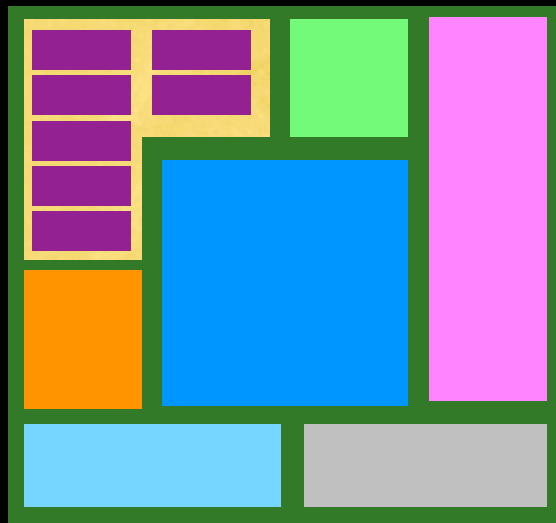


materials selection

Richard LeSar & Mark Bryden

Ames Laboratory
Simulation, Modeling, and Decision Science





materials design

Richard LeSar and *Mark Bryden*



Ames Laboratory
Simulation, Modeling, and Decision Science



A 3D CAD model of a complex mechanical part, possibly a turbine component, rendered in a color gradient from yellow to red. The red areas indicate high stress or temperature concentrations. The model is shown from a perspective view, highlighting its intricate internal and external features.

Integrated Computational Materials Engineering

A Transformational
Discipline for Improved
Competitiveness and
National Security

a new paradigm

NATIONAL RESEARCH COUNCIL
OF THE NATIONAL ACADEMIES

Materials Genome Initiative
for Global Competitiveness

June 2011

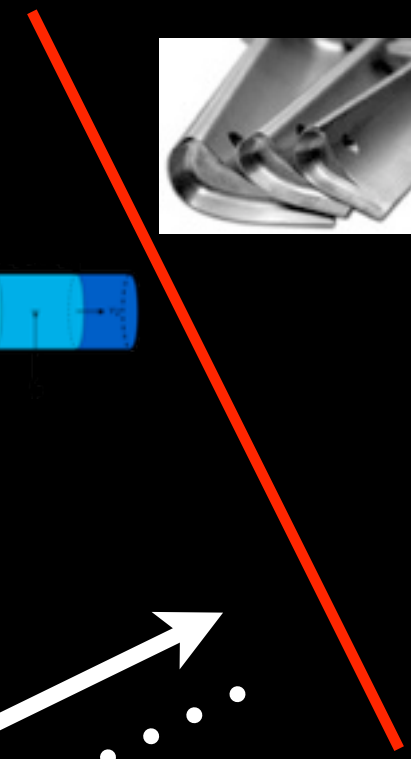
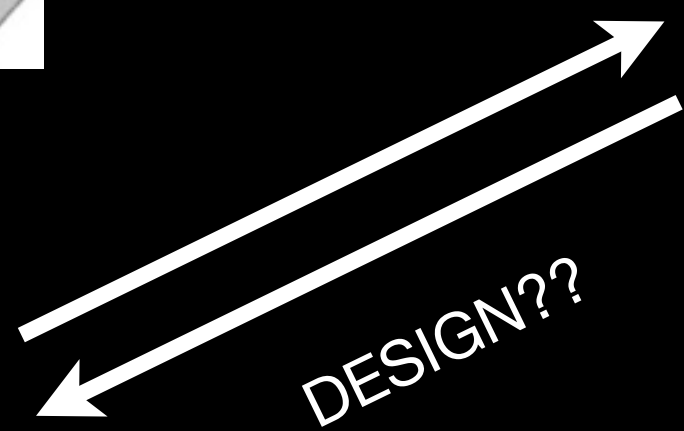
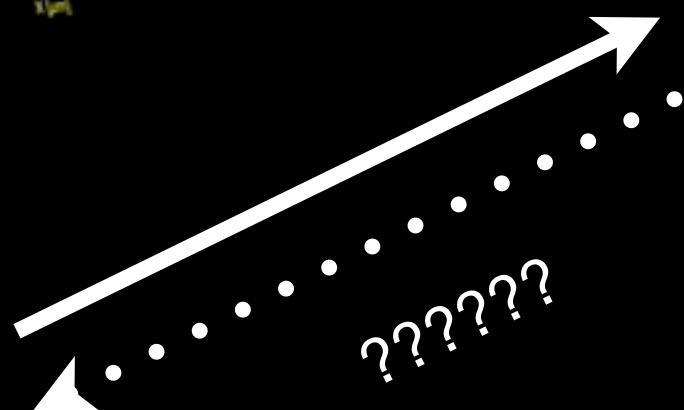
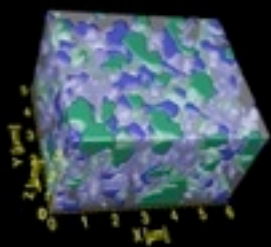
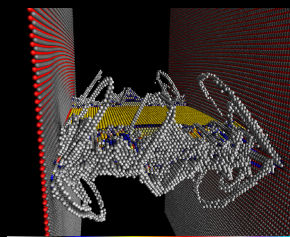
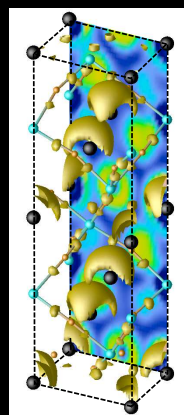


