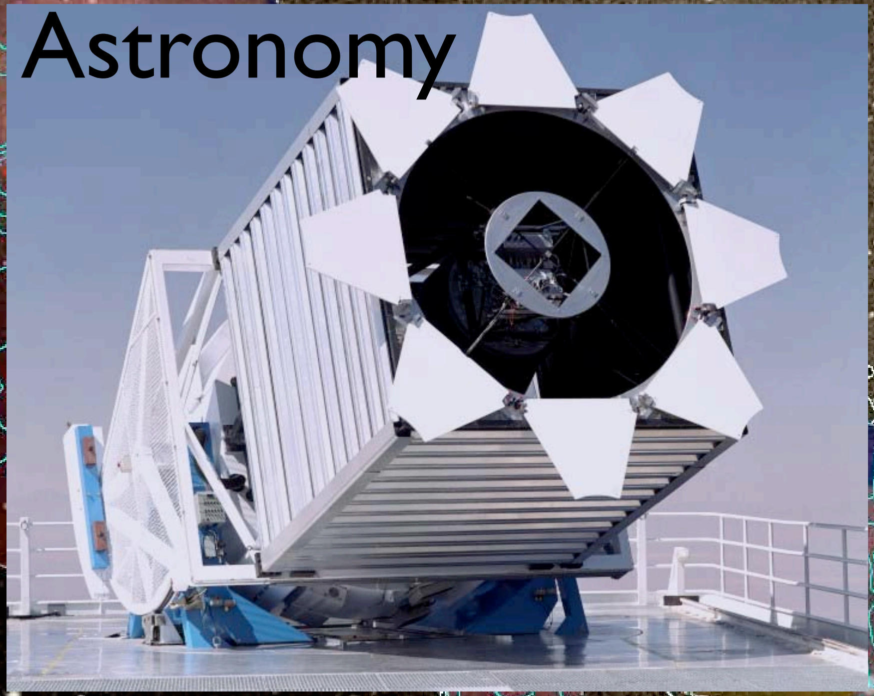
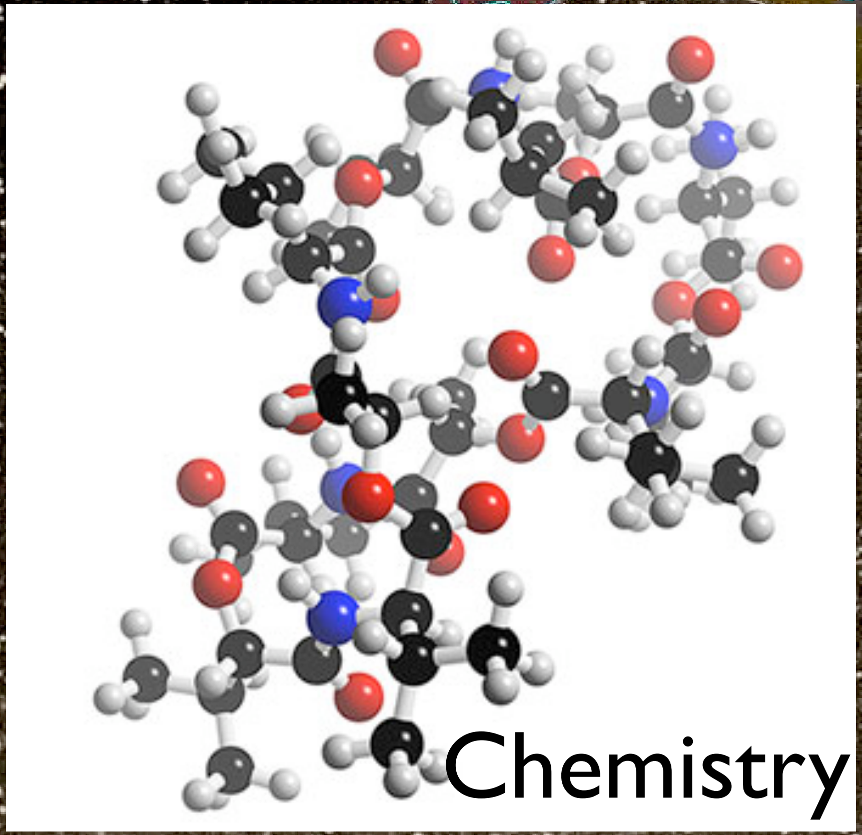
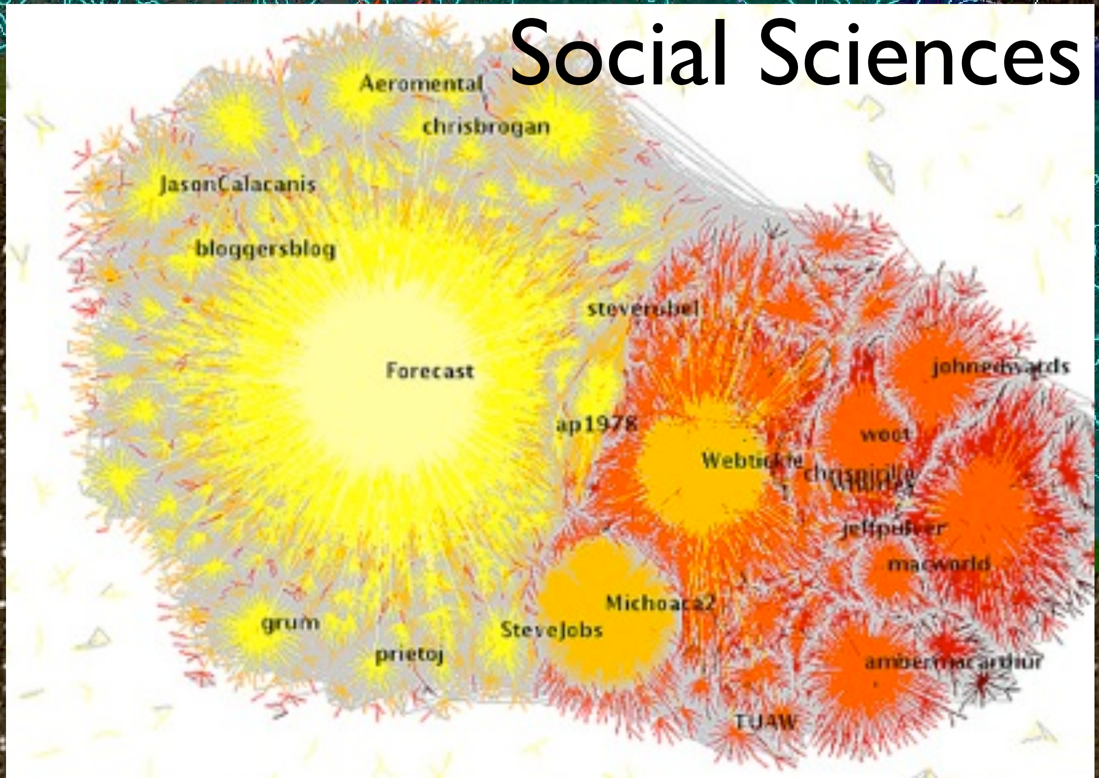
High-Throughput Science

Hanspeter Pfister, Harvard University
pfister@seas.harvard.edu

Scientific Data Explosion







Twitter Social Network © UMBC eBiquity Research Group

Computing Revolution

- Commodity energy-efficient supercomputers

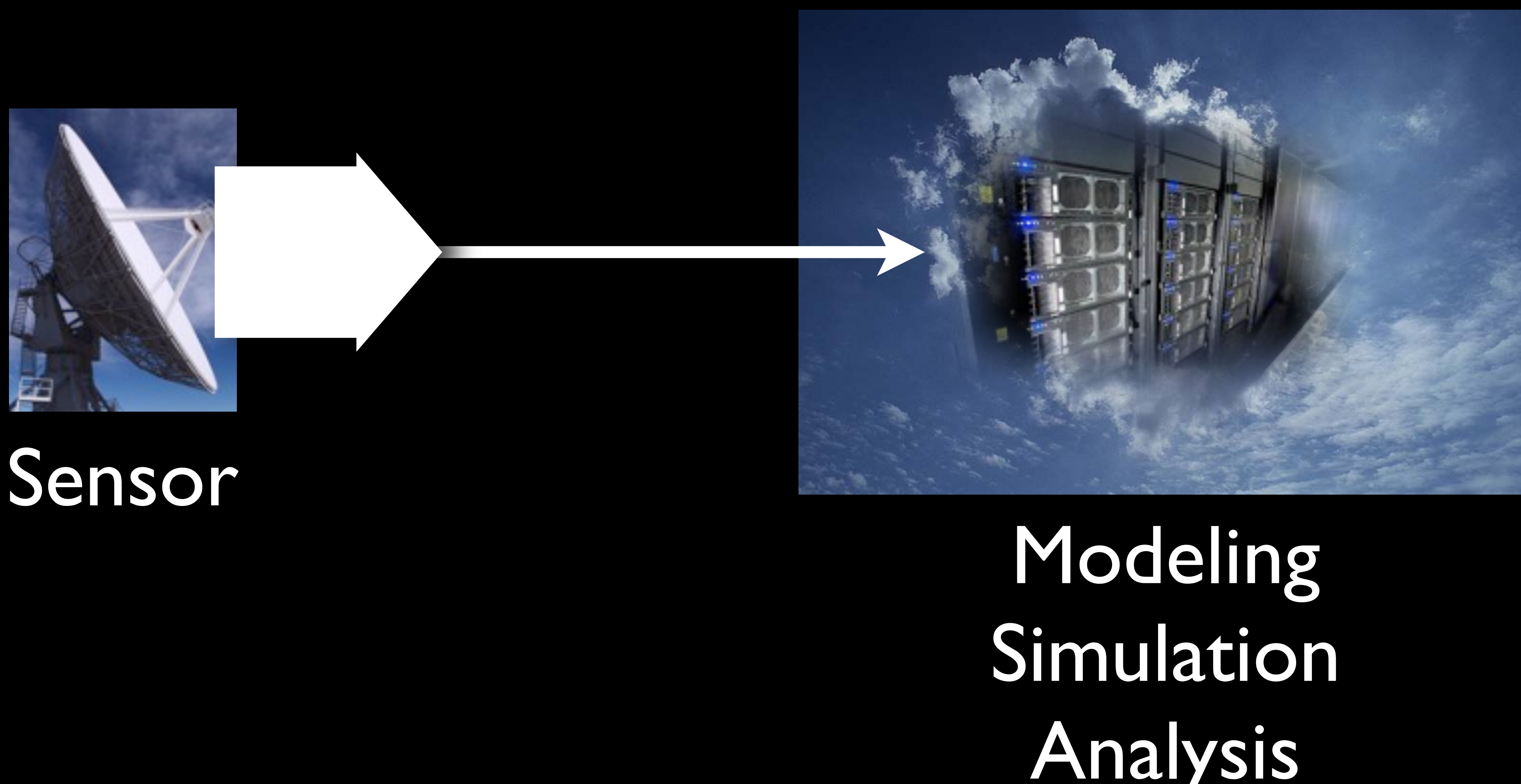
4 Teraflops @ 1400 W

Traditional

Sensor

Modeling
Simulation
Analysis

Traditional



Challenge

- Limited by communication, not processor performance [Jim Grey, Distributed Computing Economics]

Challenge

- Limited by communication, not processor performance [Jim Grey, Distributed Computing Economics]

the INQUIRER
News, reviews, facts and friction

Search

Saturday, 12 September 2009 | INQ Mobile | RSS

Pigeon protocol offers faster data delivery

The pigeon is mightier than ADSL

By **David Neal**

Thursday, 10 September 2009, 14:15

AN UNORTHODOX RACE in South Africa has revealed that it is faster to transmit 4GB of data via carrier pigeon than it is to send it over the country's main ADSL services.

Challenge

Sensor

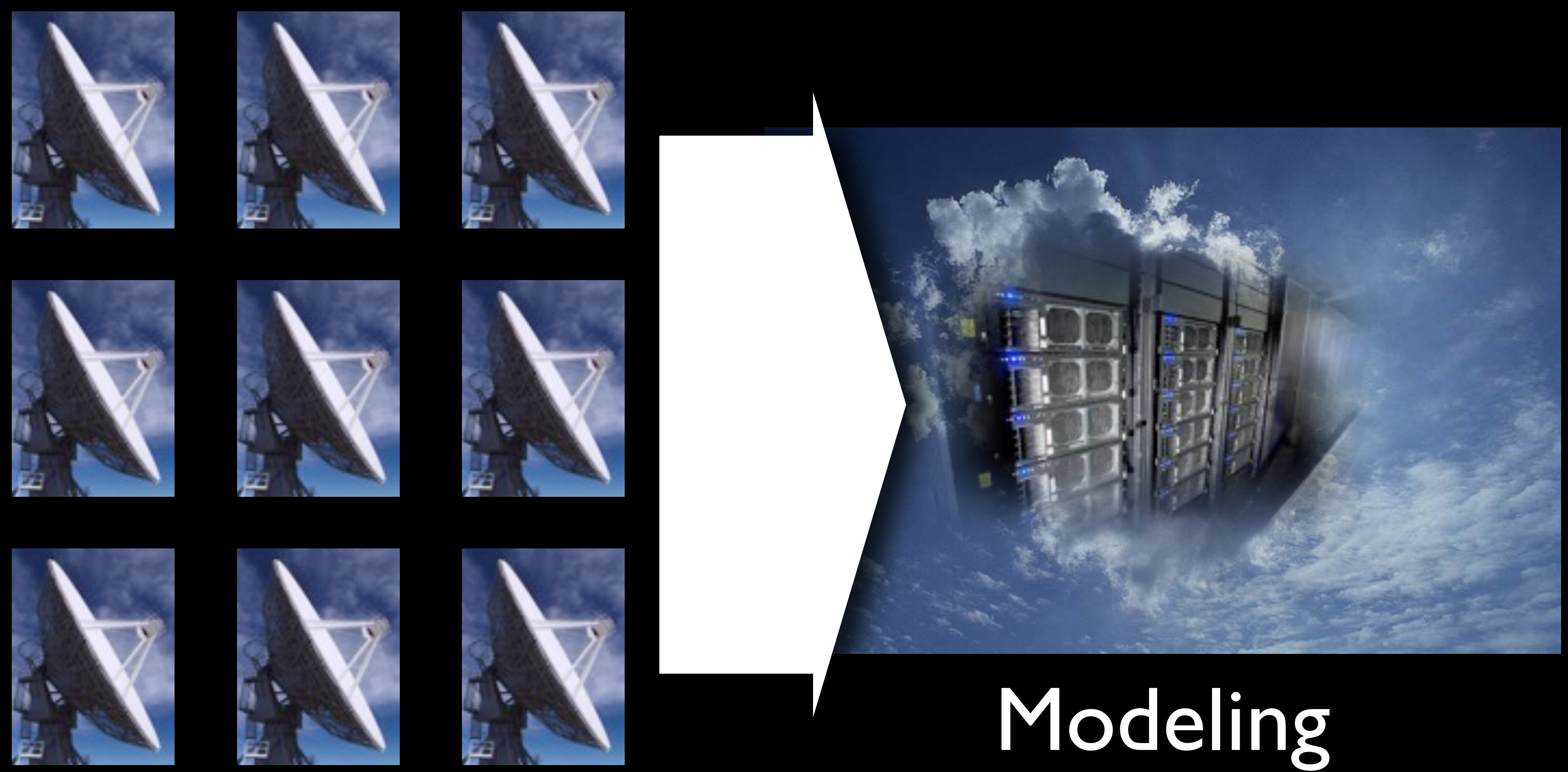
Modeling
Simulation
Analysis

Challenge

Sensor

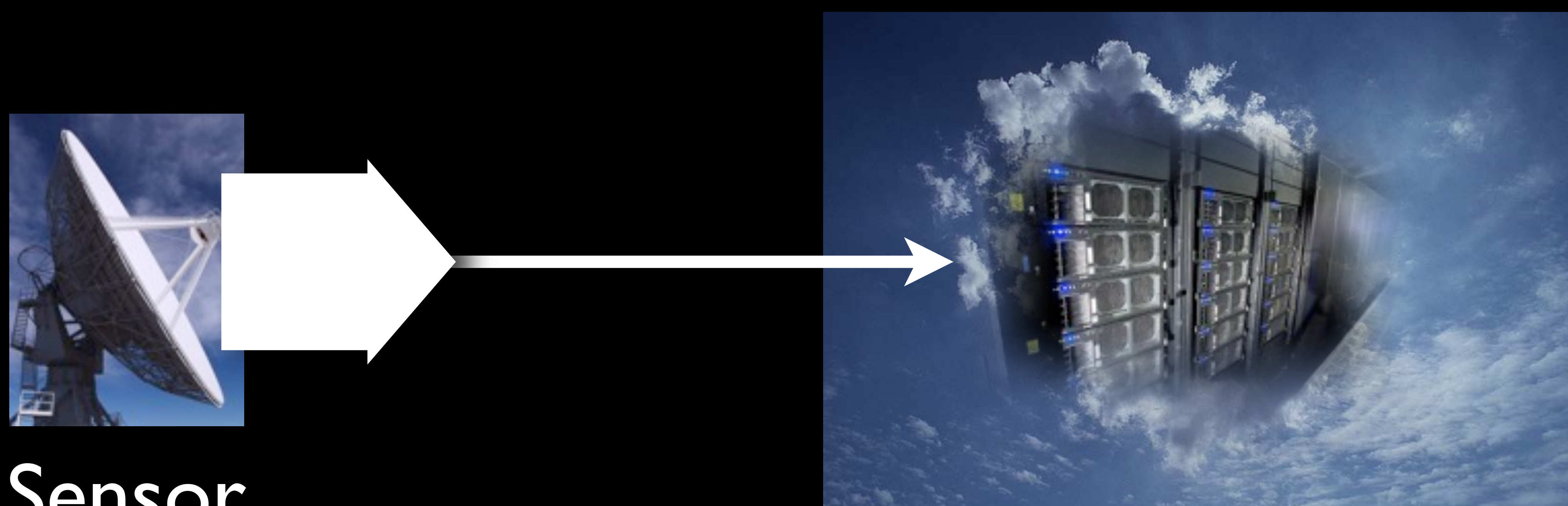
Modeling
Simulation
Analysis

Challenge



Modeling
Simulation
Analysis

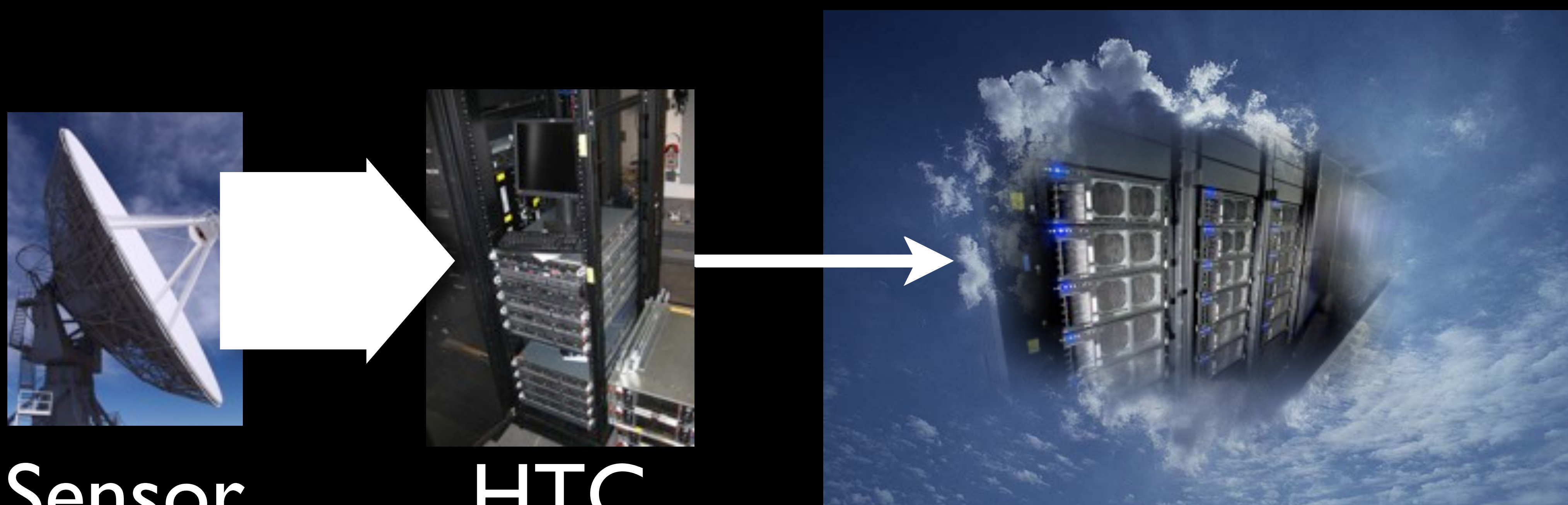
High-Throughput Computing



Sensor

Modeling
Simulation
Analysis

High-Throughput Computing



Sensor

HTC

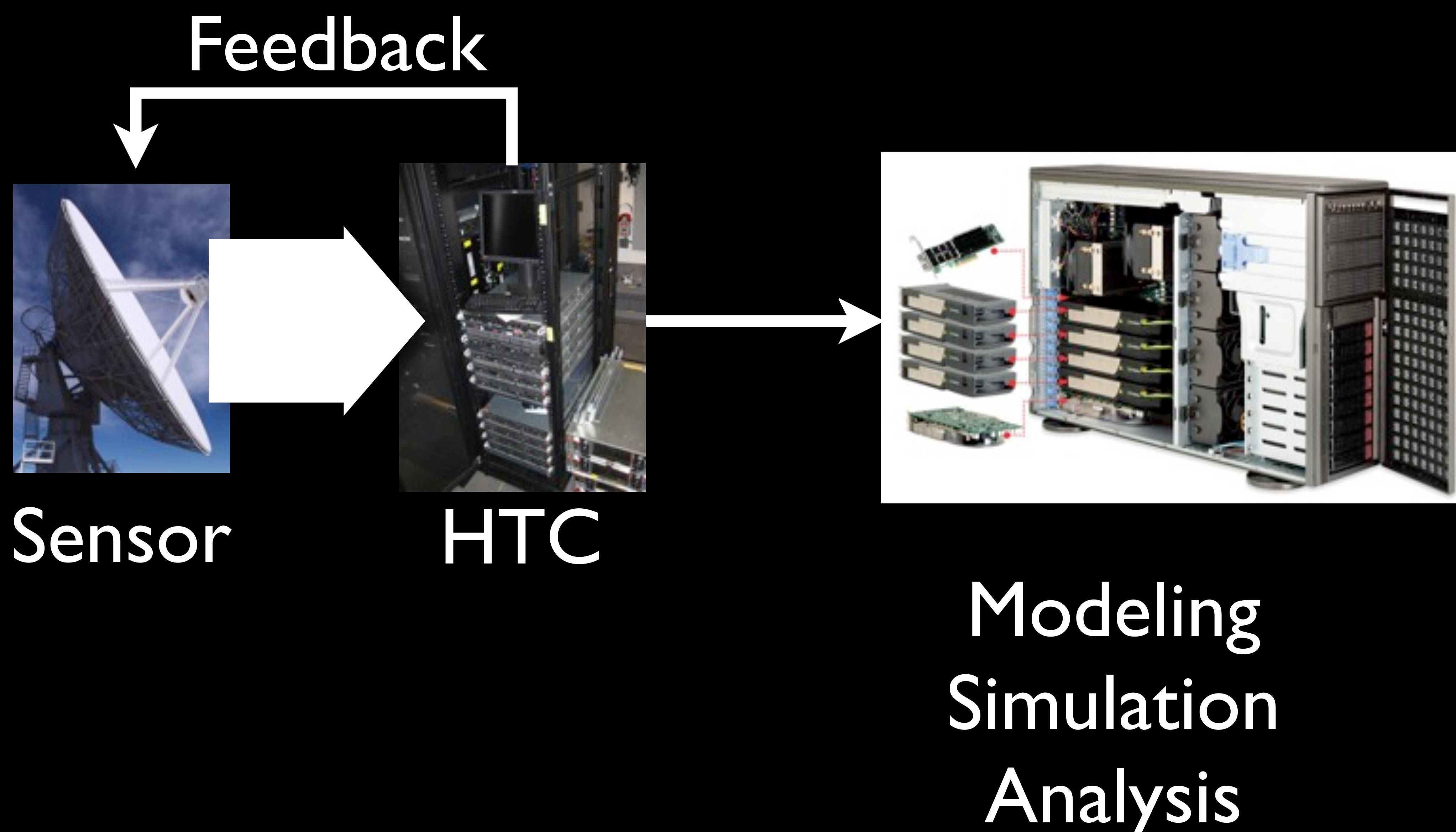
Modeling
Simulation
Analysis

High-Throughput Computing

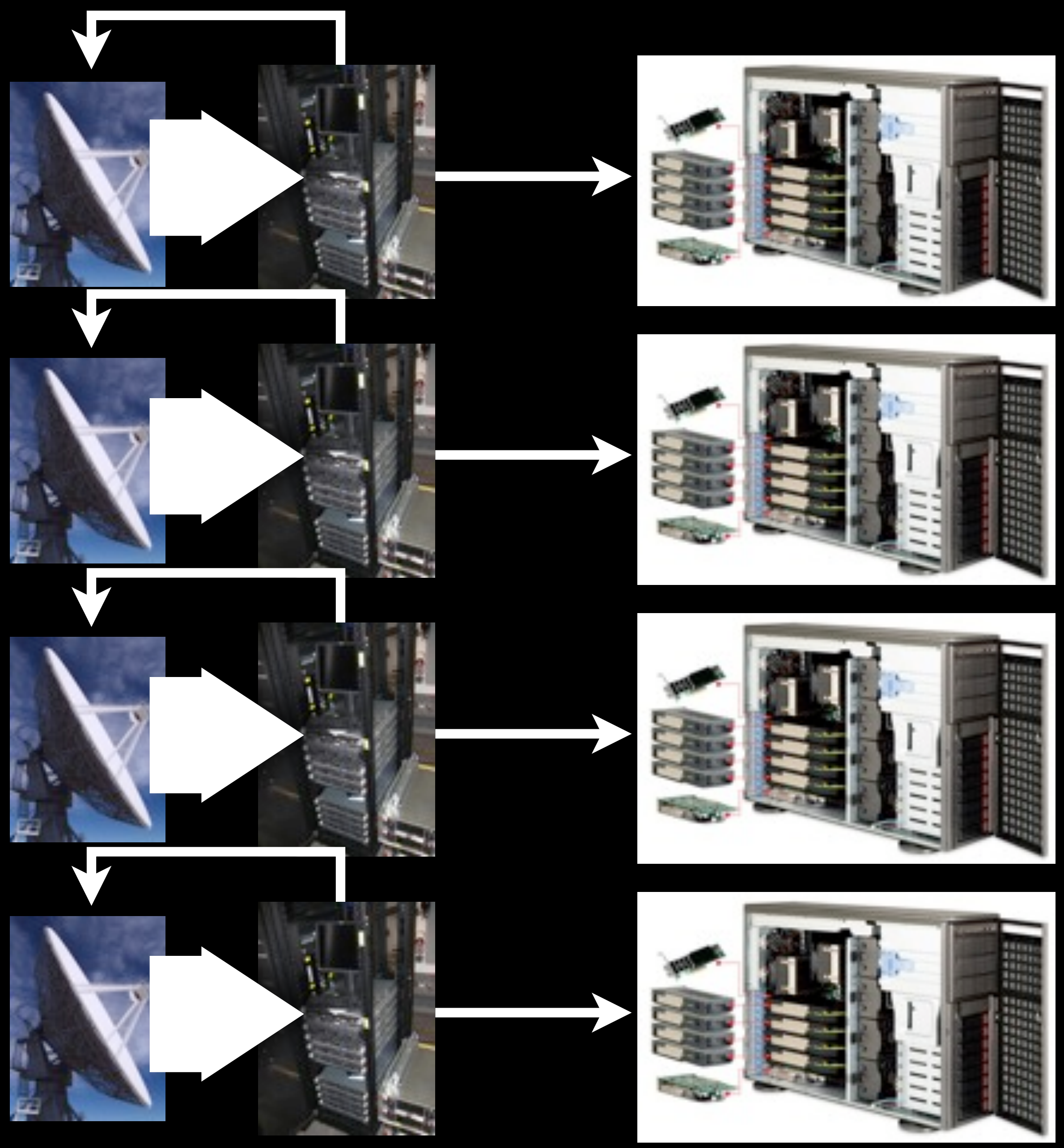
Sensor HTC

Modeling
Simulation
Analysis

High-Throughput Computing

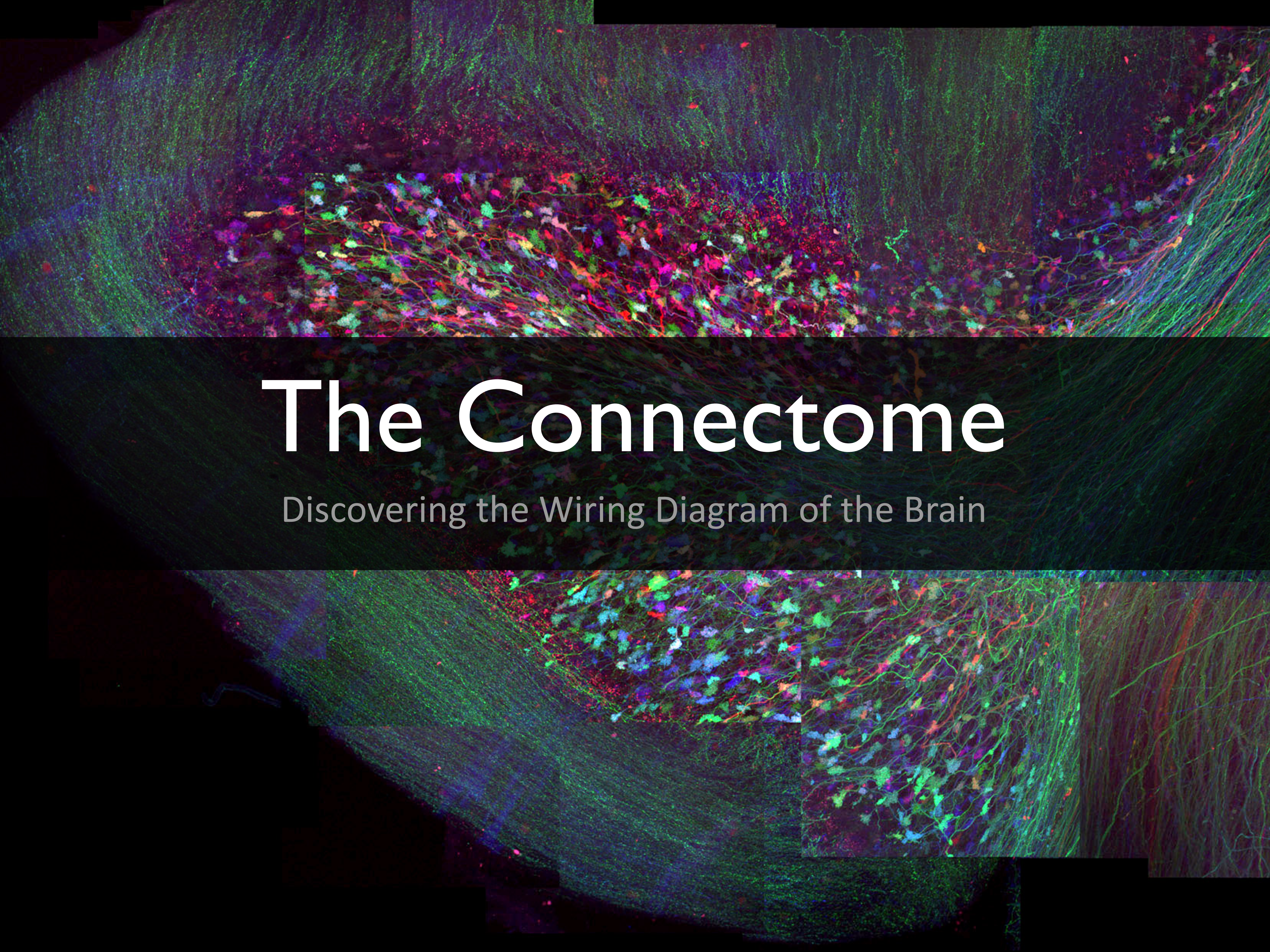


High-Throughput Computing



Outline

- How is the brain wired?
- How did the universe start?
- How does matter interact at the quantum level?
- How does the human visual system work?
- How can we prevent heart attacks?

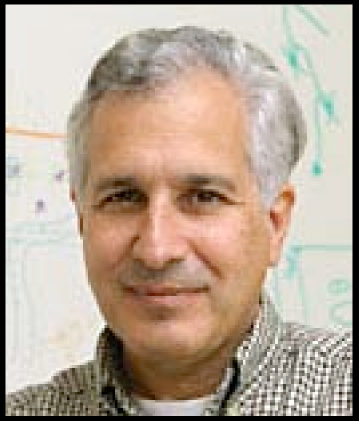


The Connectome

Discovering the Wiring Diagram of the Brain

Collaborators

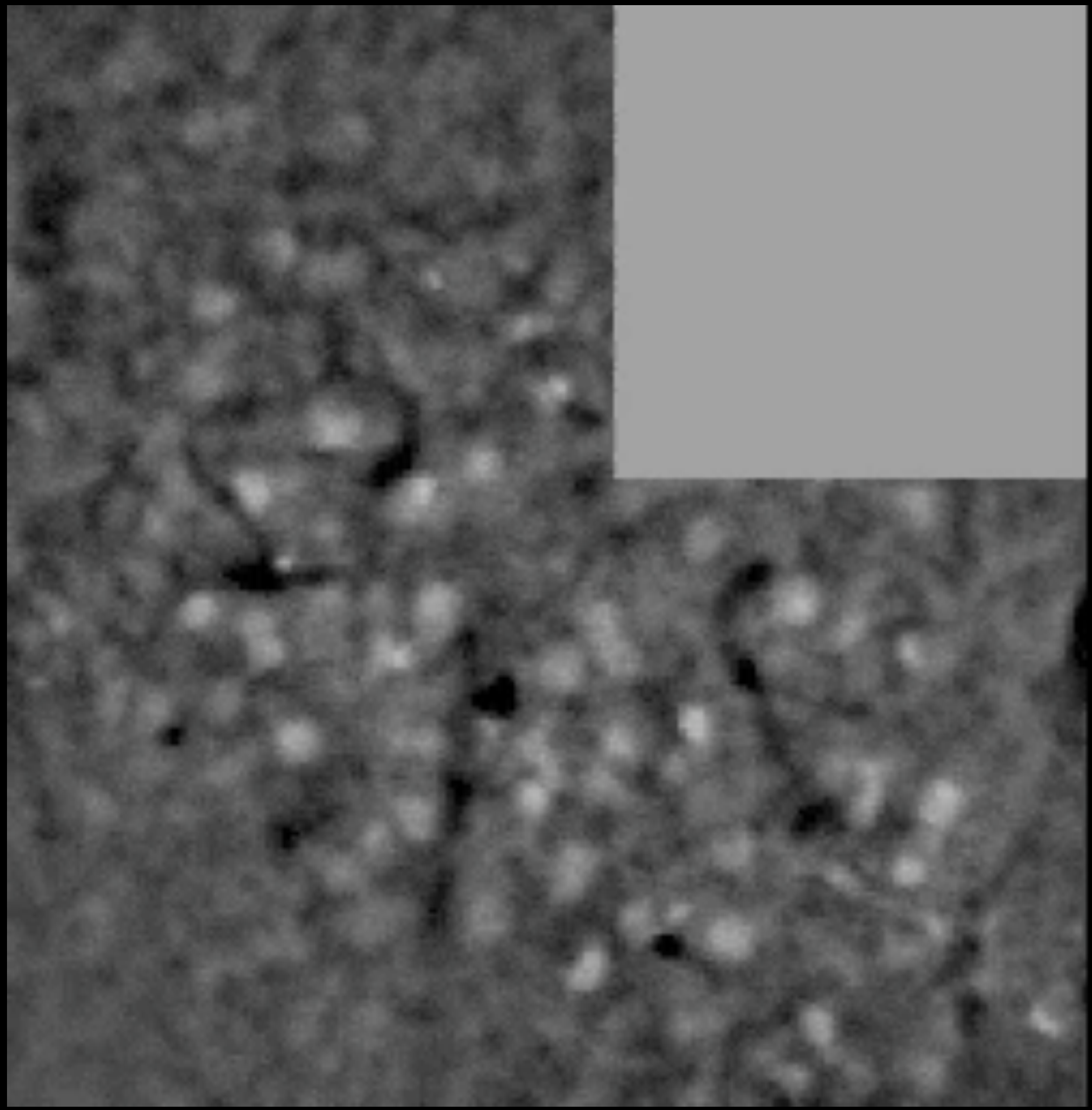
- Harvard Center for Brain Science
  - Jeff Lichtman & Clay Reid
- Kitware Inc.
  - Will Schroeder, Charles Law, Rusty Blue
- VRVis Vienna
  - Markus Hadwiger, Johanna Beyer
- SEAS
  - Amelio Vazquez, Won-Ki Jeong
  - Hanspeter Pfister






The Scientific Challenge

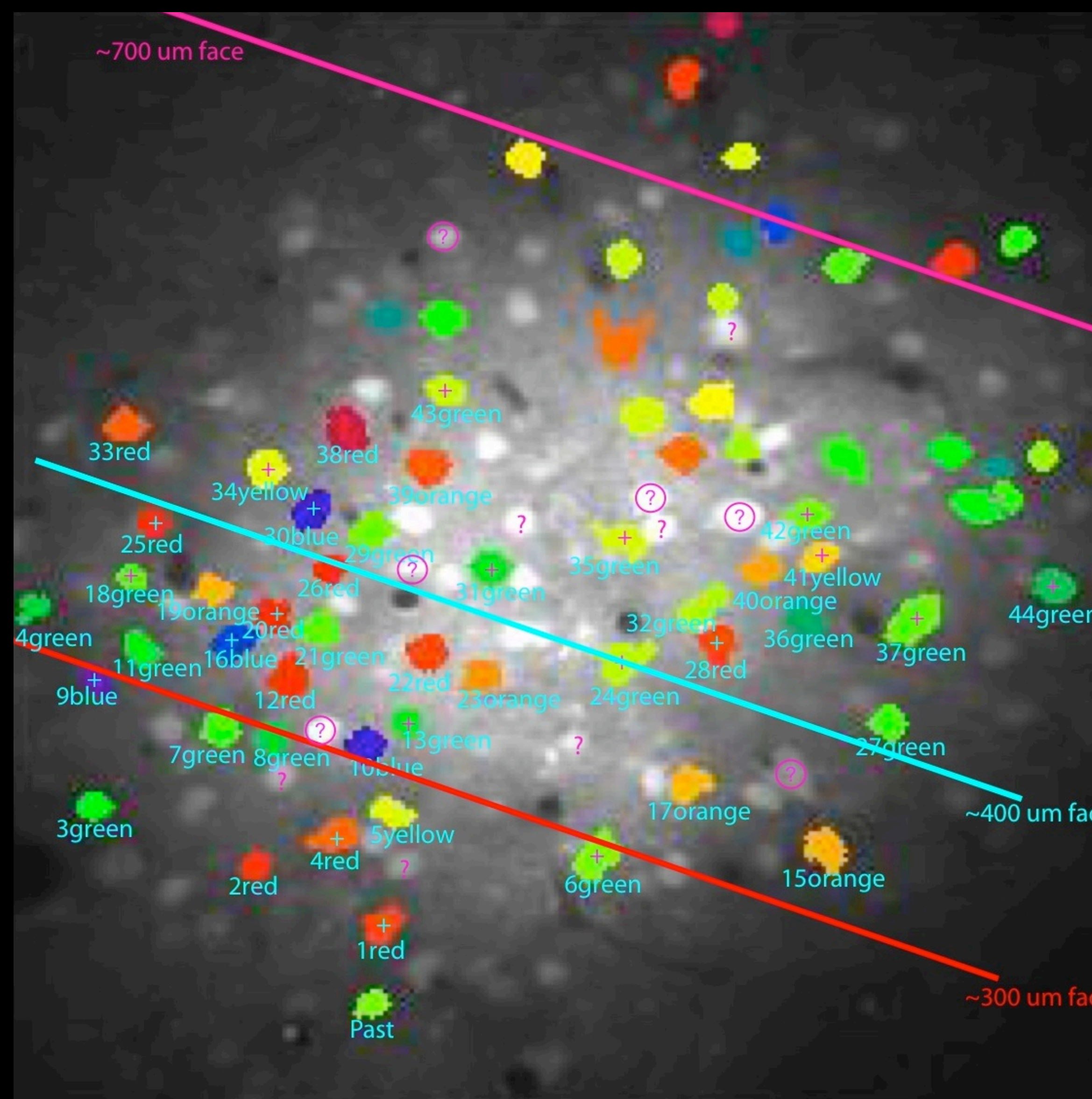
- What do large brain circuits do?



