ay/bi199: methods of computational science

visualization

visualization system+techniques

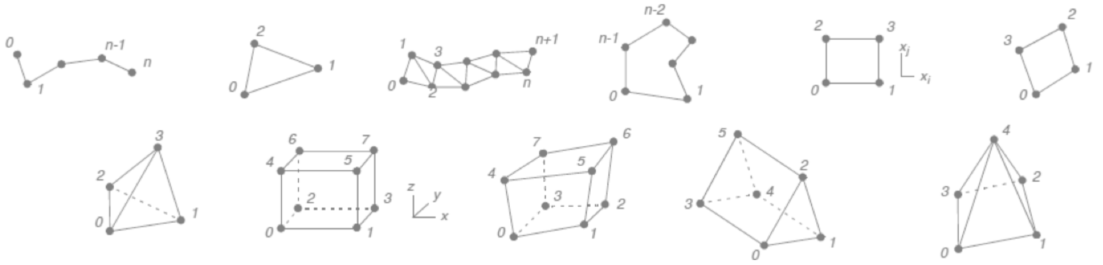
santiago v lombeyda | center for advanced computing research | caltech

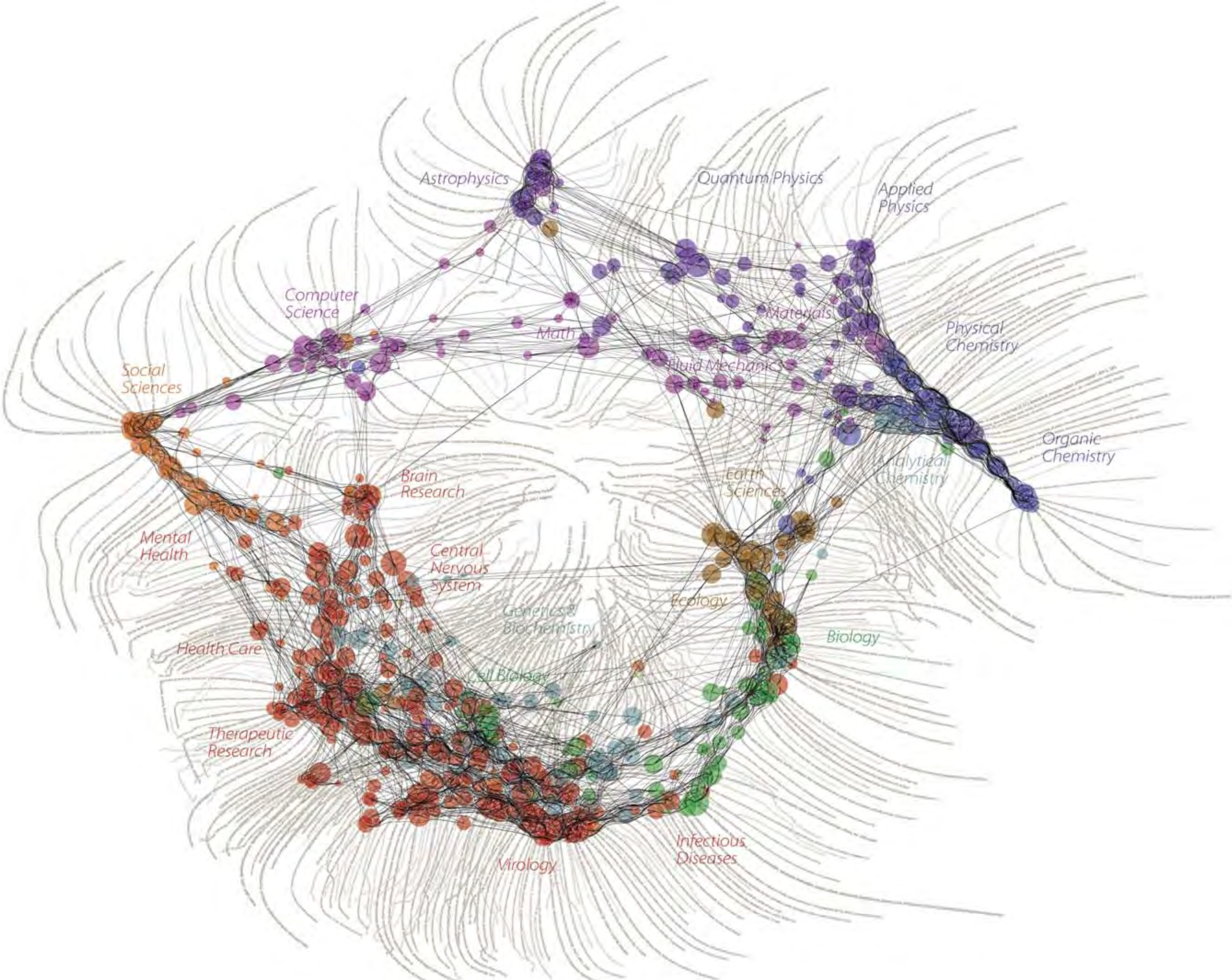
data: GEOMETRIC STRUCTURE

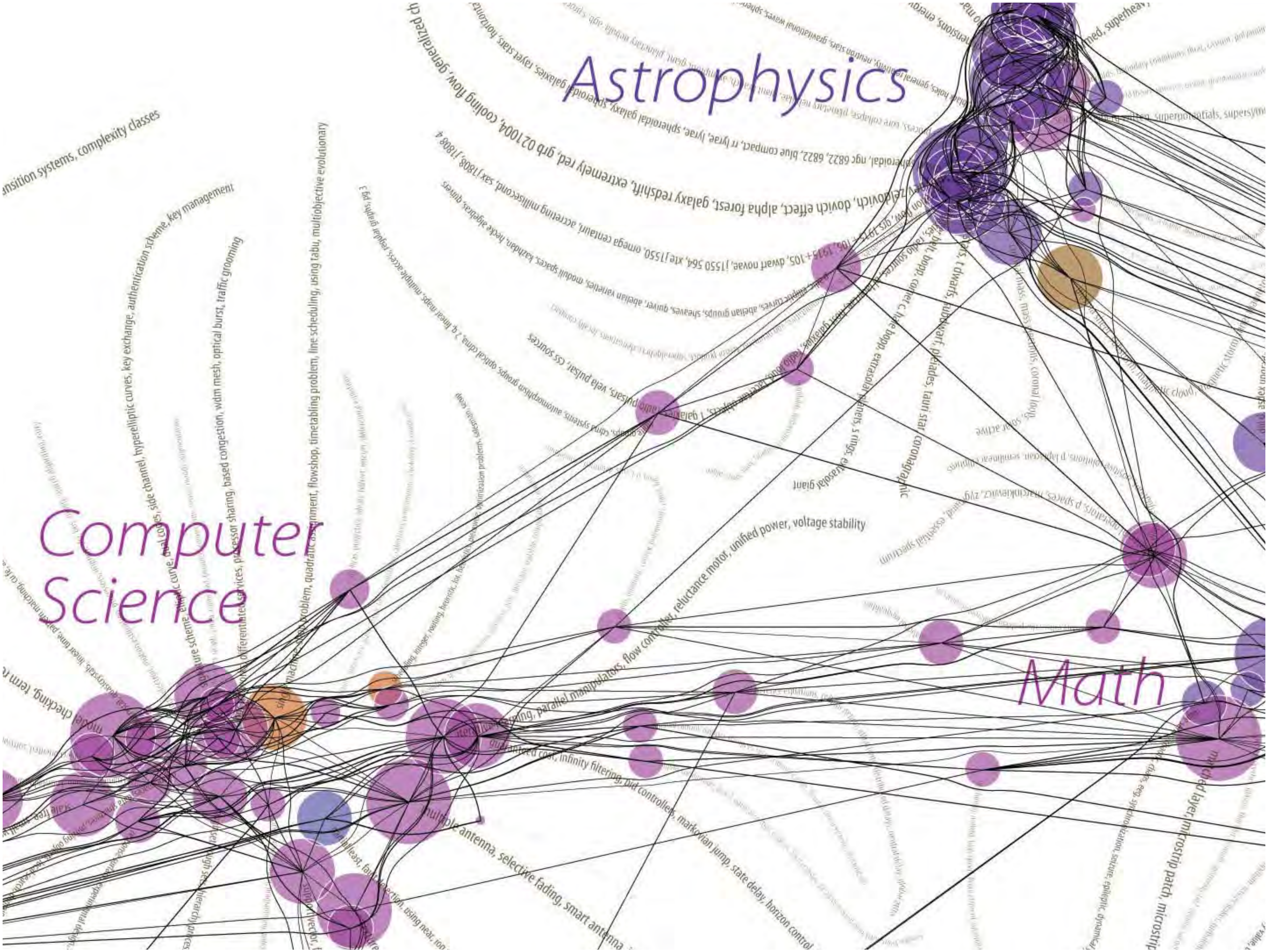
abstract

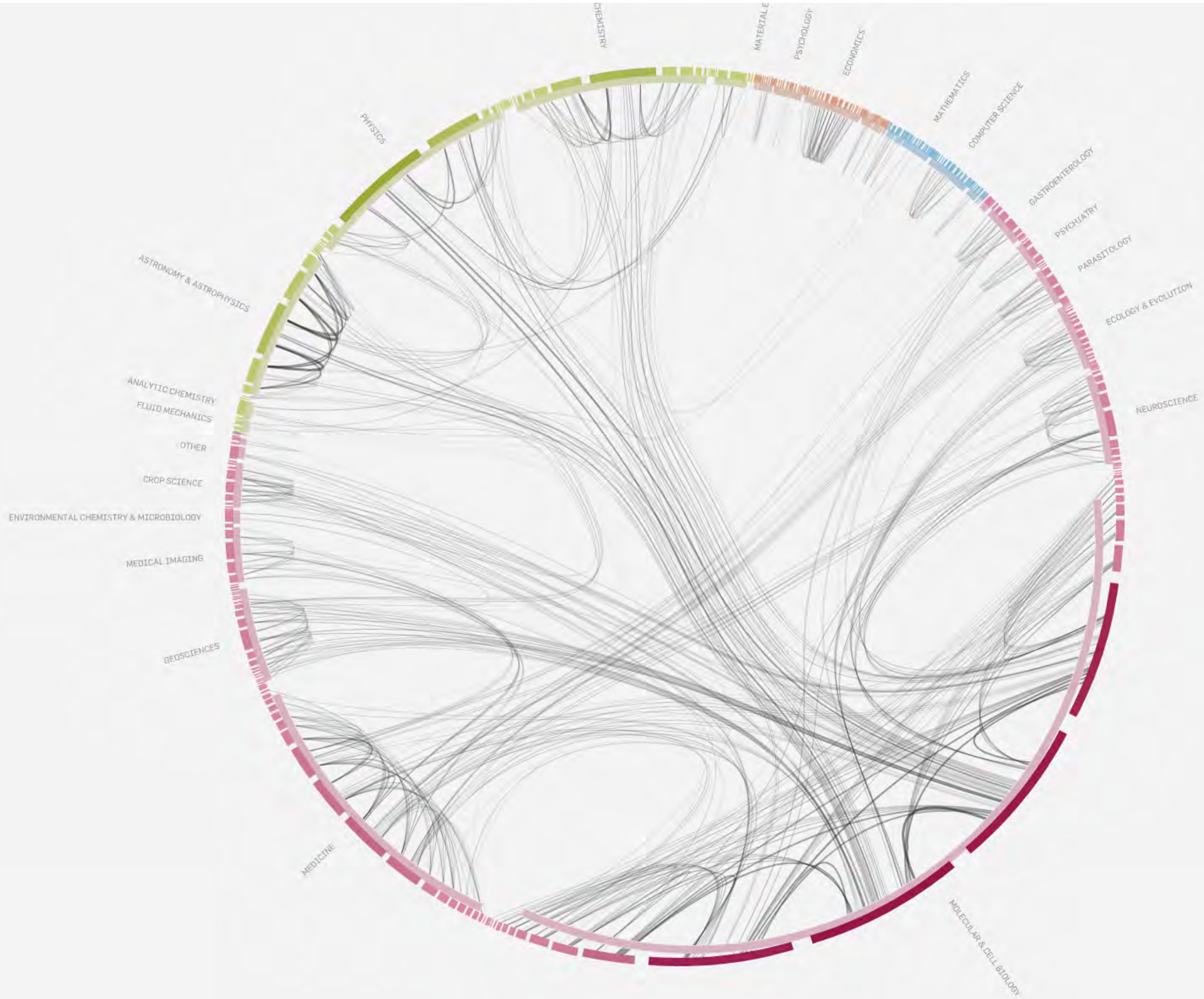
```
MPG Cylinders Horsepower Weight Acceleration Year Origin
8. 50.4 2.8 8.2 4 40. 250. 4 1500. 5500. 4 5. 30. 4 69.5 82.5 4 .8 3.2  3
18.000000 8.000000 130.000000 3504.000000 12.000000 70.000000 1.000000
15.000000 8.000000 165.000000 3693.000000 11.500000 70.000000 1.000000
18.000000 8.000000 150.000000 3436.000000 11.000000 70.000000 1.000000
16.000000 8.000000 150.000000 3433.000000 12.000000 70.000000 1.000000
17.000000 8.000000 140.000000 3449.000000 10.500000 70.000000 1.000000
... ... ... ... ... ... ... ... ...
```

2d/3d data

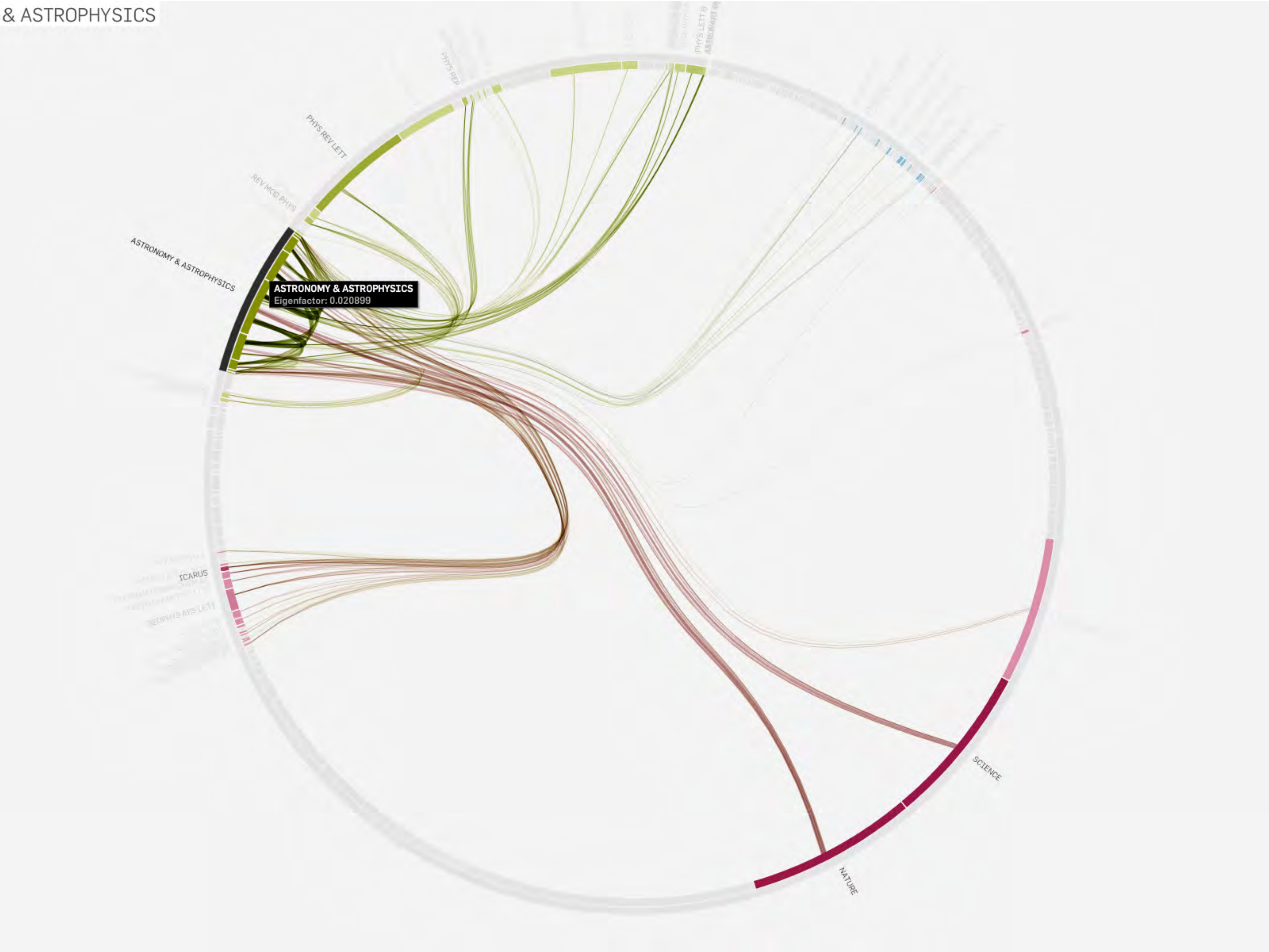


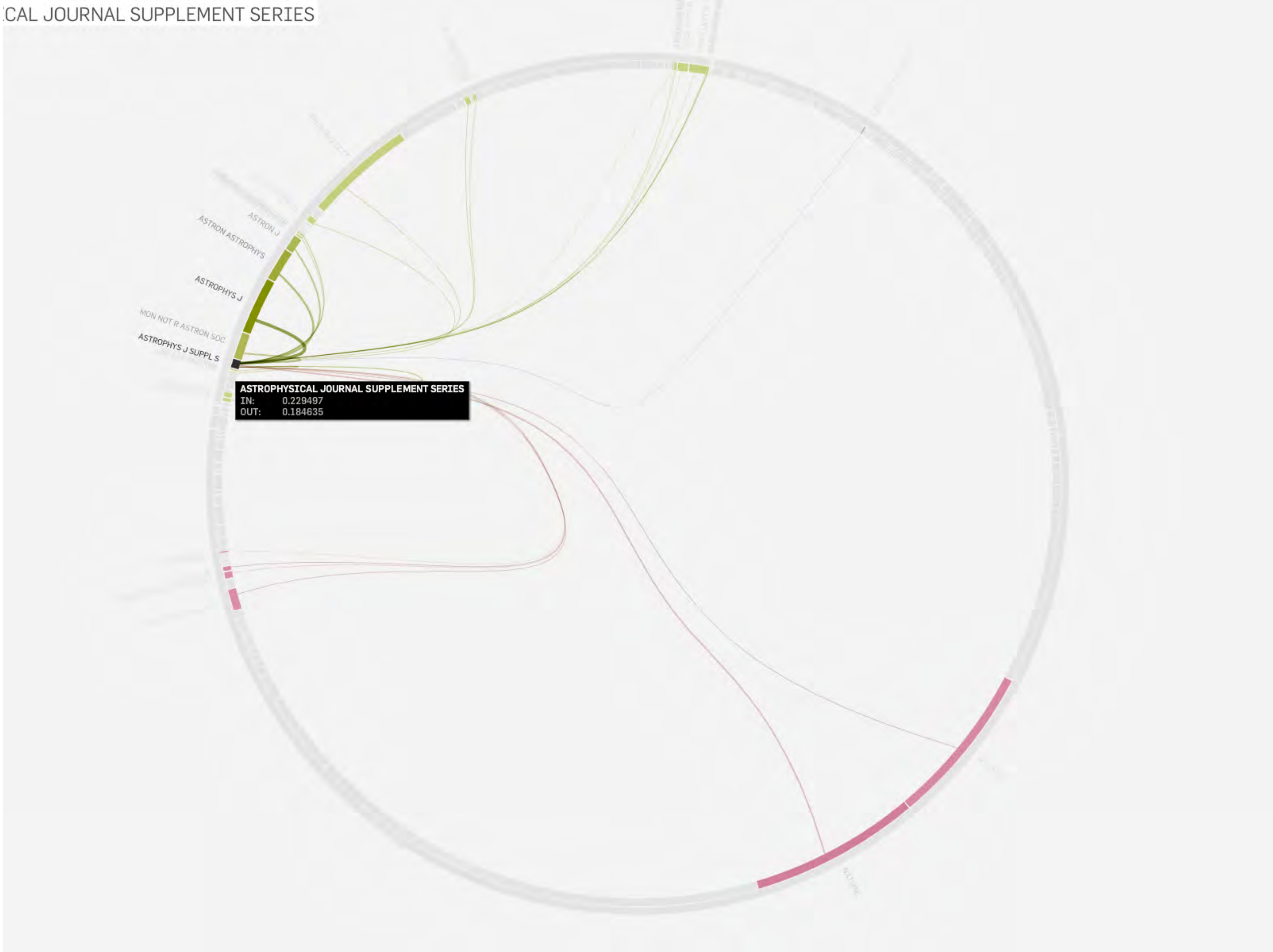

Astrophysics
Quantum Physics
Applied Physics
Computer Science
Math
Materials
Fluid Mechanics
Physical Chemistry
Social Sciences
Organic Chemistry
Analytical Chemistry
Earth Sciences
Brain Research
Mental Health
Central Nervous System
Genetics & Biochemistry
Ecology
Biology
Health Care
Cell Biology
Therapeutic Research
Infectious Diseases
Virology


Astrophysics
Computer Science
Math
ansition systems, complexity classes
side channel, hyperelliptic curves, key exchange, authentication scheme, key management
based congestion, wdm mesh, optical burst, traffic grooming
flowshop, timetabling problem, line scheduling, using tabu, multiobjective evolutionary
generalized ch, cooling flow, grb 021004, extremely red, galaxy redshift, alpha forest, dovich effect, zeldovich
spheroidal, ngc 6822, 6822, blue compact, rr lyrae, lyrae, spheroidal galaxy, spheroidal galaxies, rayet stars, horizontal
j1808 4, sax j1808, millisecond, accreting millisecond, omega centauri, xte j1550, j1550 564, dwarf novae, 105, 1915+105
abelian groups, sheaves, quiver, abelian varieties, moduli spaces, kazhdan, hecke algebras, quiver
vela pulsar, css sources
subdwarf, pleiades, faint star, coronagraphic
extrasolar giant
coronal loop, solar active
magnetic cloud, magnetic storm
superpotentials, supersym
med, superheav
parallel manipulators, flow controller, reluctance motor, unified power, voltage stability
guaranteed cost, infinity filtering, pid controllers, markovian jump, state delay, horizon control
multiple antenna, selective fading, smart antenna
matched layer, microstrip patch, microstrip
model checking, term re


CHEMISTRY
MATERIAL E
PSYCHOLOGY
ECONOMICS
MATHEMATICS
COMPUTER SCIENCE
GASTROENTEROLOGY
PSYCHIATRY
PARASITOLOGY
ECOLOGY & EVOLUTION
NEUROSCIENCE
MOLECULAR & CELL BIOLOGY
MEDICINE
GEOSCIENCES
MEDICAL IMAGING
ENVIRONMENTAL CHEMISTRY & MICROBIOLOGY
CROP SCIENCE
OTHER
FLUID MECHANICS
ANALYTIC CHEMISTRY
ASTRONOMY & ASTROPHYSICS
PHYSICS

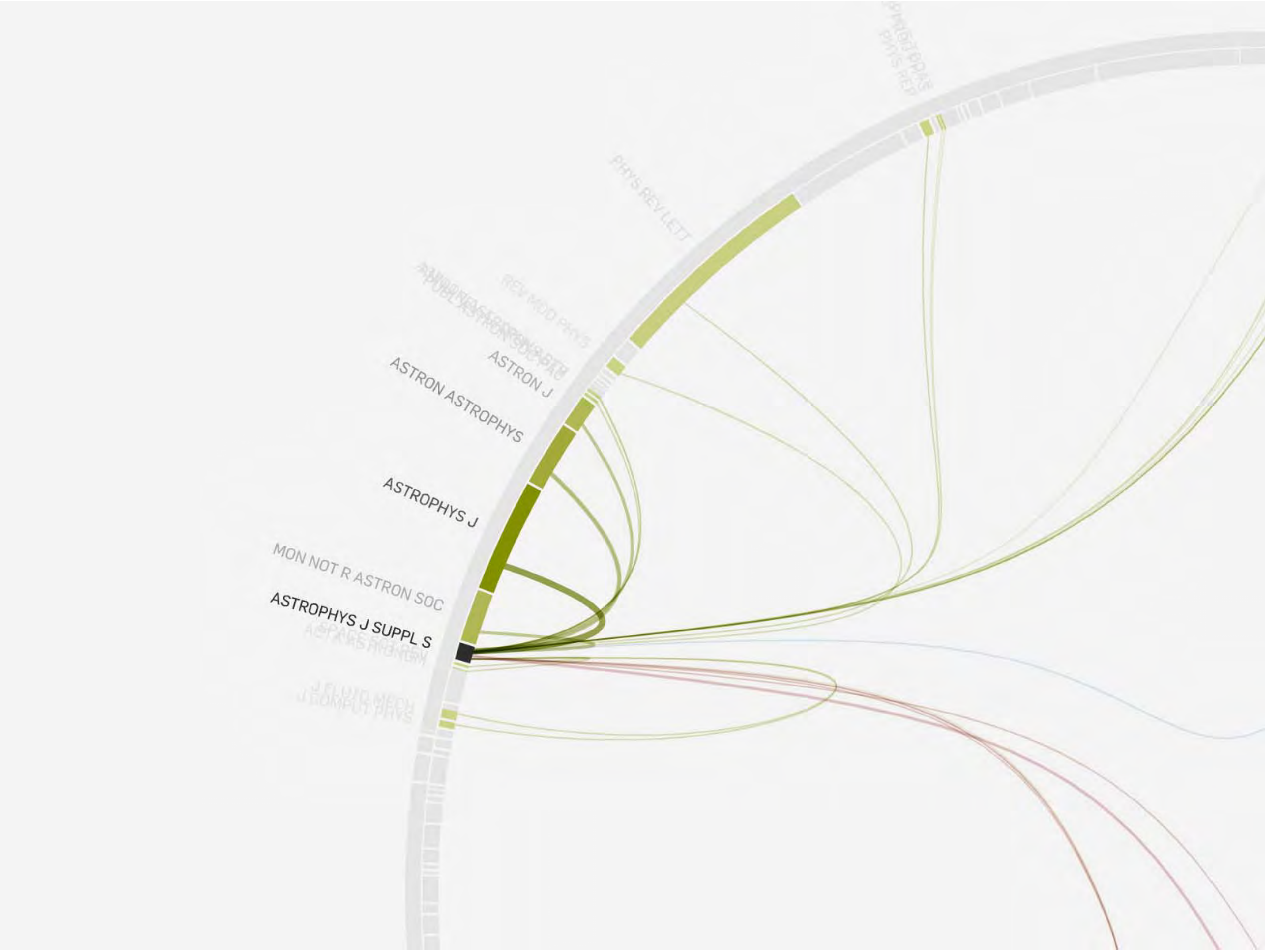
& ASTROPHYSICS





CAL JOURNAL SUPPLEMENT SERIES

ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES
IN: 0.229497
OUT: 0.184635

