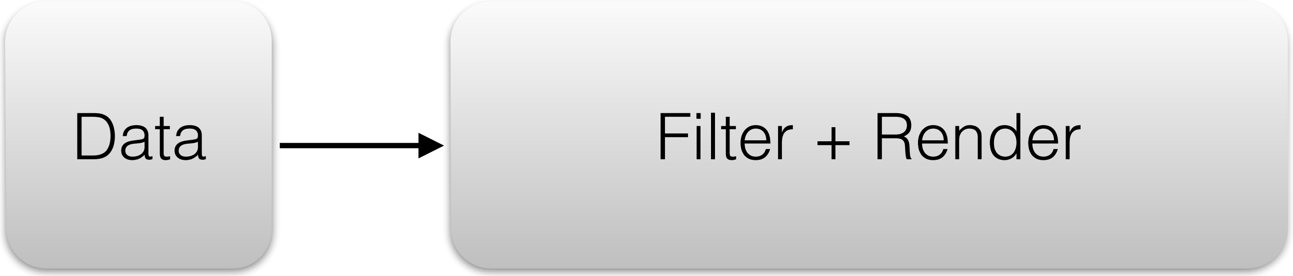
0	4	8	0
4	14	9	0
6	11	1	0
2	1	0	0



The 15 Cube Combinations



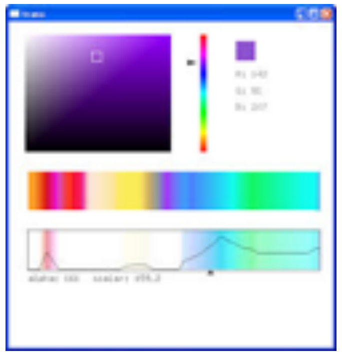
Direct visualization

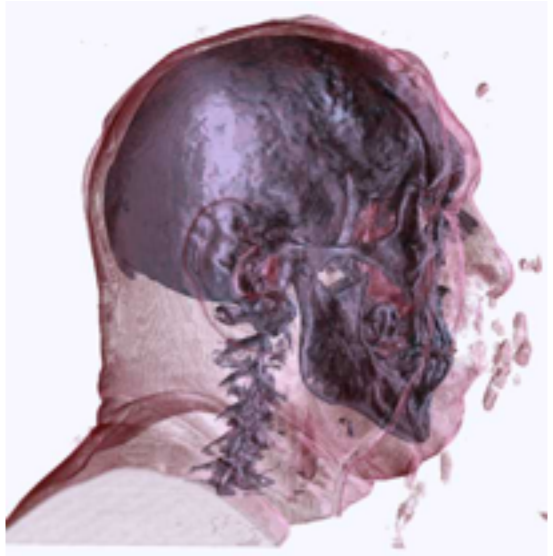


Data

Filter + Render

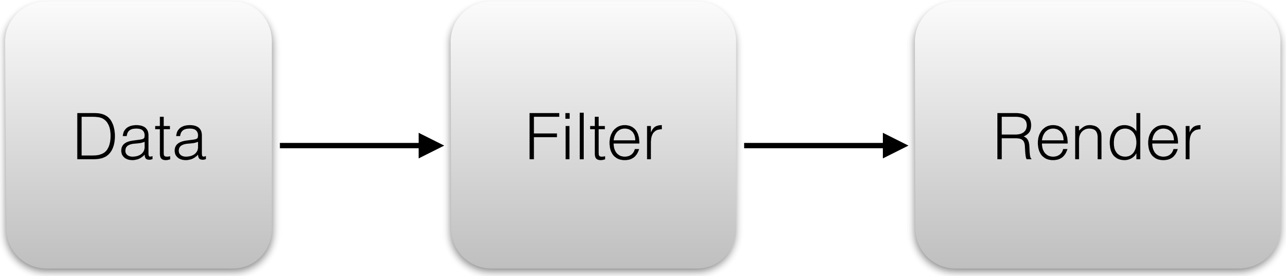
0	4	8	0
4	14	9	0
6	11	1	0
2	1	0	0





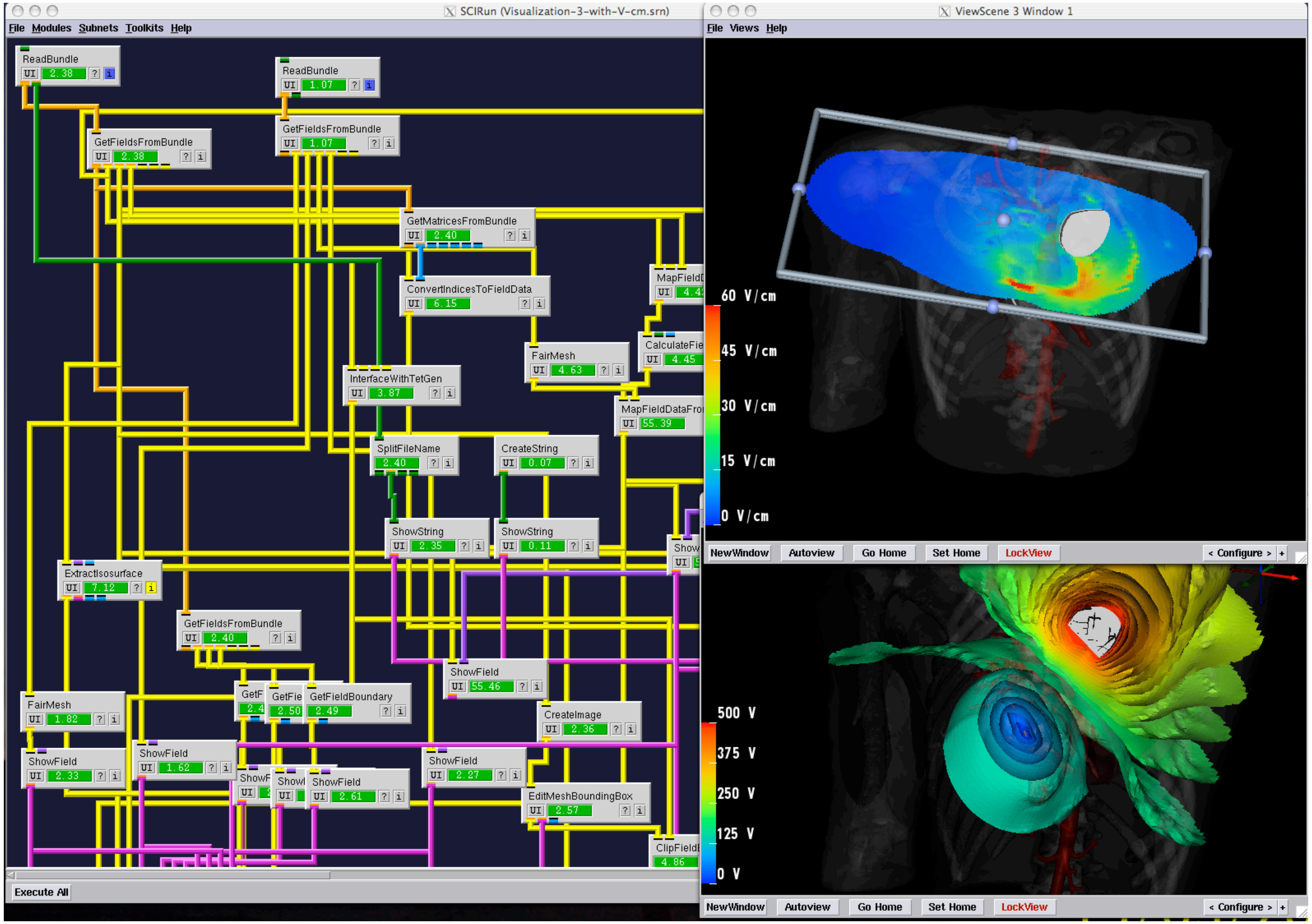
The visualization pipeline

- Even if we merge filtering and rendering, it is helpful to think of them as a chain of operations.



- Visualization workflows take the form of a flow chart, tree or network…

SCIRun



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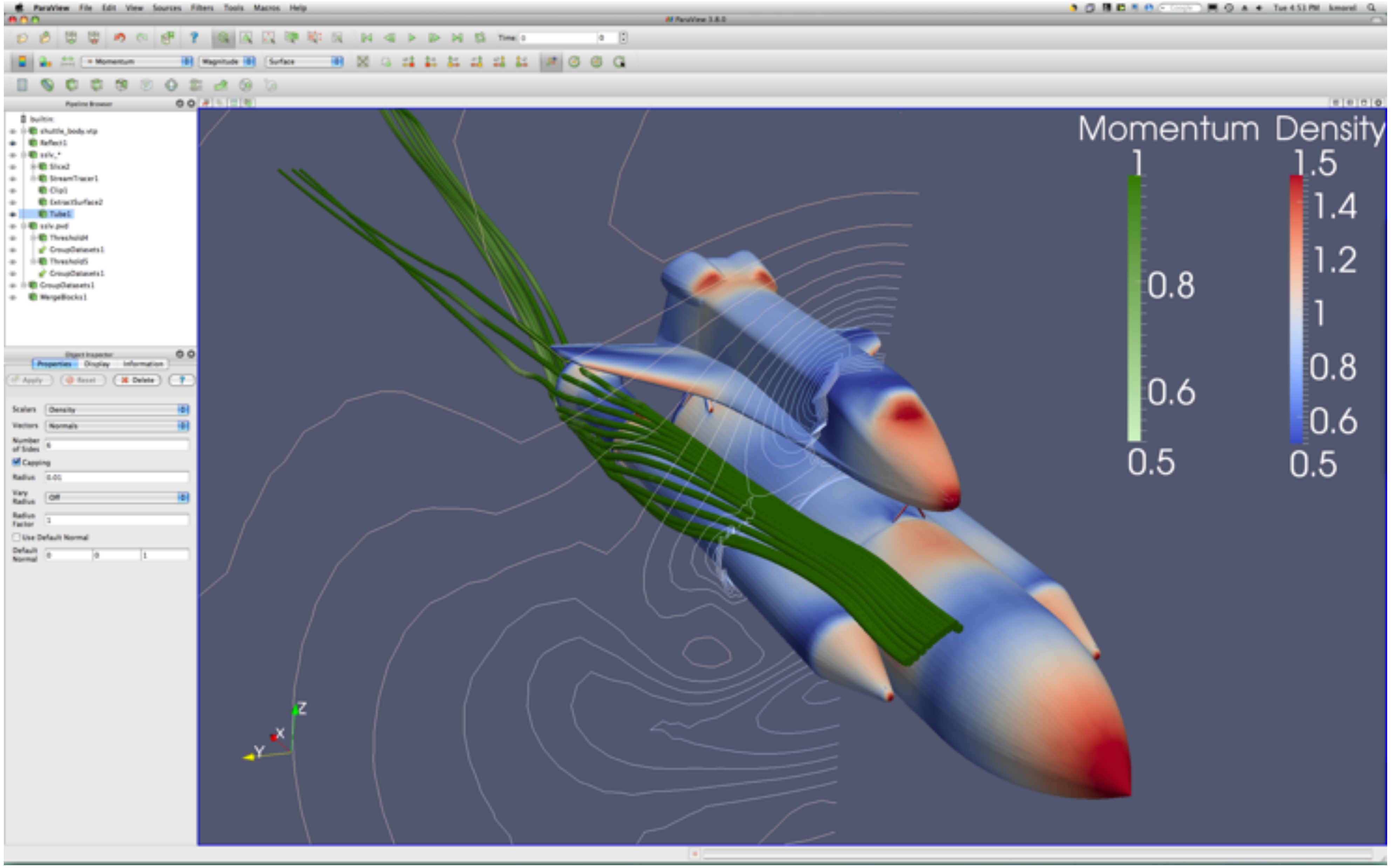
ParaView



