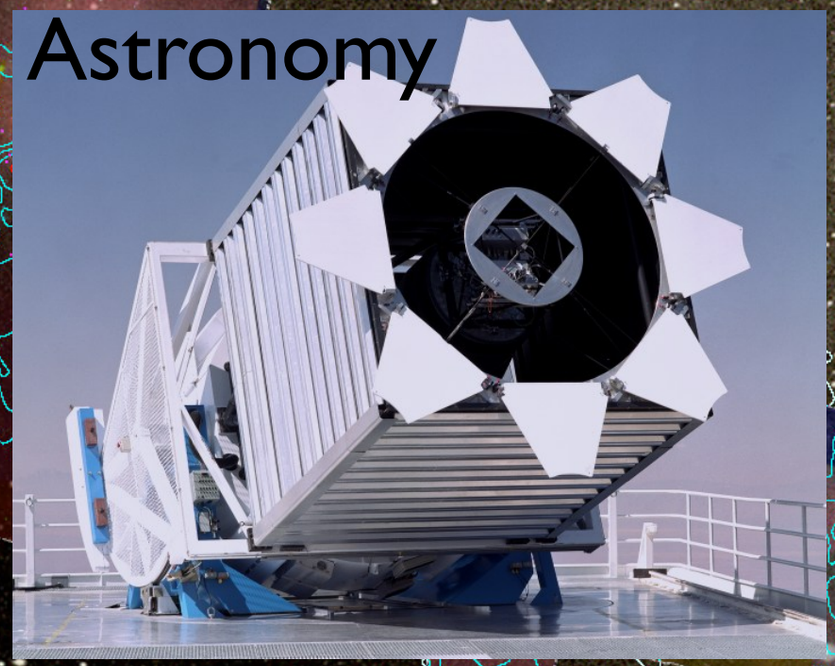
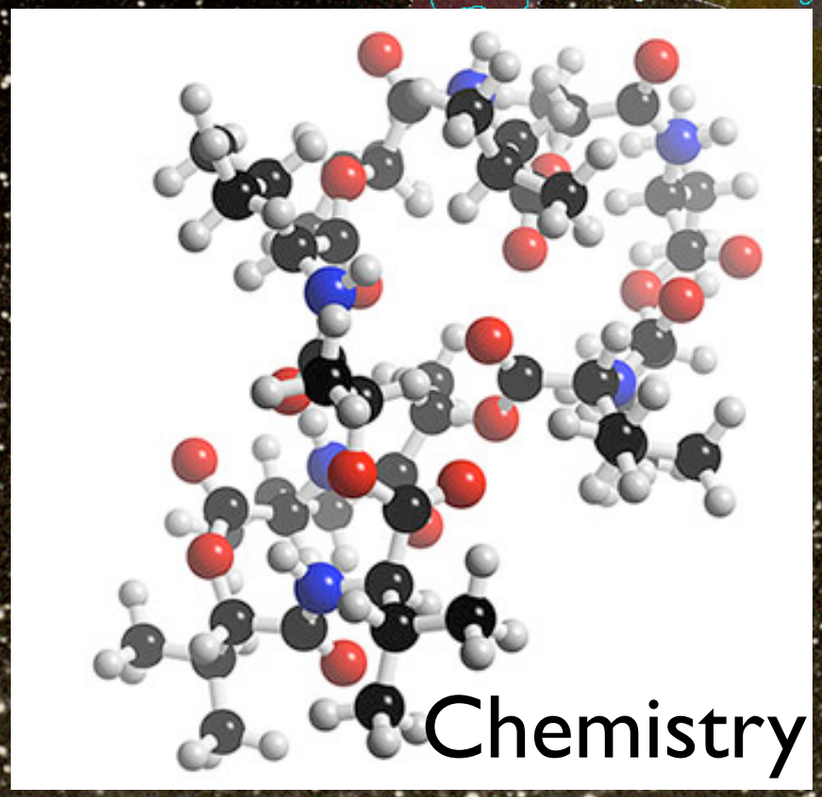
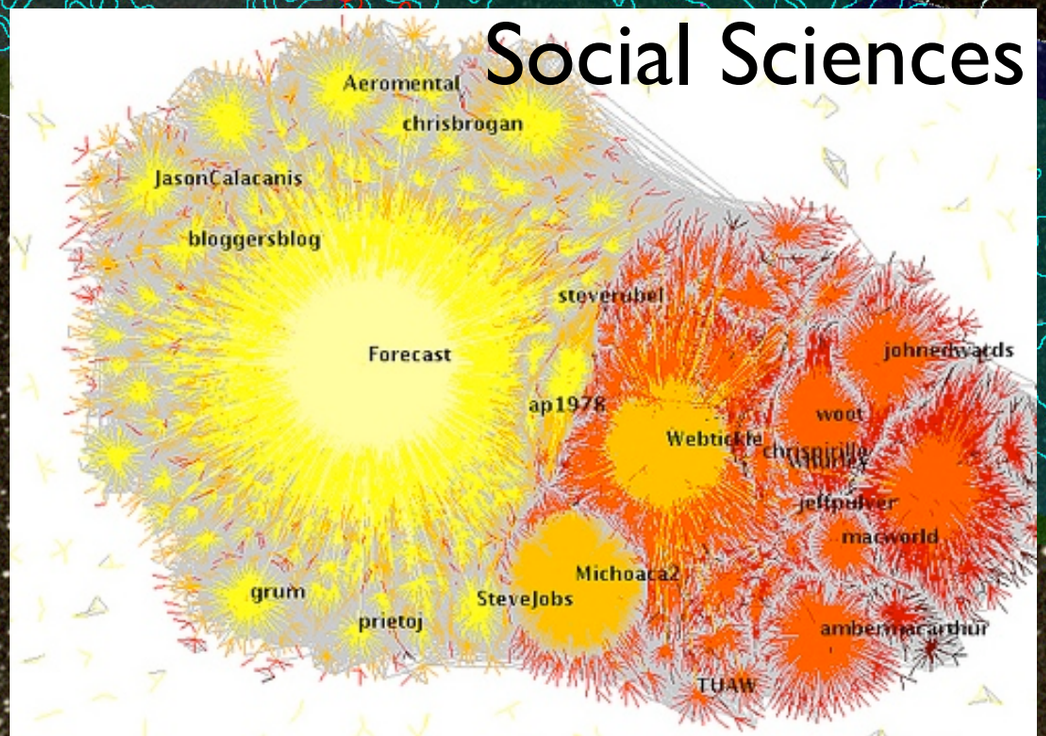
GPUs for High-Throughput Science

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

Scientific Data Explosion



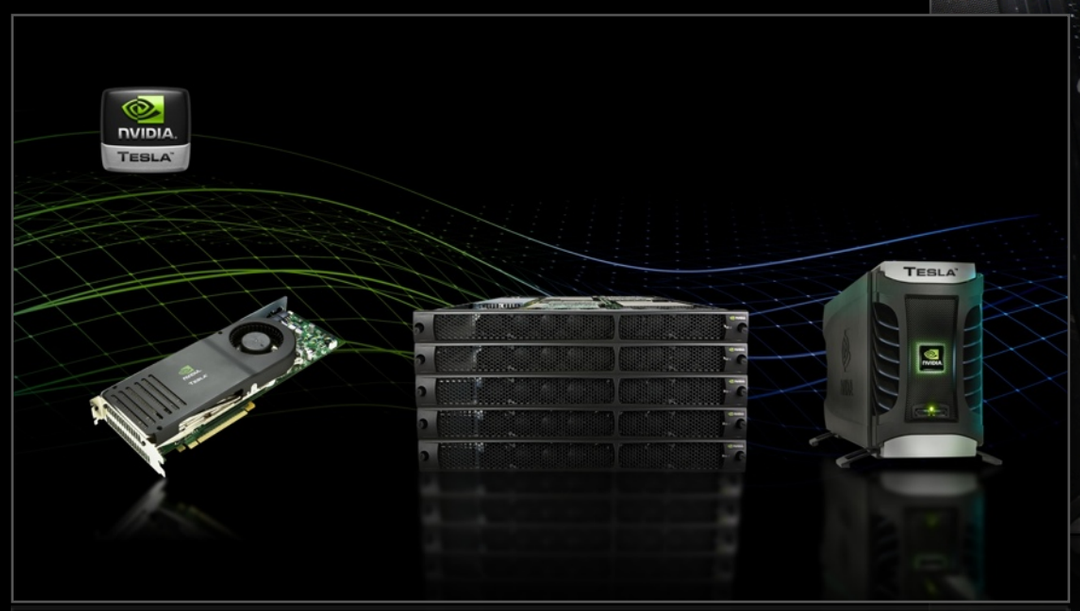




Twitter Social Network © UMBC eBiquity Research Group

Computing Revolution

- Commodity energy-efficient supercomputers



4 Teraflops @ 1400 W

SE
S
[S]
[U]