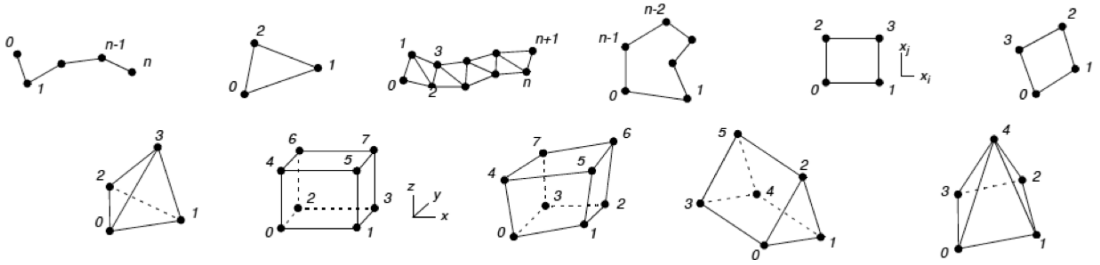

PHYS REP
PHYS REV LETT
REV MOD PHYS
PUBL ASTRON SOC PAC
ASTRON J
ASTRON ASTROPHYS
ASTROPHYS J
MON NOT R ASTRON SOC
ASTROPHYS J SUPPL S
SPACE SCI REV
ACTA ASTRONOM
J FLUID MECH
J COMPUT PHYS

data: GEOMETRIC STRUCTURE

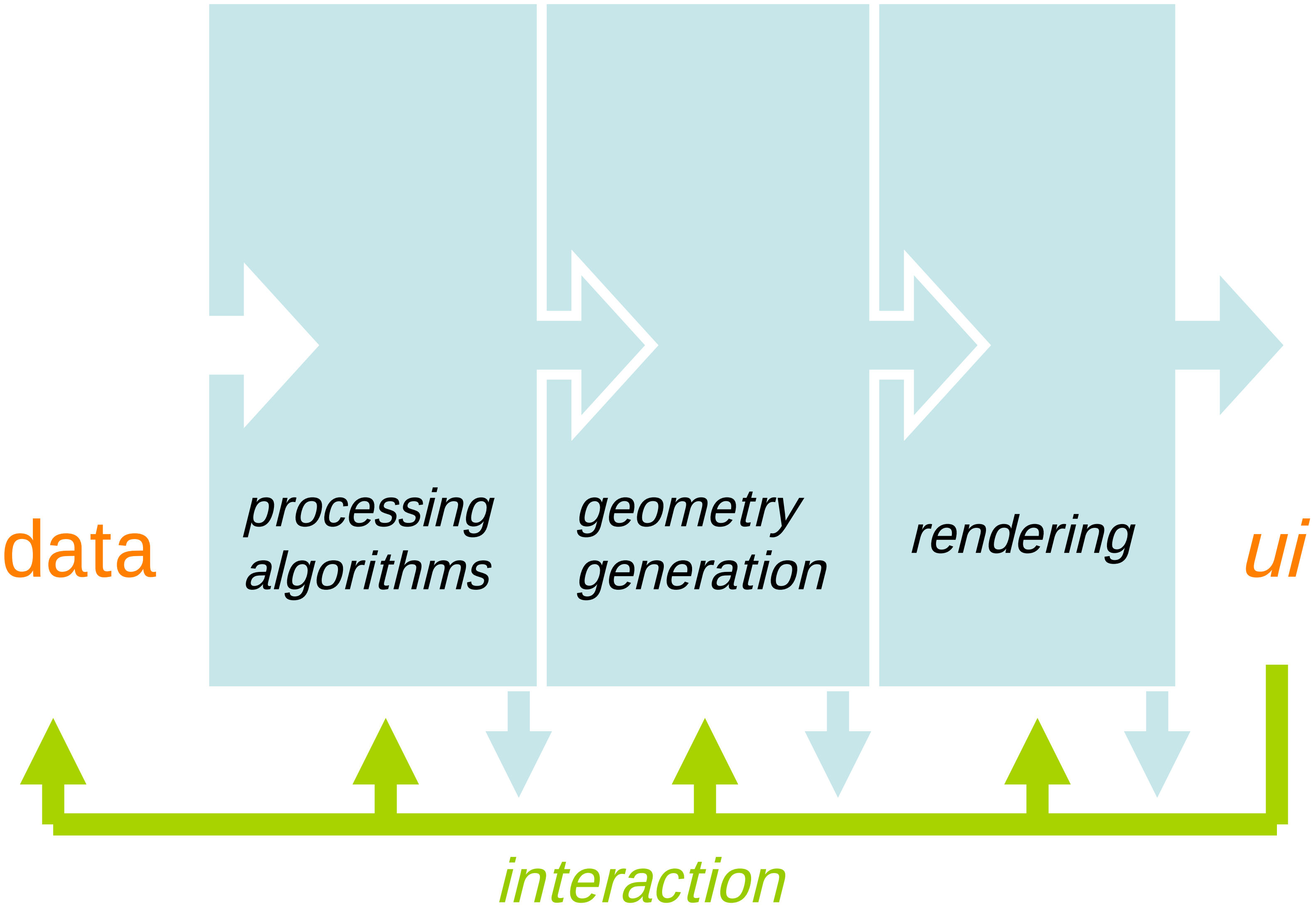
abstract

```
MPG Cylinders Horsepower Weight Acceleration Year Origin
8. 50.4 2.8 8.2 4 40. 250. 4 1500. 5500. 4 5. 30. 4 69.5 82.5 4 .8 3.2  3
18.000000 8.000000 130.000000 3504.000000 12.000000 70.000000 1.000000
15.000000 8.000000 165.000000 3693.000000 11.500000 70.000000 1.000000
18.000000 8.000000 150.000000 3436.000000 11.000000 70.000000 1.000000
16.000000 8.000000 150.000000 3433.000000 12.000000 70.000000 1.000000
17.000000 8.000000 140.000000 3449.000000 10.500000 70.000000 1.000000
... ... ... ... ... ... ... ... ...
```

2d/3d data



usual visualization engine



data

processing algorithms

geometry generation

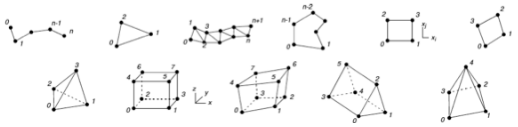
rendering

ui

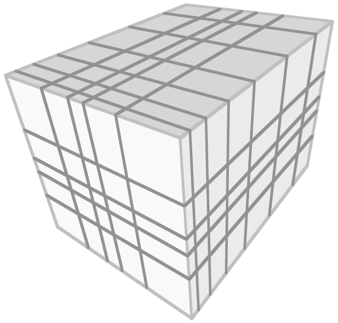
interaction

viz pipeline: *in the beginning*

DATA FORMATS



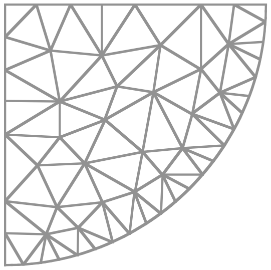
basic data types



structured grids

most basic: regular *(easy to do raw binary)*

more complex: AMR (adaptive mesh refinement)

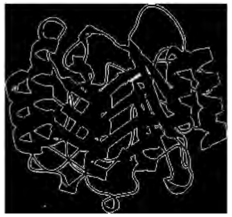


unstructured grids

points

triangle meshes

tet meshes



atomic coordinate files

PDB (protein data bank)

no standard formats

raw

vtk

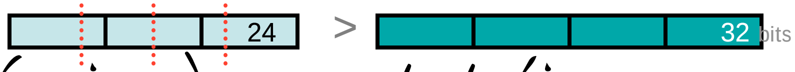
ascii or binary

new vtk

xml

== abcdefgh ijklmnop
qrstuvwx yzABCDEF
GHIJKLMN OPQRSTUV
WXYZ0123 456789+/

(64=2^6) 6 bits -> 8 bit char (*size * 4/3*)



ascii or base64 (mime) encoded binary

amr

chombo(hdf5)/silo

pdb

standard..

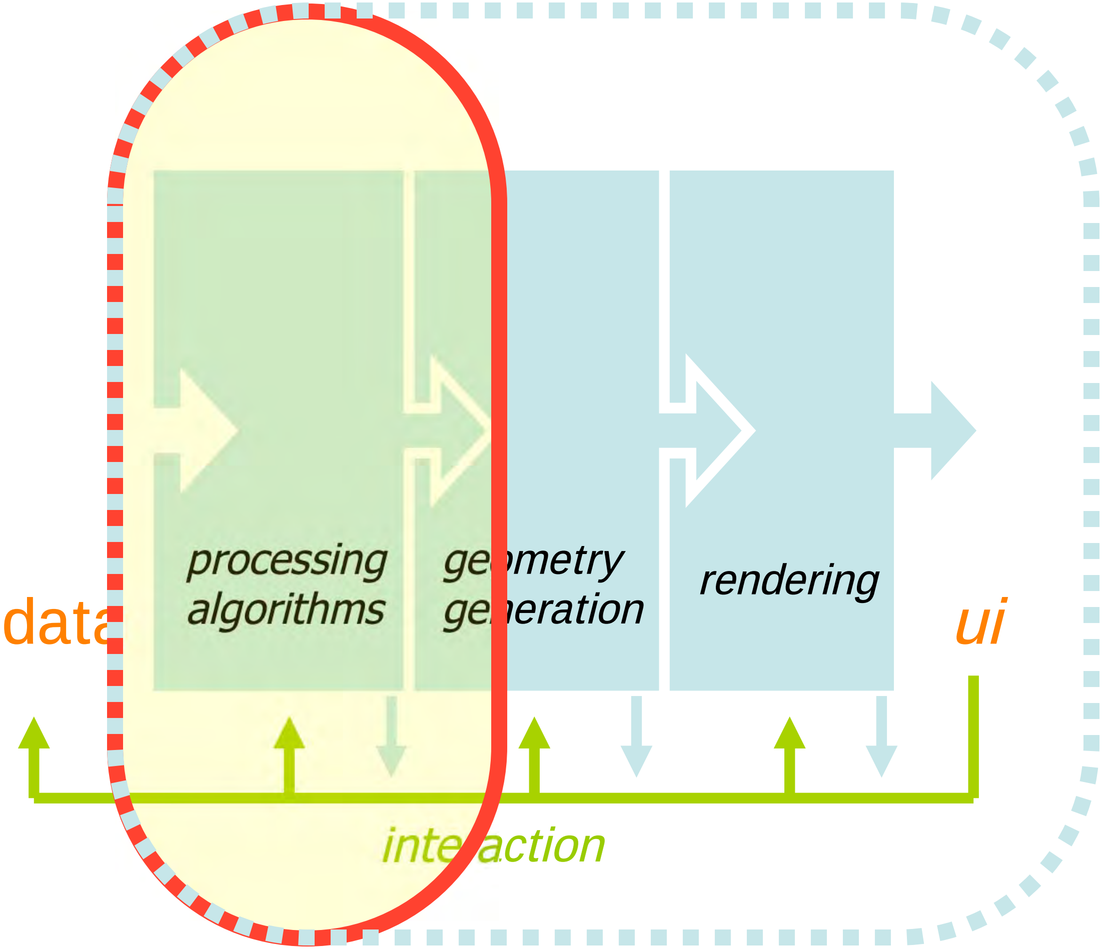
vtk sample: volume.vti

```
<?xml version="1.0"?>
<VTKFile type="ImageData" version="0.1" byte_order="LittleEndian">
<ImageData WholeExtent="0 3 0 3 0 3" Origin="0 0 0" Spacing="1 1 1">
 <Piece Extent="0 3 0 3 0 3">

  <PointData Scalars="vertexData">
   <DataArray type="Float32" Name="scalarData" format="ascii">
    0 1 2 3  1 2 3 4  2 3 4 8  3 6 9 11
    2 3 4 5  5 6 7 8  3 4 5 6  4 5 6 7
    3 4 5 6  3 4 5 6  4 5 6 7  6 7 8 9
    2 3 4 5  2 3 4 5  3 4 5 6  4 5 6 7
   </DataArray>
  </PointData>

  <CellData Scalars="cellData" Normals="cell_ normals">
   <DataArray type="Int32" Name="cellData" format="ascii">
    1 3 9  2 8 16  3 9 27
    2 3 4  6 7 8   6 9 10
    0 1 2  0 2 4   1 2 3
   </DataArray>
  </CellData>
 </Piece>
</ImageData>
</VTKFile>
```

“the” visualization toolkit



- VTK
    - c/c++
    - tcl/tk
    - python
    - java
- R

viz pipeline: *the tools*

VTK

the visualization toolkit

g.e. medical viz algorithms

➔ KITWARE

collection of filters

MARCHING CUBES *(patented)*

educational

➔ VTK book

evolved/extended

object oriented

C++

GL + Tk (UI)

now python

vtk.org

kitware.com

vtkpython

PYTHON MODULE

pyvtk

FILE MANIPULATION

vtk

visualization algorithms

- scalar
- vector
- tensor
- texture
- volumetric

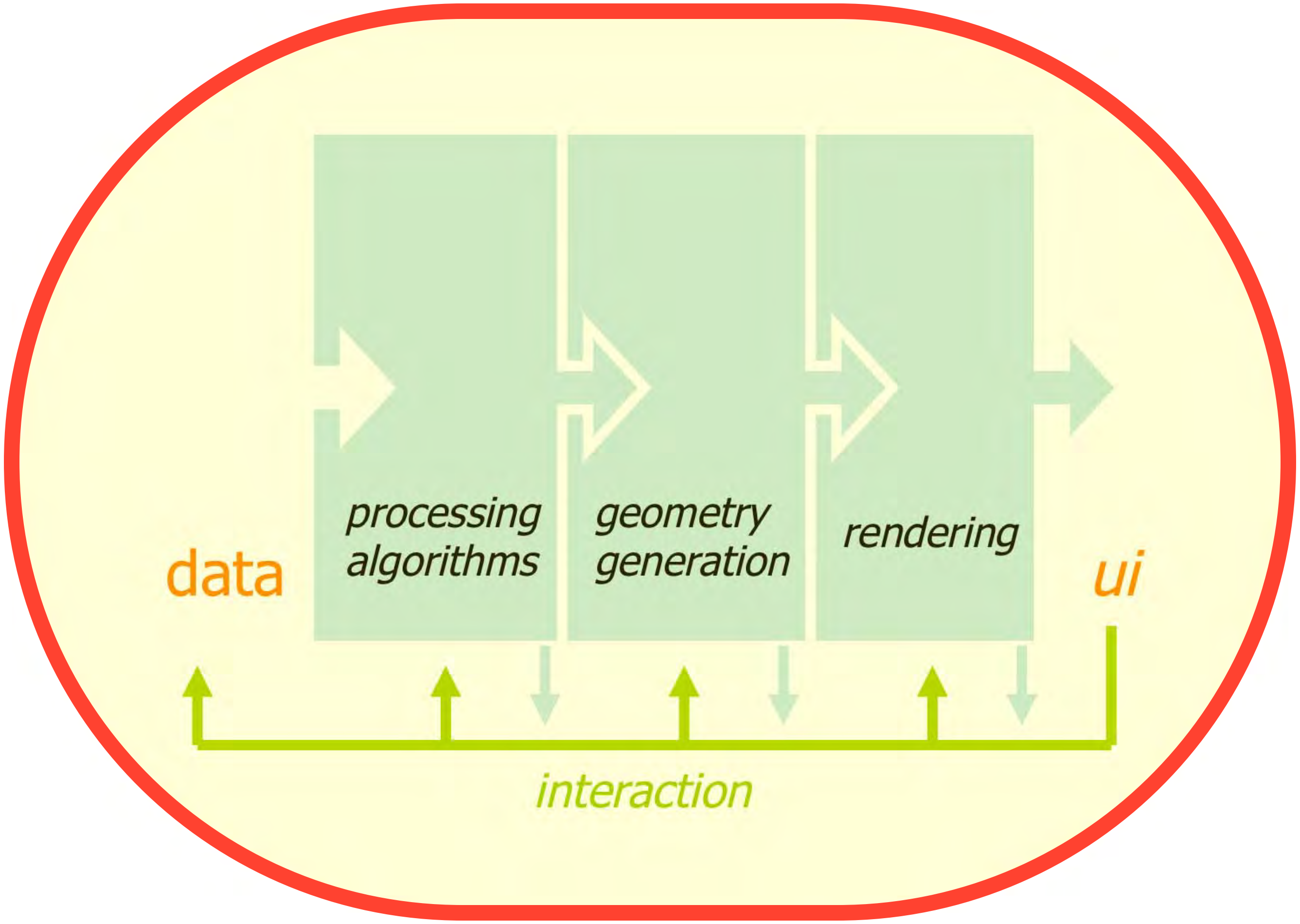
imaging algorithms

- directly integrated
- mix 2D imaging/3D graphics

modeling techniques

- implicit modeling
- polygon reduction
- mesh smoothing
- cutting
- contouring
- Delaunay triangulation

visualization system



- Paraview^{VTK}
- LLNL VisIt^{VTK}
- EnSight$^{\$}$
- Protovis^{www}
- Many Eyes^{www}
  - *Wiki based*
- Modrian^{R}, TomCat, Mollegro, ...

paraview

paraview.org

vtk based!

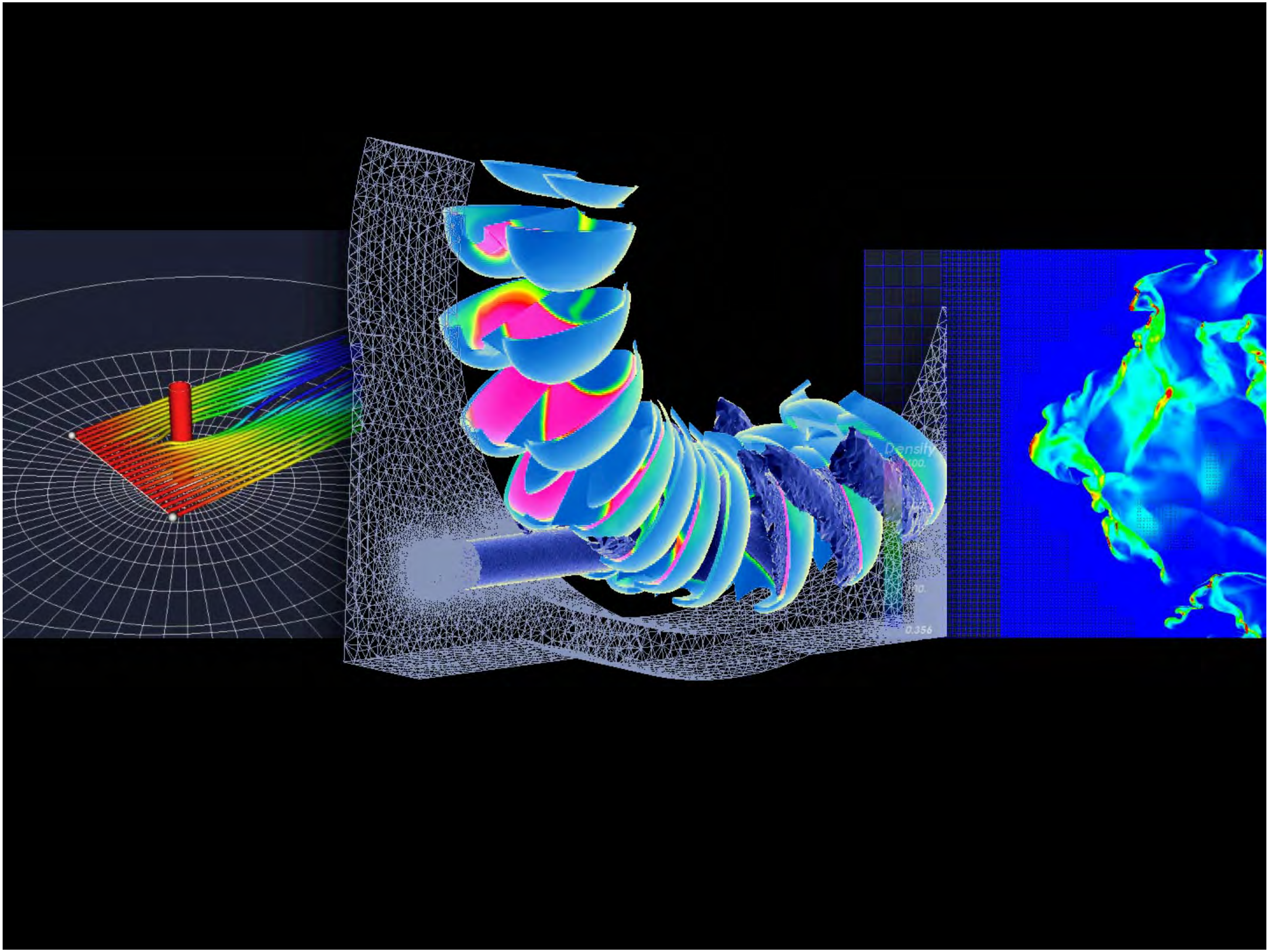
active community

- mailing list + wiki
- lead at kitware: *berk geveci*
  - sandia national lab
  - los alamos national lab, army research lab

parallel!

QT based

- starting 3.6.2 decent python scripting support


Density
100.
10.
0.356

bluntfin:

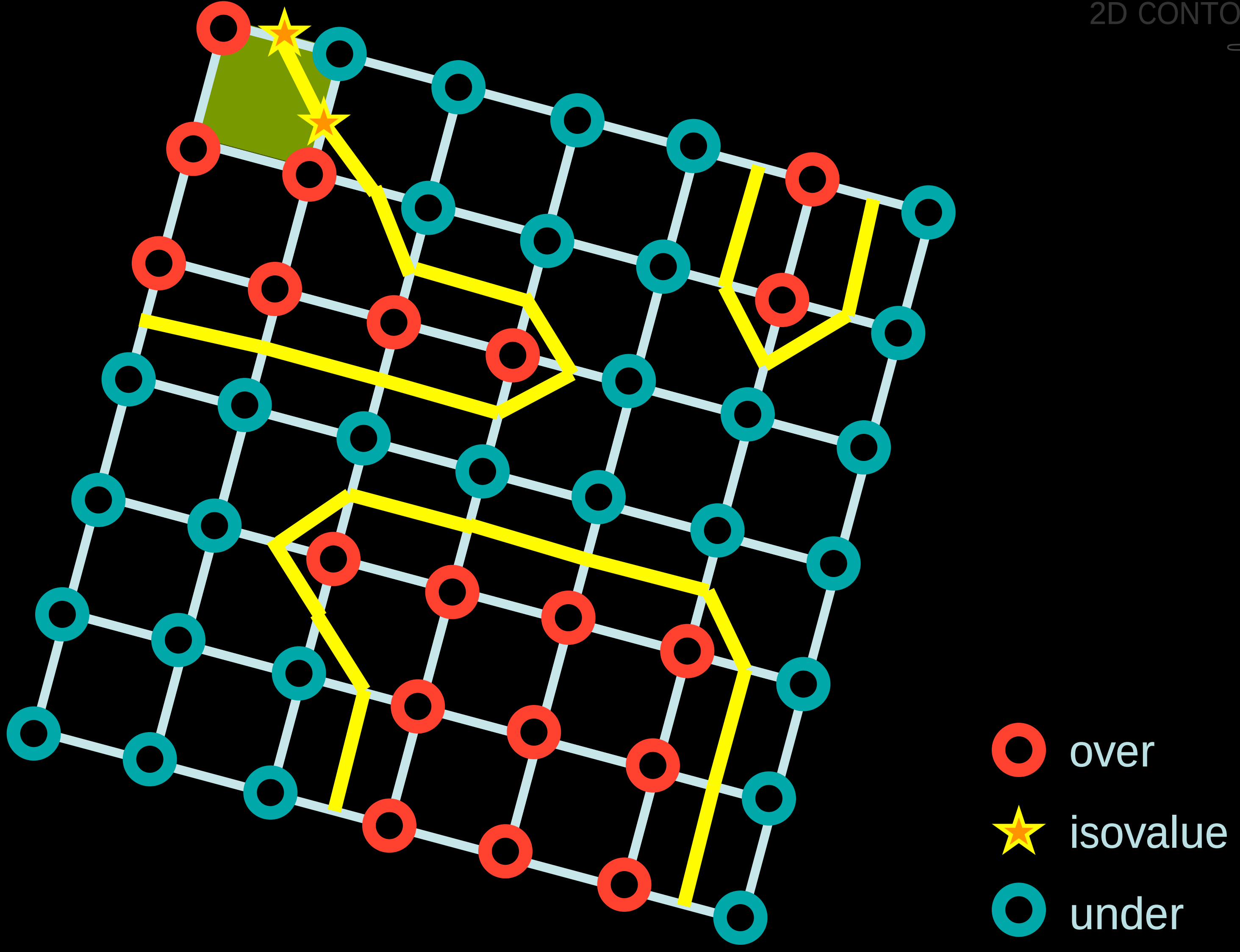
PARAVIEW

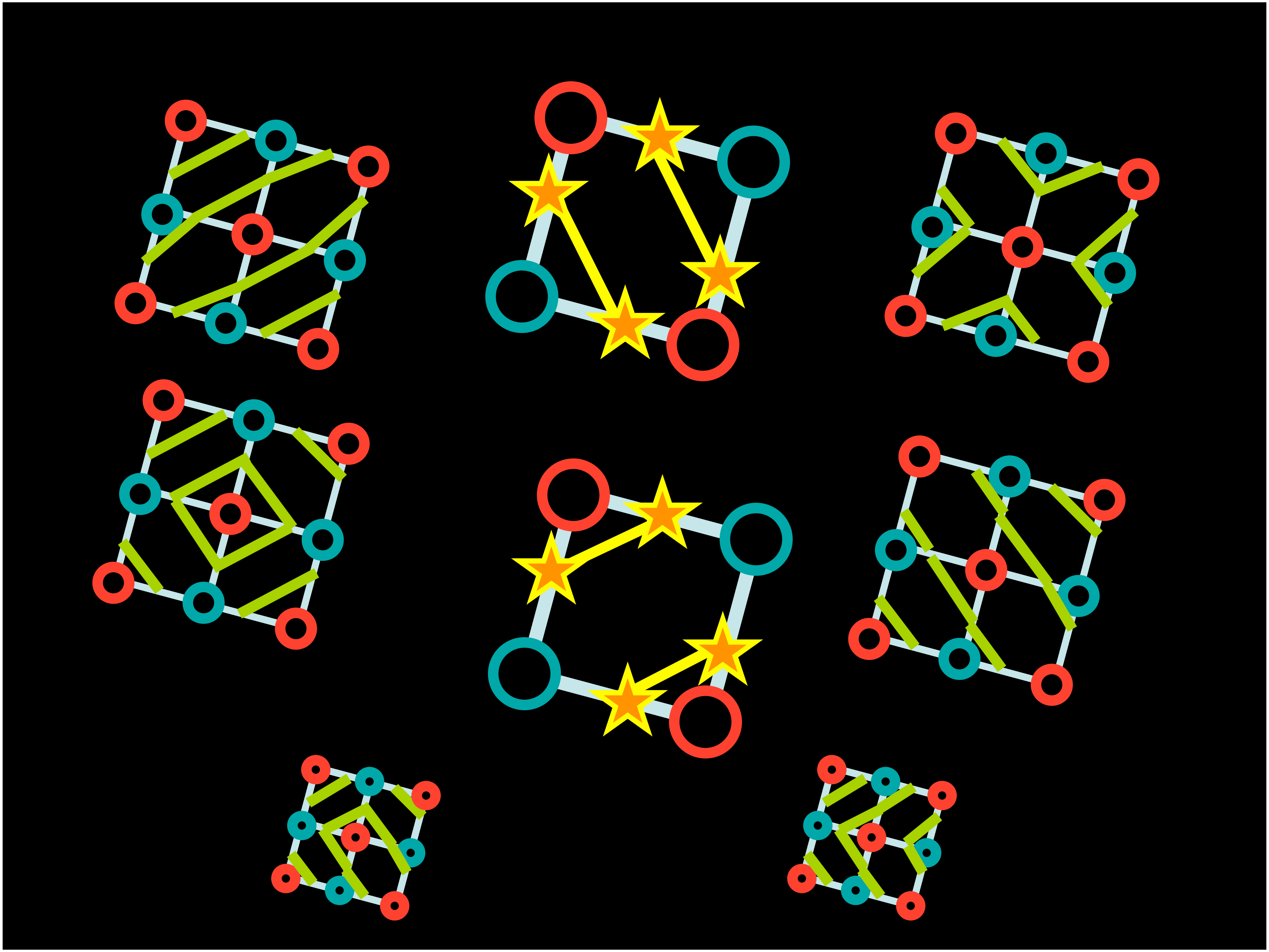
quick look

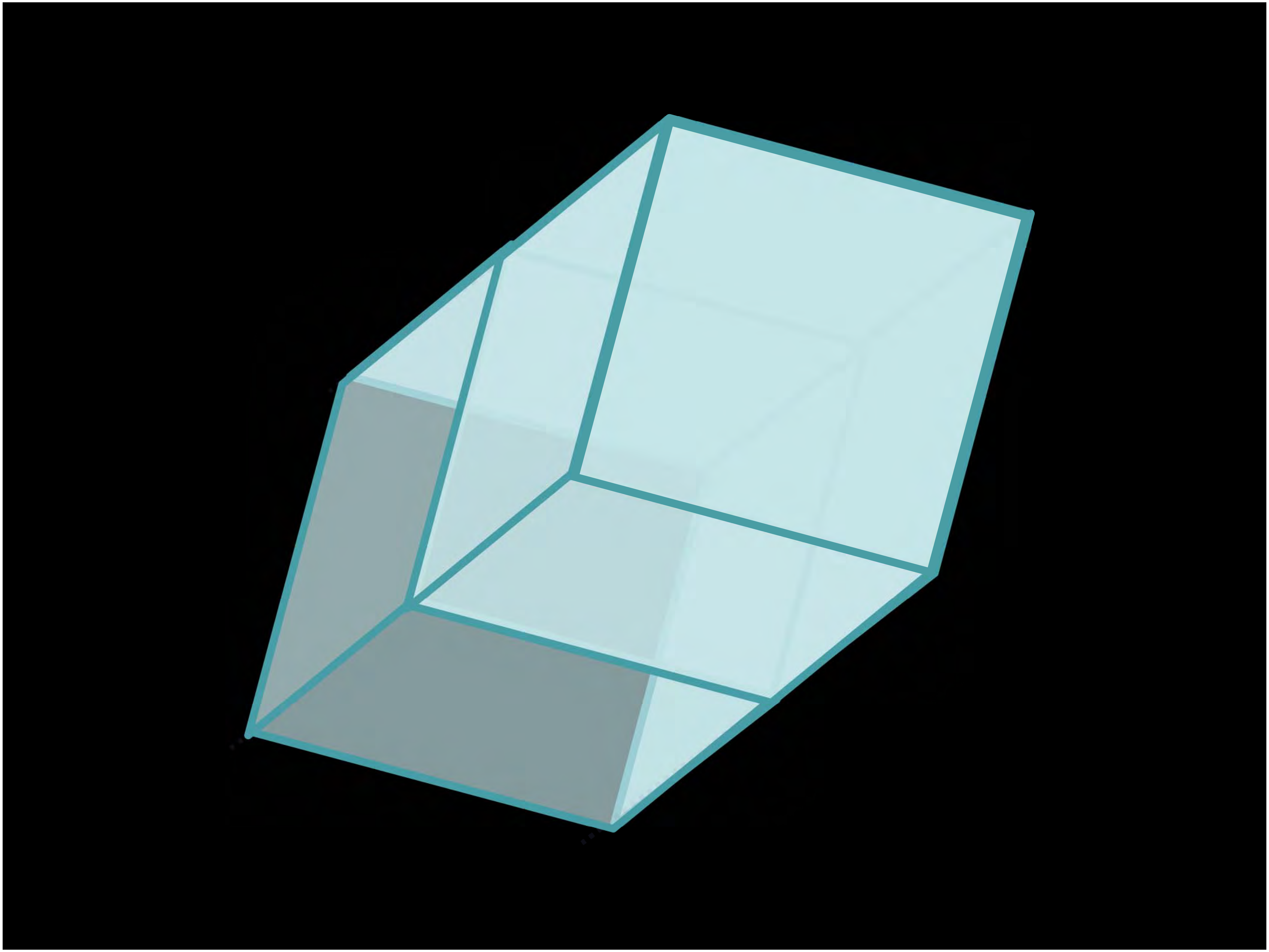
quick inside look: *marching cubes*

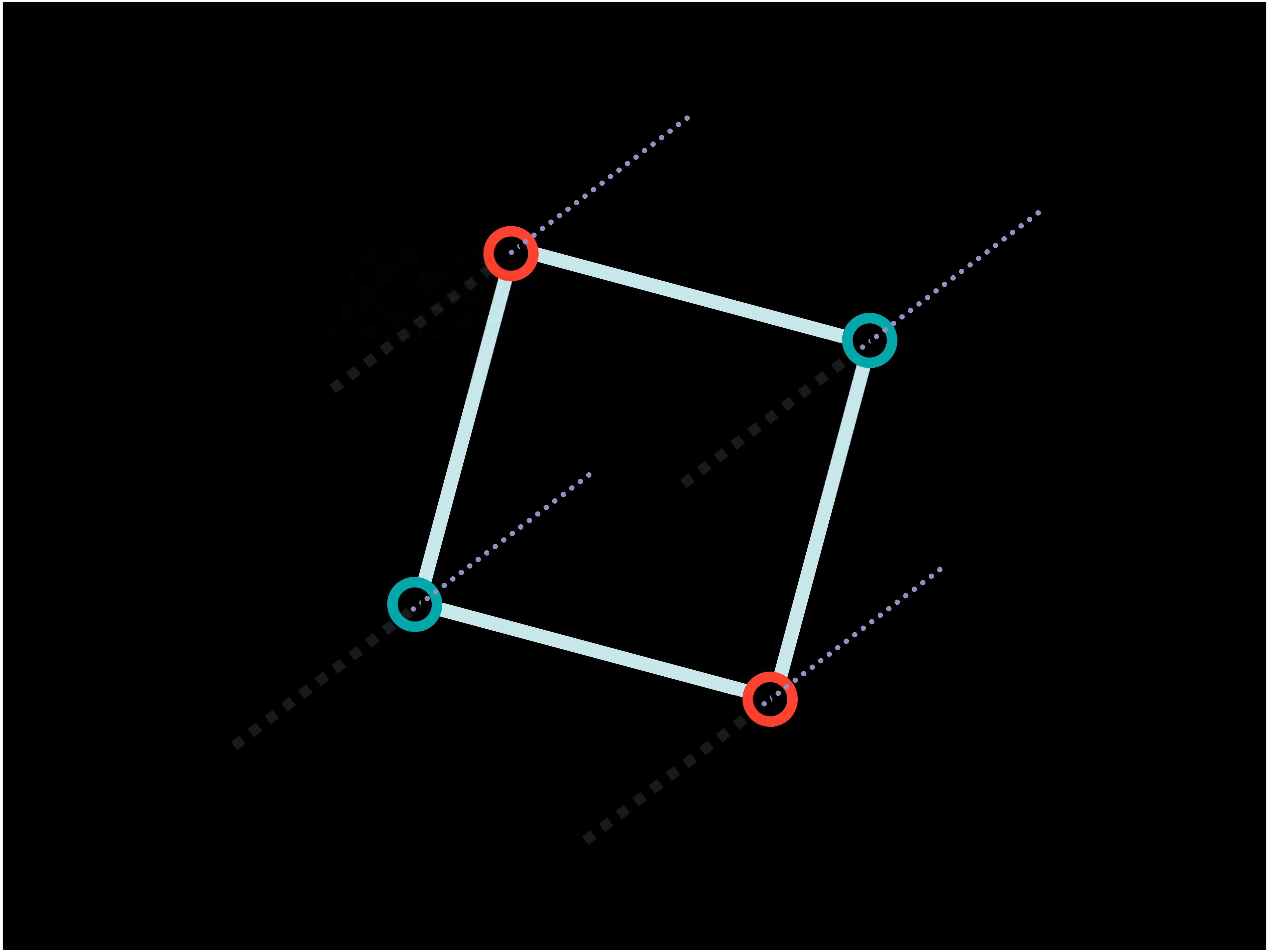
VTK

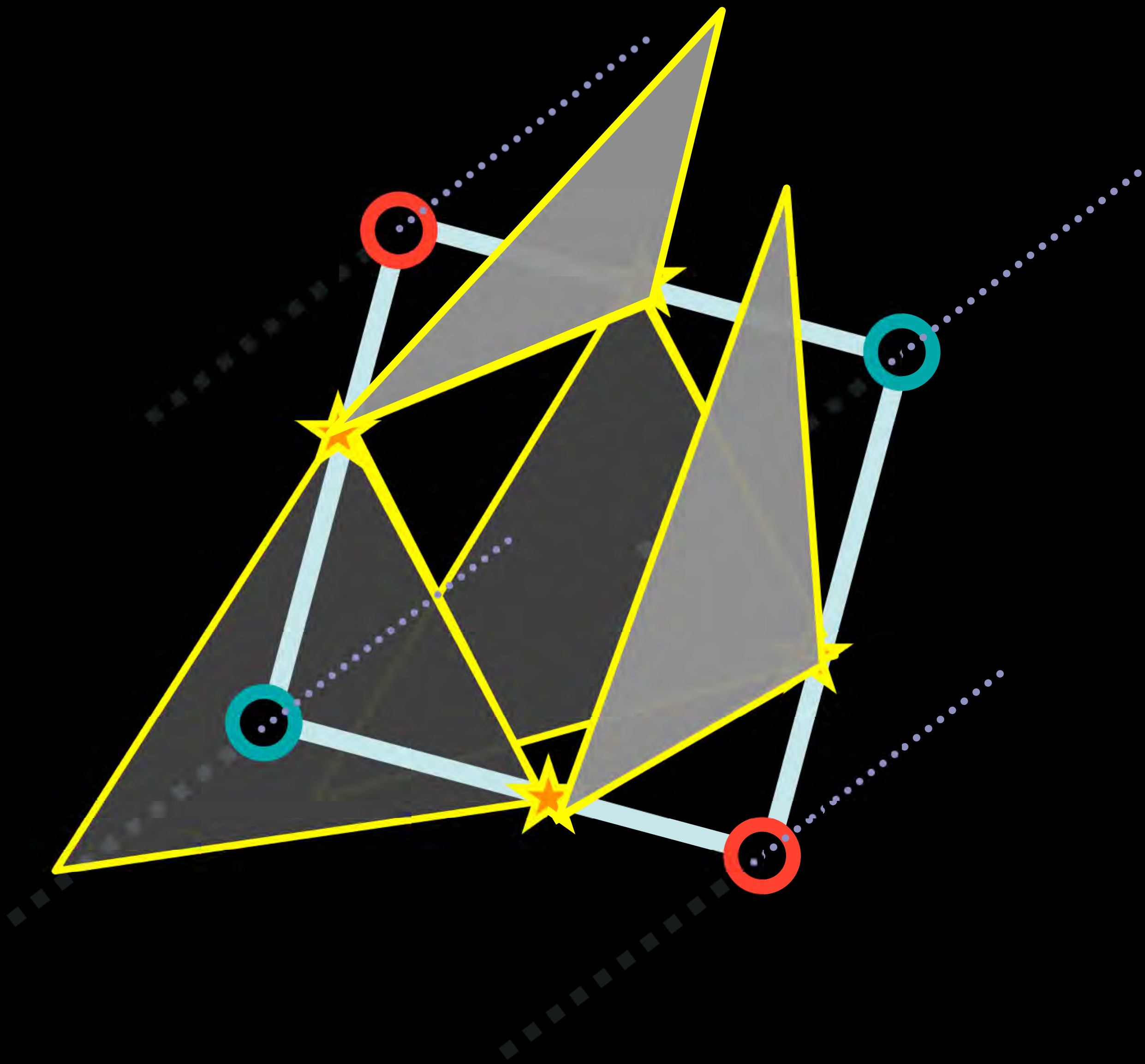
2D CONTOUR

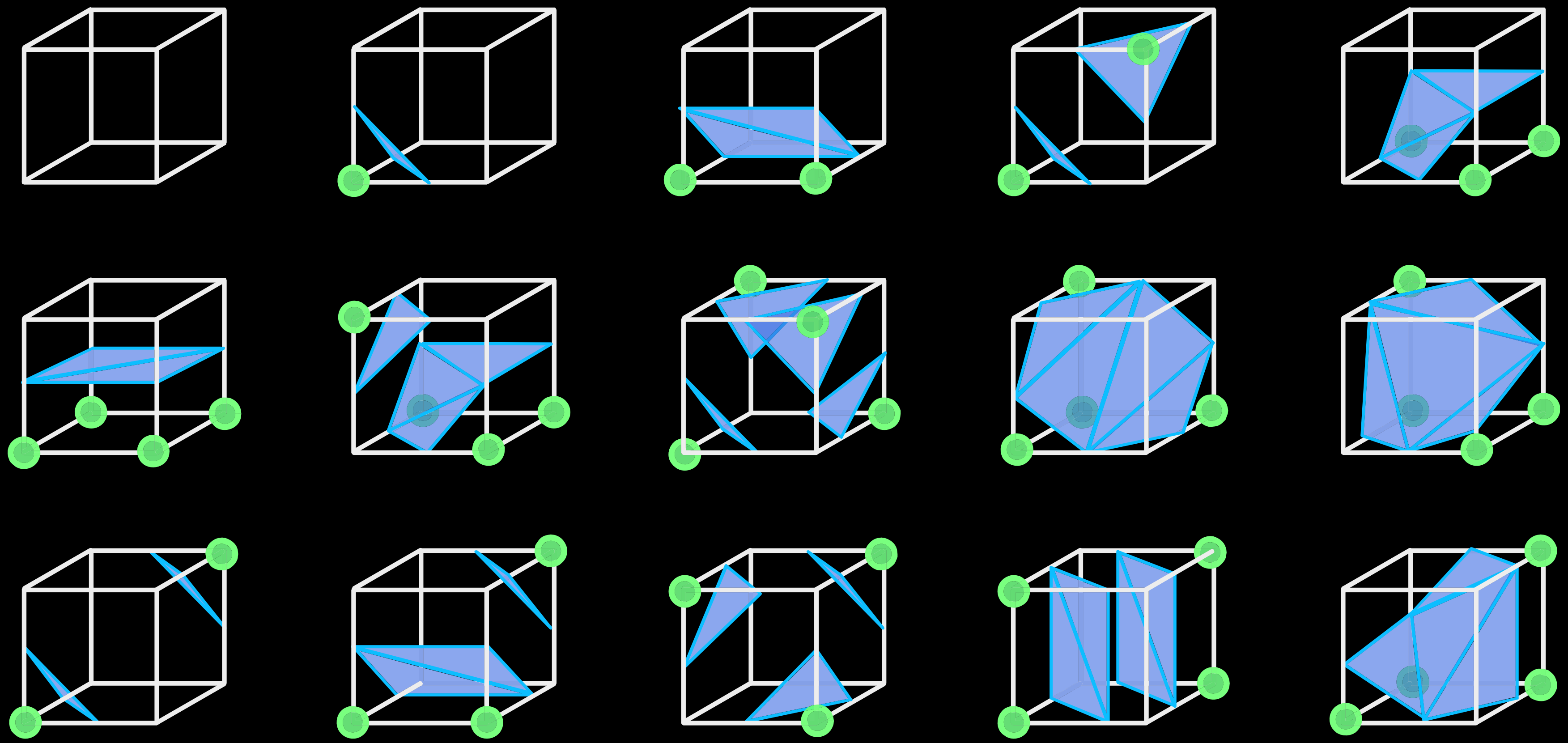




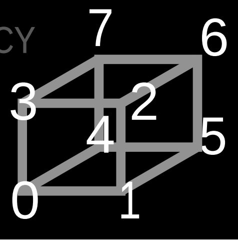








INCONSISTENCY ERROR ☝ FIX: TABLE FORCING CONSISTENCY



quick look: *techniques*

VOLUME RENDERING

project stargate:

NATIONAL LABS+SDSC

quick movie

volume rendering

VOLUMETRIC DATA

voxels: volume elements

usually regular 3D grid

scalar field

volume rendering

projected semi-transparent representation

scalar field + color transfer function (R,G,B,α)