C. Reid

The Scientific Challenge

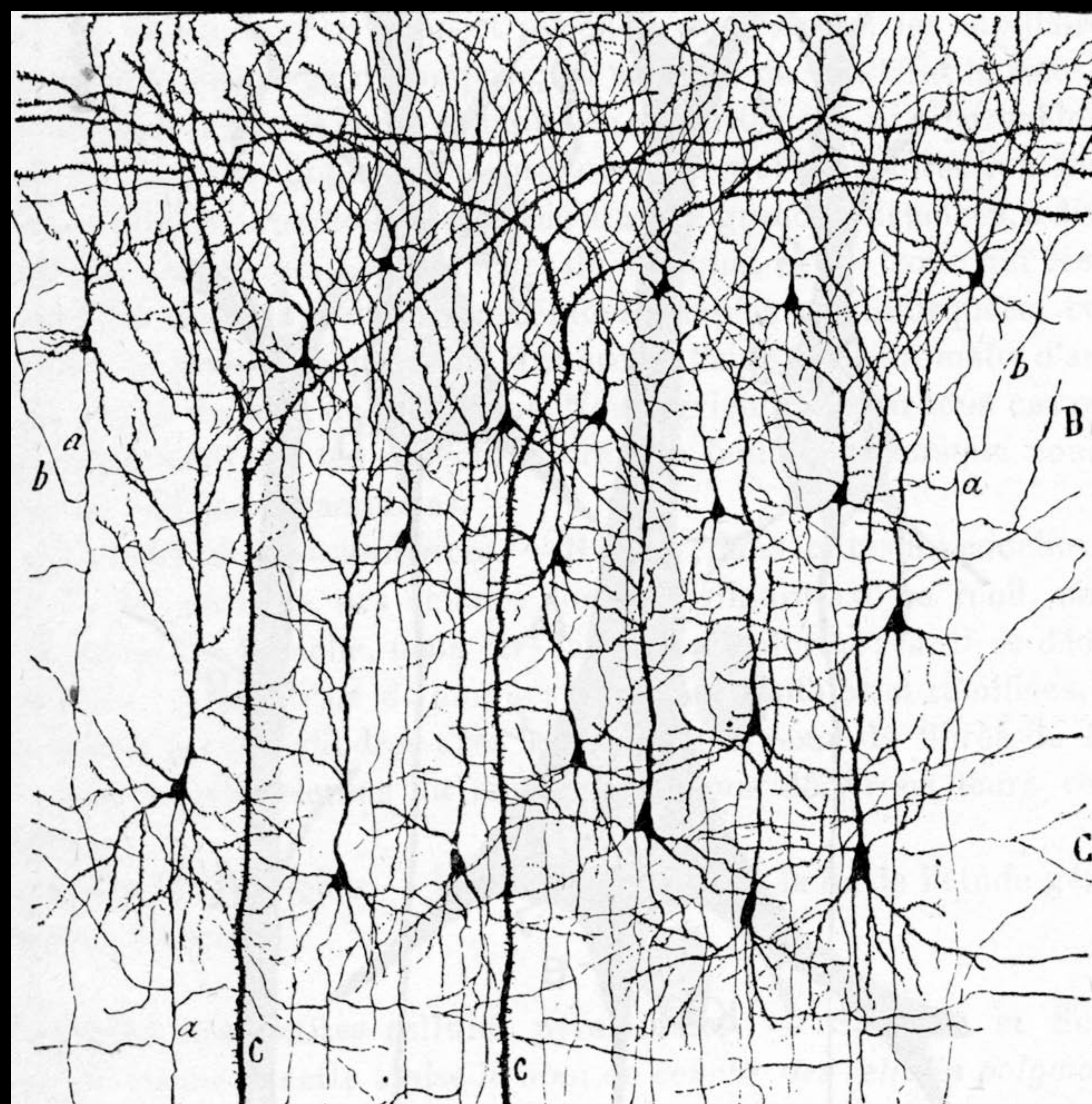
- What do large brain circuits do?



C. Reid

The Scientific Challenge

- What is their connectivity?



Ramón y Cajal, 1905

Connectome Pipeline

Connectome Pipeline

Get a brain

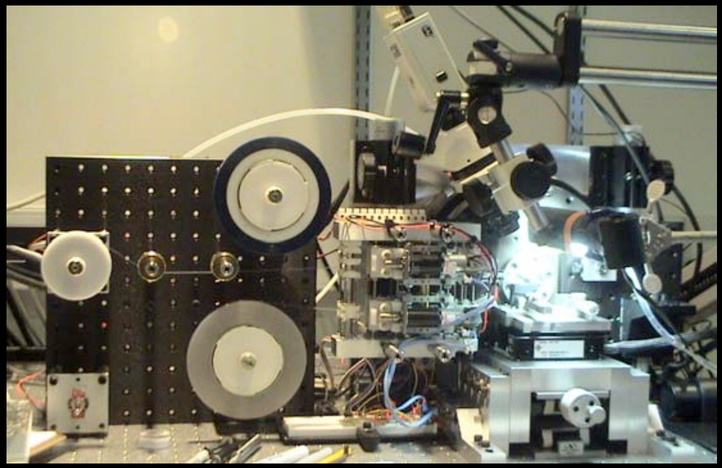
Connectome Pipeline

Get a brain → Get a piece

Connectome Pipeline

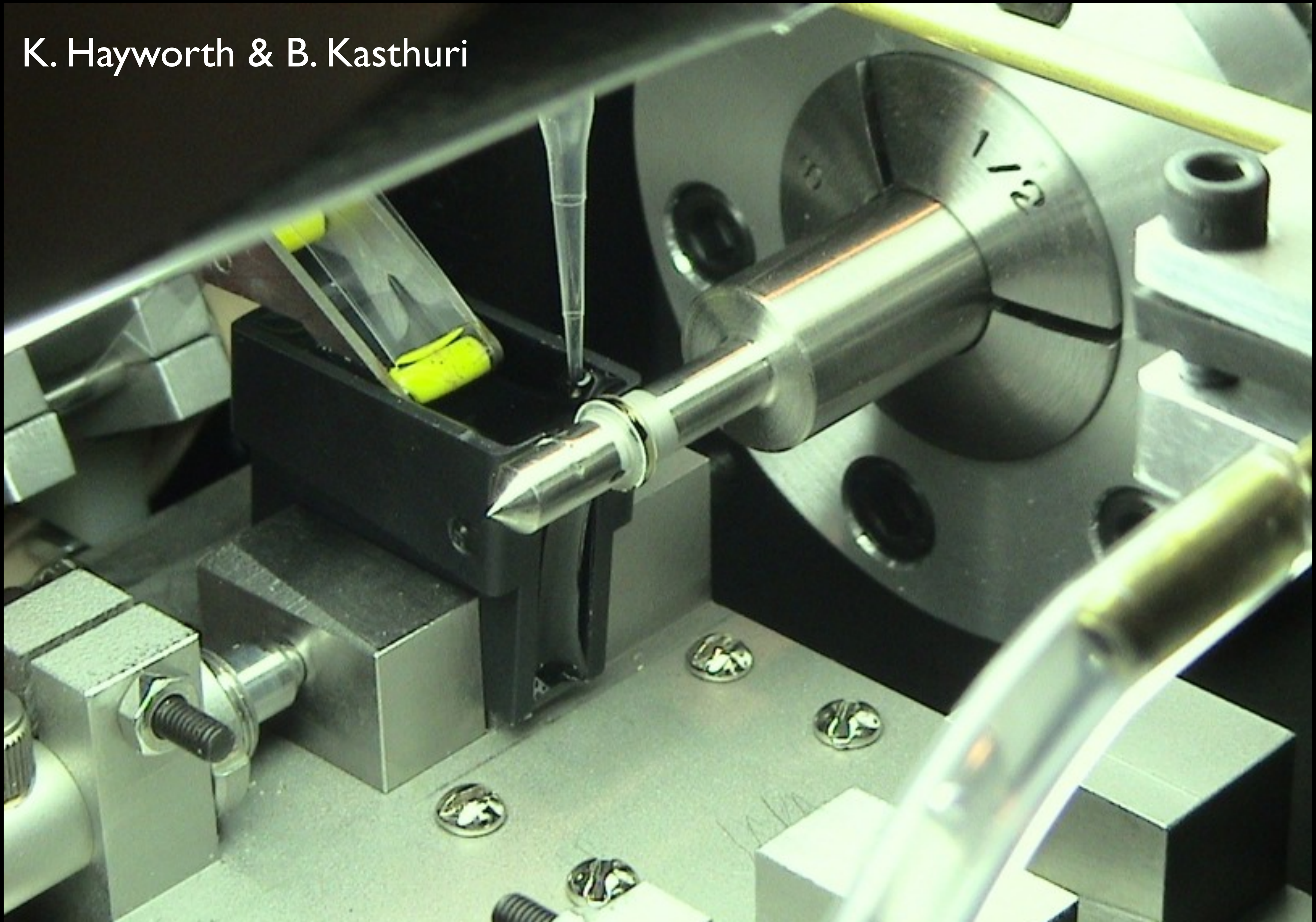
Get a brain →

Get a piece →

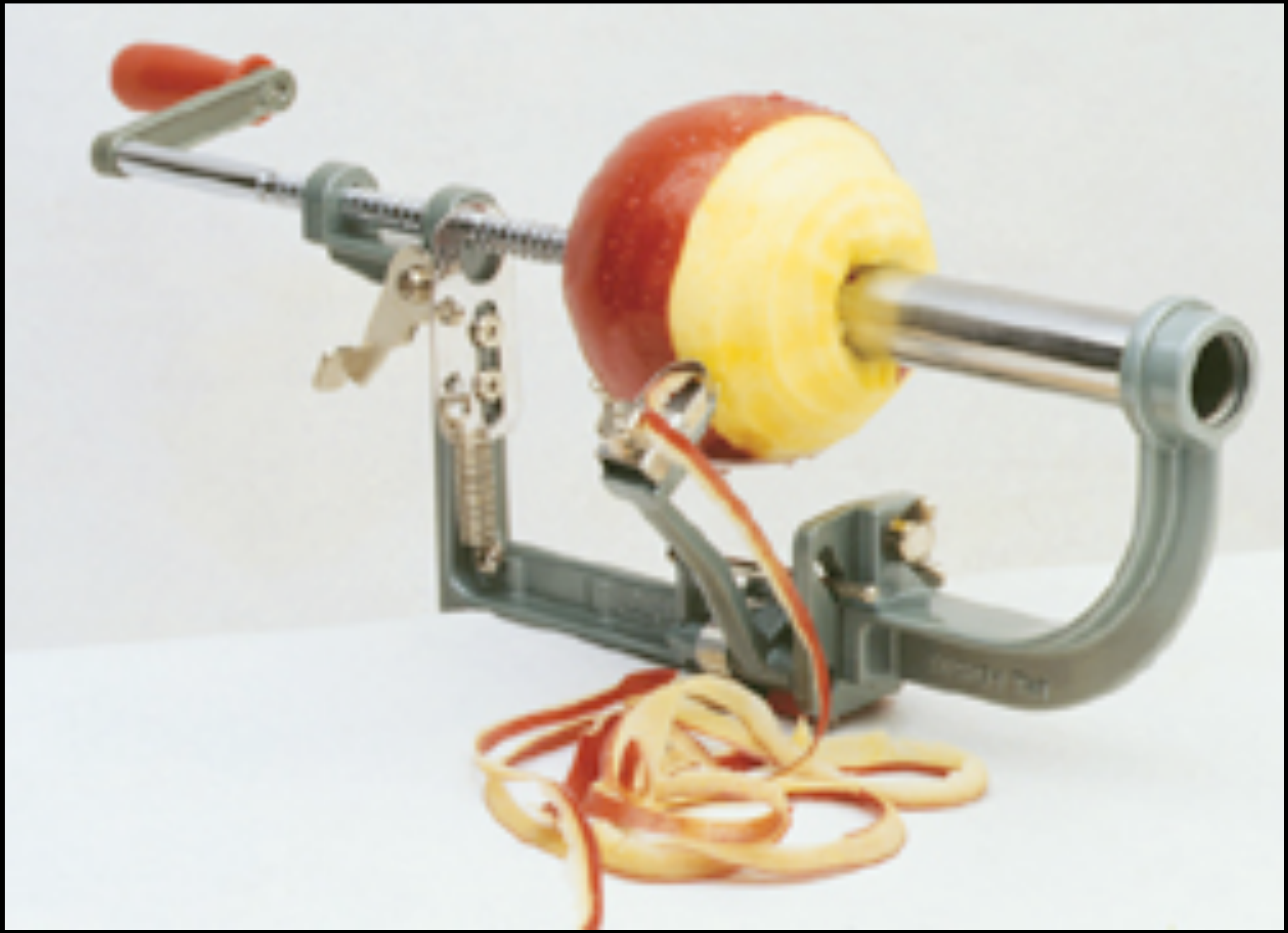


Cut it thin

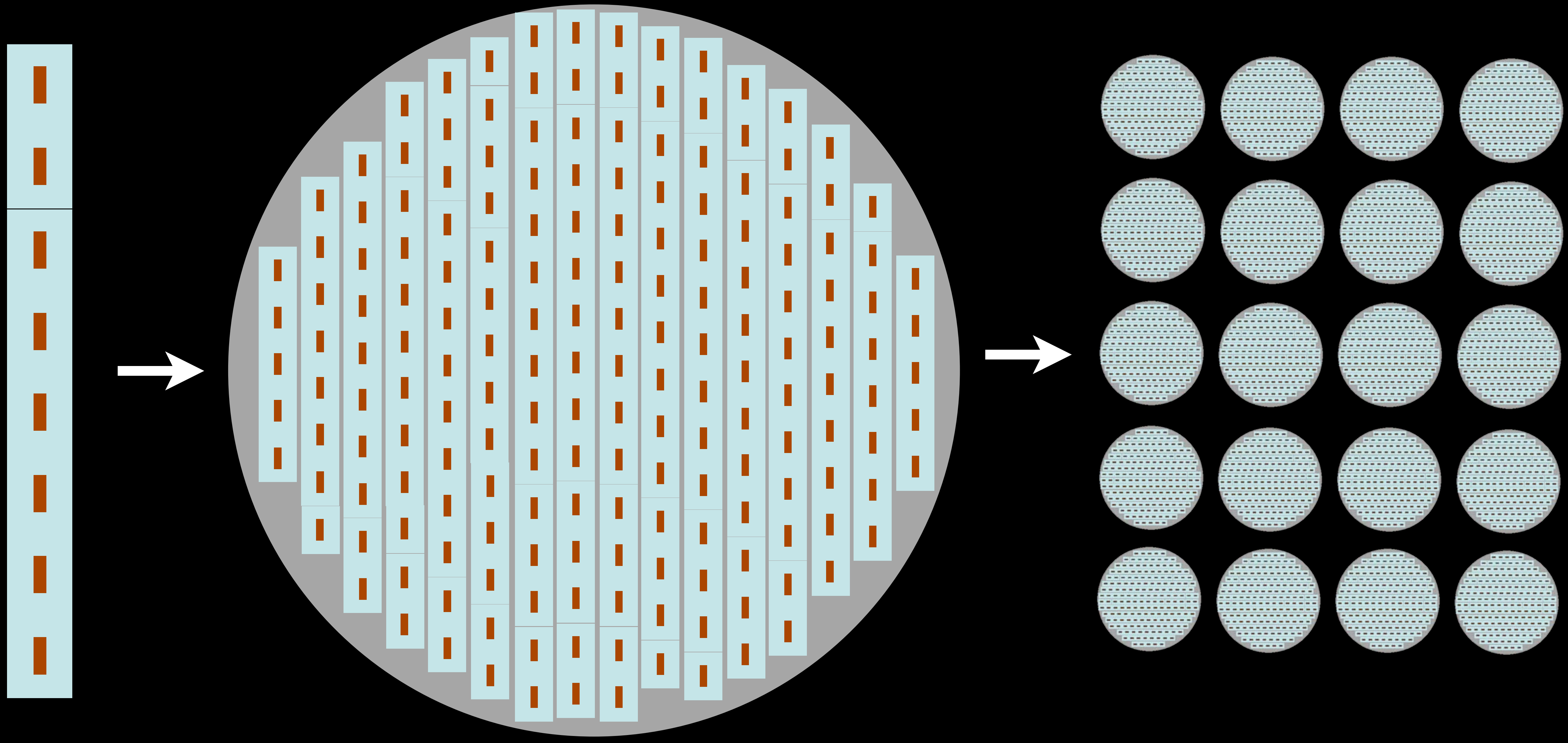
Automatic Tape-collecting Lathe Ultra Microtome



Inspiration for ATLUM



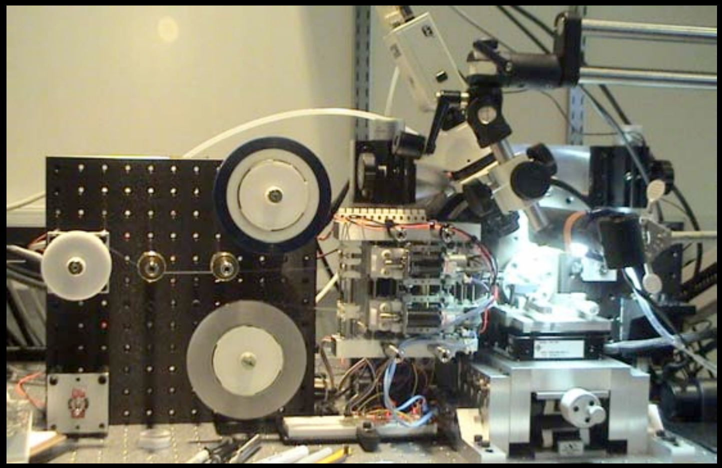
Ultrathin Section Libraries



Connectome Pipeline

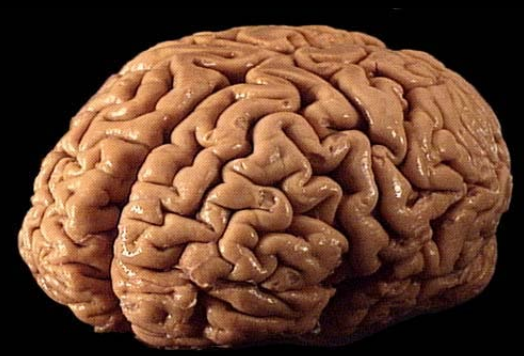
Get a brain →

Get a piece →



Cut it thin

Connectome Pipeline

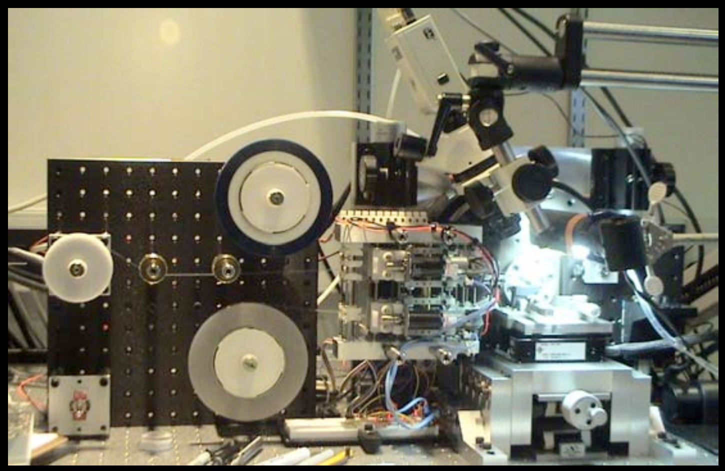


Get a brain

→

Get a piece

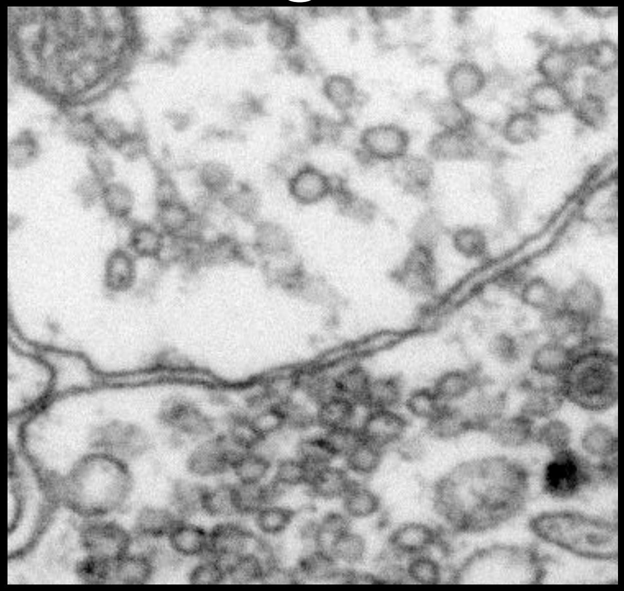
→

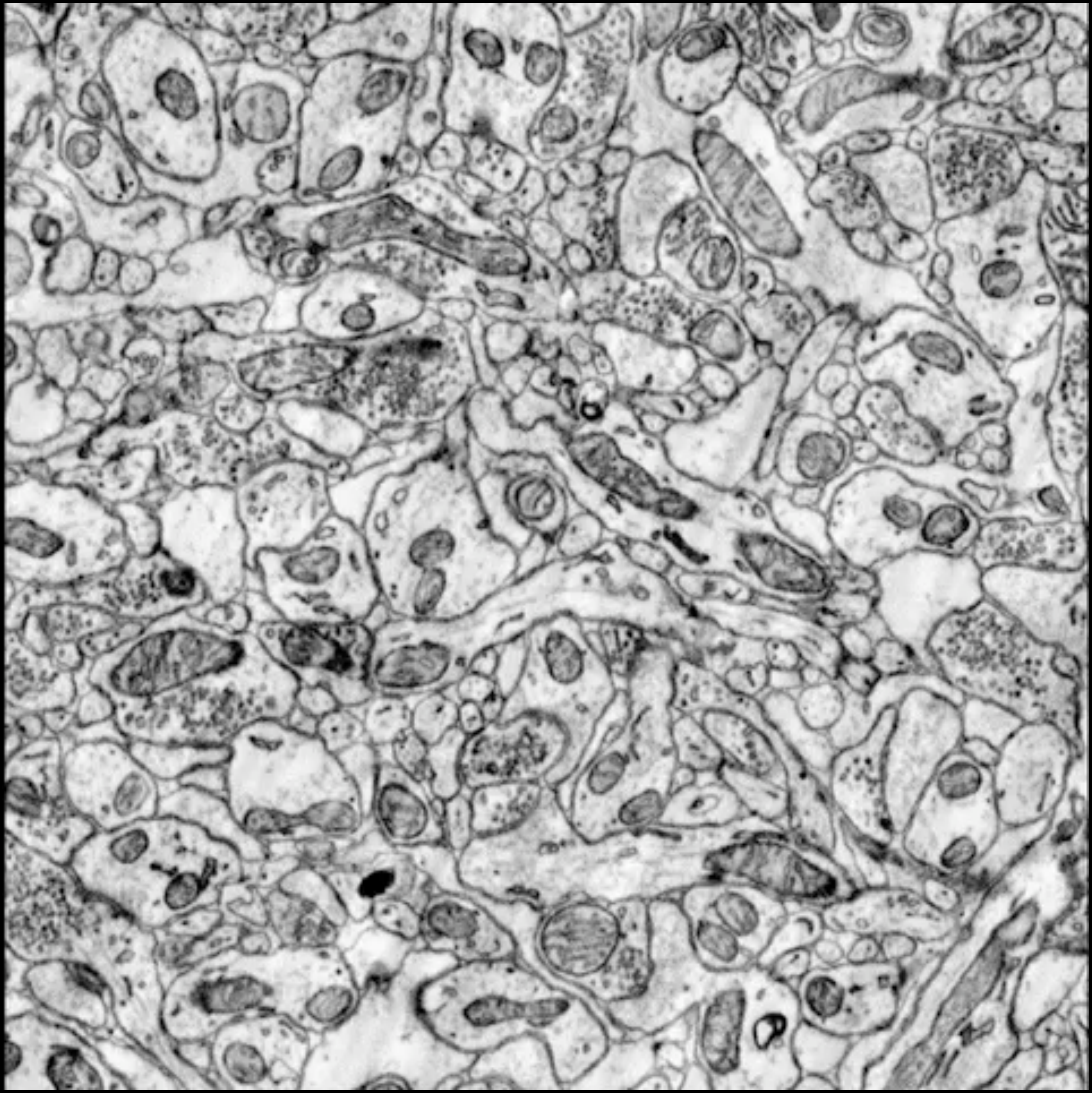


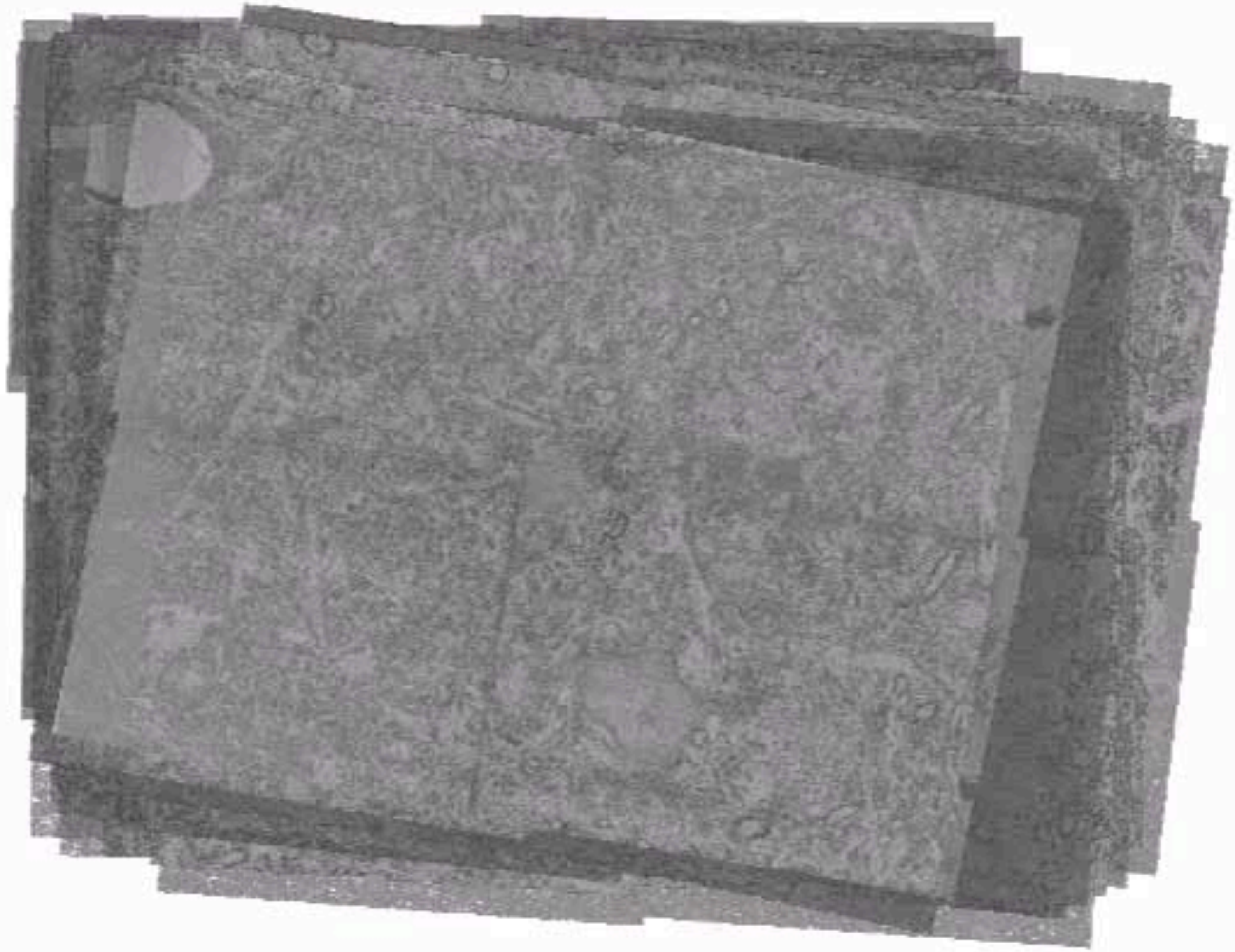
Cut it thin

↓

Image it

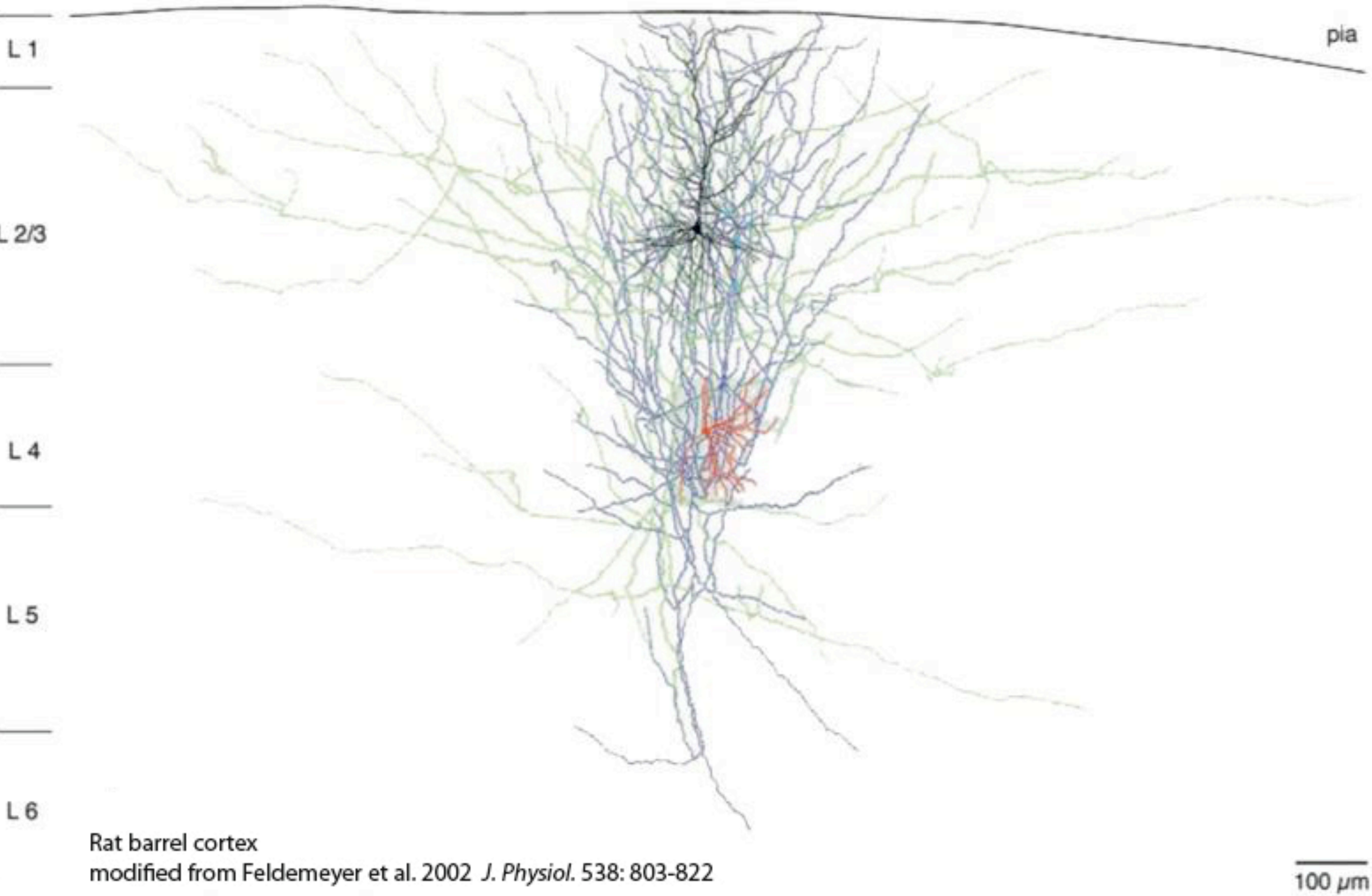






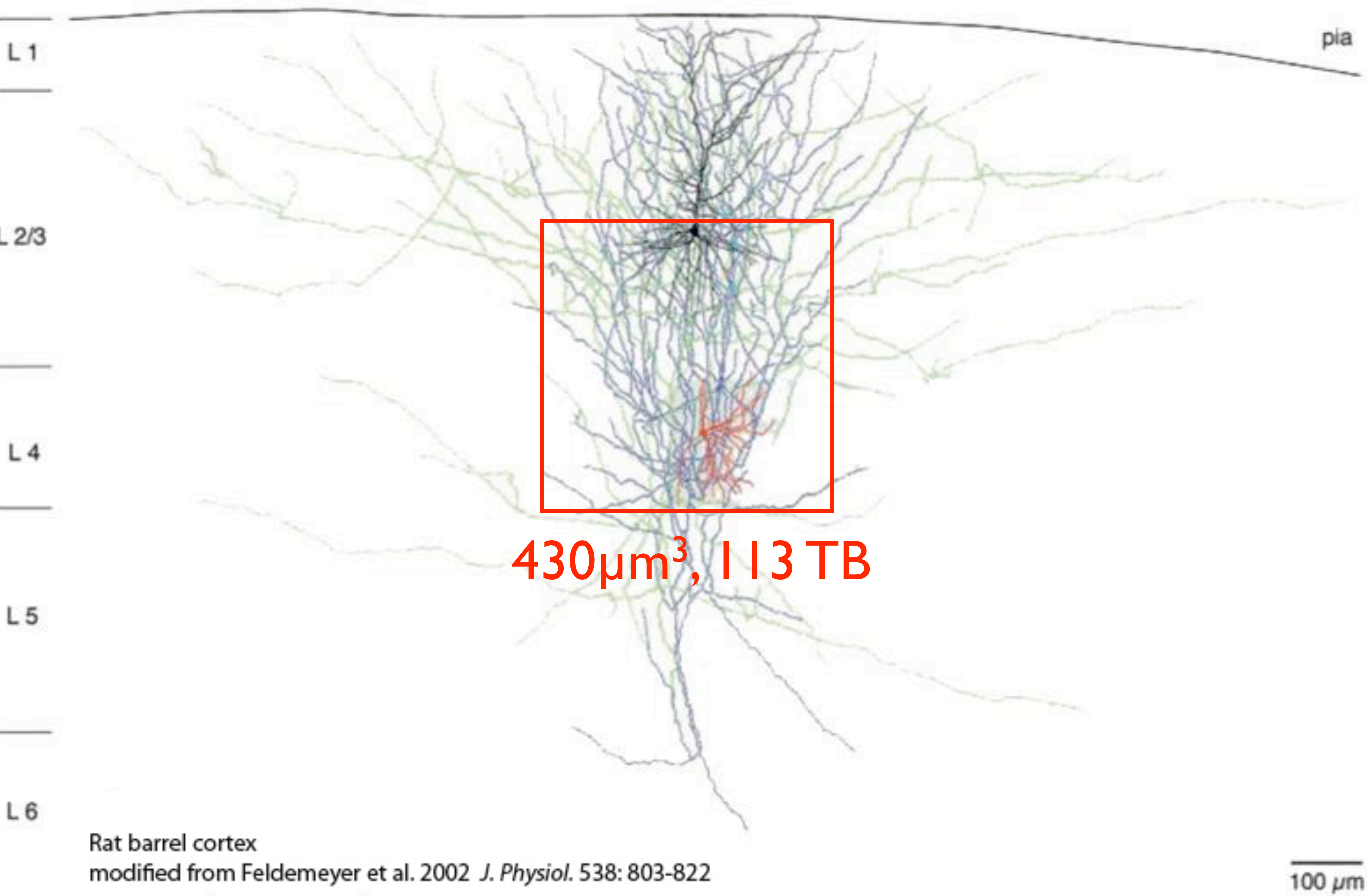
14,000 x 11,000 pixels, 300 sections = 40 GB

Imaging at 5 nm x 5 nm x 40 nm



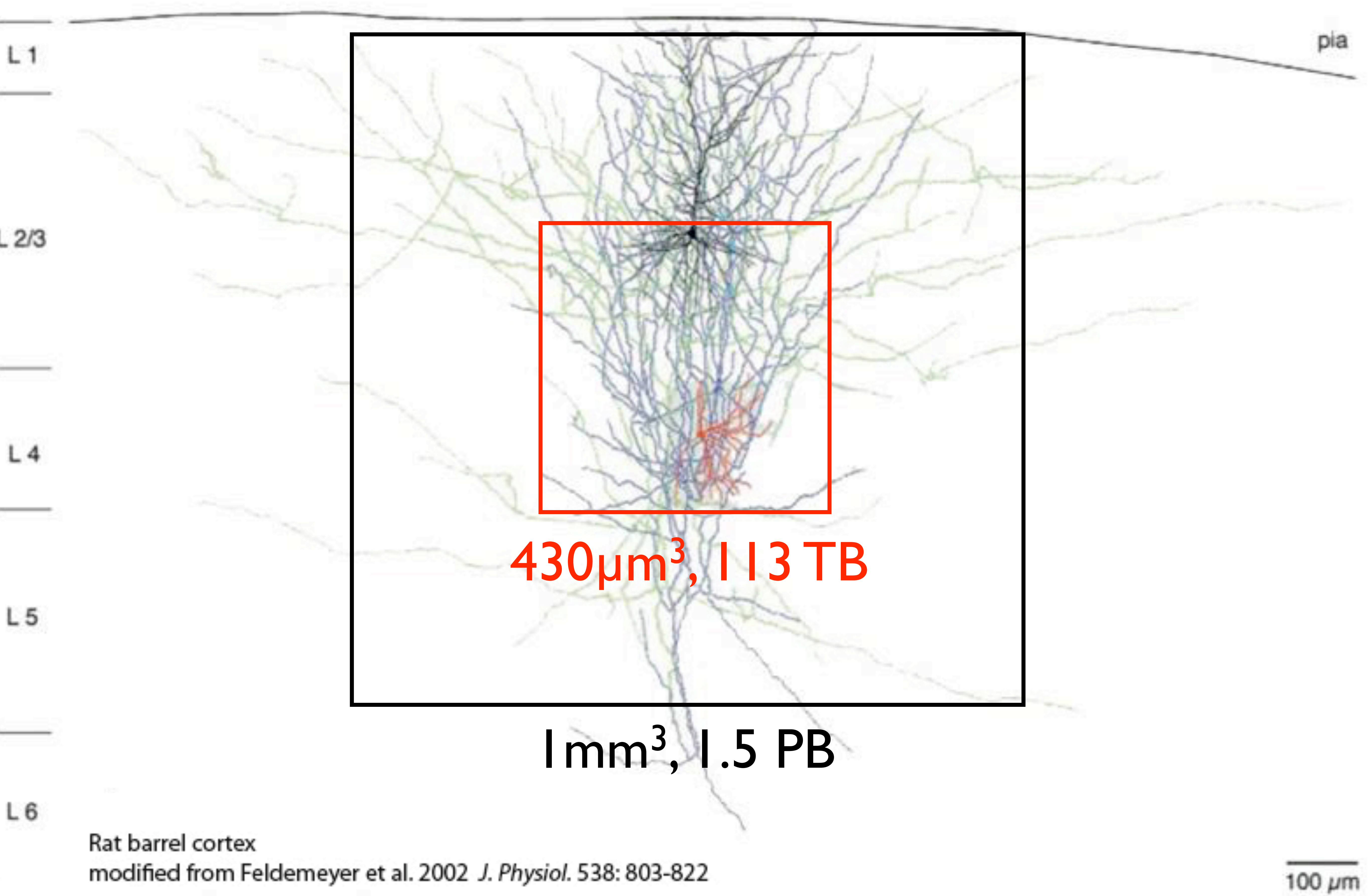
Rat barrel cortex
modified from Feldemeyer et al. 2002 *J. Physiol.* 538: 803-822