Traditional

Sensor

Modeling
Simulation
Analysis

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

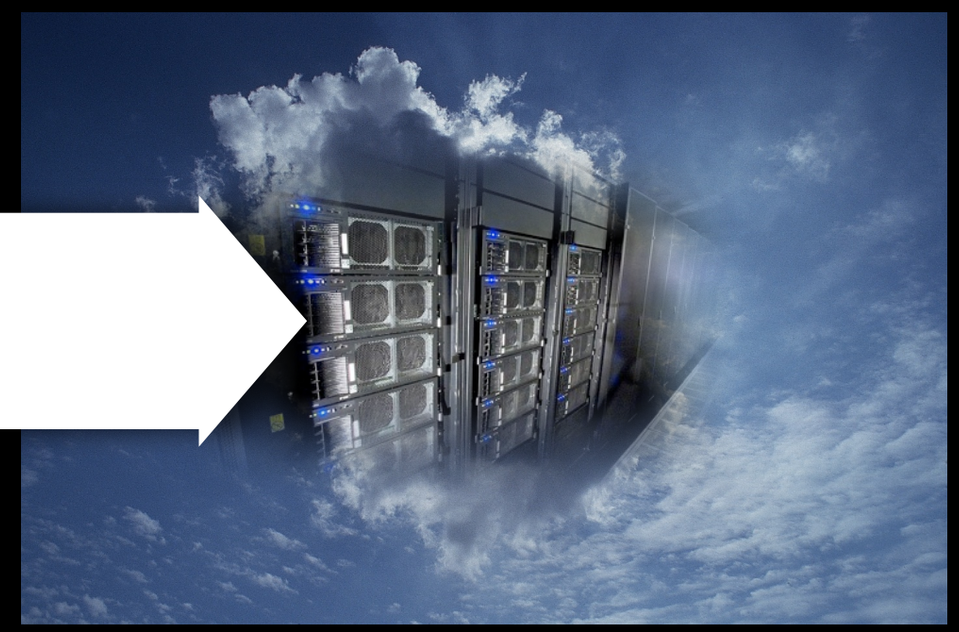
By **David Neal**

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

Modeling
Simulation
Analysis

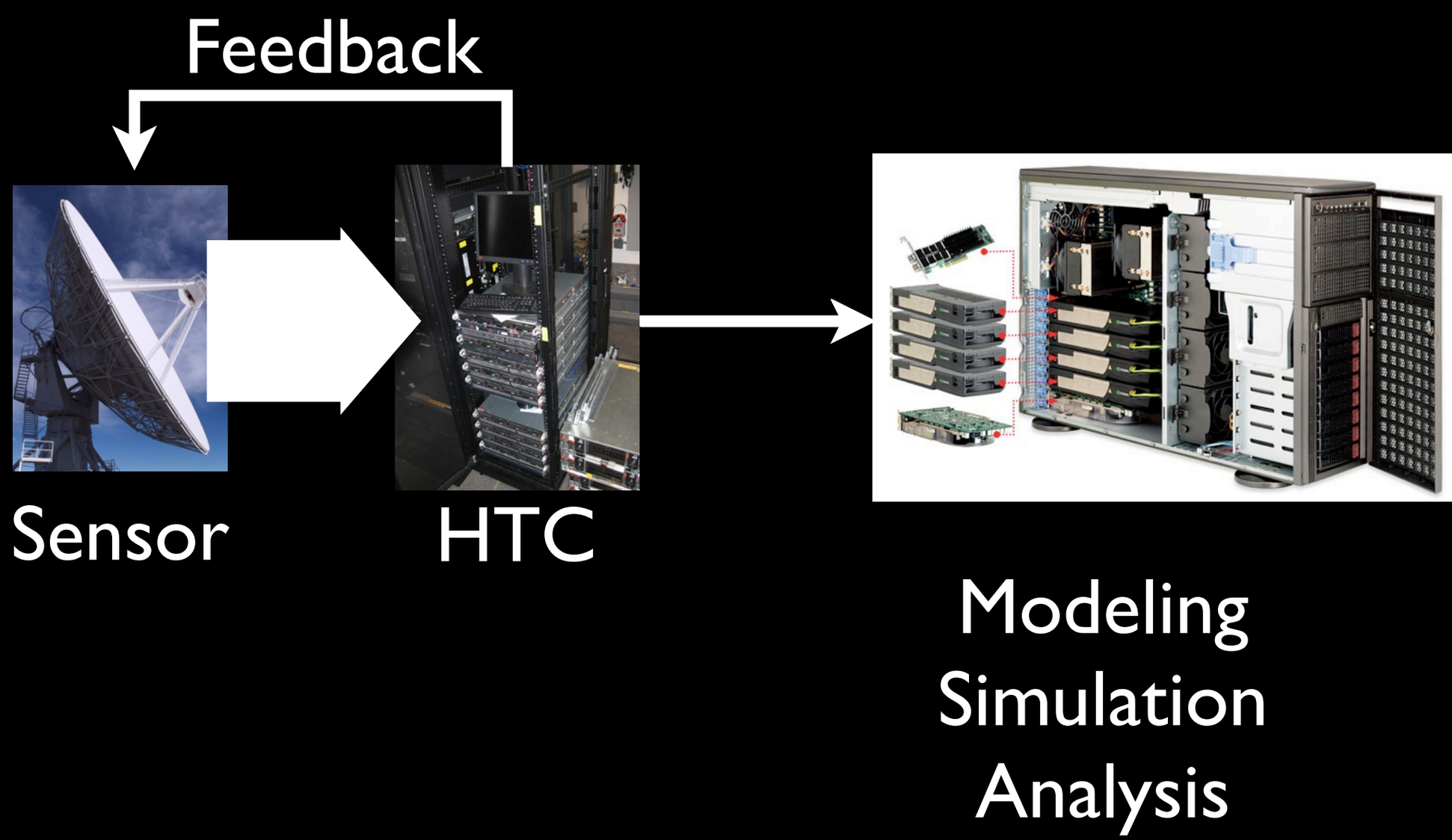
High-Throughput Computing

Sensor

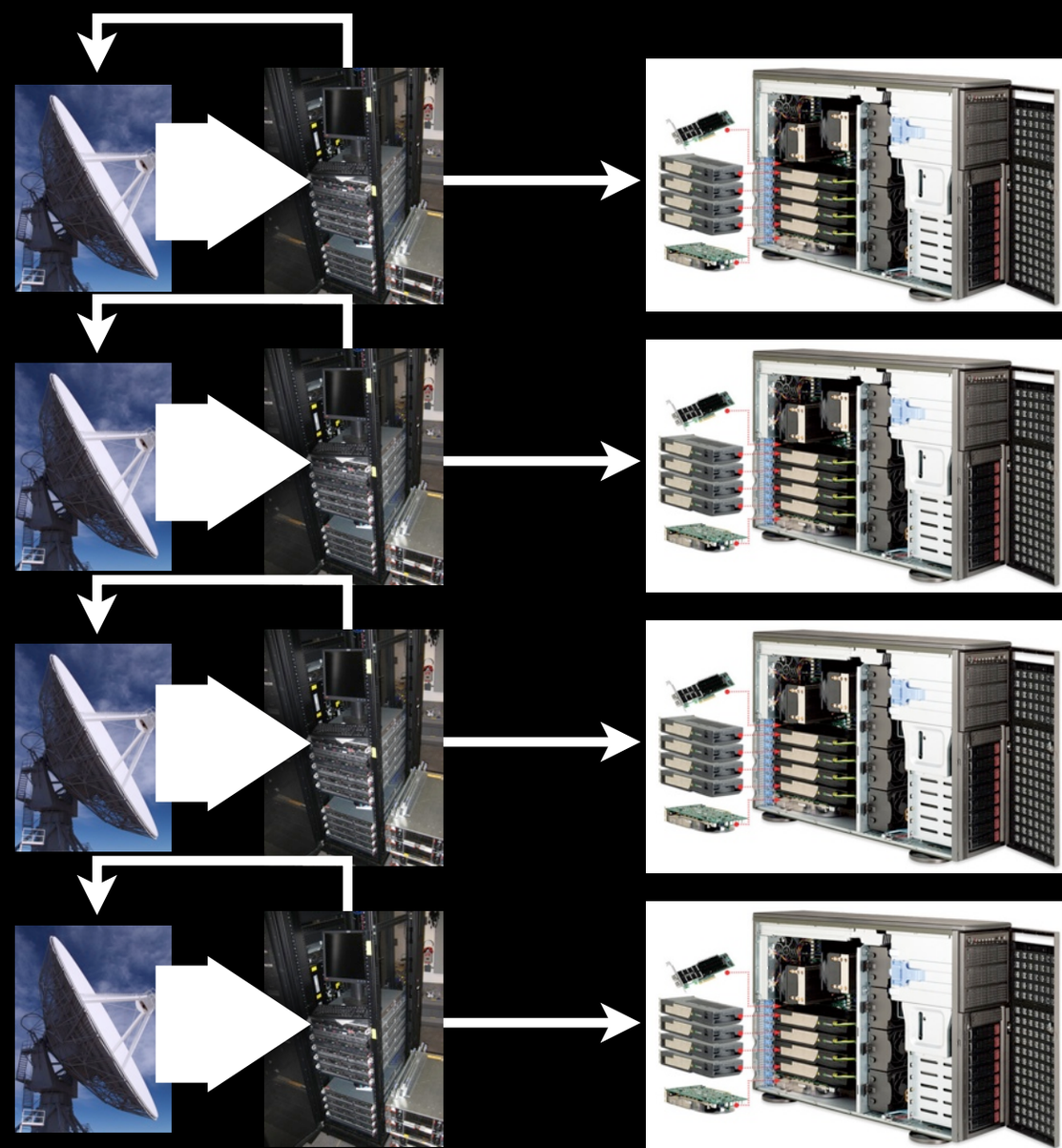
HTC

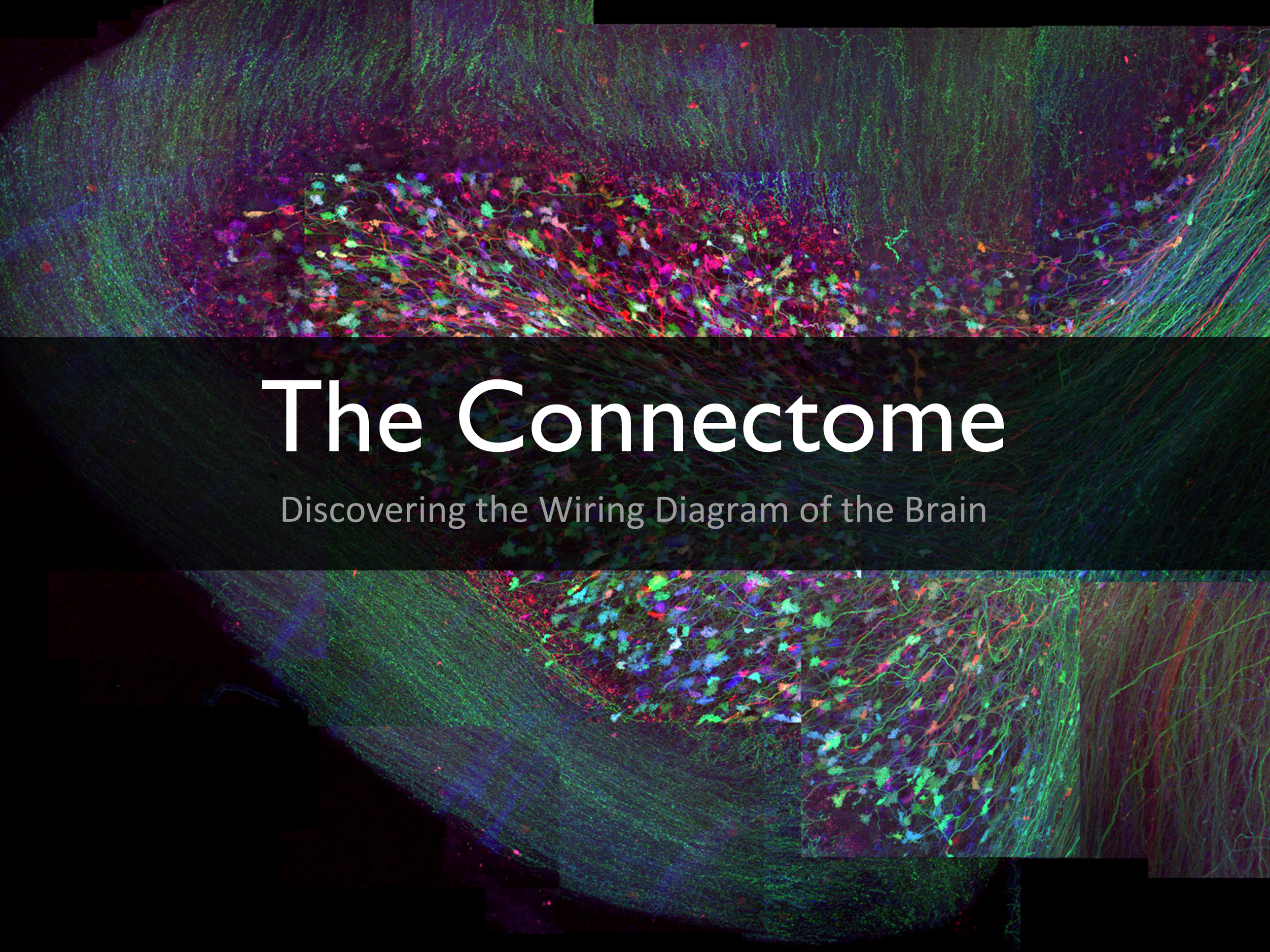
Modeling
Simulation
Analysis

High-Throughput Computing



High-Throughput Computing





The Connectome

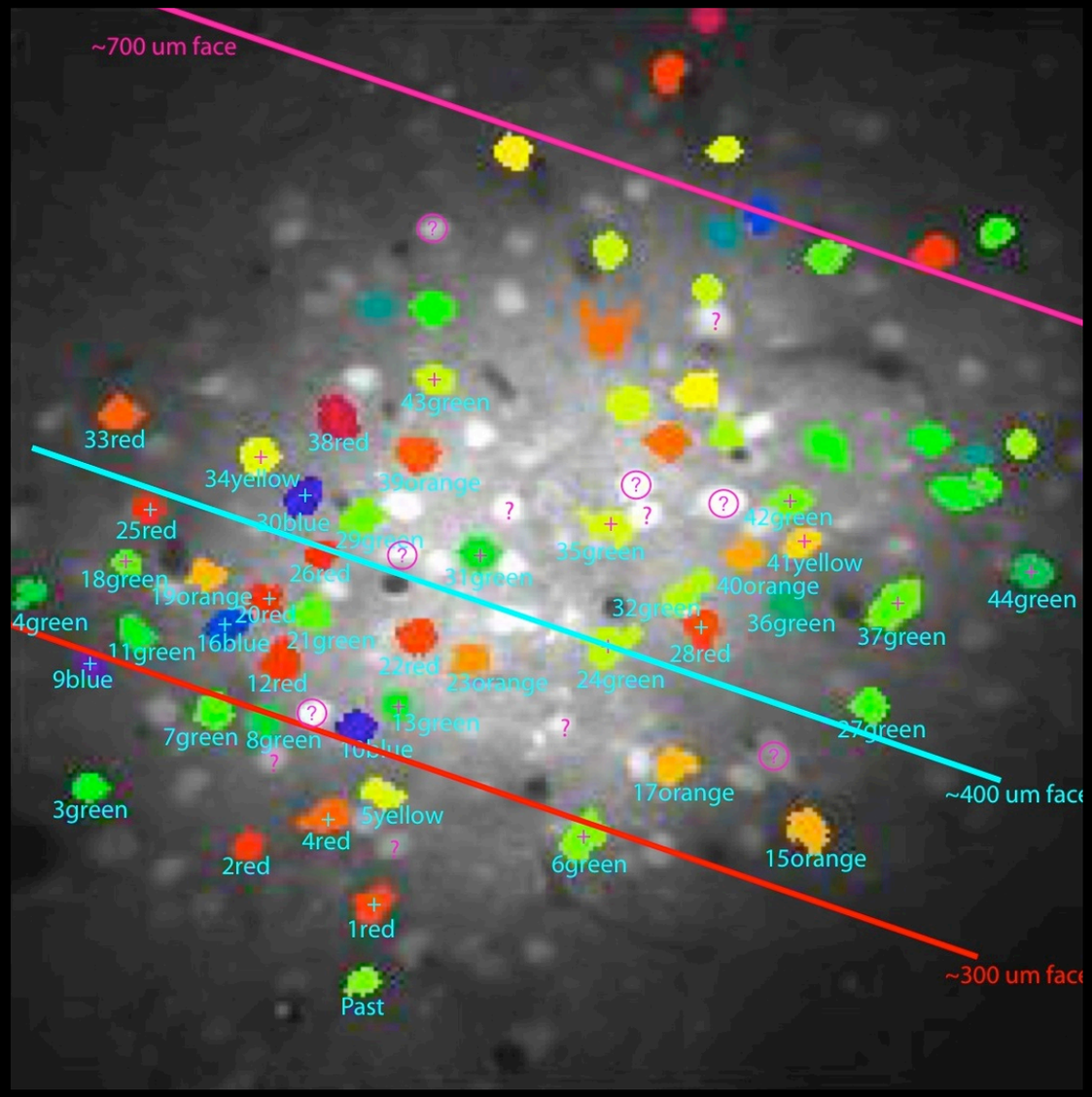
Discovering the Wiring Diagram of the Brain

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

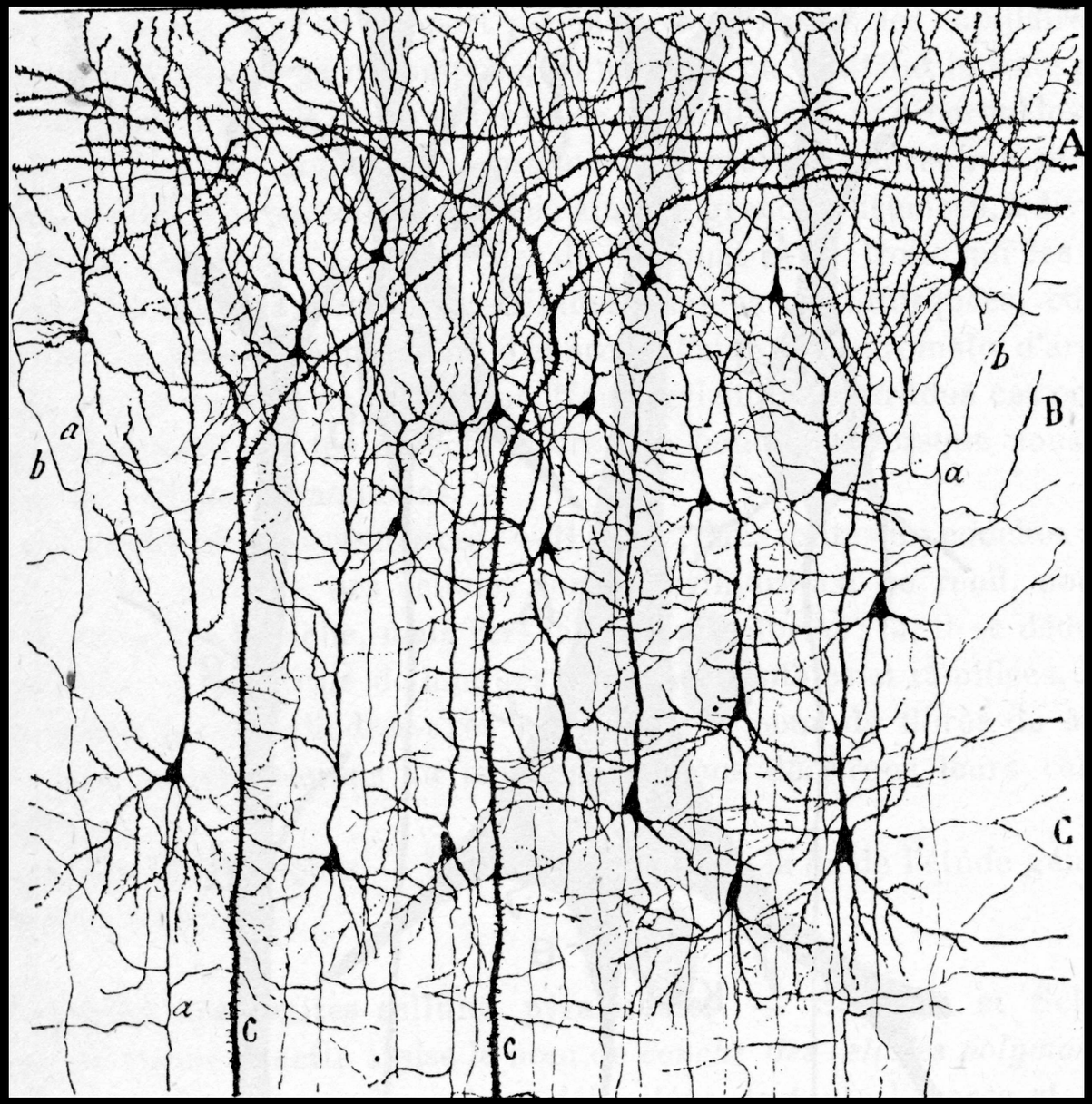
- What do large brain circuits do?



C. Reid

The Scientific Challenge

- What is their connectivity?