↓

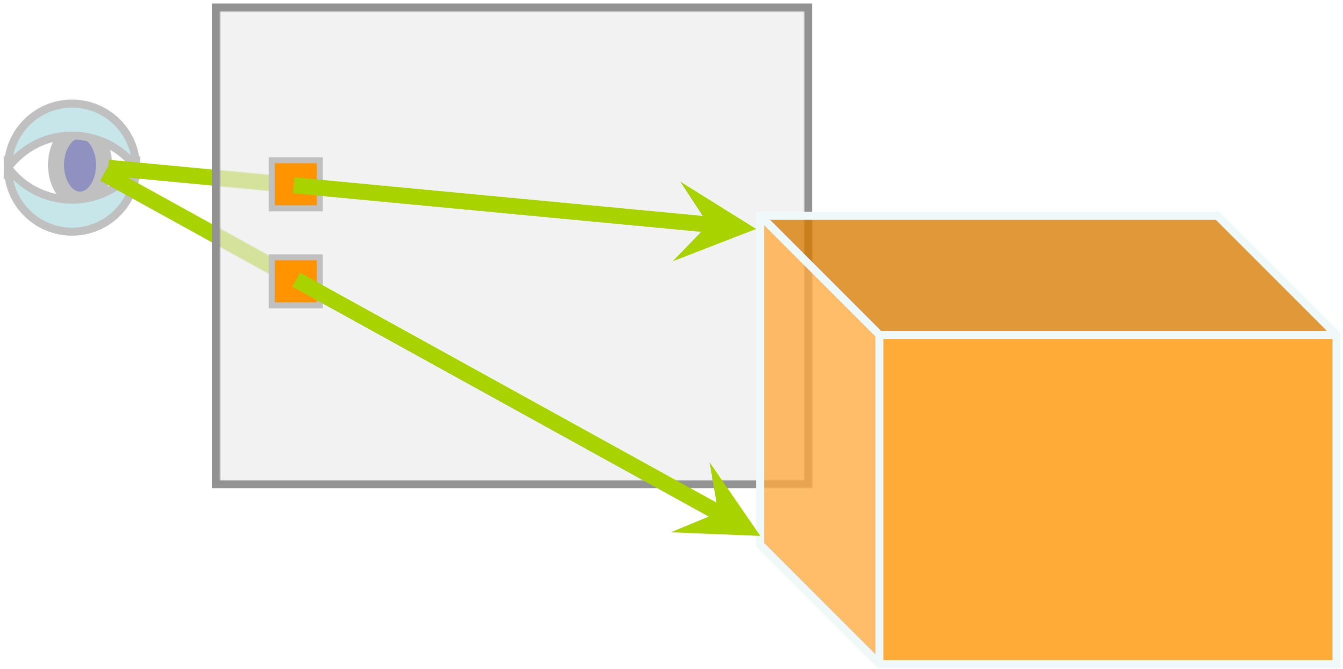
pixels

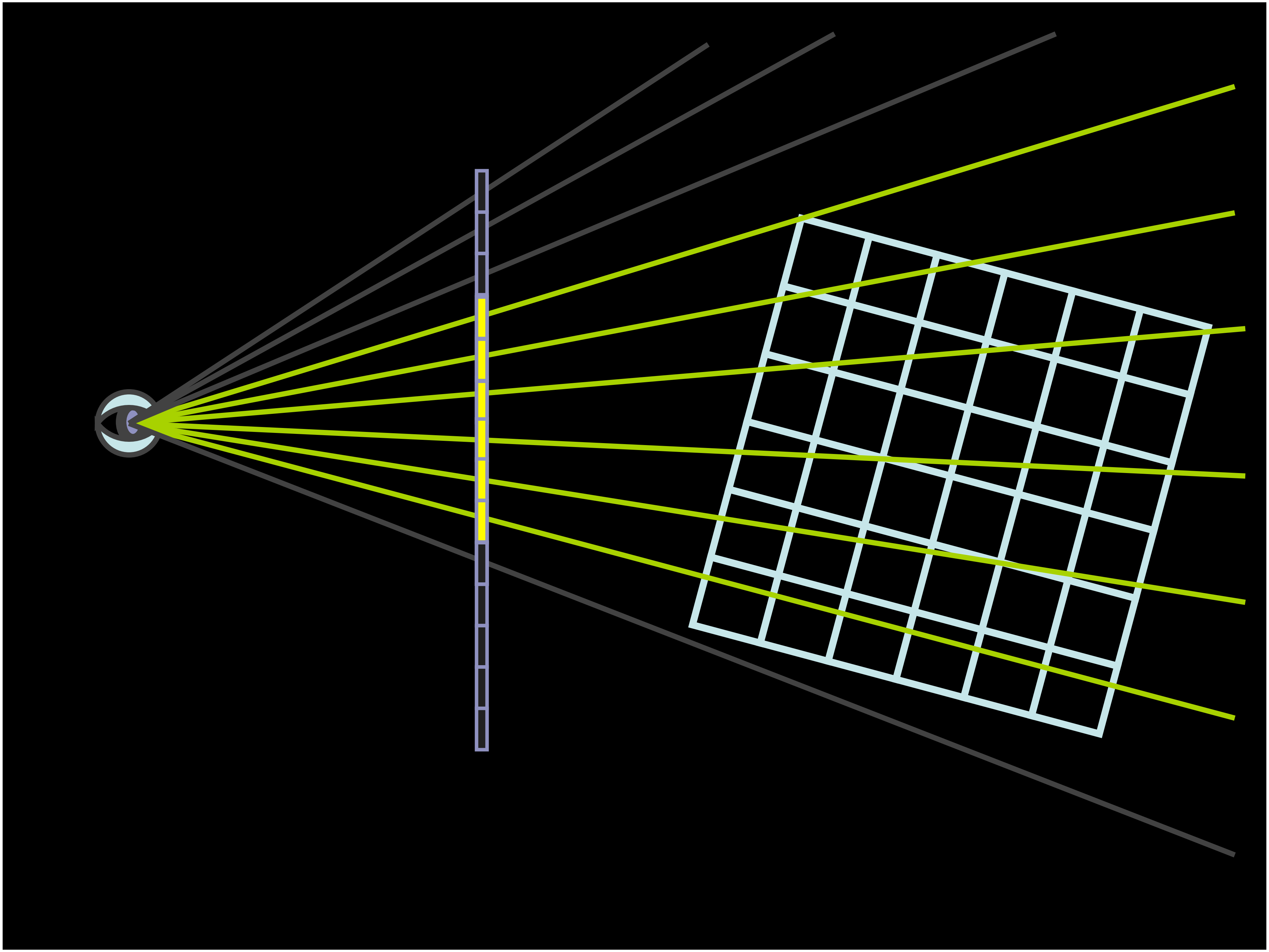
image space algorithm

object space algorithm

image space

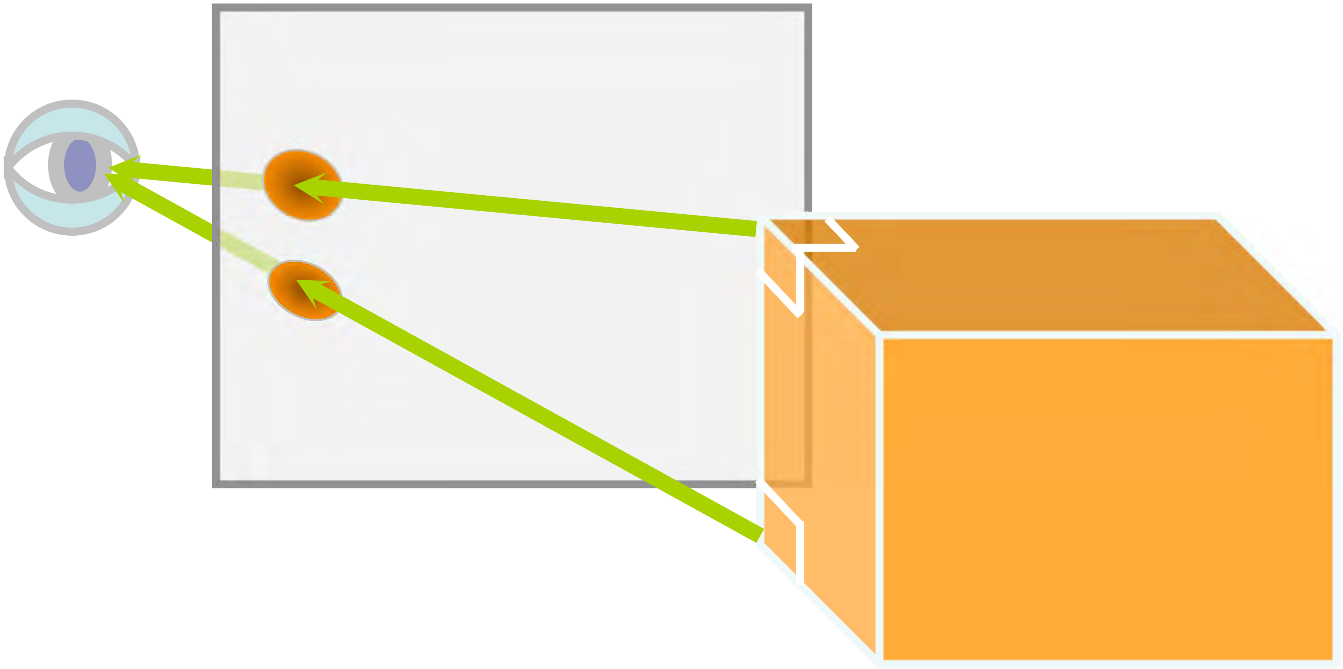
feed backward: ray casting

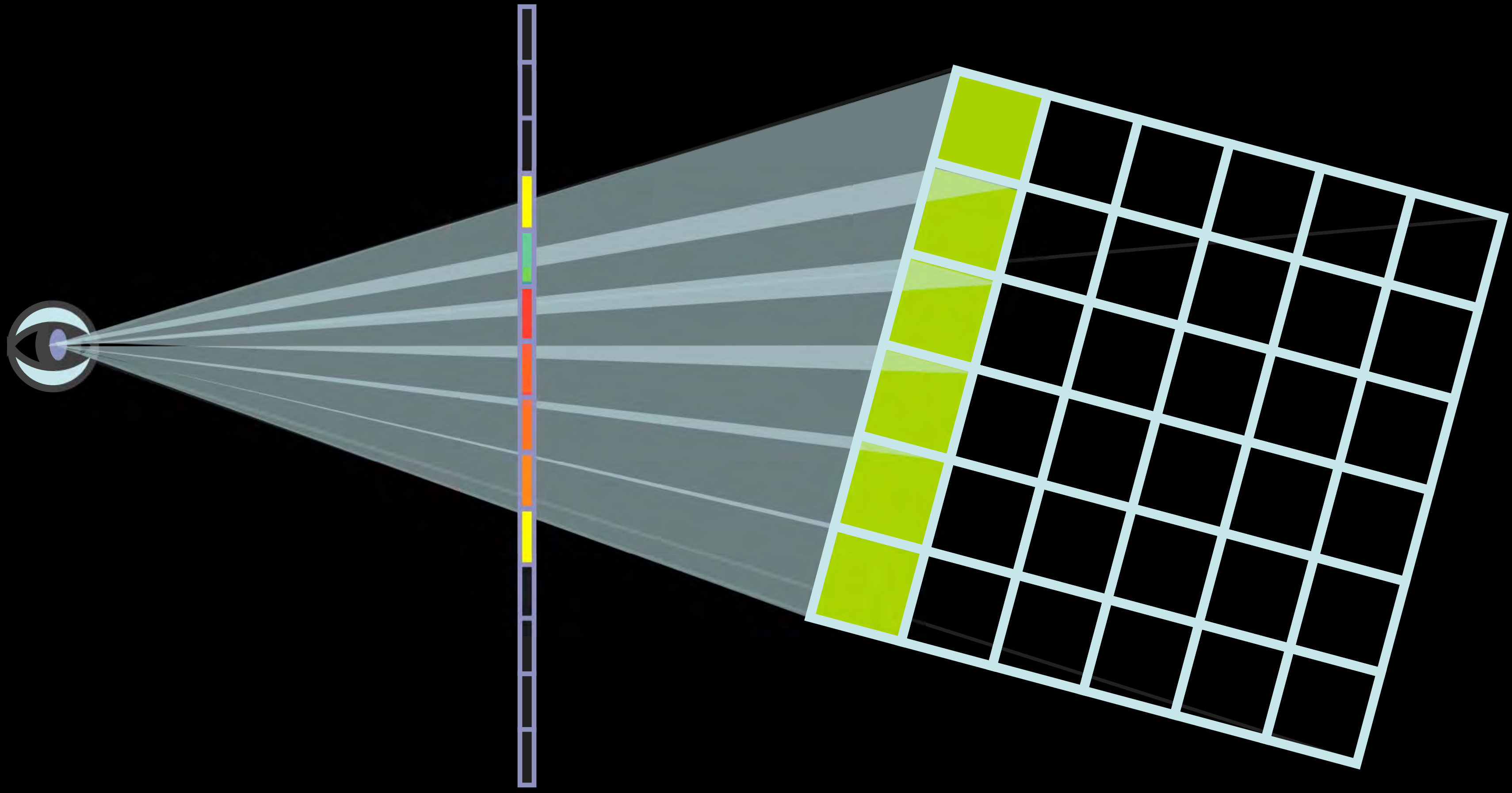




object space

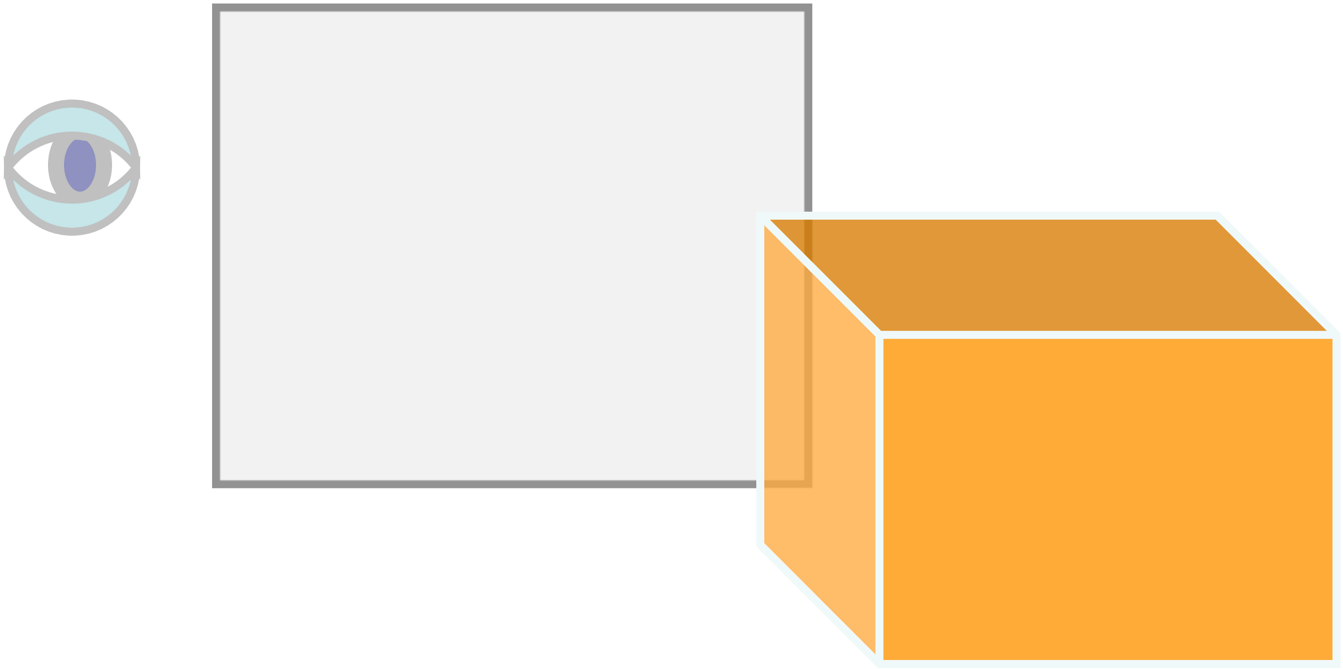
feed forward: splatting

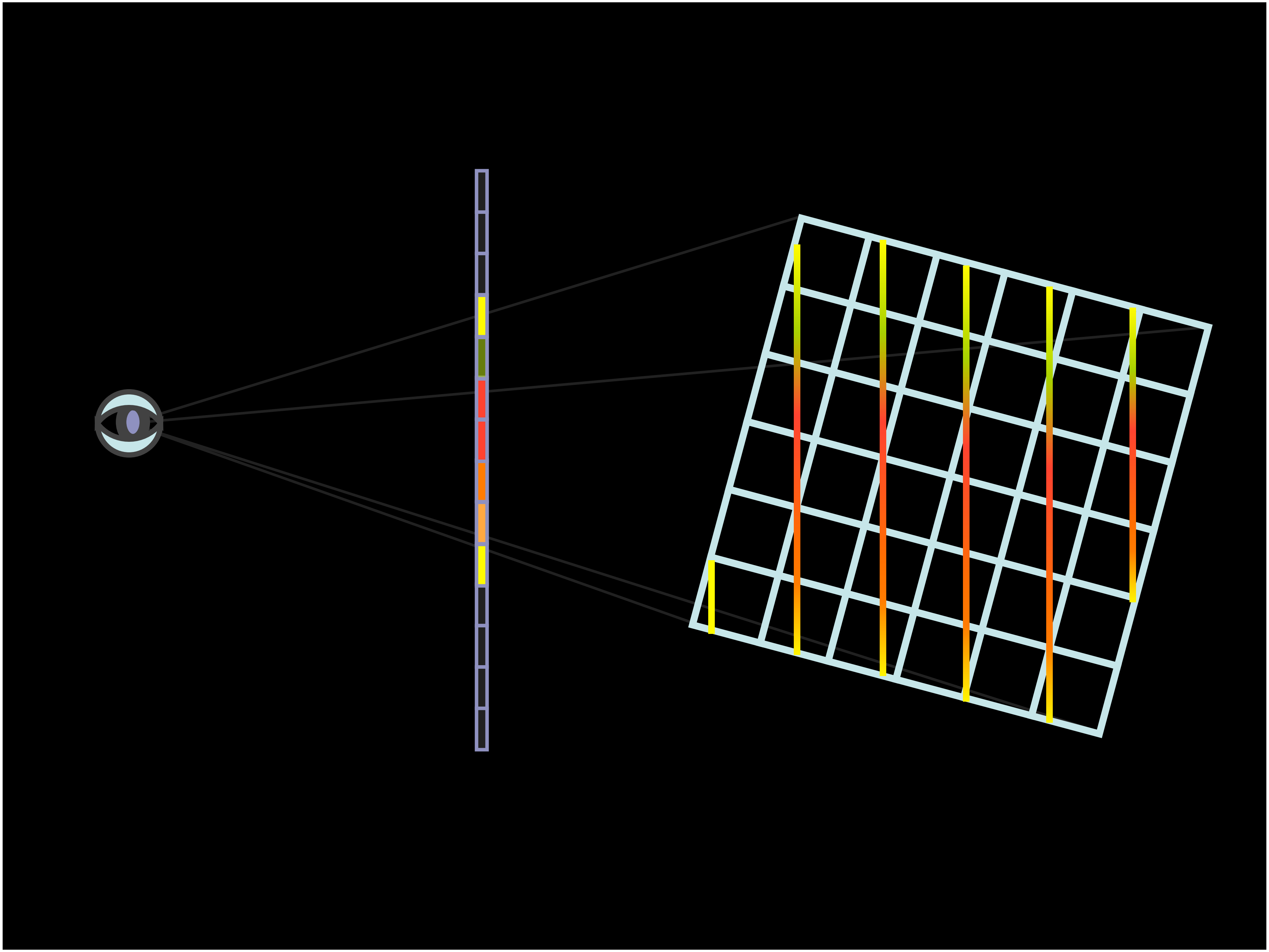




using *gpu*

triangulate slices: 3d textures

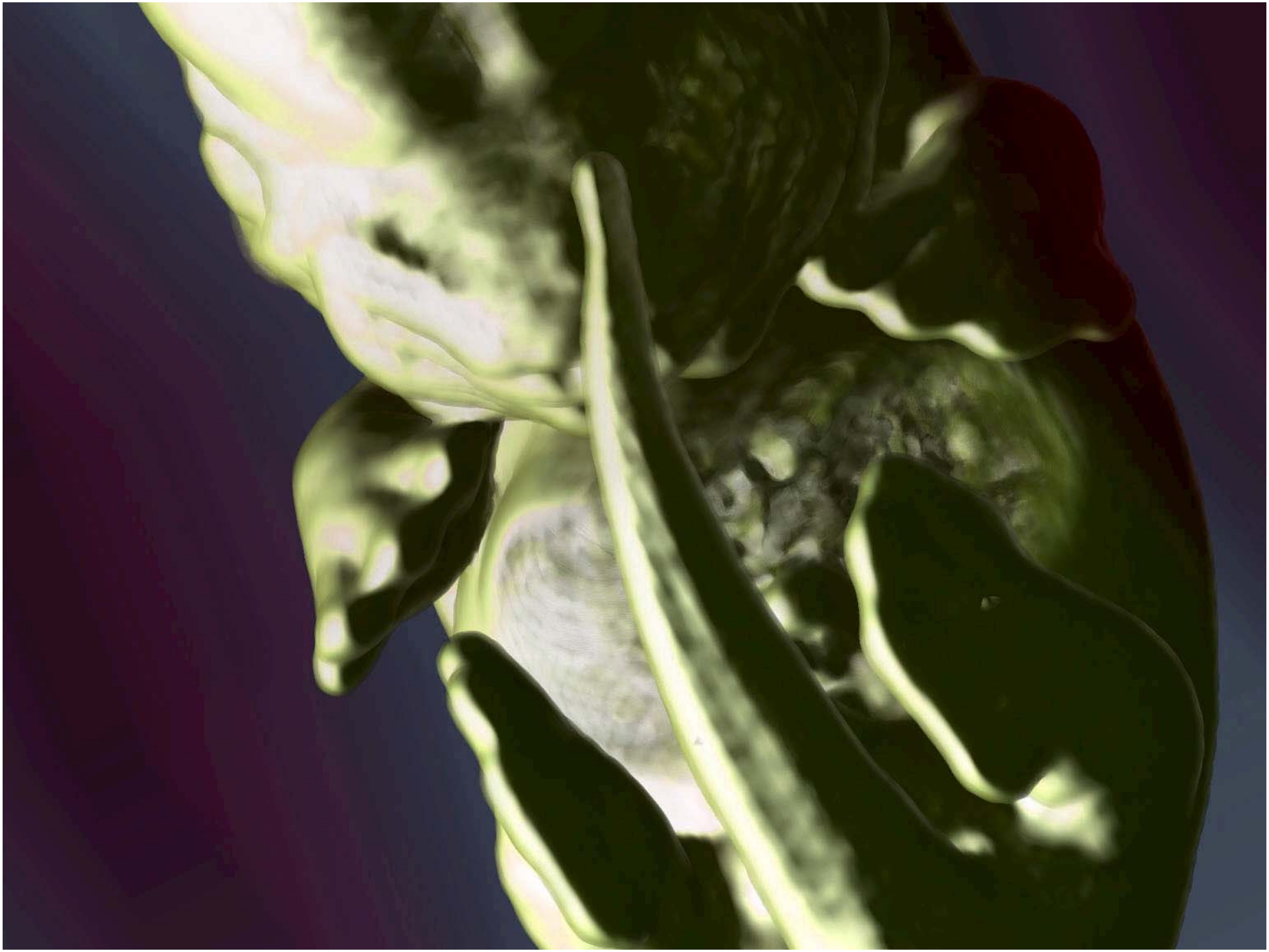




mouse ct scan:

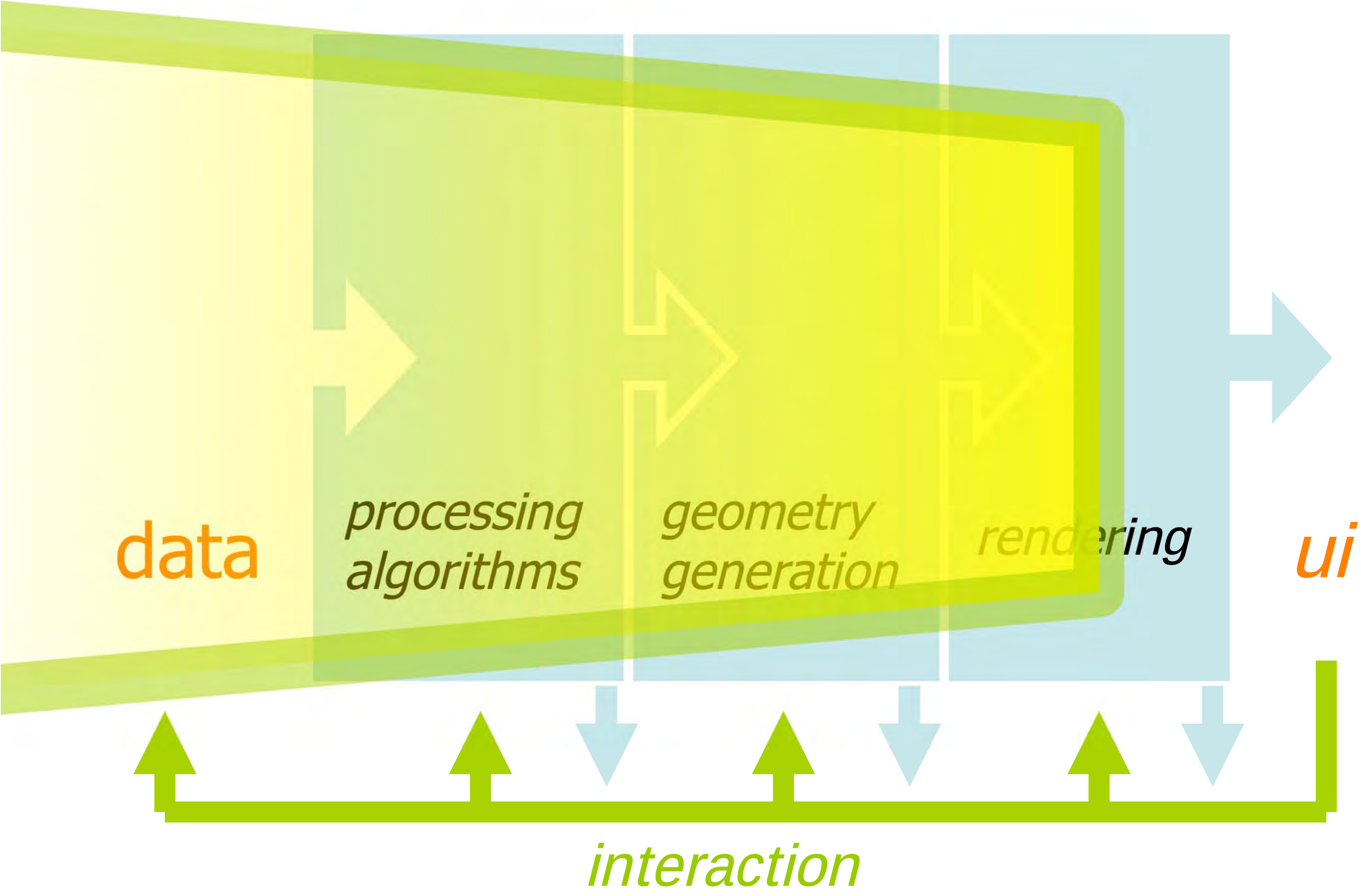
PARAVIEW

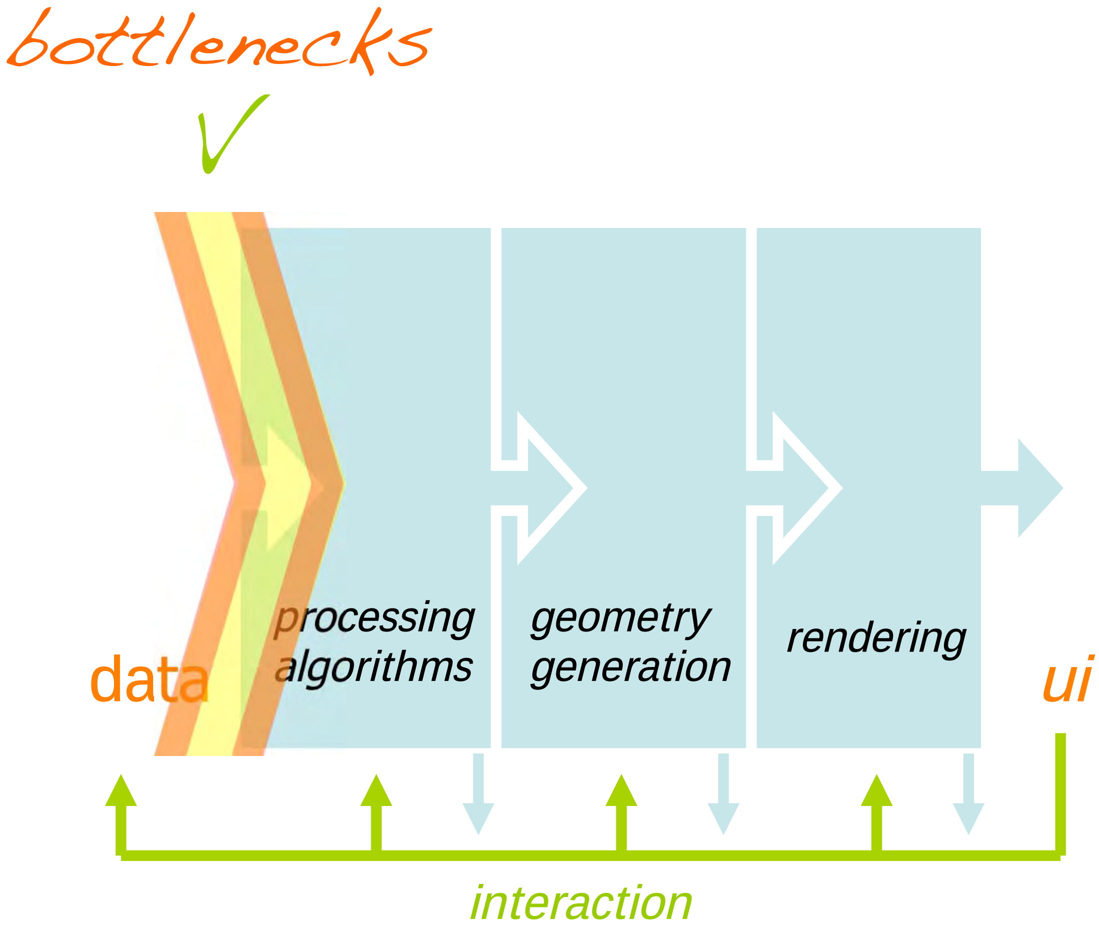
quick demo



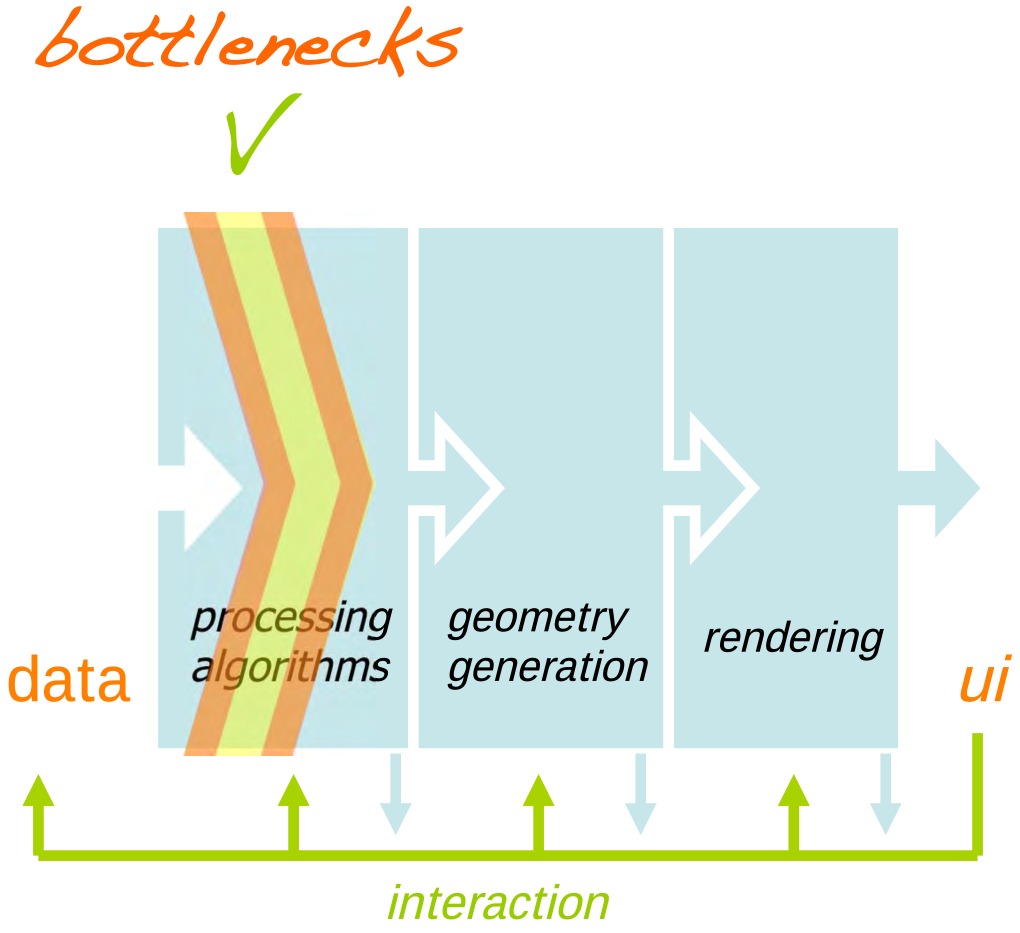
CLOSER LOOK:
BOTTLENECKS

usual visualization “engine”





- data size
- data format
  - *xml*



bottlenecks ✓

data

processing algorithms

geometry generation

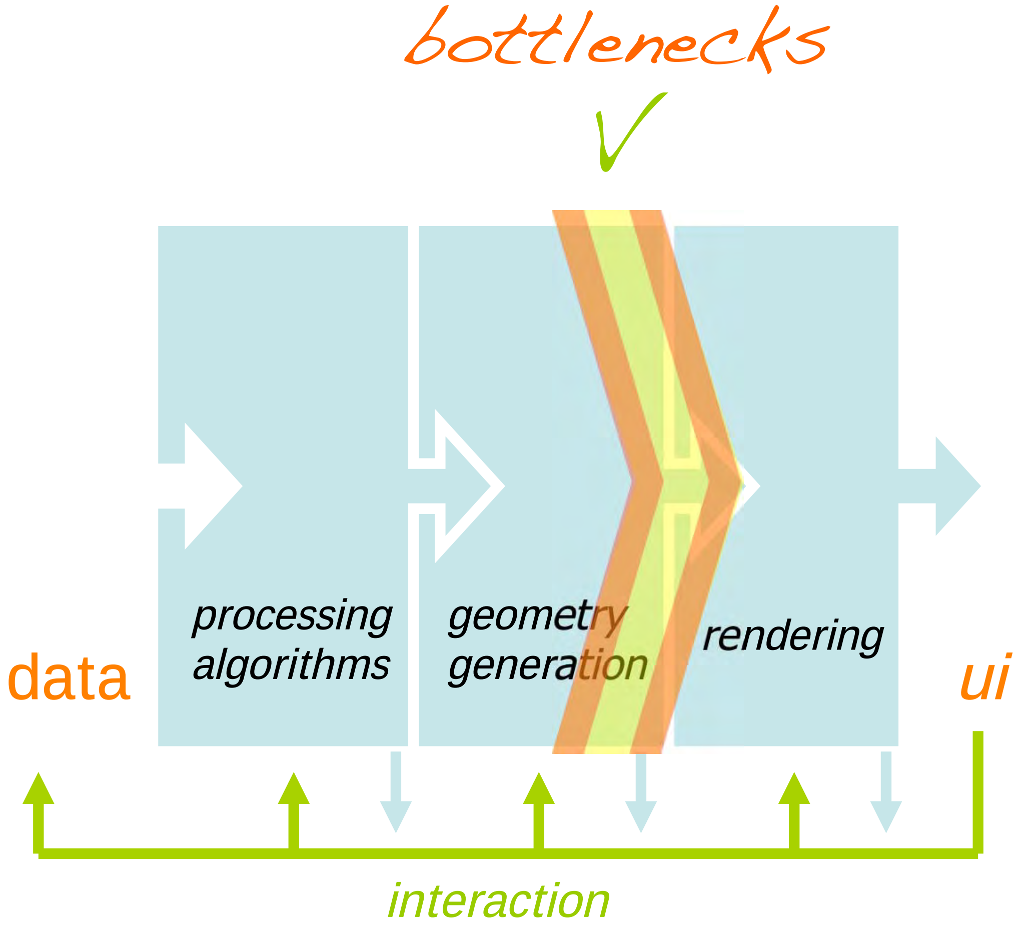
rendering

ui

interaction

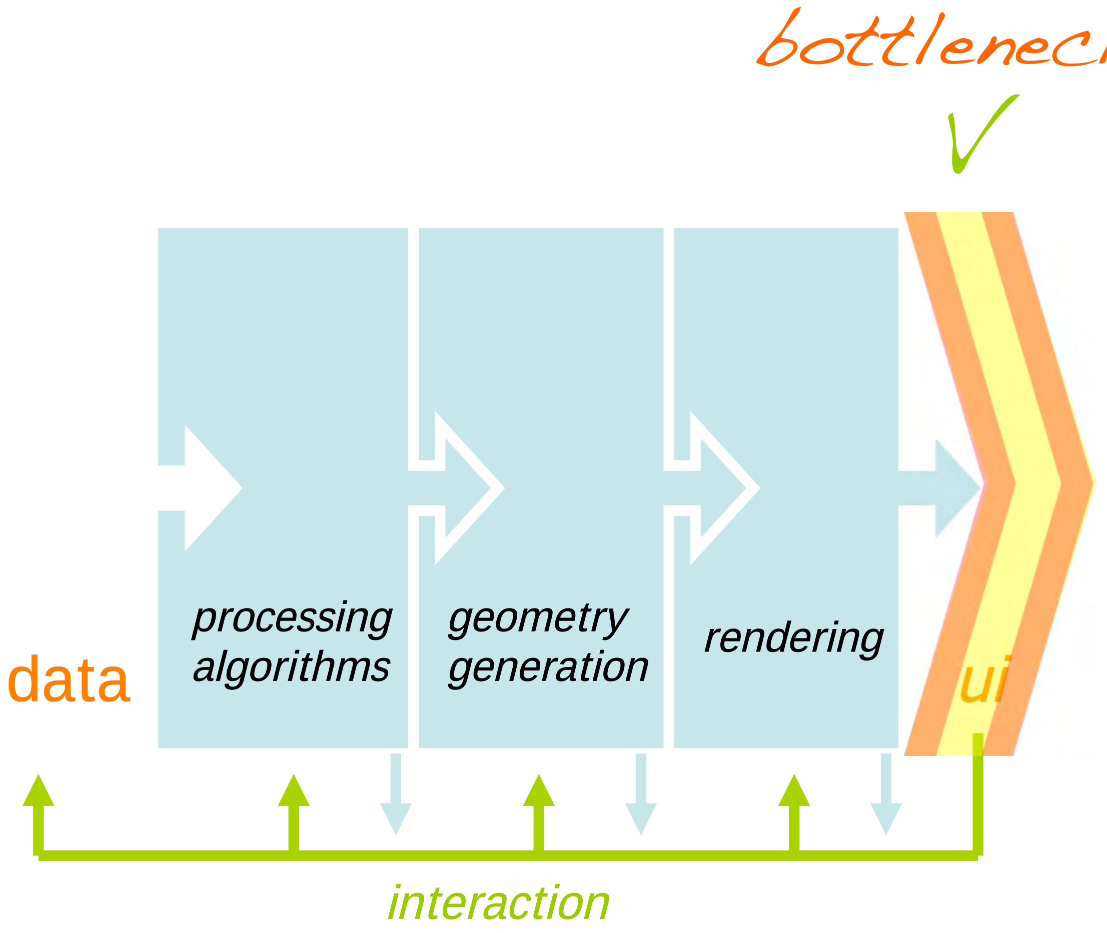
✱ computation

power



- number of records
- number of triangles

  (base rendering units)
- number voxels



bottlenecks

✓

data

processing algorithms

geometry generation

rendering

ui

interaction

- knowledge level of “end user”
- complexity of data base

bottlenecks: *addressing the problem*

lod vs parallelism

addressing throughput bottlenecks

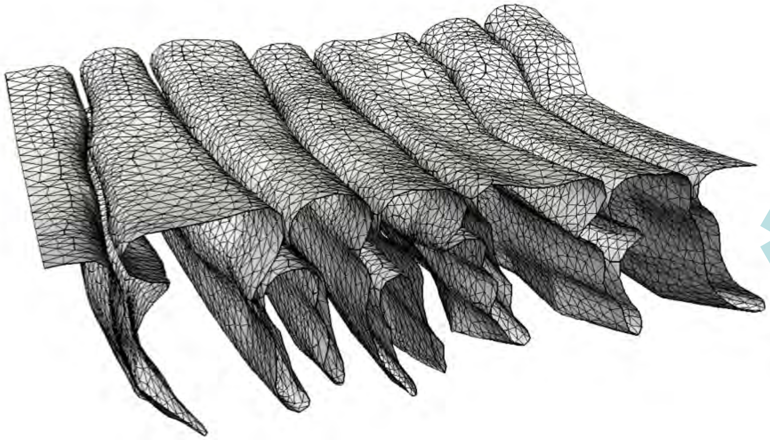
level of detail (LOD)