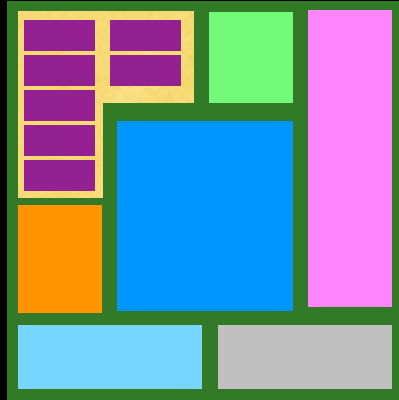
*a marriage of experiment, materials simulation,
information sciences and*

design

design

the materials challenge





three big questions ...

-
- what is the nature of multiscale design?
 - how we mathematically represent multiscale systems?
 - how do we interact with multiscale systems?

- quantitative information
- qualitative information
- metaphor
- narrative



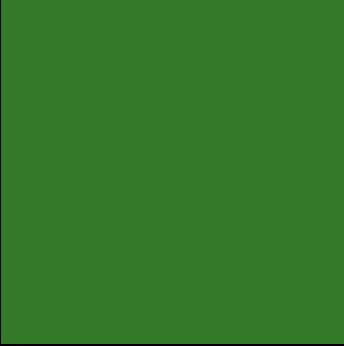
the nature of multiscale design



narrative

“Plot, then, is the first principle and, as it were, soul of tragedy, while character is secondary.”

- Aristotle, Poetics VI



nature of multiscale information and objects

- music
- the “PORS” problem
- origami
- digital manufacturing

M.M. J. 100

GRAN CASSA

VIOLE

VIOLONCELLI

CONTRABASSI

Trombe

Grande Cassa

Viole

Violoncelli

Contrabassi

Clarineti in La

Fagotti

Coro in Fa

Trombe in Do

Trombe

Grande Cassa

Arpa

Violini I.