Scalars: Density

Vectors: Normals

Number of Sides: 6

☑ Capping

Radius: 0.01

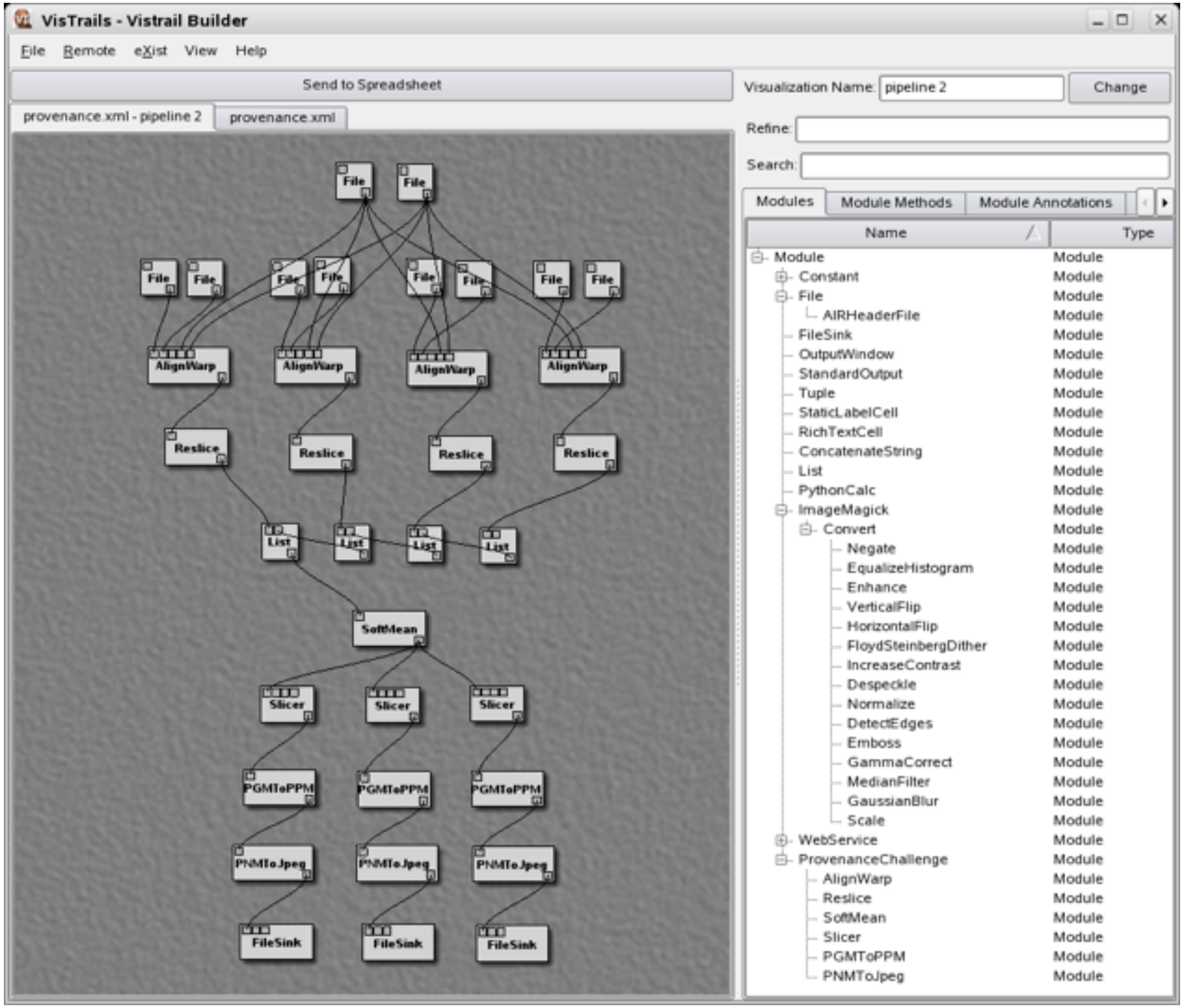
Vary Radius: Off

Radius Factor: 1

☐ Use Default Normal

Default Normal: 0 0 1

VisTrails



Visualization Name: pipeline 2

Refine:

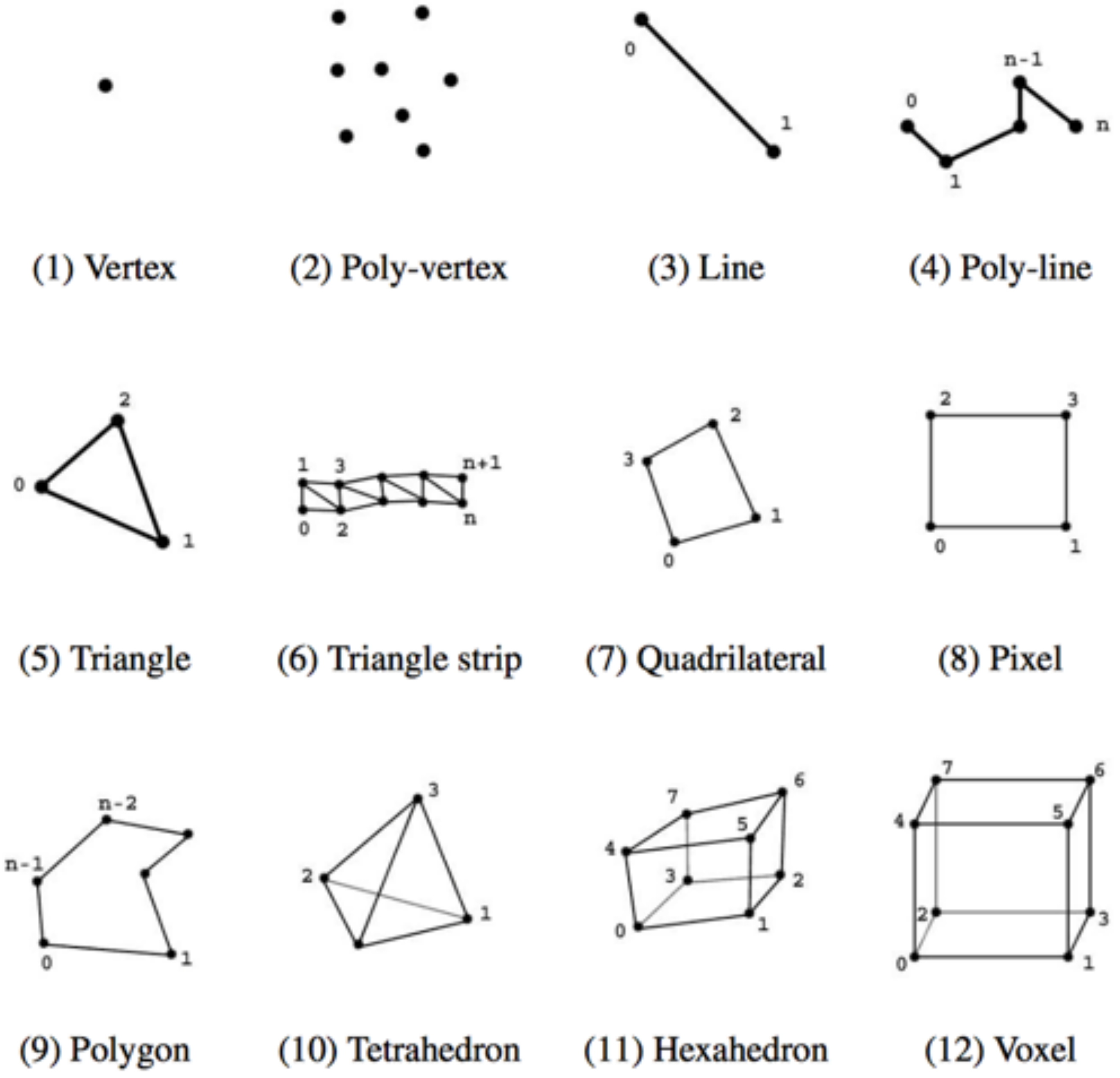
Search:

Name	Type
Module	Module
Constant	Module
File	Module
AIRHeaderFile	Module
FileSink	Module
OutputWindow	Module
StandardOutput	Module
Tuple	Module
StaticLabelCell	Module
RichTextCell	Module
ConcatenateString	Module
List	Module
PythonCalc	Module
ImageMagick	Module
Convert	Module
Negate	Module
EqualizeHistogram	Module
Enhance	Module
VerticalFlip	Module
HorizontalFlip	Module
FloydSteinbergDither	Module
IncreaseContrast	Module
Despeckle	Module
Normalize	Module
DetectEdges	Module
Emboss	Module
GammaCorrect	Module
MedianFilter	Module
GaussianBlur	Module
Scale	Module
WebService	Module
ProvenanceChallenge	Module
AlignWarp	Module
Reslice	Module
SoftMean	Module
Slicer	Module
PGMToPPM	Module
PNMToJpeg	Module

VTK

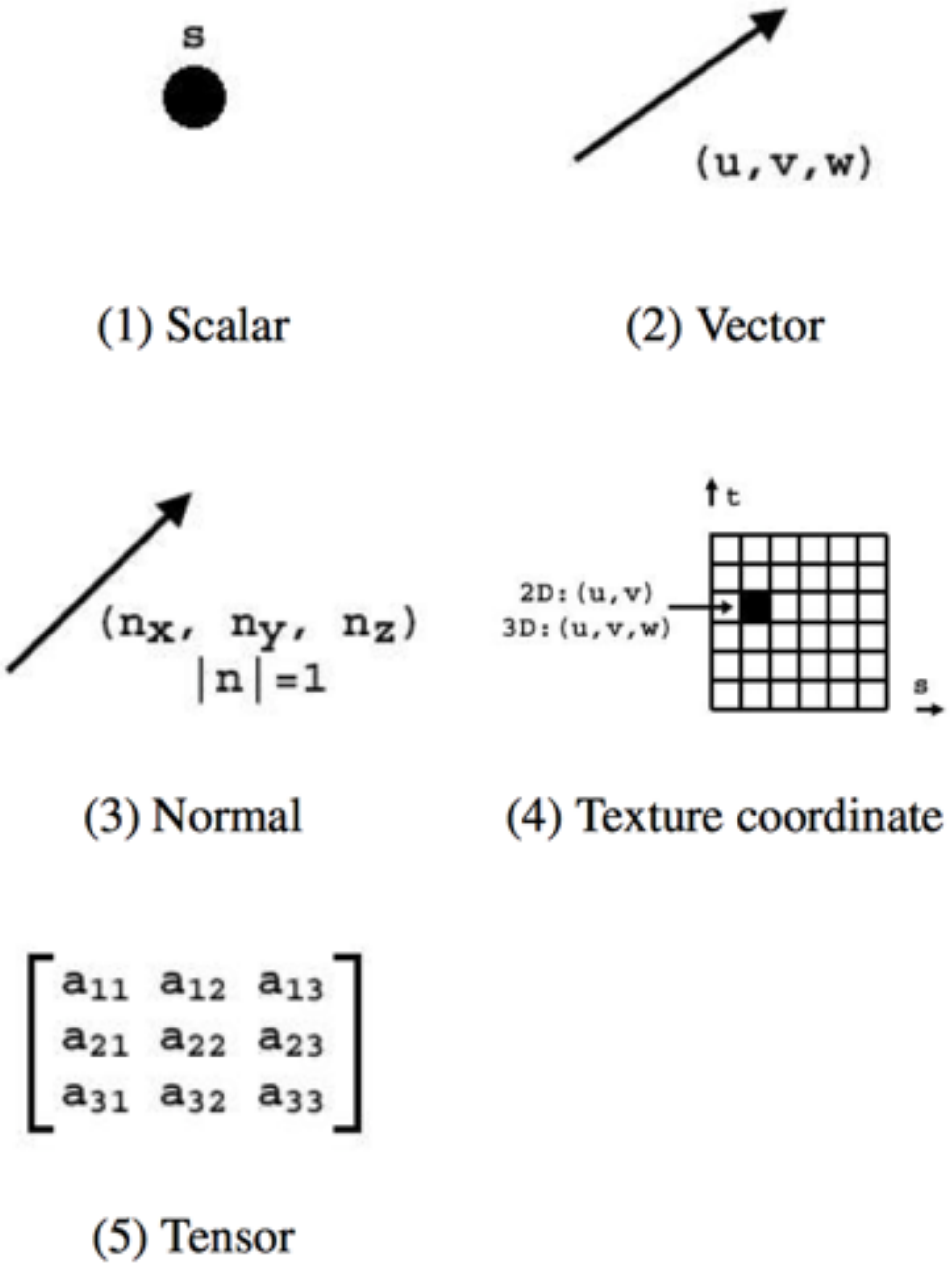
- http://www.vtk.org, open-source, developed and maintained by Kitware.
- The standard-bearer API for general-purpose scientific visualization
  - Full-fledged data model for structured, unstructured, particle data
  - Marching cubes, cut/clip planes, streamlines, etc.
  - Hundreds of other analysis filters
  - Numerous readers for common scientific formats
- Call as a library from C++, Java, Python, Tcl/Tk
- Limitations:
  - no UI — you need to code (or at least, script) your workflows.
  - No distributed rendering (see Paraview, VisIt)
  - does not exploit latest OpenGL features (OpenGL 2.x support currently in the works!)
  - filters and renderers do not support all "exotic" data structures (e.g., spectral finite elements)
  - data model can be "heavy", memory-inefficient — but it nearly always works!