Imaging at 5 nm x 5 nm x 40 nm



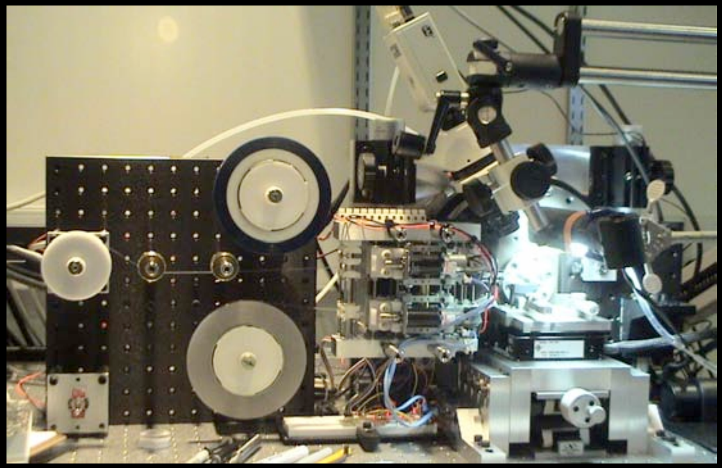
Rat barrel cortex
modified from Feldemeyer et al. 2002 *J. Physiol.* 538: 803-822

Imaging at 5 nm x 5 nm x 40 nm

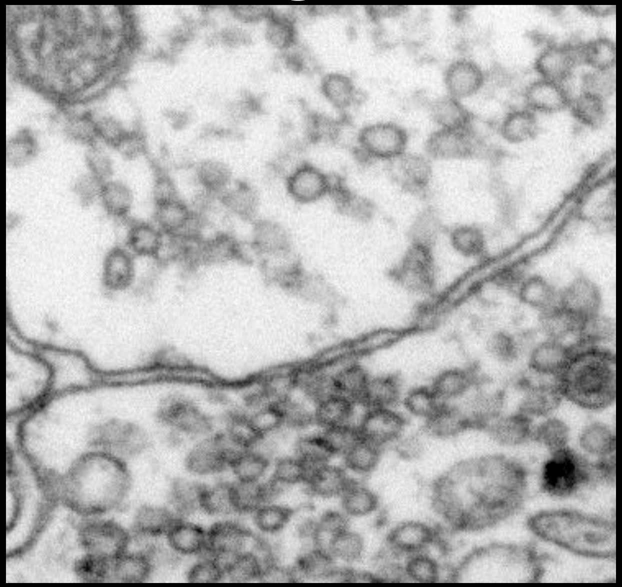


Rat barrel cortex
modified from Feldemeyer et al. 2002 *J. Physiol.* 538: 803-822

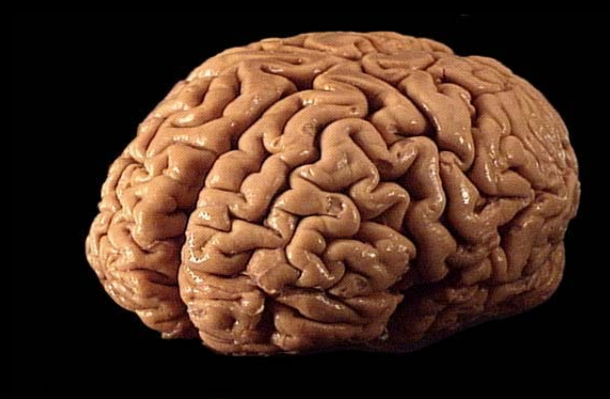
Connectome Pipeline



Get a brain → Get a piece → Cut it thin ↓ Image it

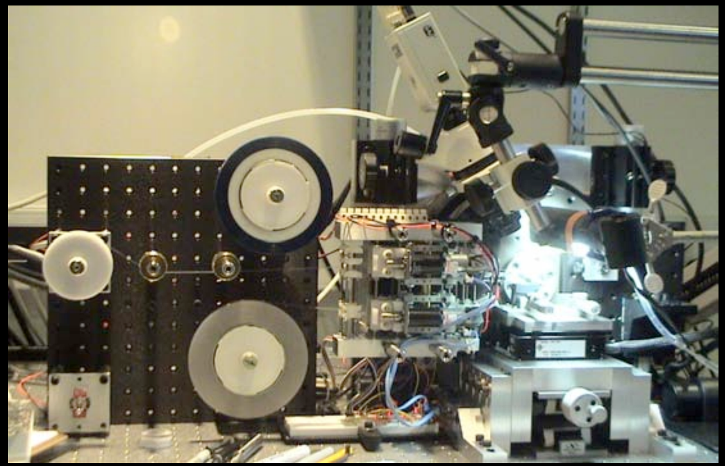


Connectome Pipeline



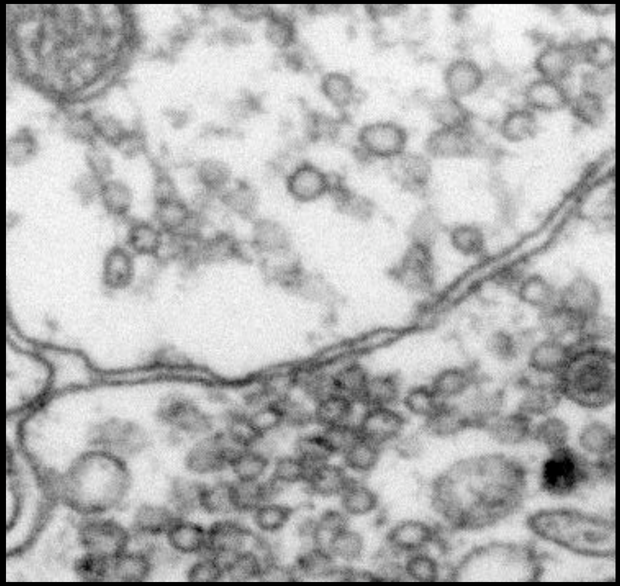
Get a brain →

Get a piece →

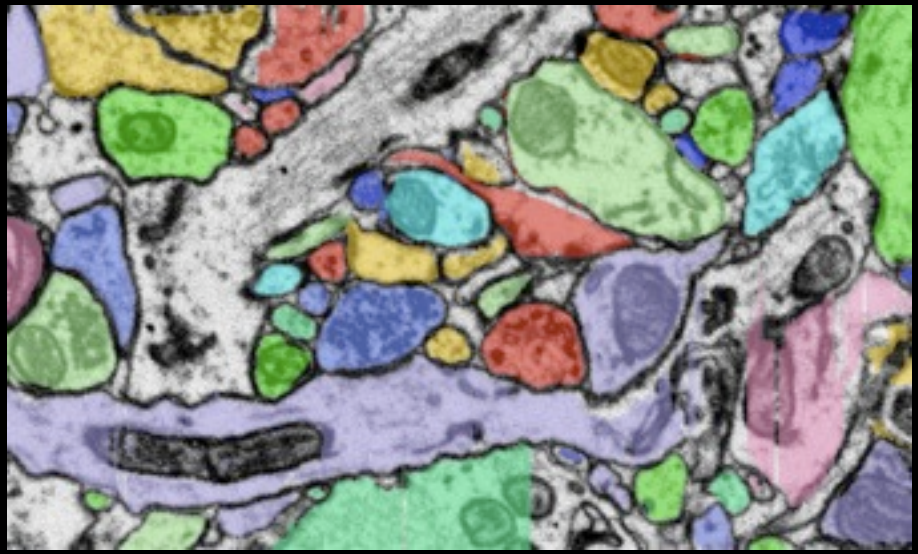


Cut it thin ↓

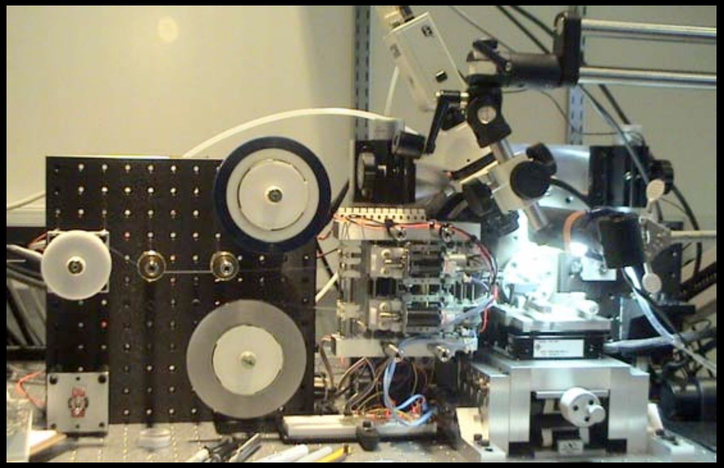
Image it ←



Reconstruct



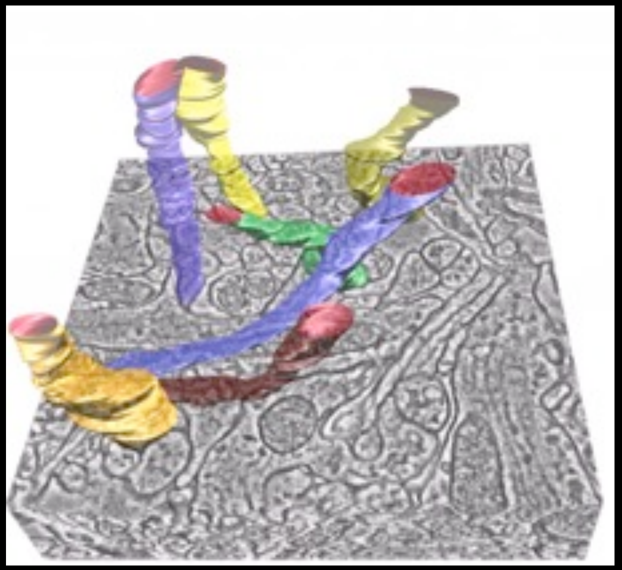
Connectome Pipeline

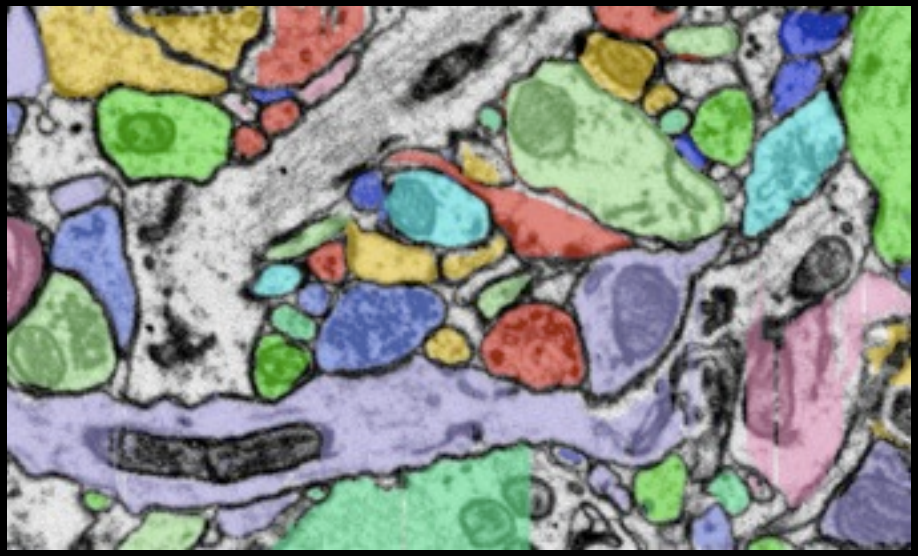


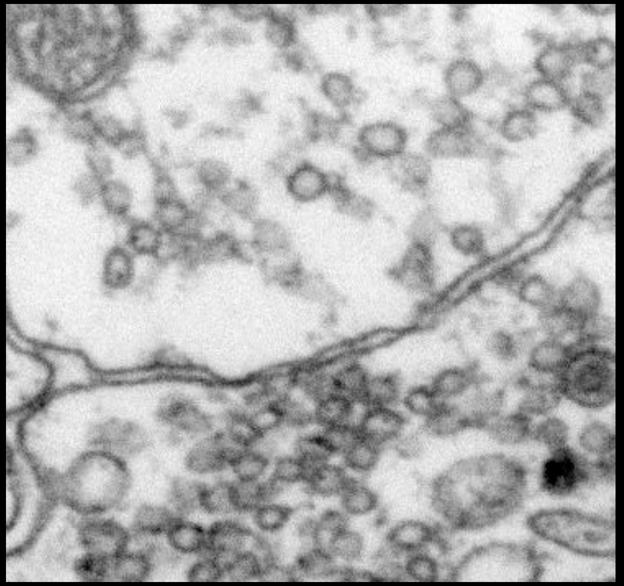
Get a brain → Get a piece → Cut it thin

↓

Visualize & Analyze ↔ Reconstruct ← Image it







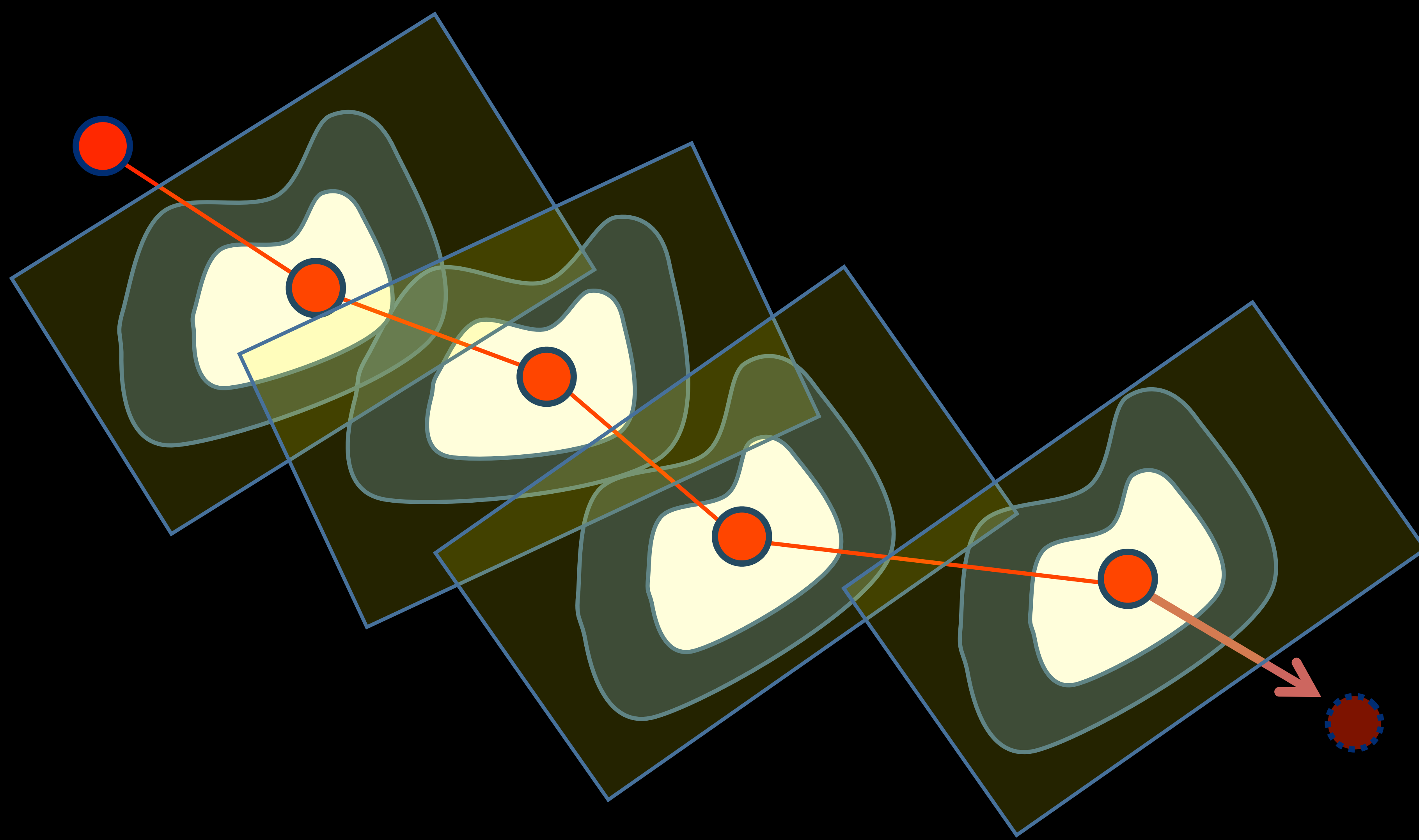
Reconstruction

- Active Ribbons [Vazquez 09]

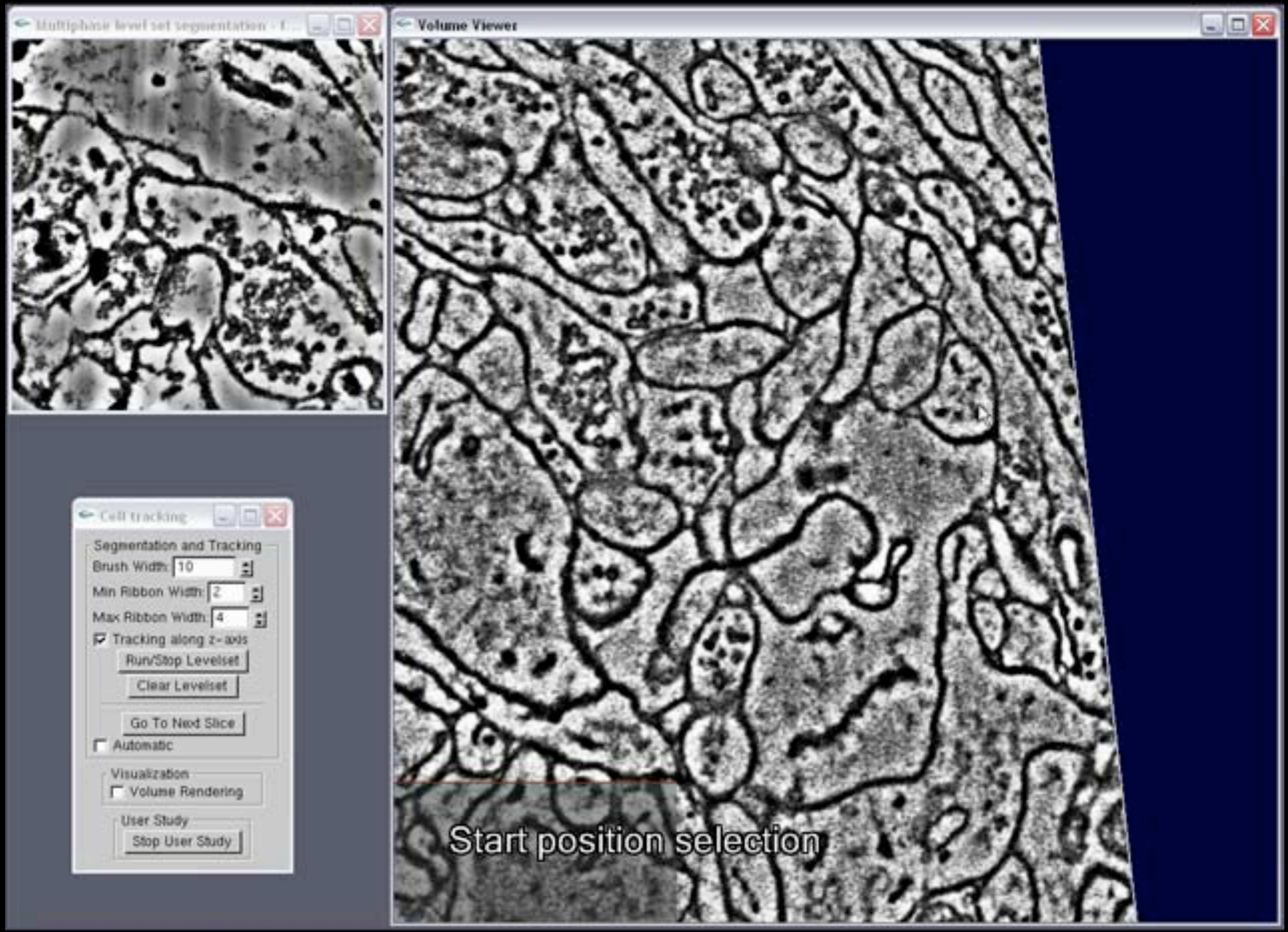
Section 1

GPU Processing

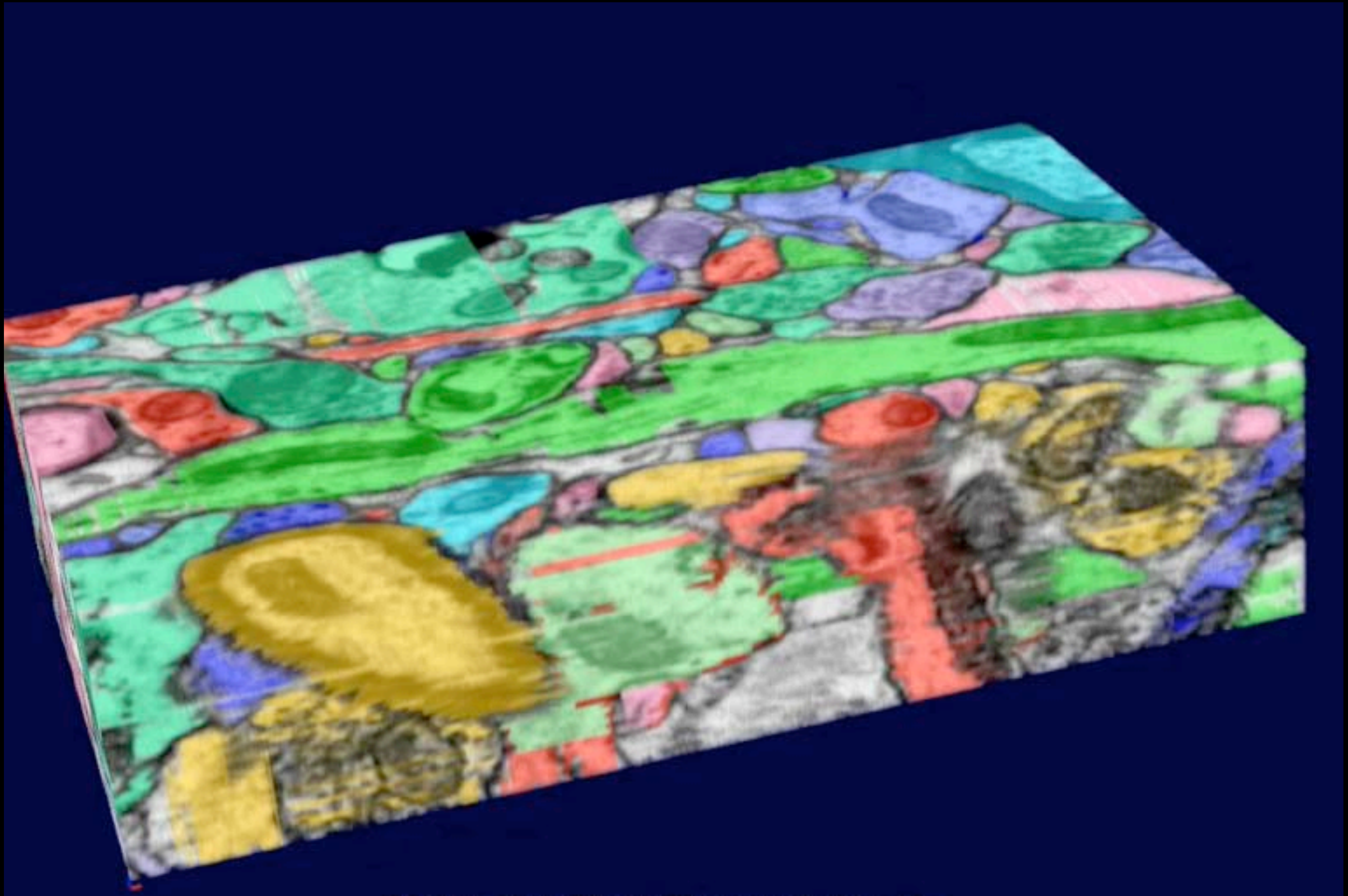
- Active Ribbons on GPUs: 23x speedup



NeuroTrace [Jeong 09]