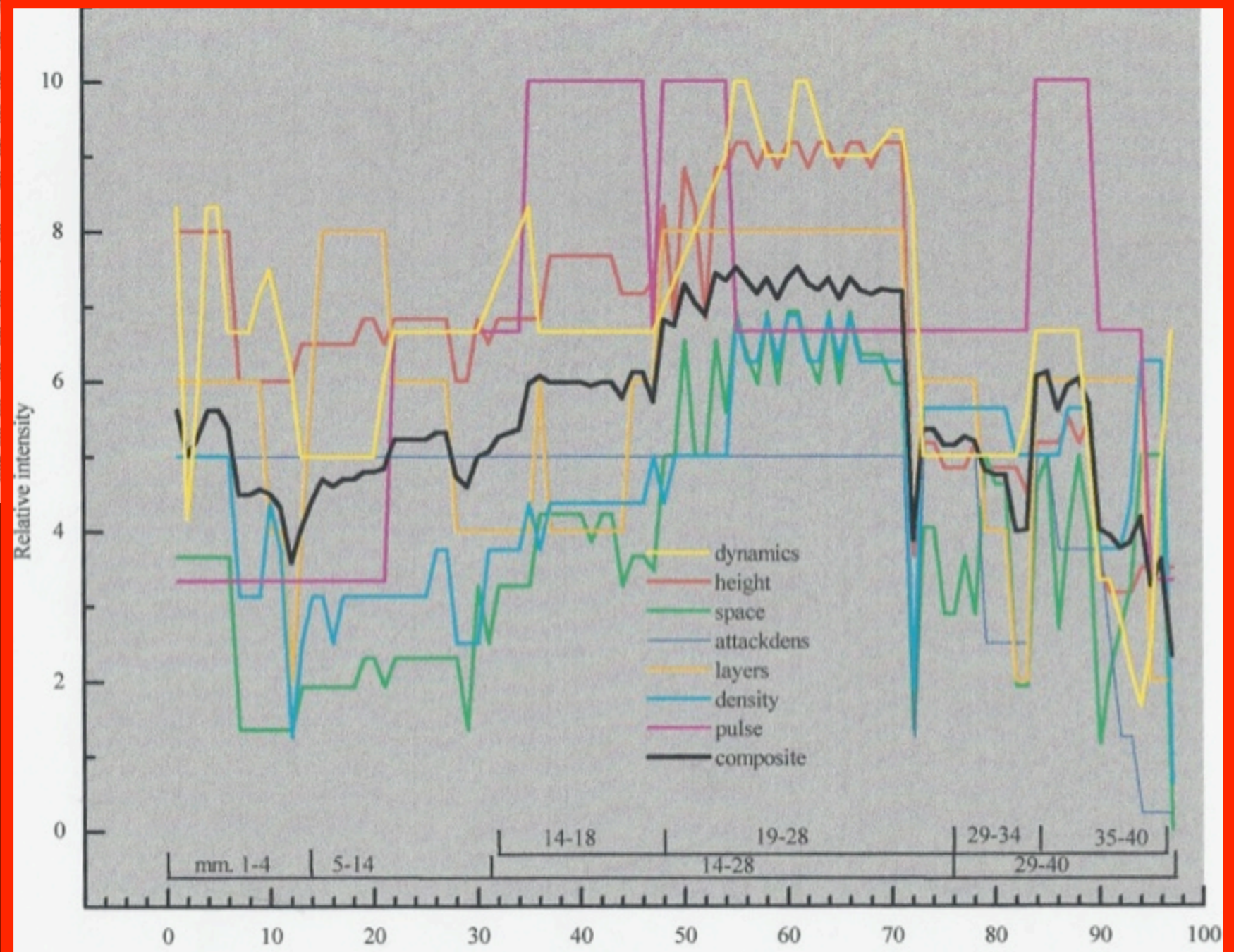
Viola

Violoncelli

Contrabassi

“What delivers me from the anguish into which an unrestricted freedom plunges me is the fact that I am always able to turn immediately to the concrete things that are here in question.”

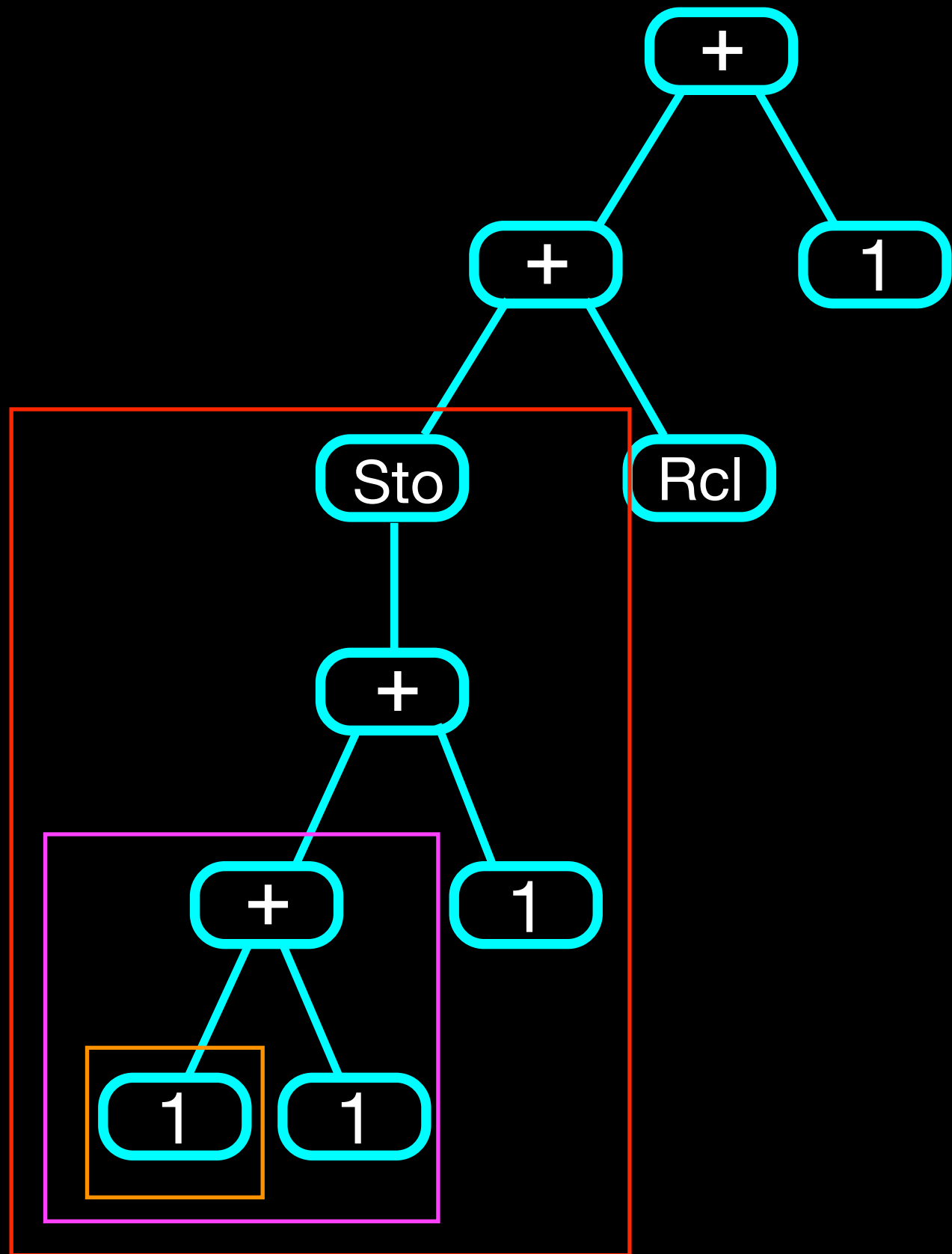
I. Stravinsky



PORS

$1 + 1 + 1(\text{sto}) + (\text{rcl}) + 1$

$= 7$



a hierarchy of scales

origami



digital manufacturing

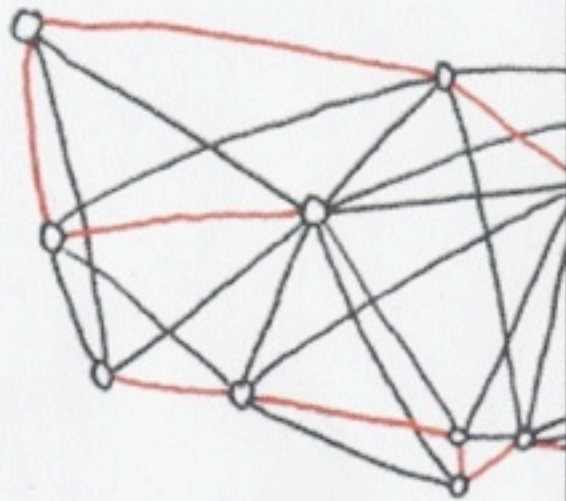


- current models are process poor
- combinatorics for information share
- sparse matrix theory for linkage
- respecting the question being asked