Cell types in VTK



S. Bruckner, “Data Structures in the Visualization Toolkit.”

Attribute types in VTK



(1) Scalar

(2) Vector

(3) Normal

(4) Texture coordinate

(5) Tensor

S. Bruckner, “Data Structures in the Visualization Toolkit.”

Simple data flow in VTK

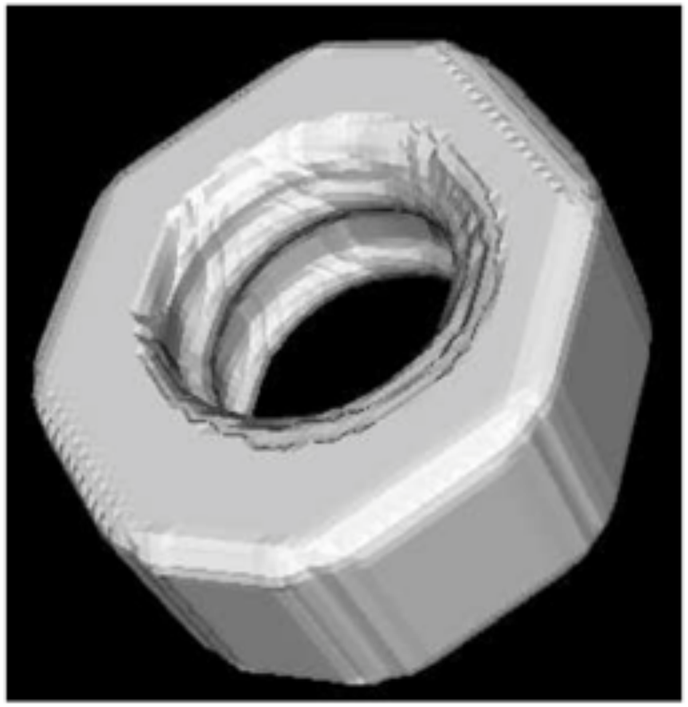


Figure 7: Resulting image for program 3.2

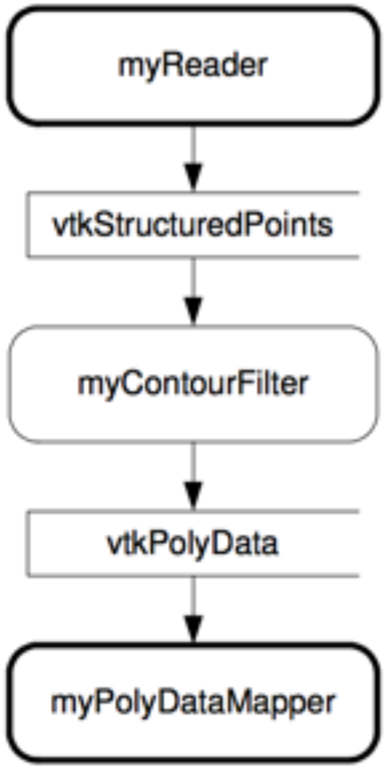


Figure 8: Data-flow chart for program 3.2

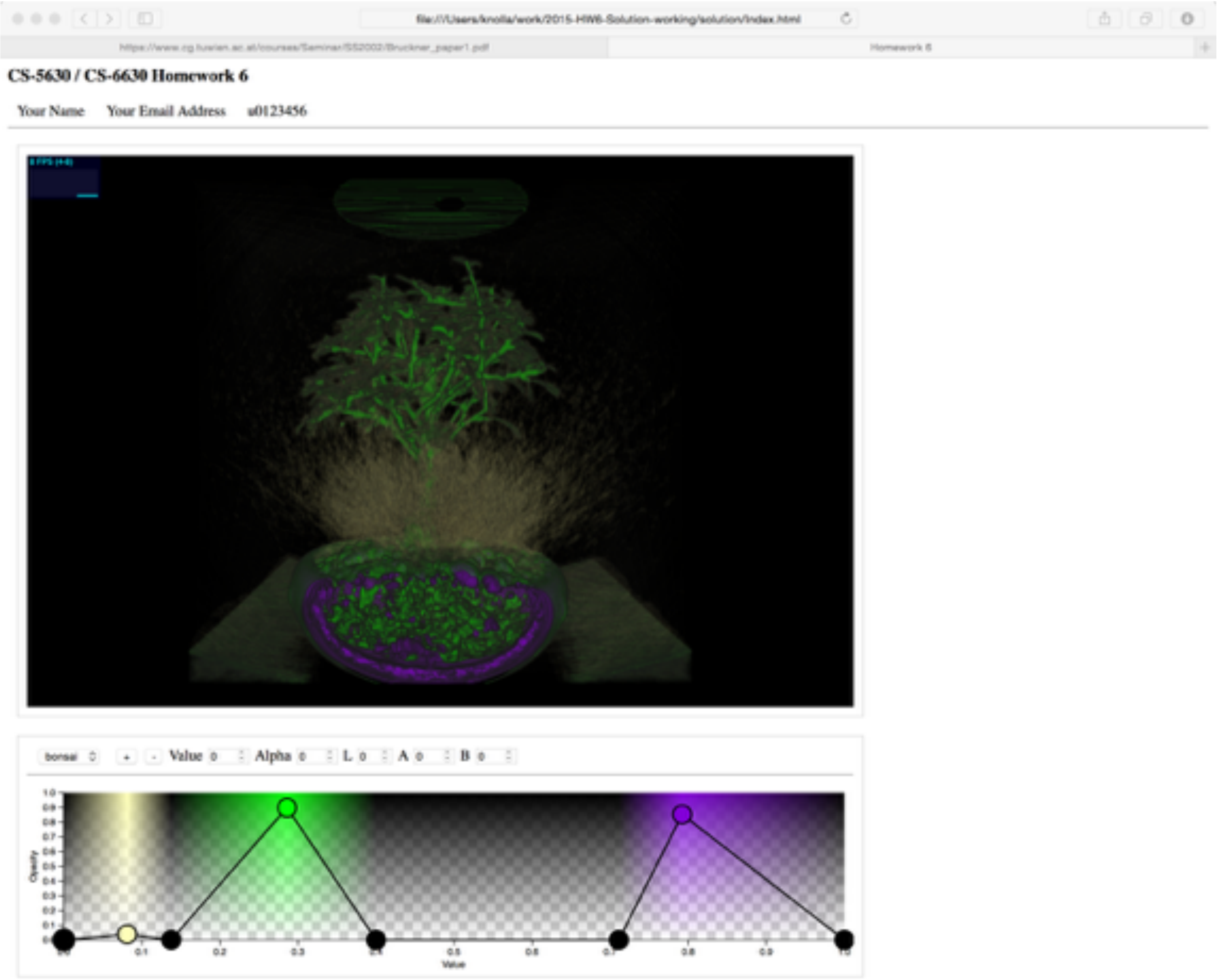
S. Bruckner, "Data Structures in the Visualization Toolkit."

In practice…

- Most of the time, we want to visualize one or two scalar fields at a time, in 2D or 3D
- The type of visualization we do depends more on **context** than the MxN chart of fields, or even type of data. E.g.,
  - Volume rendering for 3D continuous phenomena
  - Heatmaps in 2D, GIS
  - Glyphs to represent explicit geometry (e.g. molecular vis, vectors or tensors)
  - Geometric abstractions and special geometry where appropriate (ribbons, streamlines, etc.)
- More on these later!

Homework 6 preview

- volume rendering in WebGL and Javascript
- D3 transfer function editor
- (extra credit) phong lighting



file:///Users/knolla/work/2015-HW6-Solution-working/solution/index.html
https://www.cg.tuwien.ac.at/courses/Seminar/SS2002/Bruckner_paper1.pdf
Homework 6

CS-5630 / CS-6630 Homework 6

Your Name Your Email Address u0123456

Value 0 Alpha 0 L 0 A 0 B 0

Opacity
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Value

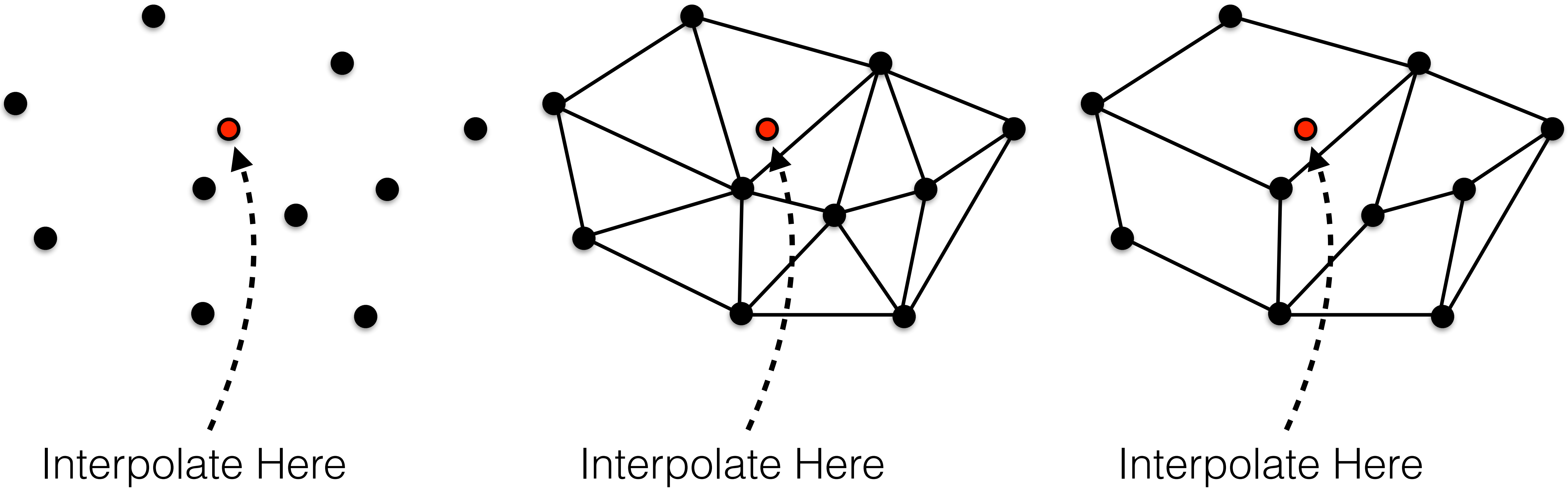
Next sci-vis lecture: Oct 22

- Interpolation
- Isosurfaces and Marching cubes
- Volume rendering
- Introduction to GLSL / ELSL (for HW6).