- requires pre-processing
- requires larger storage *(original+...)*

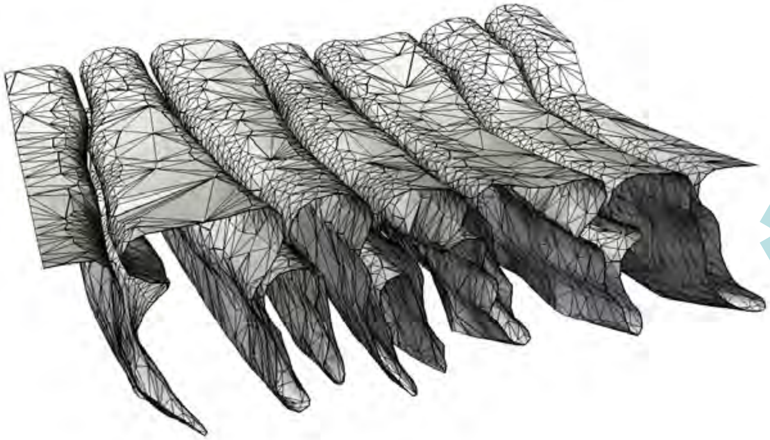
parallel processing/rendering

- requires a parallel system
- increases sw complexity
- less likely to be "portable"

lod: decimation

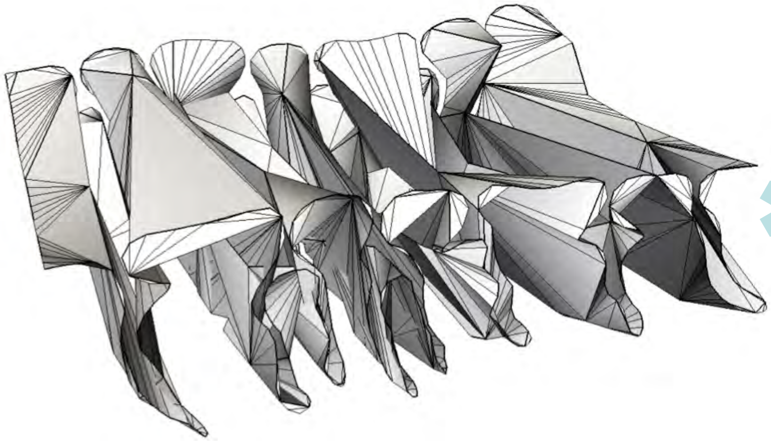


25365



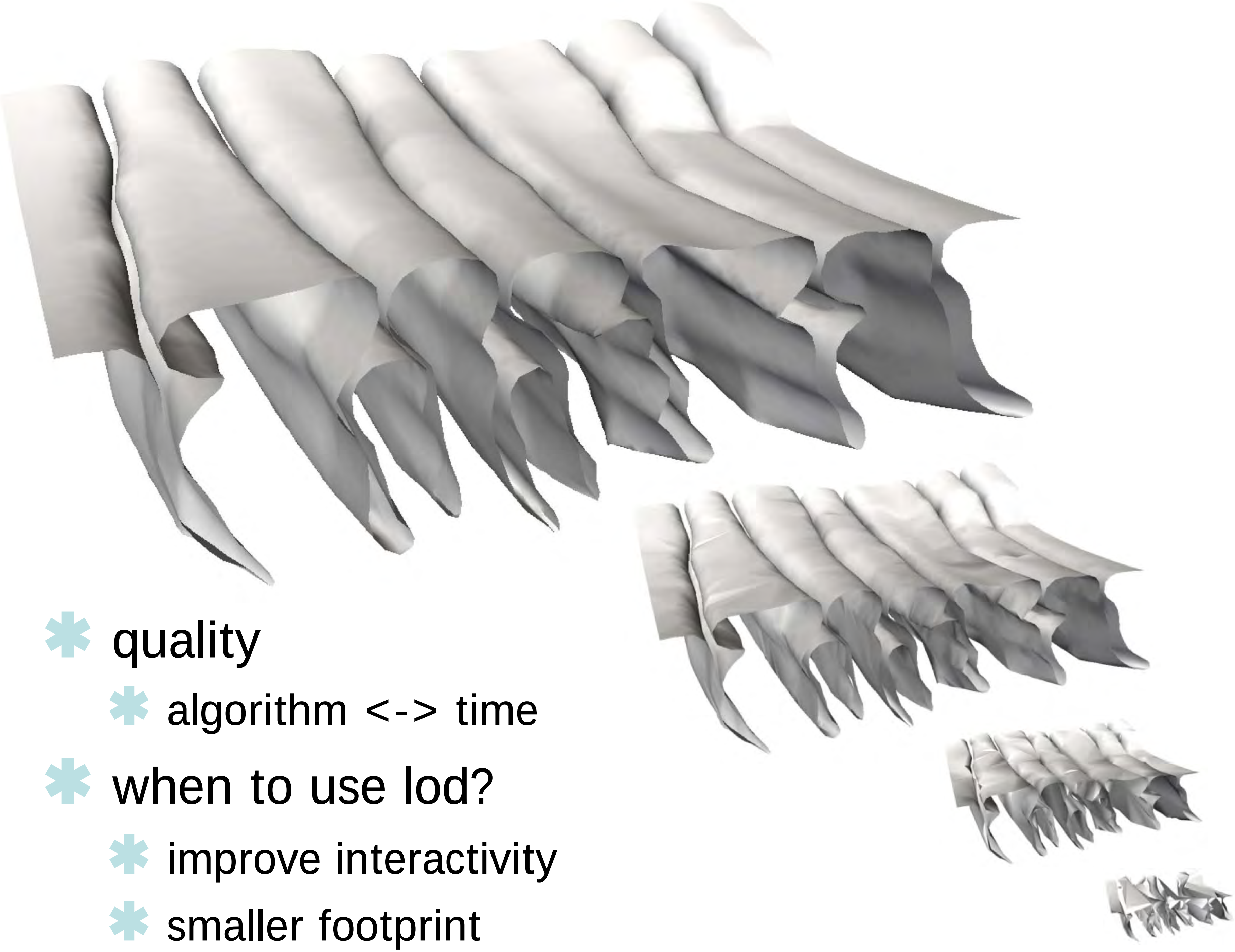
12681

50%

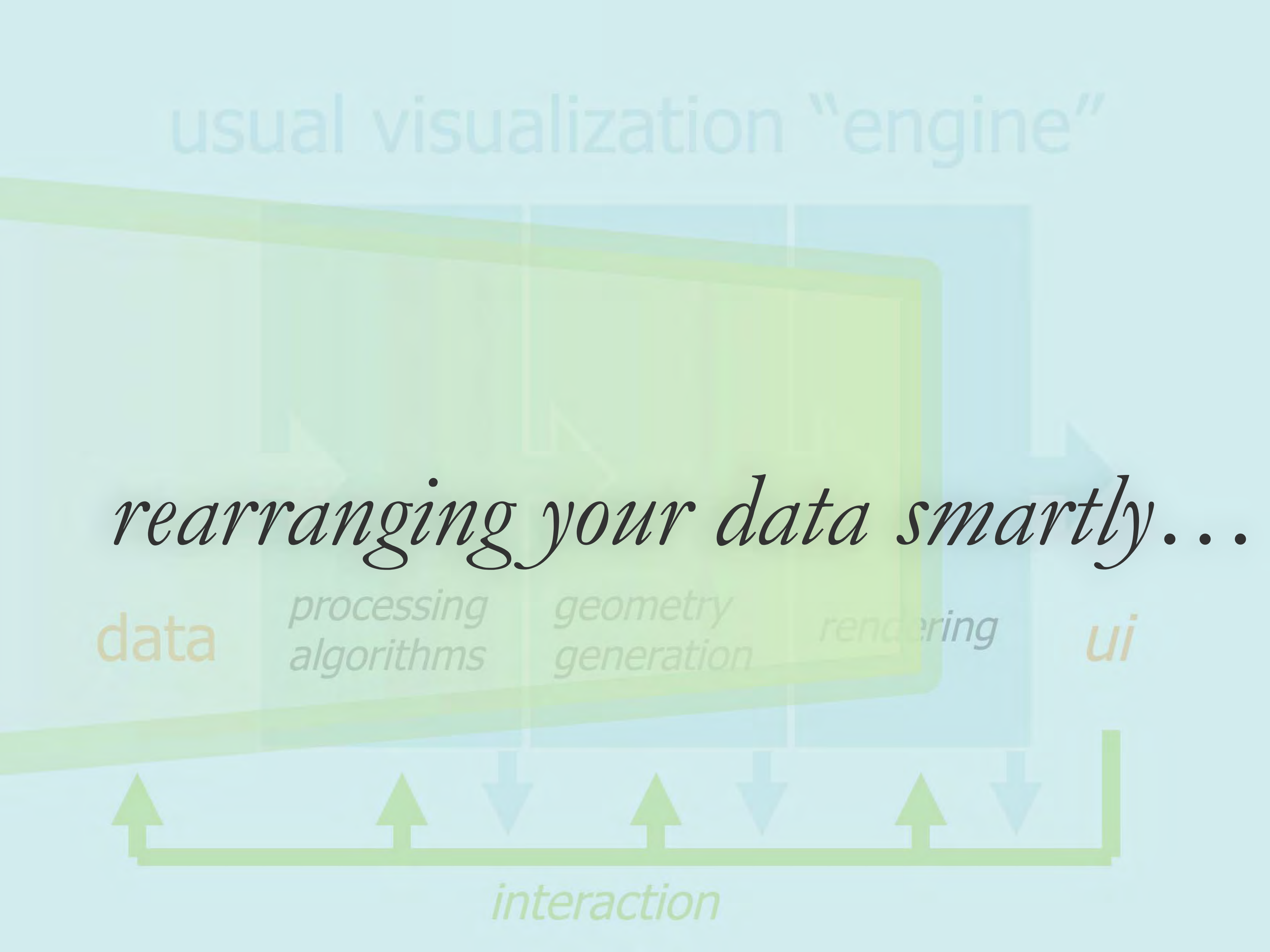


1011

4%

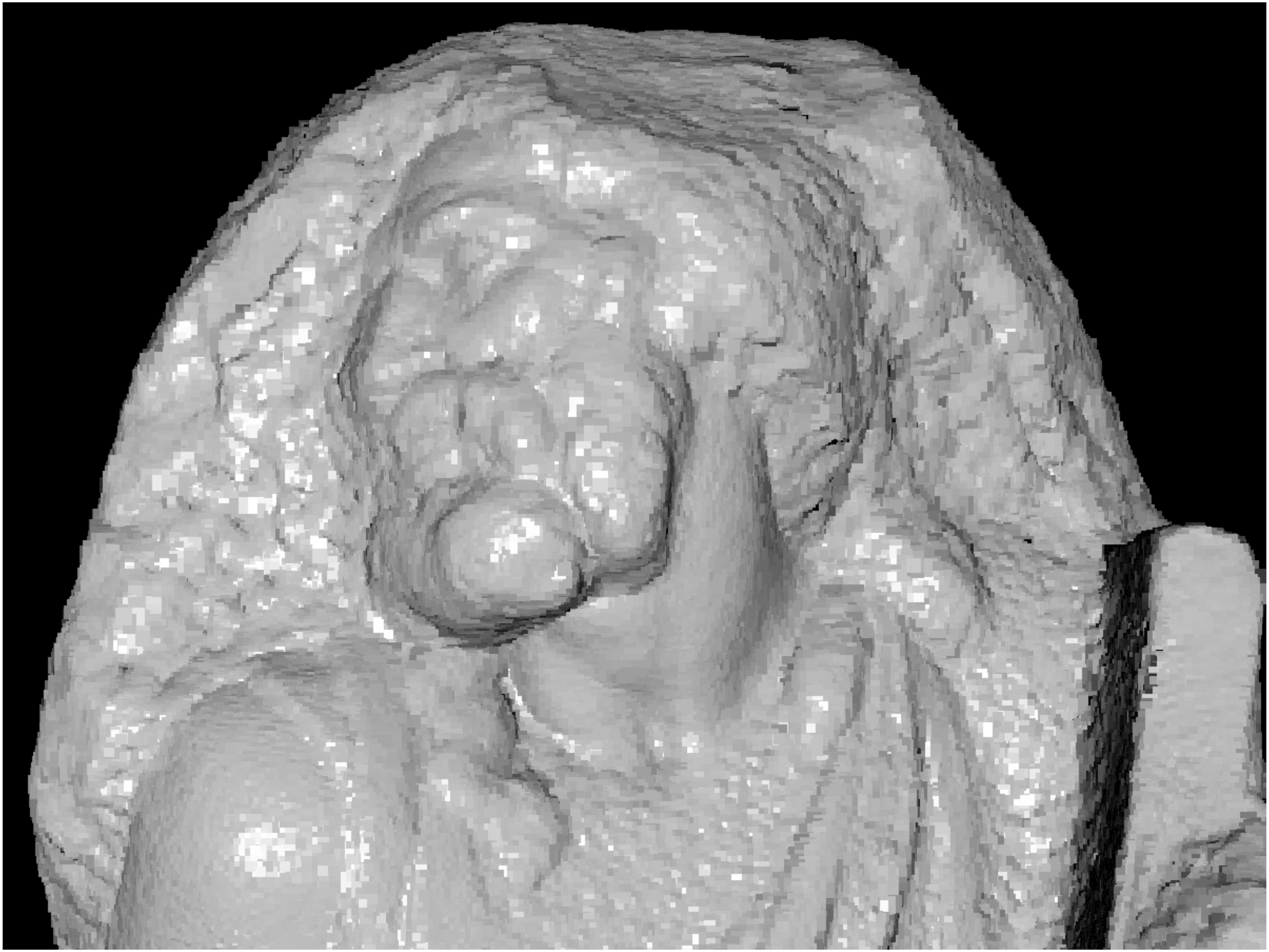


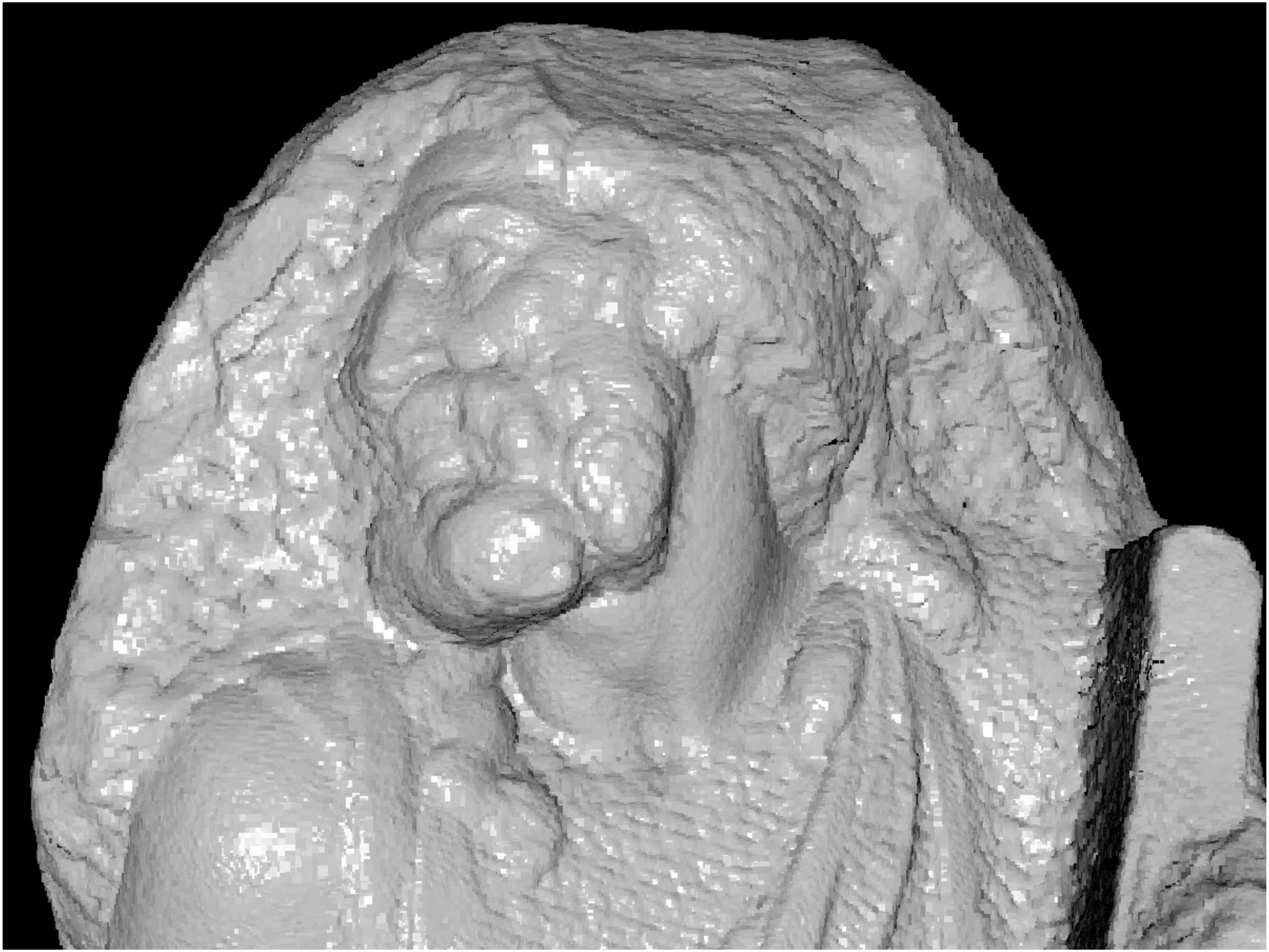
- quality
  - algorithm <-> time
- when to use lod?
  - improve interactivity
  - smaller footprint

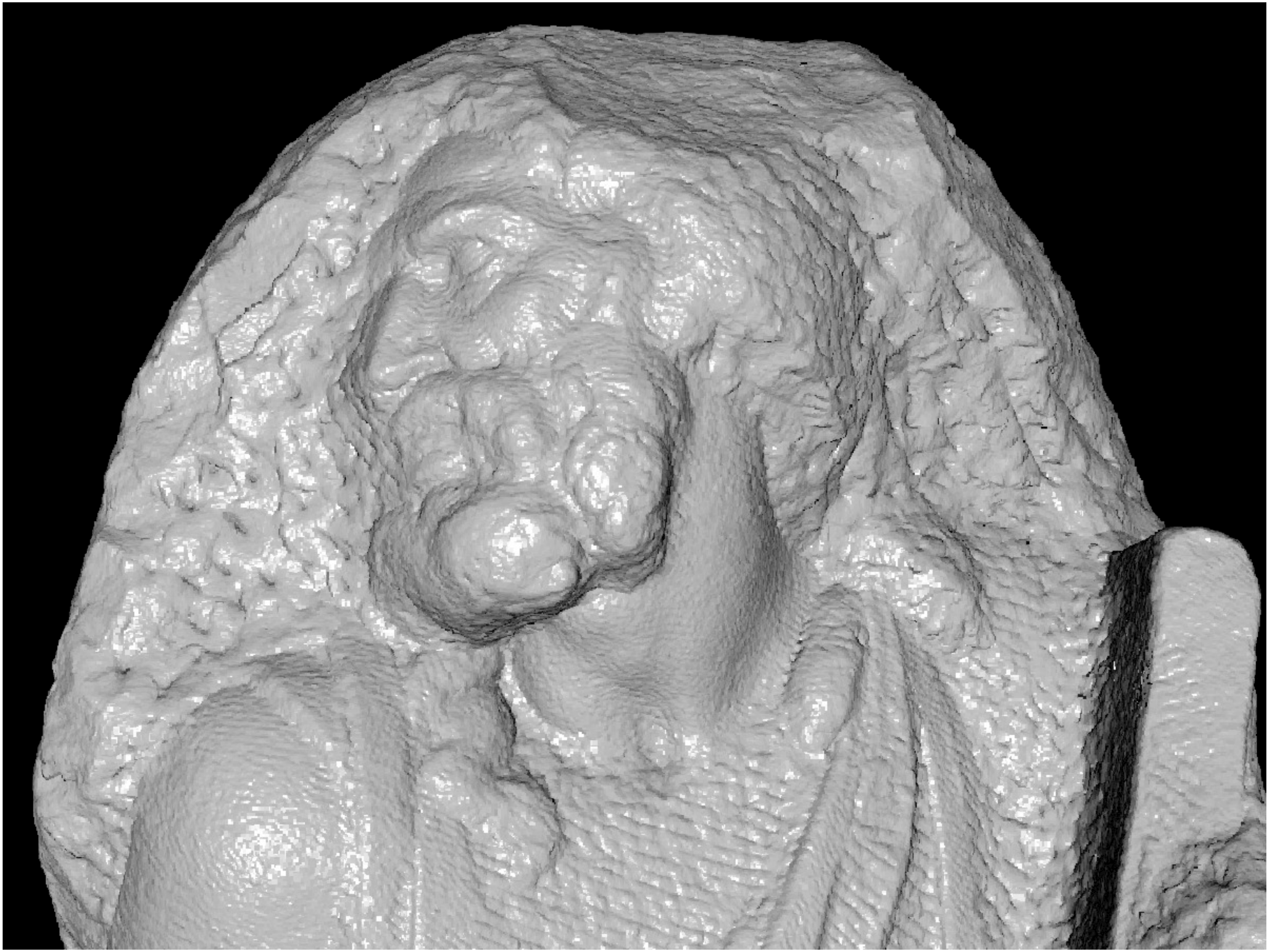


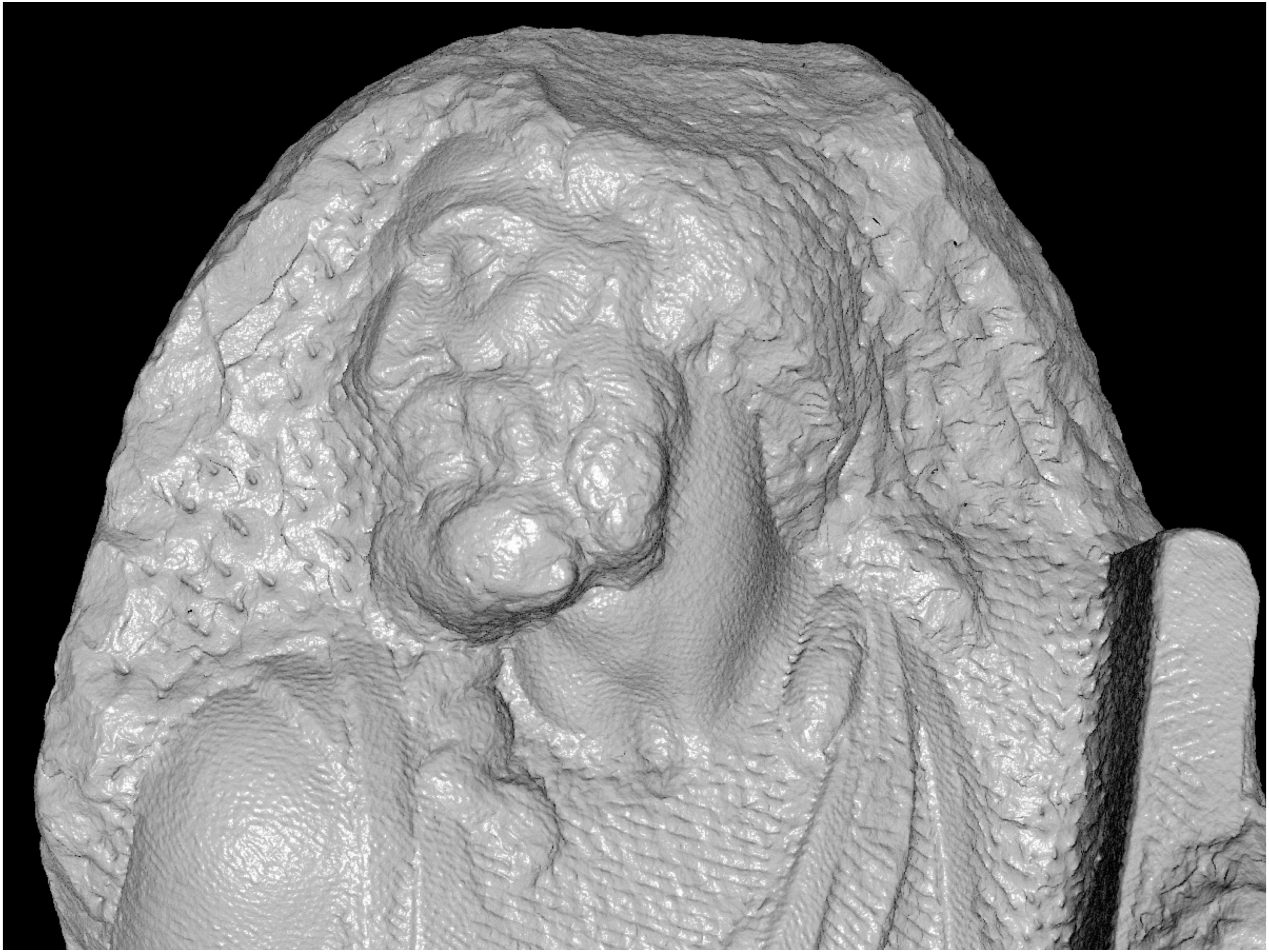
rearranging your data smartly…

stanford: qsplat



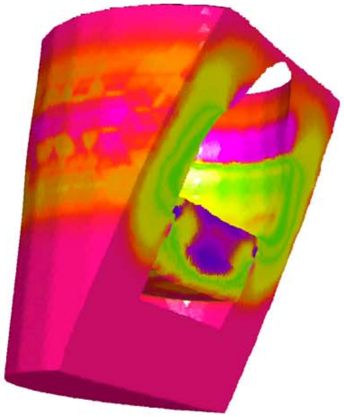


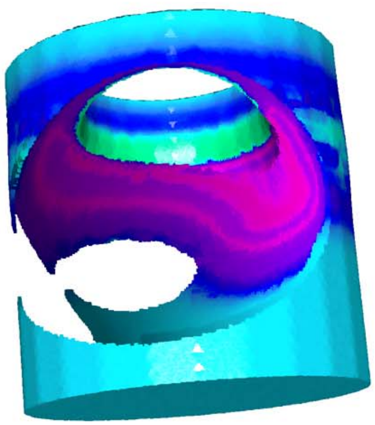


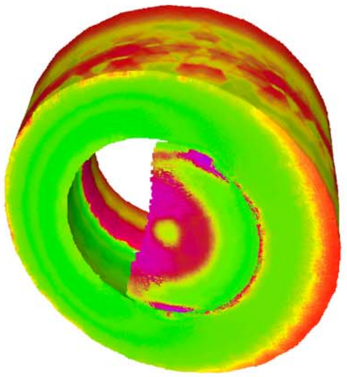


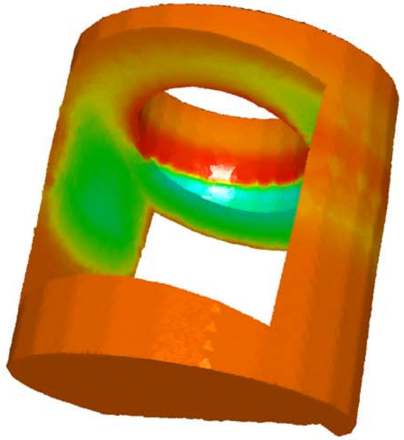
extending to volumetric data: tetsplat

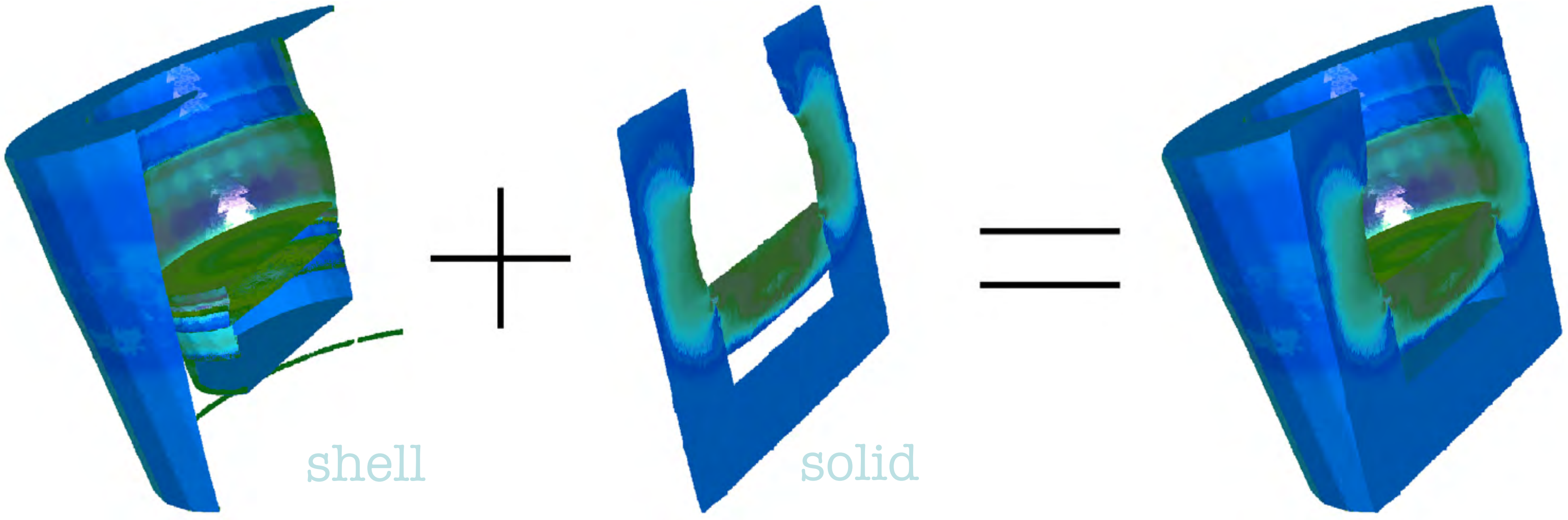
exploring the shock-test cannister











bottlenecks: *addressing the problem*

lod vs parallelism

addressing throughput bottlenecks

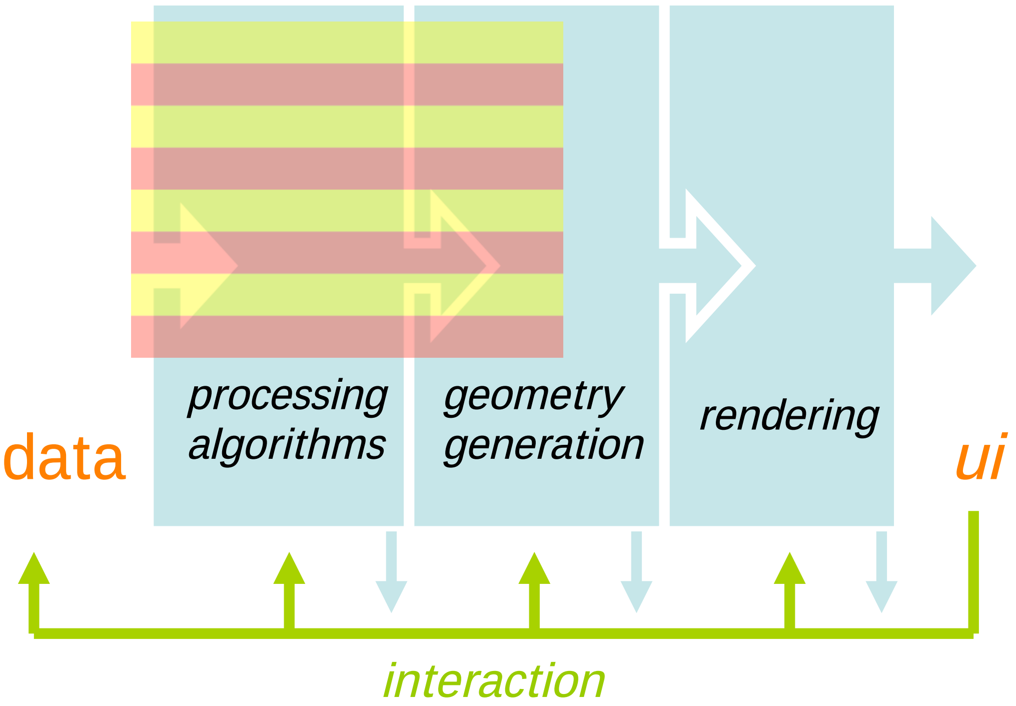
level of detail (LOD)