mathematical representation

BRUTE-FORCE
SOLUTION:
 $O(n!)$



DYNAMIC
PROGRAMMING
ALGORITHMS:
 $O(n^2 2^n)$



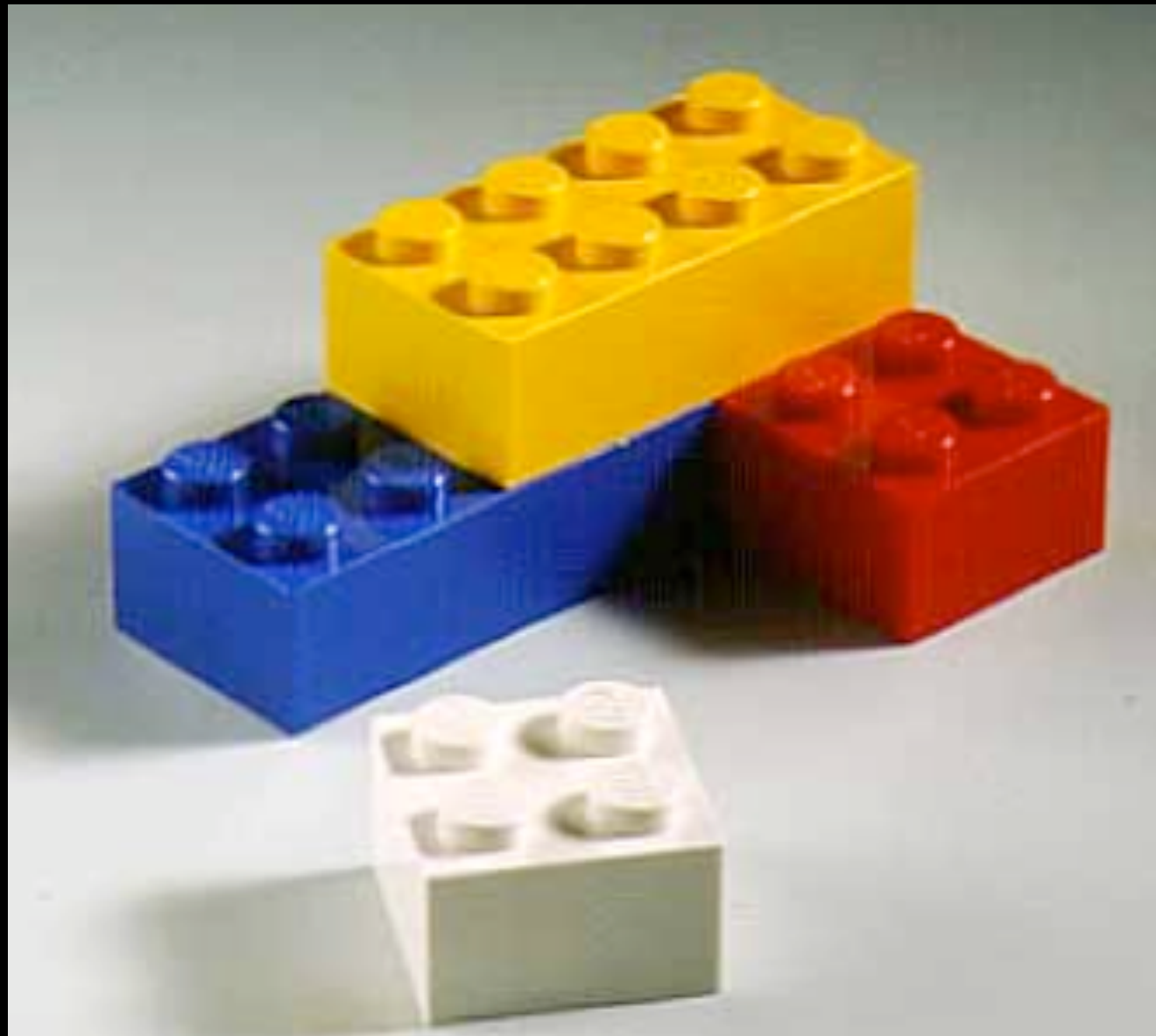
SELLING ON EBAY:
 $O(1)$

STILL WORKING
ON YOUR ROUTE?