Interpolation

Mesh Choice Impacts How the Continuous Data is Interpreted

- Two key questions:
    - Sampling, or the choice of where attributes are measured
    - Interpolation, or how to model the attributes in the rest of space



Interpolation

- **Continuous** reconstruction of **discrete** input data

position

$$F : \mathbb{R}^n \longrightarrow \mathbb{R}^m$$

$$(\mathbf{x}_i, f_i)$$

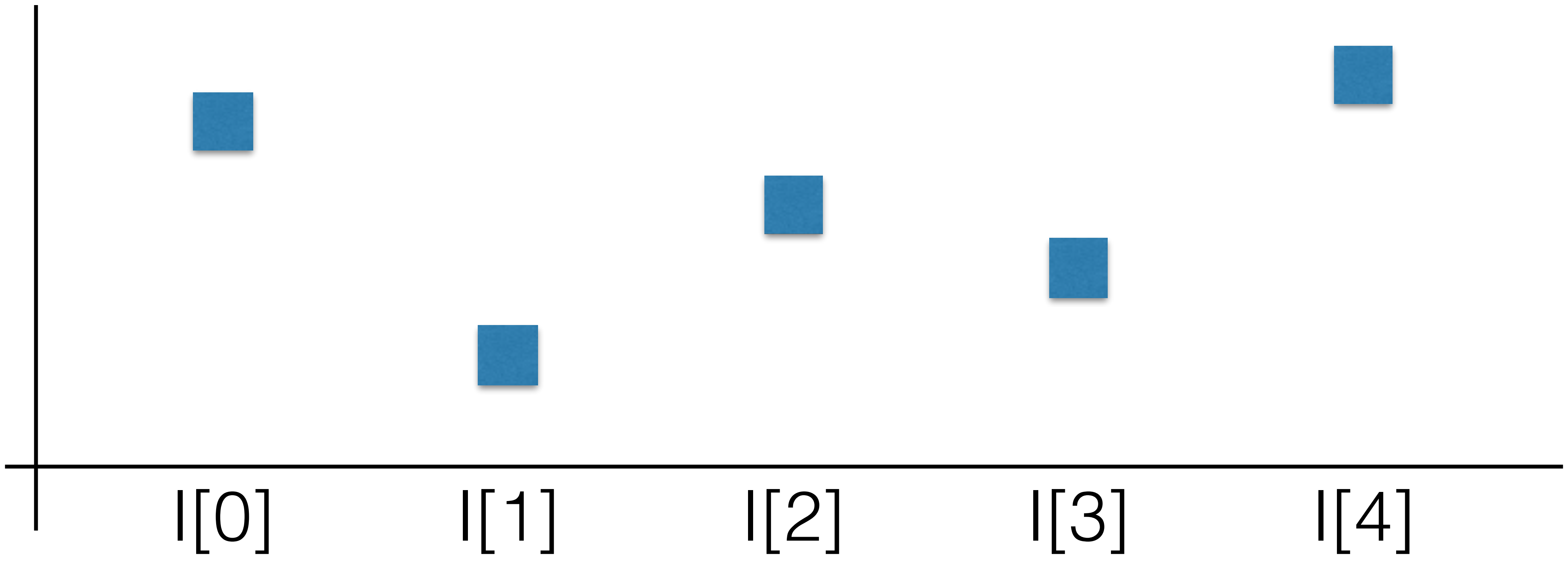
value

$$\forall i \in \{1, .., n\}, F(\mathbf{x}_i) = f_i$$

- Depends on grid structure (when available)
- Interpolation vs. approximation

Nearest Neighbor Interpolation

- Consider a 1-dimensional, grayscale image I spread horizontally
- What value is I[1.3] ?



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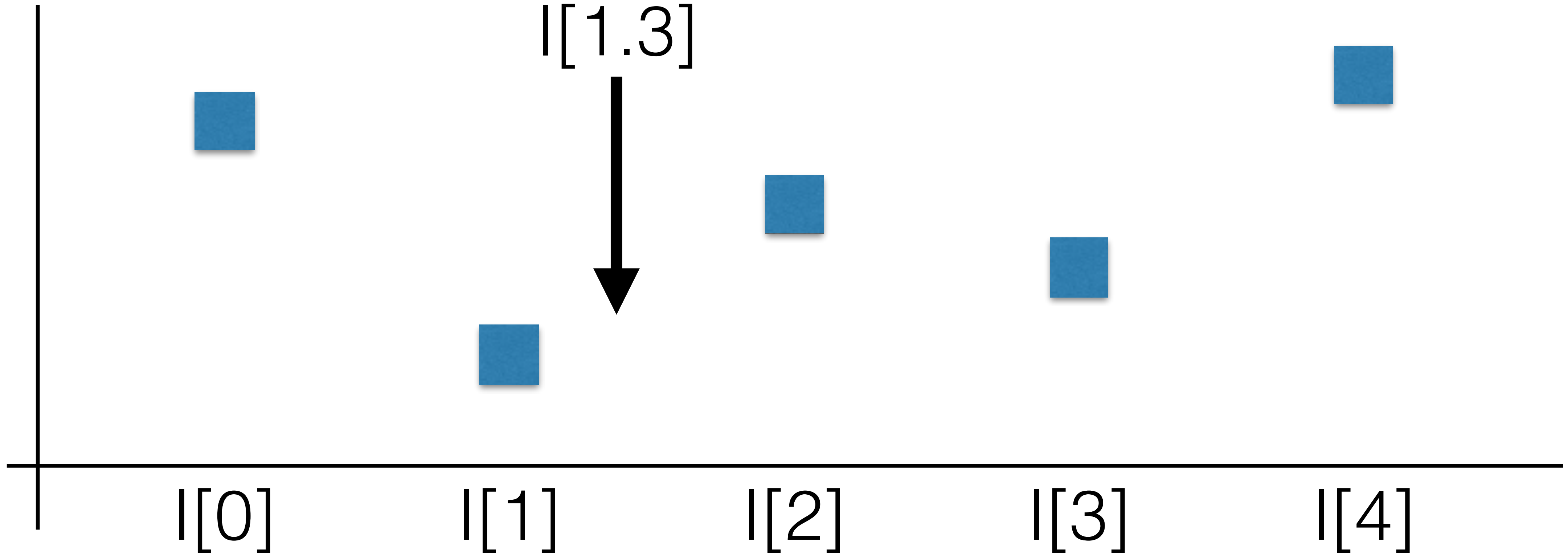

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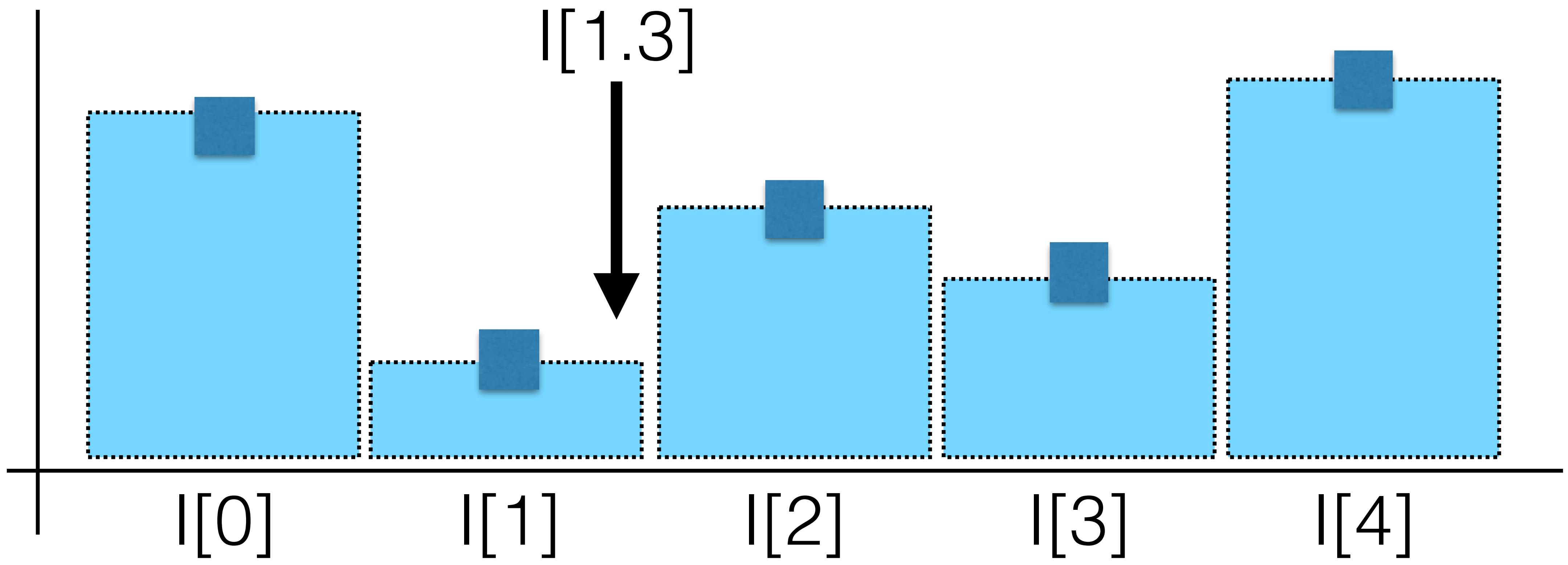
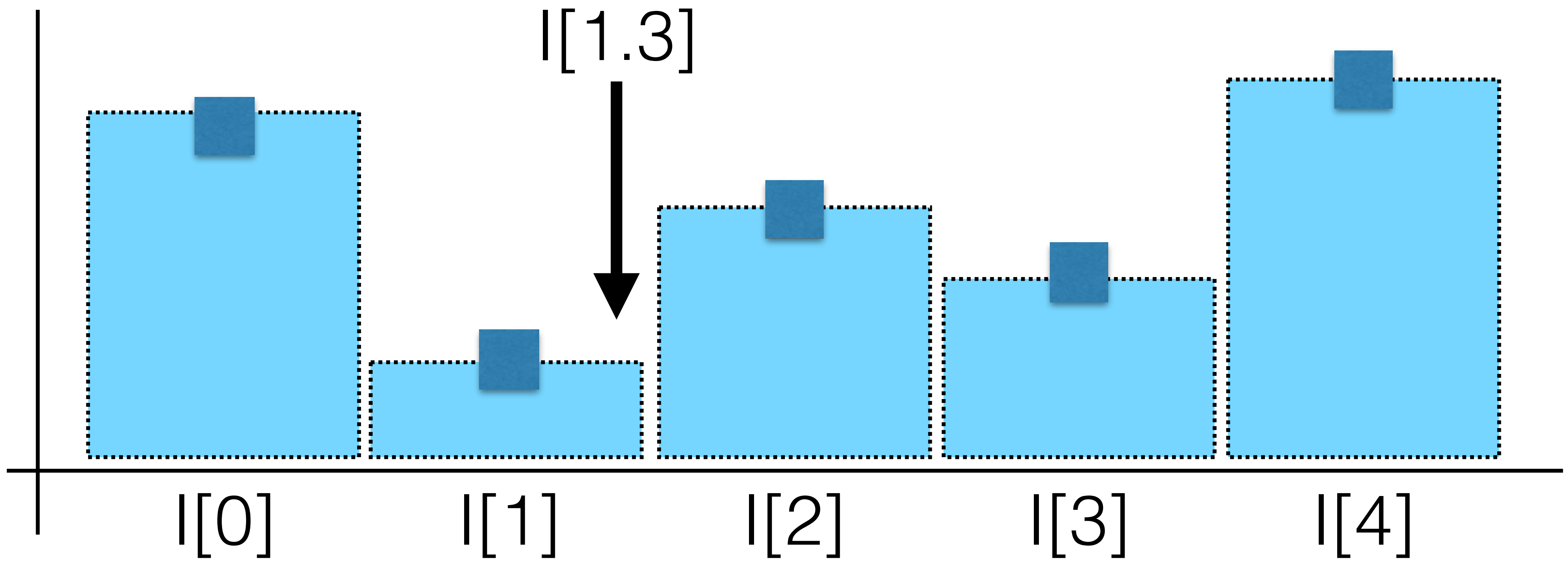