* requires pre-processing
* requires larger storage

parallel processing/rendering

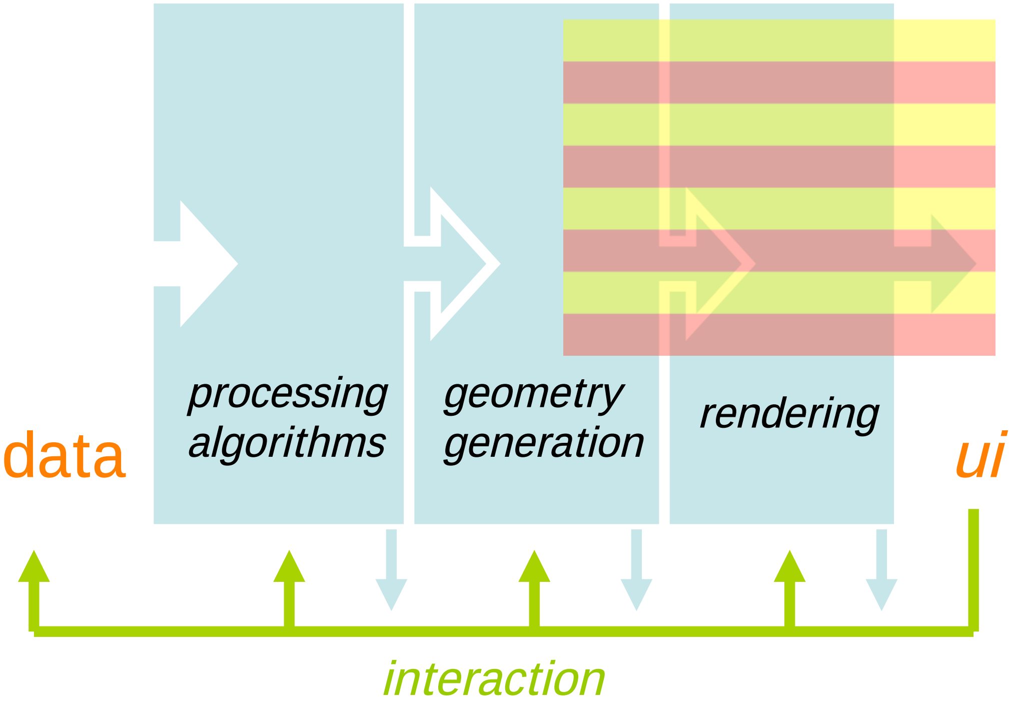
* requires a parallel system
* increases sw complexity
* less likely to be "portable"

>> parallel viz >>

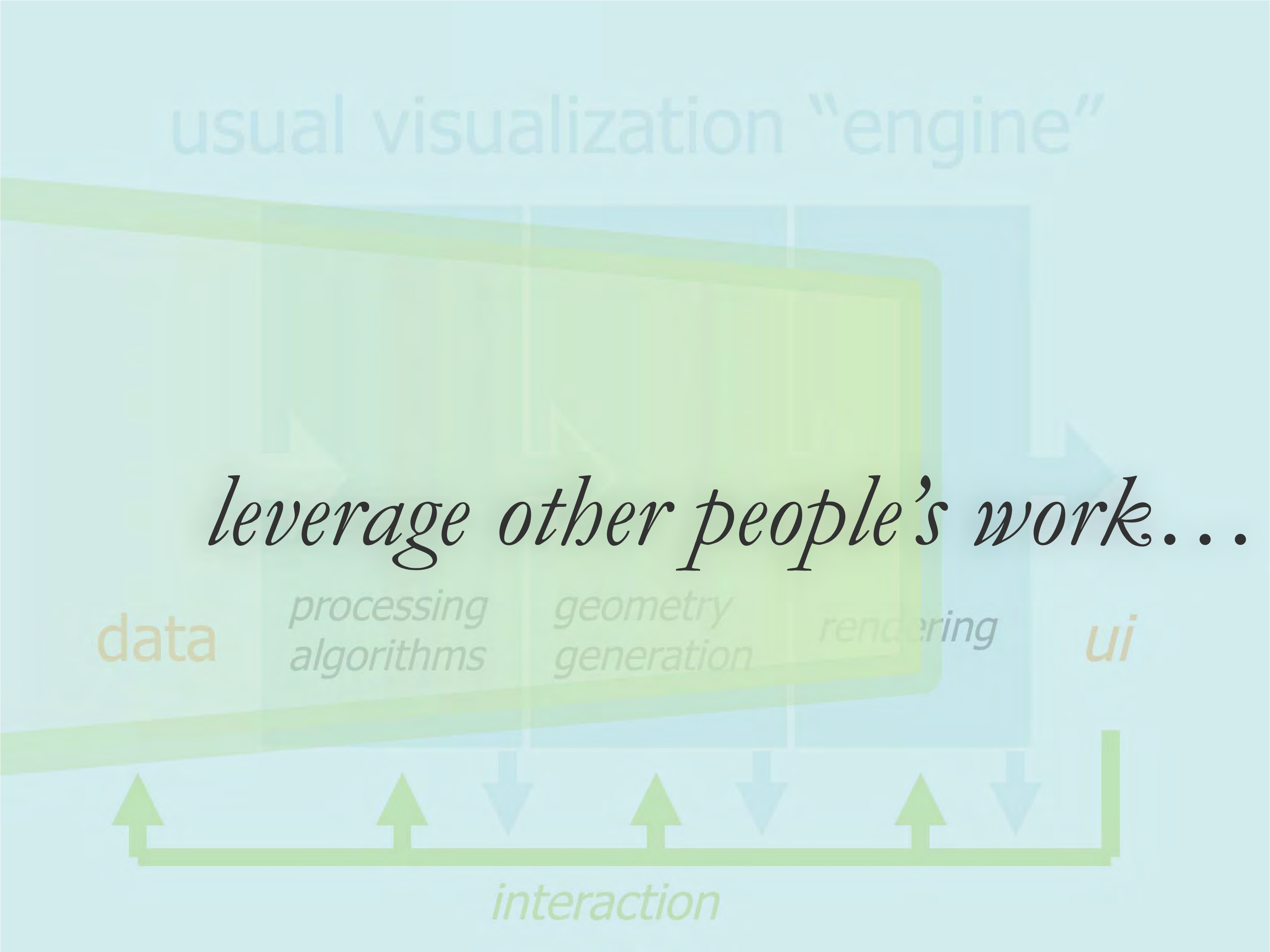


- + cpus
  - data?
  - seams?

>> parallel viz >>



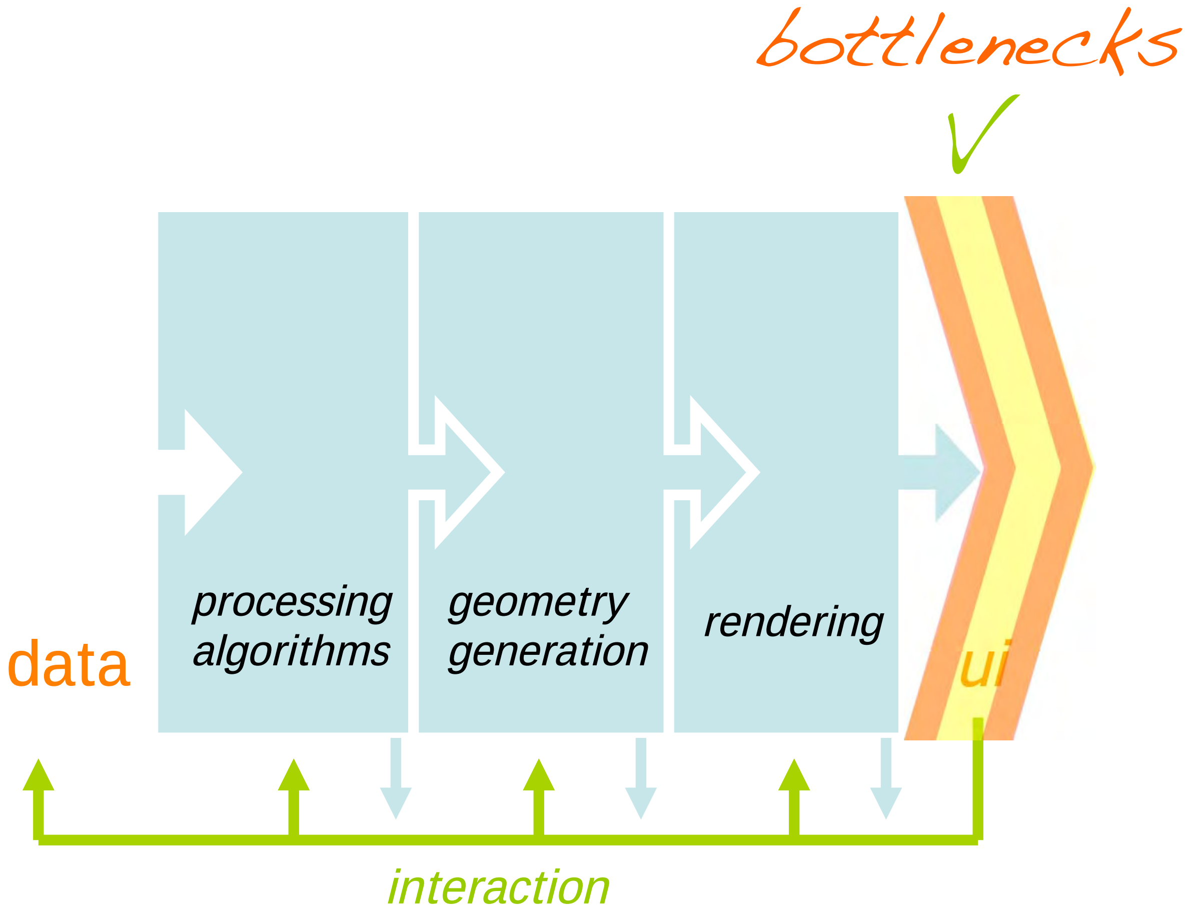
- + gpus
- screen?
- space?



leverage other people's work…

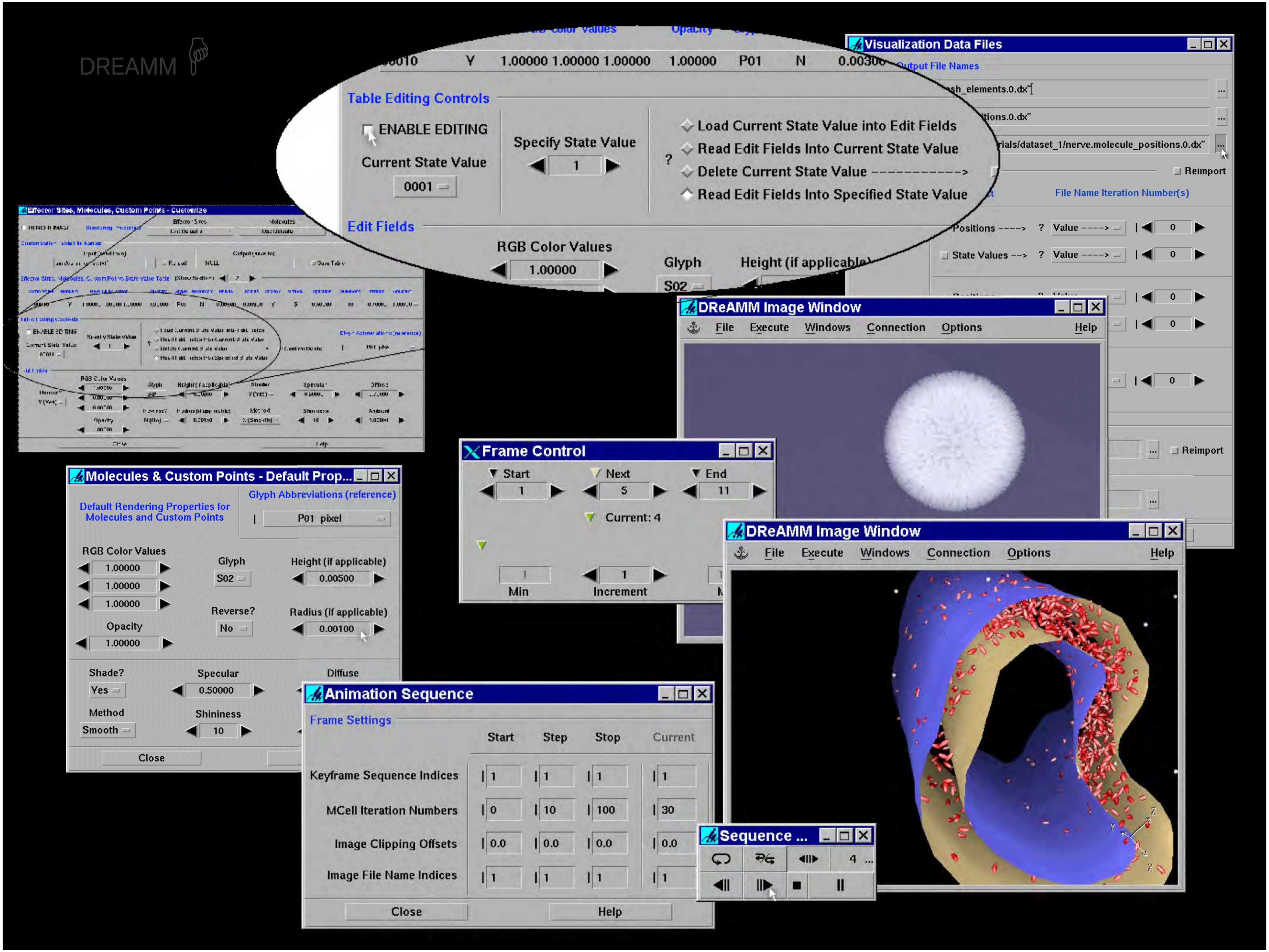
bottlenecks: *addressing the problem*

ui


bottlenecks
✓
data
processing algorithms
geometry generation
rendering
ui
interaction

case study: *gui design*

mcell viewer



...0010 Y 1.00000 1.00000 1.00000 1.00000 P01 N 0.00300

Table Editing Controls

□ ENABLE EDITING

Current State Value: 0001

Specify State Value: 1

- ◇ Load Current State Value into Edit Fields
- ◇ Read Edit Fields Into Current State Value
- ◇ Delete Current State Value ------------>
- ◆ Read Edit Fields Into Specified State Value

Edit Fields

RGB Color Values: 1.00000

Glyph: S02

Height (if applicable)

Visualization Data Files

Output File Names

...sh_elements.0.dx"

...tions.0.dx"

...rials/dataset_1/nerve.molecule_positions.0.dx"

□ Reimport

File Name Iteration Number(s)

Positions ----> ? Value ----> 0

□ State Values --> ? Value ----> 0

0

0

0

□ Reimport

Frame Control

Start	Next	End
1	5	11

Current: 4

Min: 1

Increment: 1

Molecules & Custom Points - Default Properties

Default Rendering Properties for Molecules and Custom Points

Glyph Abbreviations (reference): P01 pixel

RGB Color Values: 1.00000, 1.00000, 1.00000

Glyph: S02

Height (if applicable): 0.00500

Reverse?: No

Radius (if applicable): 0.00100

Opacity: 1.00000

Shade?: Yes

Specular: 0.50000

Diffuse

Method: Smooth

Shininess: 10

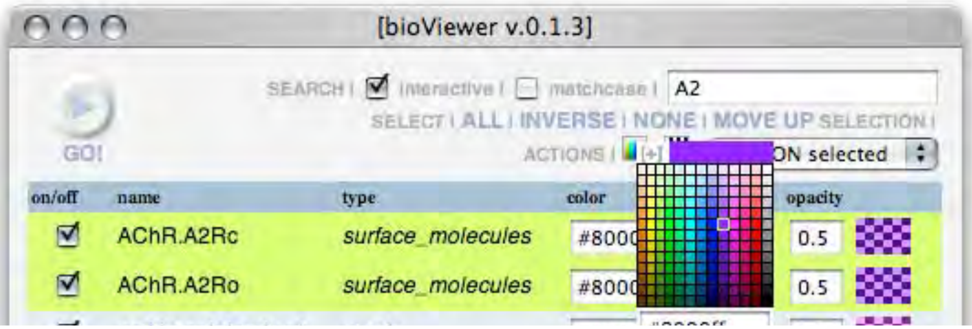
Animation Sequence

Frame Settings

	Start	Step	Stop	Current
Keyframe Sequence Indices	1	1	1	1
MCell Iteration Numbers	0	10	100	30
Image Clipping Offsets	0.0	0.0	0.0	0.0
Image File Name Indices	1	1	1	1

Sequence ...: 4

GUI

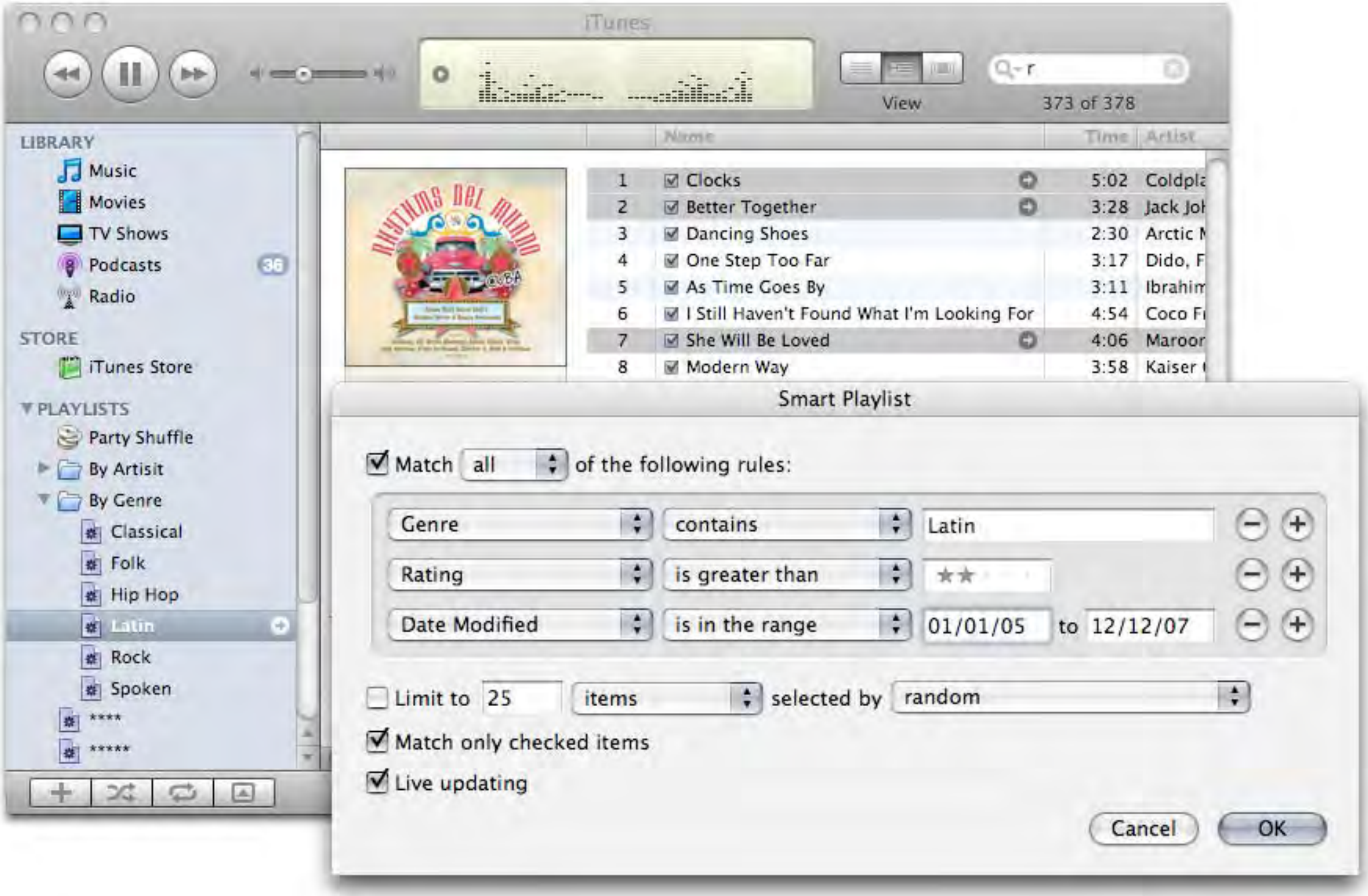

[bioViewer v.0.1.3]

SEARCH | ☑ interactive | □ matchcase | A2

SELECT | ALL | INVERSE | NONE | MOVE UP SELECTION |

ACTIONS | ON selected

on/off	name	type	color	opacity
☑	AChR.A2Rc	*surface_molecules*	#800	0.5
☑	AChR.A2Ro	*surface_molecules*	#800	0.5



	Name	Time	Artist
1	☑ Clocks	5:02	Coldpla
2	☑ Better Together	3:28	Jack Joh
3	☑ Dancing Shoes	2:30	Arctic M
4	☑ One Step Too Far	3:17	Dido, F
5	☑ As Time Goes By	3:11	Ibrahim
6	☑ I Still Haven't Found What I'm Looking For	4:54	Coco F
7	☑ She Will Be Loved	4:06	Maroon
8	☑ Modern Way	3:58	Kaiser (

Smart Playlist

☑ Match all of the following rules:

Genre contains Latin

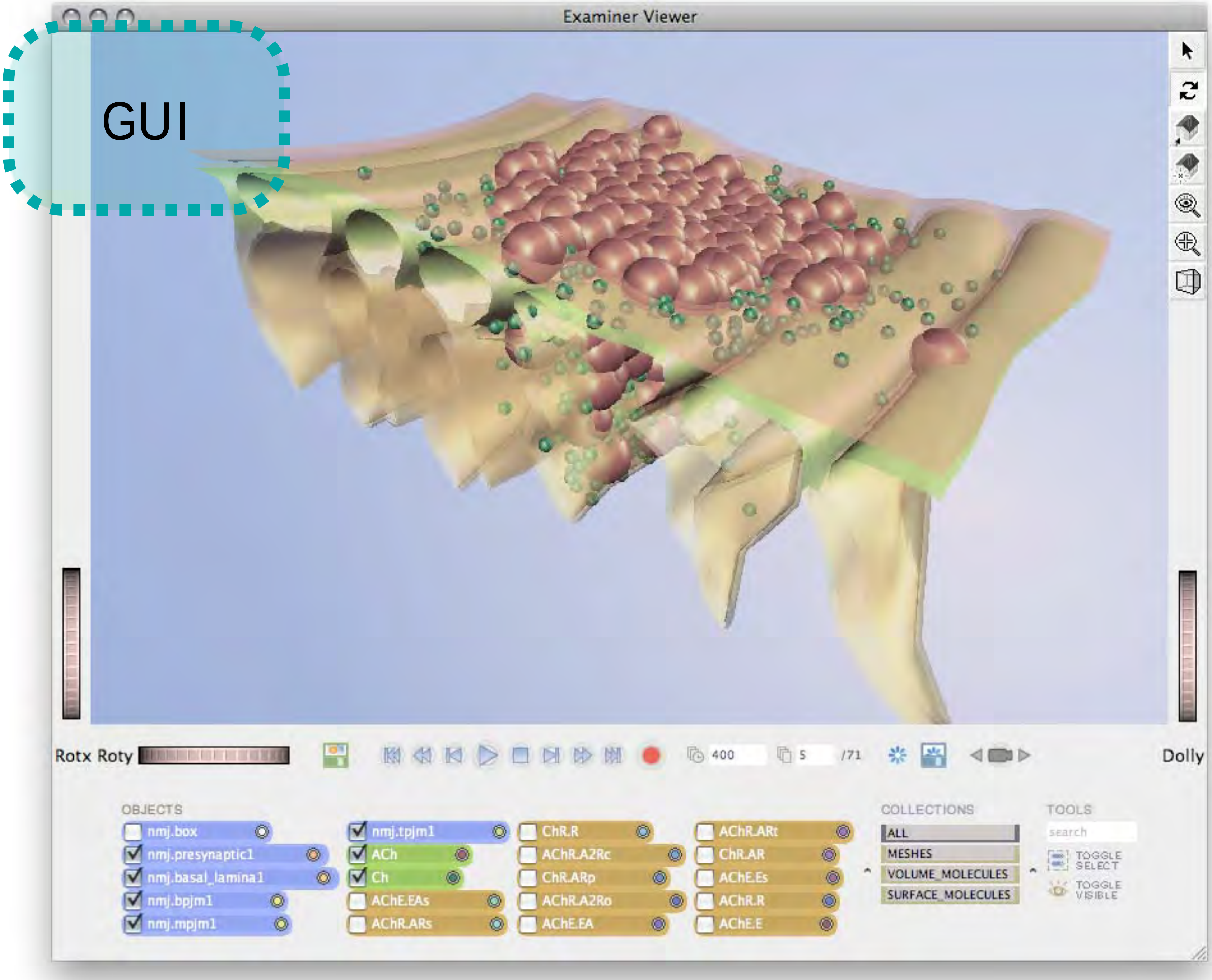
Rating is greater than ★★

Date Modified is in the range 01/01/05 to 12/12/07

□ Limit to 25 items selected by random

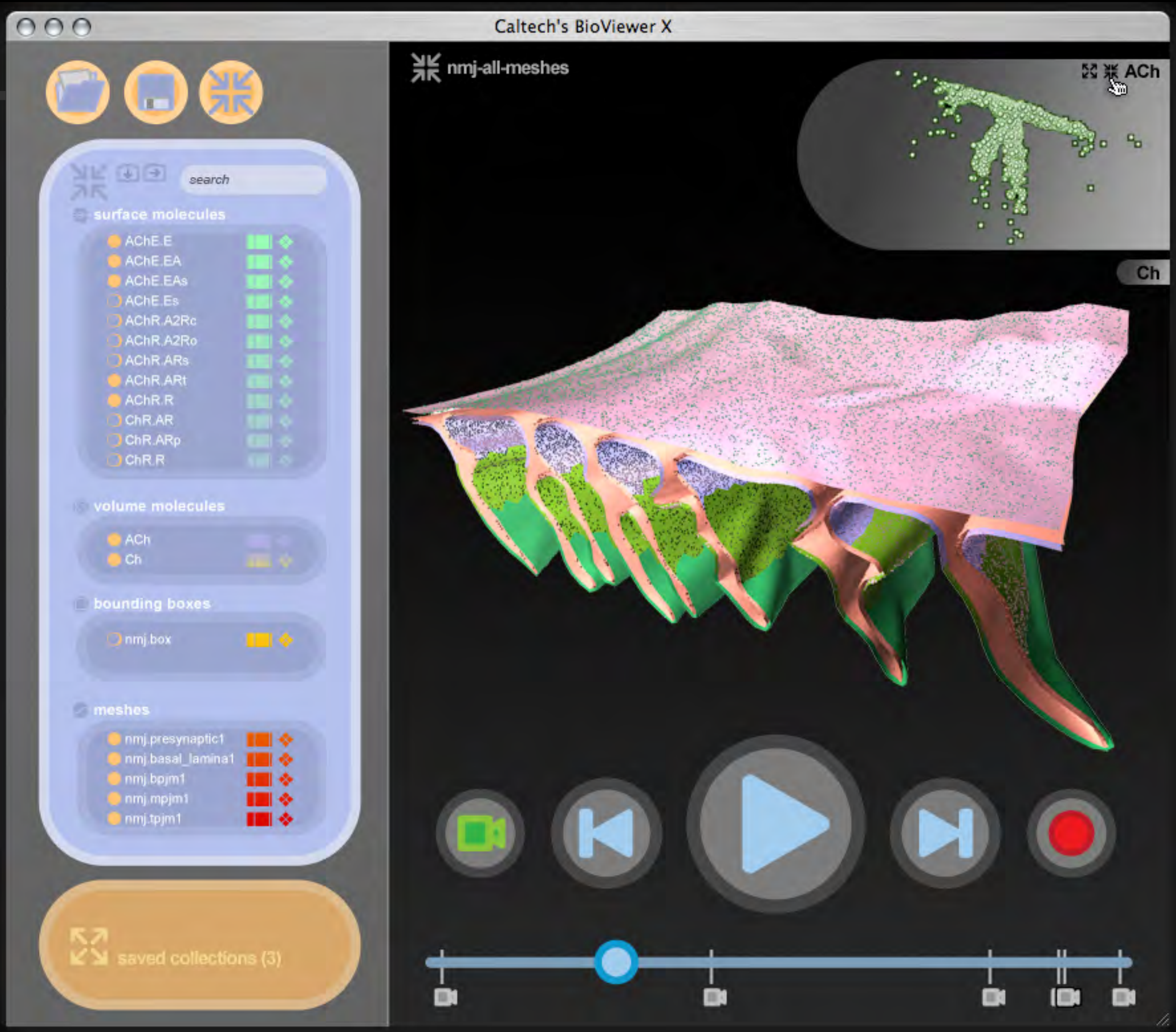
☑ Match only checked items

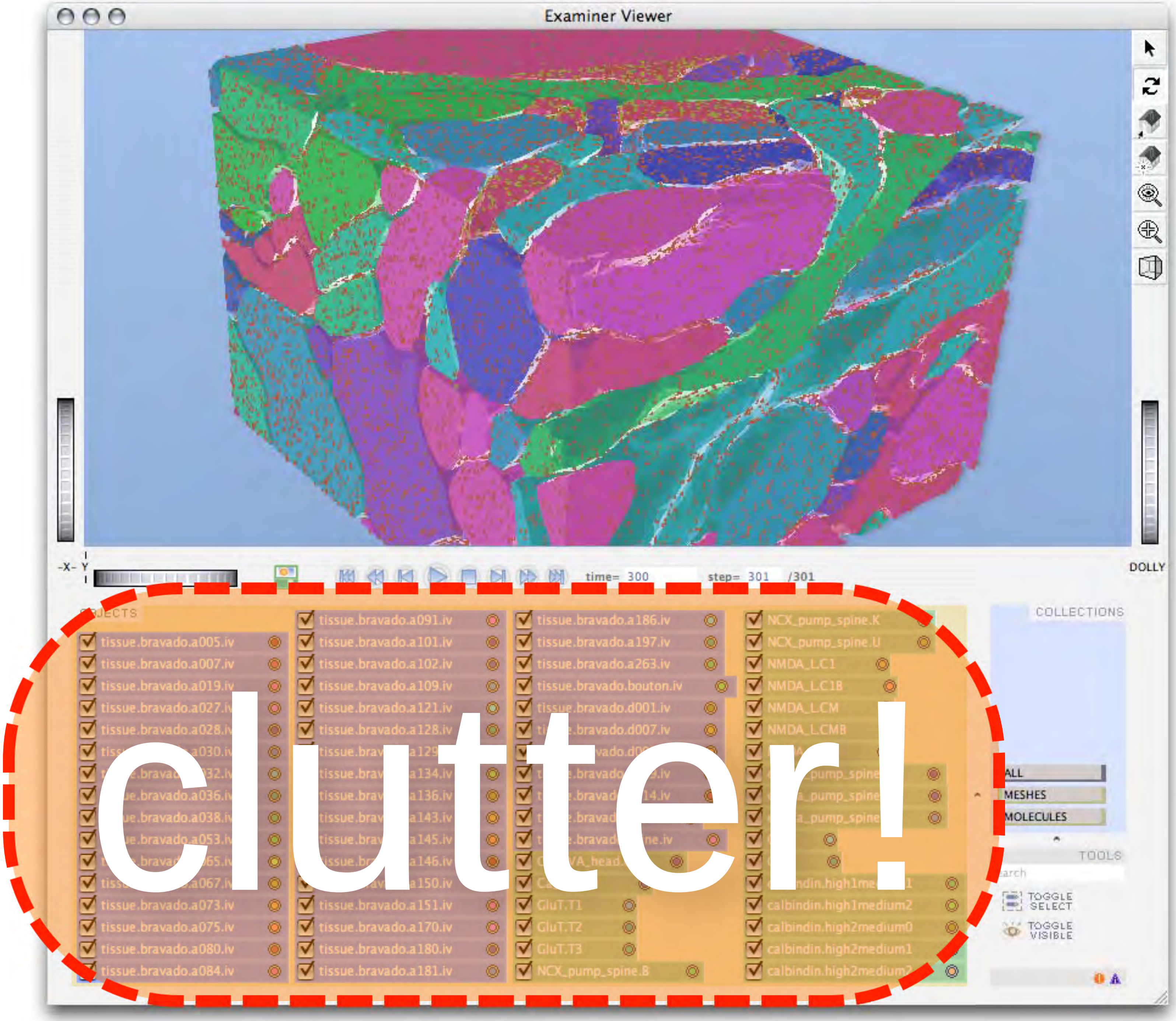
☑ Live updating


Examiner Viewer
Rotx Roty
400
5
/71
Dolly
OBJECTS
□ nmj.box
☑ nmj.presynaptic1
☑ nmj.basal_lamina1
☑ nmj.bpjm1
☑ nmj.mpjm1
☑ nmj.tpjm1
☑ ACh
☑ Ch
□ AChE.EAs
□ AChR.ARs
□ ChR.R
□ AChR.A2Rc
□ ChR.ARp
□ AChR.A2Ro
□ AChE.EA
□ AChR.ARt
□ ChR.AR
□ AChE.Es
□ AChR.R
□ AChE.E
COLLECTIONS
ALL
MESHES
VOLUME_MOLECULES
SURFACE_MOLECULES
TOOLS
search
TOGGLE SELECT
TOGGLE VISIBLE