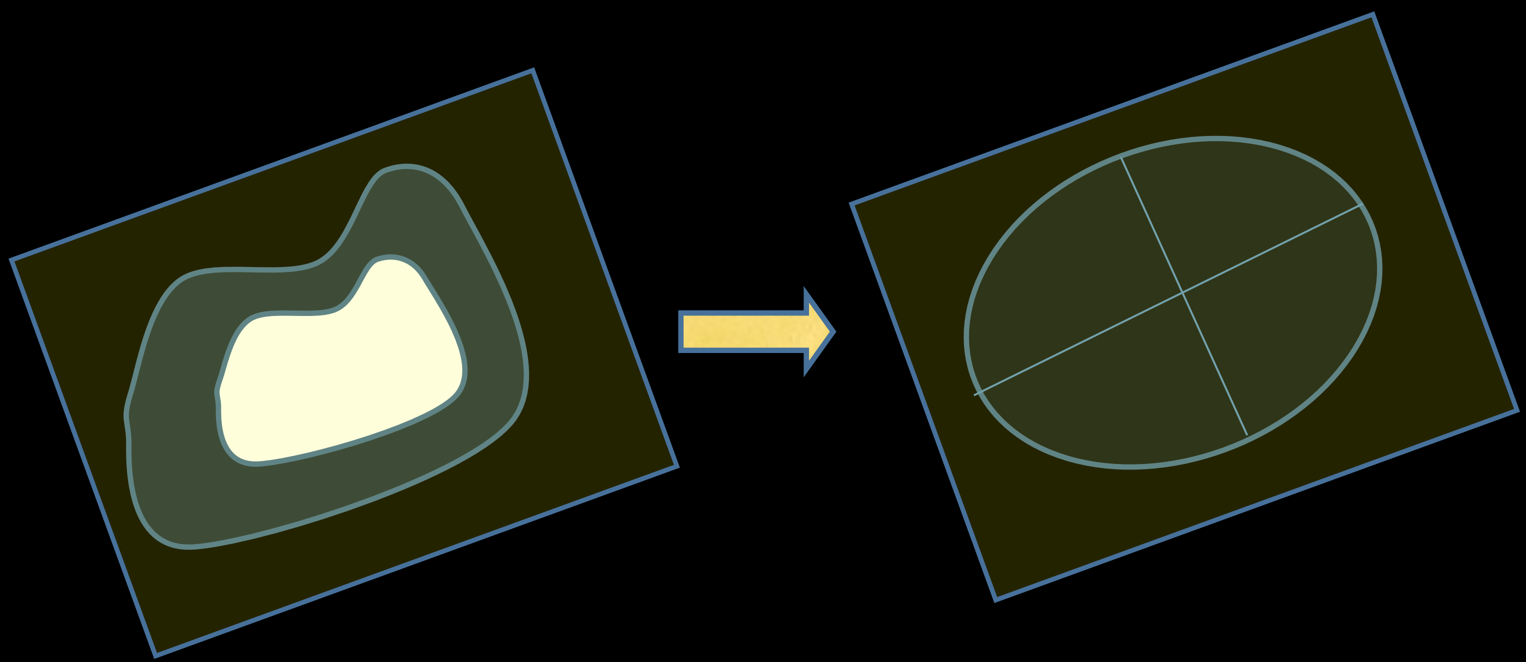
Visualization



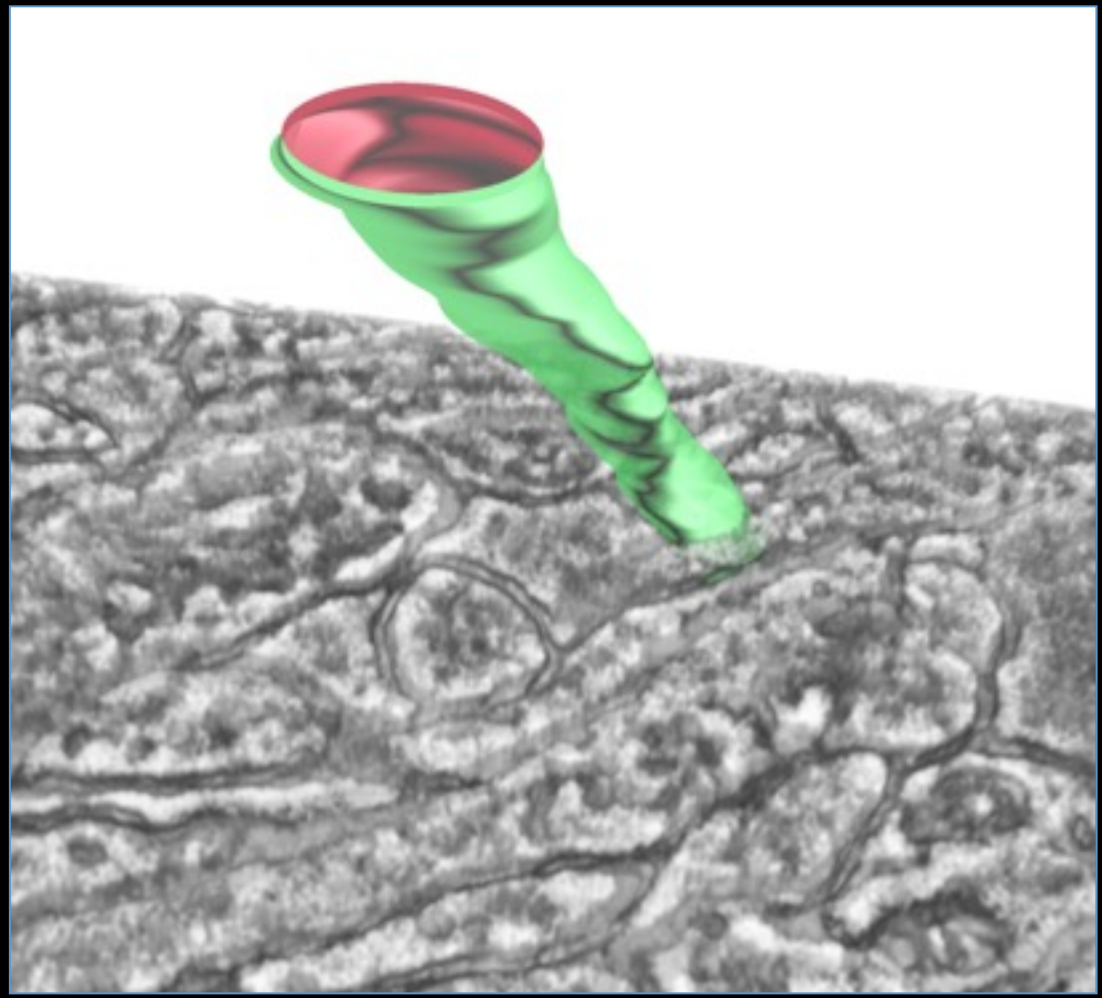
Volume rendring of segmented axons

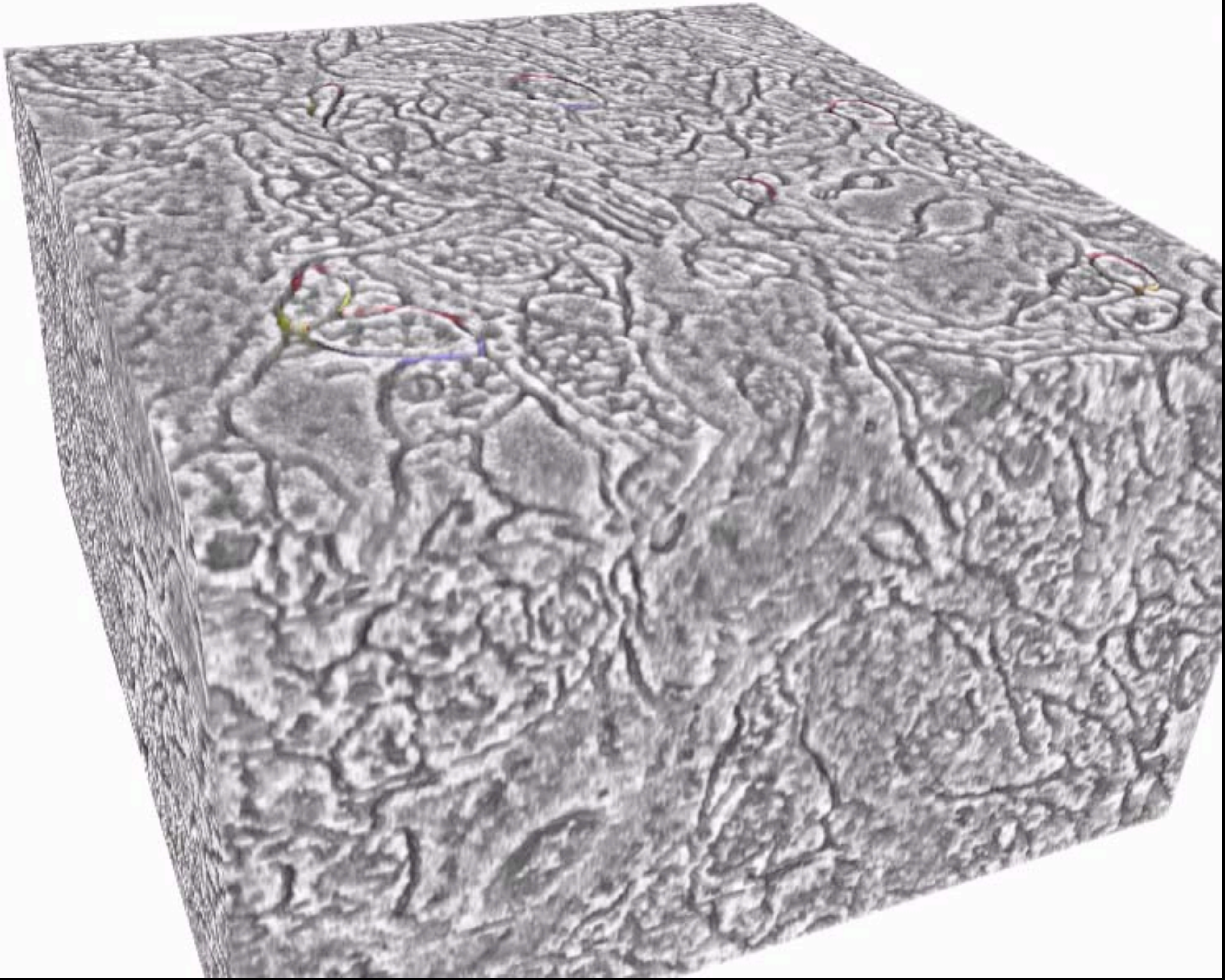
Visualization

- Elliptical approximation of ribbons

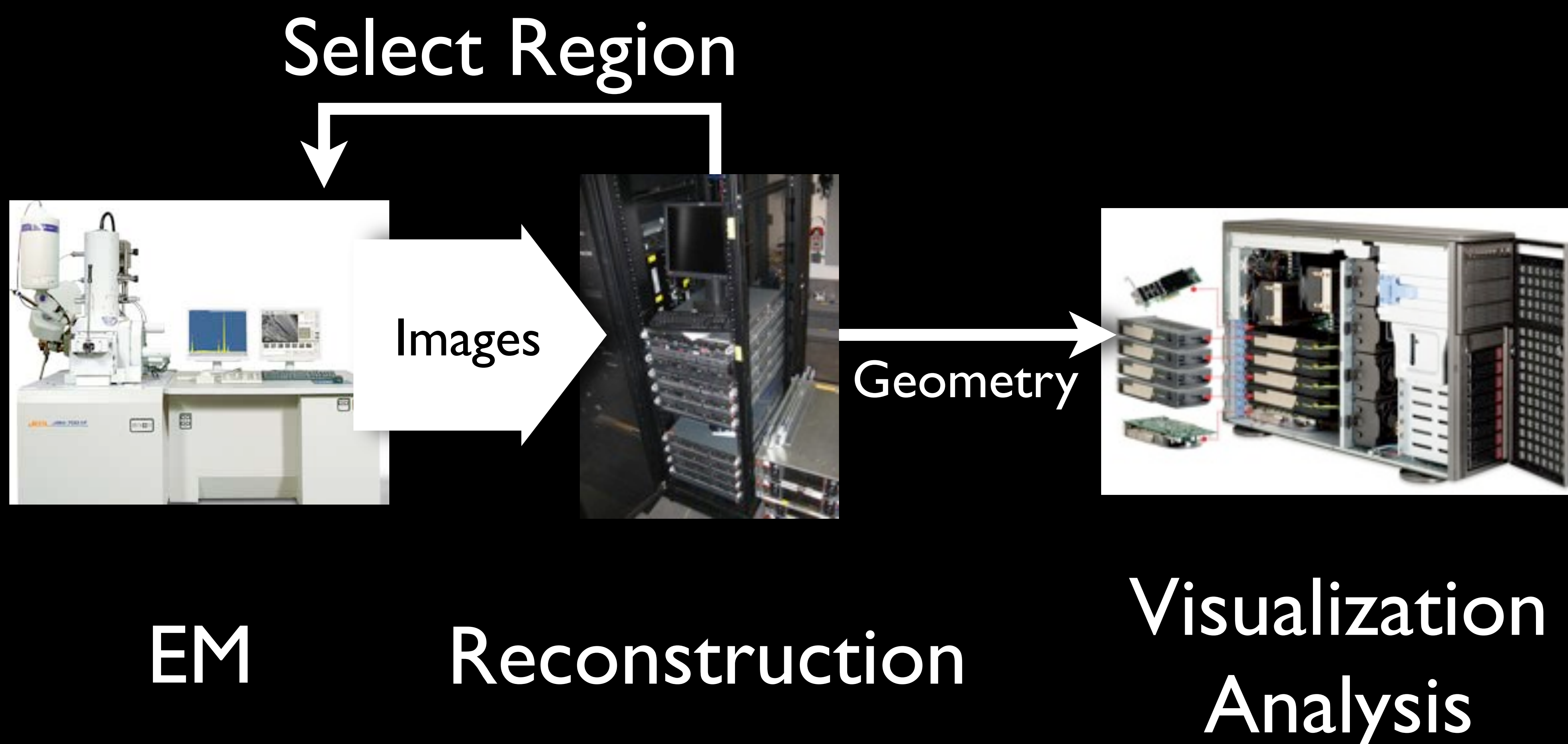


Compression ratio = ~ 1000

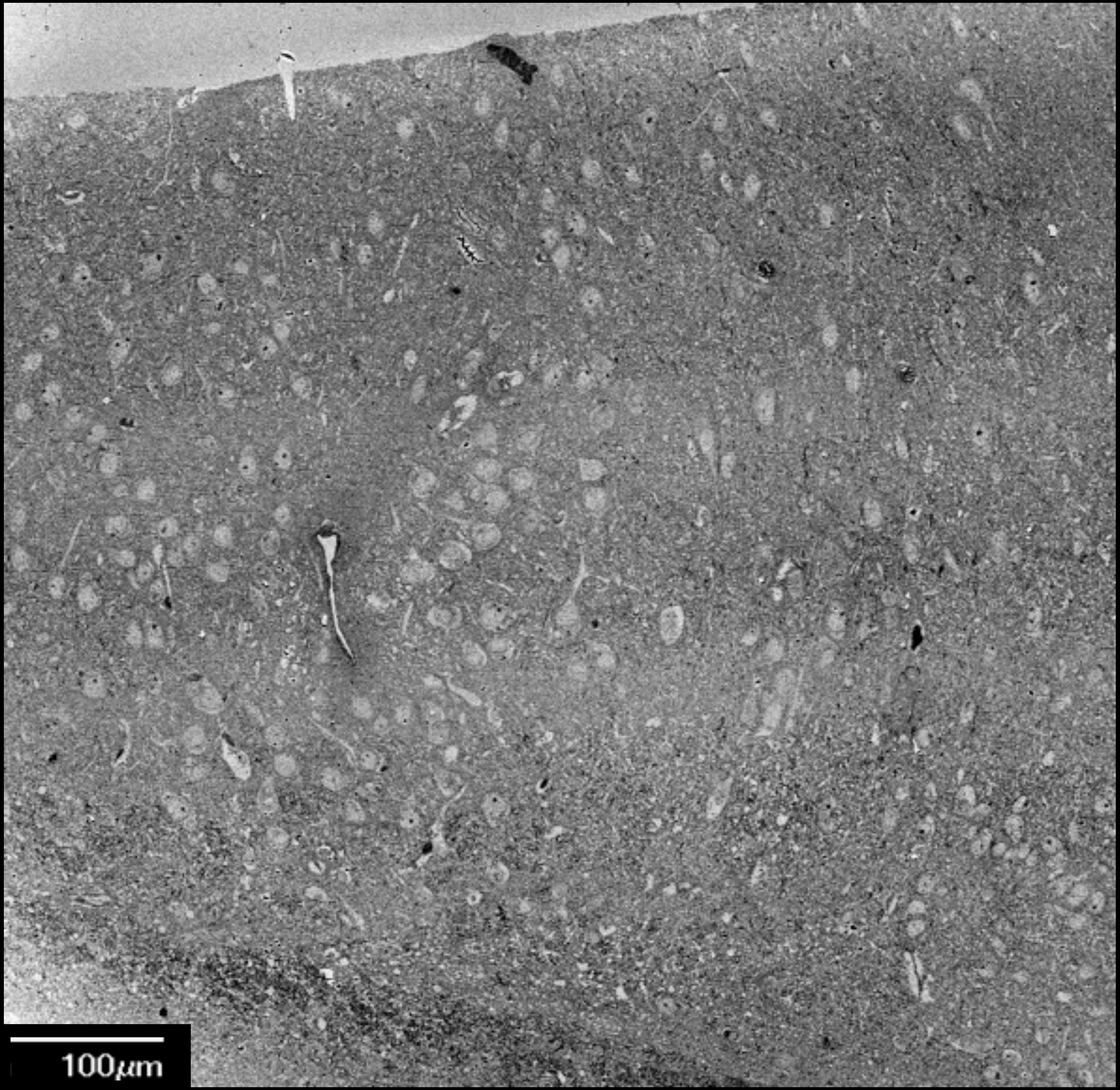




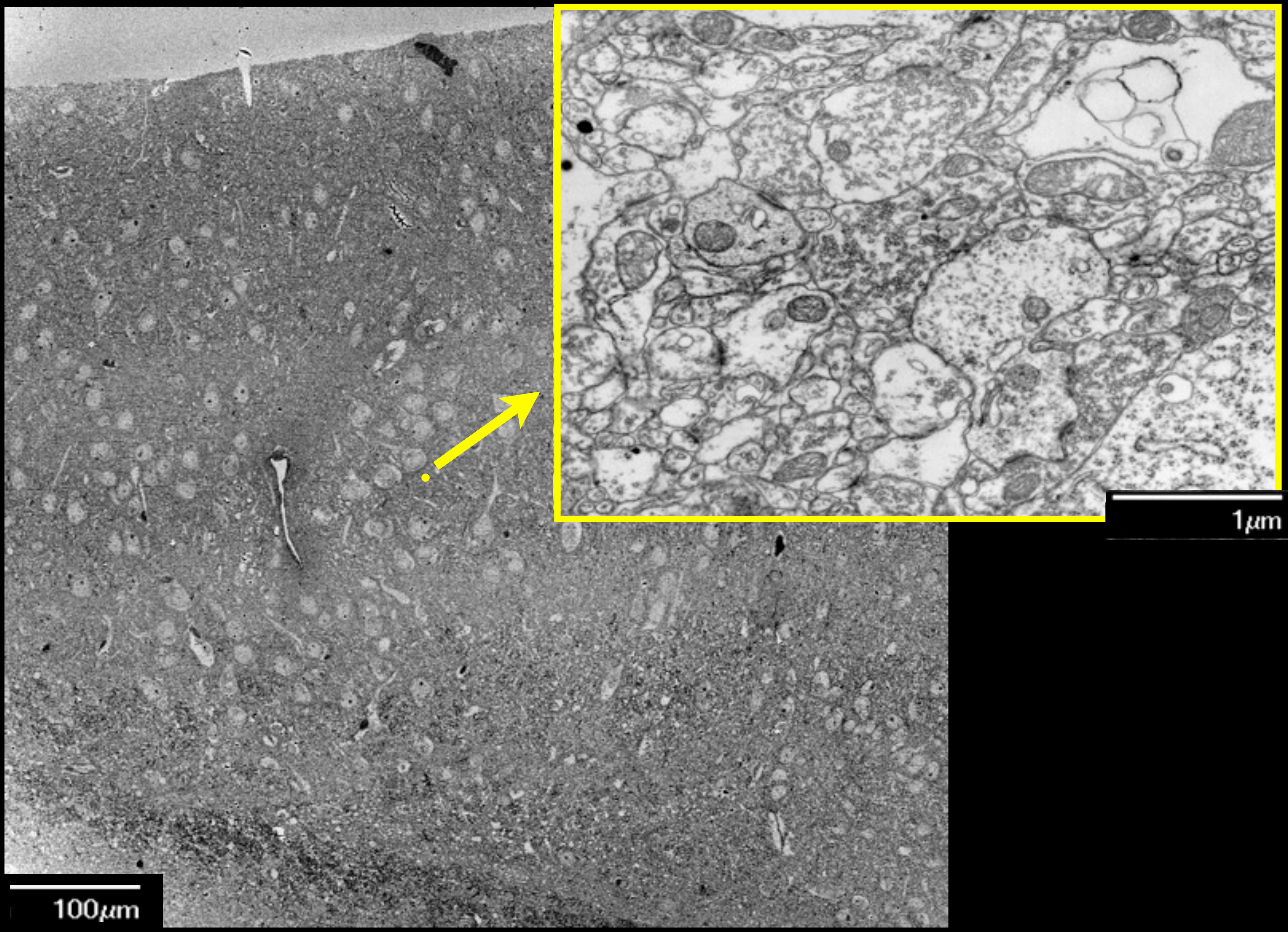
High-Throughput Neuroscience



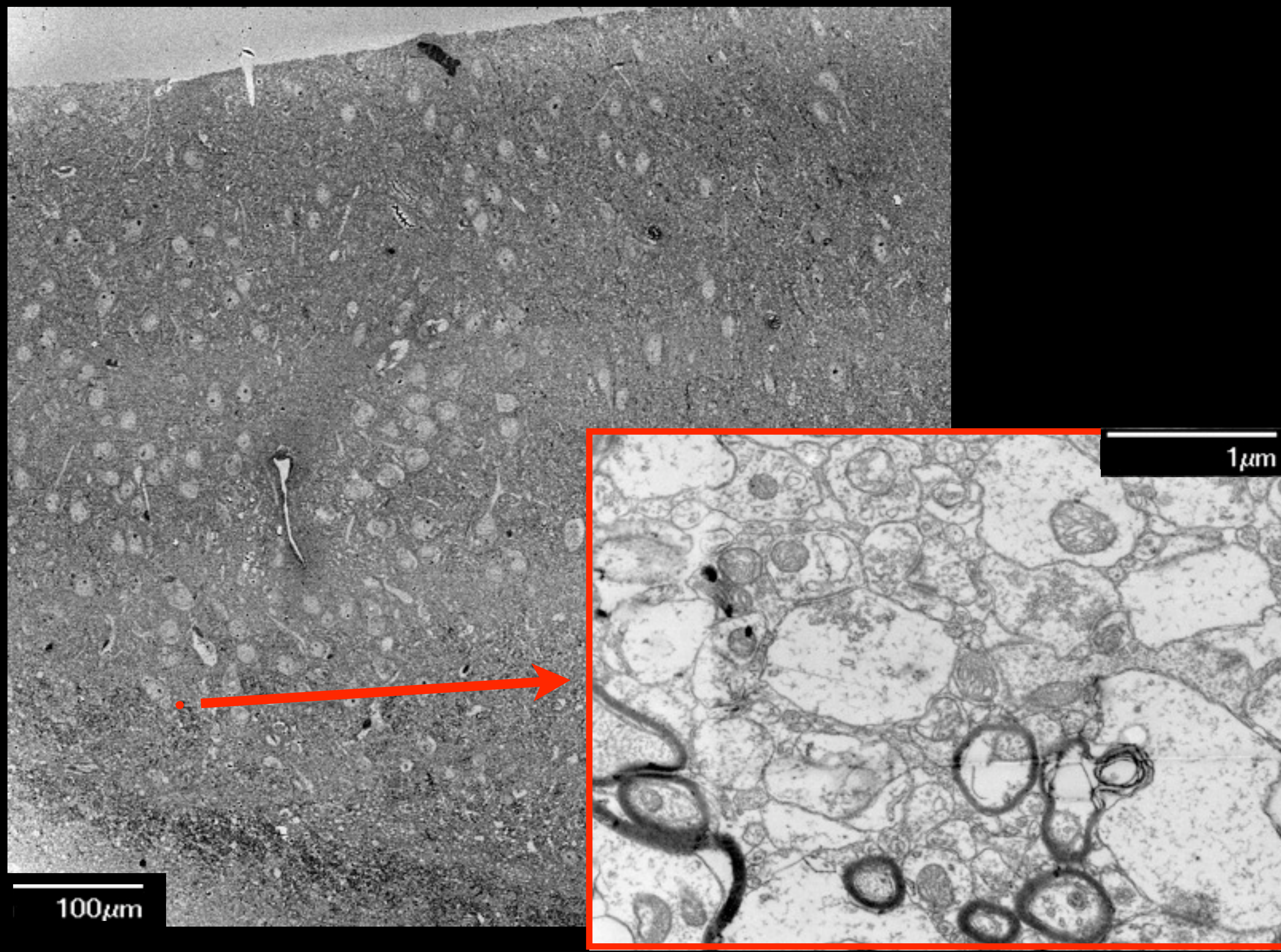
Multi-Scale Imaging



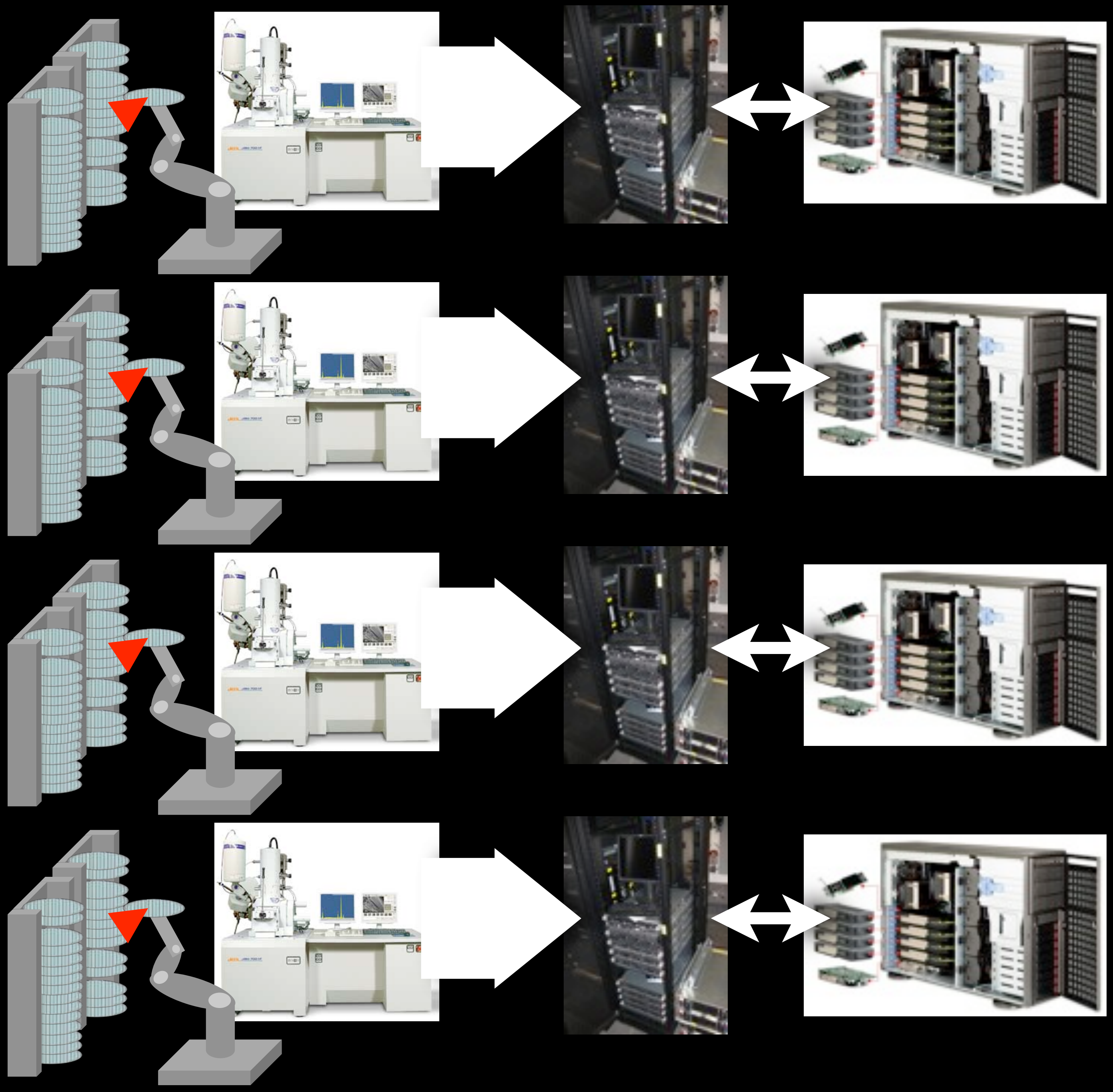
Multi-Scale Imaging



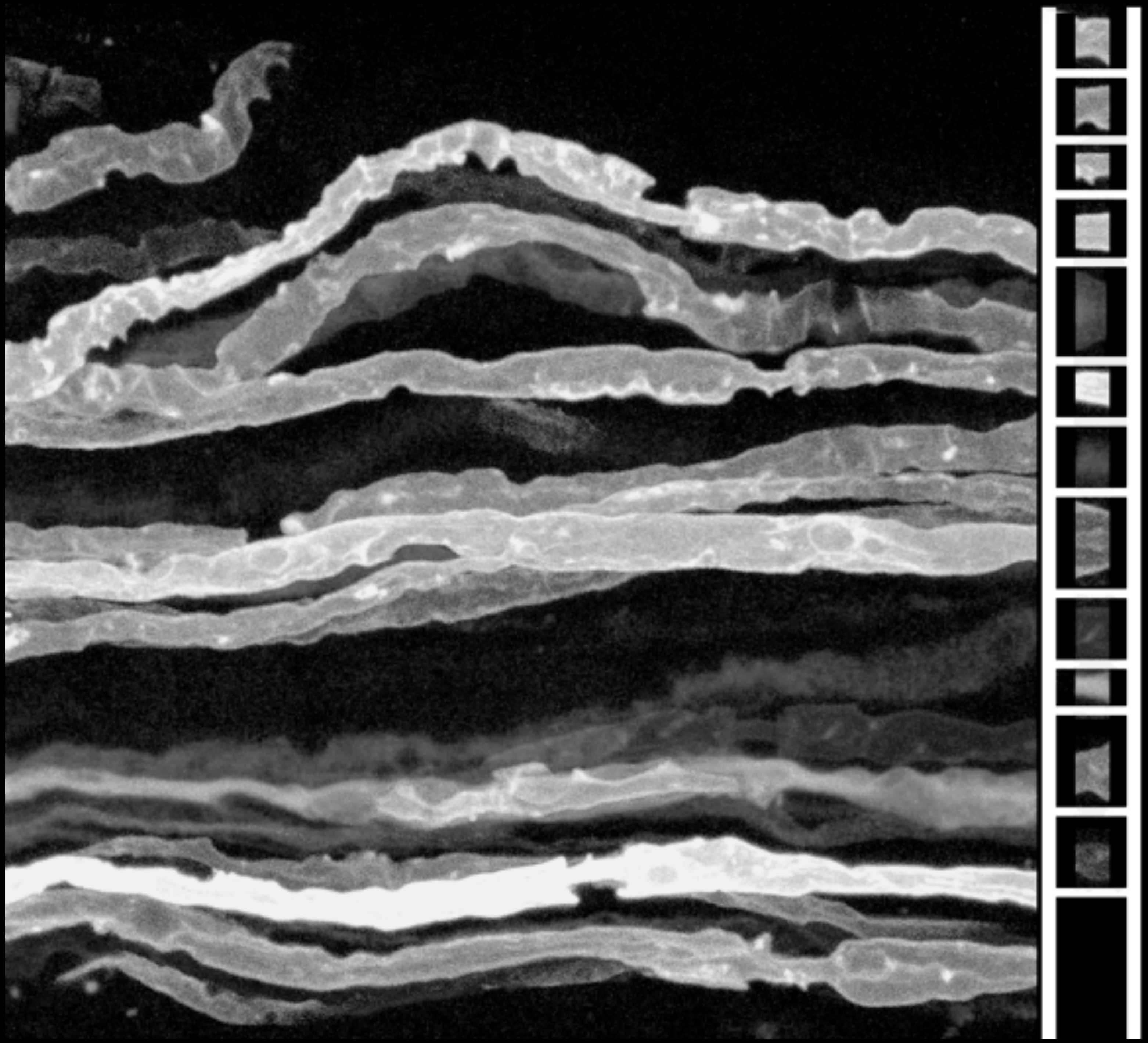
Multi-Scale Imaging



Scalable

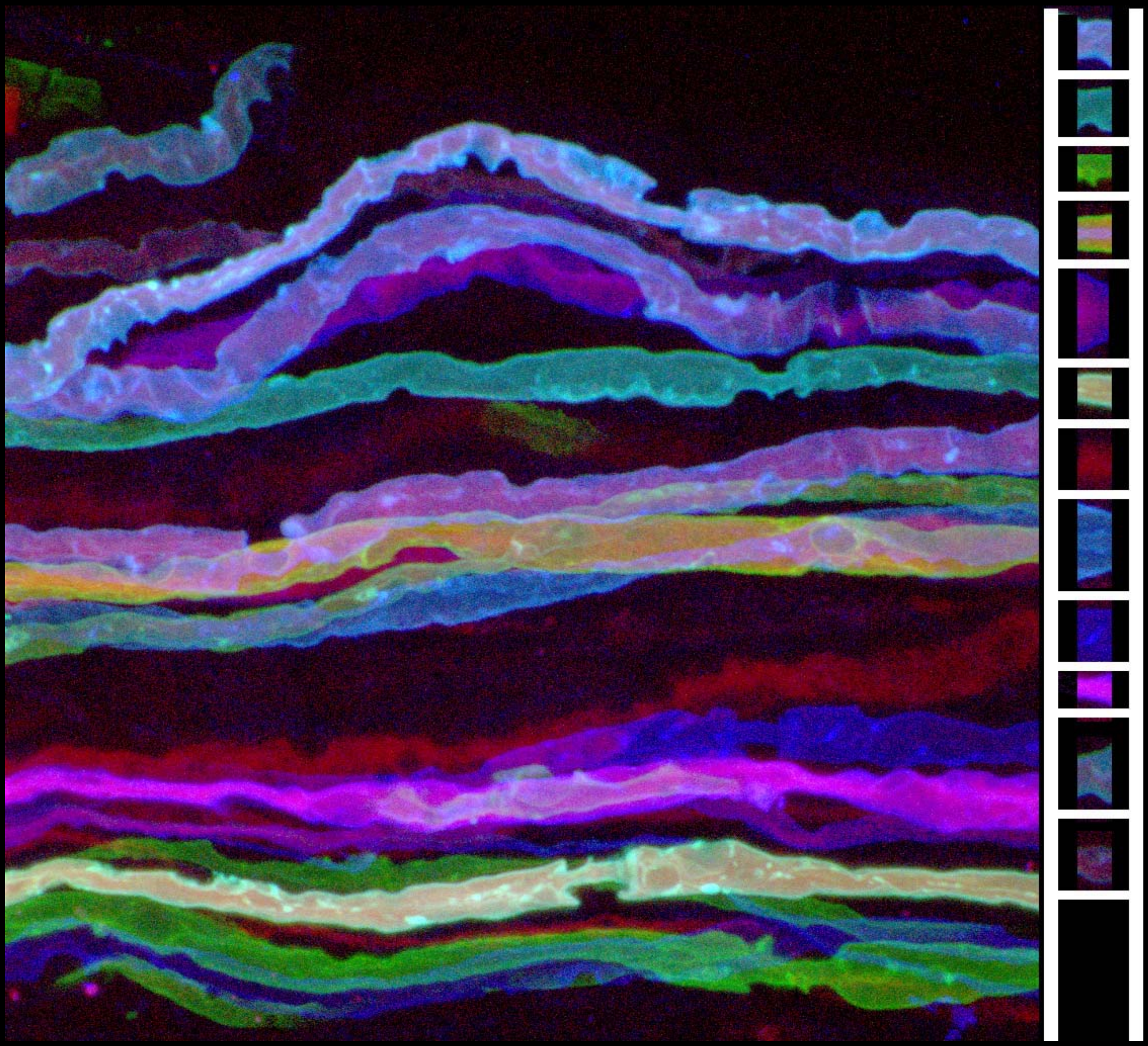


The Future

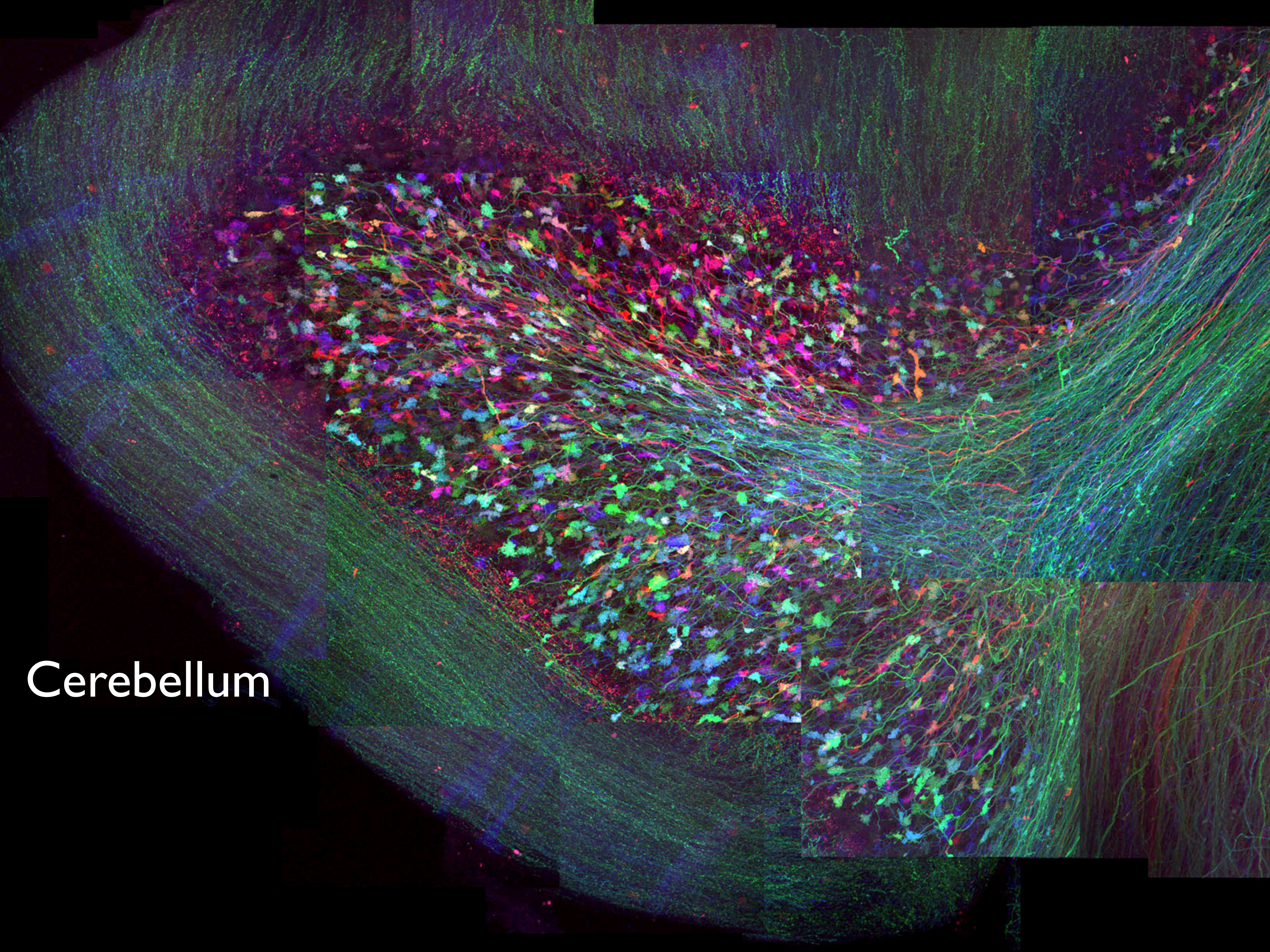


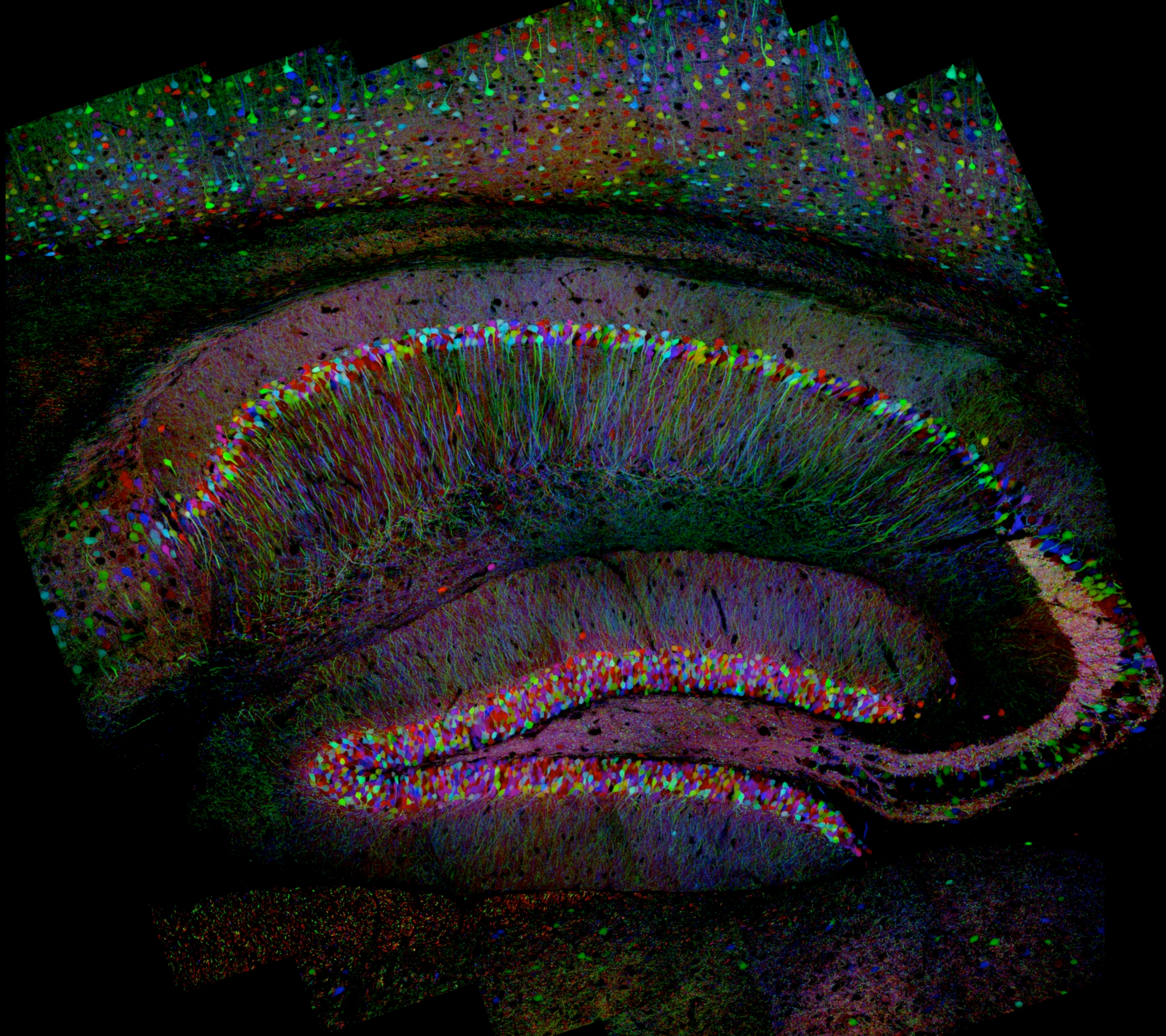
J. Livet

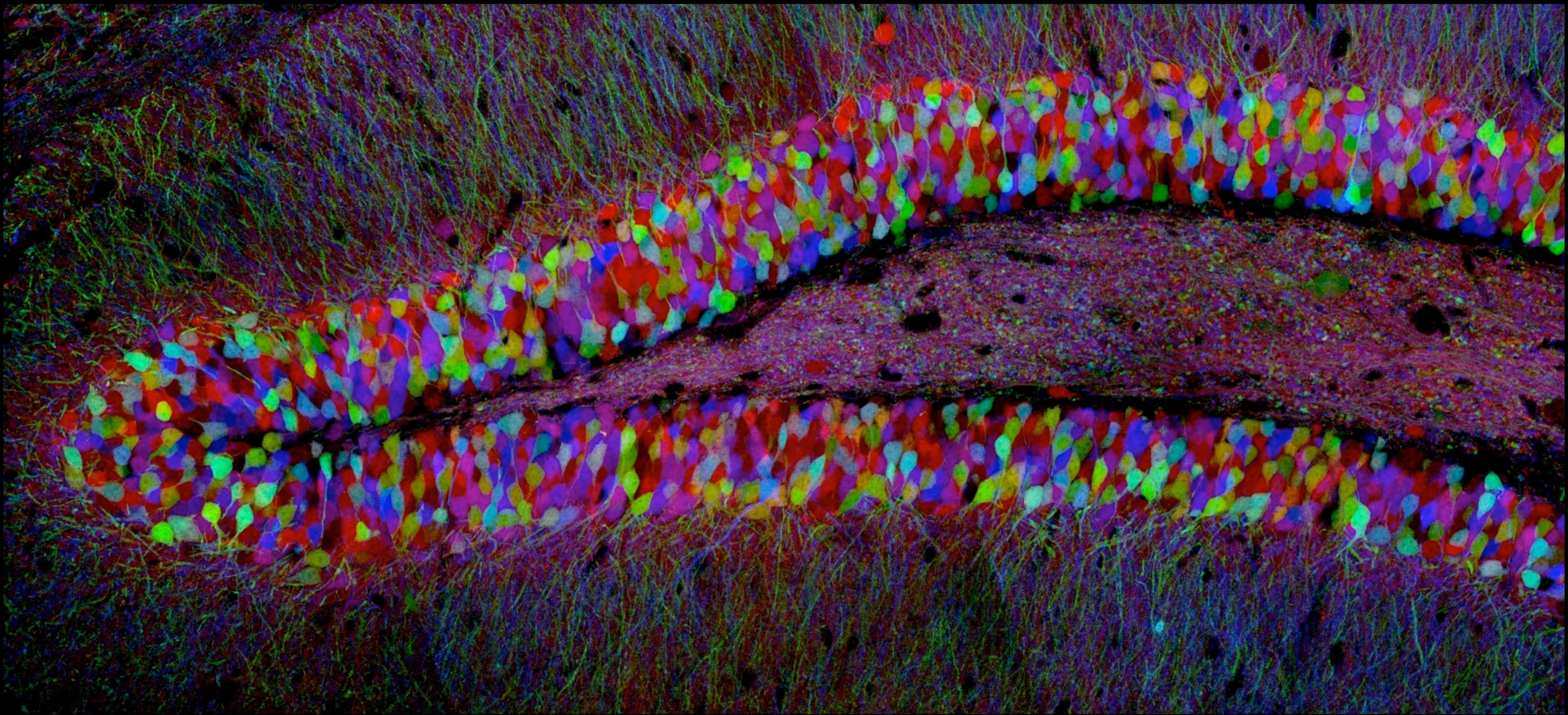
Brainbow



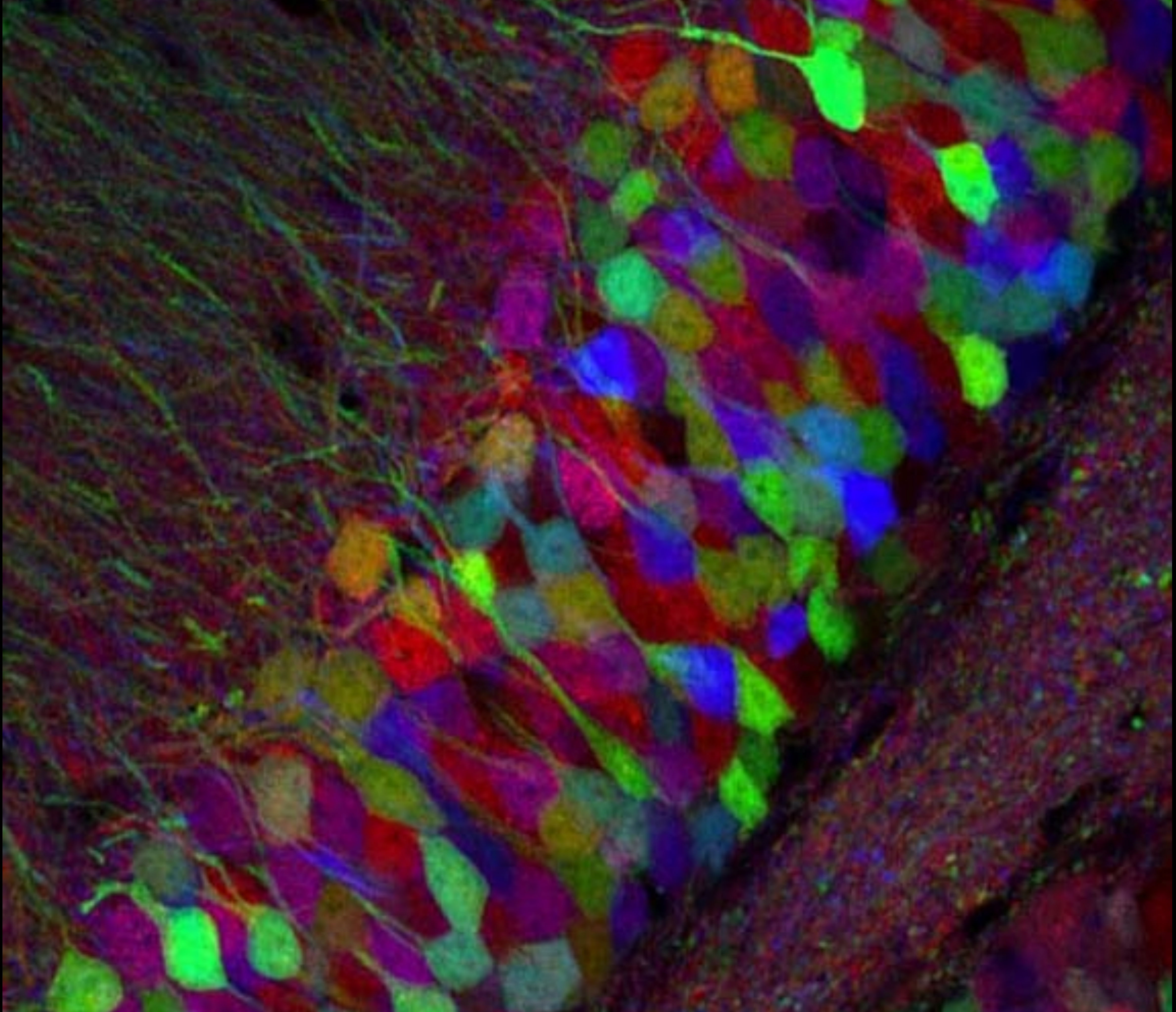
J. Livet


Cerebellum





Hippocampus




Convergent evolution?

More Information

Won-Ki Jeong
Reconstructing the Brain: Extracting Neural Circuitry with CUDA and MPI
Session Id#1075
Friday 4 pm Empire

The MWA

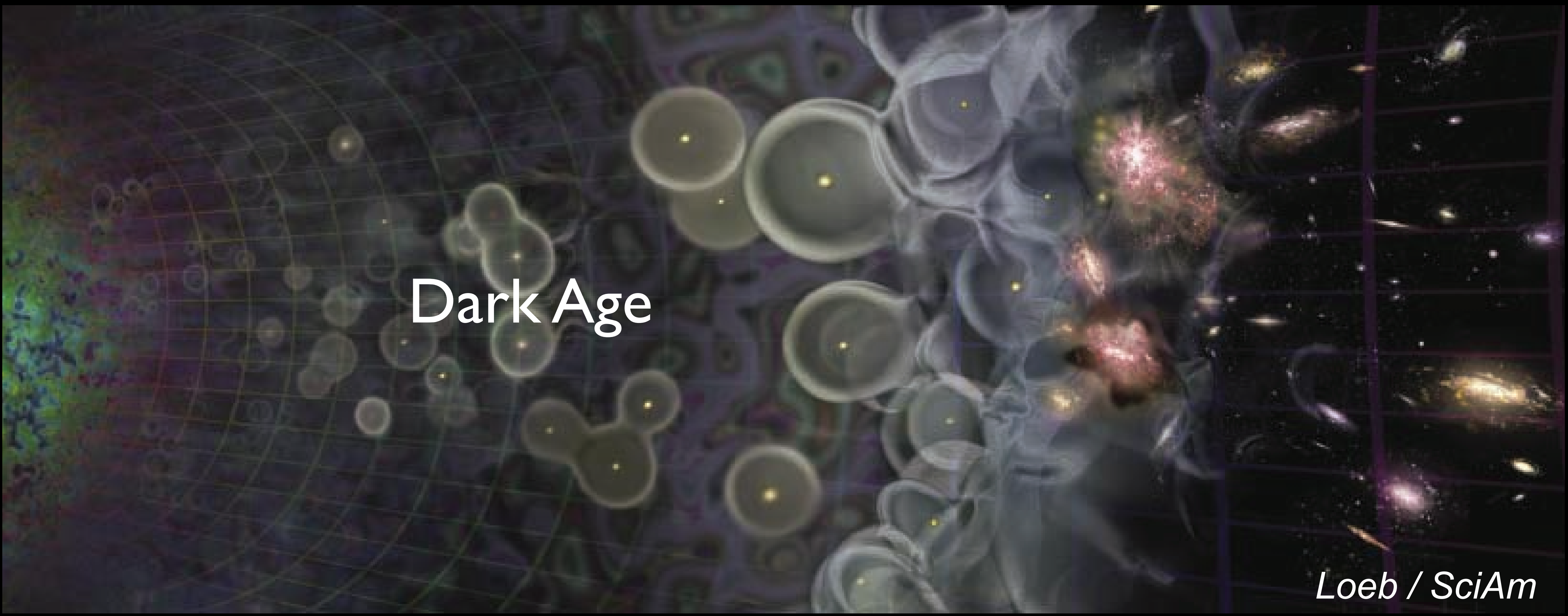
Outback Supercomputing

Collaborators

- Harvard Center for Astrophysics
  - Lincoln Greenhill
  - Daniel Mitchell
  - Stephen Ord
  - Randall Wayth
- SEAS
  - Kevin Dale, Richard Edgar
  - Hanspeter Pfister

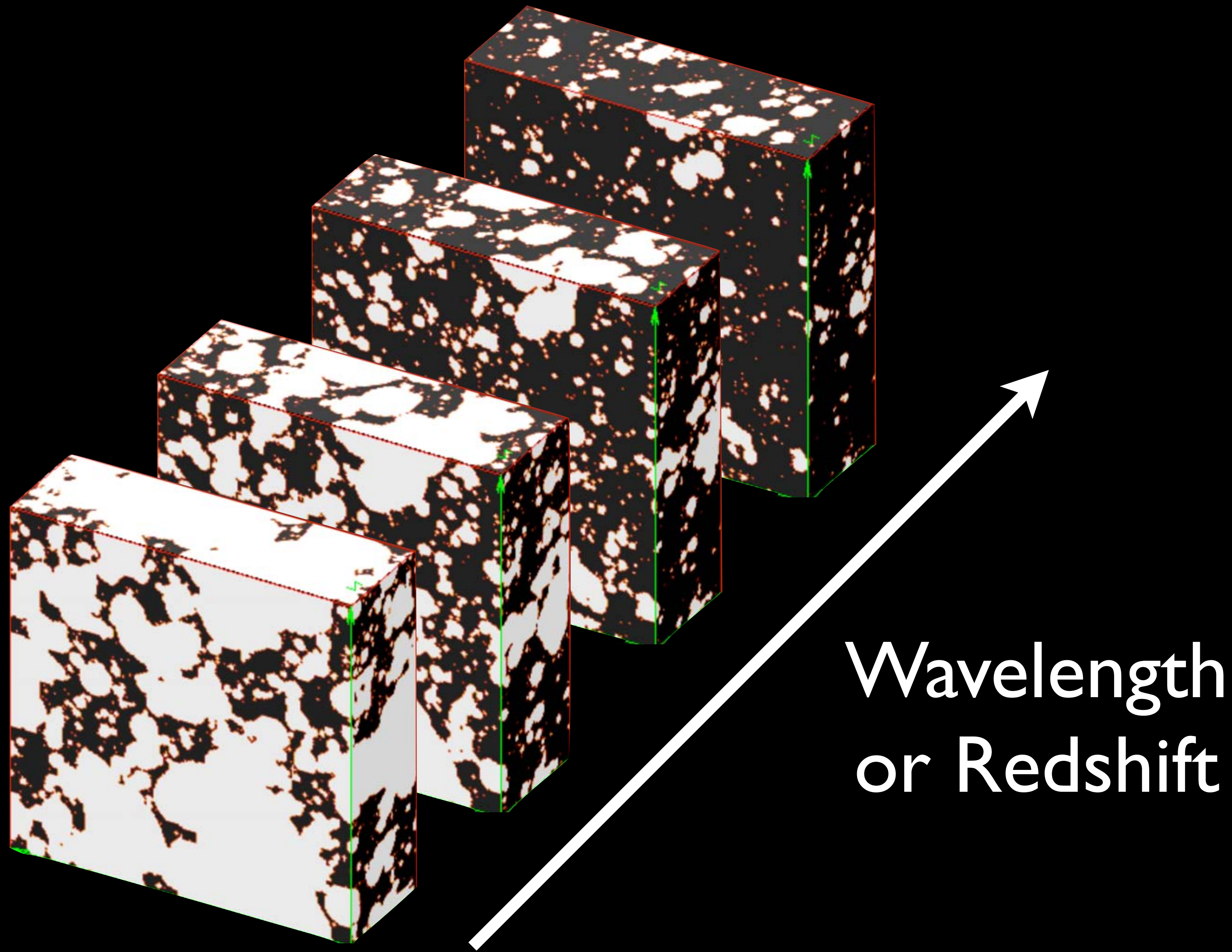
The Scientific Challenge

- What happened through the 1 billion years of the universe's dark ages?