Nearest Neighbor Interpolation

- Consider a 1-dimensional, grayscale image I spread horizontally
- What value is I[1.3] ?
  - I[1.3] = I[round(1.3)] = I[1]



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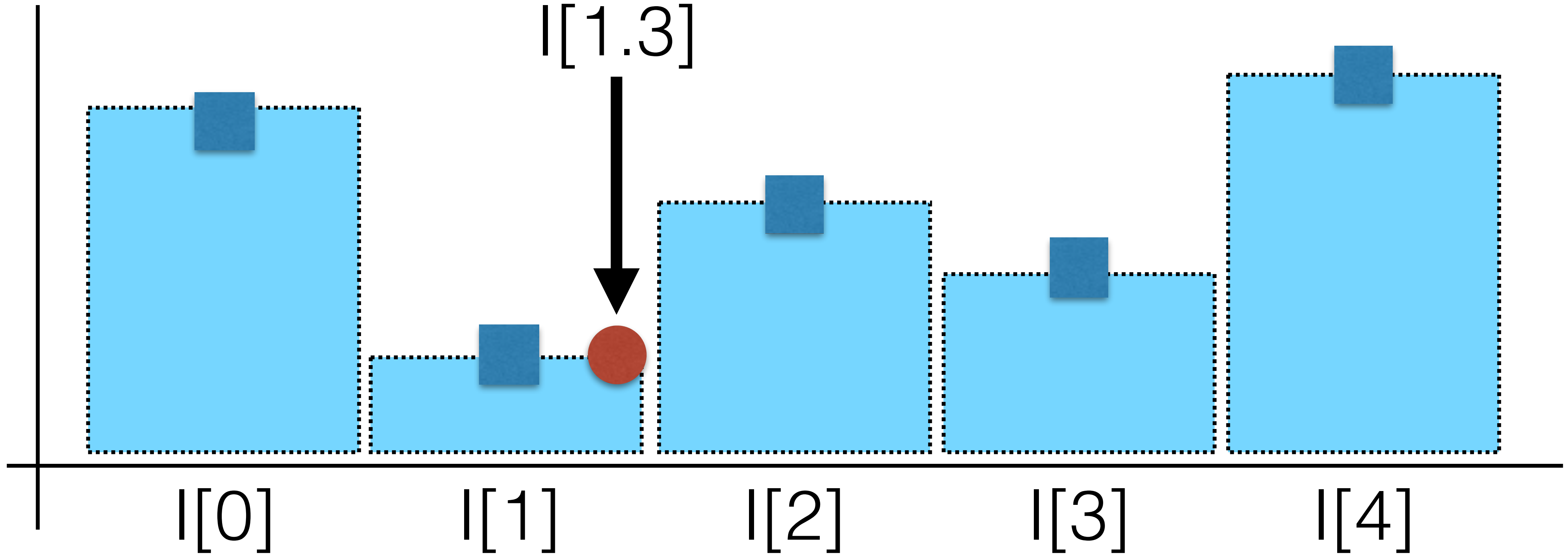

Linear Interpolation

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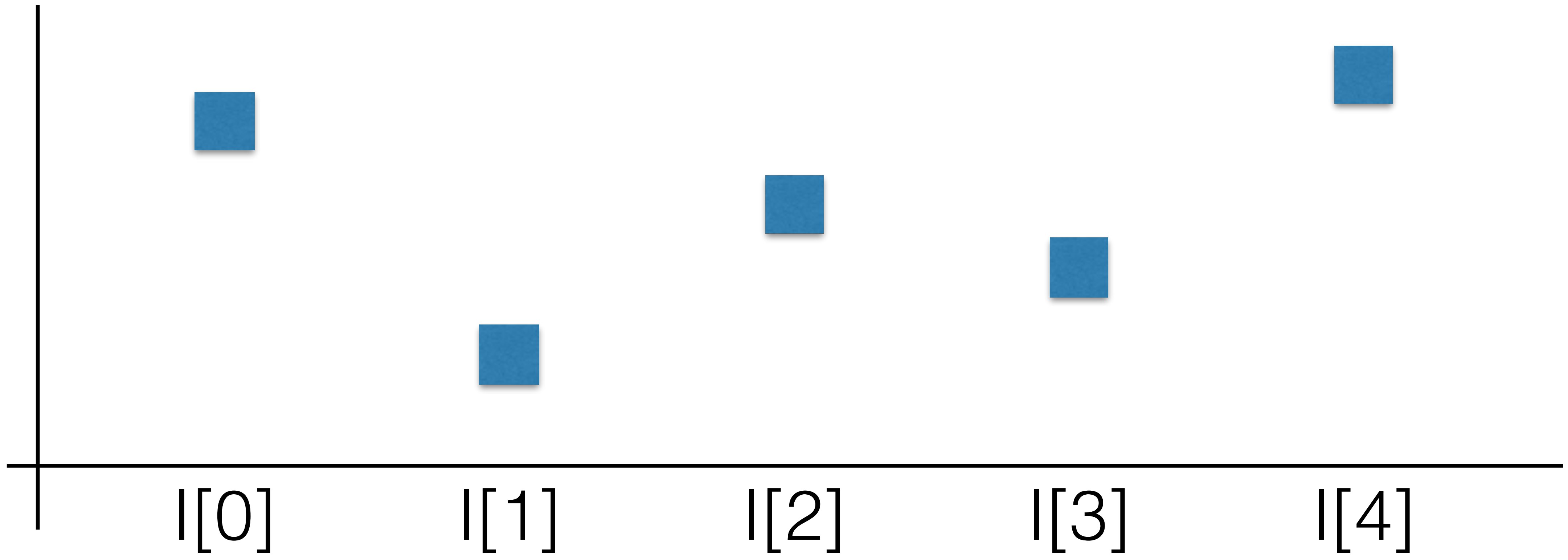

Linear Interpolation

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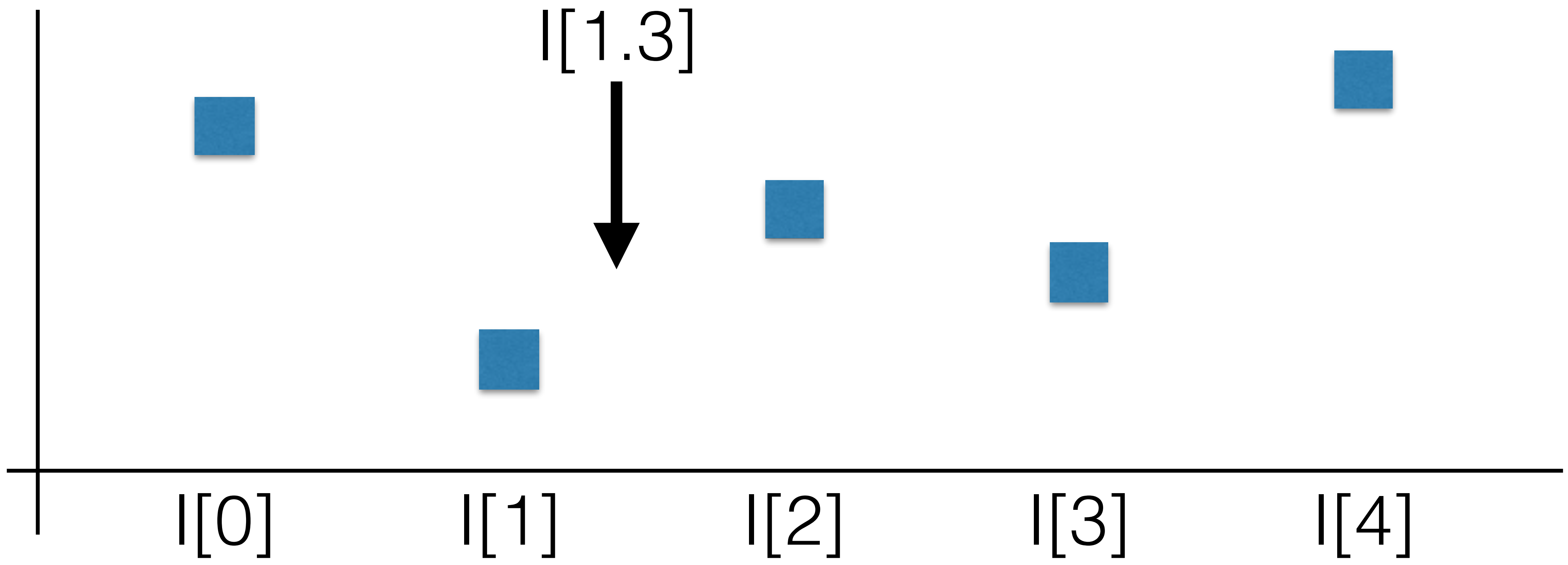

Linear Interpolation

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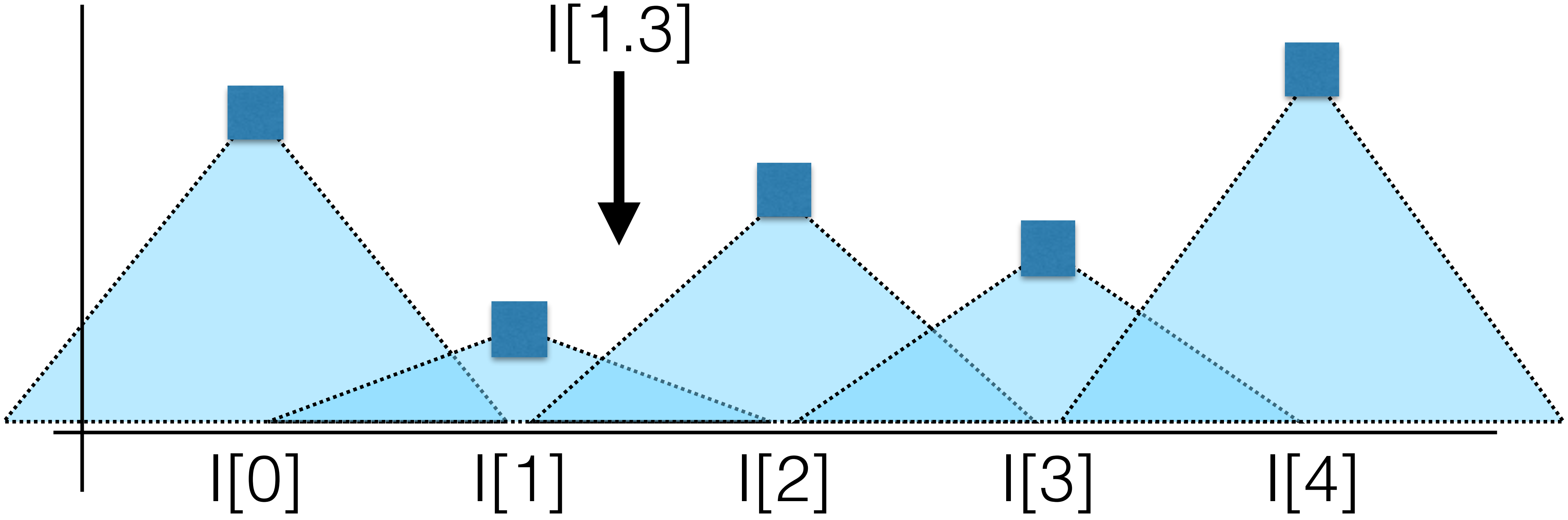