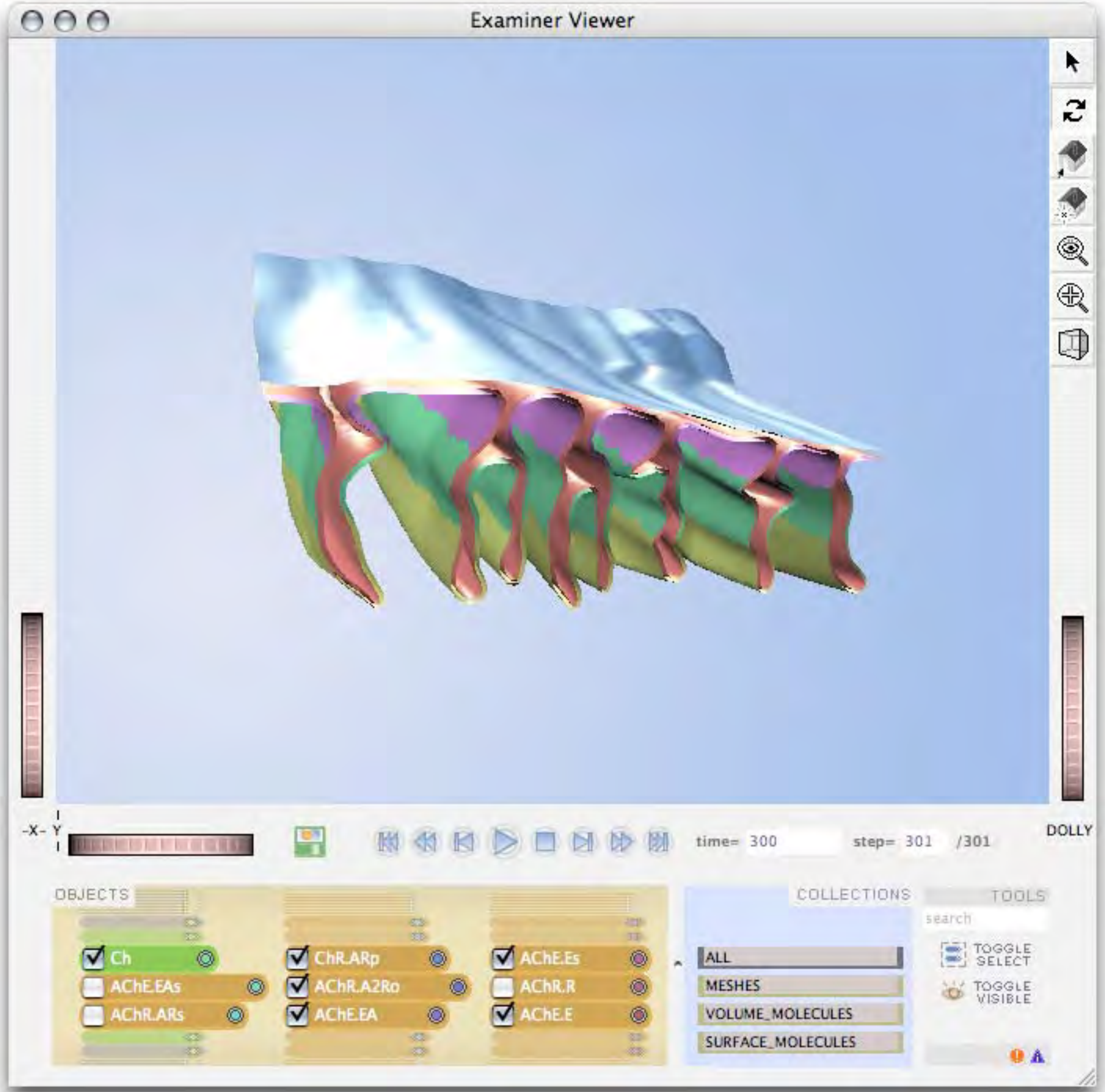
GUI

ultimate tool mockup




Examiner Viewer
-X- Y
DOLLY
time= 300
step= 301 /301
OBJECTS
☑ tissue.bravado.a005.iv
☑ tissue.bravado.a007.iv
☑ tissue.bravado.a019.iv
☑ tissue.bravado.a027.iv
☑ tissue.bravado.a028.iv
☑ tissue.bravado.a073.iv
☑ tissue.bravado.a075.iv
☑ tissue.bravado.a080.iv
☑ tissue.bravado.a084.iv
☑ tissue.bravado.a091.iv
☑ tissue.bravado.a101.iv
☑ tissue.bravado.a102.iv
☑ tissue.bravado.a109.iv
☑ tissue.bravado.a121.iv
☑ tissue.bravado.a128.iv
☑ tissue.bravado.a151.iv
☑ tissue.bravado.a170.iv
☑ tissue.bravado.a180.iv
☑ tissue.bravado.a181.iv
☑ tissue.bravado.a186.iv
☑ tissue.bravado.a197.iv
☑ tissue.bravado.a263.iv
☑ tissue.bravado.bouton.iv
☑ tissue.bravado.d001.iv
☑ GluT.T1
☑ GluT.T2
☑ GluT.T3
☑ NCX_pump_spine.B
☑ NCX_pump_spine.K
☑ NCX_pump_spine.U
☑ NMDA_LC1
☑ NMDA_LC1B
☑ NMDA_LCM
☑ NMDA_LCMB
☑ calbindin.high1medium2
☑ calbindin.high2medium0
☑ calbindin.high2medium1
☑ calbindin.high2medium2
COLLECTIONS
ALL
MESHES
MOLECULES
TOOLS
TOGGLE SELECT
TOGGLE VISIBLE

clutter!



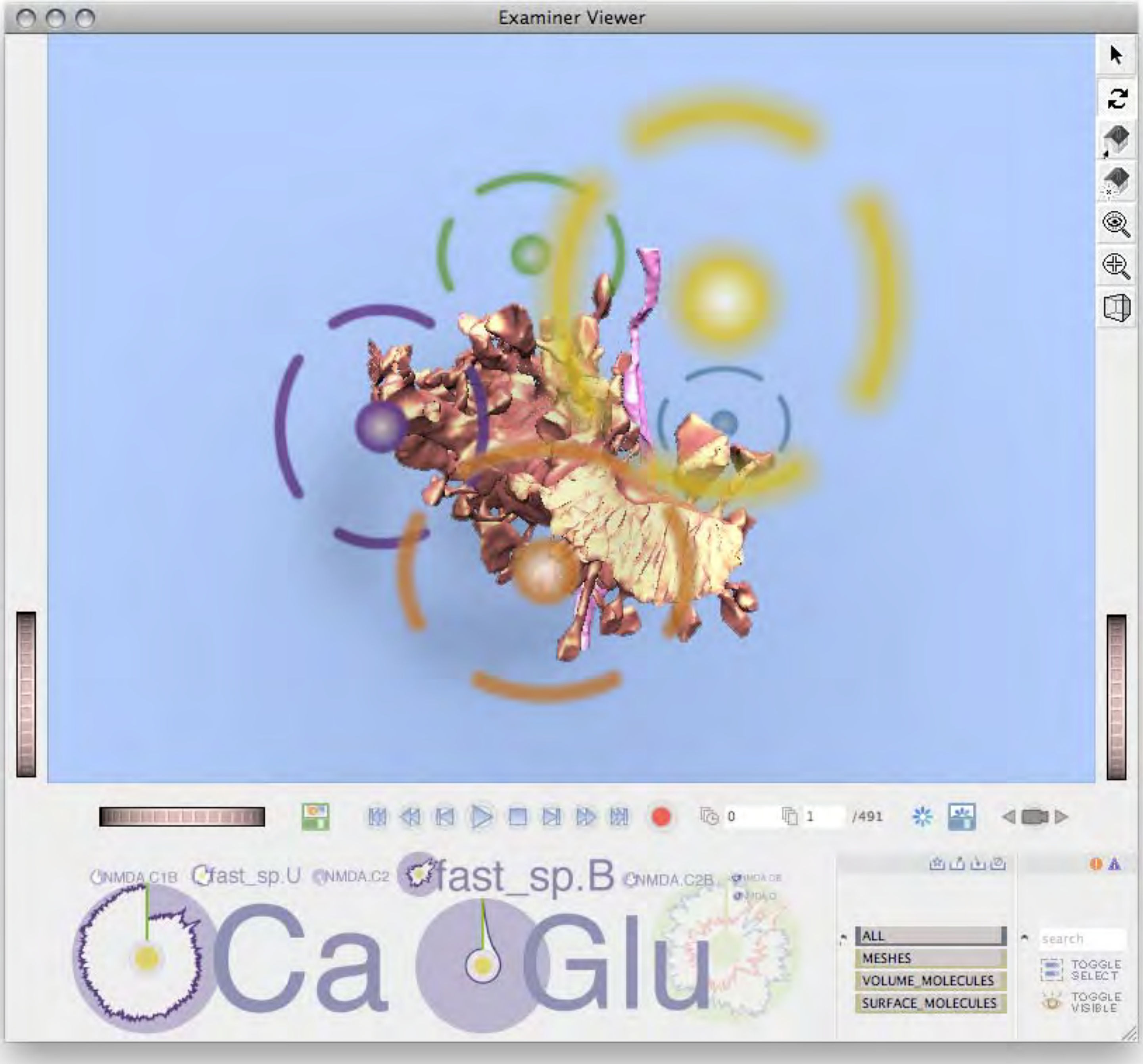
time= 300 step= 301 /301

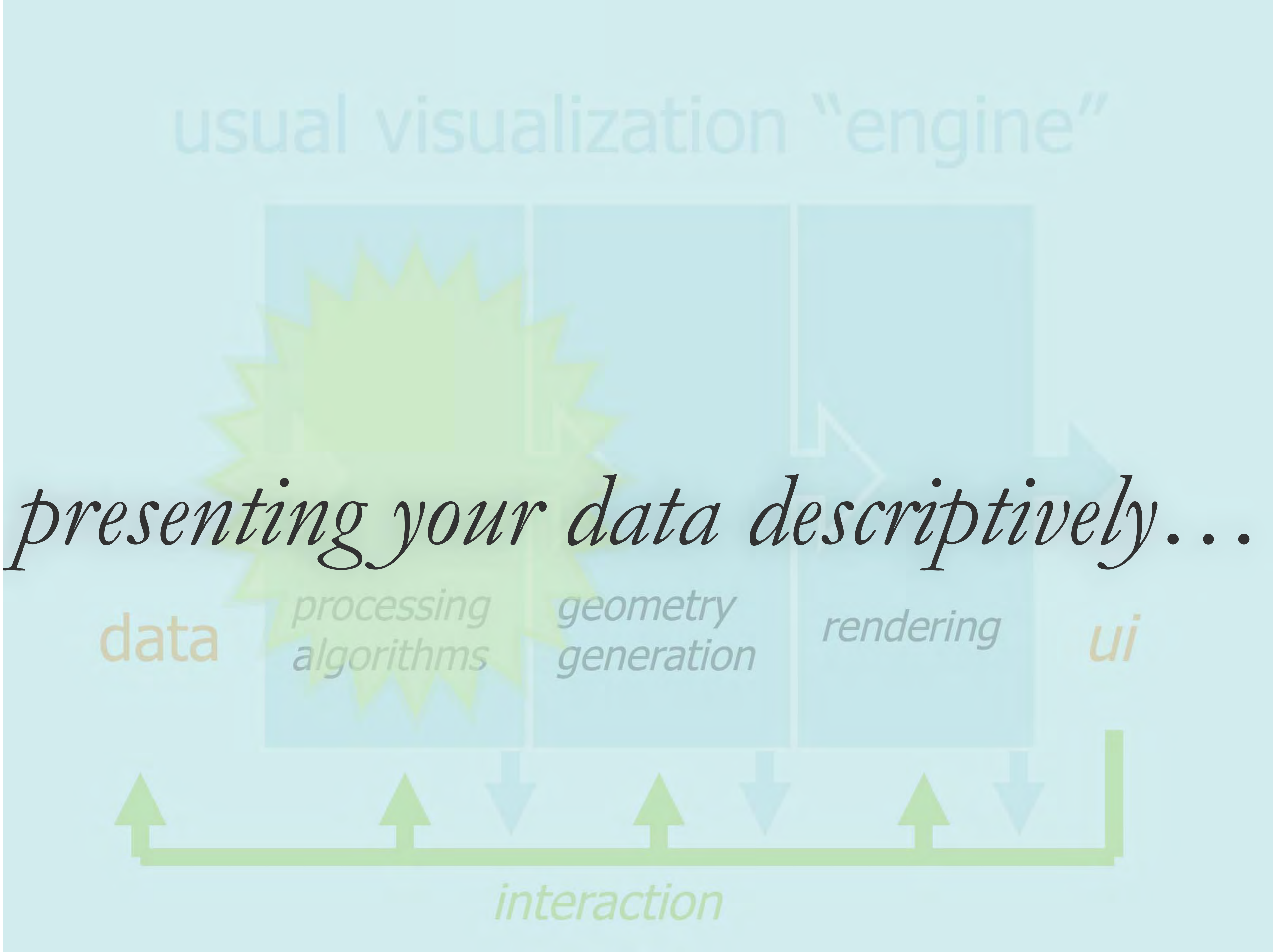
☑ Ch
□ AChE.EAs
□ AChR.ARs
☑ ChR.ARp
☑ AChR.A2Ro
☑ AChE.EA
☑ AChE.Es
□ AChR.R
☑ AChE.E

ibm: wordle

visualization
data
bottlenecks
based
engine
parallel
advanced
python
requires
research
lombeyda
vtk
computing
center
system
STRUCTURE
GEOMETRIC
abstract
usual
caltech
space
santiago
representation
VTK
number
techniques
DataArray
type
object
binary
ascii
ImageData
complexity
volume
sample
lab
purpose
nmj
standard
meshes
PointData
cellData
case
increases
preprocessing
ParaviewVTK
study
agrawala
LLNL
interaction
looking
version
intuitive
Mollegro
grids
wiki
BIO
base
rendering
mapping
Many
tools
gui
know
likely
throughput
vs
java
c/c++
volumetric
algorithms
regular
topics
viz
visualize
ray
EyesWWW
less
analysis
storage
VTKFile
DATA
larger
format
basic
Java
VisItVTK
raw
CellData
detail
QT
portable
want
maneesh
voxels
original+
quick
design
LOD
Scalars
xml
Name
addressing
field
image
interactive
sketch
toolkit
lod
user
MCELL
scalar
pipeline
ModrianR
understandable
ProtovisWWW
PARAVIEW
TomCat
national
level
algorithm
look
Wiki
feed
infovis
tcl/tk
EnSight
sw
Piece
processing/rendering
OpenInventor
www.infovis-wiki.net

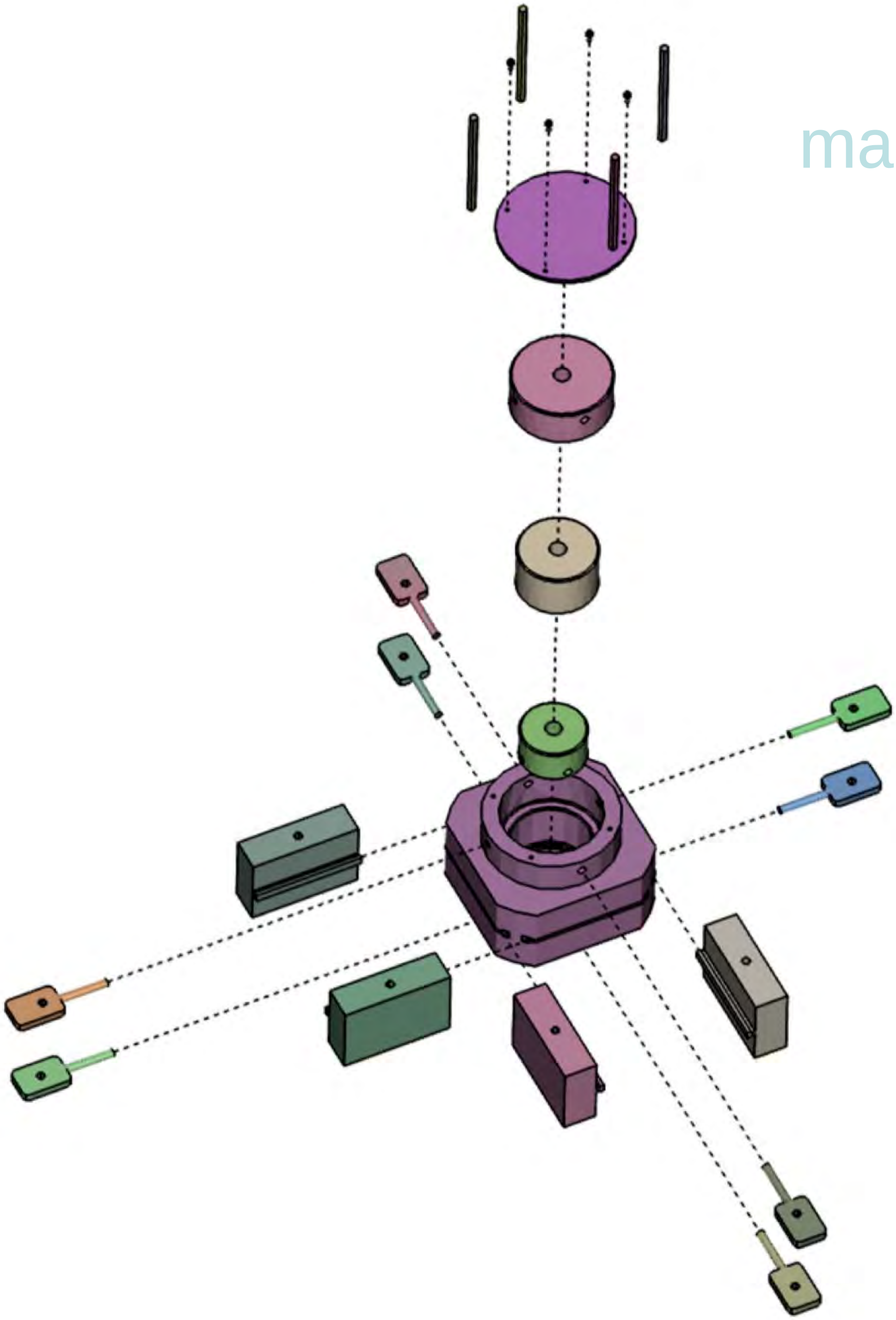
ibm: wordle


Examiner Viewer
0
1
/491
NMDA.C1B
fast_sp.U
NMDA.C2
fast_sp.B
NMDA.C2B
Ca
Glu
ALL
MESHES
VOLUME_MOLECULES
SURFACE_MOLECULES
search
TOGGLE SELECT
TOGGLE VISIBLE



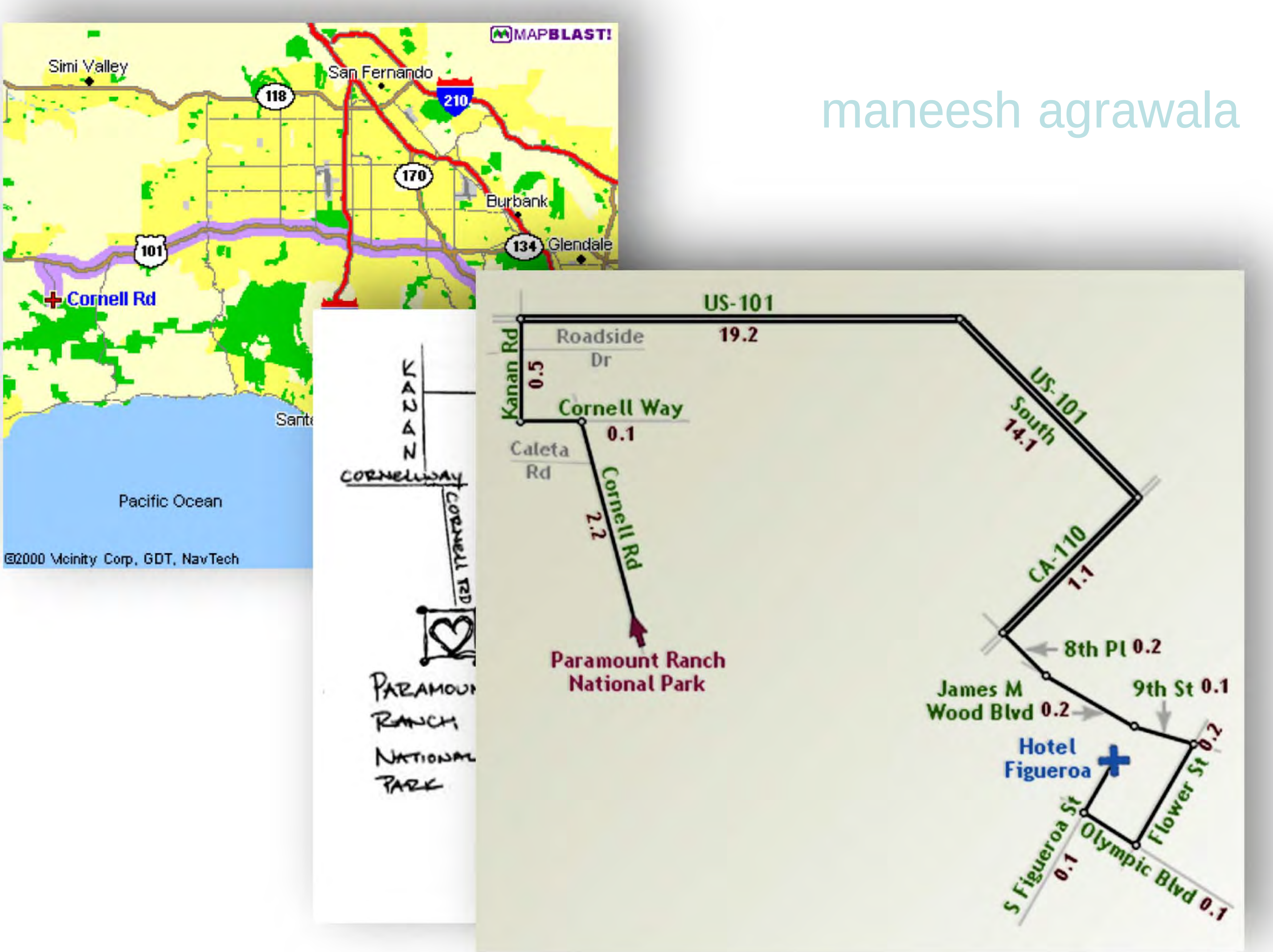
presenting your data descriptively…

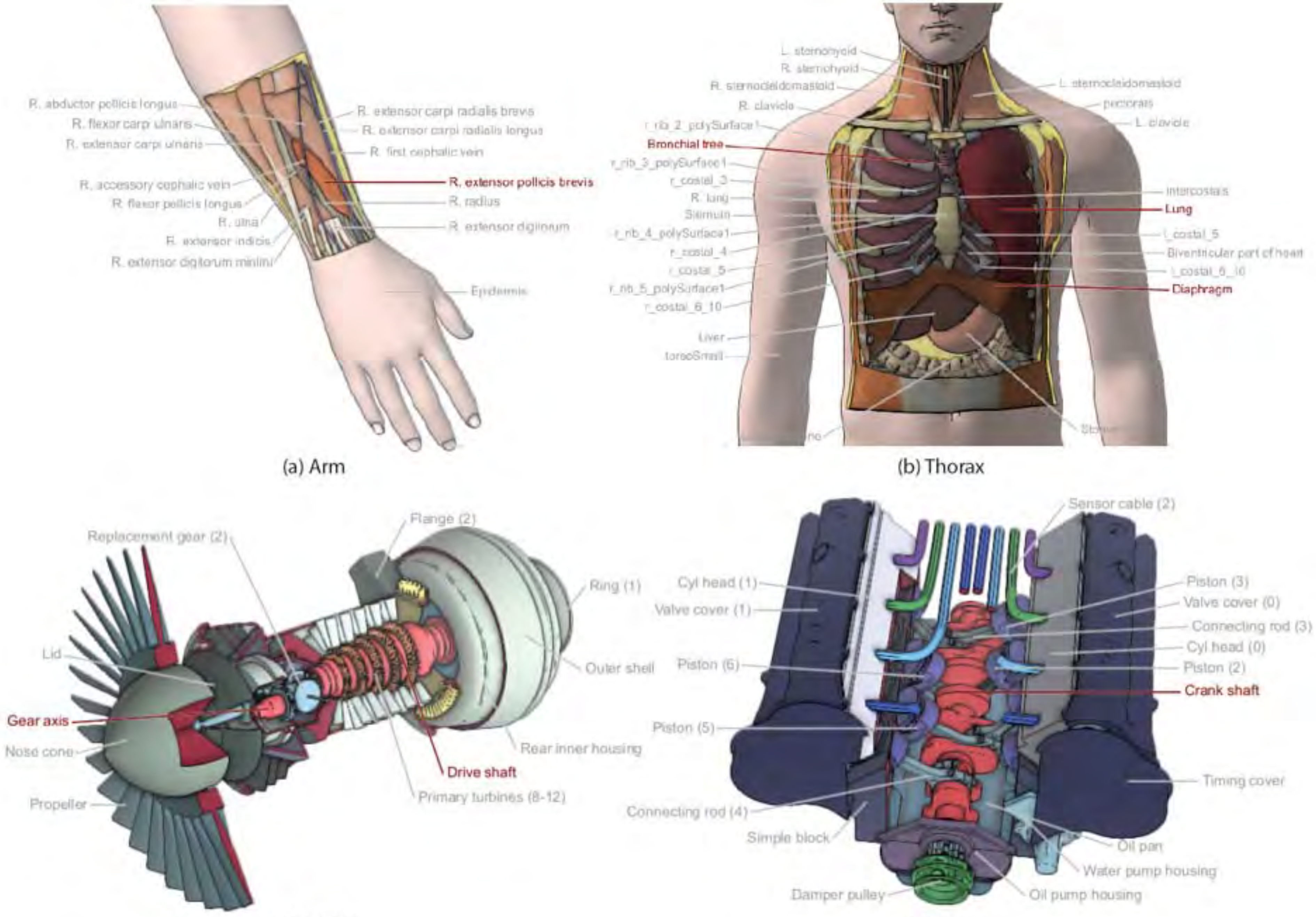
advanced: *techniques*
interactive cutaways