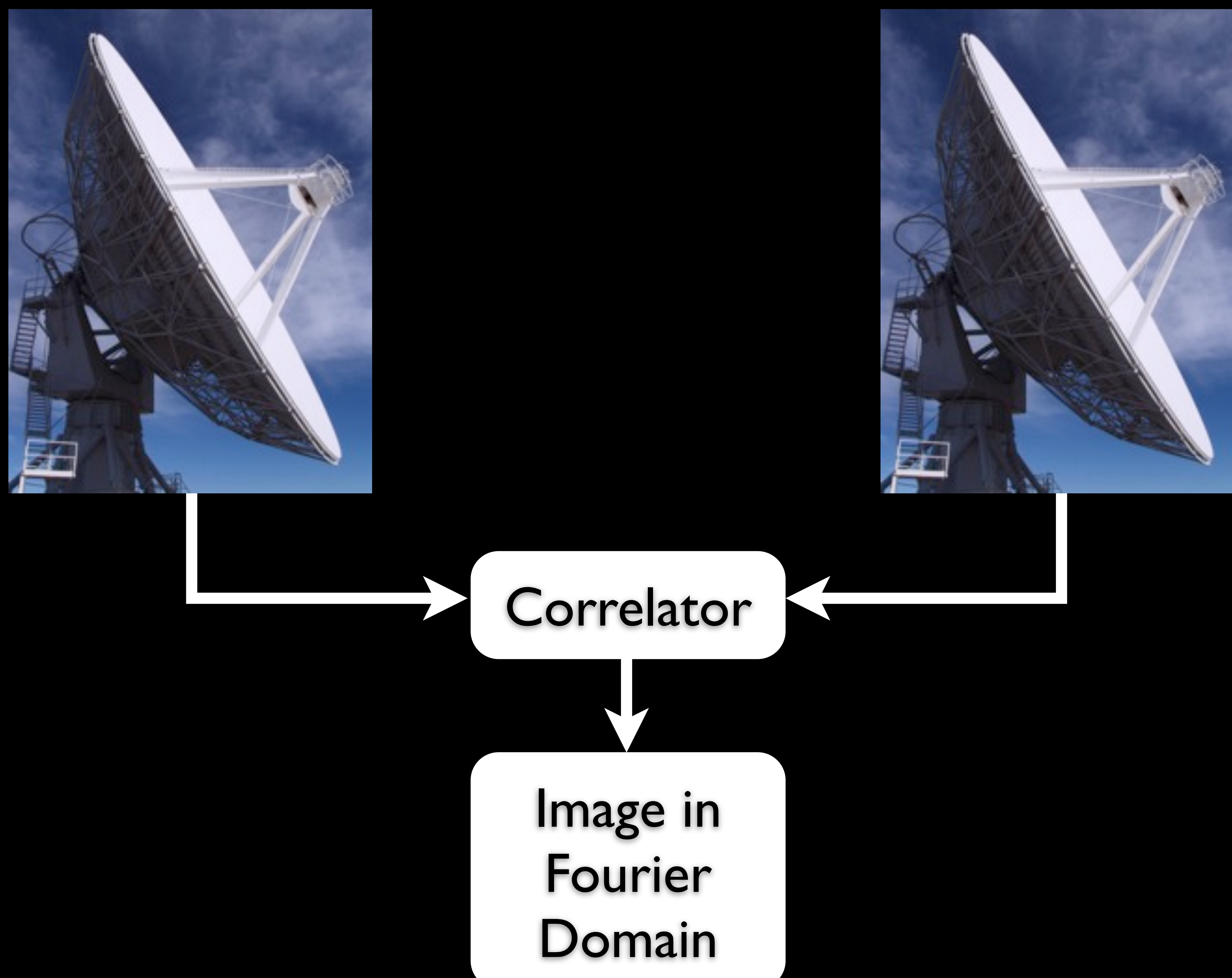


~300,000 ~1 bio

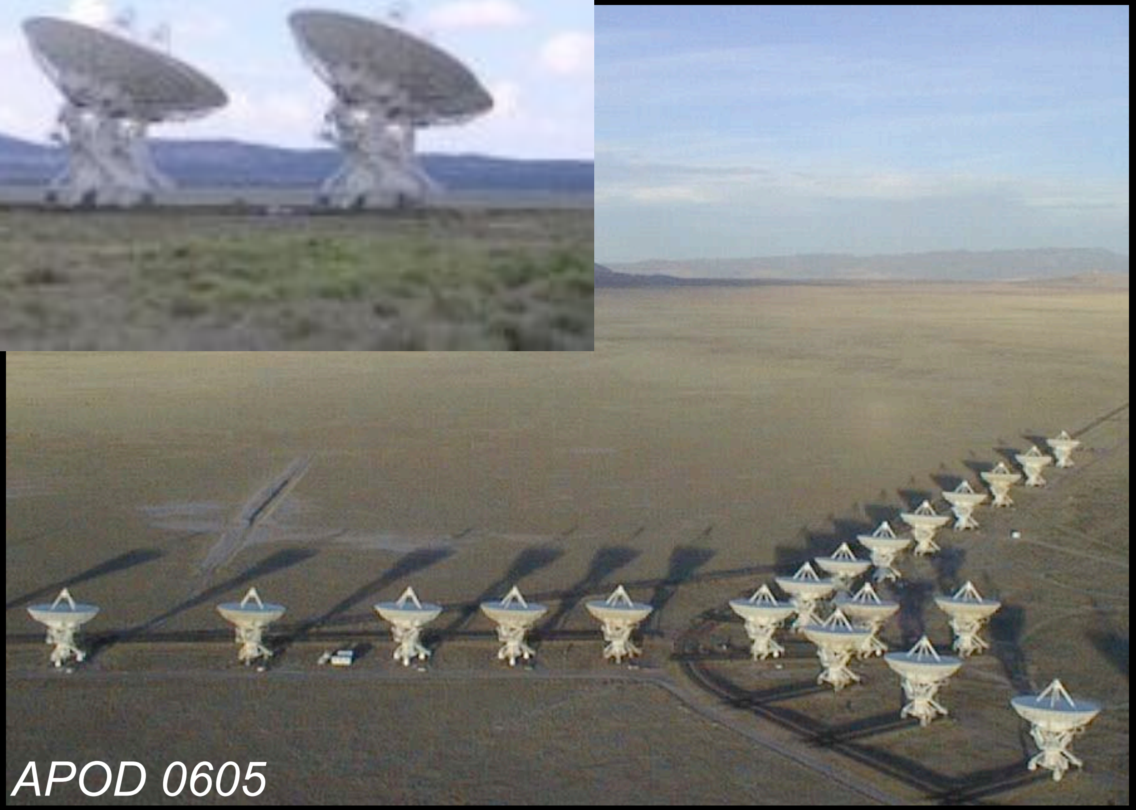
3D Tomography



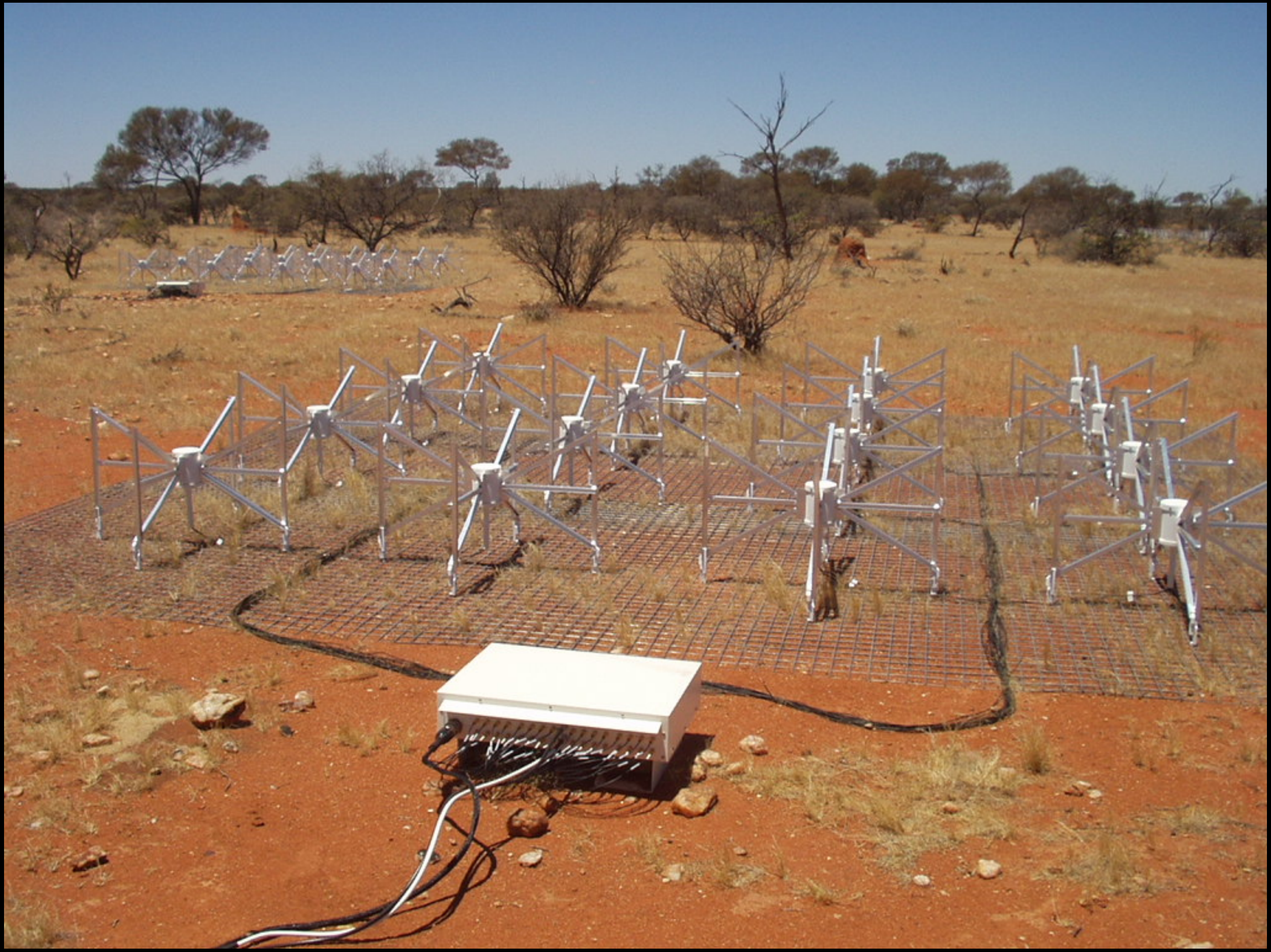
Radio Interferometry



From this...

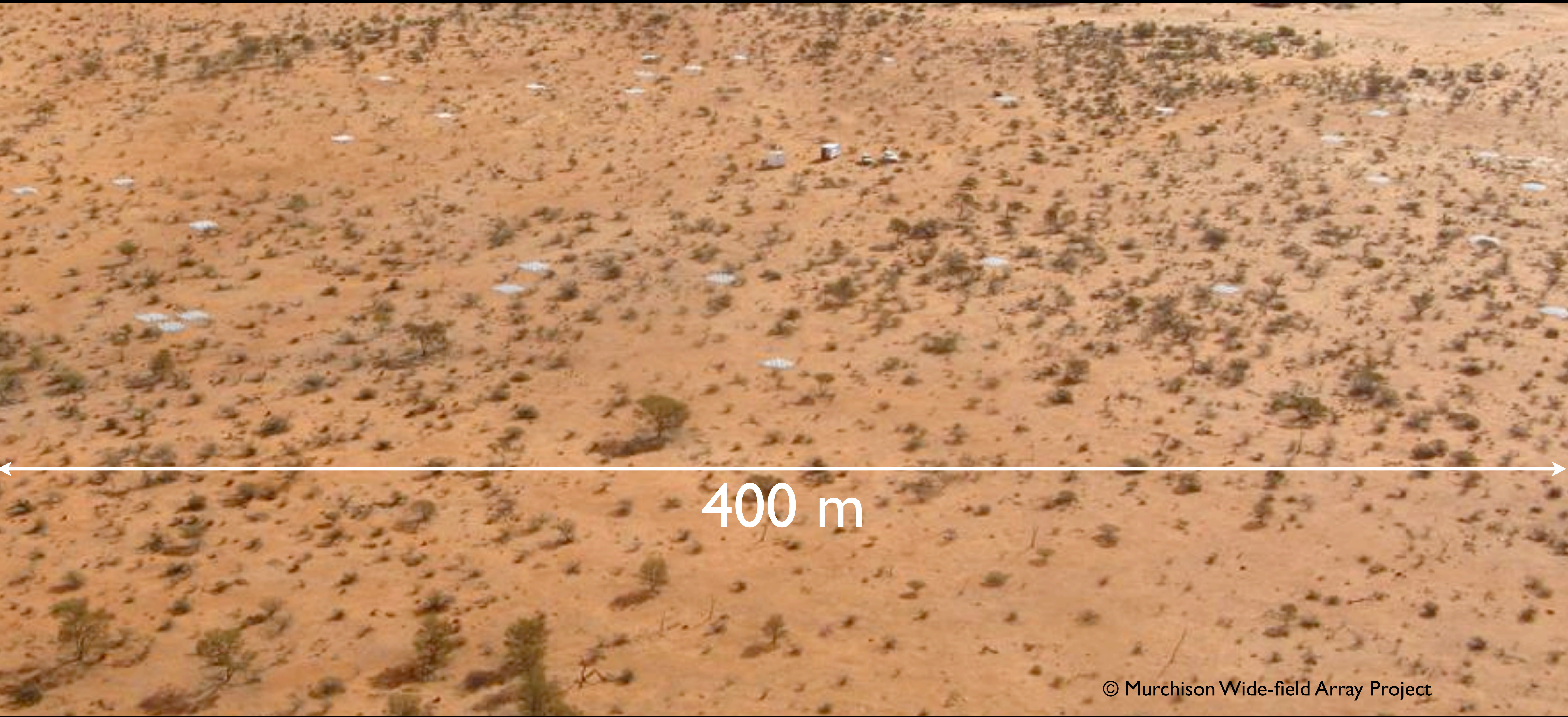


...to this



MWA

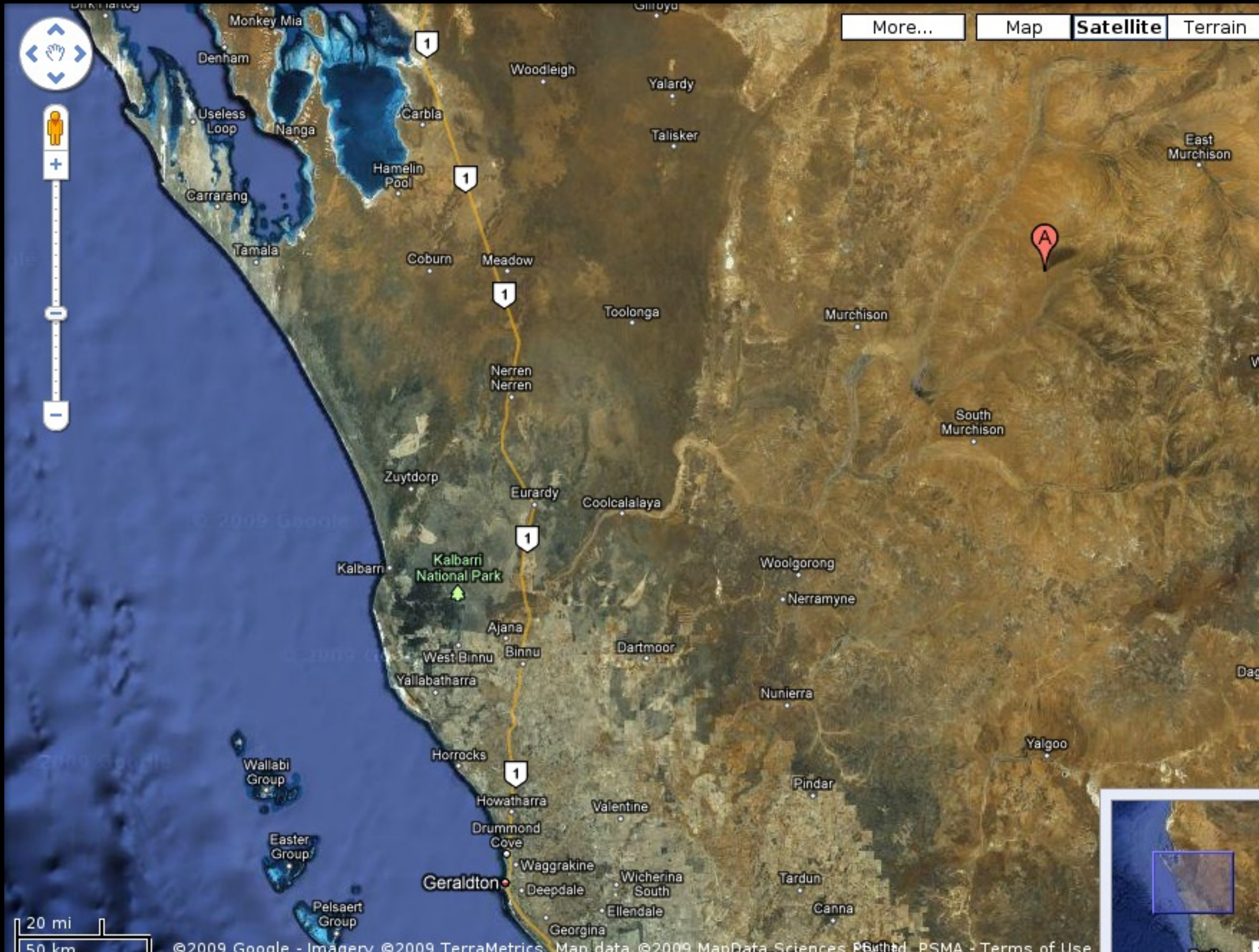
- 32 antenna prototype
- Eventually 512 antennas on 1 km^2




Nowhere (Middle of)
300 km
THANK YOU FOR BEING RADIO QUIET

Outback Computing

- Max. ambient on site: 50° C / 122° F



More...
Map
Satellite
Terrain
Monkey Mia
Denham
Useless Loop
Nanga
Carbla
Woodleigh
Yalardy
Talisker
Hamelin Pool
Carrarang
Tamala
Coburn
Meadow
Toolonga
Murchison
East Murchison
A
Nerren Nerren
South Murchison
Zuytdorp
Eurardy
Coolcalalaya
Kalbarri
Kalbarri National Park
Woolgorong
Nerramyne
Ajana
Binnu
West Binnu
Dartmoor
Yallabatharra
Nunierra
Yalgoo
Horrocks
Pindar
Wallabi Group
Howatharra
Valentine
Drummond Cove
Easter Group
Waggrakine
Geraldton
Deepdale
Wicherina South
Tardun
Ellendale
Canna
Pelsaert Group
Georgina
Perth
20 mi
50 km
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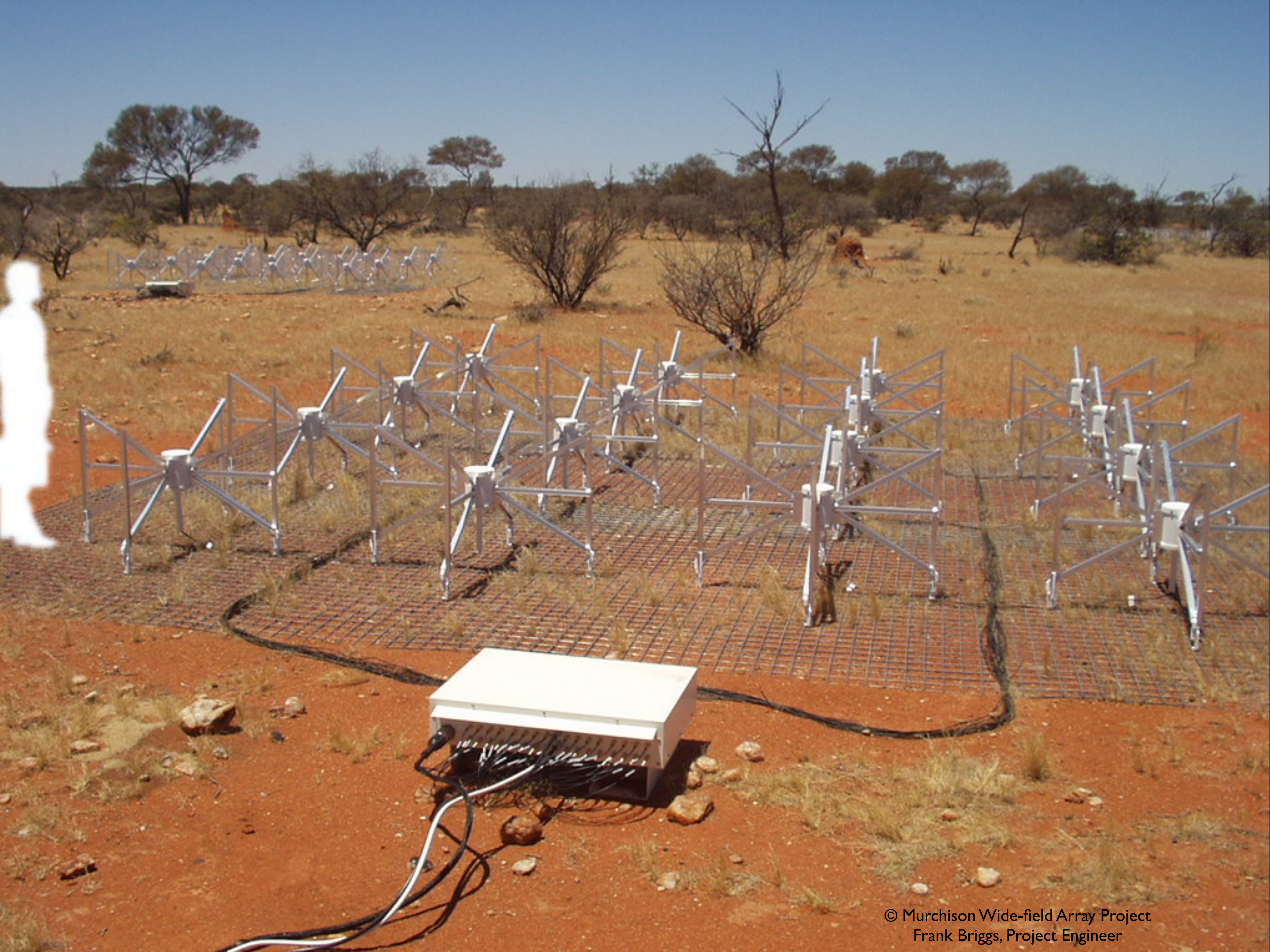
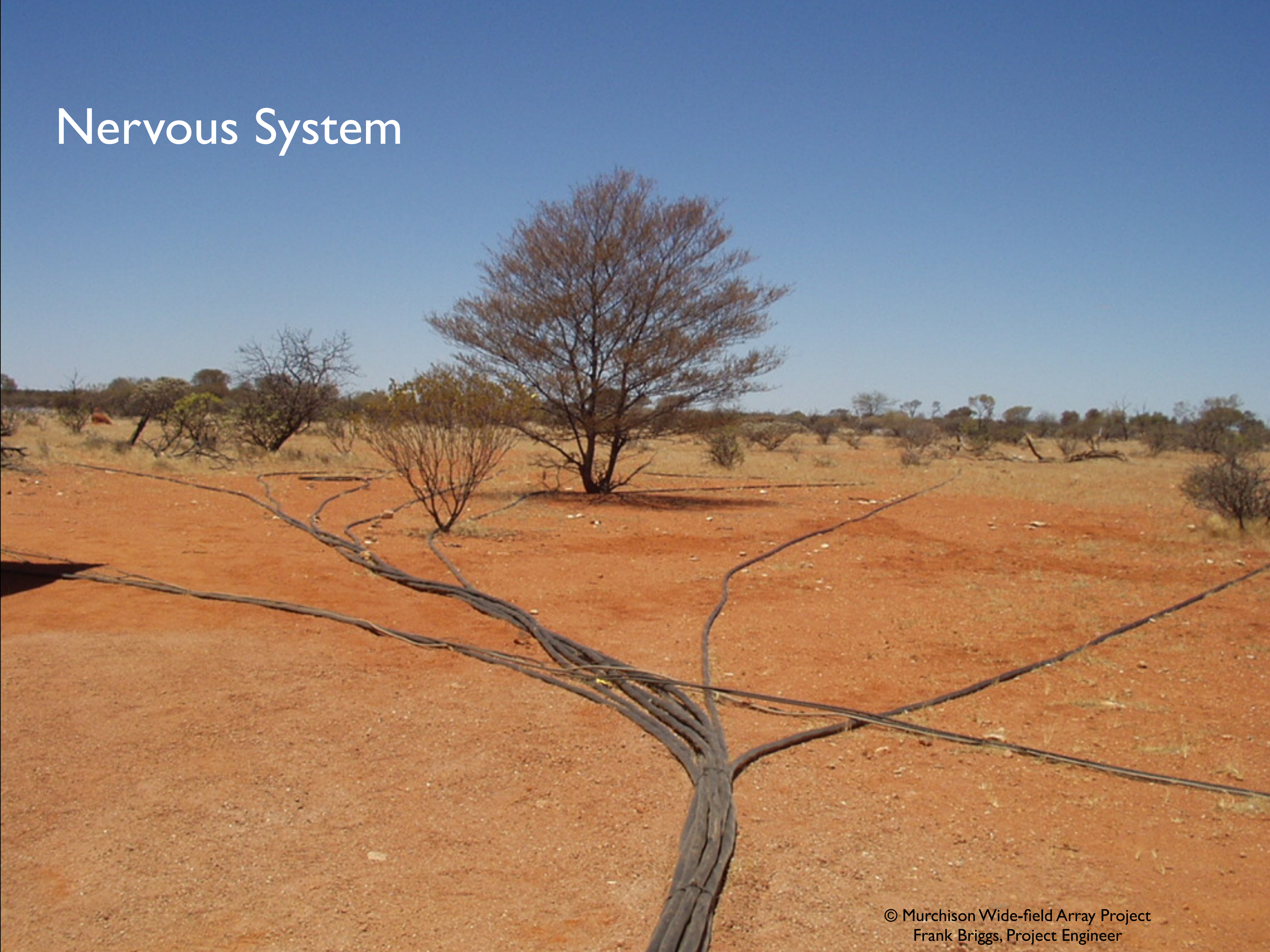
324 Mullewa Carnarvon Rd, Murchison, WA, Australia
Address is approximate
Mullewa Carnarvon Rd


© Murchison Wide-field Array Project
Frank Briggs, Project Engineer


Nervous System
© Murchison Wide-field Array Project
Frank Briggs, Project Engineer

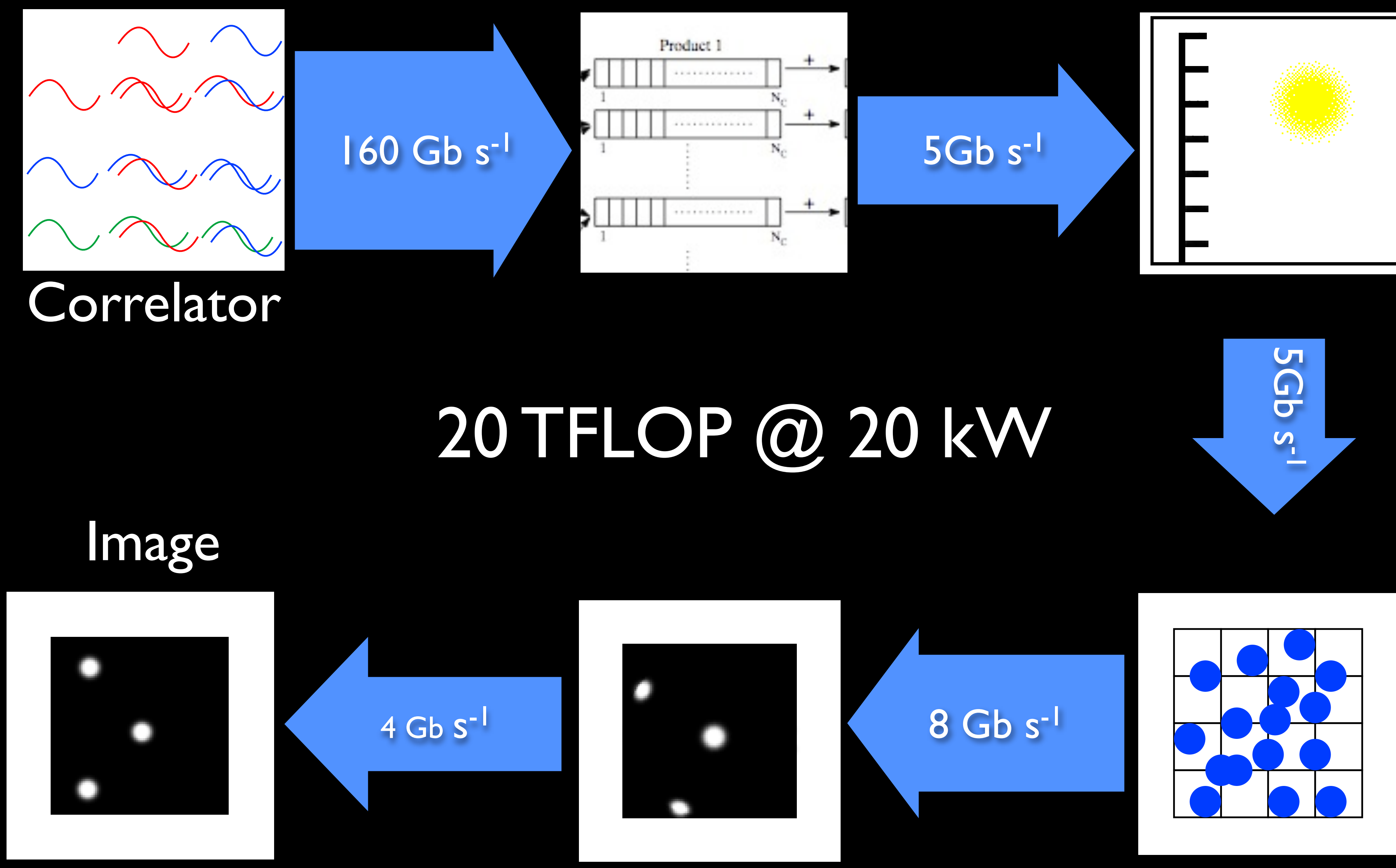
Supercomputing Center

Who is the GPU expert?

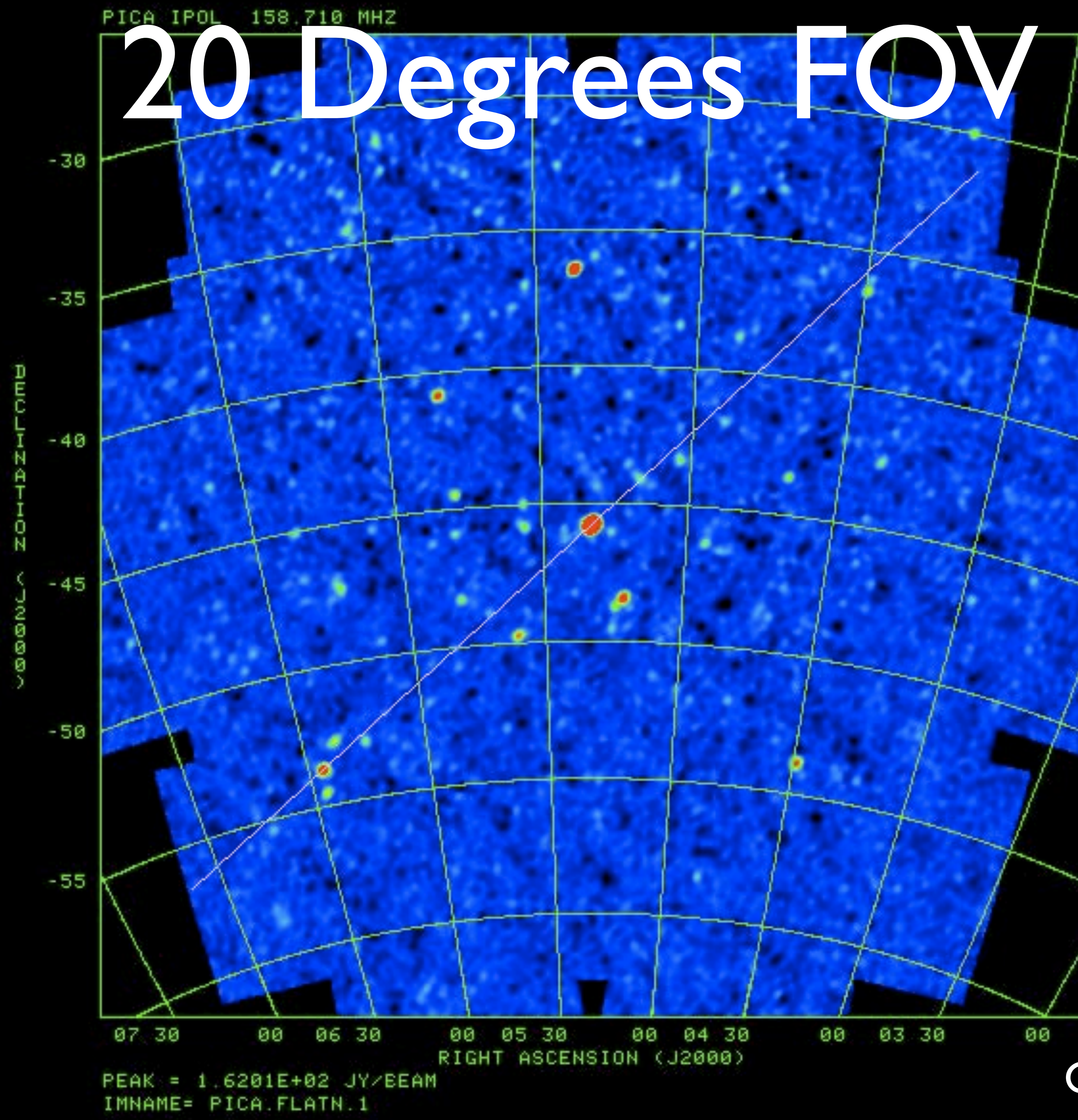
Who is the GPU expert?