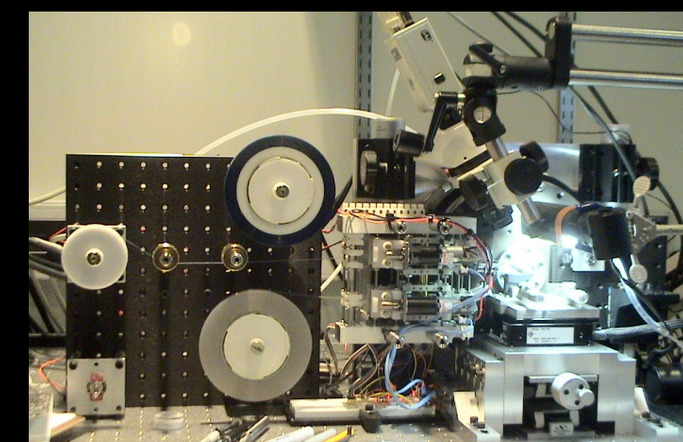


Ramón y Cajal, 1905

Connectome Workflow

Get a brain →

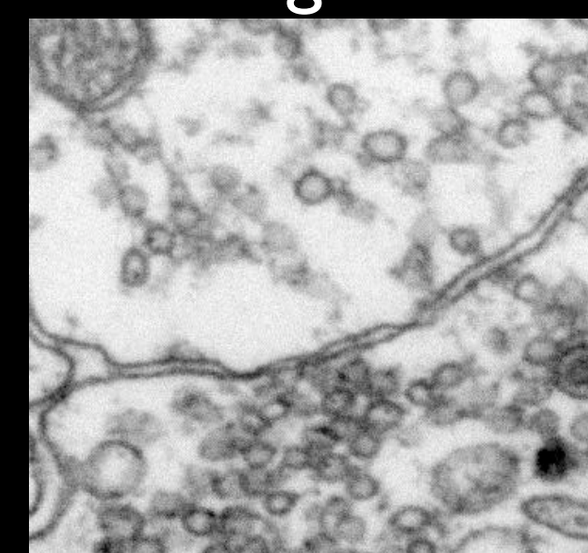
Get a piece →



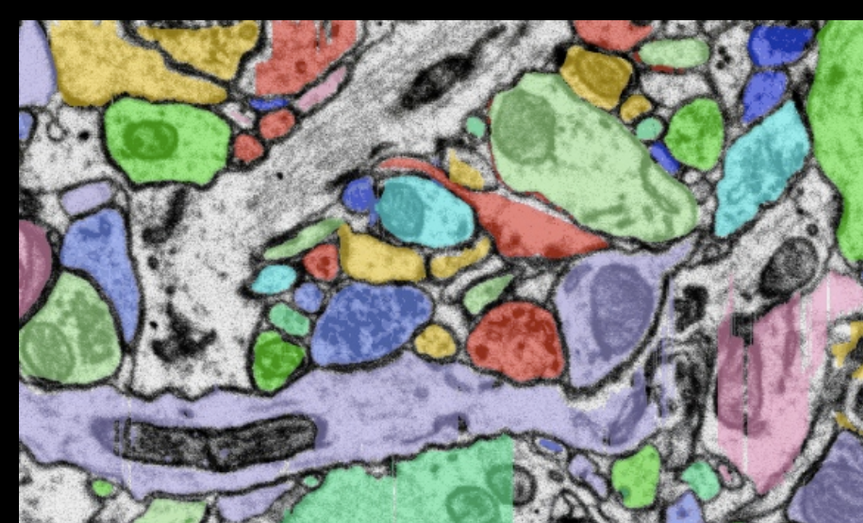
Cut it thin

↓

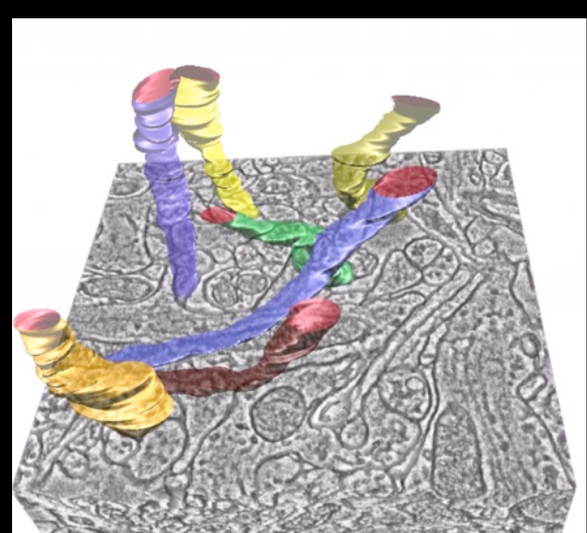
Image it ←



Reconstruct ↔

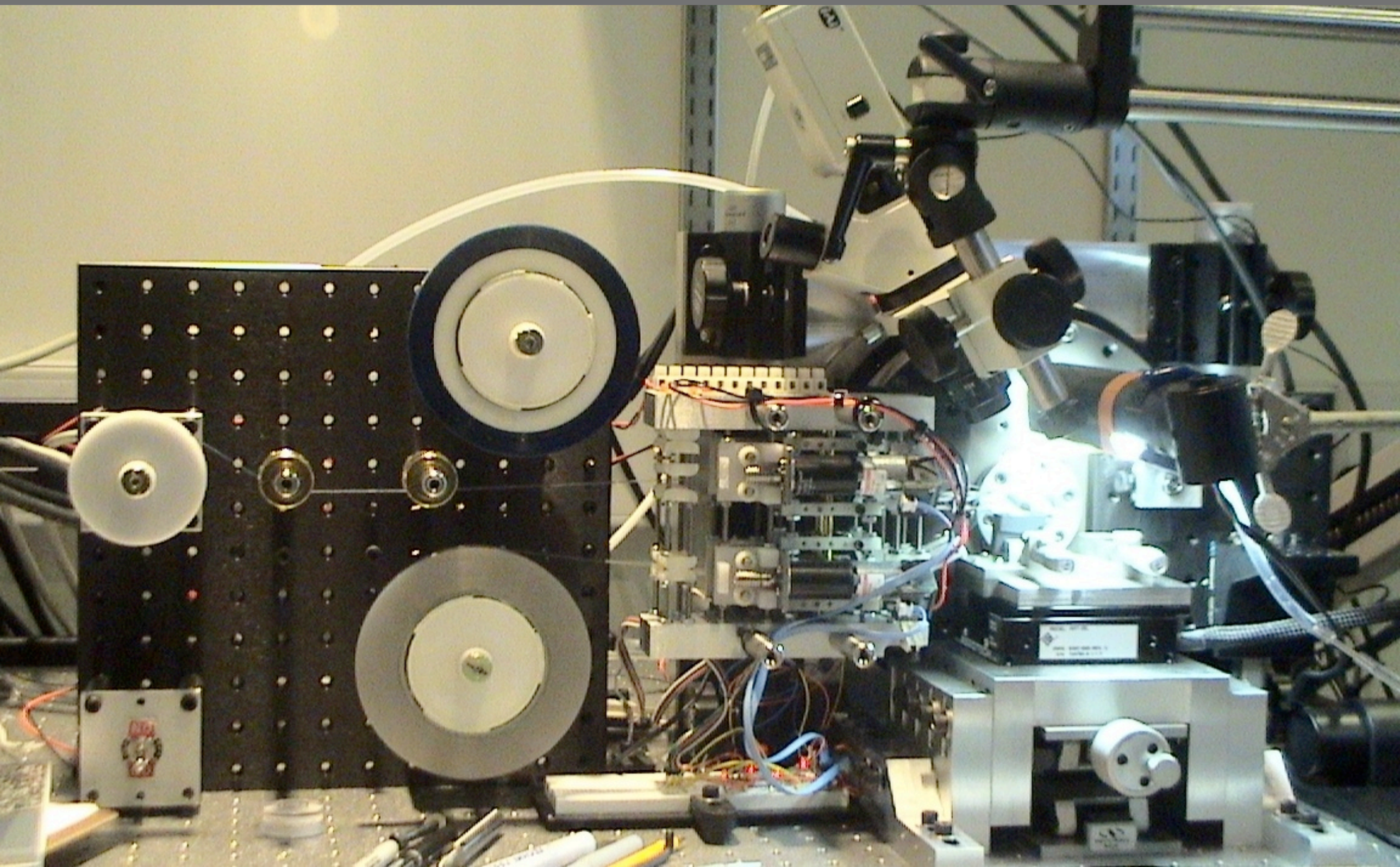


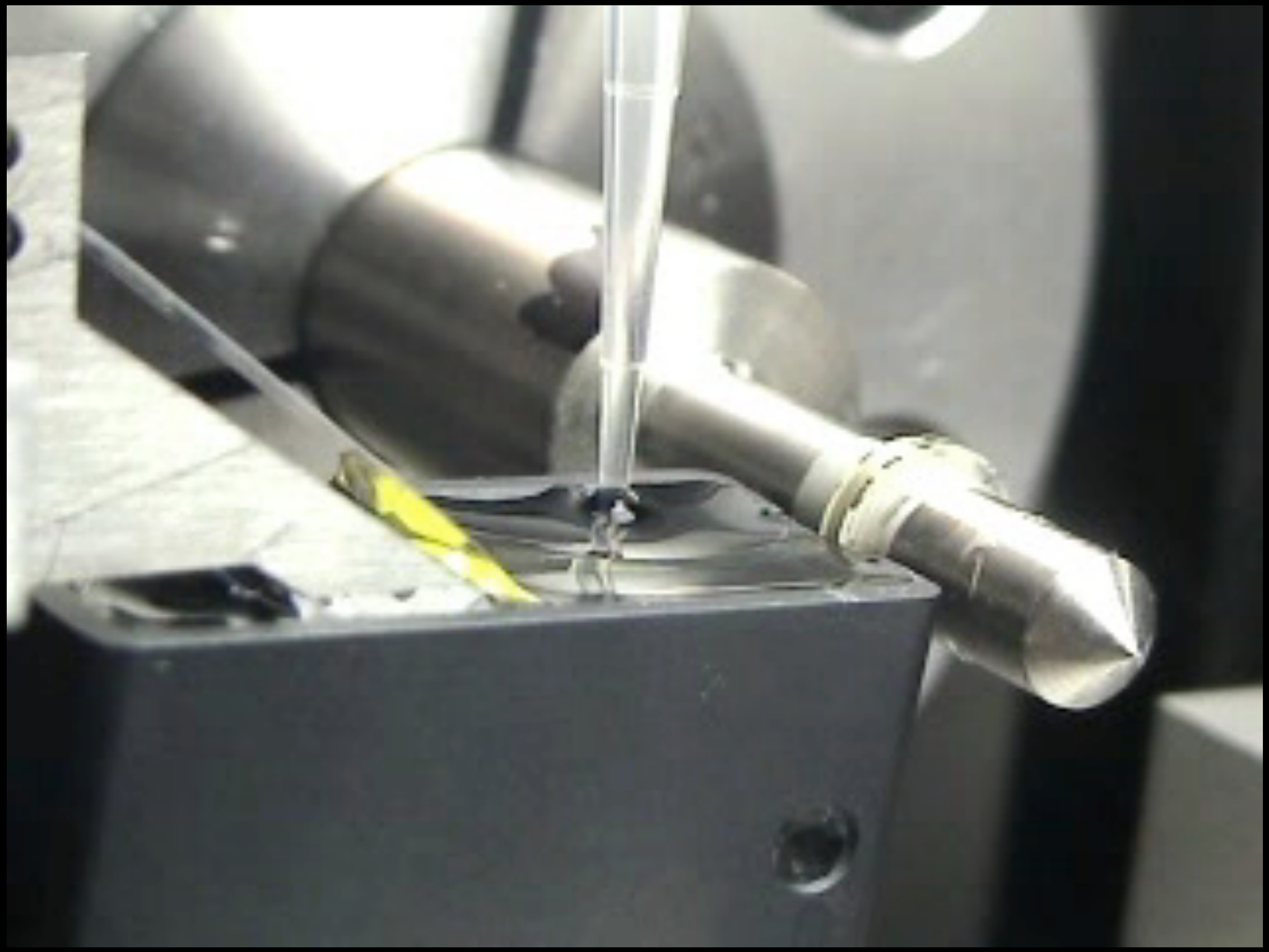
Visualize & Analyze



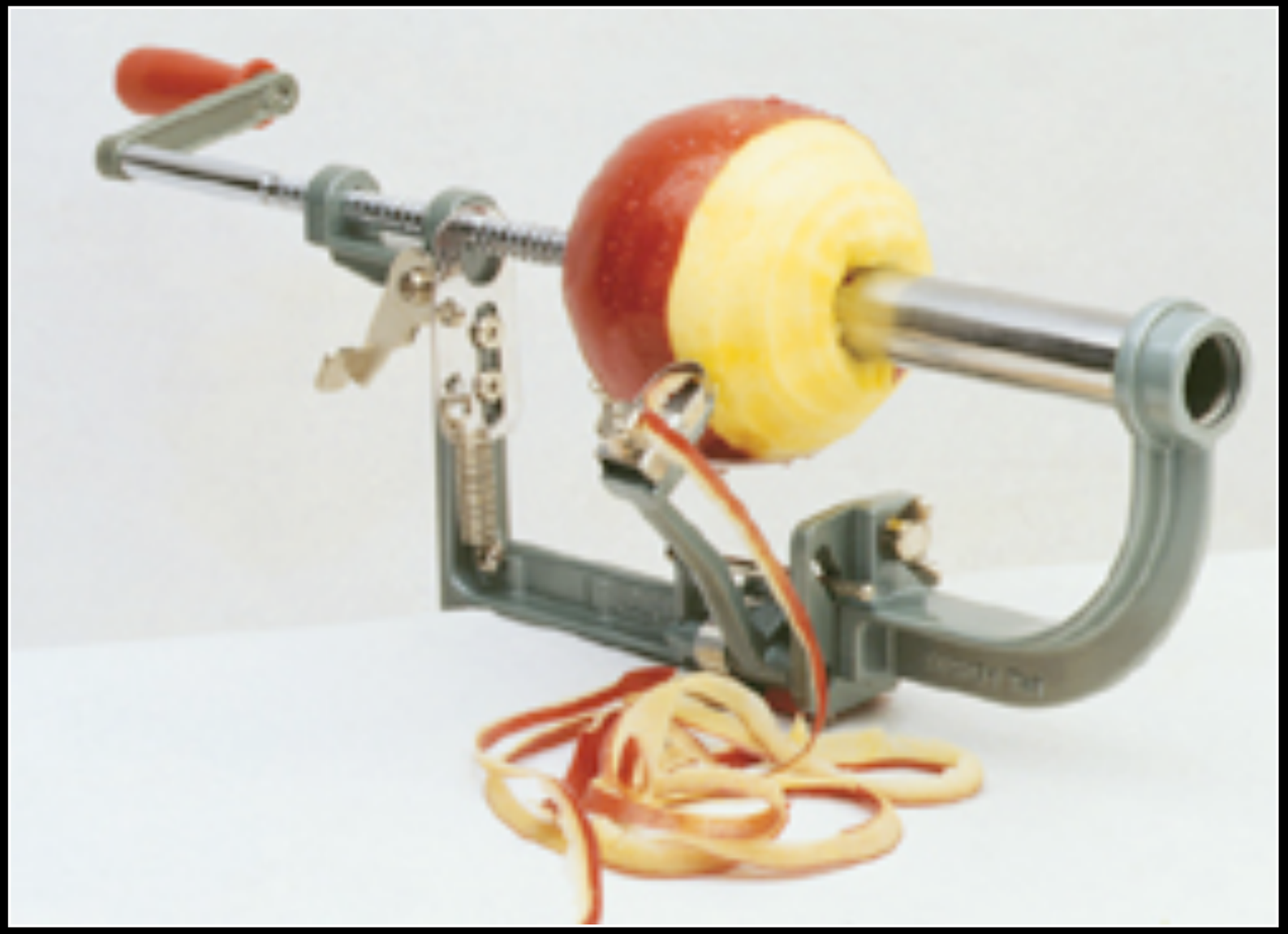
Brain on Tape: Automatic Tape-collecting UltraMicrotomes

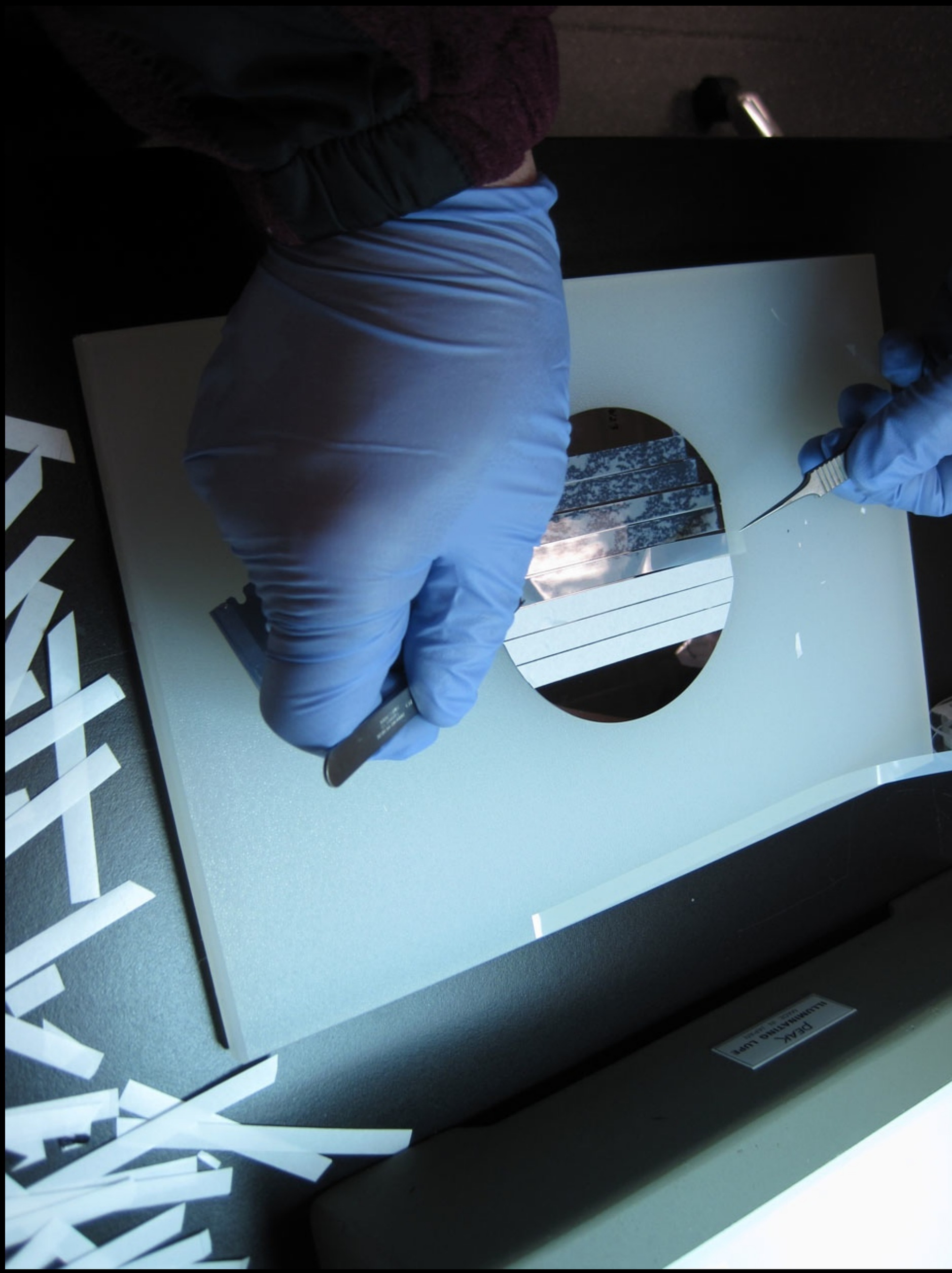
Ken Hayworth & Bobby Kasthuri



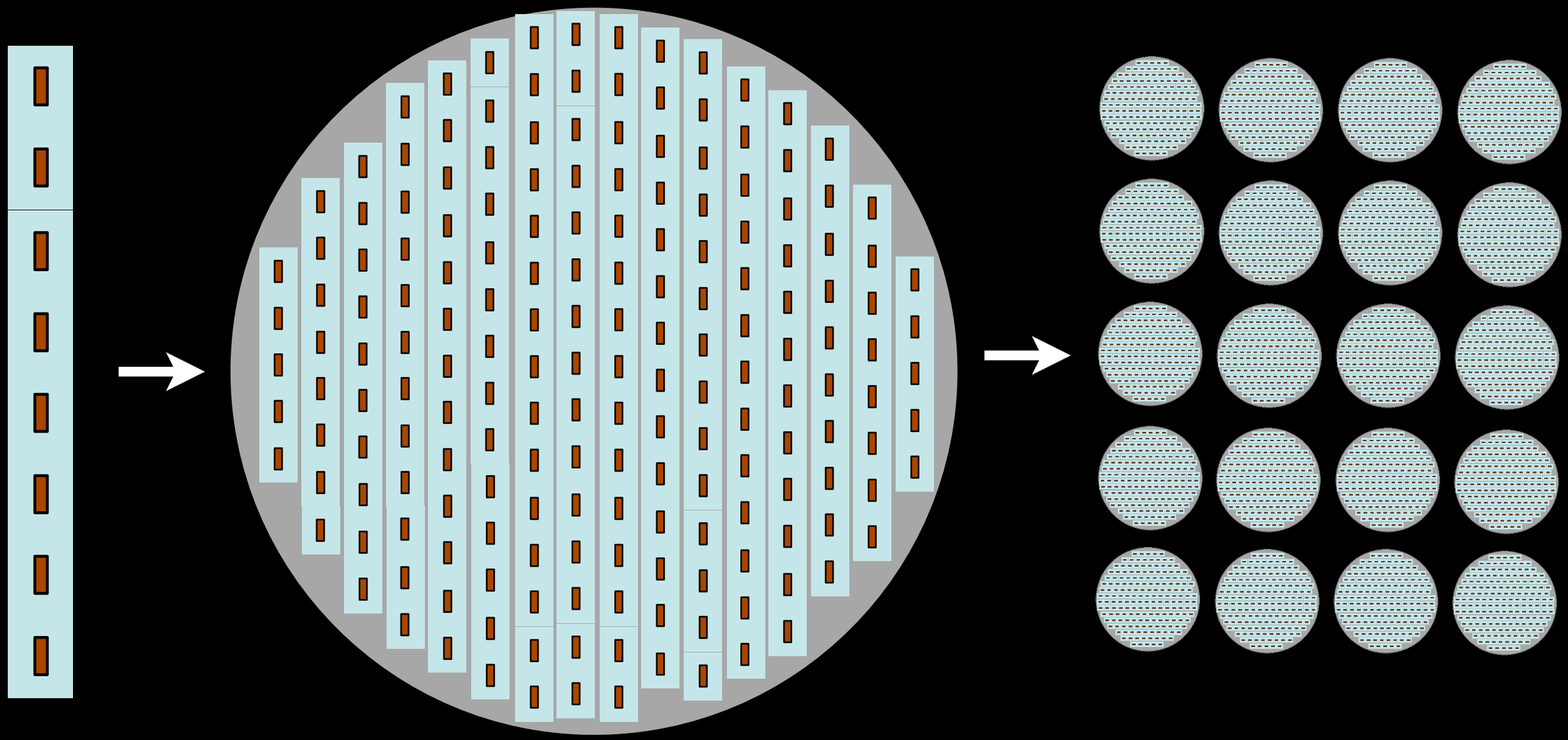


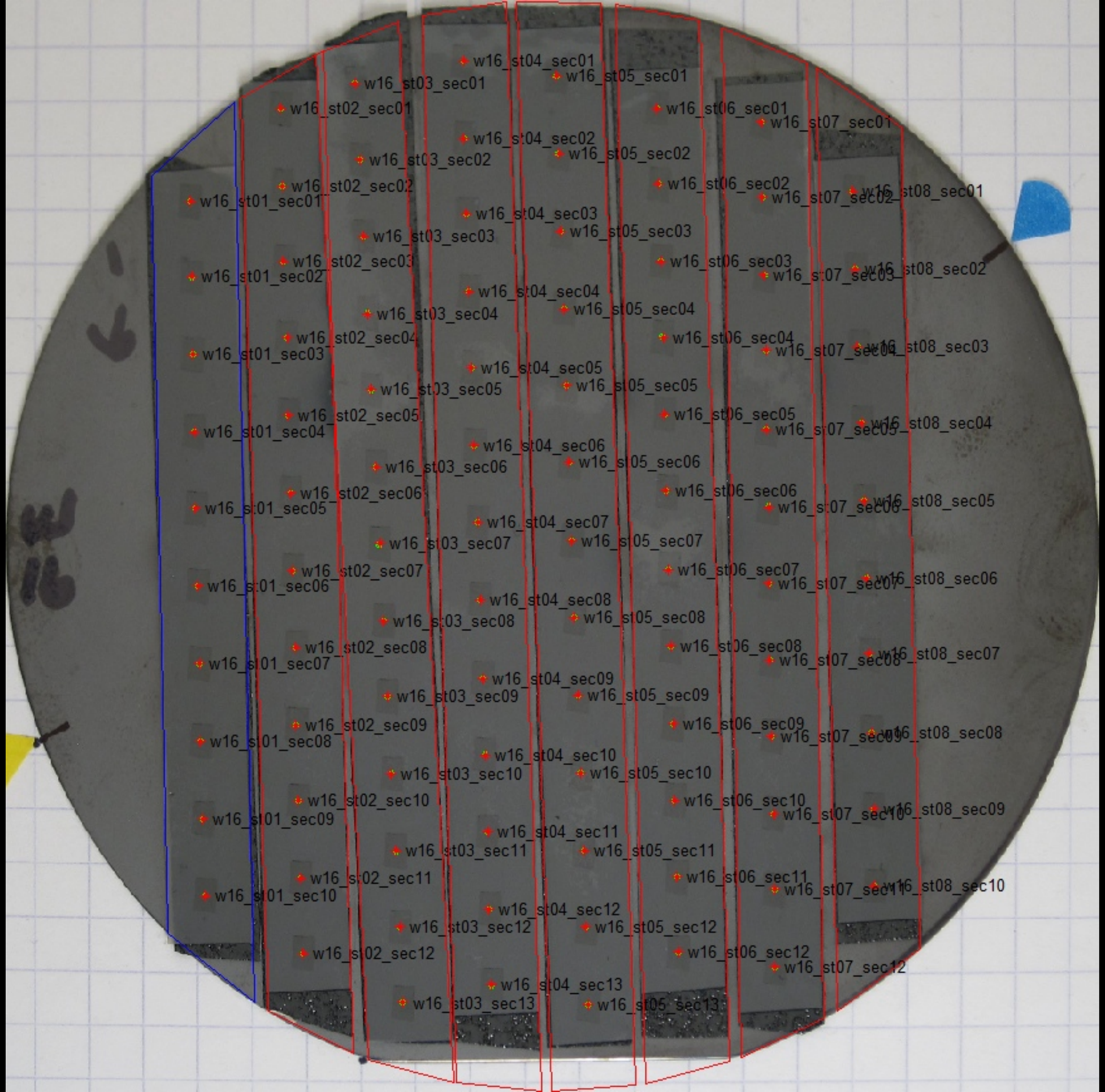
Inspiration for ATLUM




PEAK
ILLUMINATING LIFE

Ultrathin Section Libraries




w16_st04_sec01
w16_st05_sec01
w16_st03_sec01
w16_st02_sec01
w16_st06_sec01
w16_st07_sec01
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w16_st02_sec12
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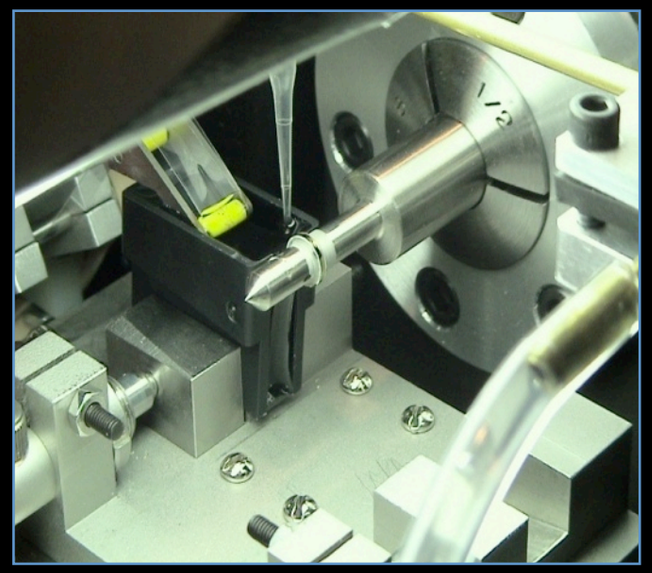
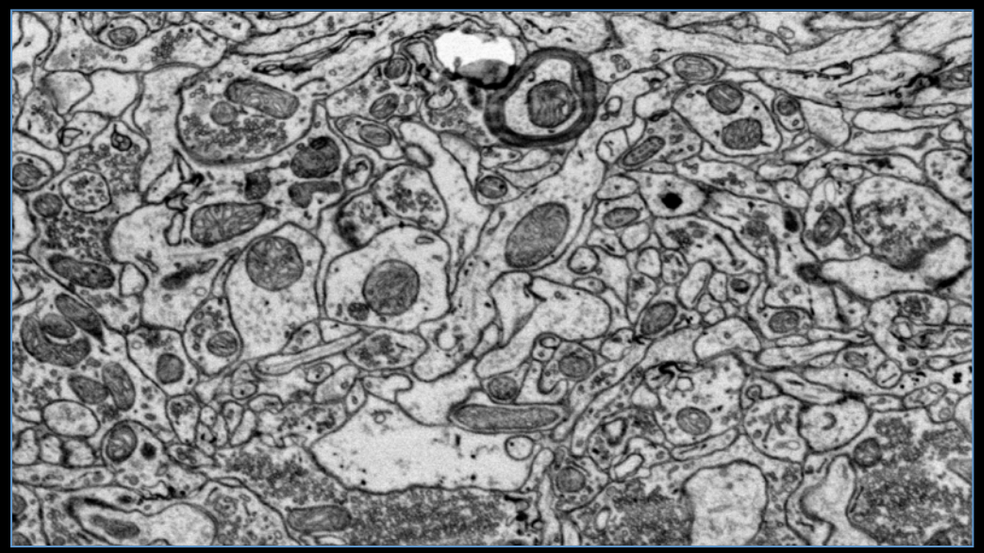
w16_st03_sec13