maneesh agrawala

maneesh agrawala



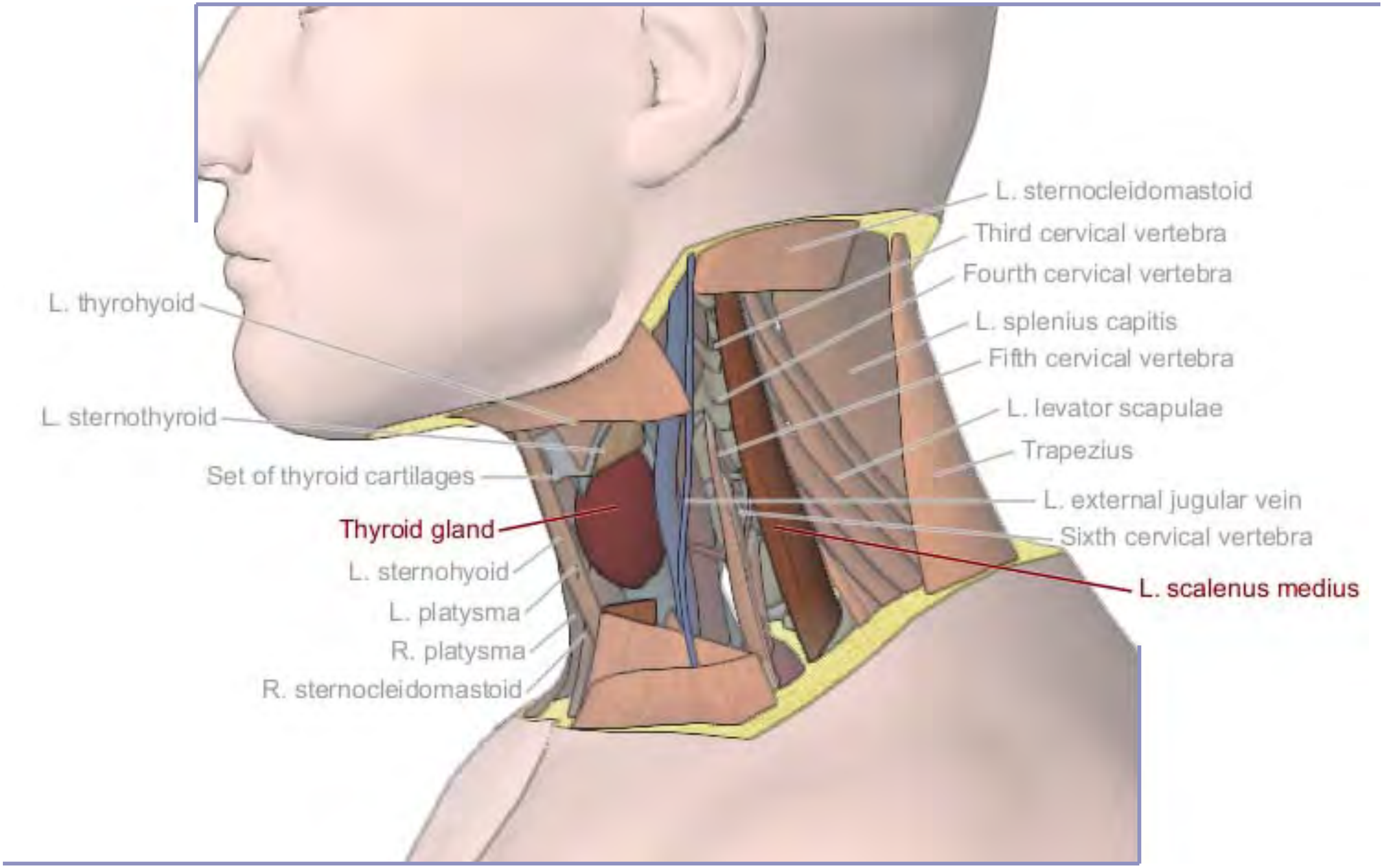


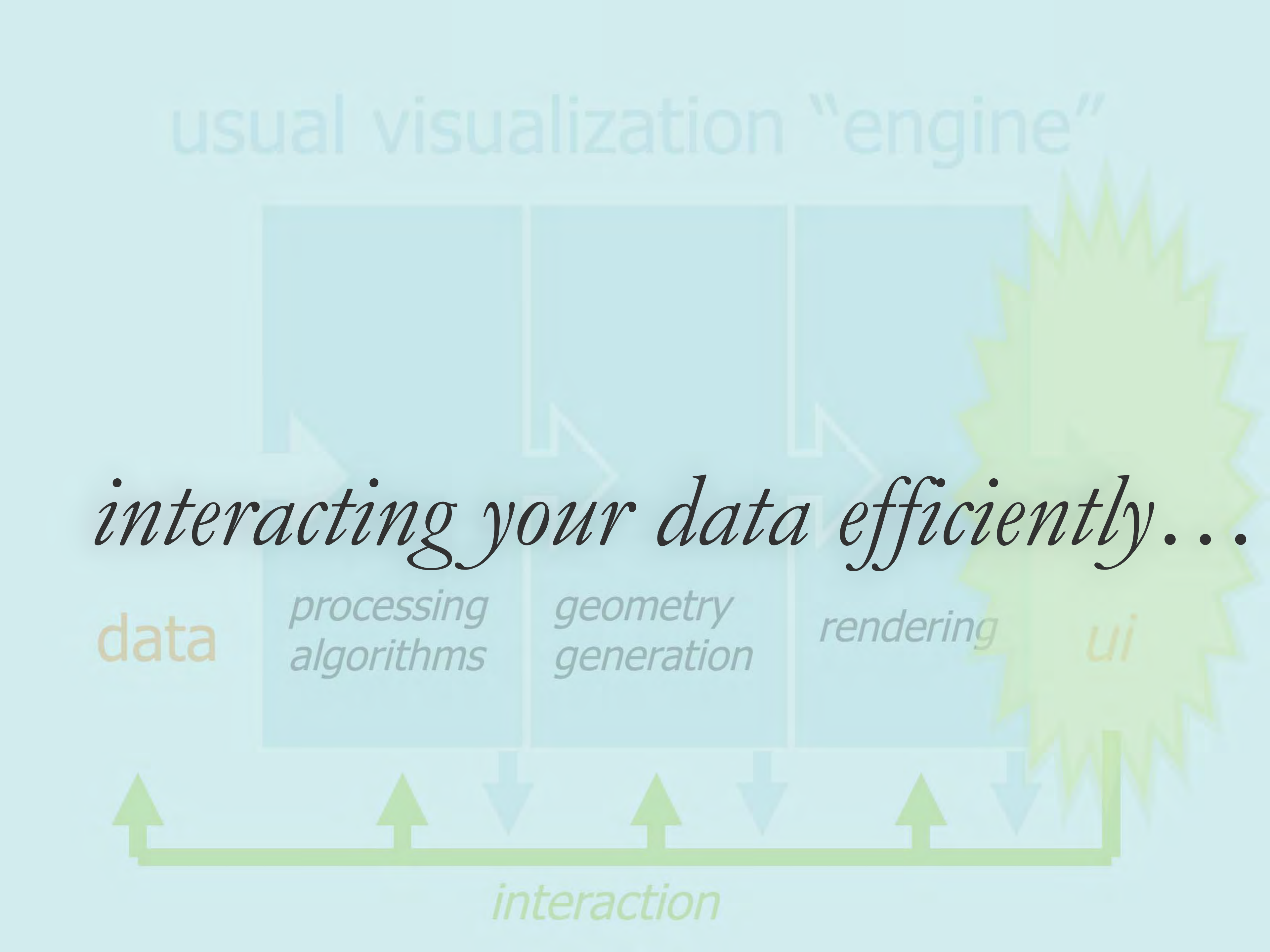
(a) Arm

(b) Thorax

(c) Turbine

(d) Engine


L. sternocleidomastoid
Third cervical vertebra
Fourth cervical vertebra
L. thyrohyoid
L. splenius capitis
Fifth cervical vertebra
L. sternothyroid
L. levator scapulae
Trapezius
Set of thyroid cartilages
L. external jugular vein
Thyroid gland
Sixth cervical vertebra
L. sternohyoid
L. scalenus medius
L. platysma
R. platysma
R. sternocleidomastoid

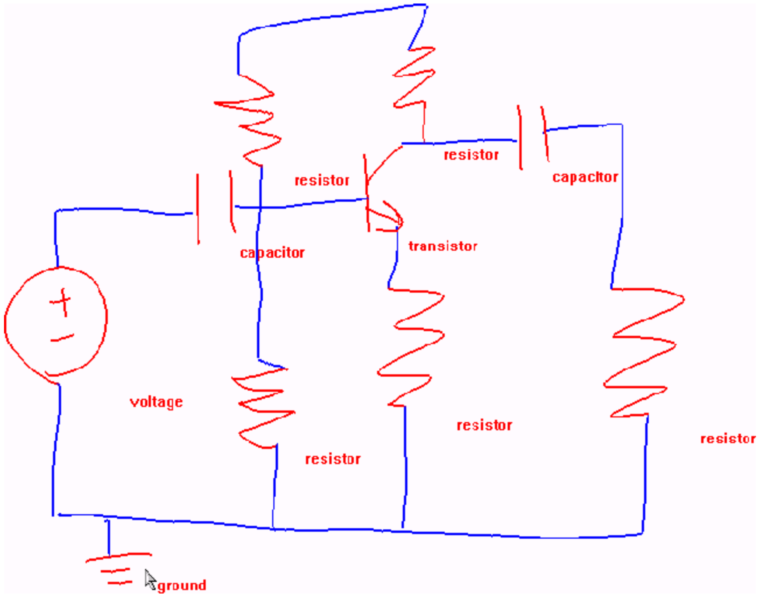


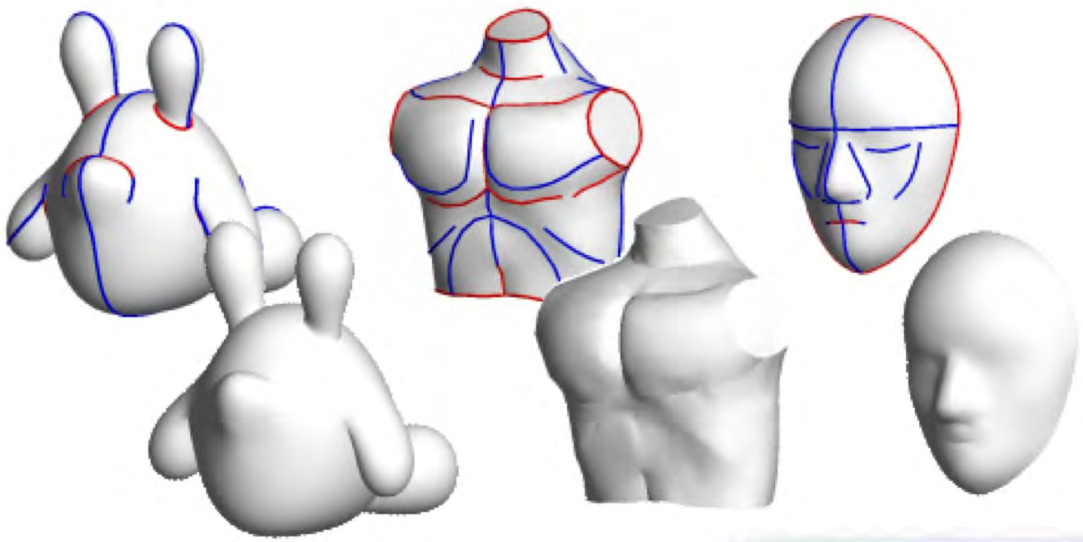
interacting your data efficiently…

advanced: *techniques*
sketch-based uis

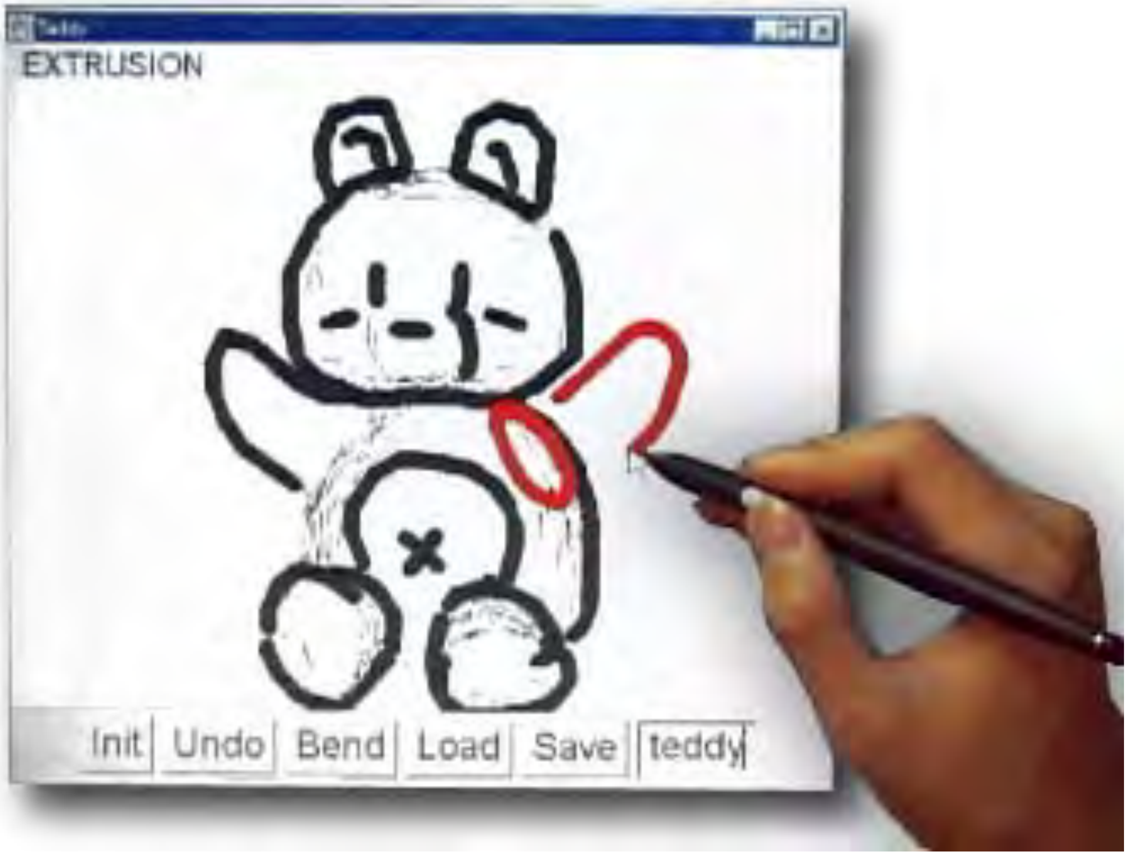
sketch based interfaces

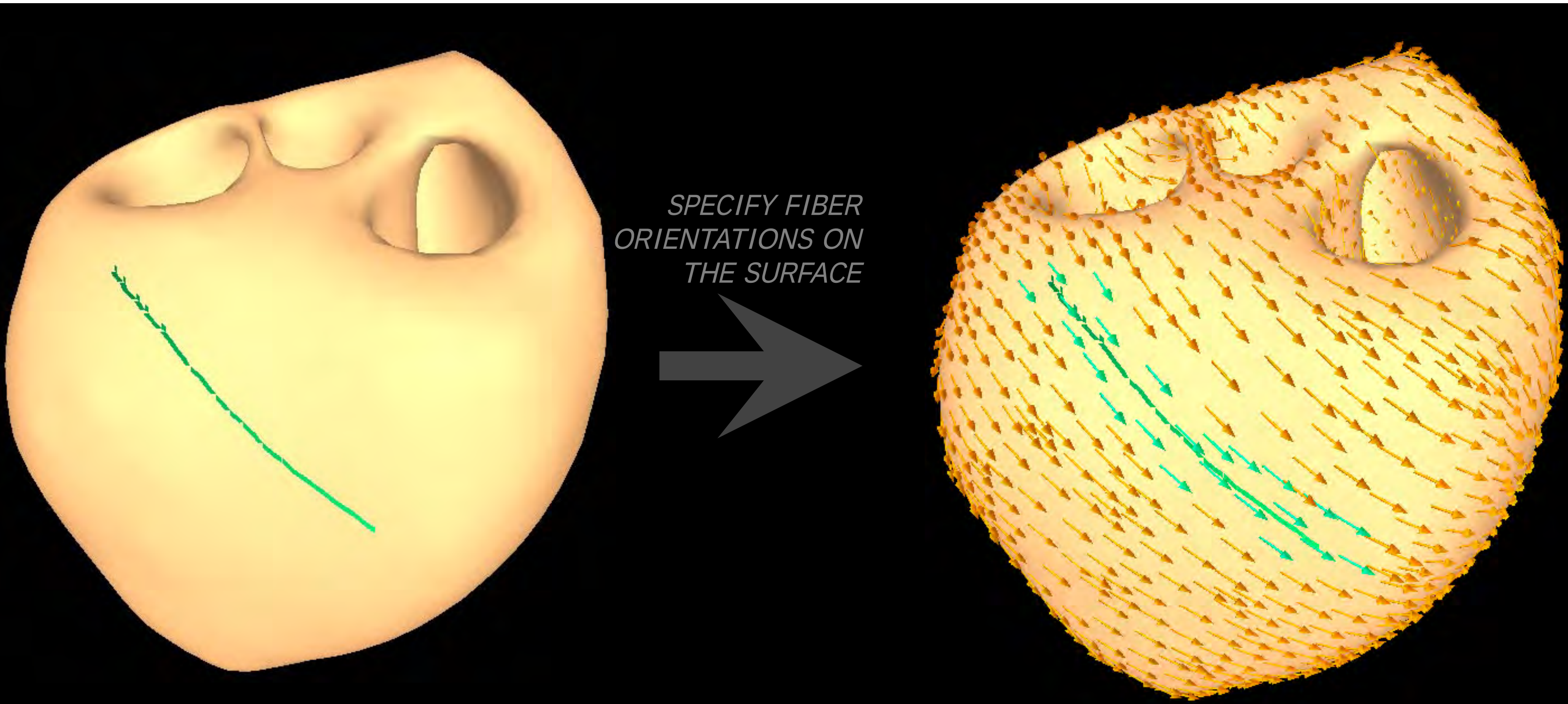
- buttons/menus -> sketch lines
  - i.e. direct interaction!
- more intuitive
- more efficient
- more elegant





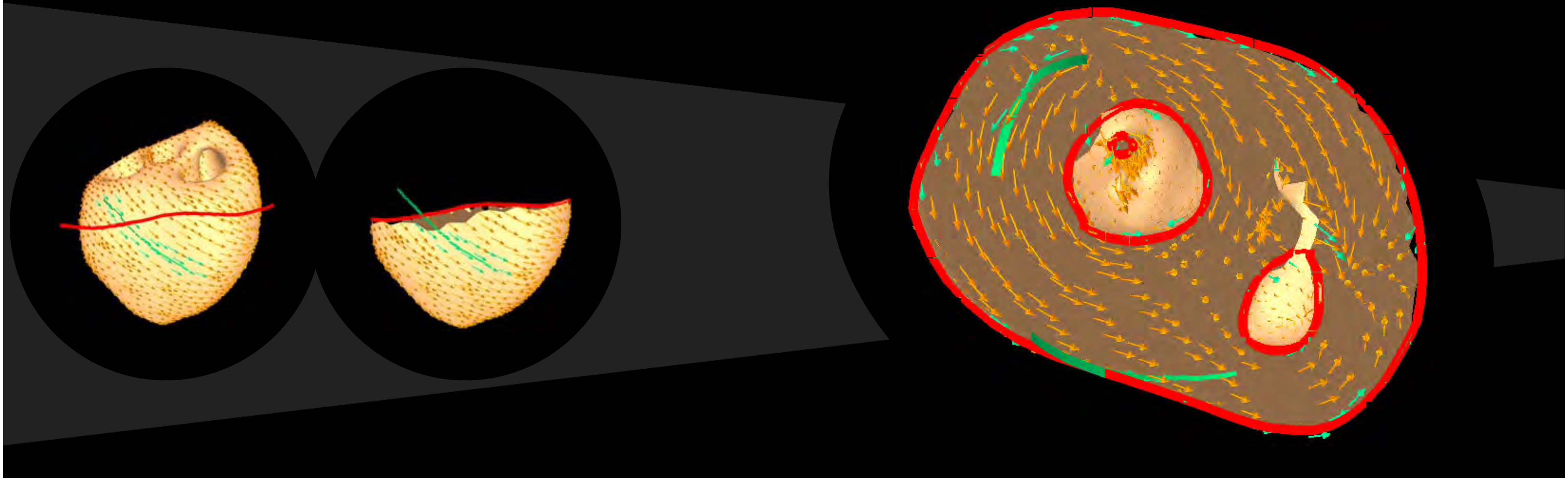
takeo igarashi





SPECIFY FIBER ORIENTATIONS ON THE SURFACE

MYOCARDIAL FIBER ORIENTATIONS FOR ELECTROPHYSIOLOGICAL SIMULATION OF THE HEART



√ carefully crafted

visual exploration ☛ answer questions

(even if questions are not clearly defined?)

☛ tools address specific task/question

(visualization is bound by tools... right?)

+ cross referencing

+ interactivity

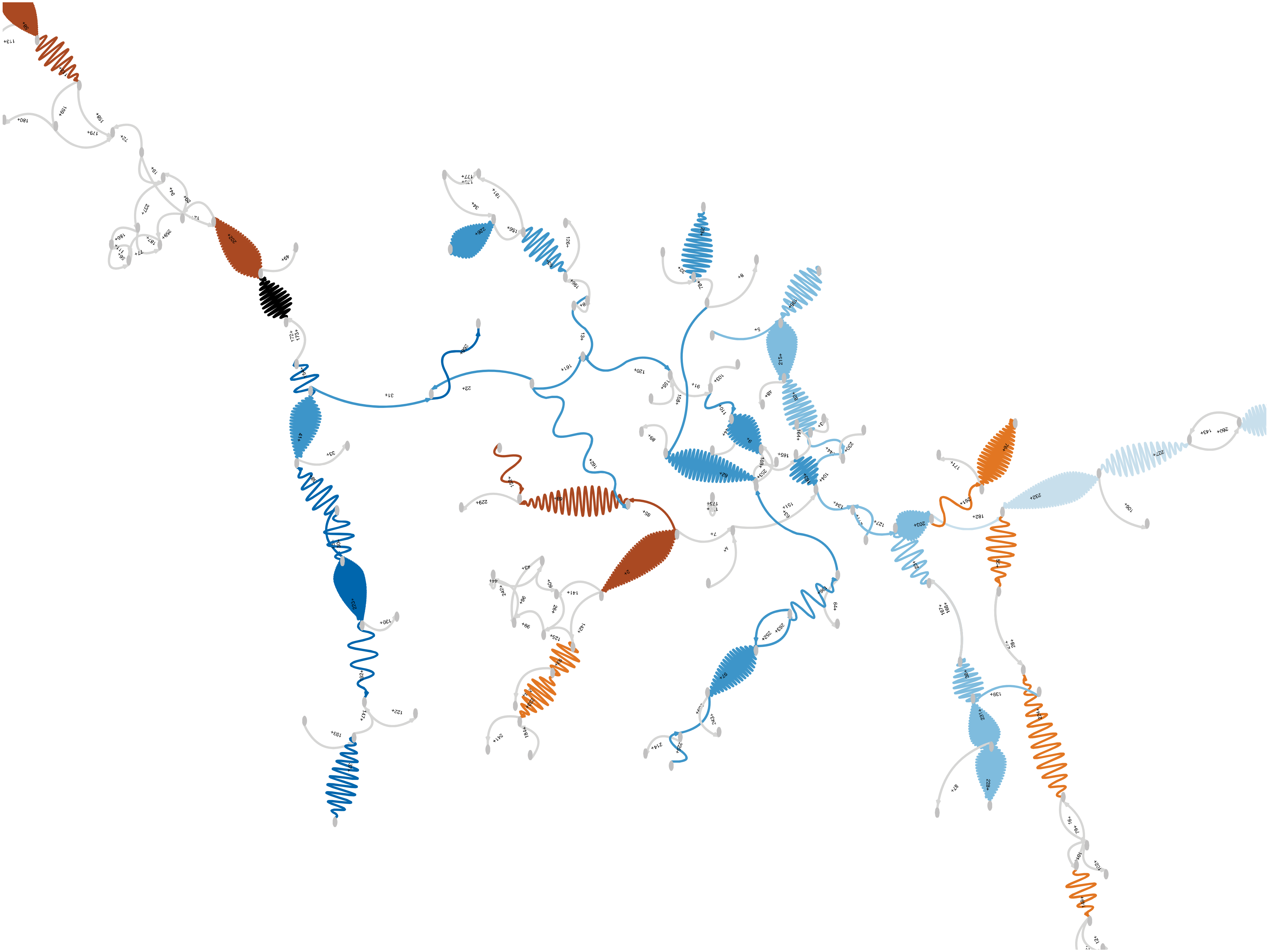
☛ *broader* set of questions addressable

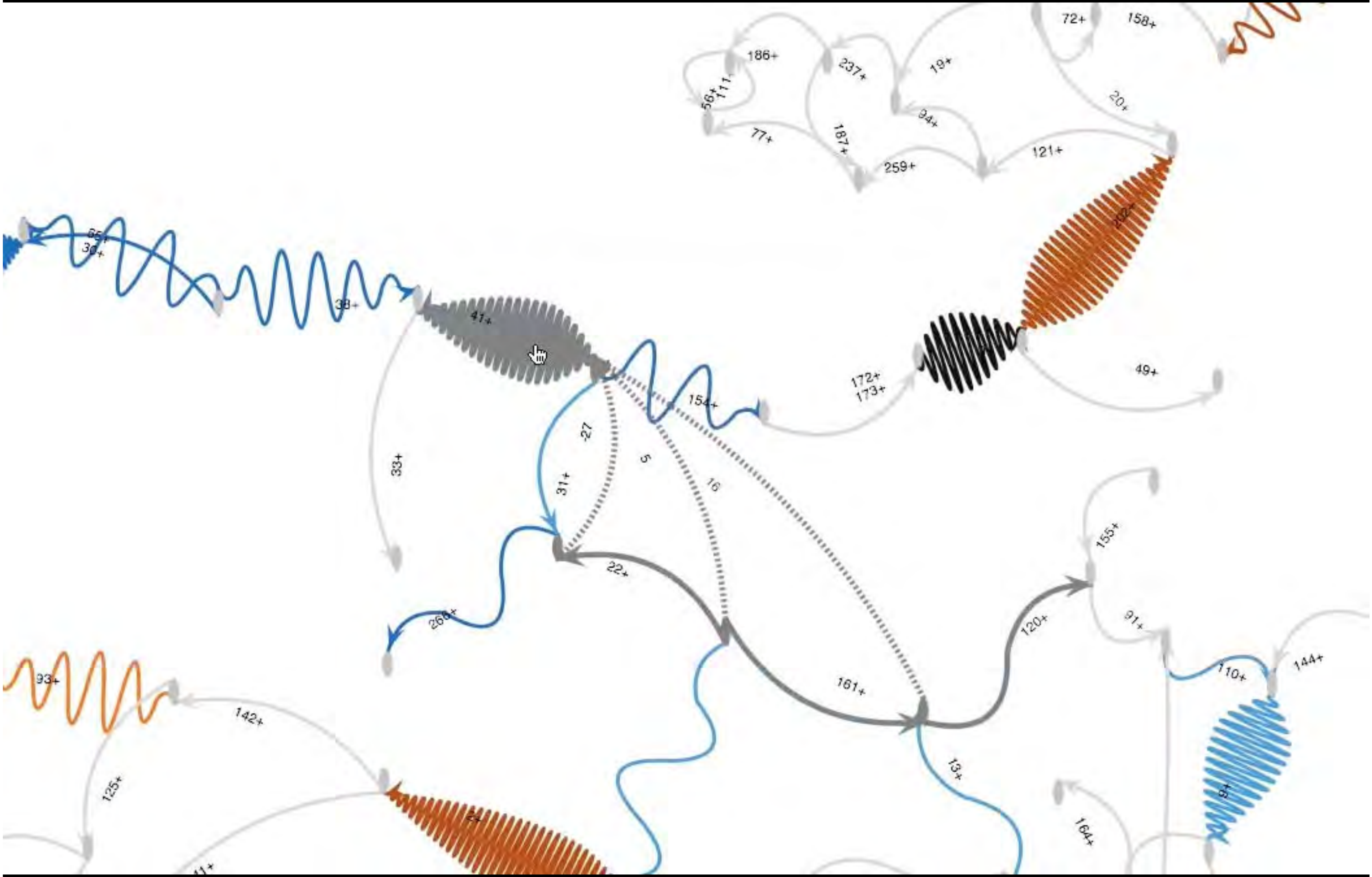
ay/bi199: methods of computational science

visualization

visualization system+techniques

santiago v lombeyda | center for advanced computing research | caltech




72+
158+
186+
237+
19+
56+
111+
20+
94+
77+
187+
121+
259+
202+
65+
30+
38+
41+
172+
173+
49+
154+
27
5
16
33+
31+
155+
22+
266+
120+
91+
110+
144+
93+
161+
142+
13+
125+
9+
2+
164+
41+