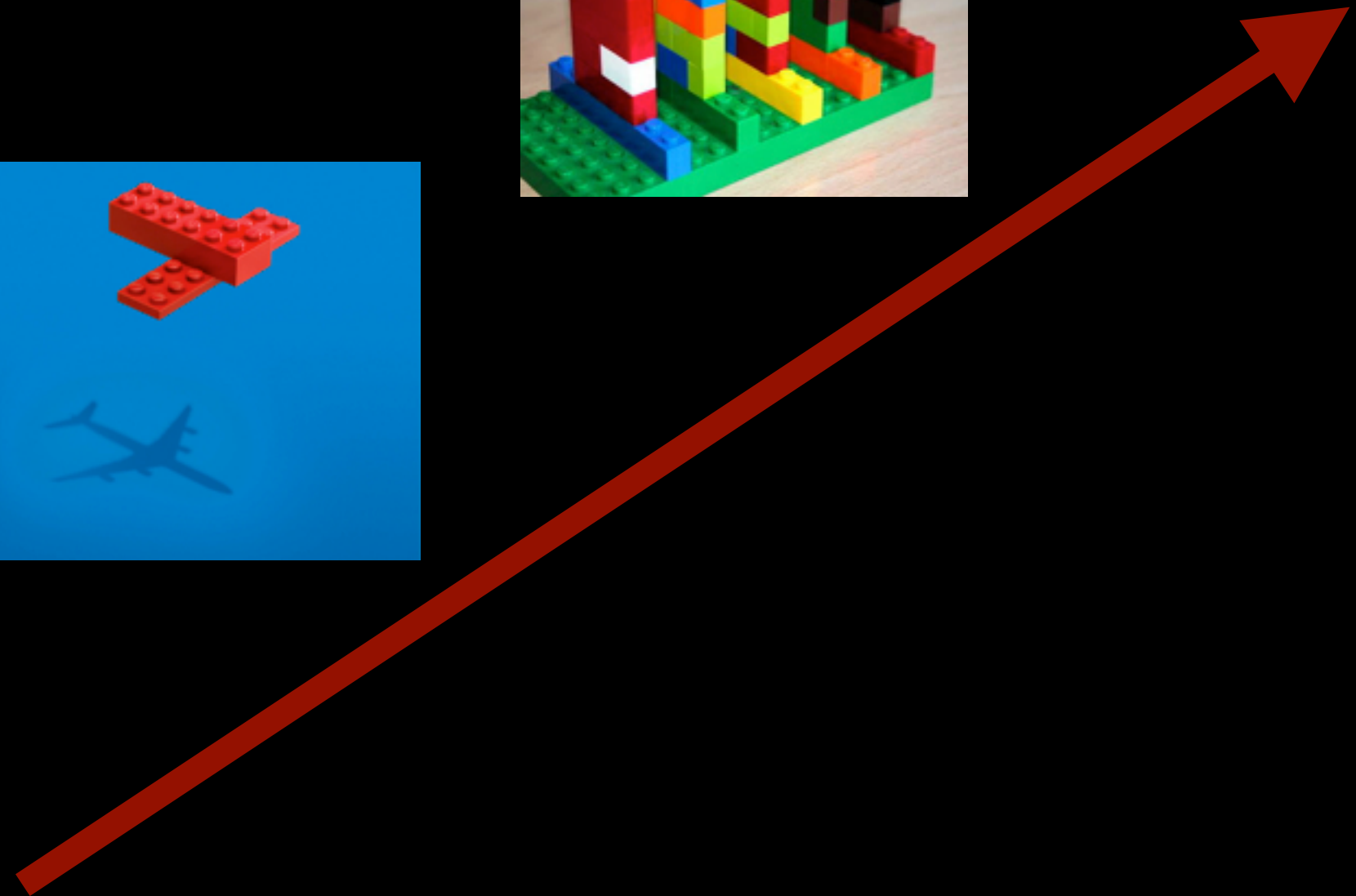
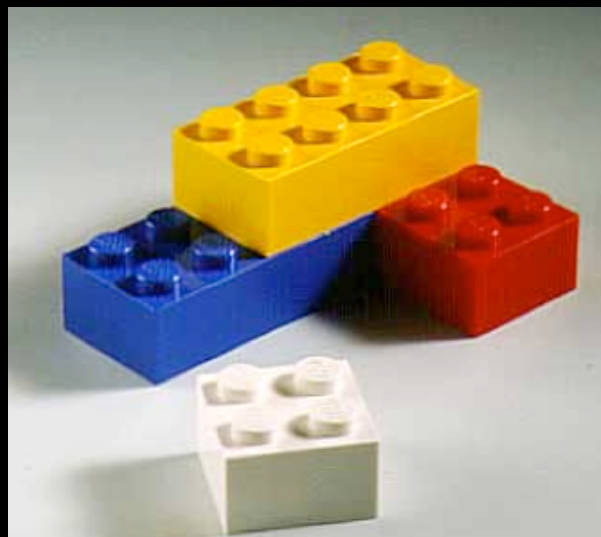
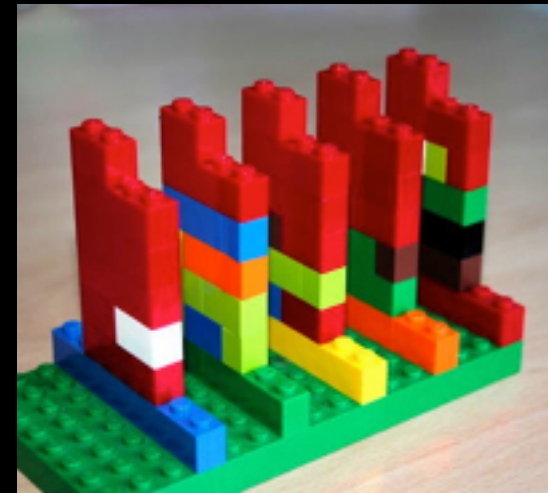
SHUT THE
HELL UP.