The Data Challenge



3 nm x 3 nm x 30 nm

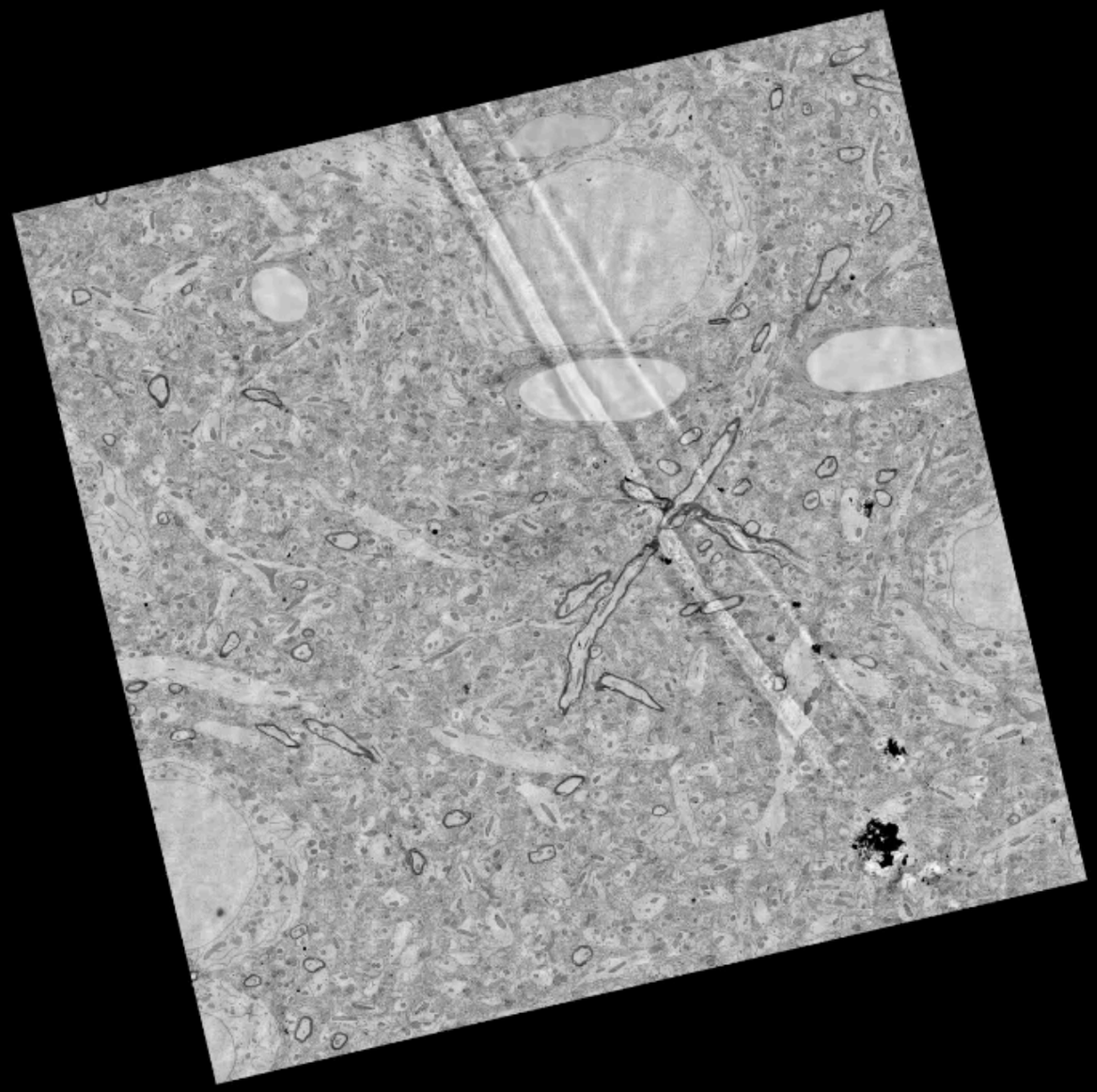


2M

1M

- Mouse thalamus ~= 1 mm^3 ~= 1 petabyte

NeuroTrace



Interactive navigation of 1TB brain dataset

W. Jeong et al., IEEE TVCG 2009

Active Ribbons

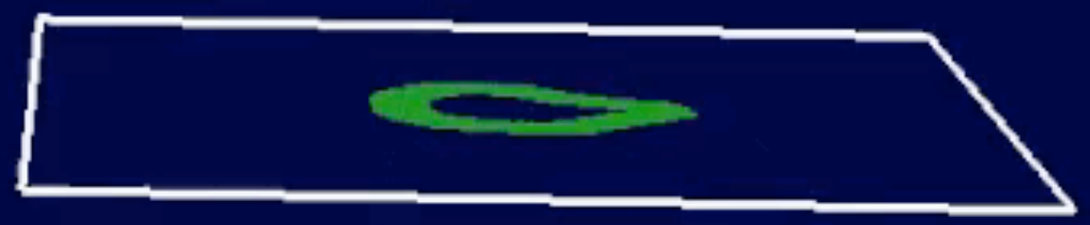
Section 1

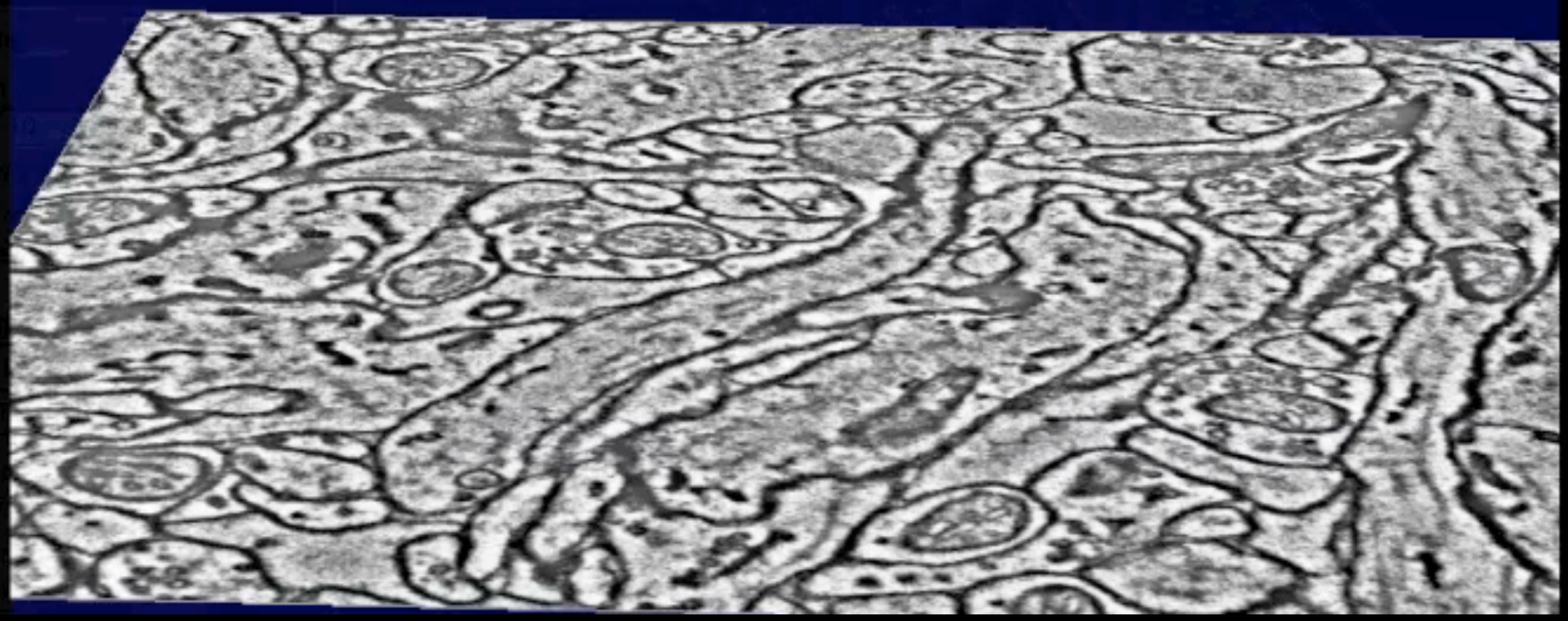
A. Vazquez et al., CVPR 2009

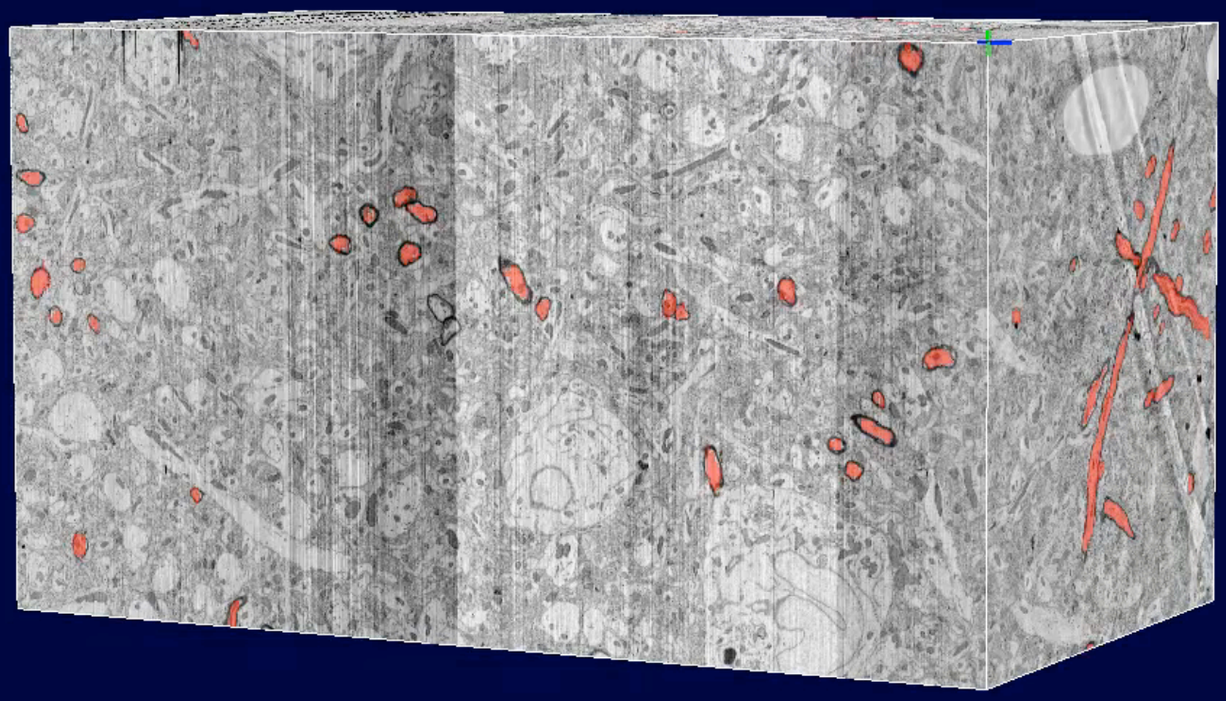
GPU Processing

- Active Ribbons on GPUs: 23x speedup

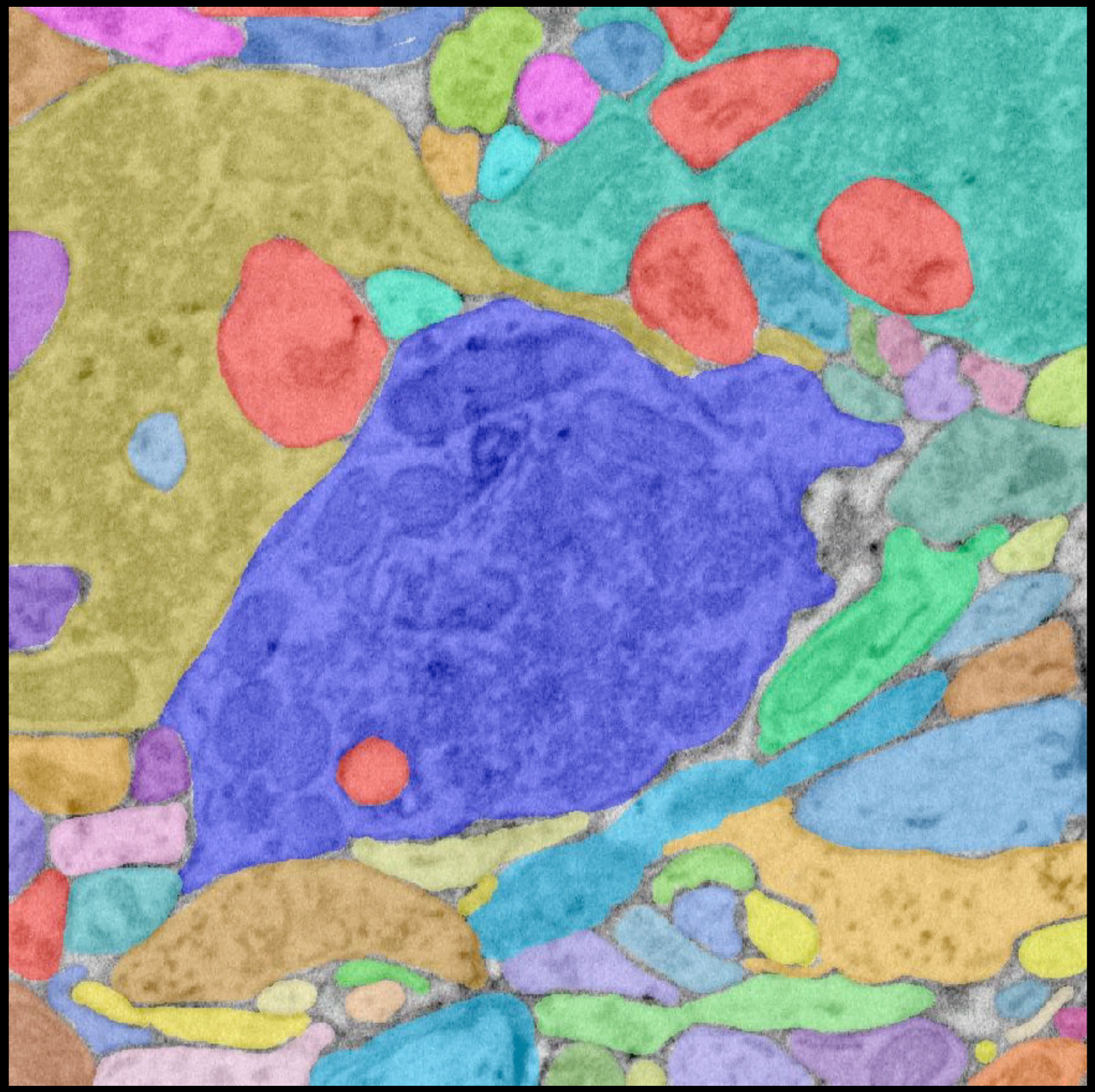
W. Jeong et al., IEEE TVCG 2009







“Temporal” Coherence

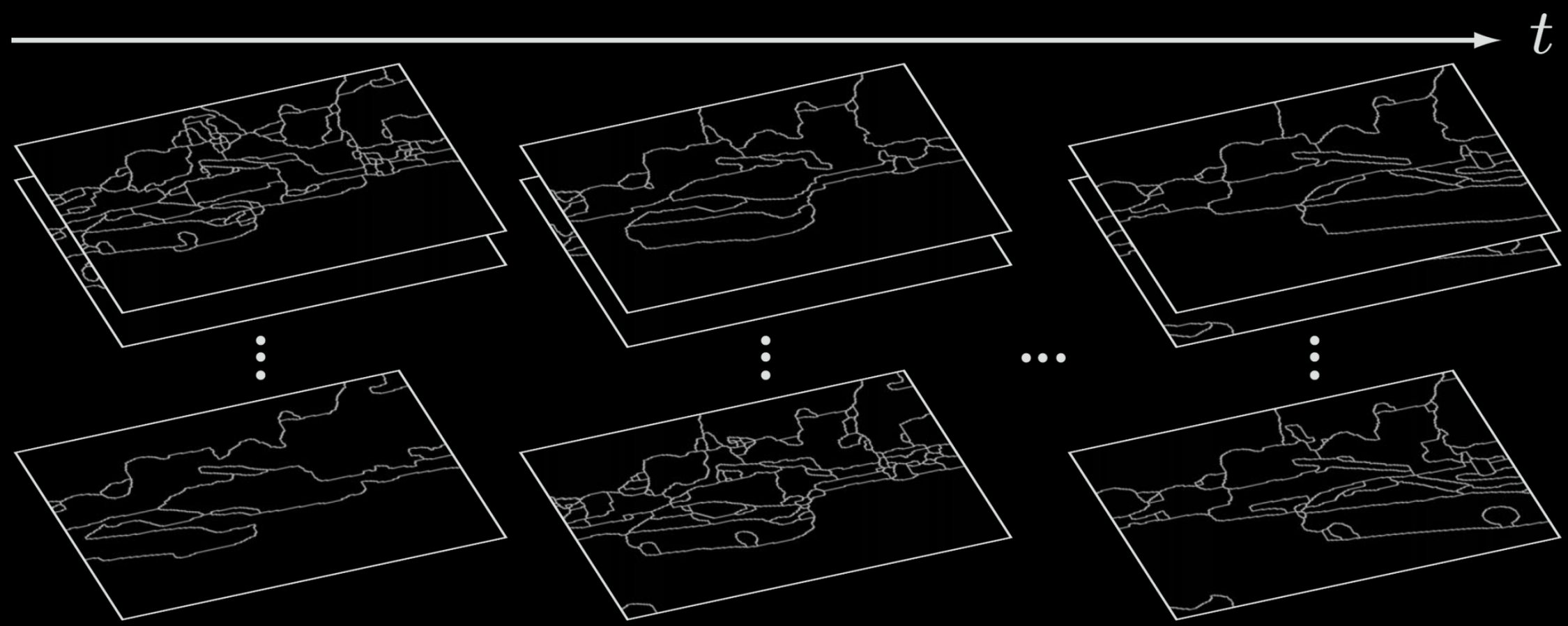


D. Berger, MIT

Multiple Hypothesis Video Segmentation

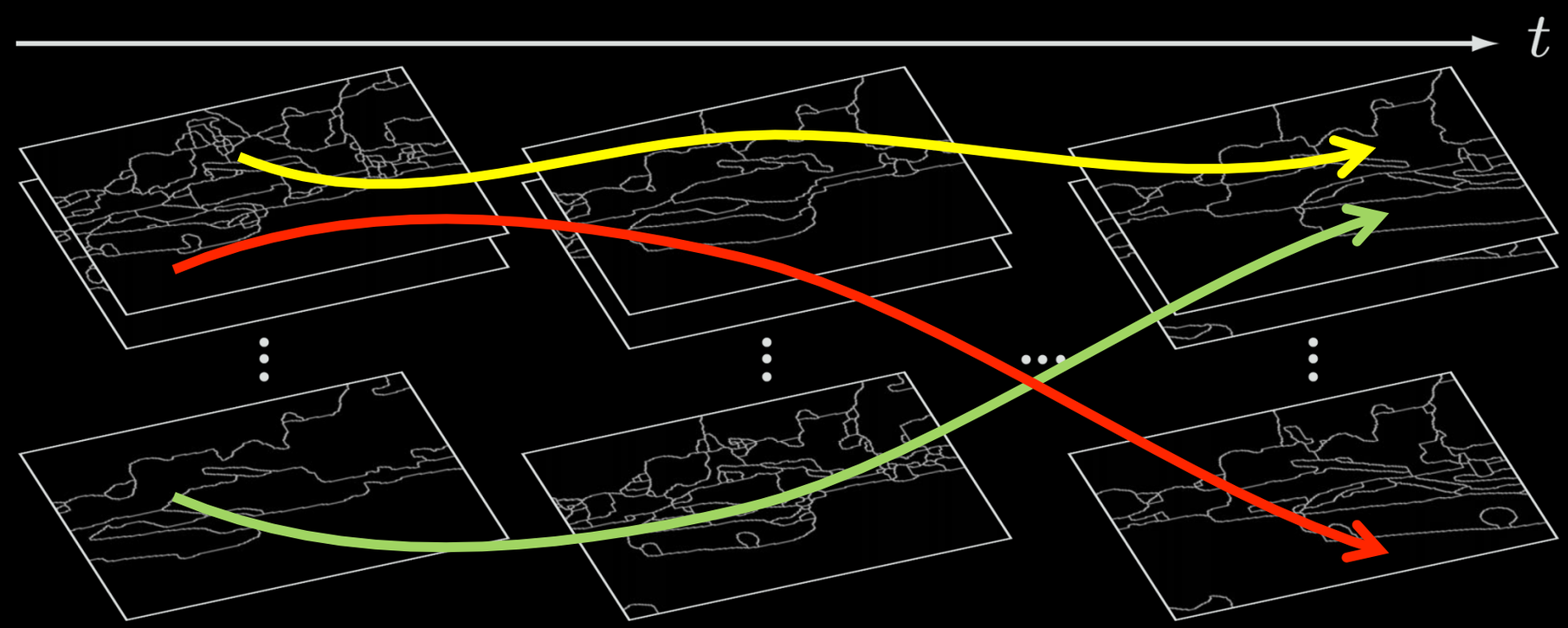
A. Vazquez et al., ECCV 2010

Multiple Hypothesis Video Segmentation



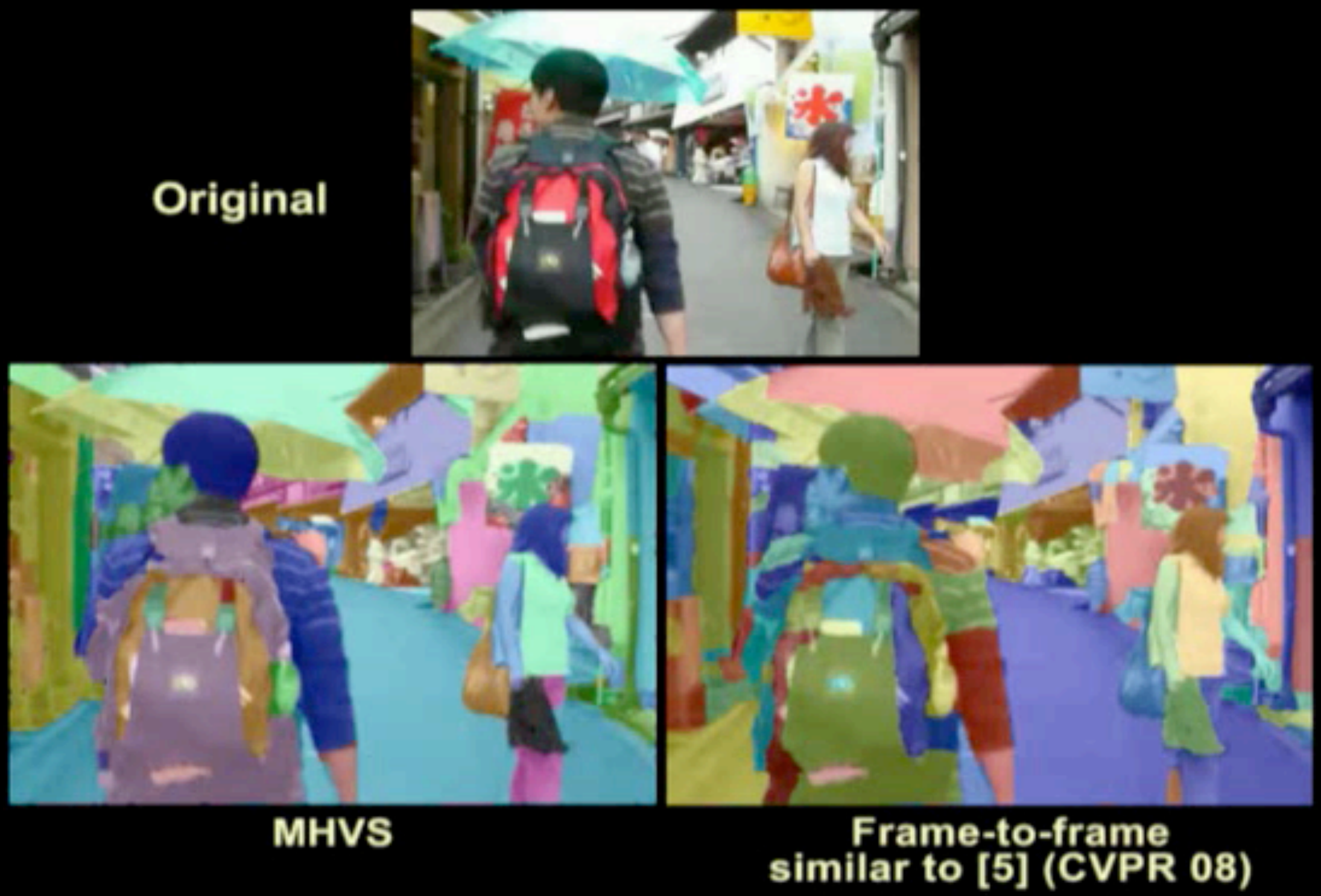
Multiple Possible Segmentations per Frame
(gPb-OWT-UCM etc.)