Life Support

MWA Pipeline

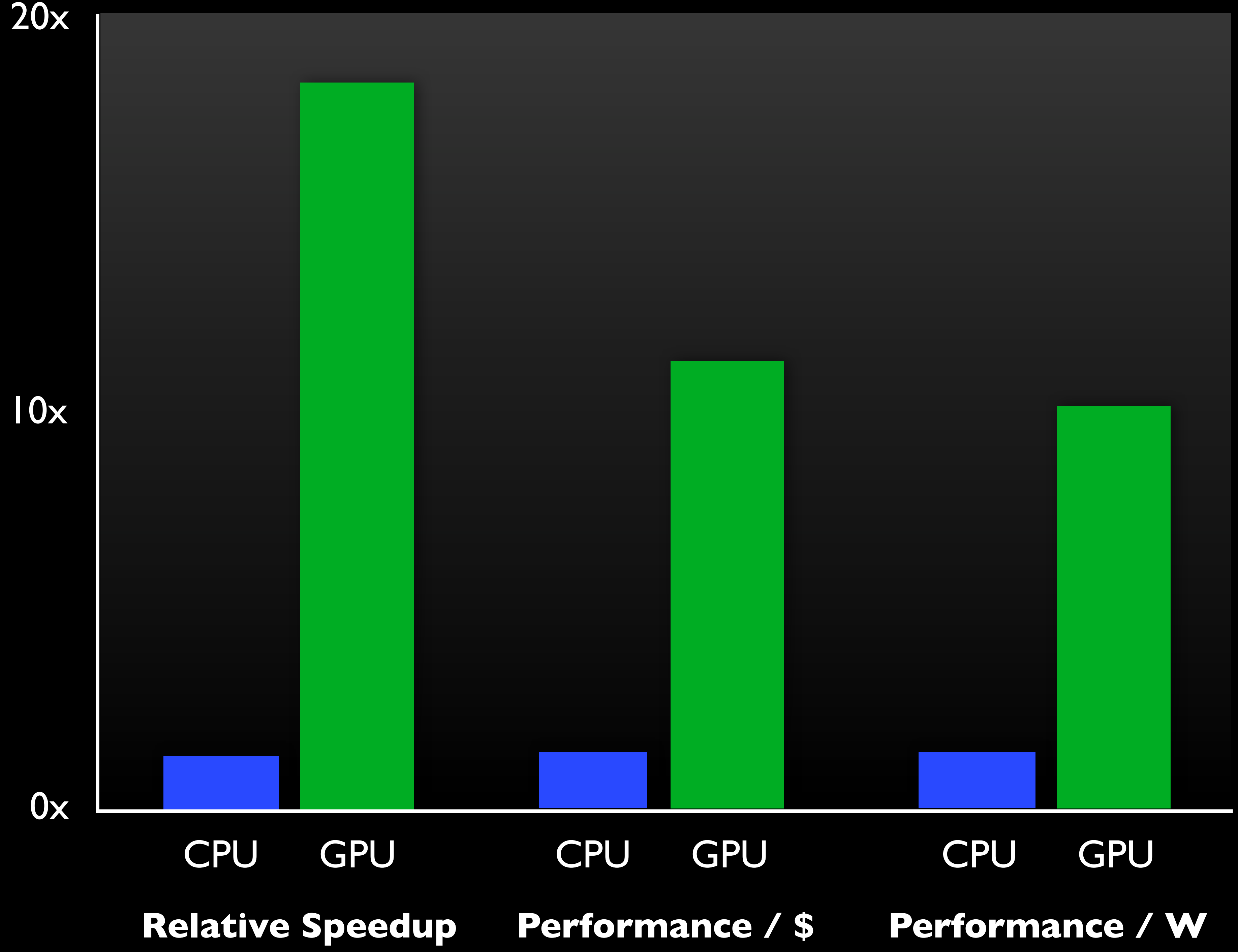


20 Degrees FOV

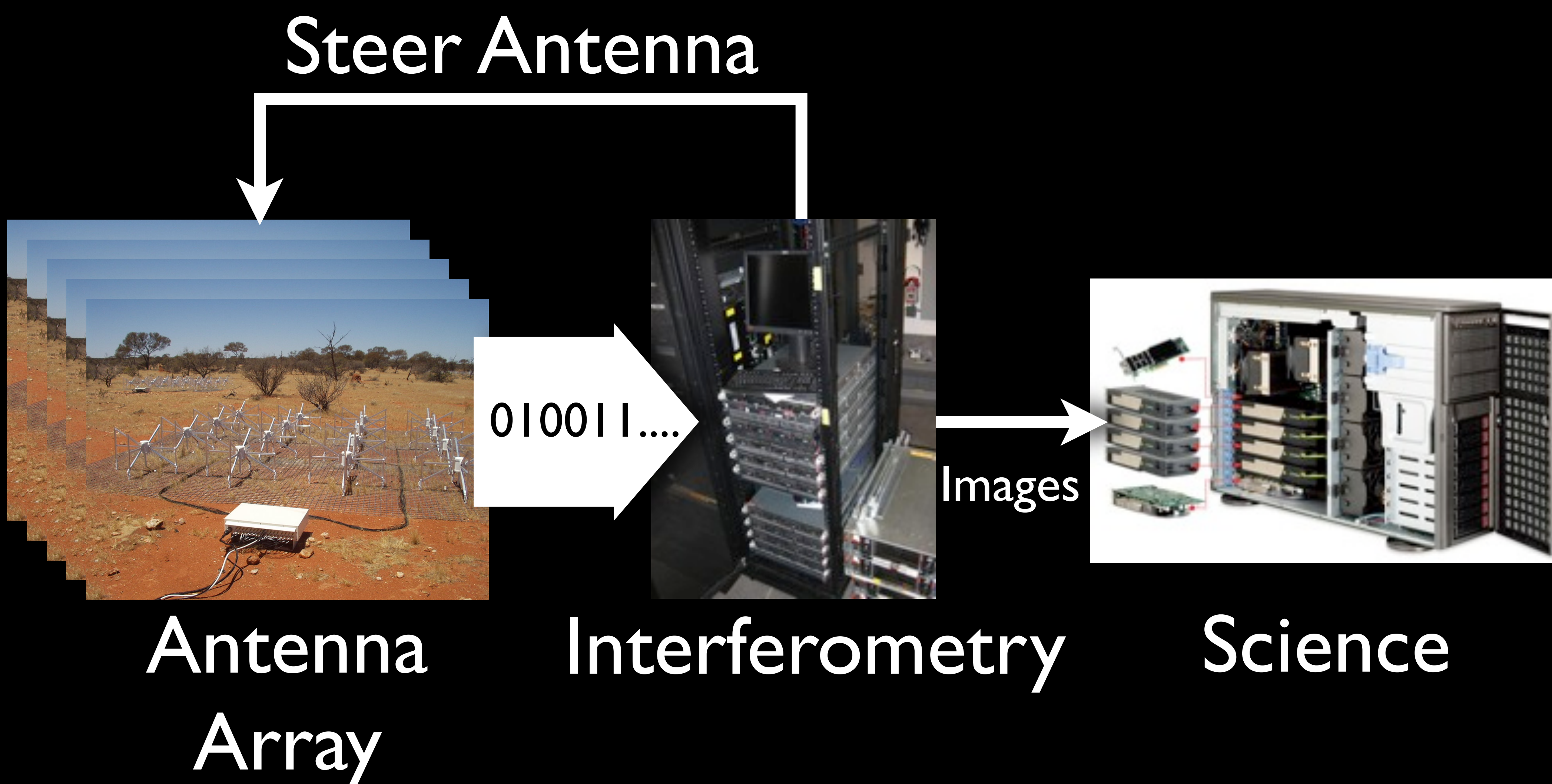


C. Williams, MIT

Real Time System

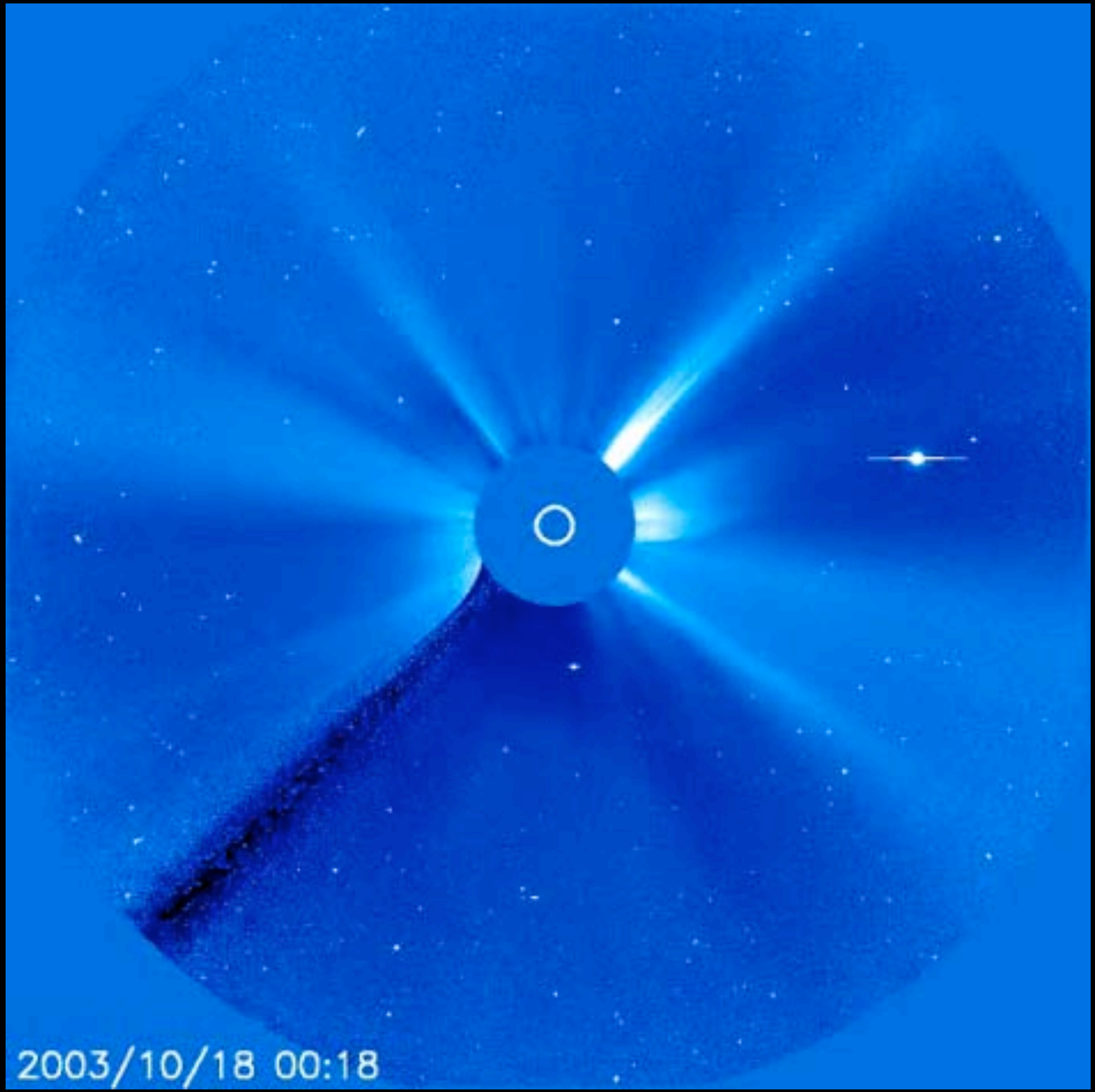


High-Throughput Radio Astronomy



Real-Time Steering

- Predict solar flares and coronal mass ejections

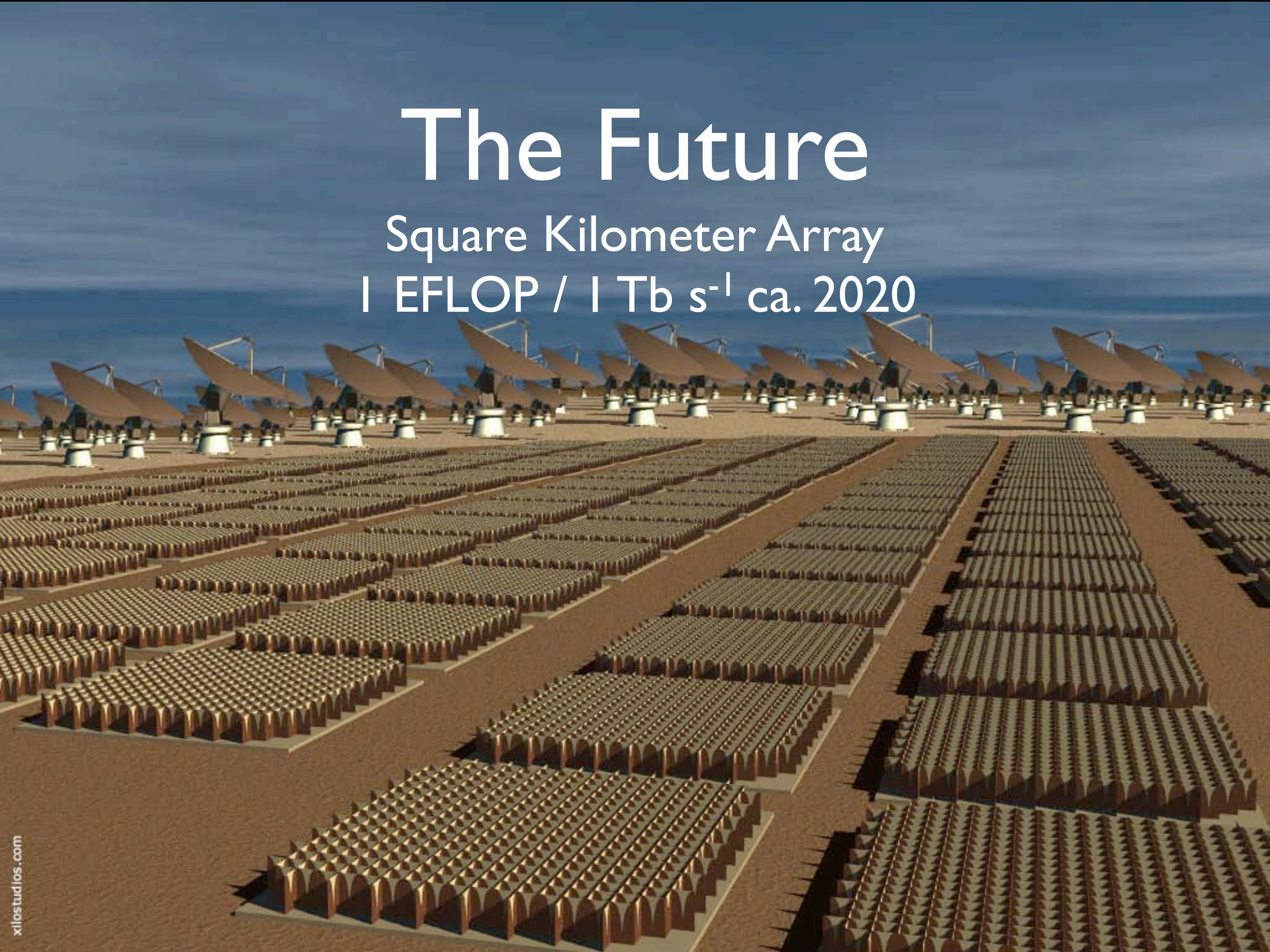


SOHO/EIT (ESA & NASA)

The Future

Square Kilometer Array

1 EFLOP / 1 Tb s^{-1} ca. 2020

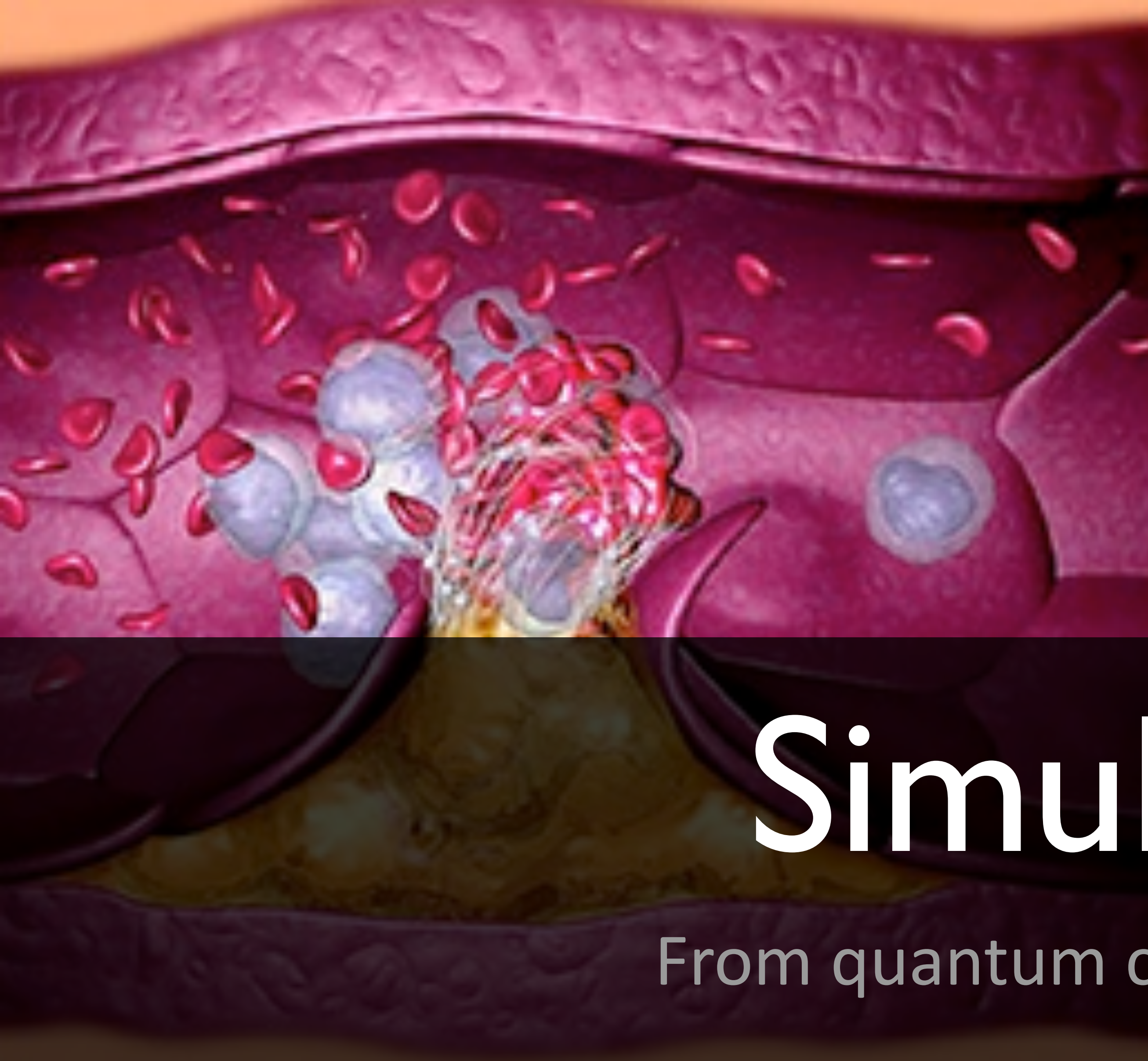


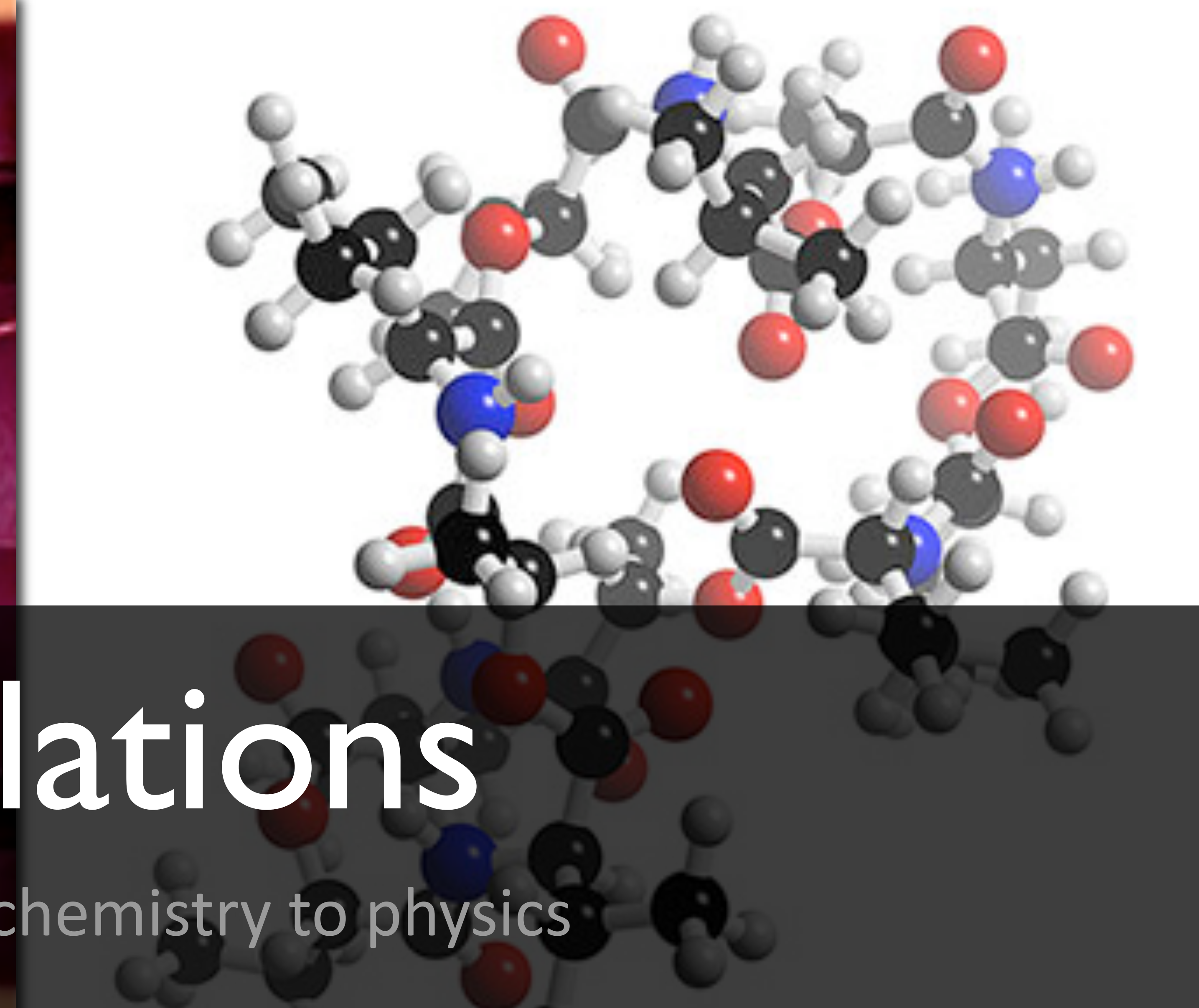
More Information

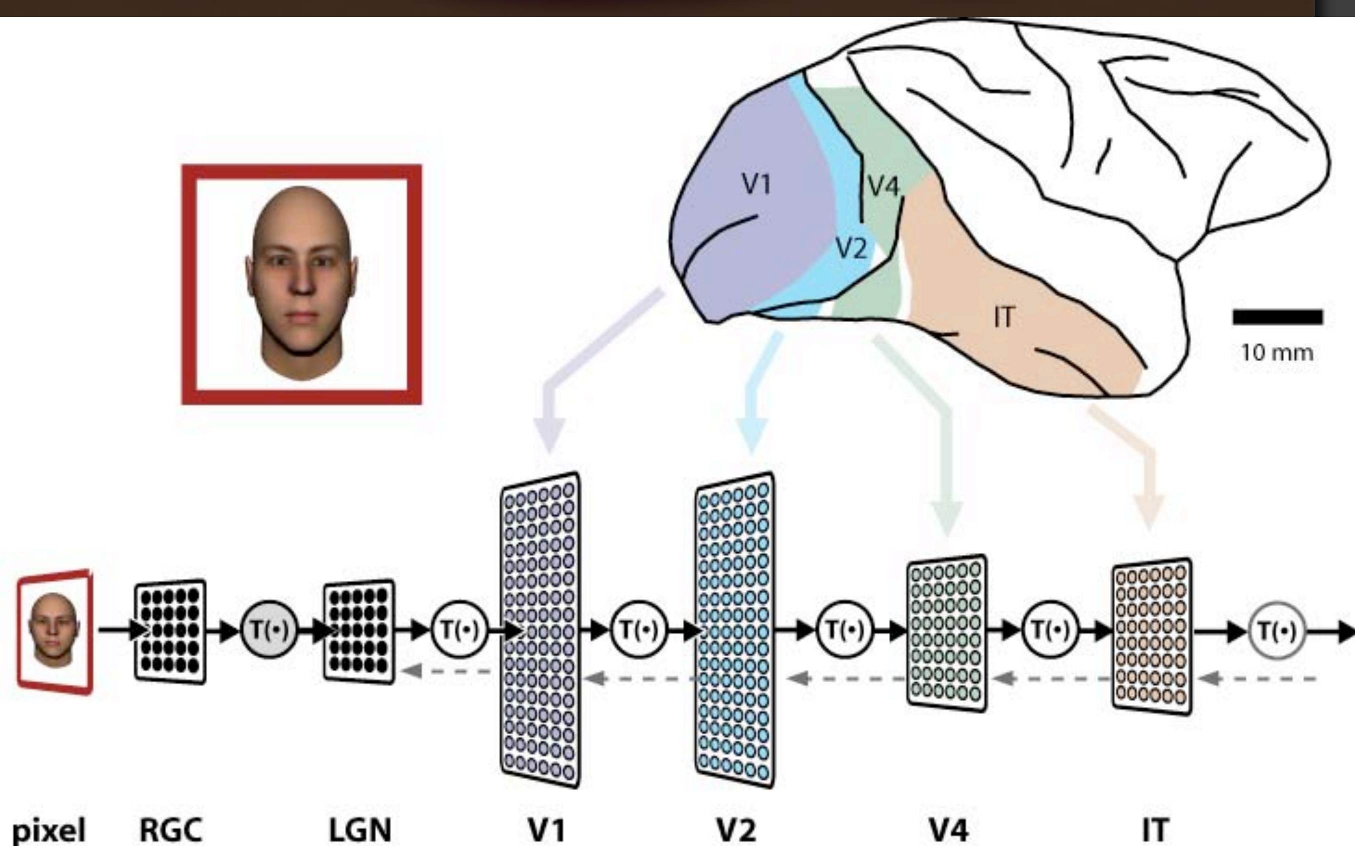
Richard Edgar
Diesel-Powered GPU Computing: Enabling a Real-Time Radio Telescope in the Australian Outback
Session Id#1065
Friday 3 pm California

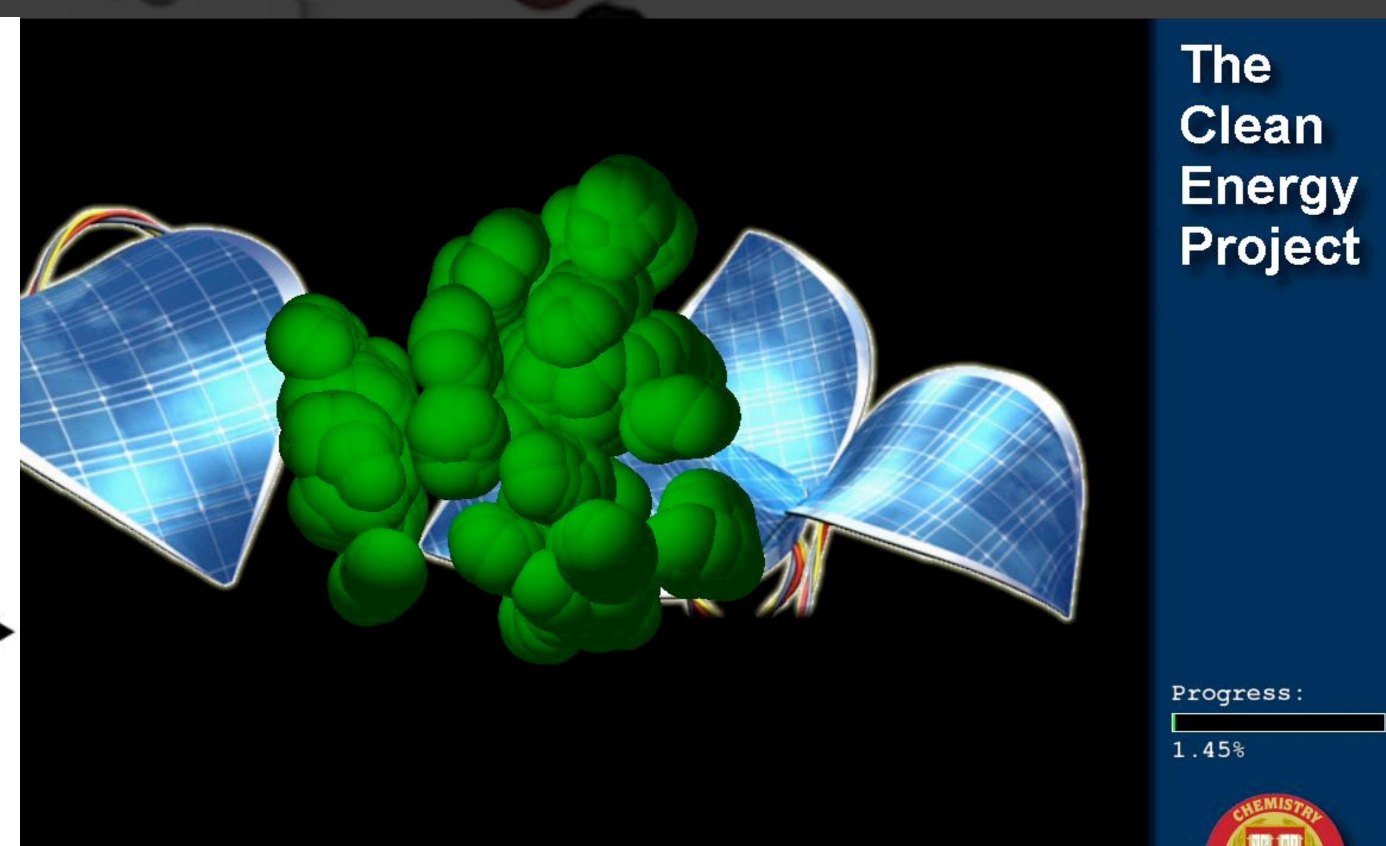
Simulations

From quantum chemistry to physics









Quantum Chemistry

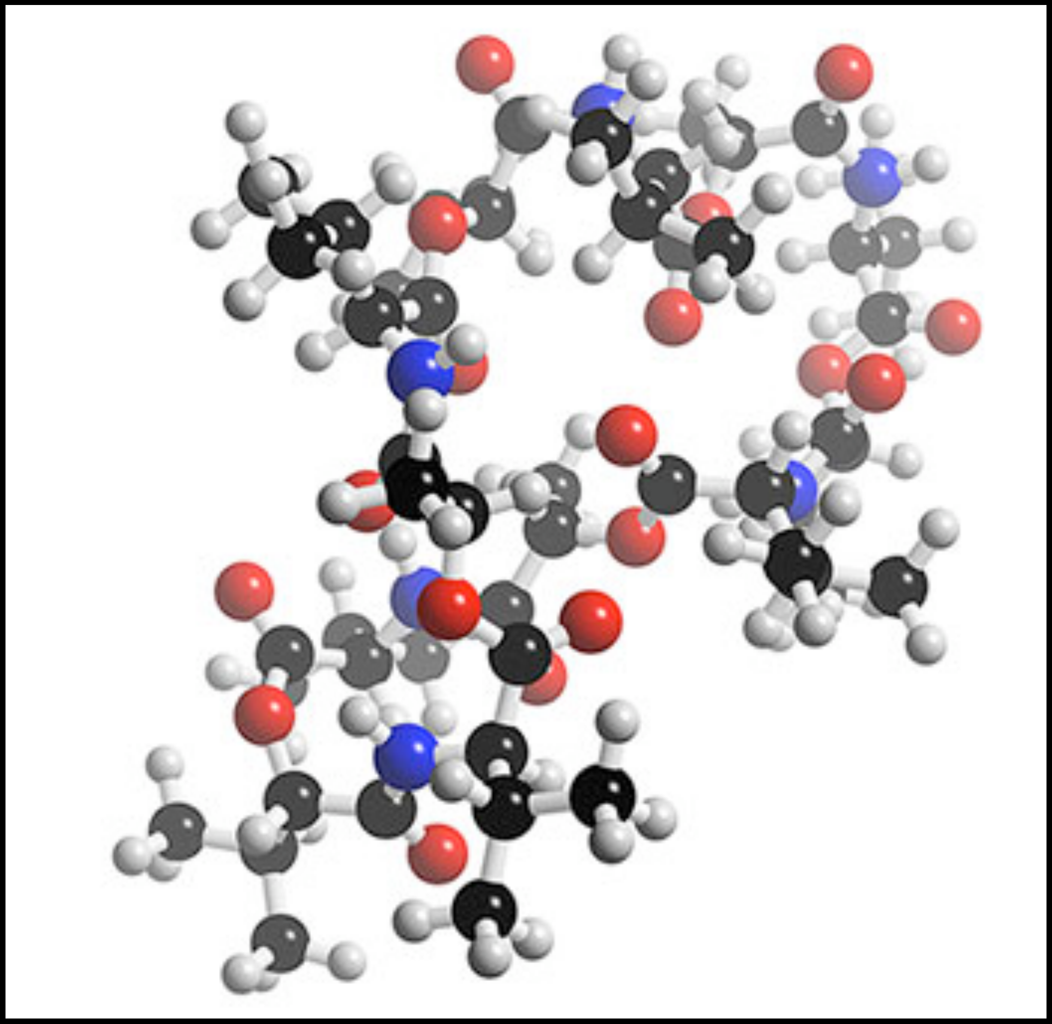
- Alan Aspuru-Guzik
- Mark Watson
- Richard Edgar
- Kenta Hongo
- Roberto Olivares
- Leslie Vogt
- Sean Kermes



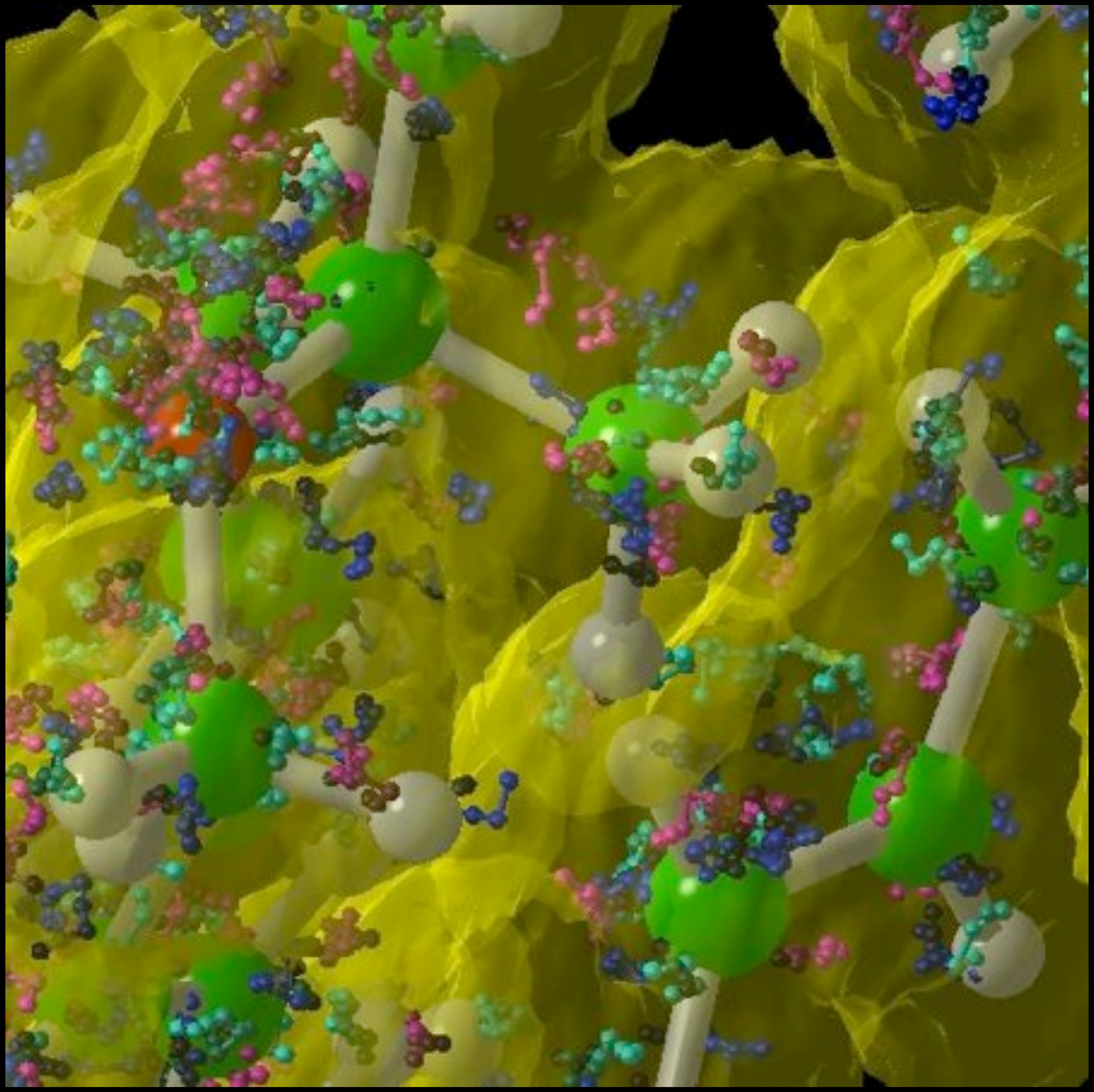



The Scientific Challenge

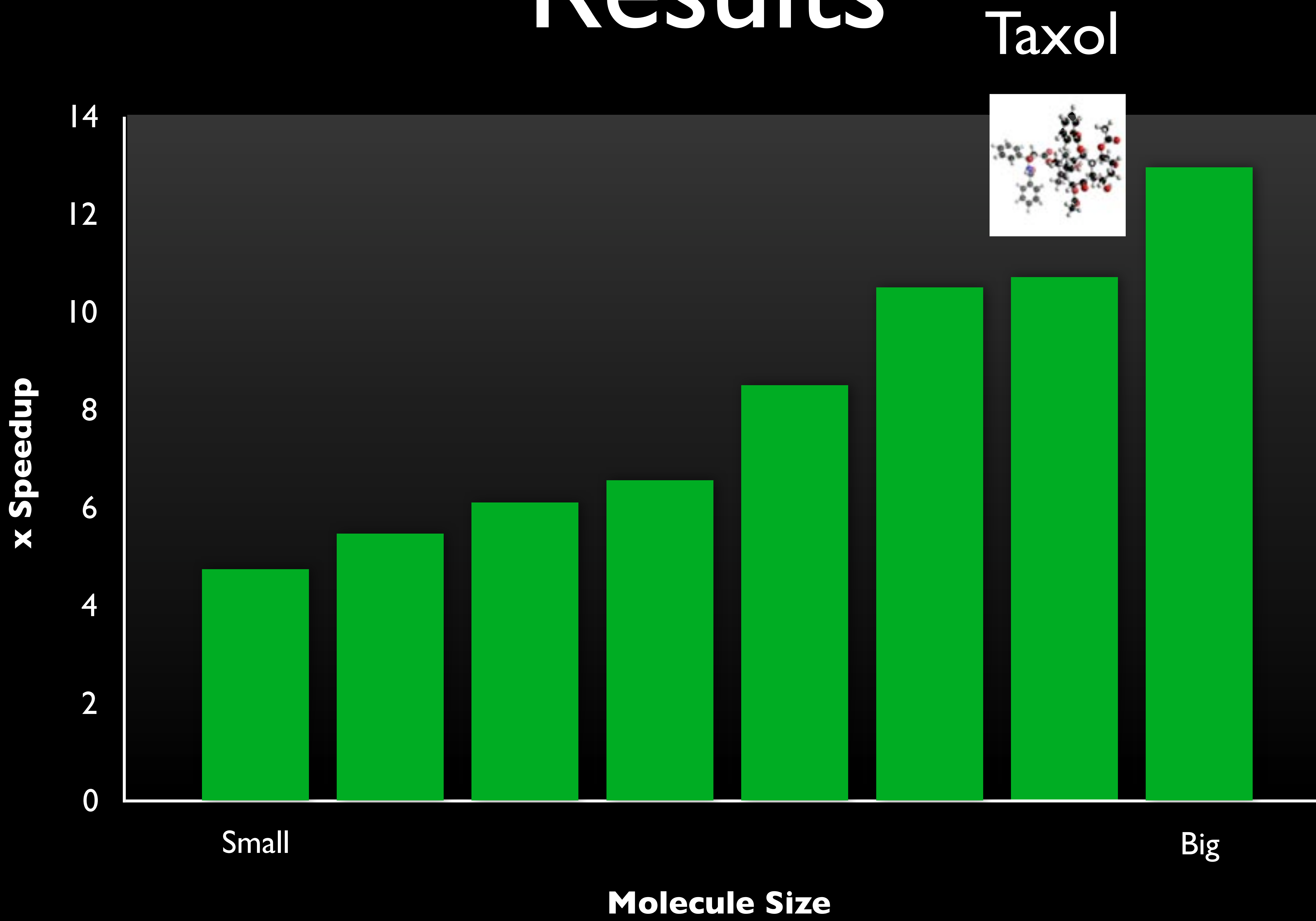
- Determine properties of organic molecules