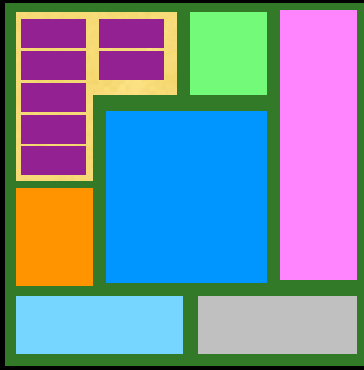


the traveling salesman problem

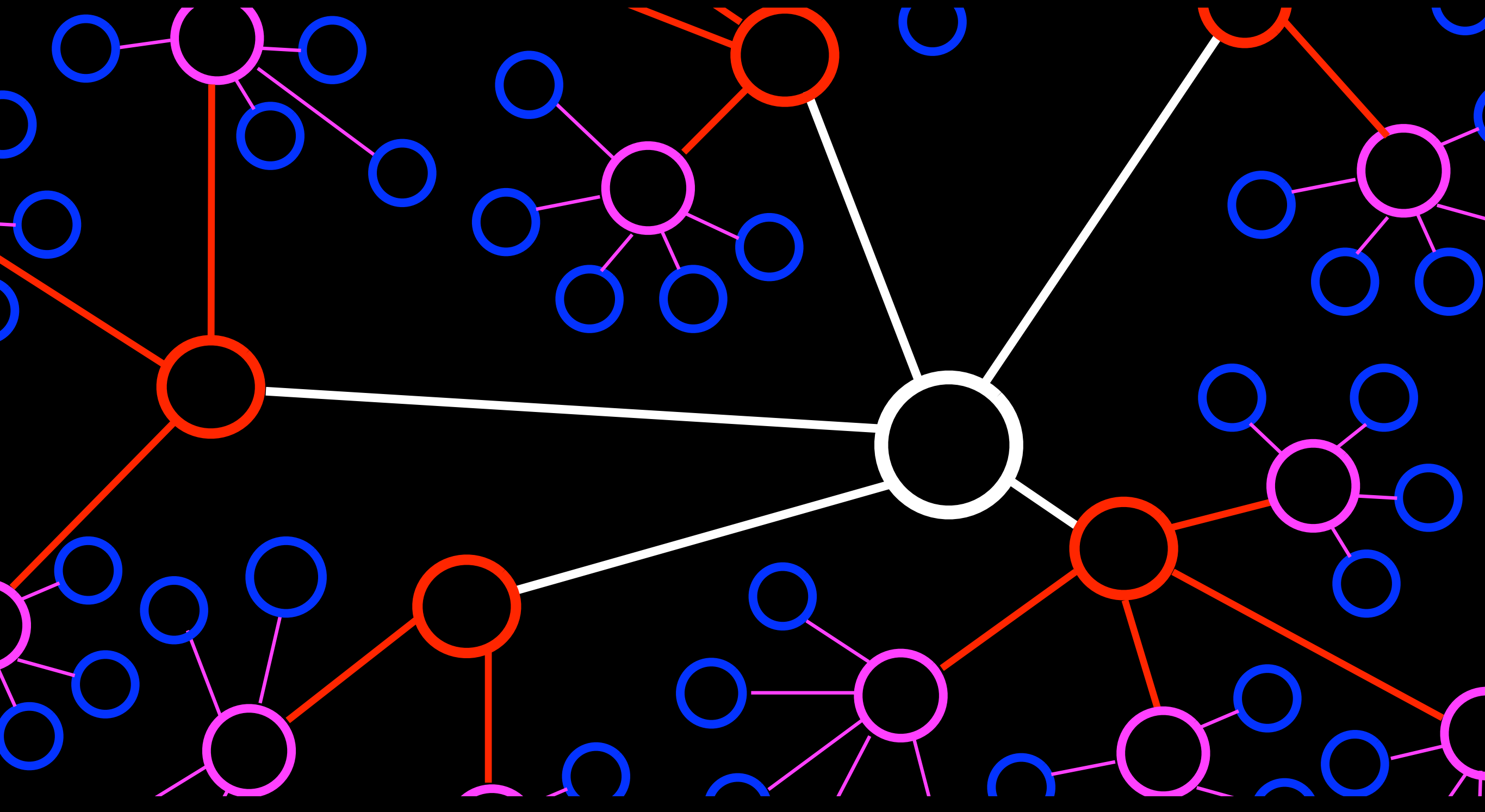


building blocks
(objects)





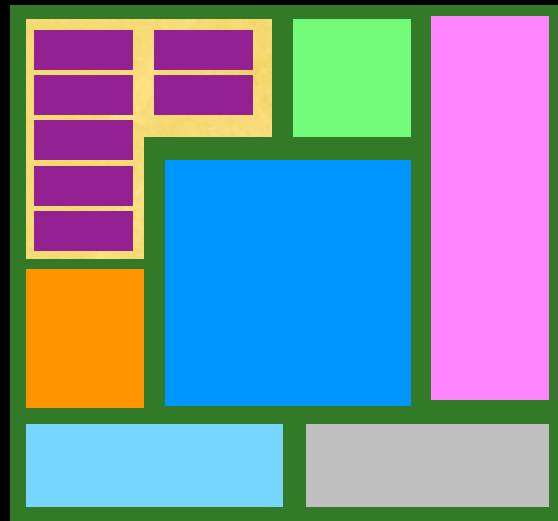
fully coupled, complex system management