Multiple Hypothesis Video Segmentation



Enumerate multiple trajectory hypotheses
Solve with higher-order MRF & graph cuts

Qualitative Evaluation



High-Throughput Neuroscience

Select Region

Images

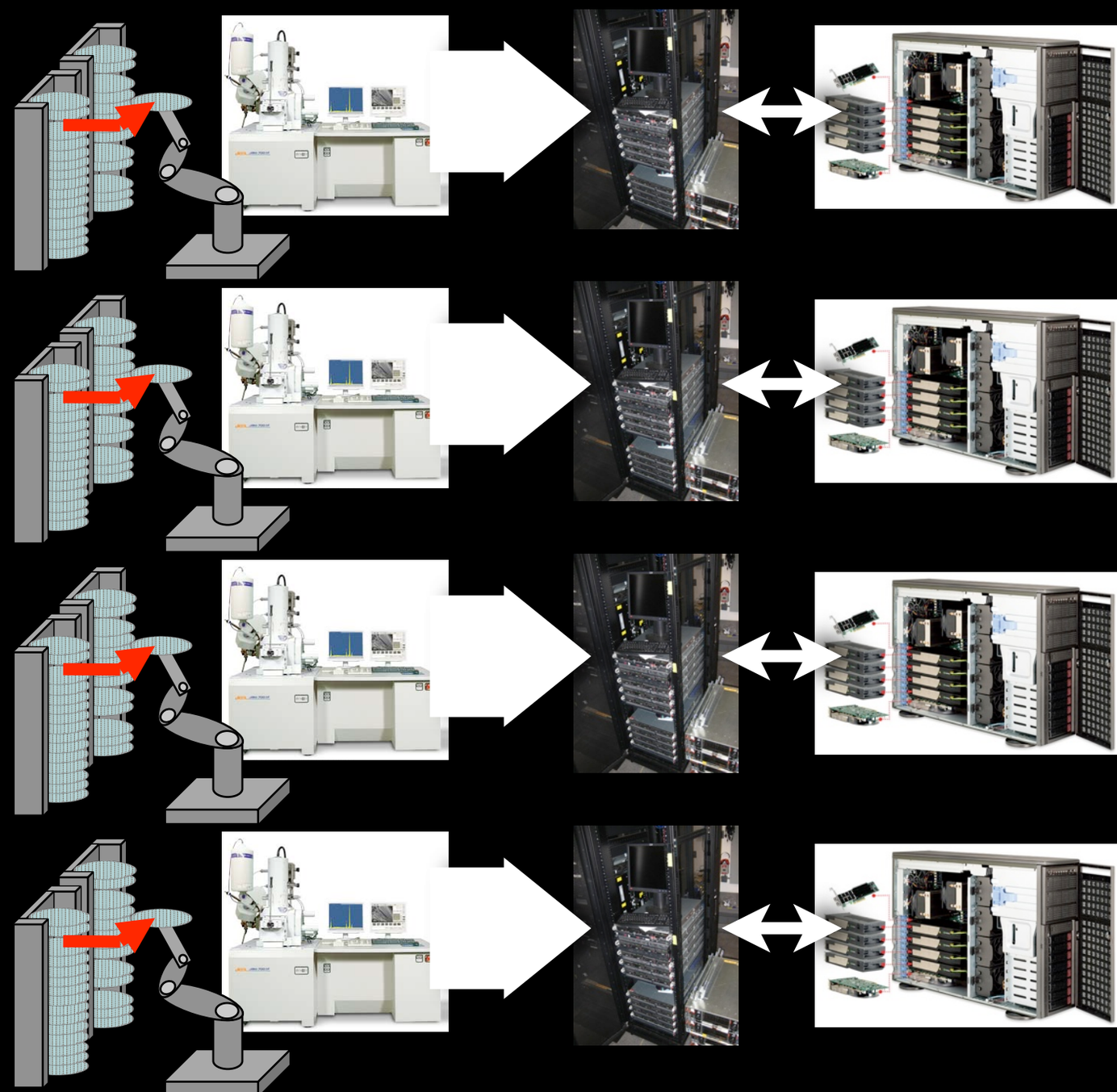
Geometry

EM

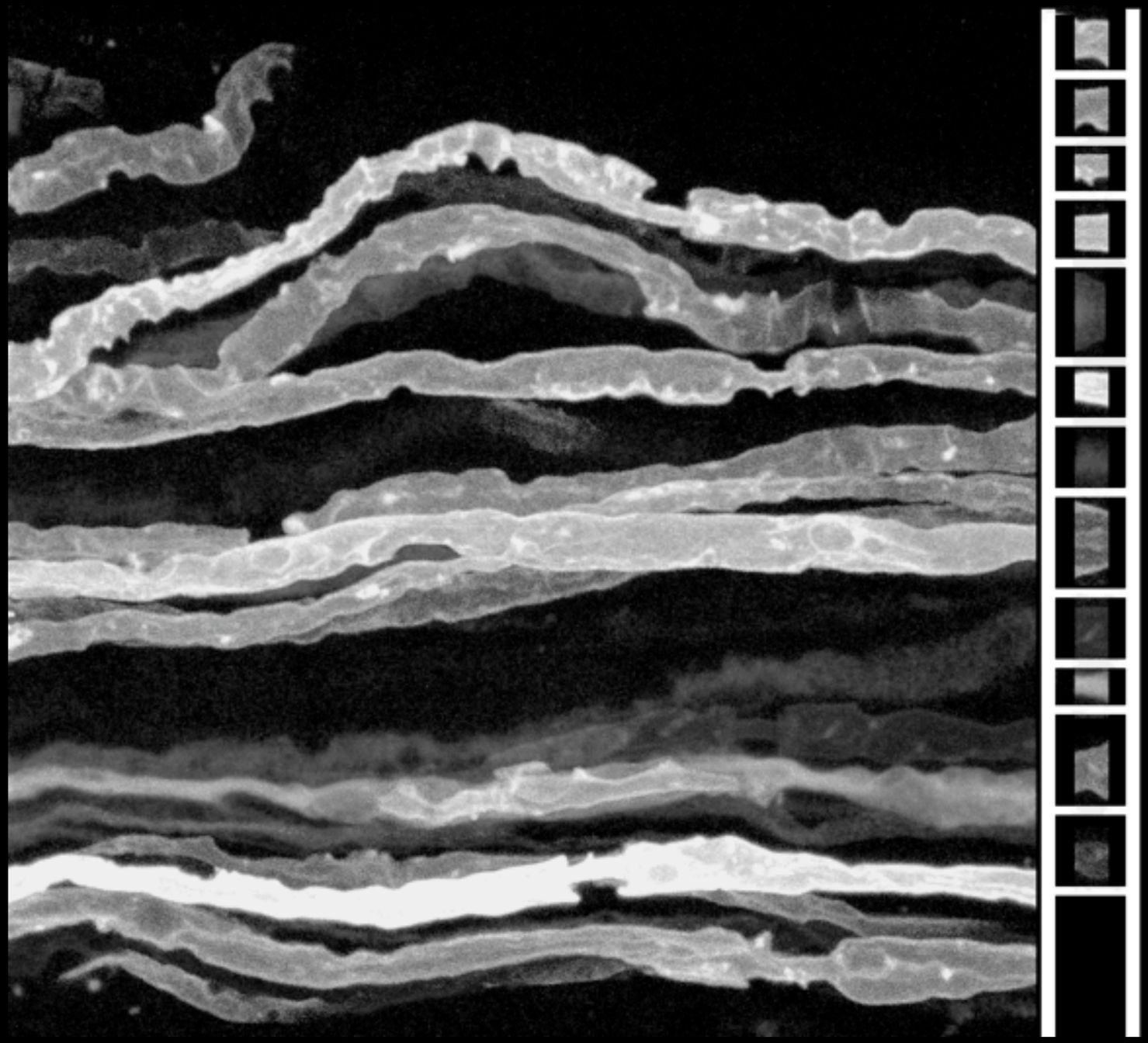
Reconstruction

Visualization
Analysis

Scalable

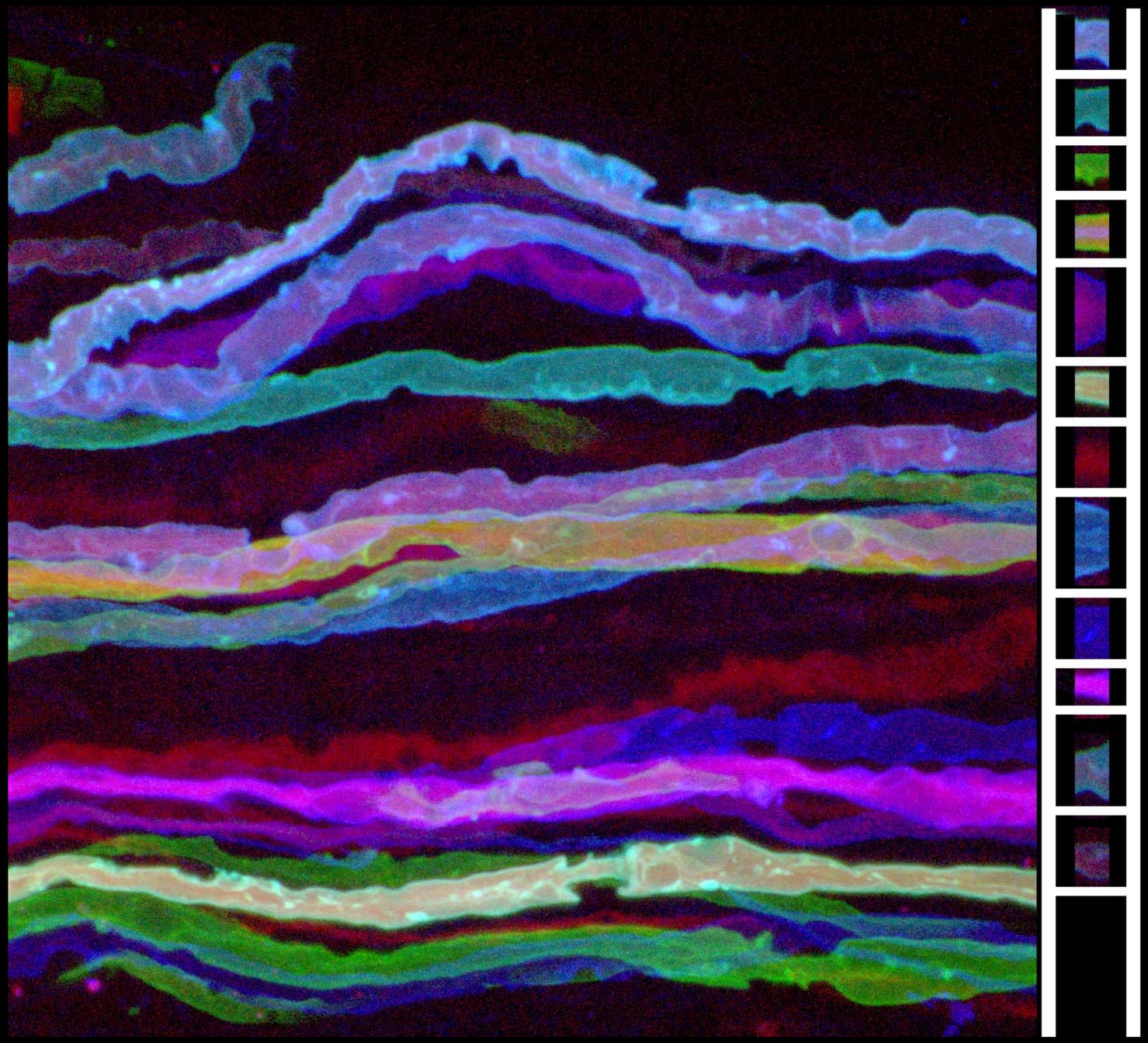


The Future

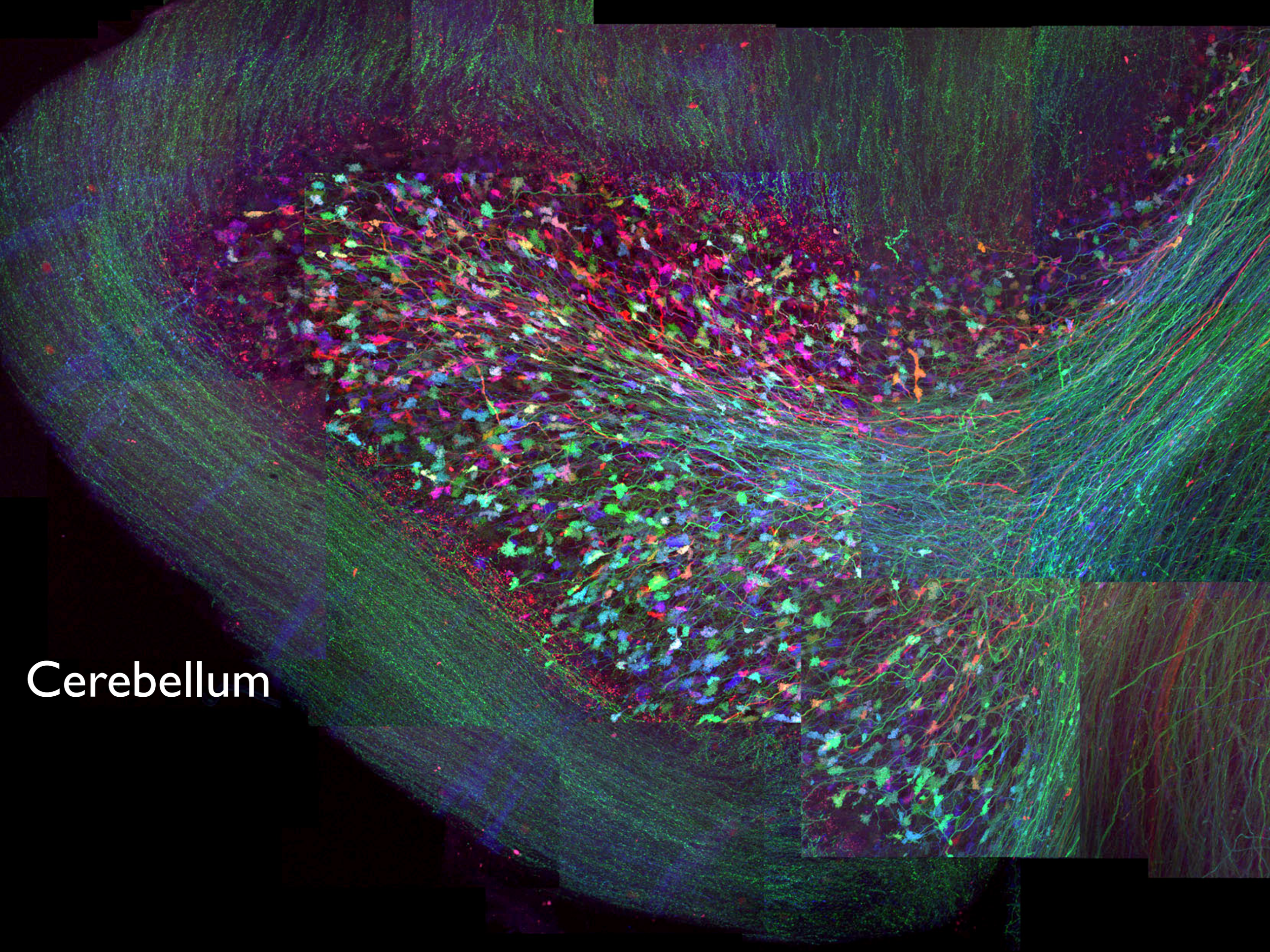


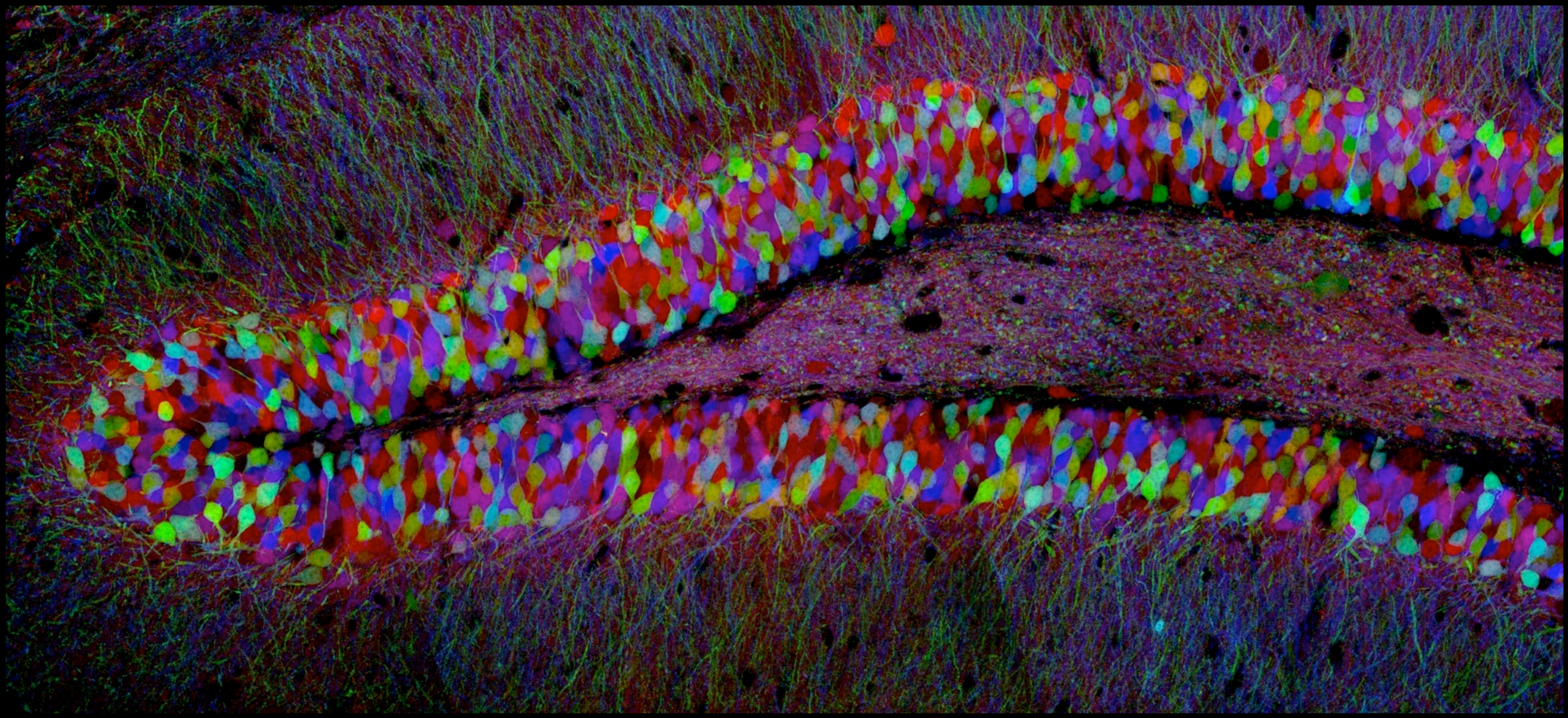
J. Livet

Brainbow



J. Livet


Cerebellum



Hippocampus

Convergent evolution?

Outline

- How is the brain wired?
- How did the universe start?
- How can we prevent heart attacks?