Quantum Many-Body Problems

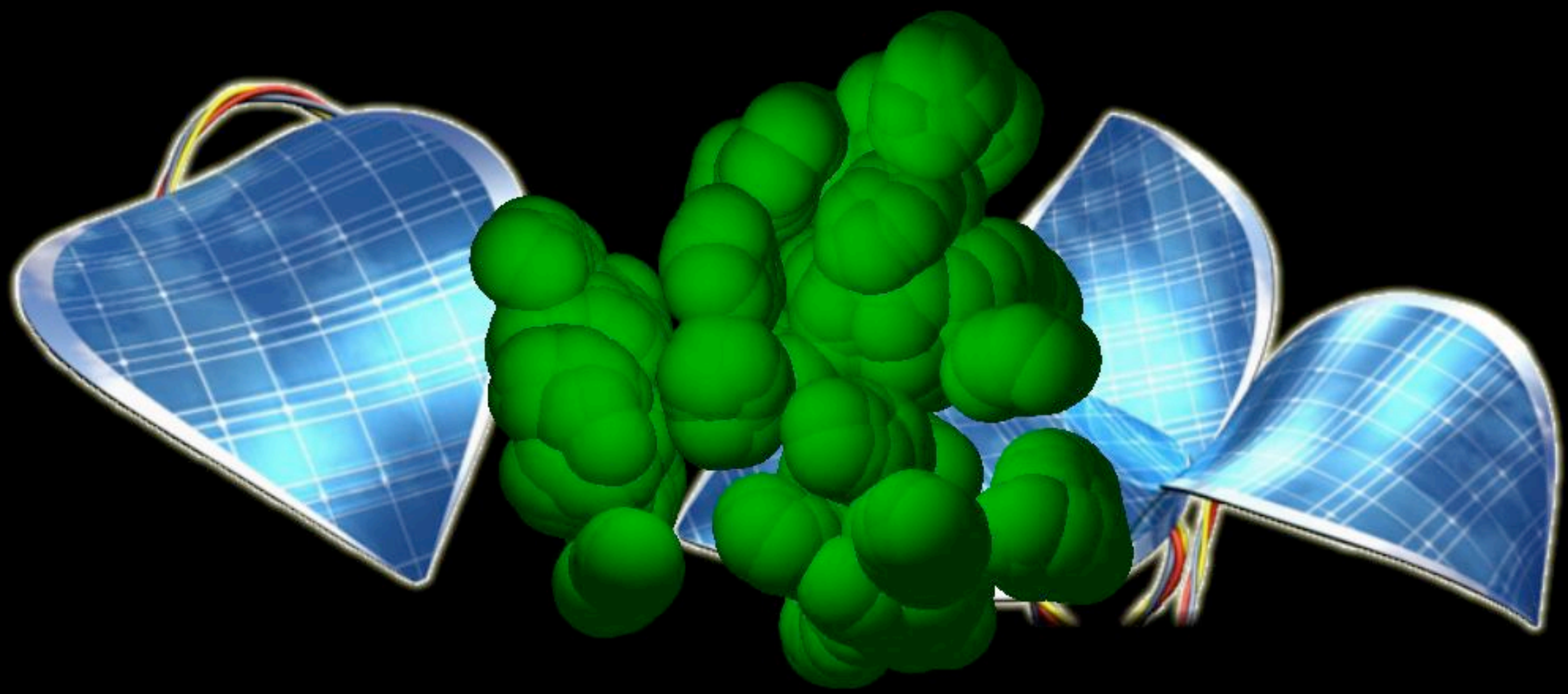


Results

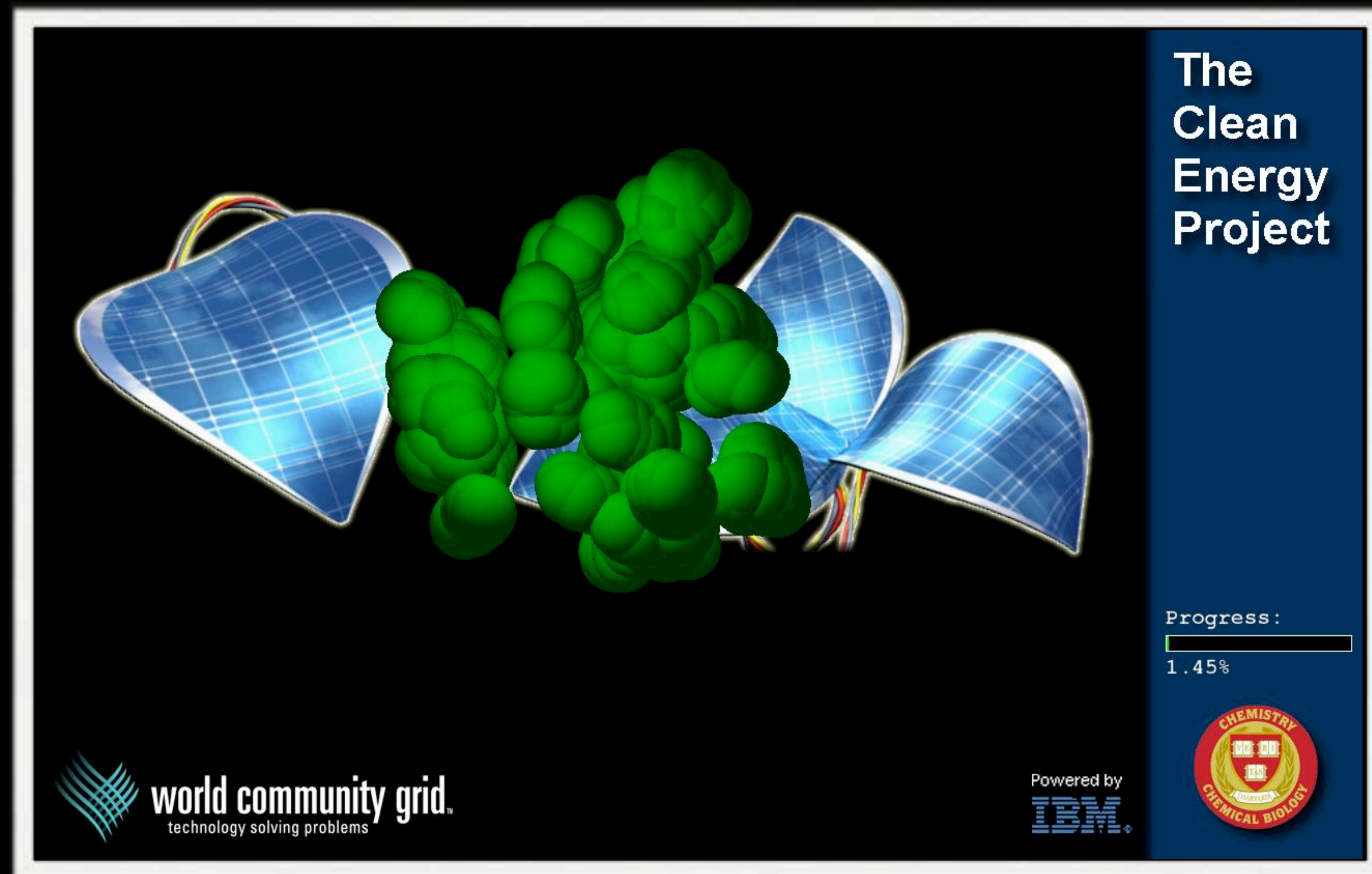


The Future

- Improve organic photovoltaic materials



Volunteer Computing



Relevant Talk

David Anderson
Volunteer Computing for GPUs: Petaflops for Free
Session Id#1010
Thursday 3 pm California

Visual Neuroscience

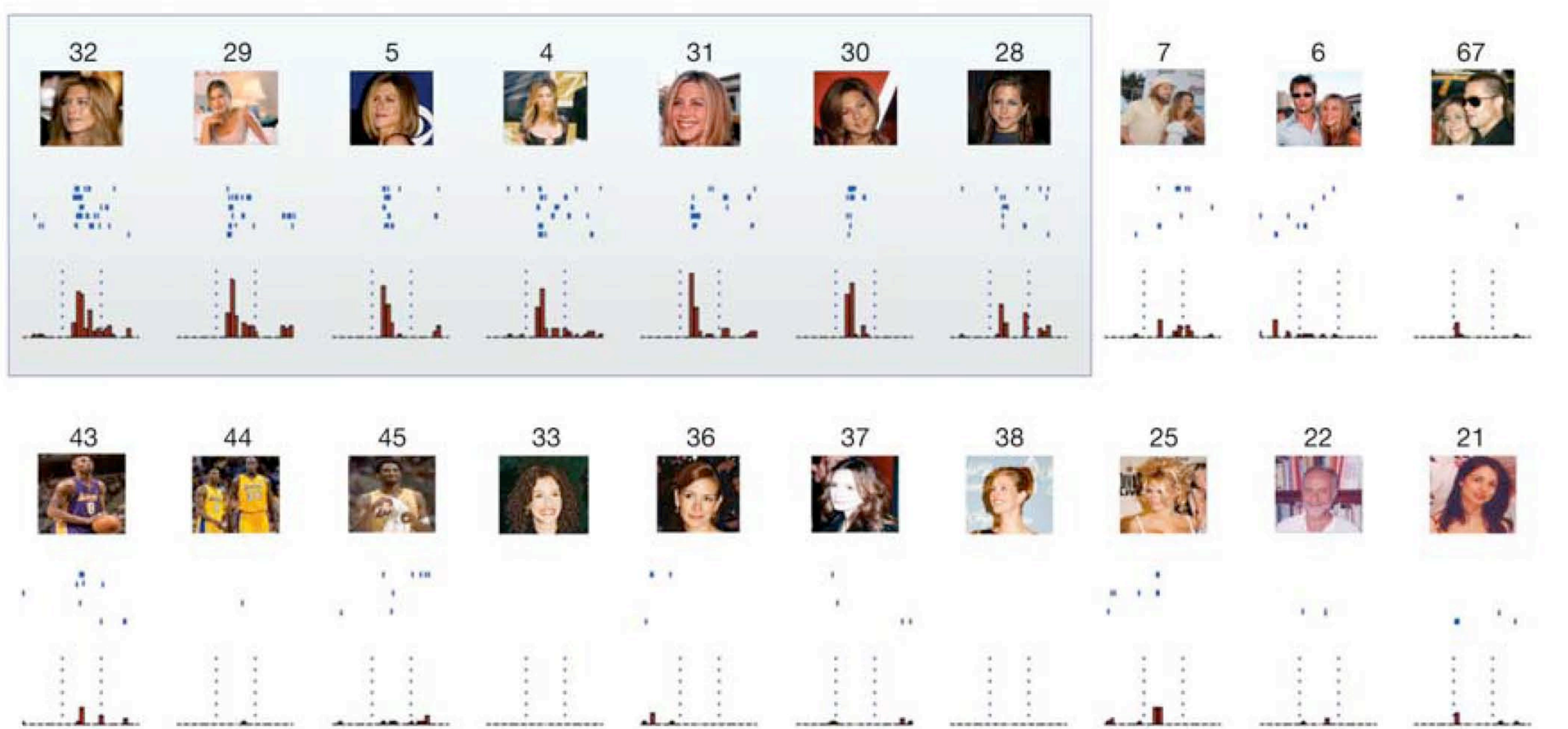
- David Cox, The Rowland Institute at Harvard

- Nicolas Pinto, MIT

- Jim DiCarlo, MIT

The Scientific Challenge

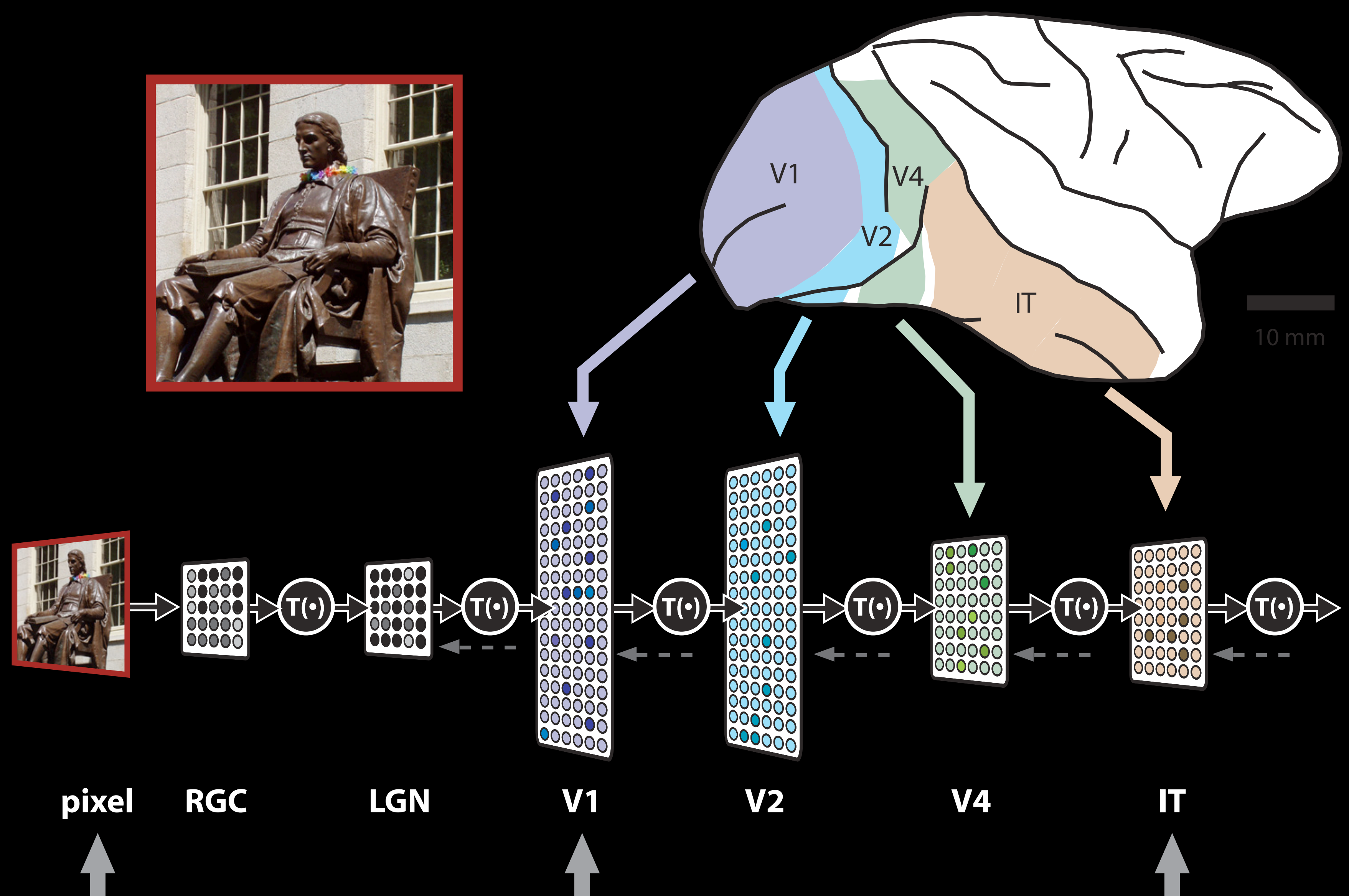
- How does the brain perform object recognition?



Quian Quiroga, Reddy, Kreiman, Koch and Fried, Nature, 2005

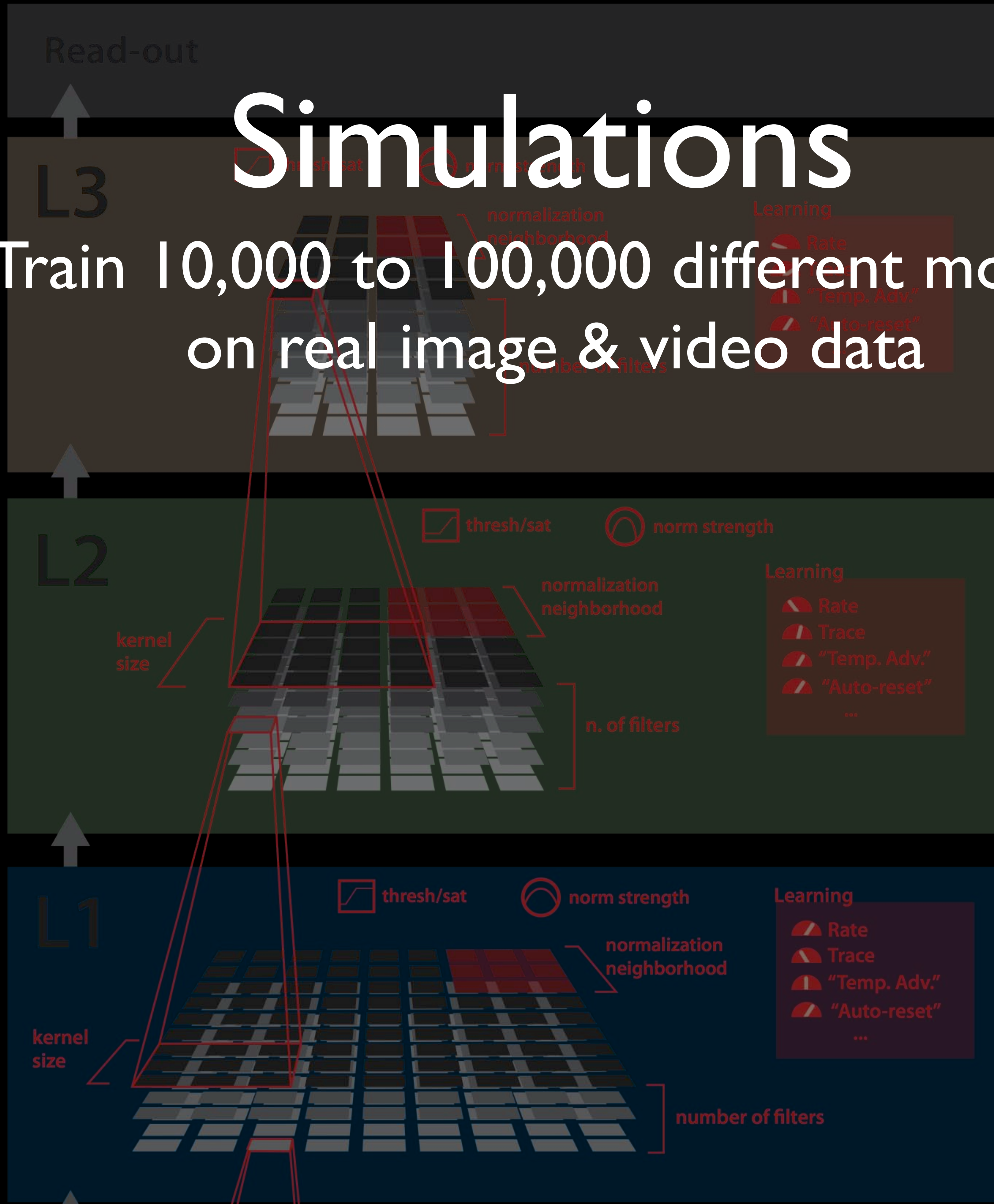
The Scientific Challenge

- What are good models of the human visual system, and what are their parameters?



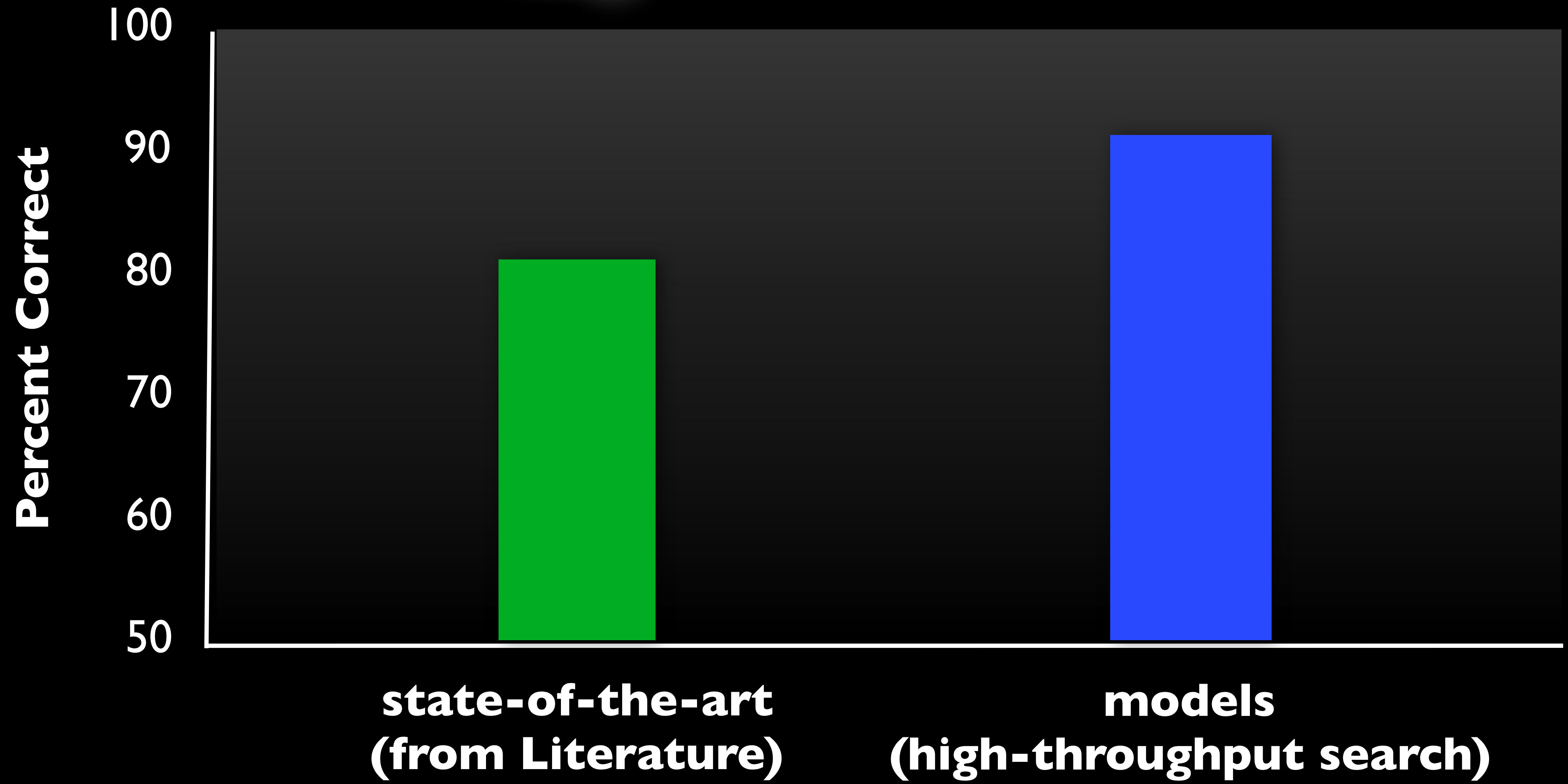
Simulations

Train 10,000 to 100,000 different models
on real image & video data

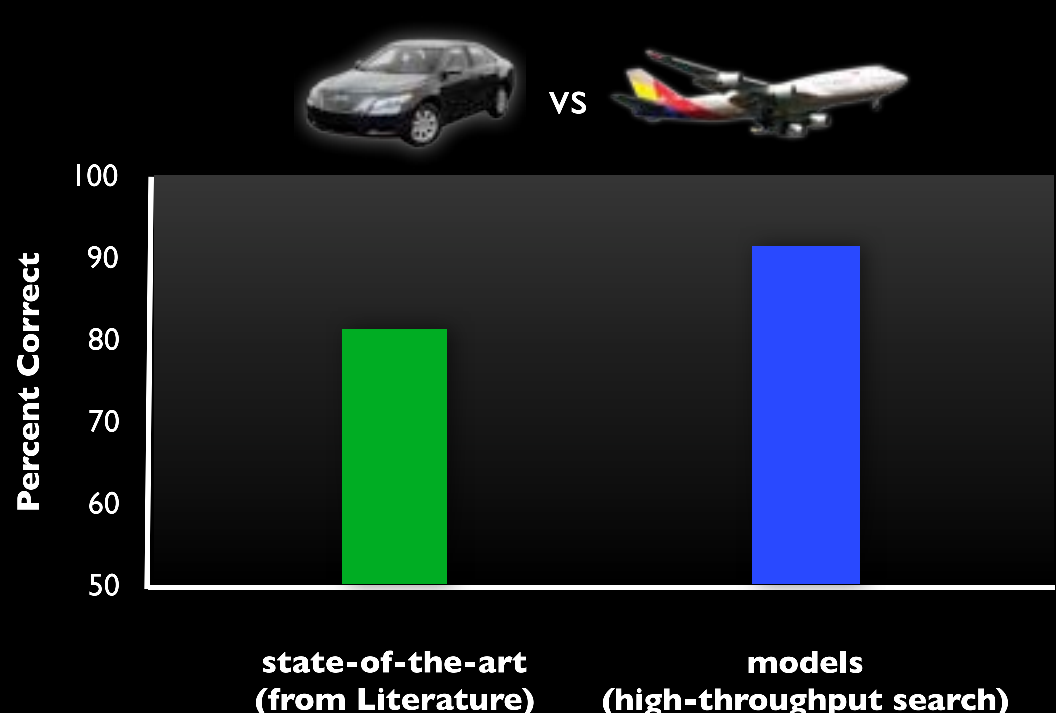


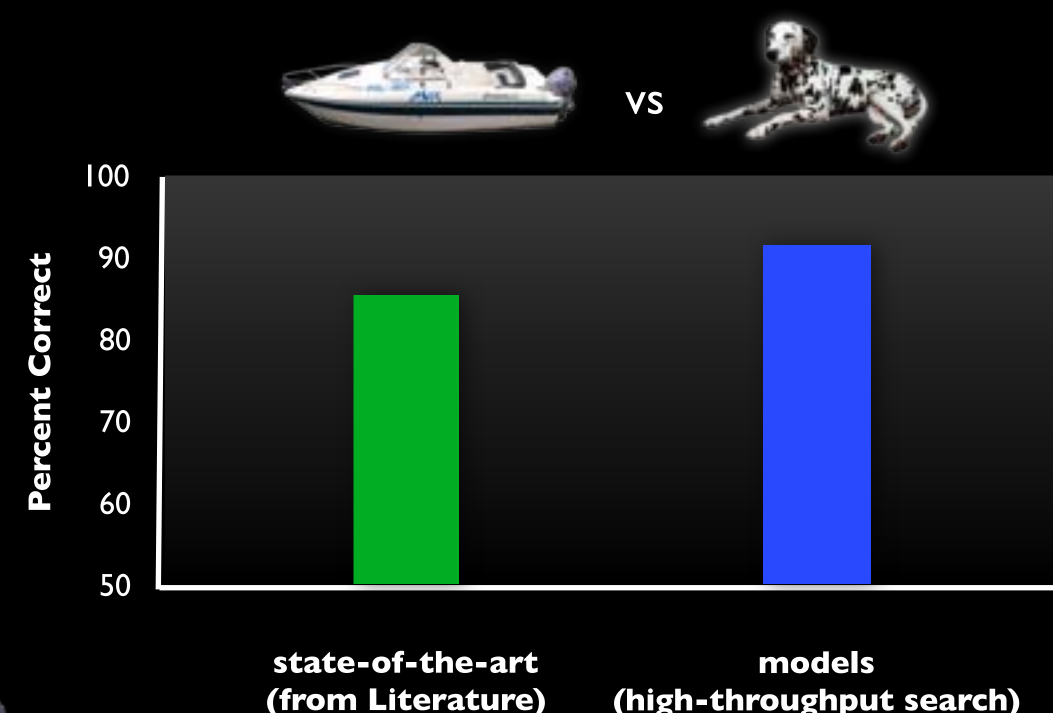
Performance

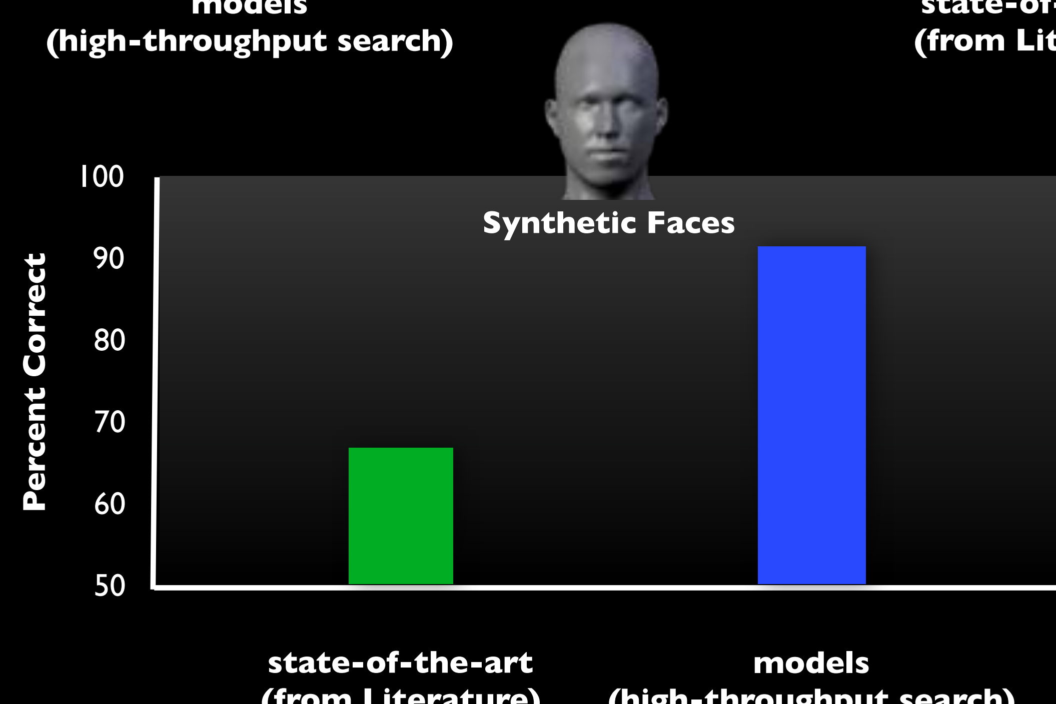
vs



Performance

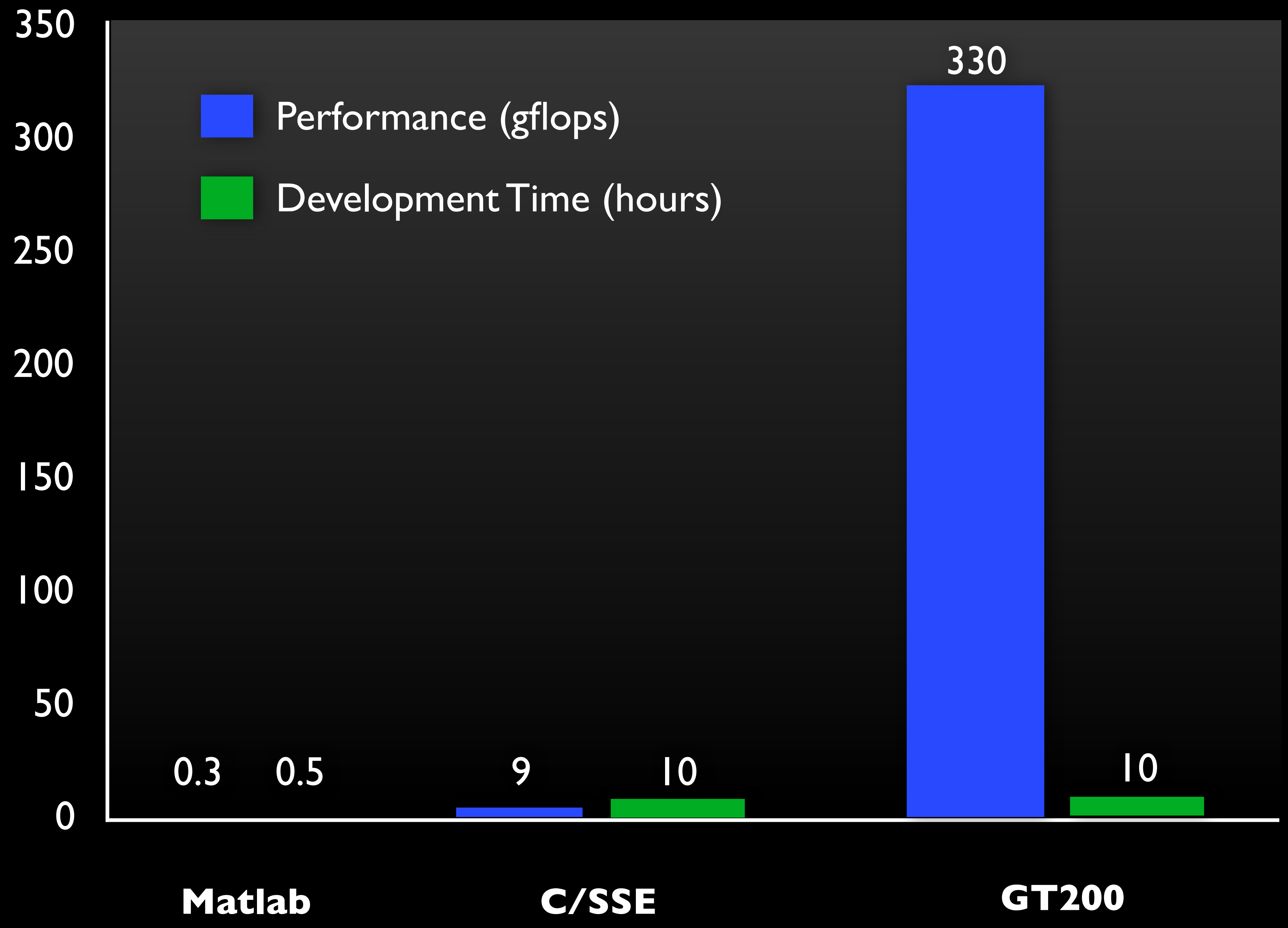






Results

3D Filterbank Convolution

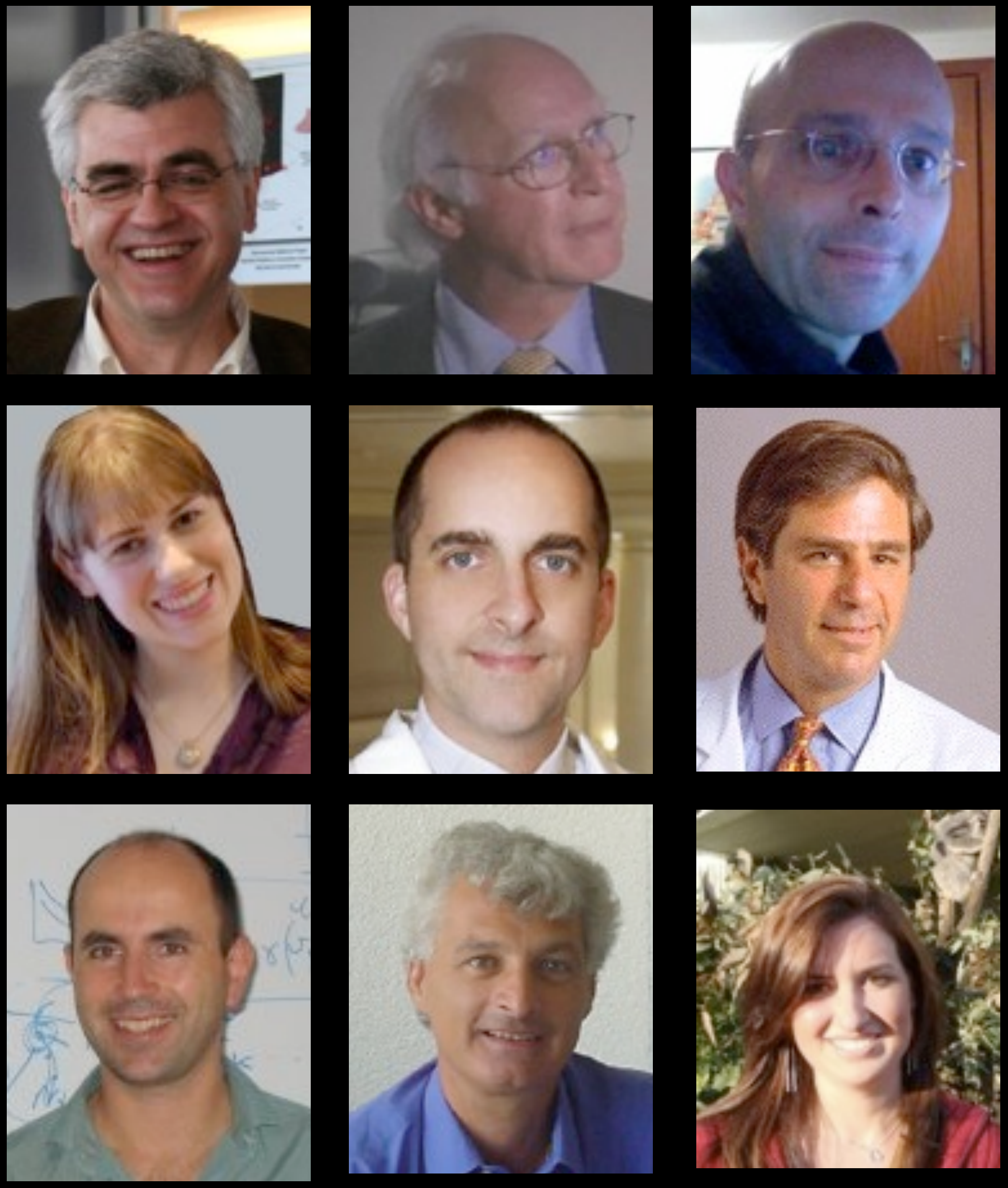


More Information

Nicolas Pinto
Unlocking Biologically-Inspired Computer Vision: a High-Throughput Approach
Session Id#1434
Thursday 5 pm Garden

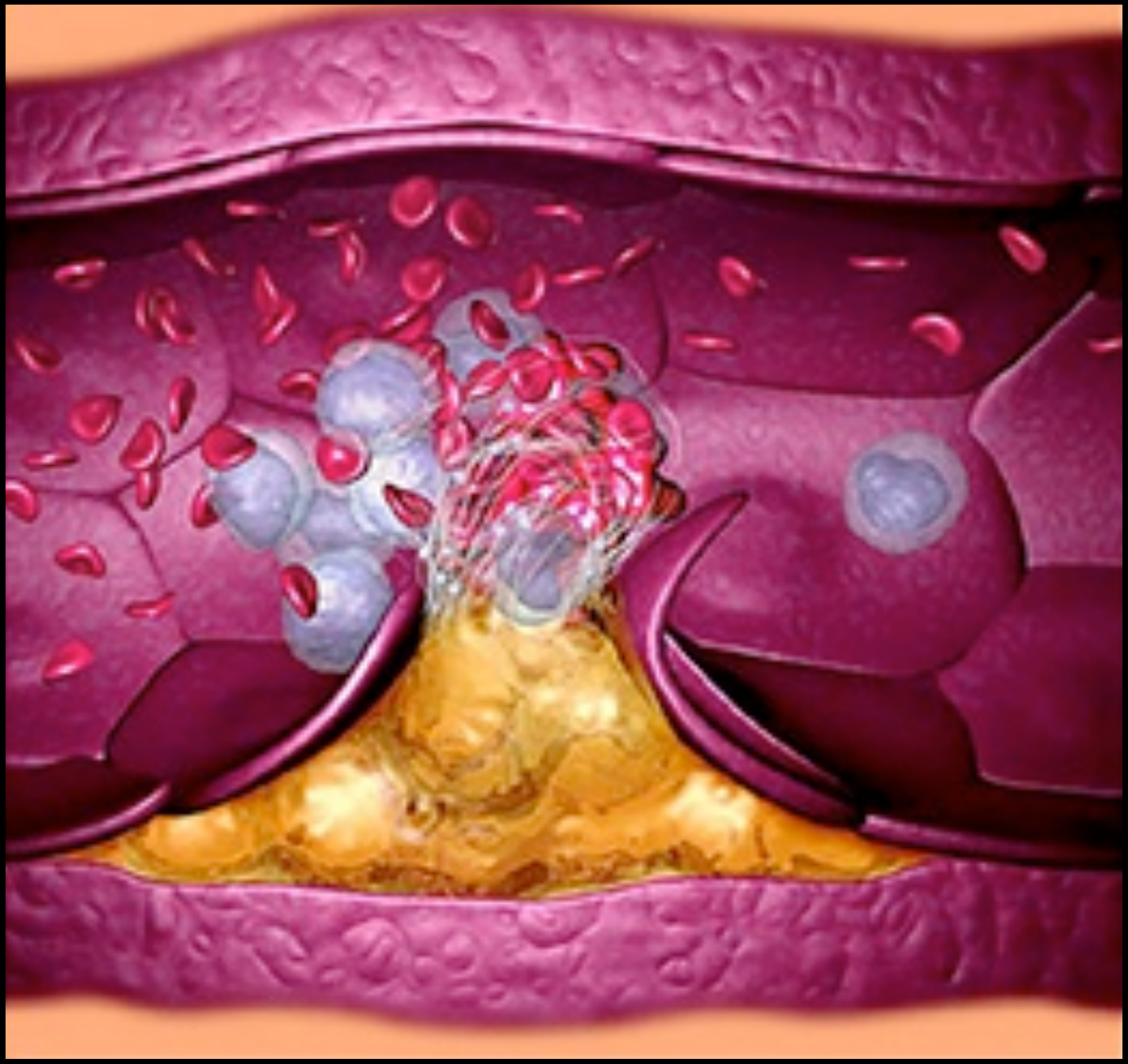
Multiscale Hemodynamics

Massimo Bernaschi - Michelle Borkin - Ahmet Coskun - Charles Feldman - Efthimios Kaxiras - Simone Melchionna - Dimitris Mitsouras - Hanspeter Pfister - Frank Rybicki - Joy Sircar - Michael Steigner - Peter Stone - Sauro Succi - Frederick Welt - Amanda Whitmore