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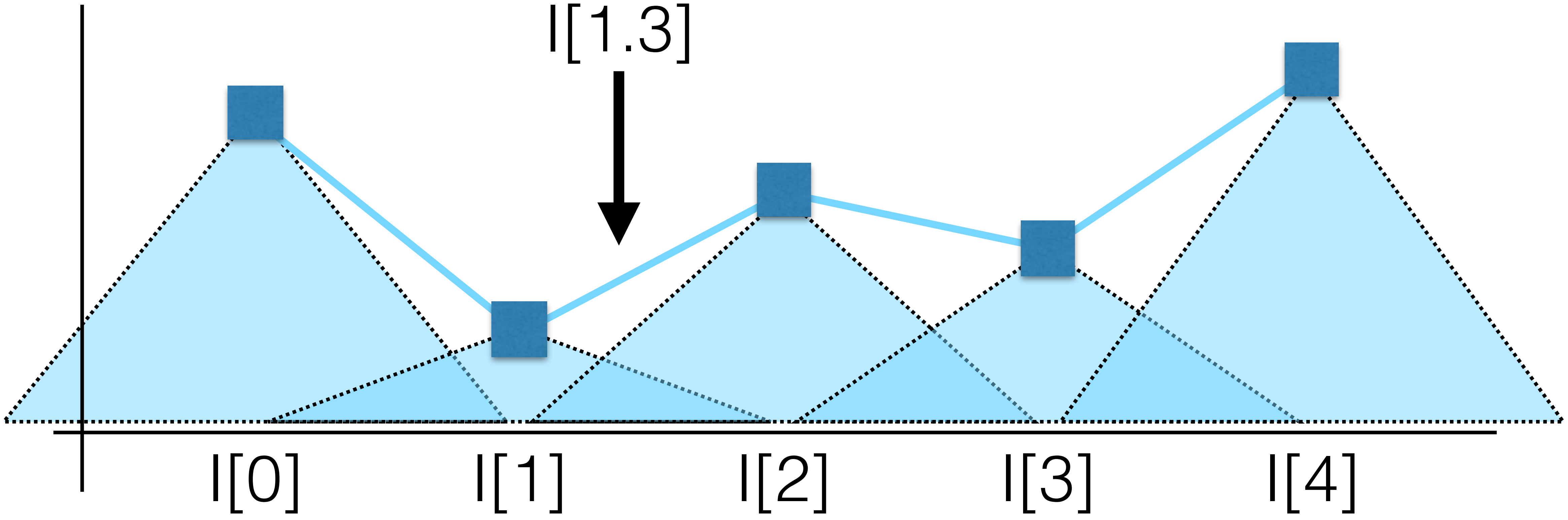
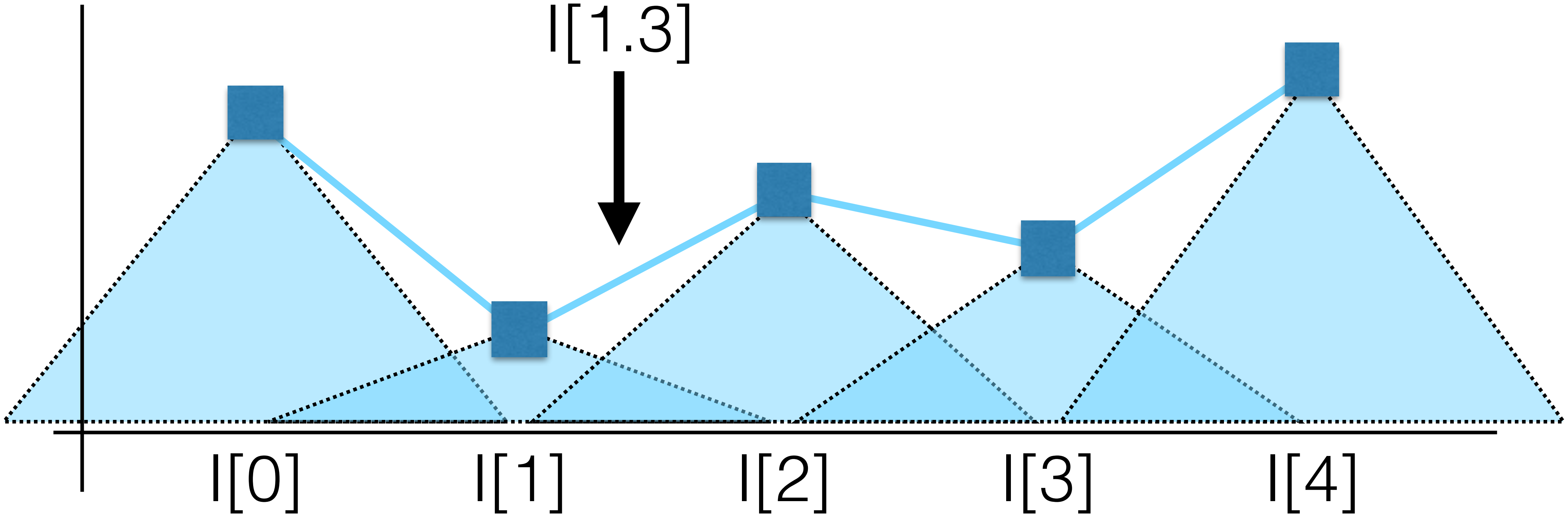


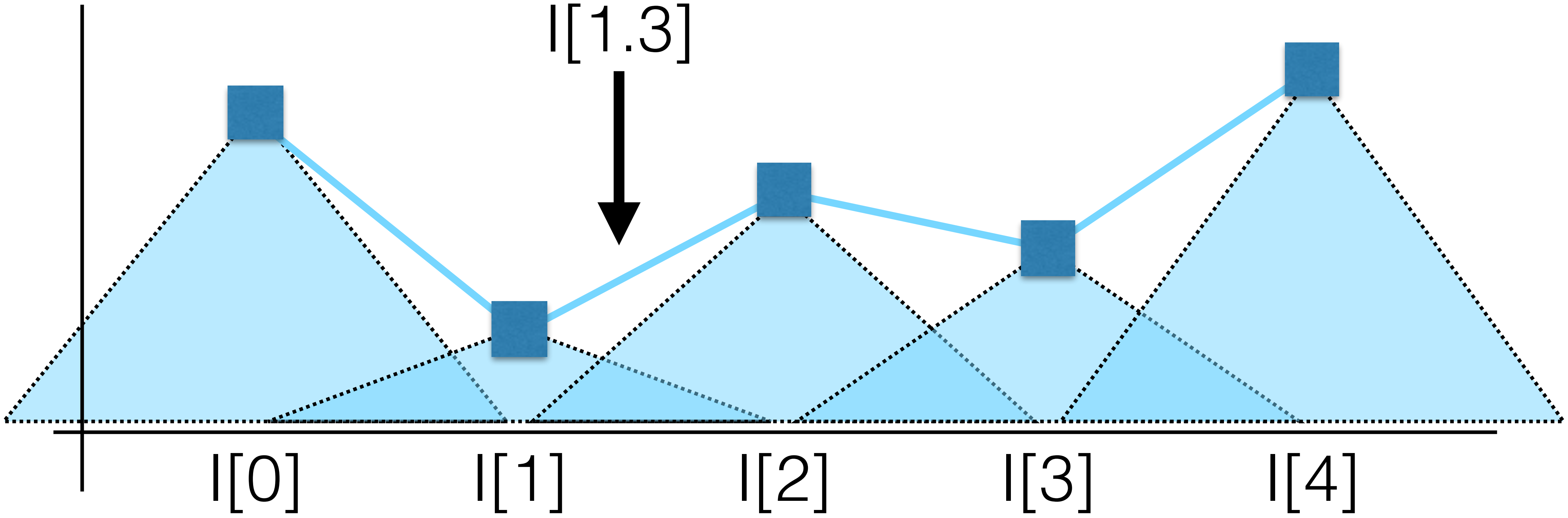
Linear Interpolation

- Consider a 1-dimensional, grayscale image I spread horizontally
- What value is I[1.3] ?
  - Let s = 1.3 - round(1.3)



Linear Interpolation

- Consider a 1-dimensional, grayscale image I spread horizontally
- What value is I[1.3] ?
    - Let s = 1.3 - round(1.3)
    - I[1.3] = 0.7*I[1] + 0.3*I[2] = (1-s)*I[1] + s*I[2]