The MWA

Outback Supercomputing

Collaborators

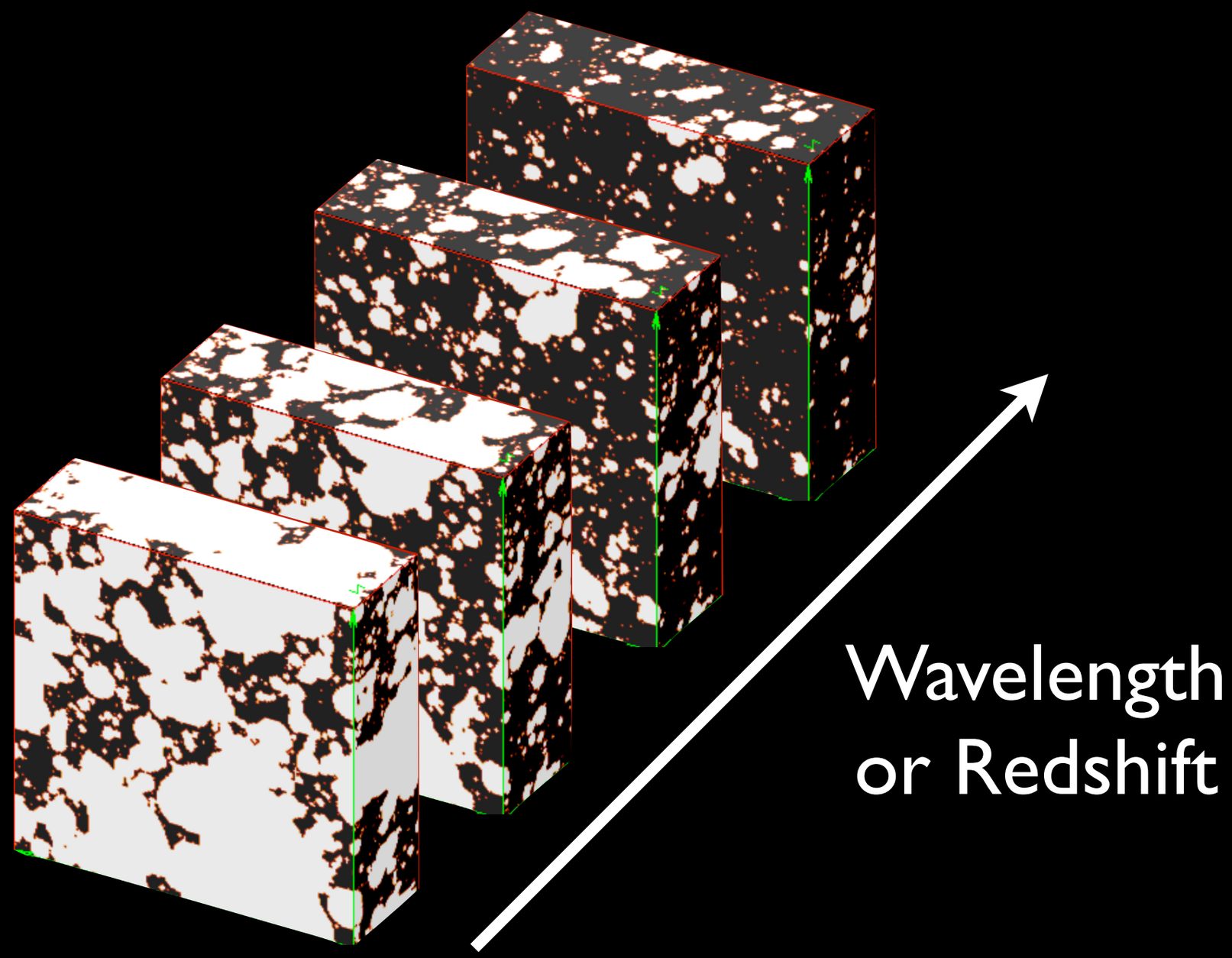
- Harvard Center for Astrophysics
  - Lincoln Greenhill
  - Daniel Mitchell
  - Stephen Ord
  - Randall Wayth
- SEAS
  - Kevin Dale, Richard Edgar
  - Hanspeter Pfister

The Scientific Challenge

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

~300,000 ~1 bio

3D Tomography

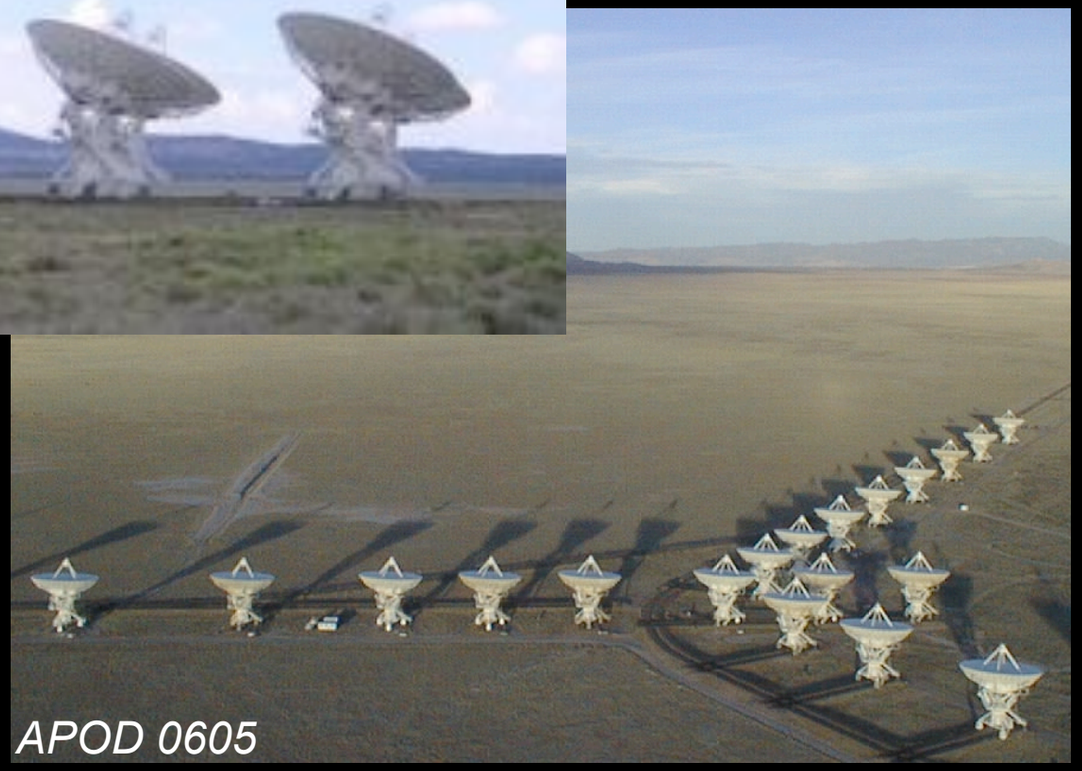


Radio Interferometry

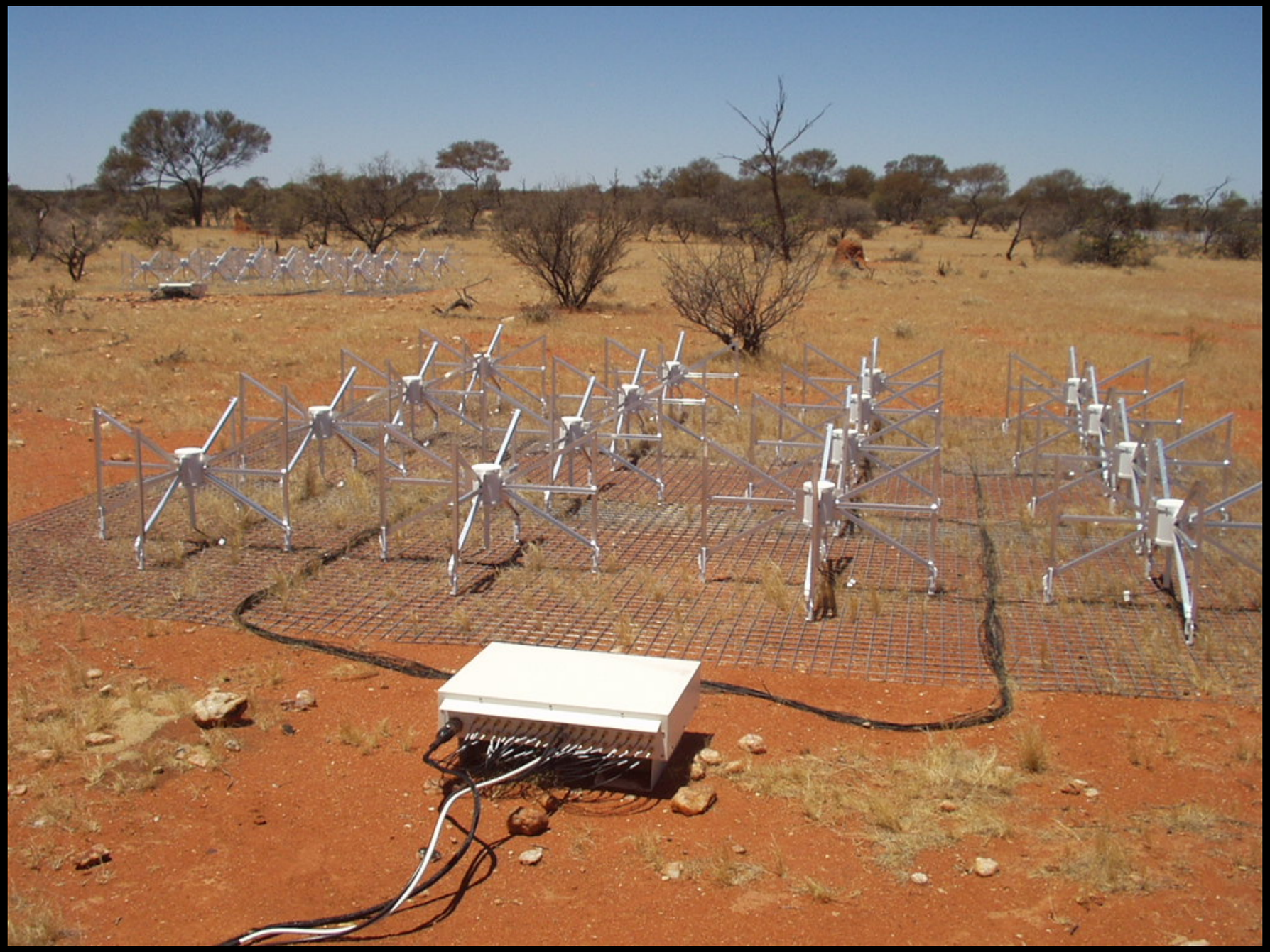
Correlator

Image in Fourier Domain

From this...



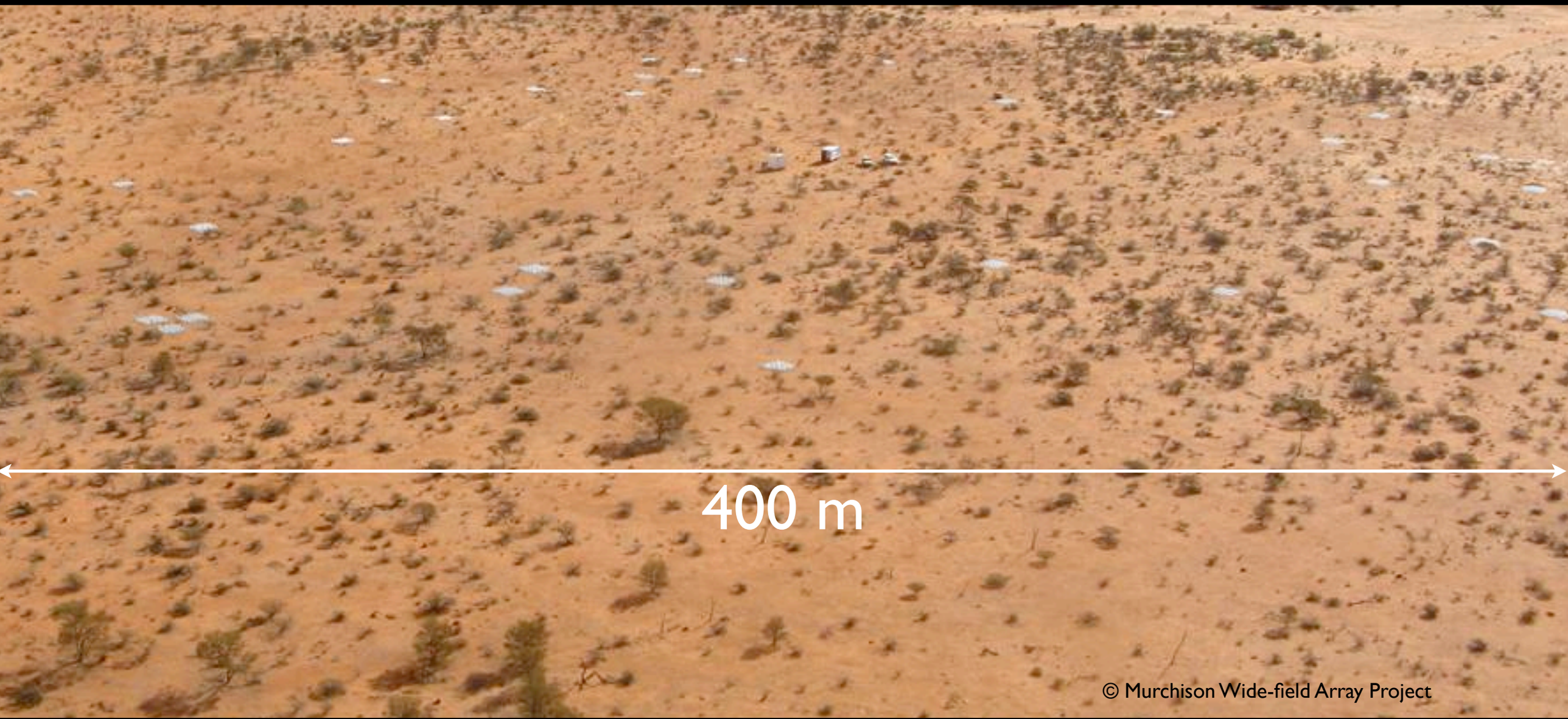
...to this



© Murchison Wide-field Array Project

MWA

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

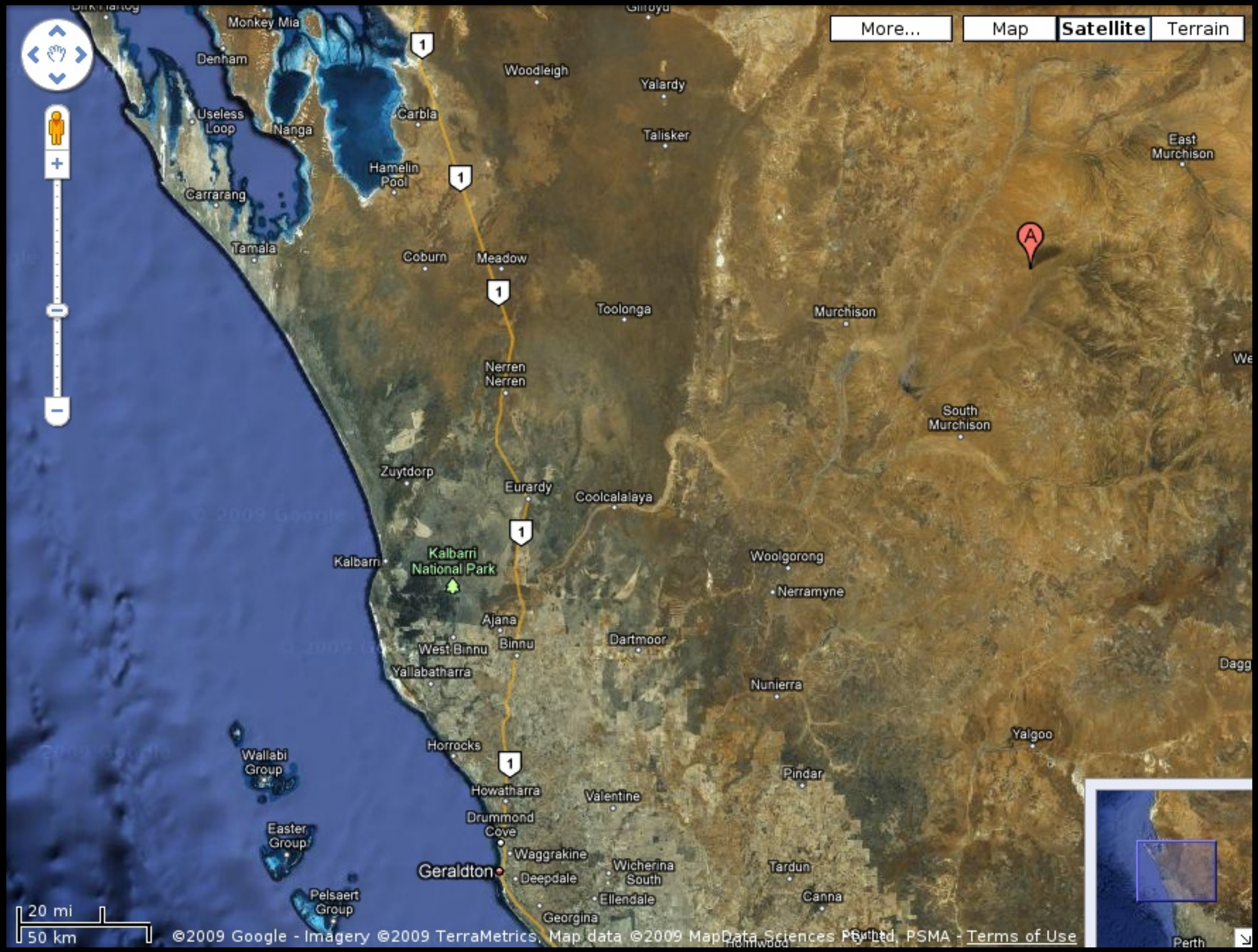


© Murchison Wide-field Array Project

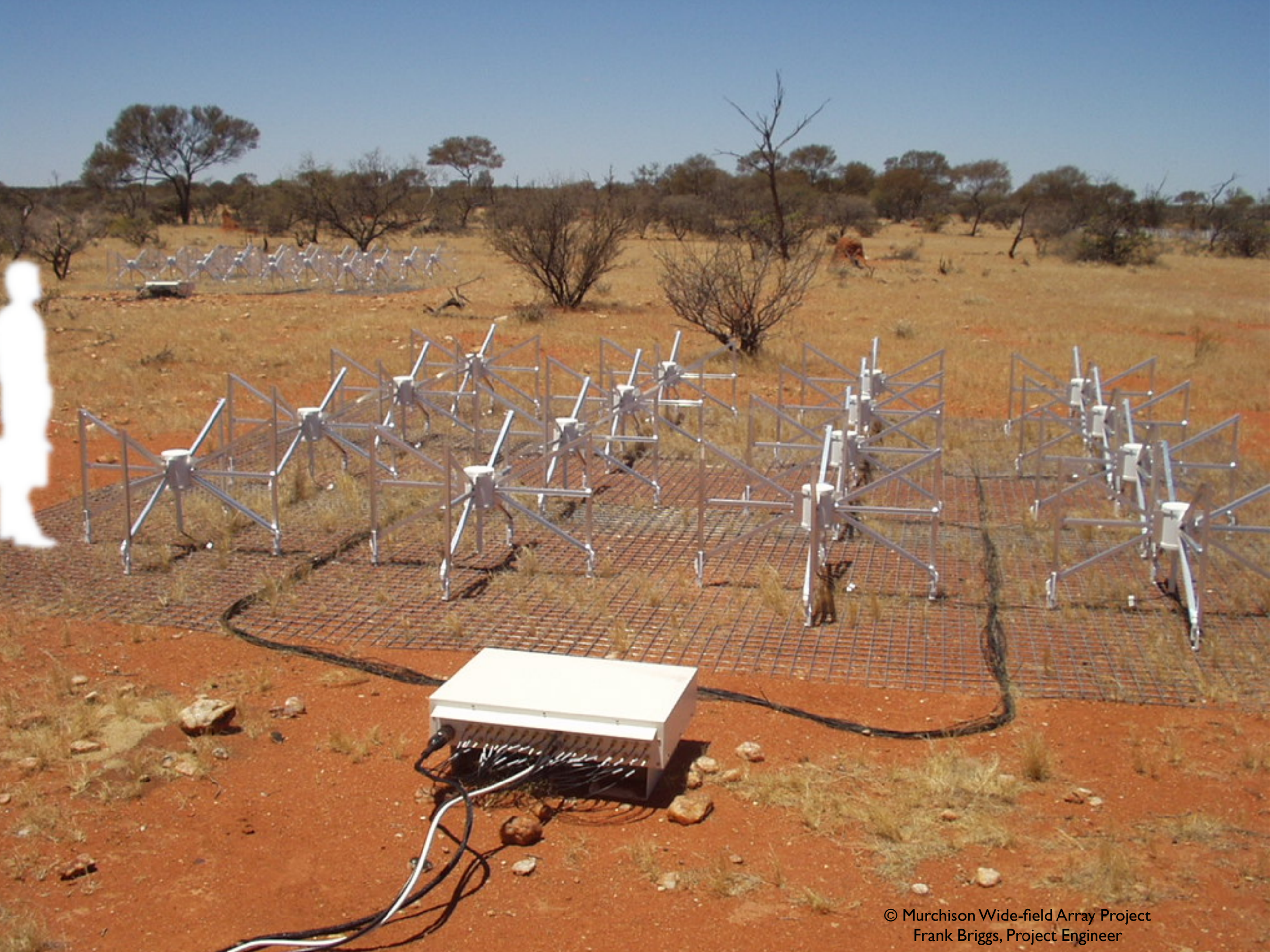
Nowhere (Middle of)
300 km
THANK YOU FOR BEING RADIO QUIET