The Scientific Challenge

- Predict and prevent heart attacks

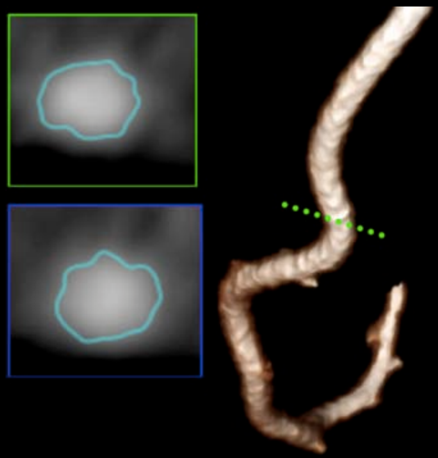


Hemodynamics Pipeline

CT Patient Data

Hemodynamics Pipeline

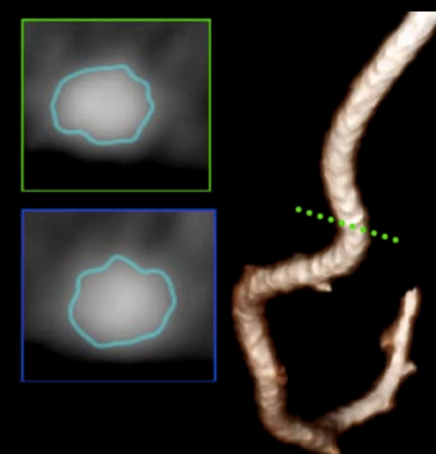
CT Patient Data →



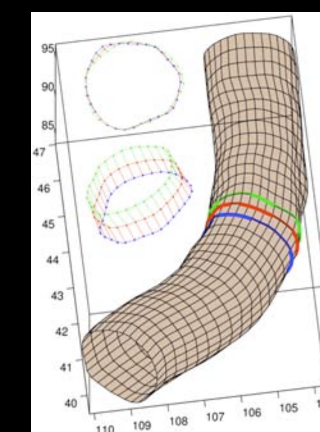
Reconstruction

Hemodynamics Pipeline

CT Patient Data →

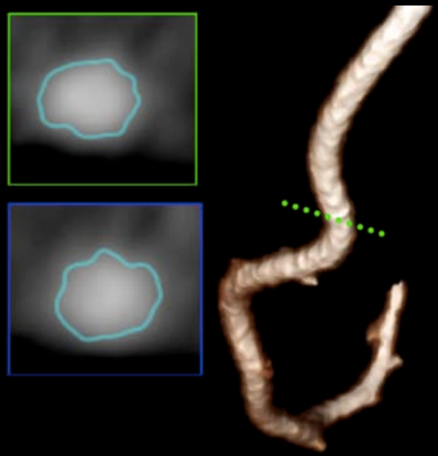


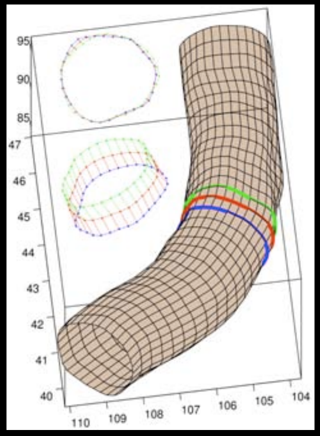
Reconstruction →



Post-Processing

Hemodynamics Pipeline

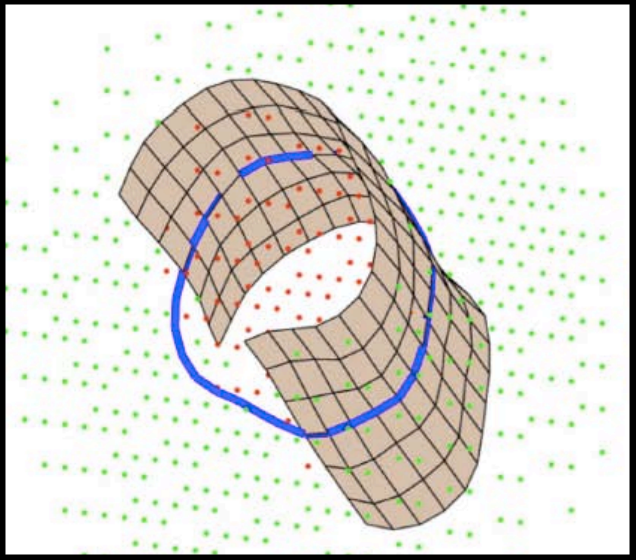




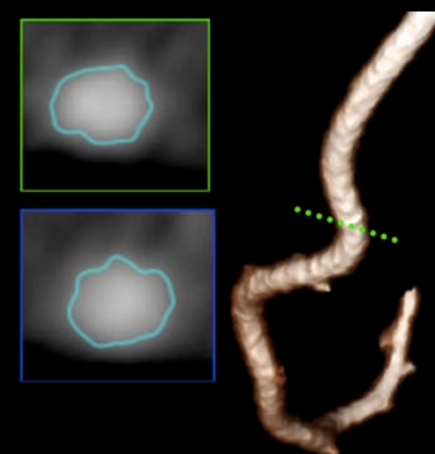
CT Patient Data → Reconstruction → Post-Processing

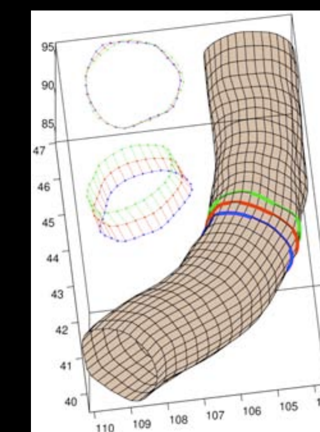
↓

Lattice Boltzman &
Molecular Dynamics



Hemodynamics Pipeline

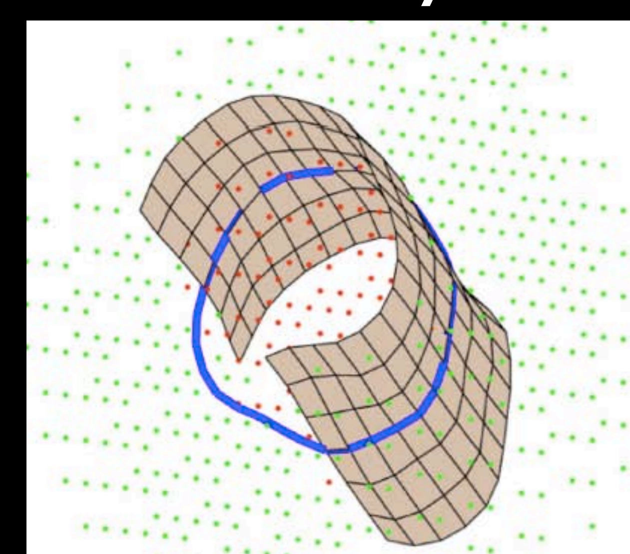




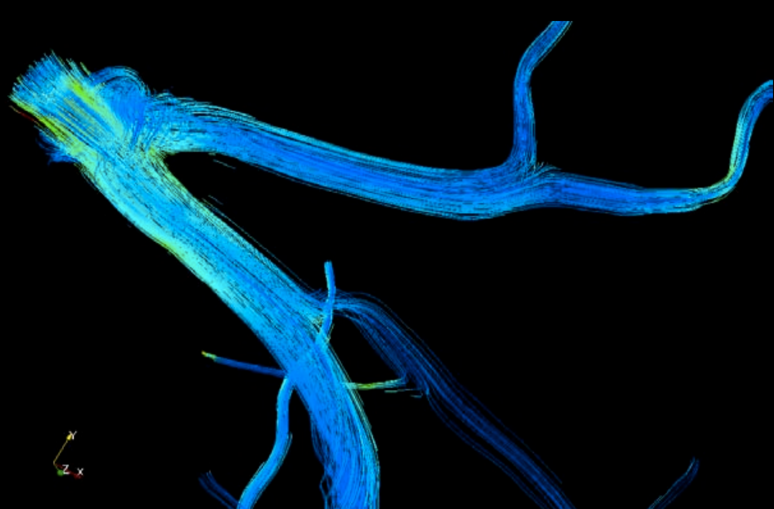
CT Patient Data → Reconstruction → Post-Processing

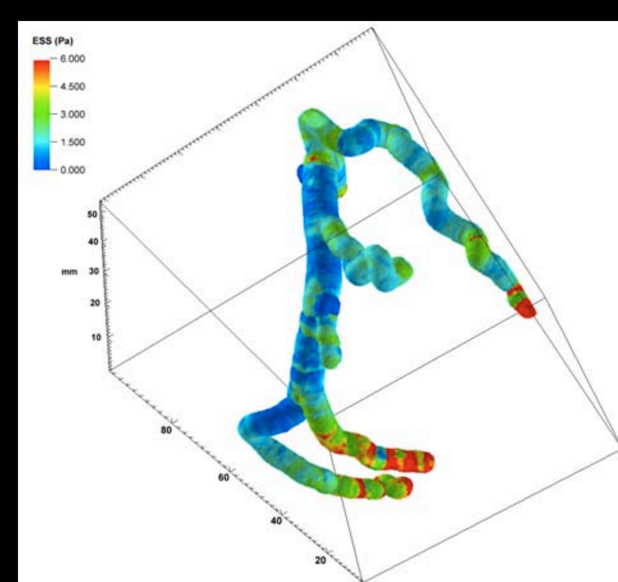
↓

Lattice Boltzman &
Molecular Dynamics

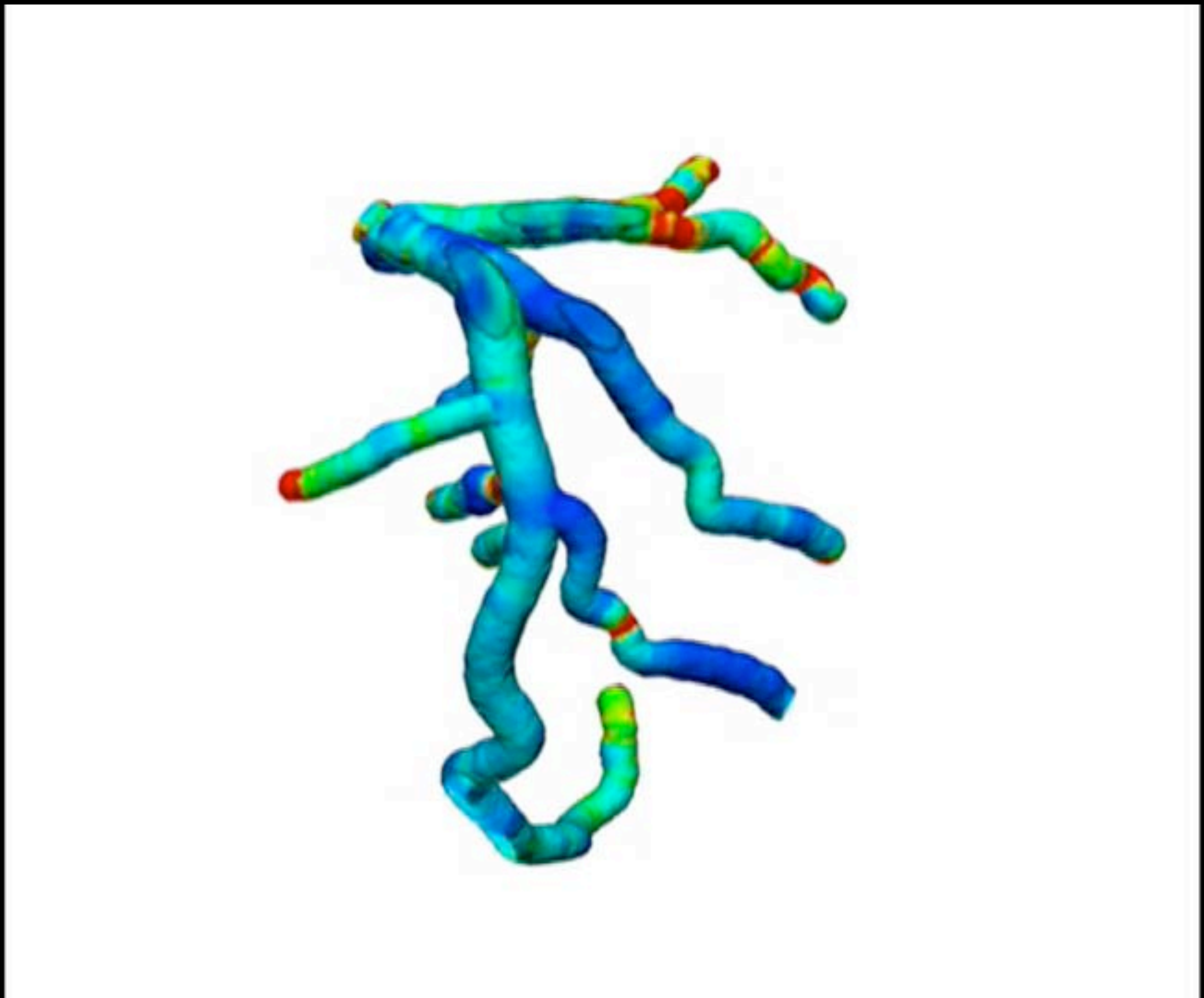


Visualization & Analysis ←

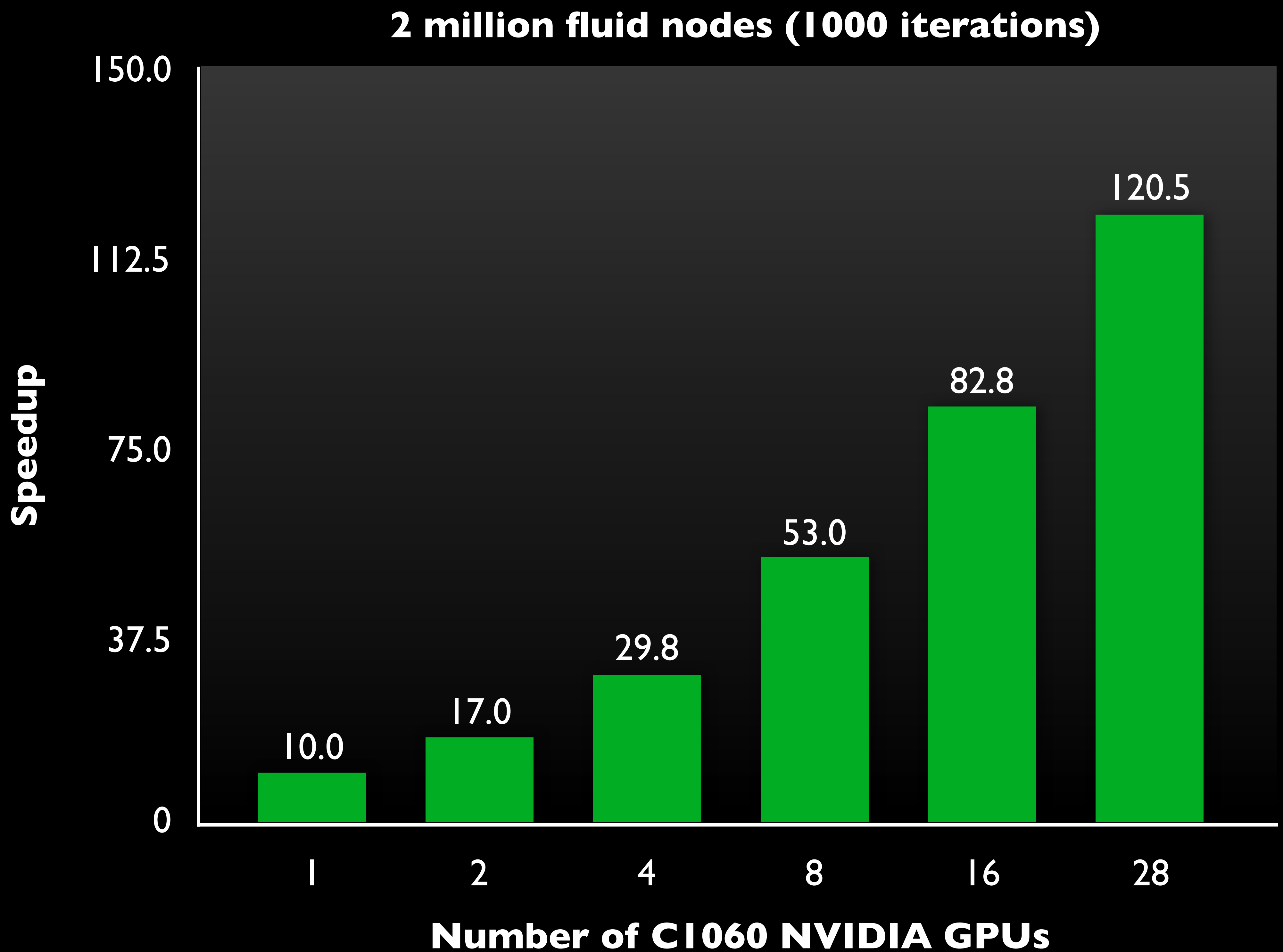




Multiscale Hemodynamics



Results



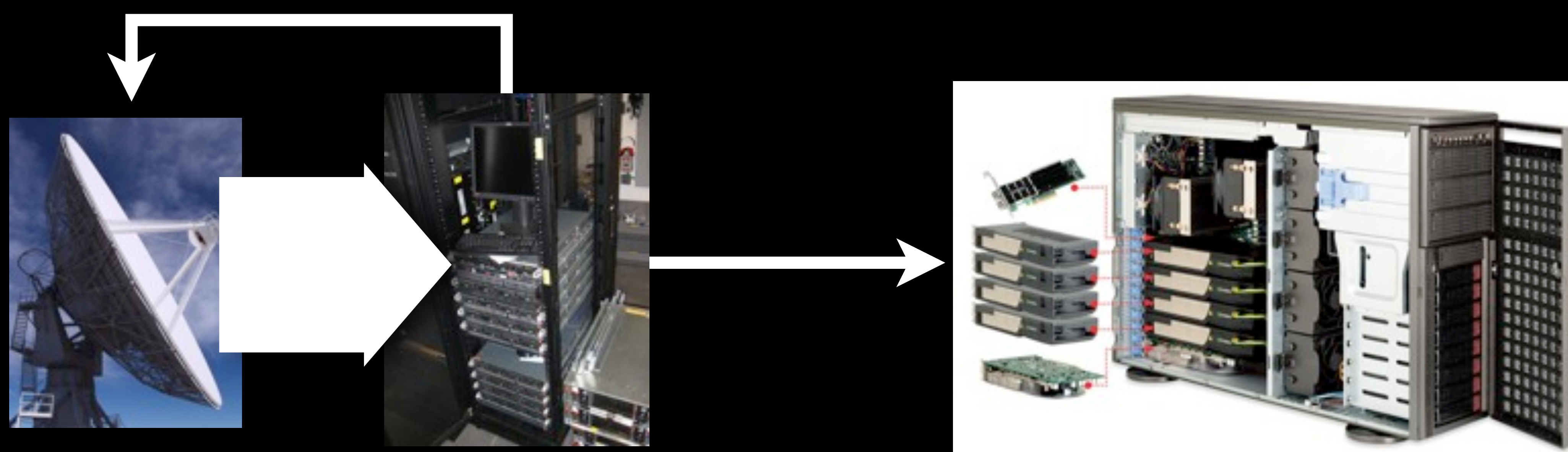
2 million fluid nodes (1000 iterations)
150.0
112.5
75.0
37.5
0
Speedup
10.0
17.0
29.8
53.0
82.8
120.5
1
2
4
8
16
28
Number of C1060 NVIDIA GPUs

The Future

- Minimally invasive early detection

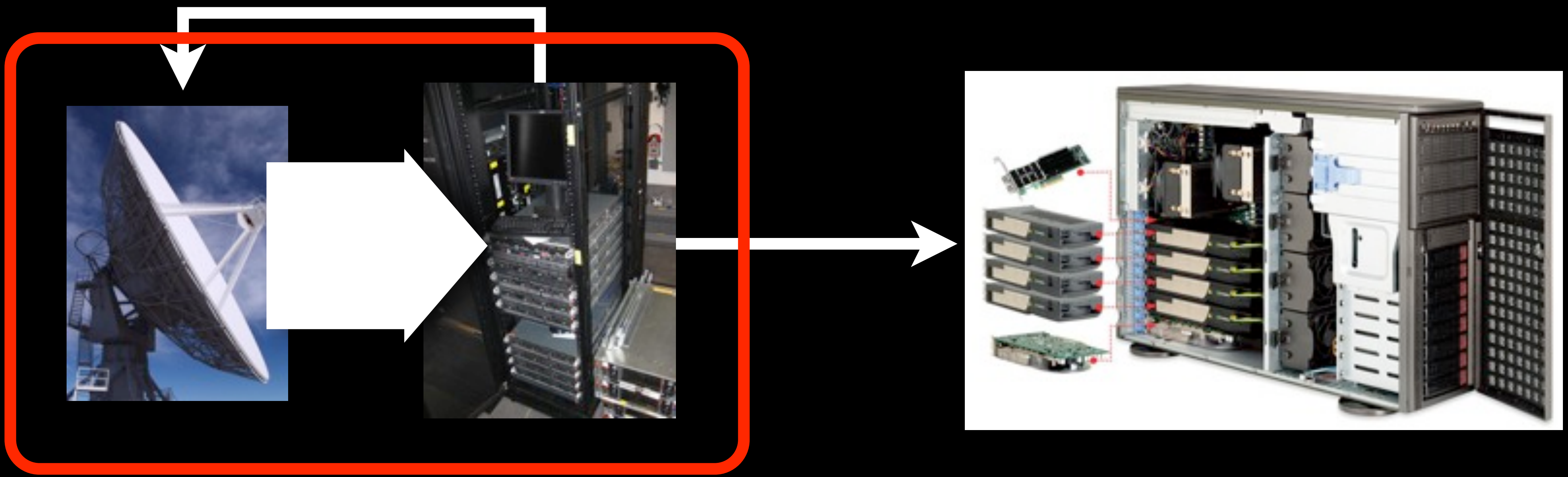
UCLA Medical Center Newsletter

HTC Lessons



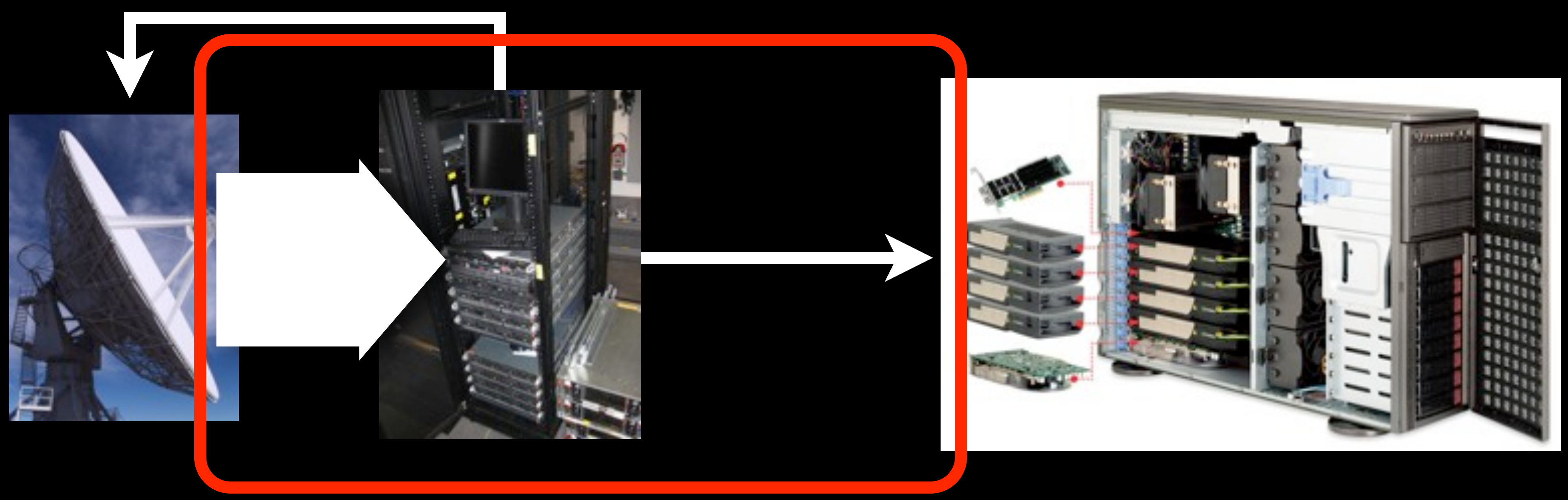
HTC Lessons

- Move the computation to the source



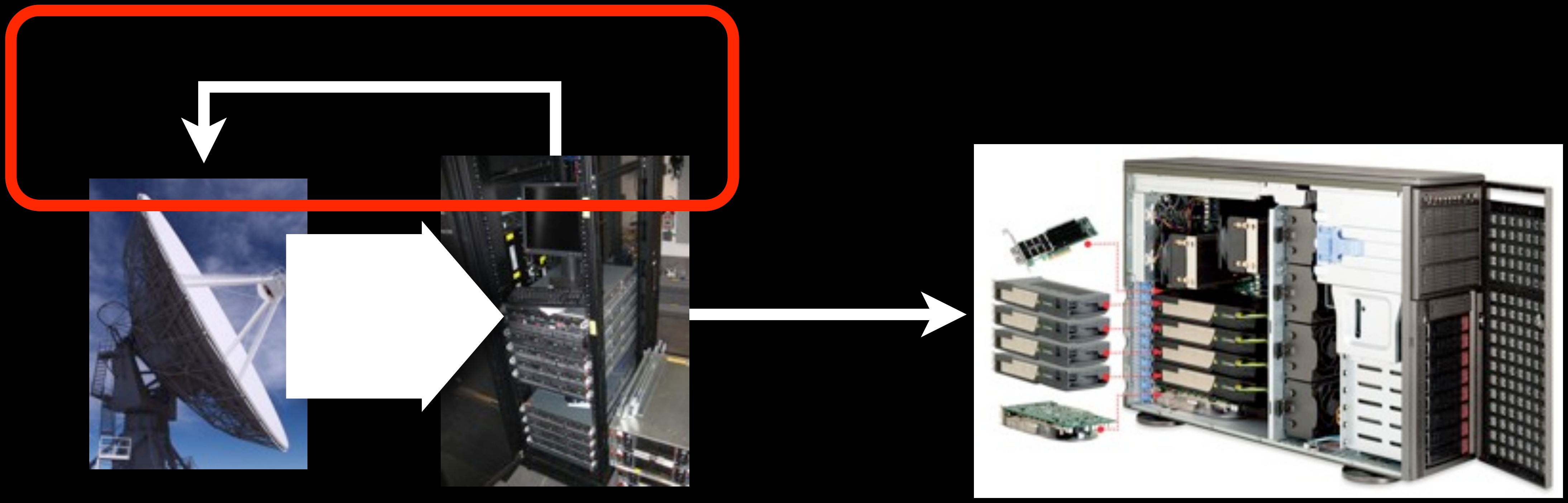
HTC Lessons

- Quickly reduce the data to its essentials



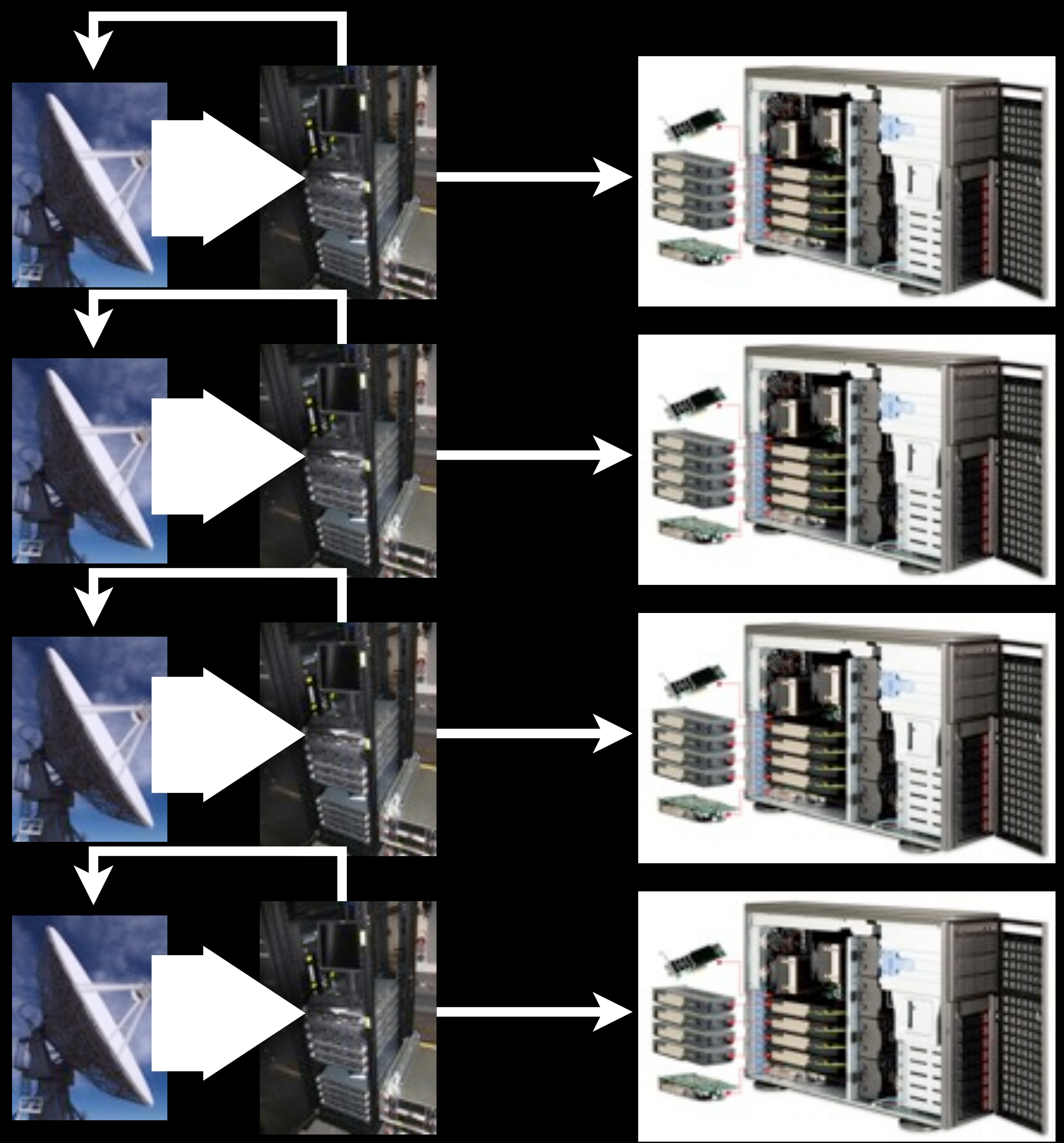
HTC Lessons

- Use feedback to optimize the acquisition



HTC Lessons

- Provides scalable and power efficient systems



Higher-Level Programming Models

Higher-Level Programming Models

- Domain Specific Languages (DSLs)

Higher-Level Programming Models

- Domain Specific Languages (DSLs)
- E.g., Tensor Contraction Engine (TCE)

$$T1_{bcdf} = \sum_{el} B_{befl} \times D_{cdel}$$
$$T2_{bcjk} = \sum_{df} T1_{bcdf} \times C_{dfjk}$$
$$S_{abij} = \sum_{ck} T2_{bcjk} \times A_{acik}$$

(a) Formula sequence

```
T1=0; T2=0; S=0;
for b, c, d, e, f, l
  [ T1bcdf += Bbefl Dcdel
for b, c, d, f, j, k
  [ T2bcjk += T1bcdf Cdfjk
for a, b, c, i, j, k
  [ Sabij += T2bcjk Aacik
```

(b) Direct implementation (unfused code)

```
S = 0;
for b, c
  T1f = 0; T2f = 0;
  for d, f
    for e, l
      [ T1f += Bbefl Dcdel
    for j, k
      [ T2fjk += T1f Cdfjk
  for a, i, j, k
    [ Sabij += T2fjk Aacik
```

(c) Memory-reduced implementation (fused)

[Baumgartner et al. 05]

Scalable Programming Models

Plug & Play Parallel High-Throughput I/O

- Serial:
  - USB 3.0 (5 Gbp s-1)?
  - Intel Light Peak (100 Gbp s^{-1})?
- Parallel?

HTC Appliances

HTC Appliances

Surveillance

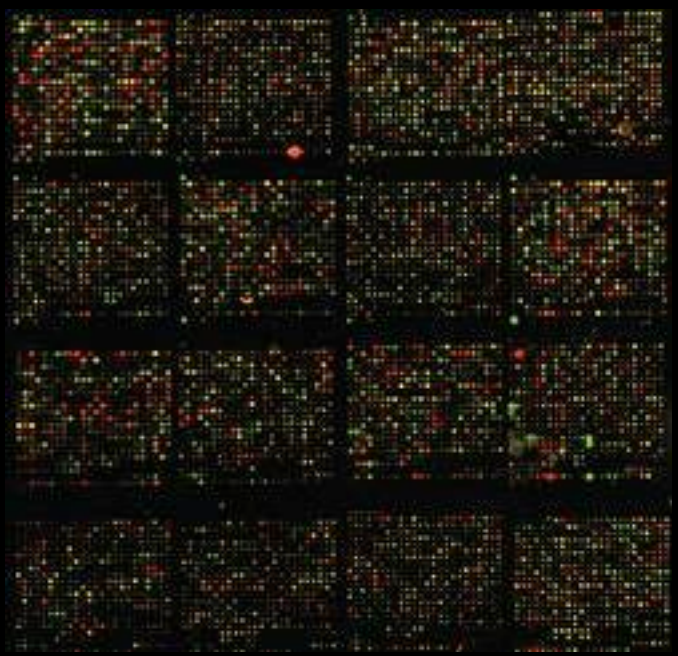
Cars

Video Conferencing

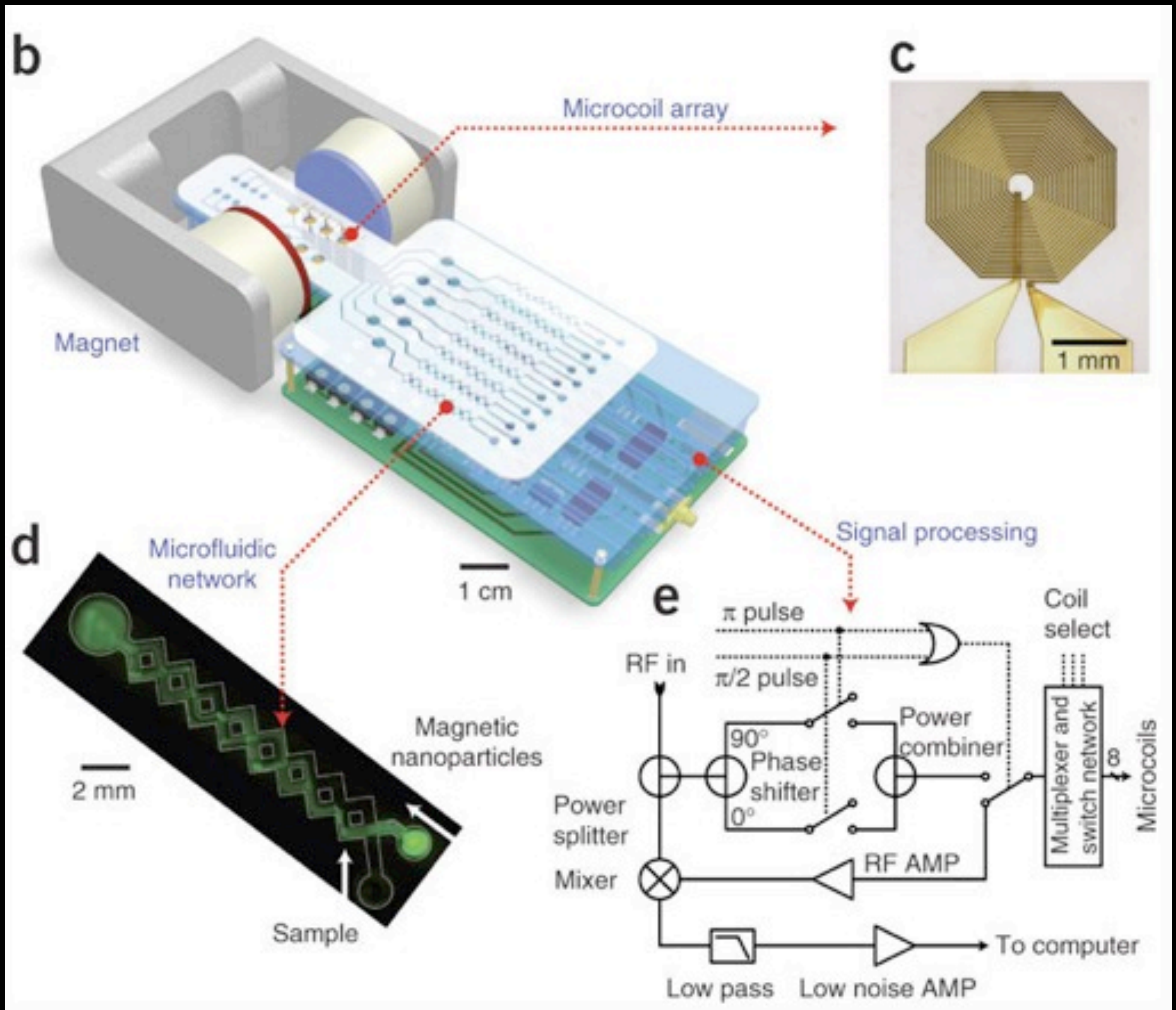
Broadcast

Chip Sensors

Gene Array Chips

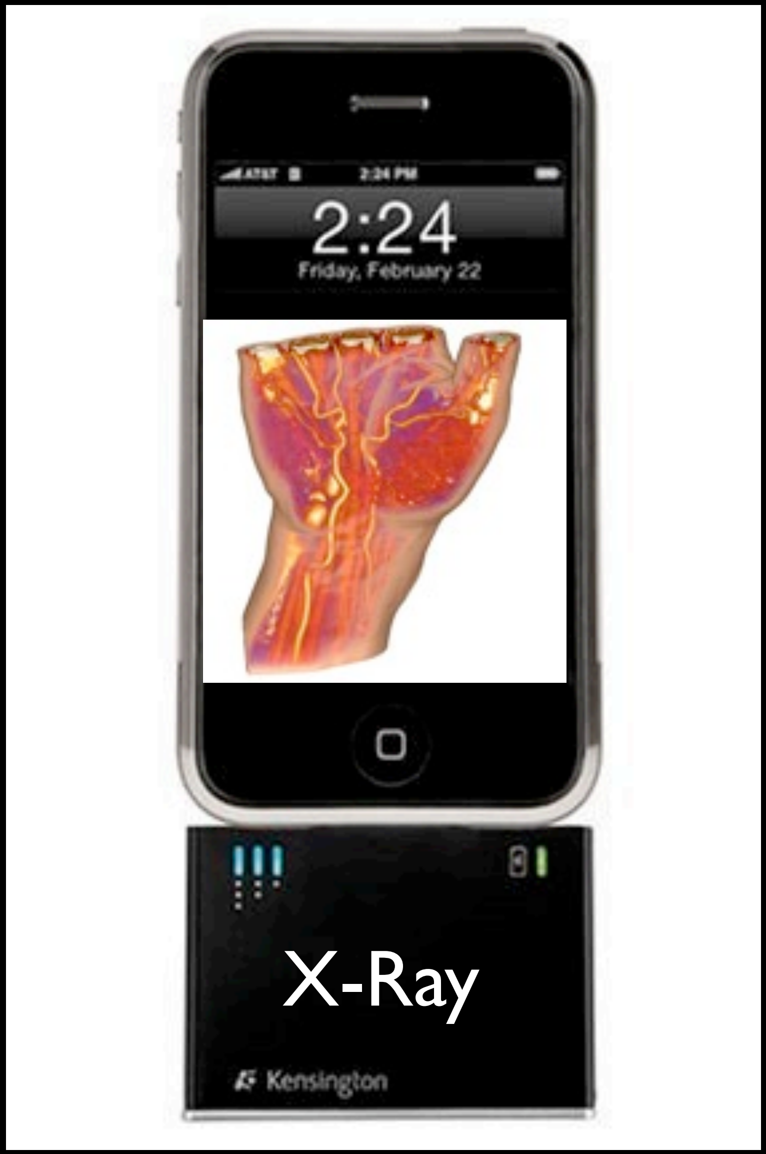


Chip-NMR Biosensor



Hakho Lee, Eric Sun, Donhee Ham & Ralph Weissleder, SEAS & HMS

Tricorders



21st Century

23rd Century

Acknowledgements

- NVIDIA
- Microsoft
- NSF CDI PHY-0835713, Austrian Research Promotion Agency FFG, Vienna Science and Technology Fund WWTF