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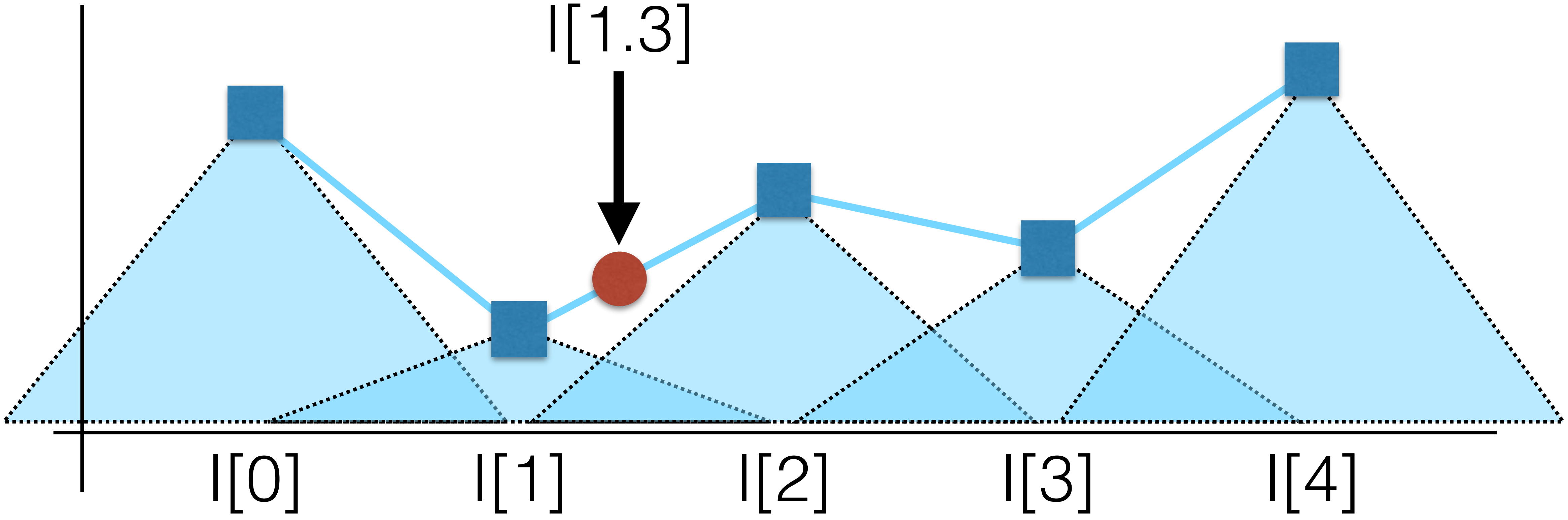
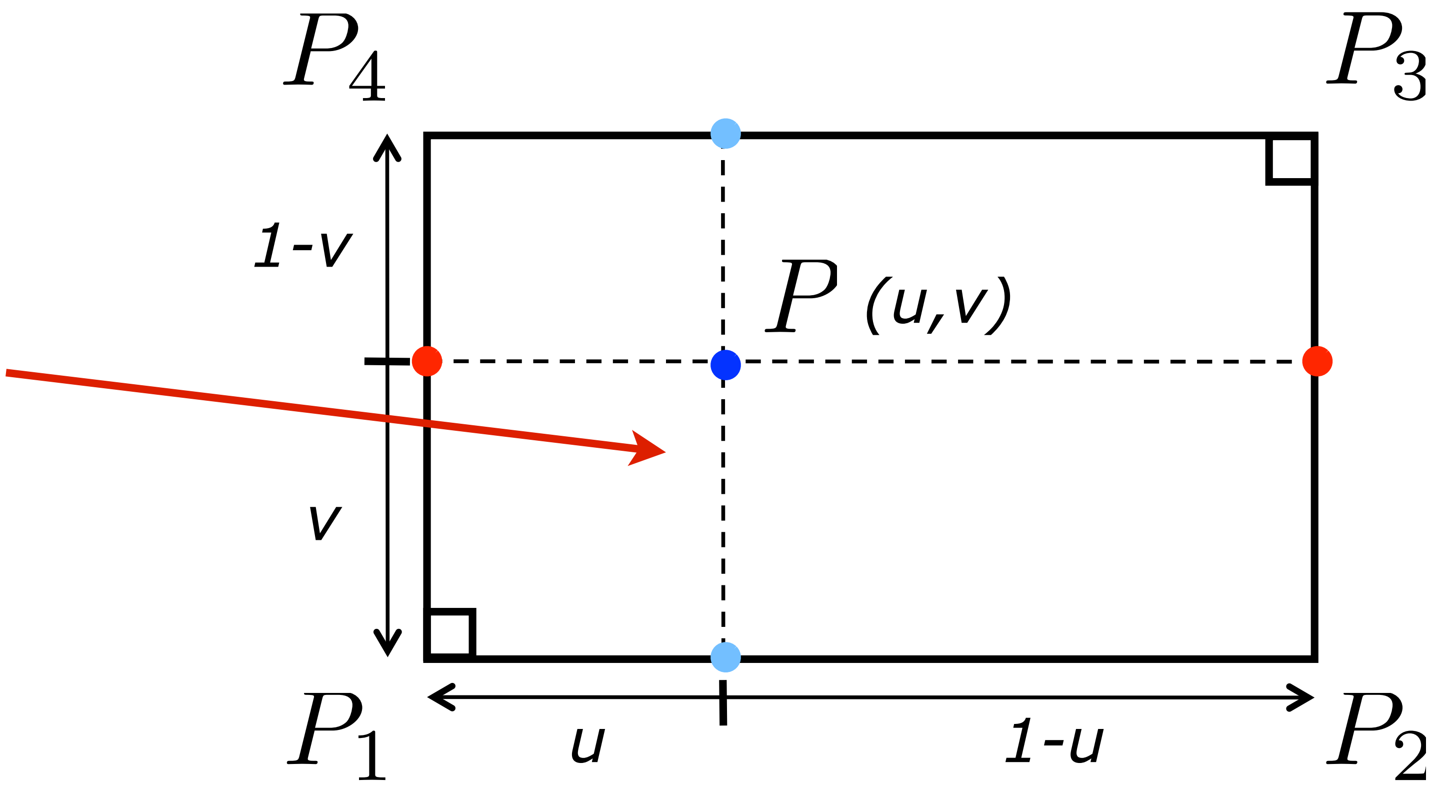


Bilinear Interpolation

- In rectangle

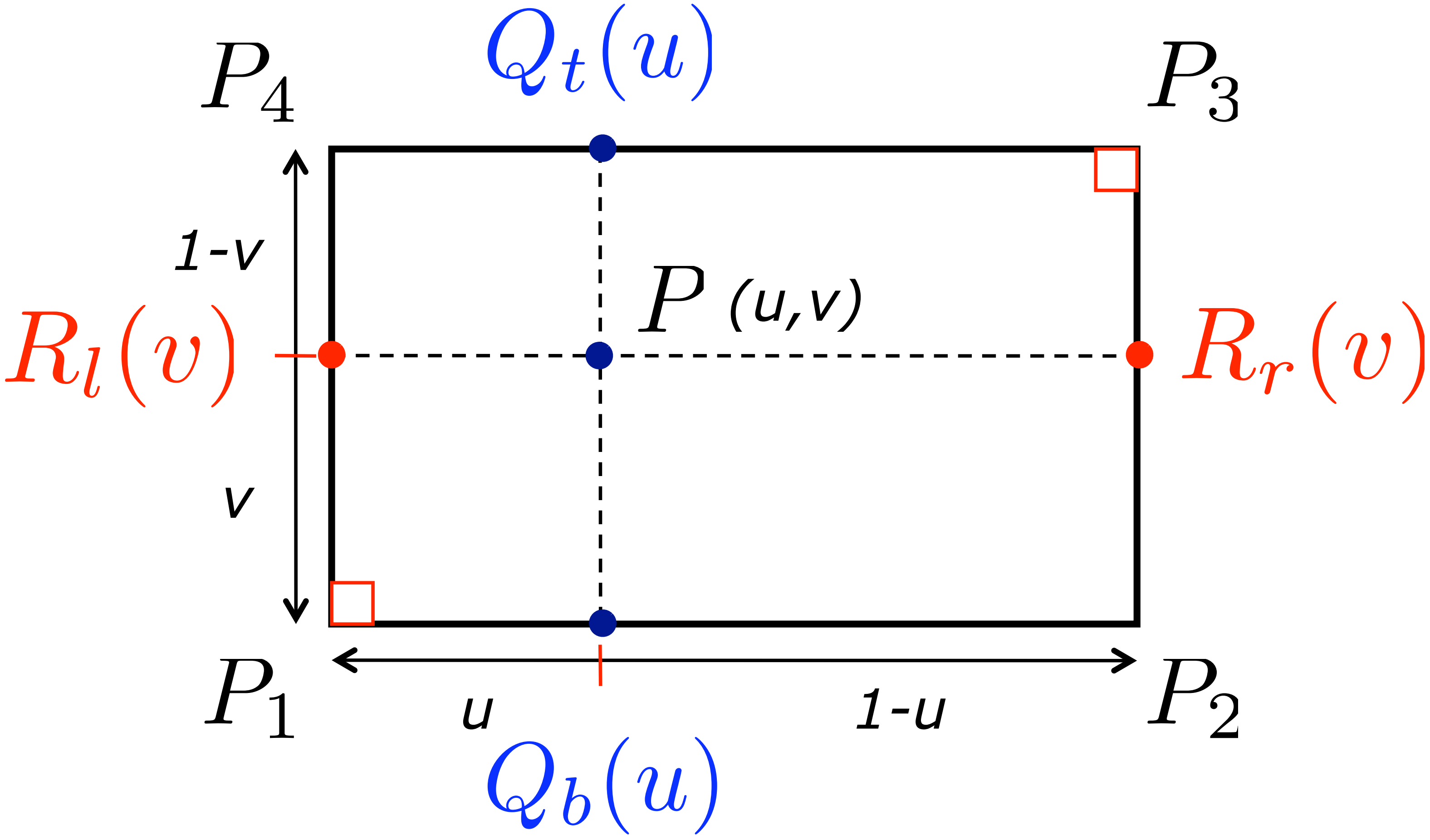
Combination of two consecutive linear interpolation



Bilinear Interpolation

- In rectangle

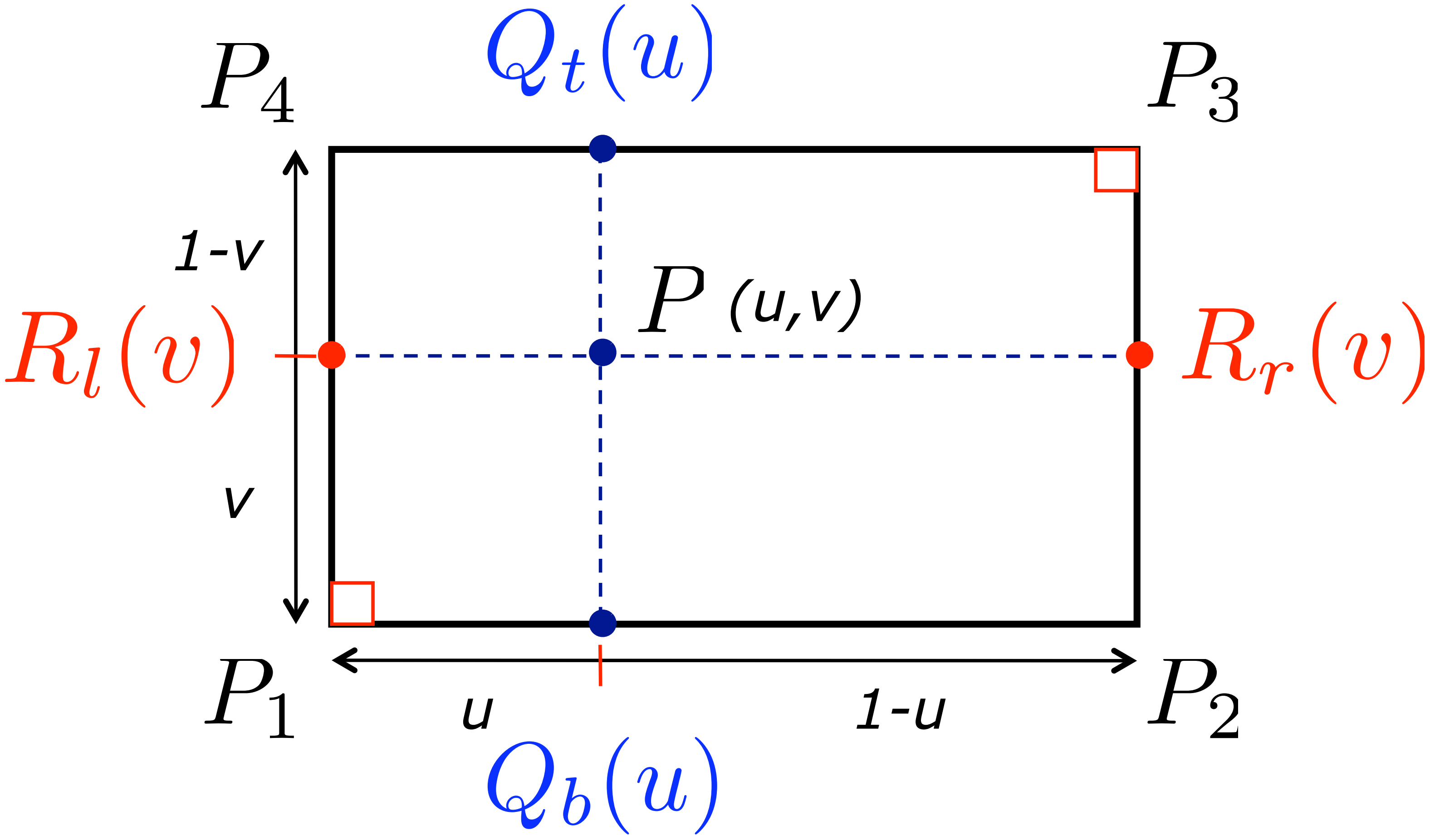
$$\boxed{\begin{aligned} P &= (1-v)Q_b(u) + vQ_t(u) \\ &= (1-u)R_l(v) + uR_r(v) \end{aligned}}$$