- visualization
- integrated computational environment
- design workbench
- merged environments for simulation & analysis



interaction with multiscale systems



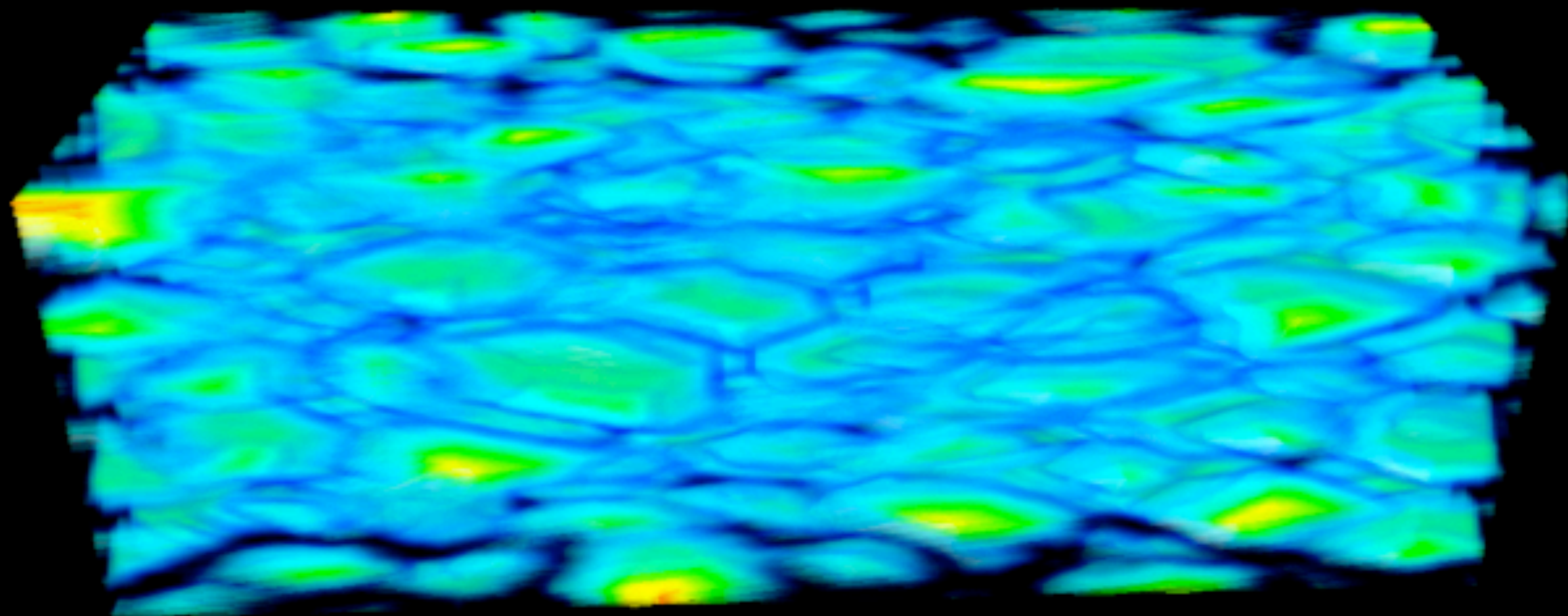
visualization needs

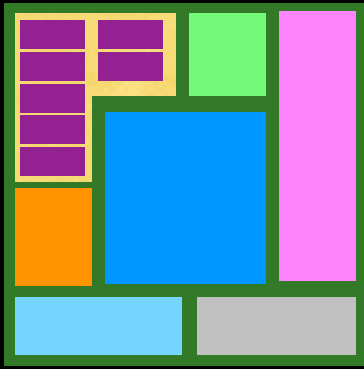
- render very large datasets interactively
- colorize and filter on any attribute set interactively