Outback Computing

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

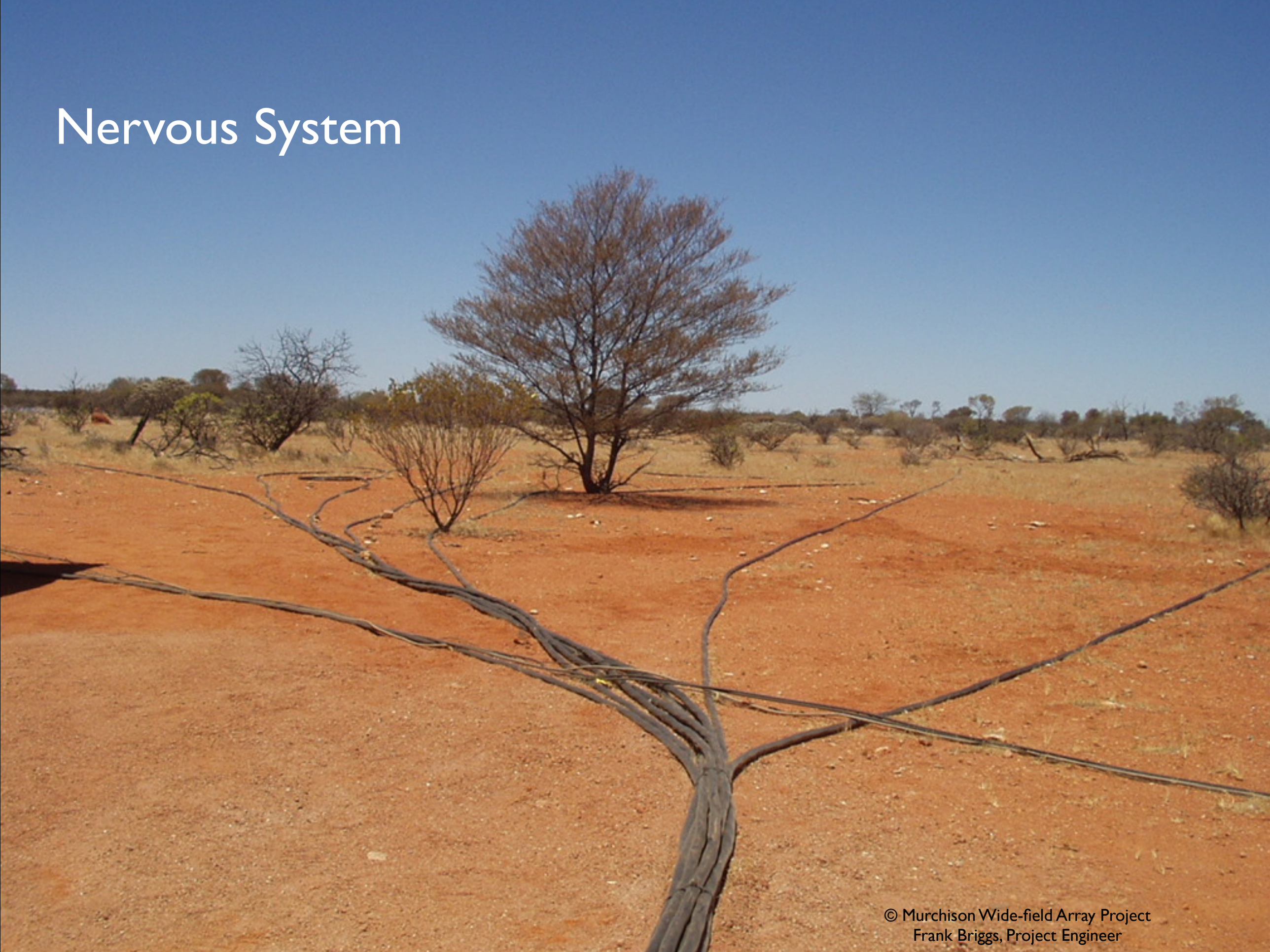

More...
Map
Satellite
Terrain
Monkey Mia
Denham
Useless Loop
Nanga
Carbla
Hamelin Pool
Carrarang
Tamala
Woodleigh
Yalardy
Talisker
East Murchison
Coburn
Meadow
Toolonga
Murchison
Nerren Nerren
South Murchison
Zuytdorp
Eurardy
Coolcalalaya
Kalbarri
Kalbarri National Park
Woolgorong
Nerramyne
Ajana
West Binnu
Binnu
Dartmoor
Yallabatharra
Nunierra
Yalgoo
Horrocks
Wallabi Group
Pindar
Howatharra
Valentine
Drummond Cove
Easter Group
Waggrakine
Geraldton
Deepdale
Wicherina South
Tardun
Pelsaert Group
Ellendale
Canna
Georgina
20 mi
50 km
©2009 Google - Imagery ©2009 TerraMetrics, Map data ©2009 MapData Sciences Pty Ltd, PSMA - Terms of Use
Perth

N
324 Mullewa Carnarvon Rd, Murchison, WA, Australia
Address is approximate
Mullewa Carnarvon Rd
© 2009 Google
Report a problem



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

Nervous System



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

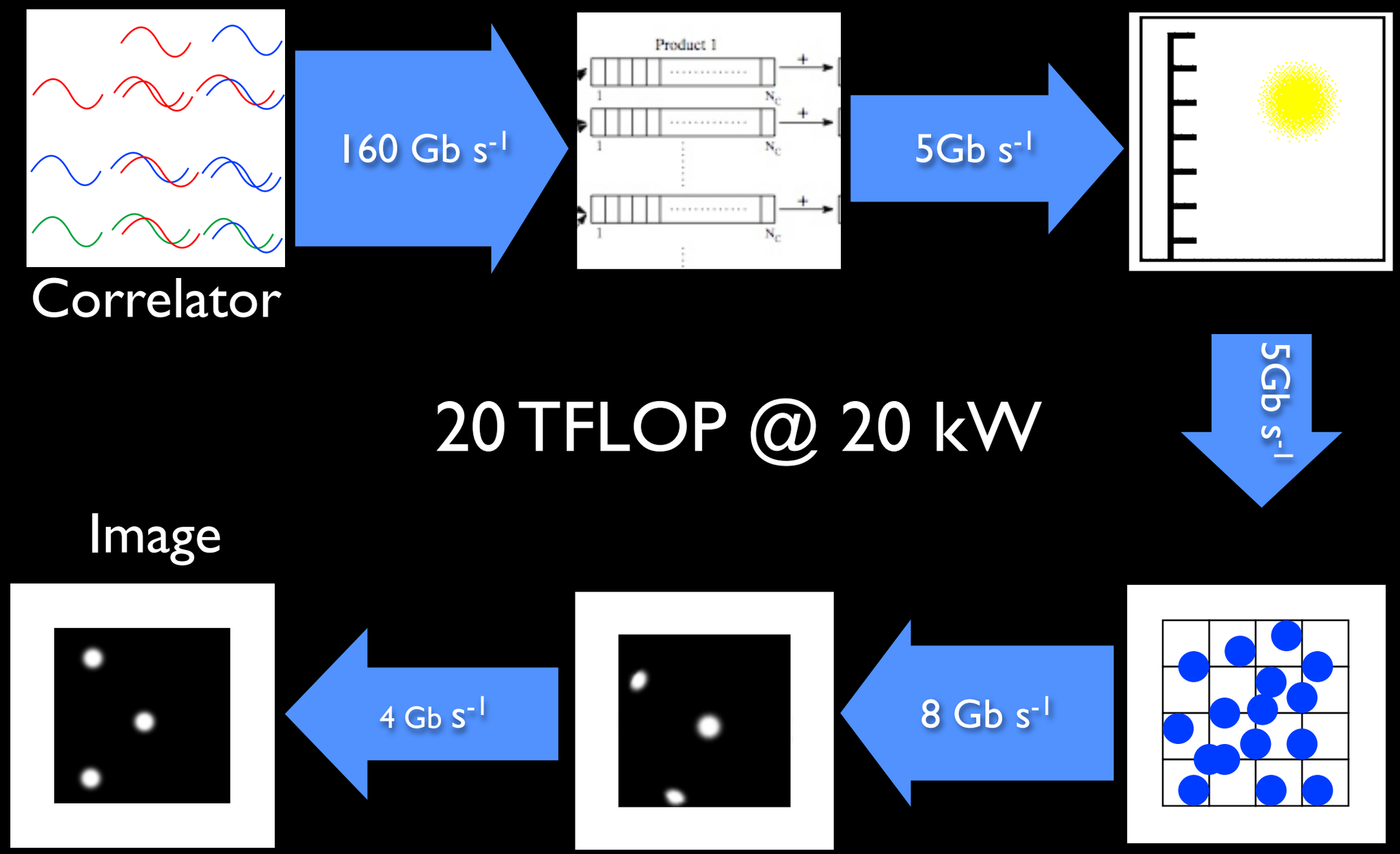
Supercomputing Center

Who is the GPU expert?

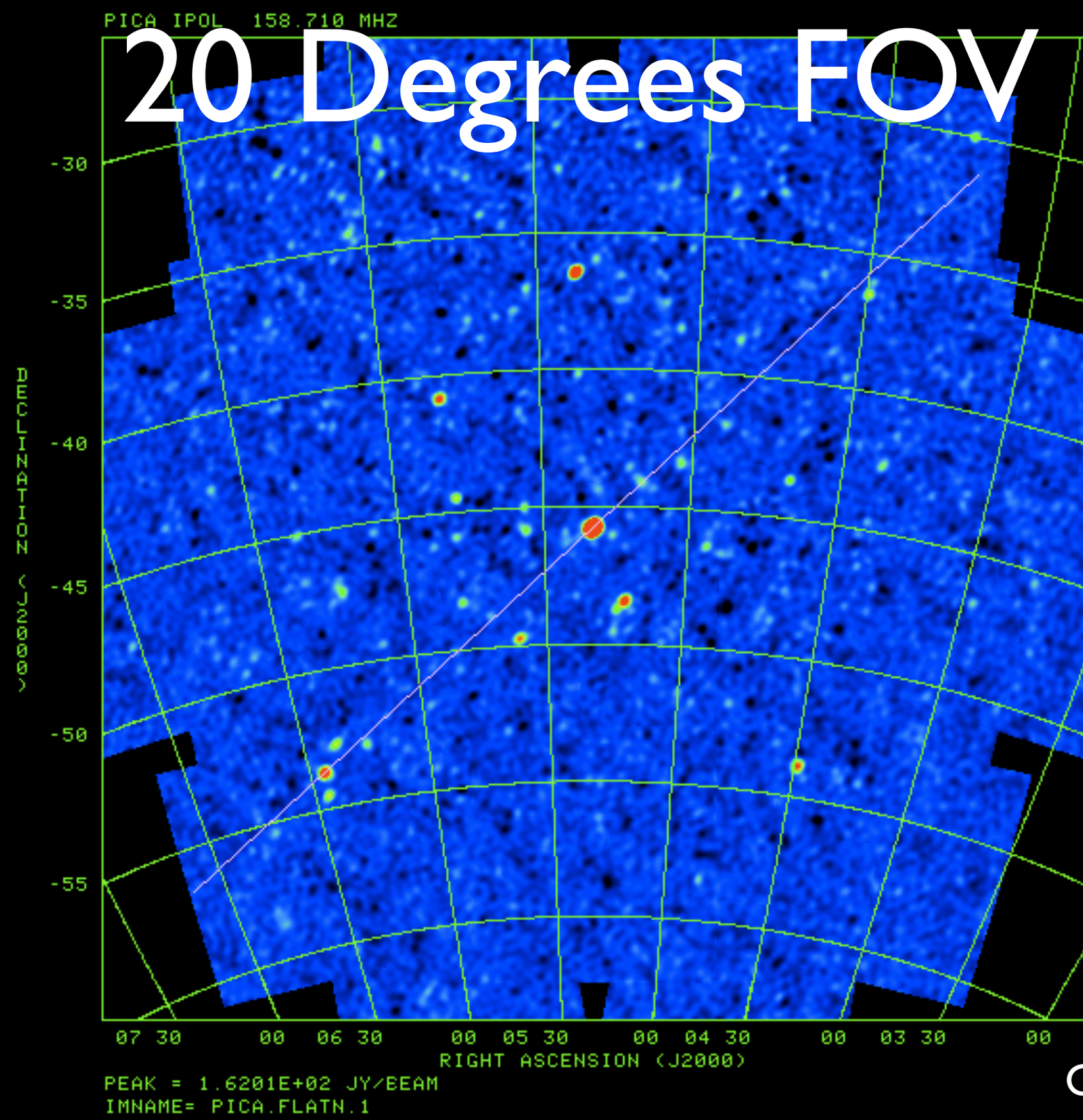
Life Support

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

MWA Pipeline

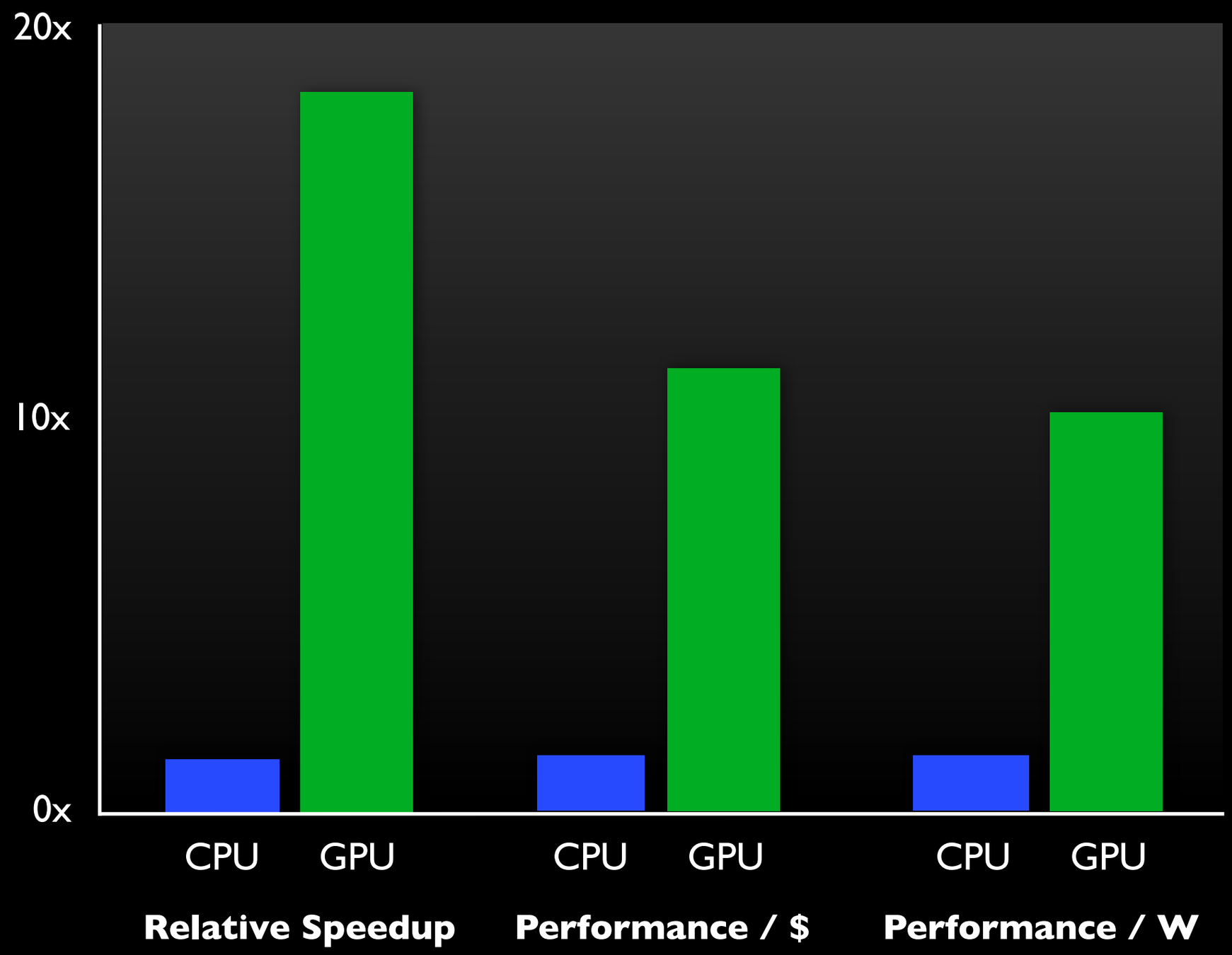


20 Degrees FOV

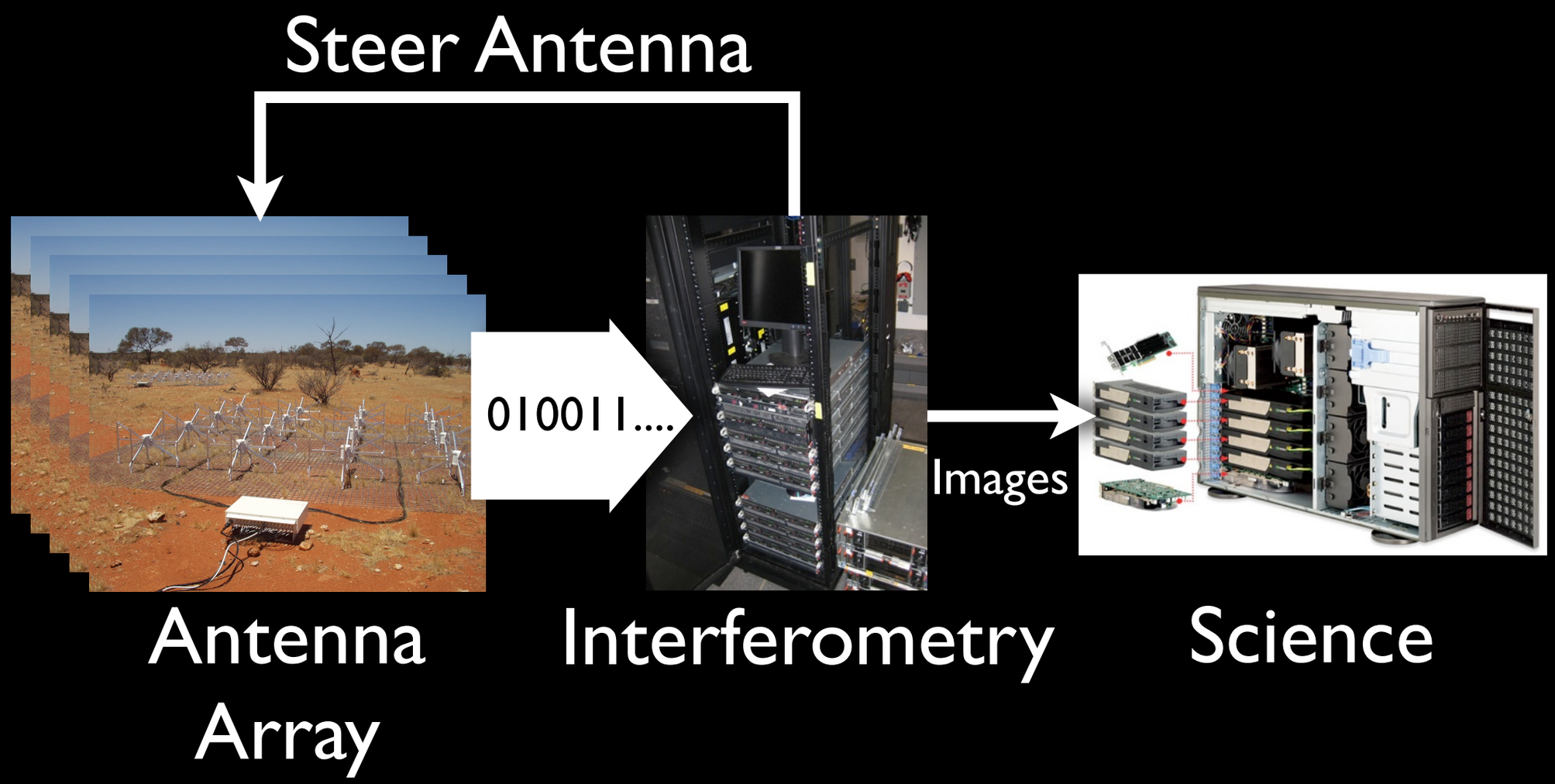


C. Williams, MIT

Real Time System

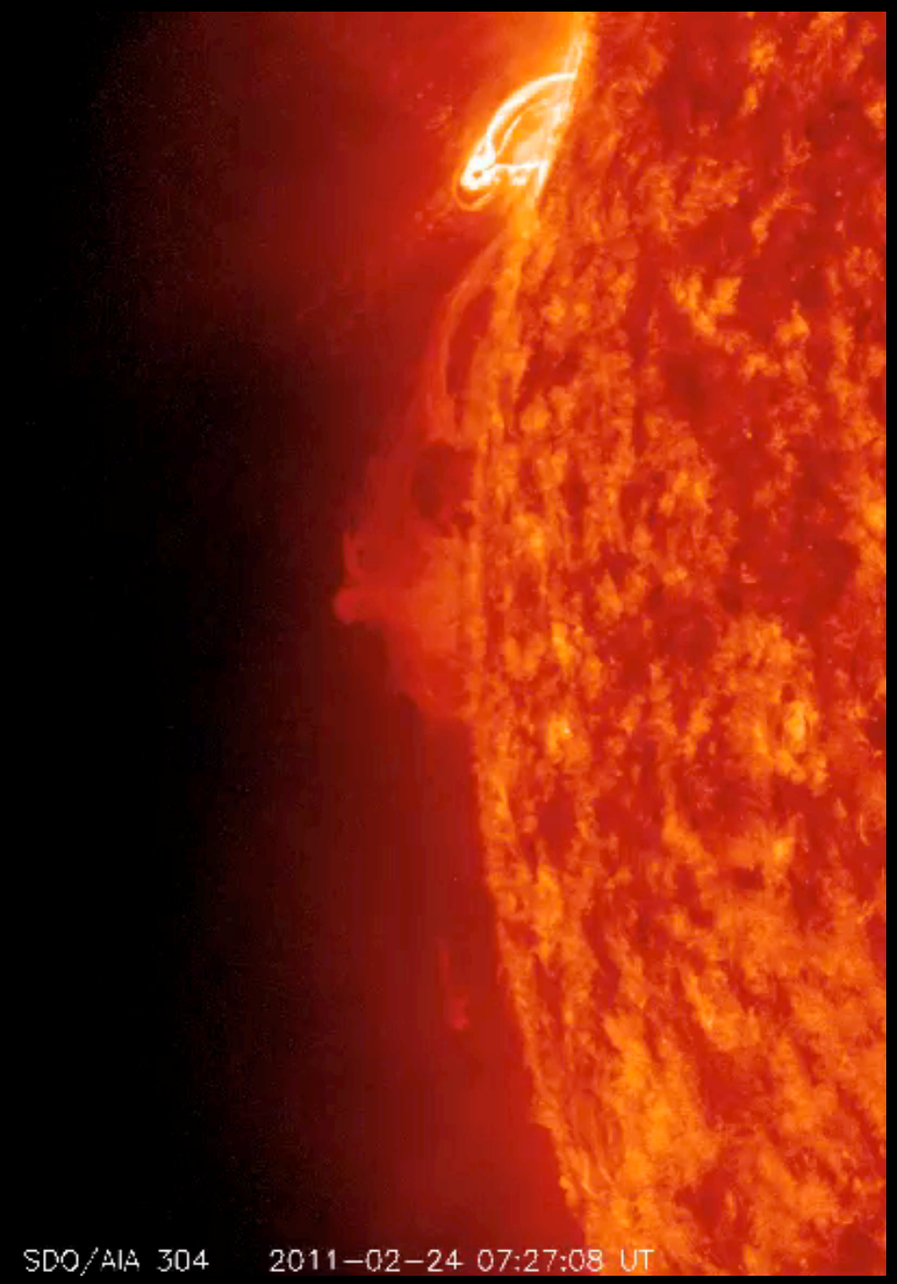


High-Throughput Radio Astronomy



Real-Time Steering

- Predict solar flares and coronal mass ejections



SDO (NASA)