Bilinear Interpolation

- In rectangle

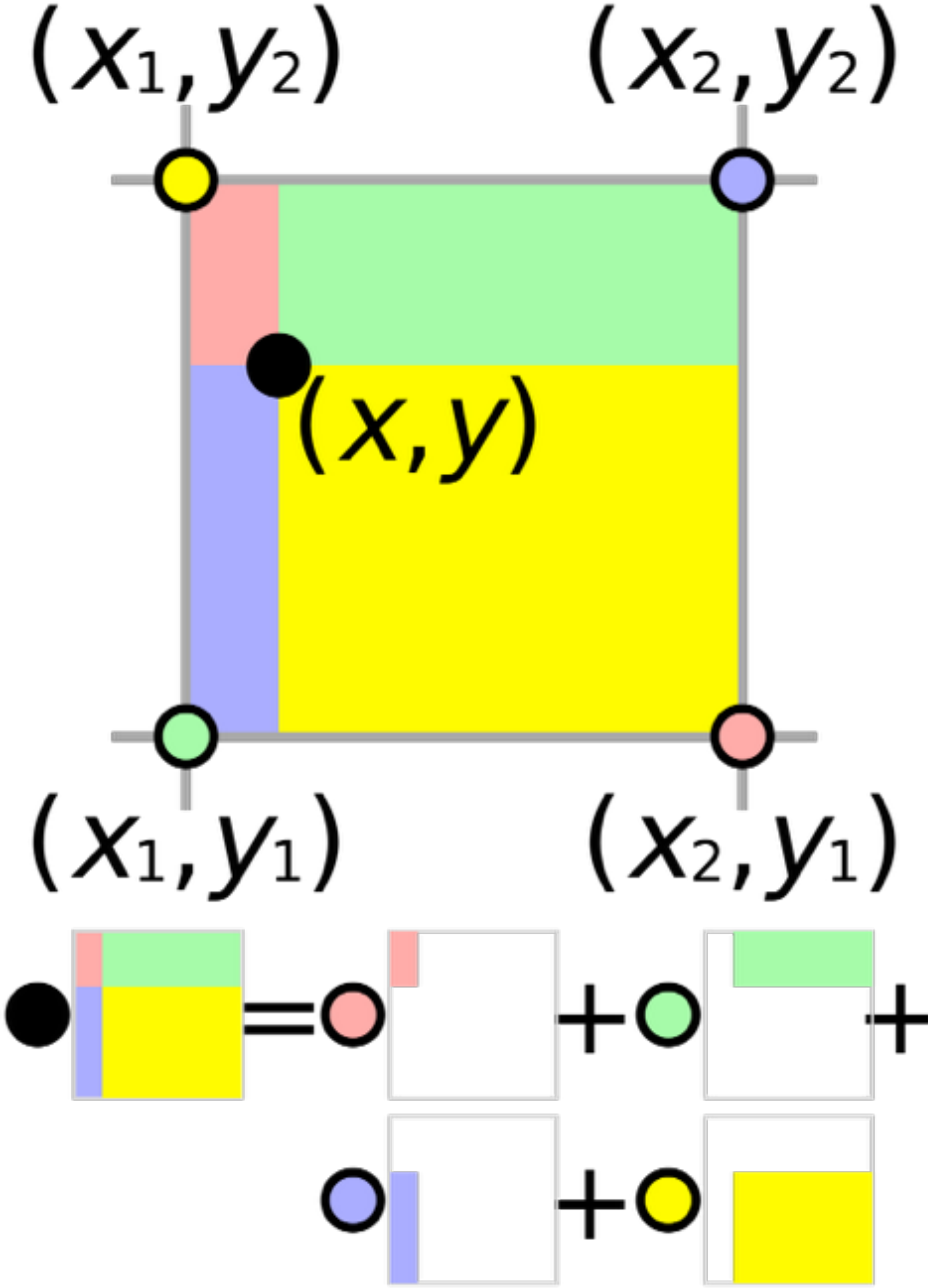
$$\boxed{\begin{aligned} P = P_1 + u(P_2 - P_1) + v(P_4 - P_1) \\ +uv(P_1 - P_2 + P_3 - P_4) \end{aligned}}$$



Bilinear Interpolation

- Alternate interpretation is a weighted sum of the four pixel values

- Weights defined by the area opposite each corner



http://en.wikipedia.org/wiki/Bilinear_interpolation

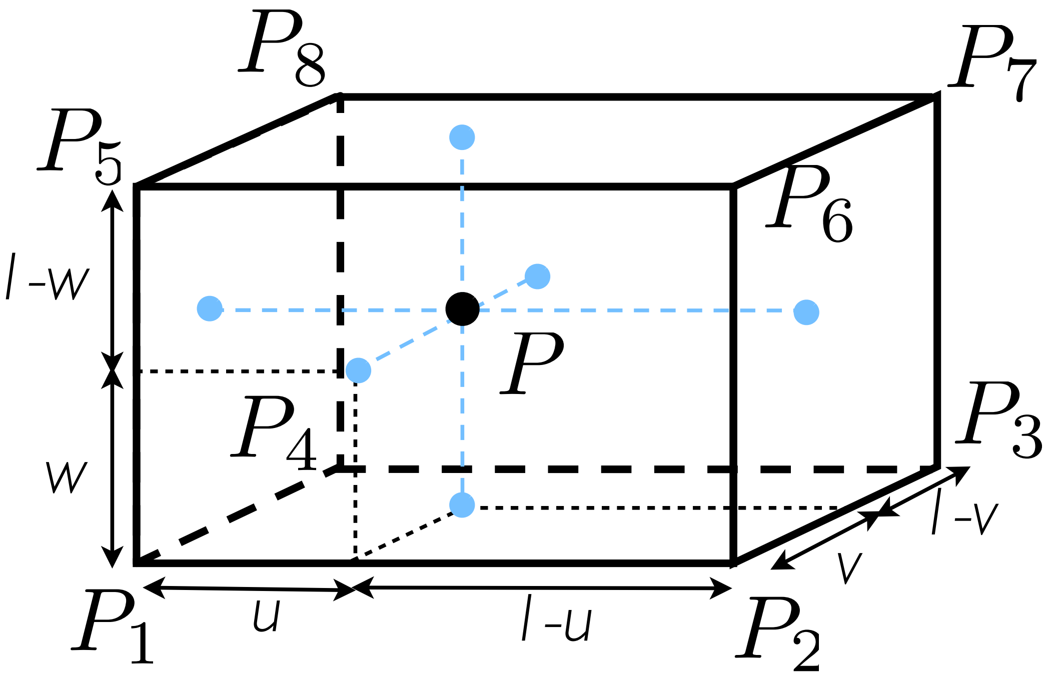
Trilinear Interpolation

- In a cuboid (axis parallel)
  - general formula

$$\phi(x,y,z) = axyz + bxy + cxz + dyz + ex + fy + gz + h$$

  - with local coordinates

$$\begin{aligned} P = P_1 & \\ & +u(P_2 - P_1) \\ & +v(P_4 - P_1) \\ & +w(P_5 - P_1) \\ & +uv(P_1 - P_2 + P_3 - P_4) \\ & +uw(P_1 - P_2 + P_6 - P_5) \\ & +vw(P_1 - P_4 + P_8 - P_5) \\ & +uvw(P_1 - P_2 + P_3 - P_4 + P_5 - P_6 + P_7 - P_8) \end{aligned}$$



Easier formula for trilinear interpolation

$$f(x,y,z) = \sum_{i,j,k=\{0,1\}} x_i y_j z_k \, v_{ijk}$$

Where $x_0 = i+1-x, x_1 = x-i$, ditto for y and z

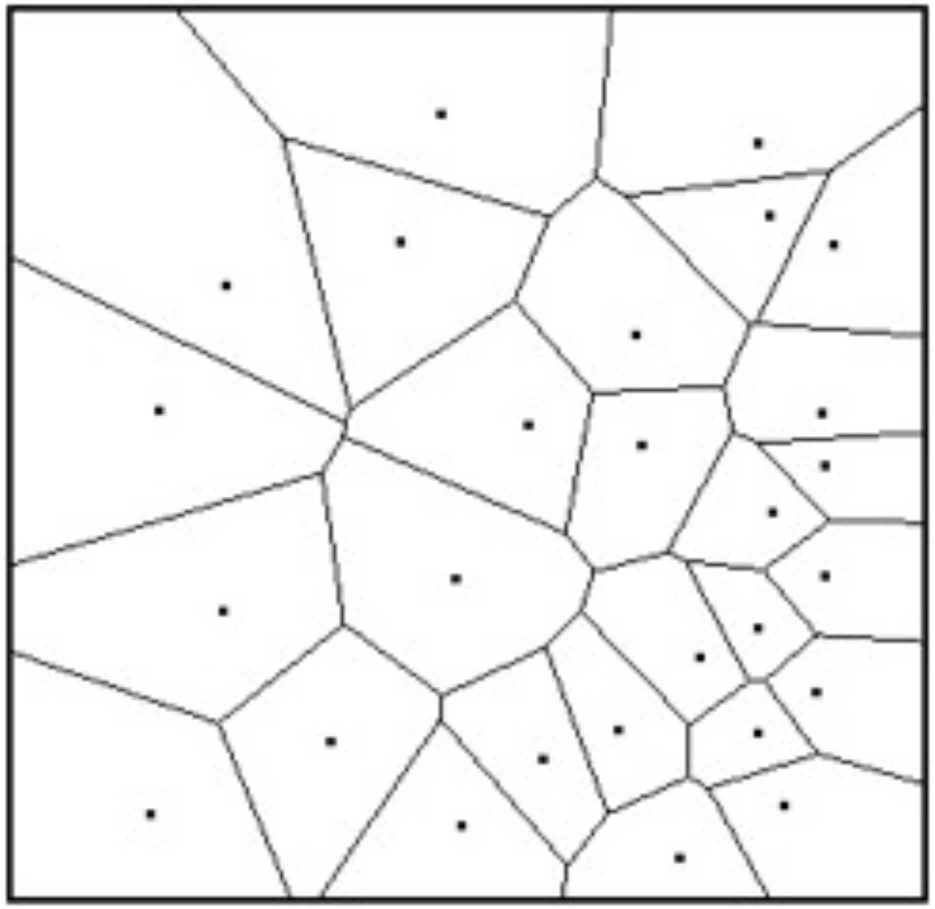
And v_{ijk} is the value of the voxel at that vertex.

Even easier: pseudocode for trilinear interpolation

Just 7 linear interpolations!

```
#define lerp(a,b,t)  (1-t) * a + t*b

//Given voxel vertices vXXX and the (x,y,z) position within the voxel [0,1]^3

//lerp along z direction.
float v000_z = lerp(v000, v001, z);
float v010_z = lerp(v010, v011, z);
float v100_z = lerp(v100, v101, z);
float v110_z = lerp(v110, v111, z);

//lerp along y direction
float v000_yz = lerp(v000_z, v010_z, y);
float v100_yz = lerp(v100_z, v110_z, y);

//lerp along x direction
return lerp(v000_yz, v100_yz, x);
```

Neighbor interpolation



Voronoi diagram

But Also...

- Higher-order interpolation schemes
  - splines, local polynomial fit (interpolation, least sq., ...)
  - smooth reconstruction kernels (on uniform grids)