*common sphere rendering techniques cannot
achieve these goals*



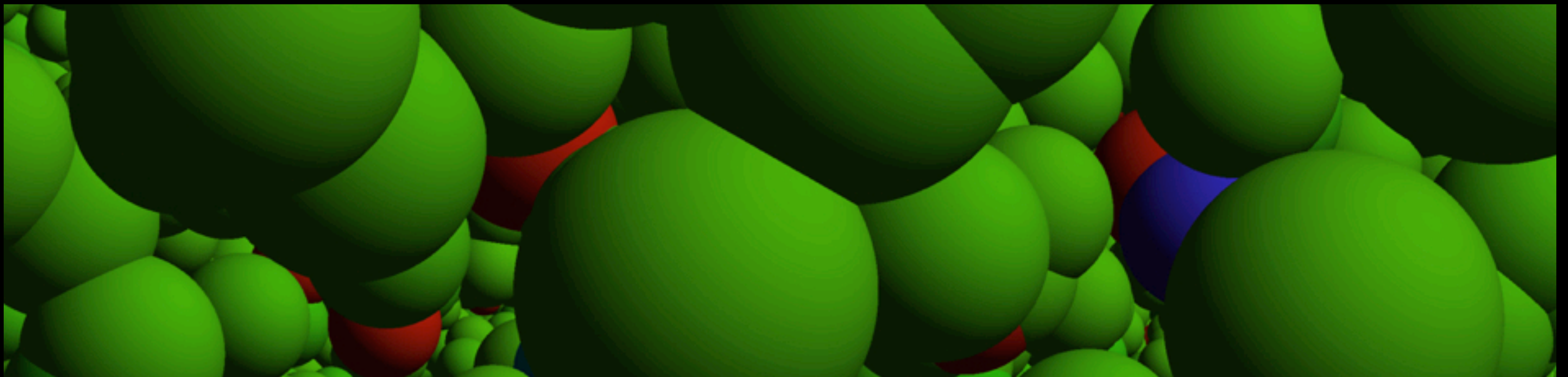
- 100+ million points
- any data source
- any visualization platform
- any compute platform

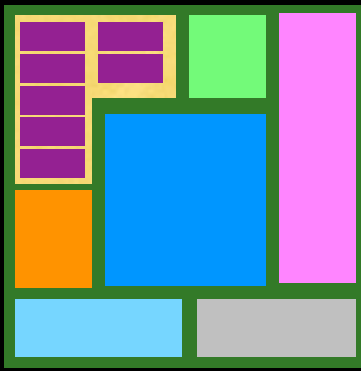




a multiscale design laboratory

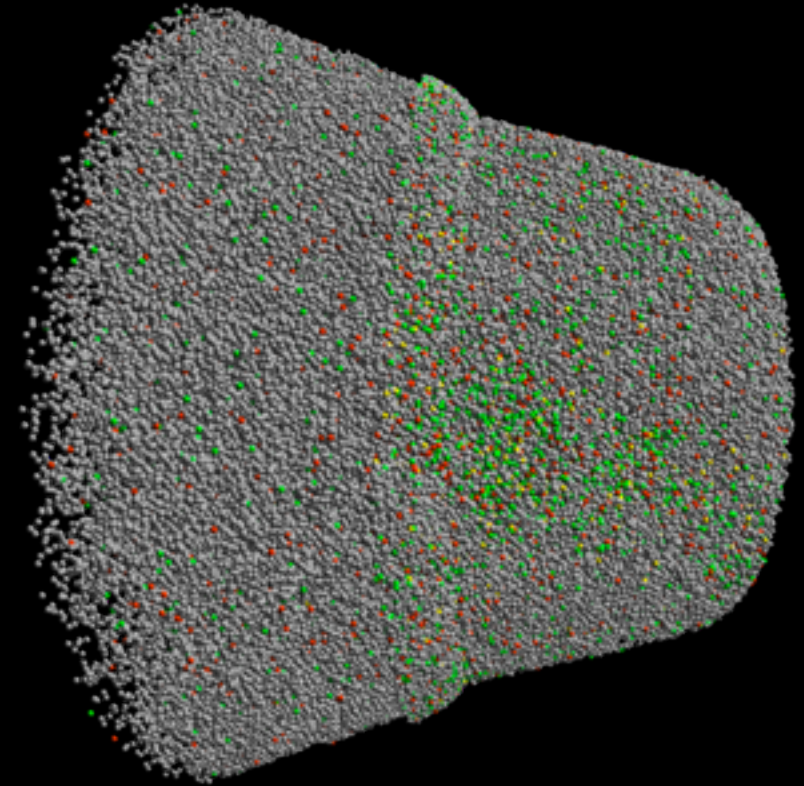
*fostering collaborative design
across scales*

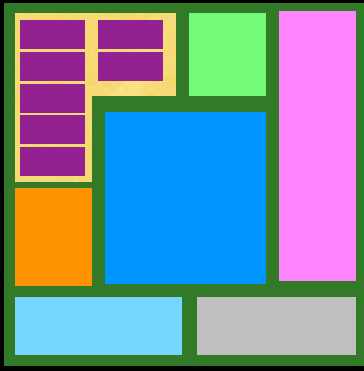




visualization of atomic systems

- experimental data, including atom probe tomography
- atomistic simulations
- render up to 10 million atoms *interactively* with current graphics cards (on a Macintosh)
- render 70+ M with new cards





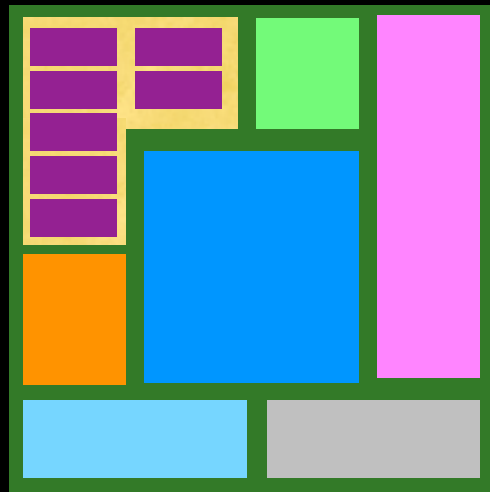
“replaying” atom probe data collection





design

... at the emerging intersection between
information, computation, and complexity



questions