The Future

Square Kilometer Array

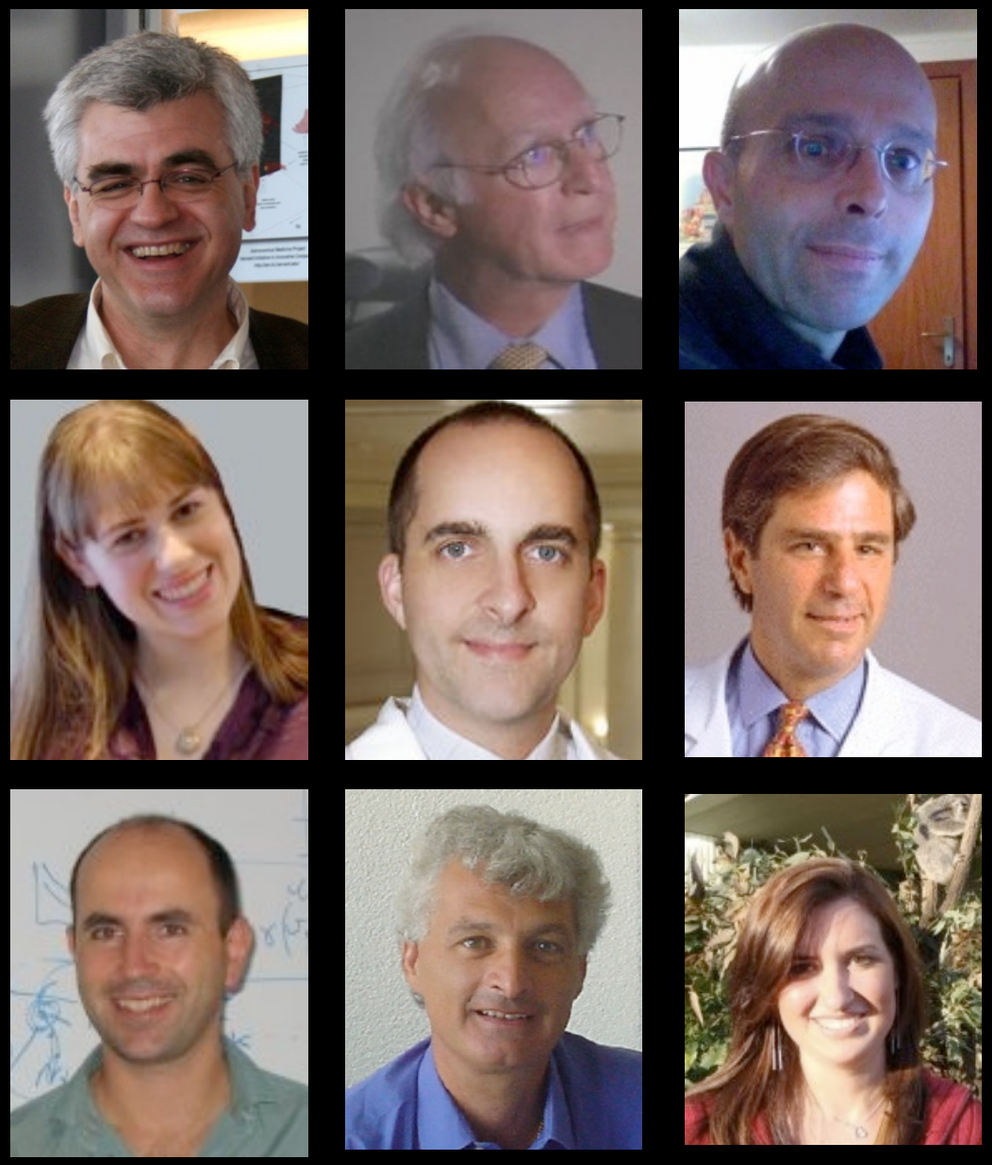
1 EFLOP / 1 Tb s^{-1} ca. 2020

Multiscale Hemodynamics

Predicting & Preventing Heart Attacks

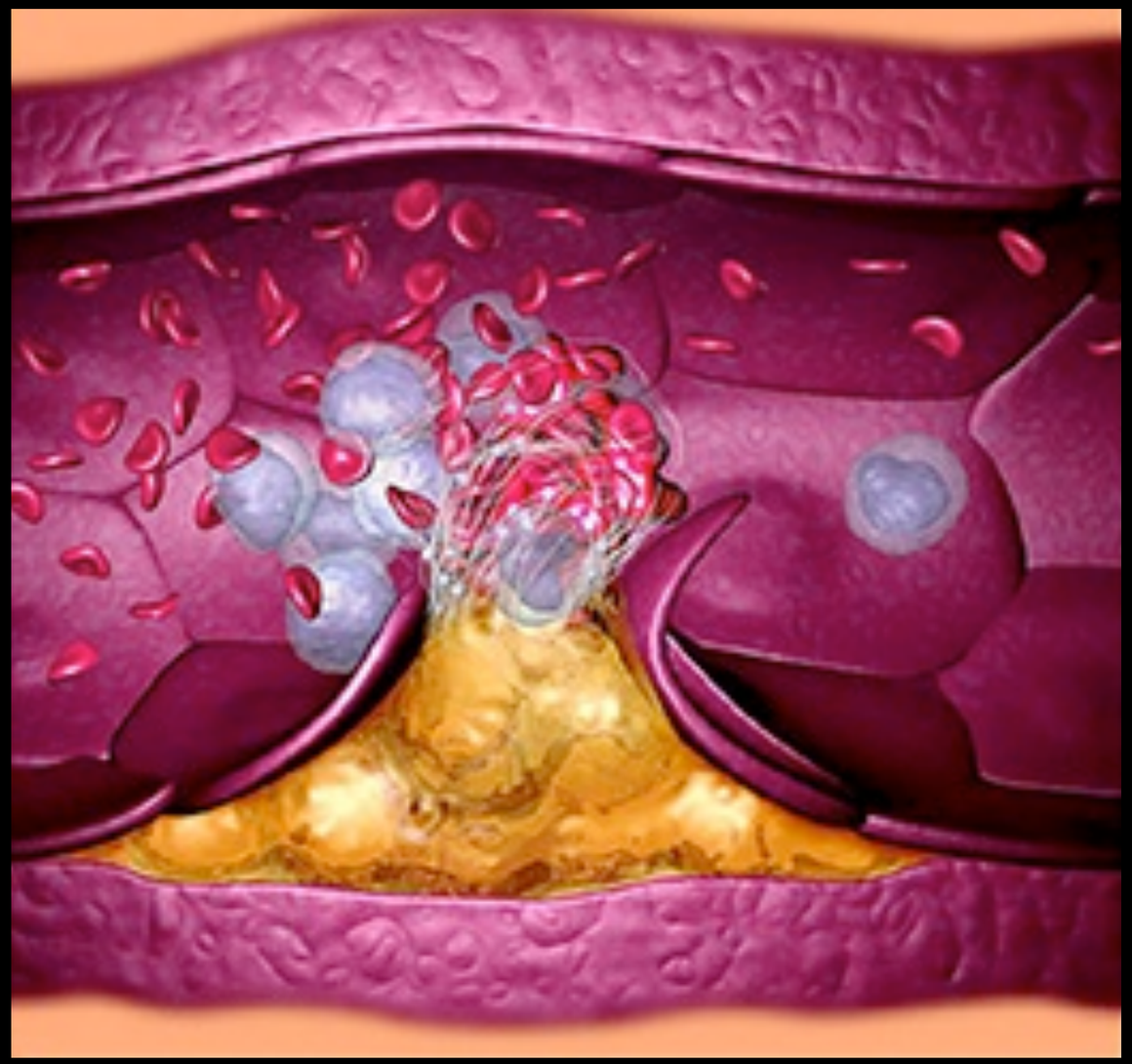
Multiscale Hemodynamics

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

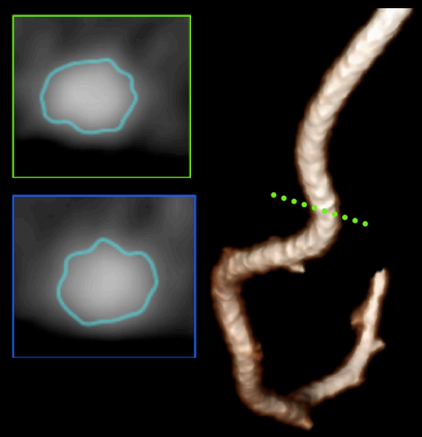


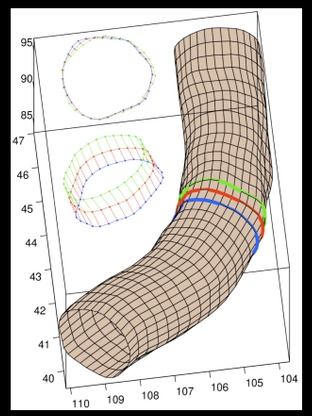
The Scientific Challenge

- Predict and prevent heart attacks



Hemodynamics Pipeline



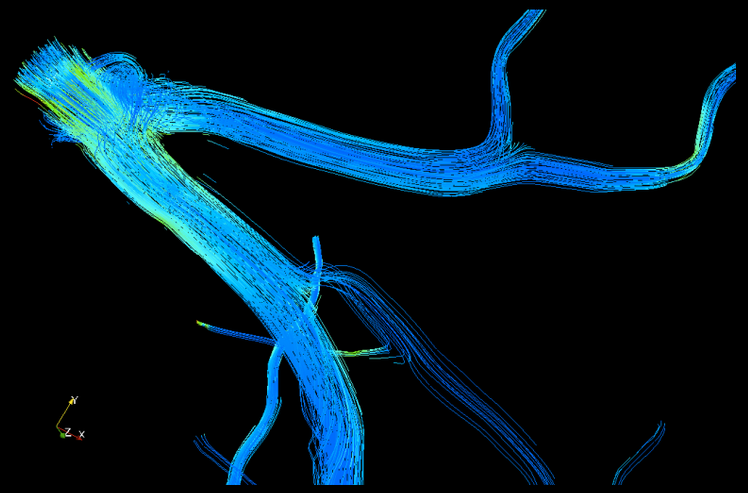


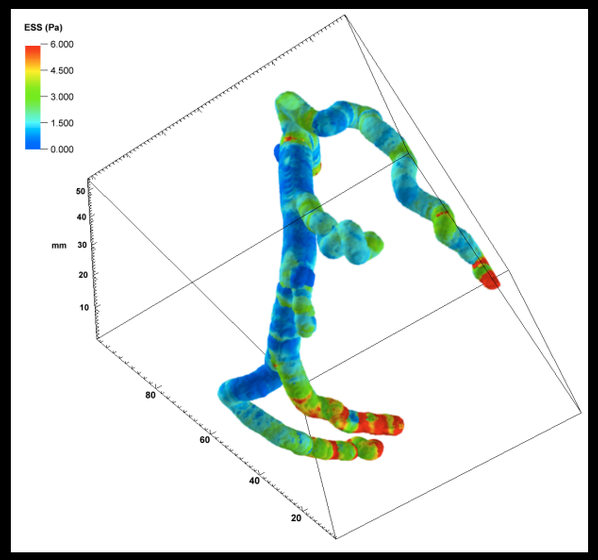
CT Patient Data → Reconstruction → Post-Processing

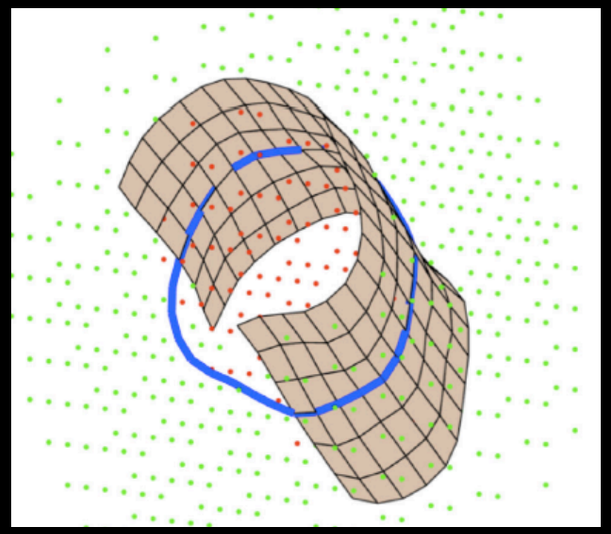
↓

Lattice Boltzman & Molecular Dynamics

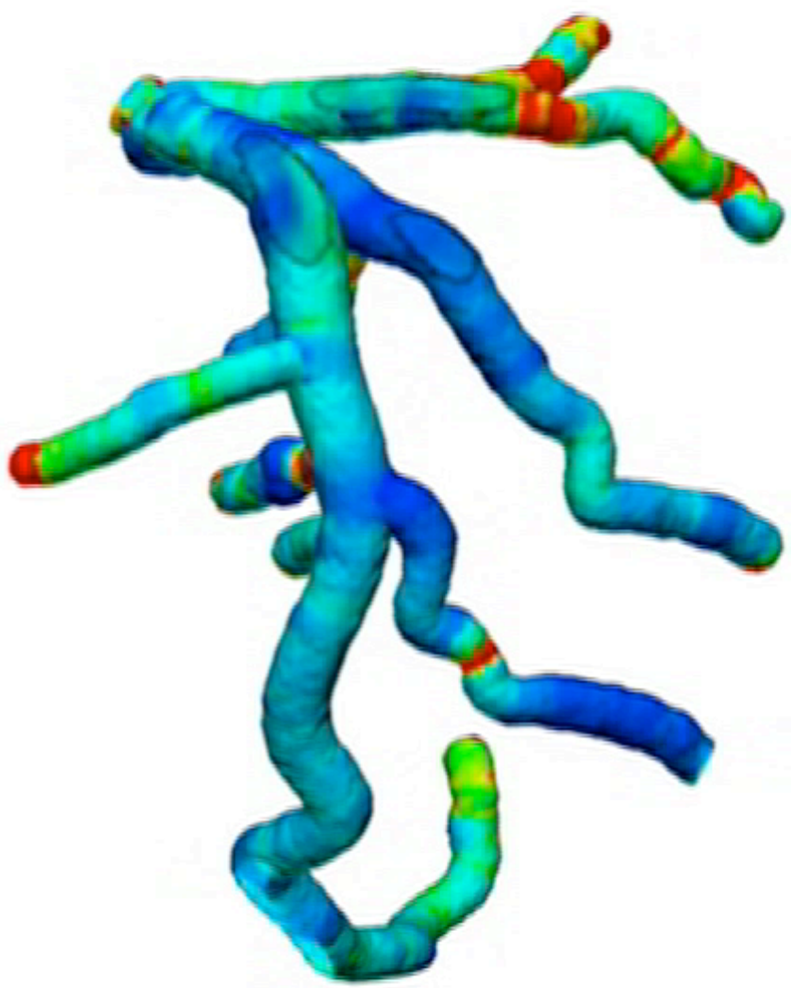
← Visualization & Analysis



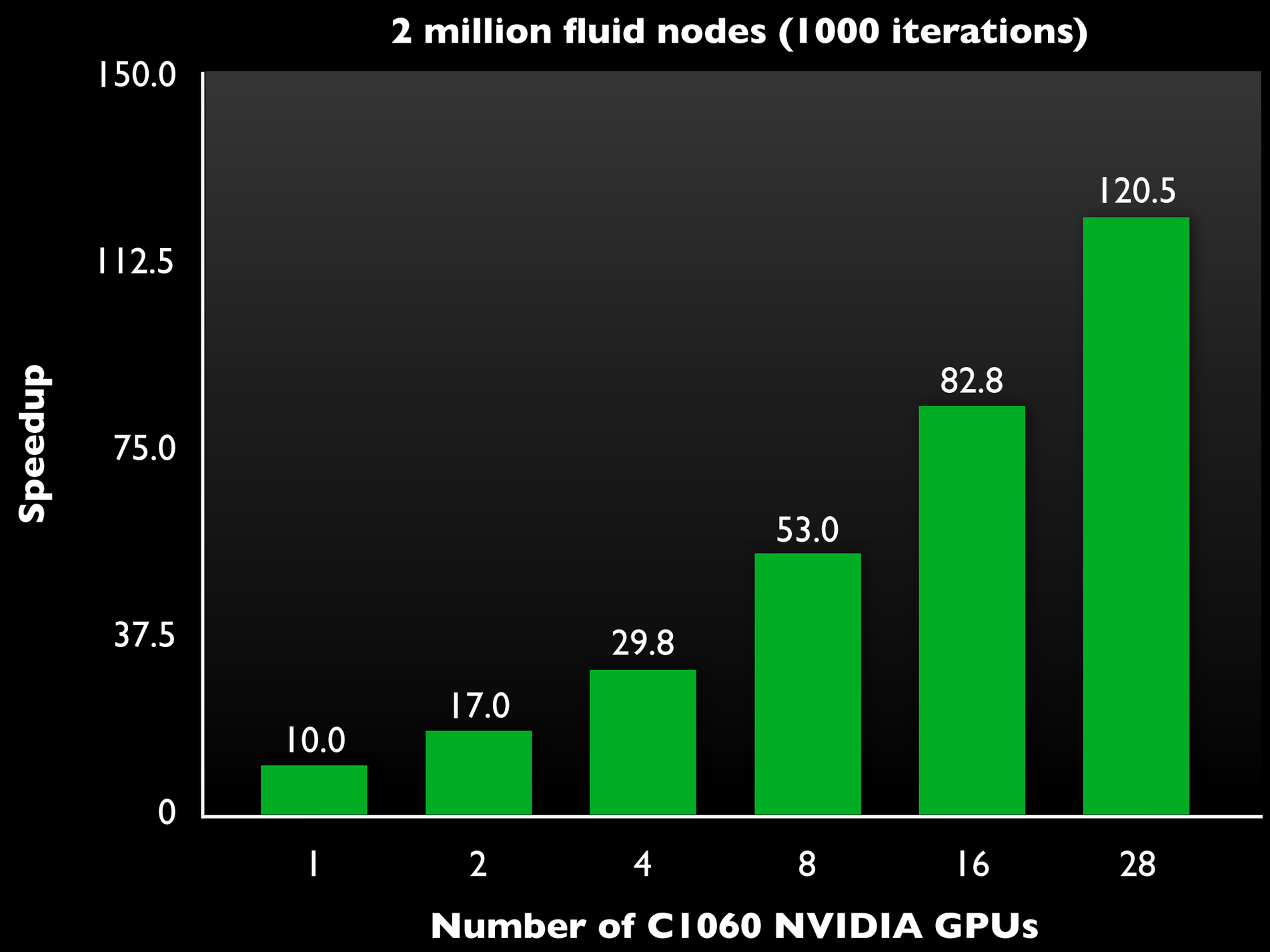




Multiscale Hemodynamics



Results

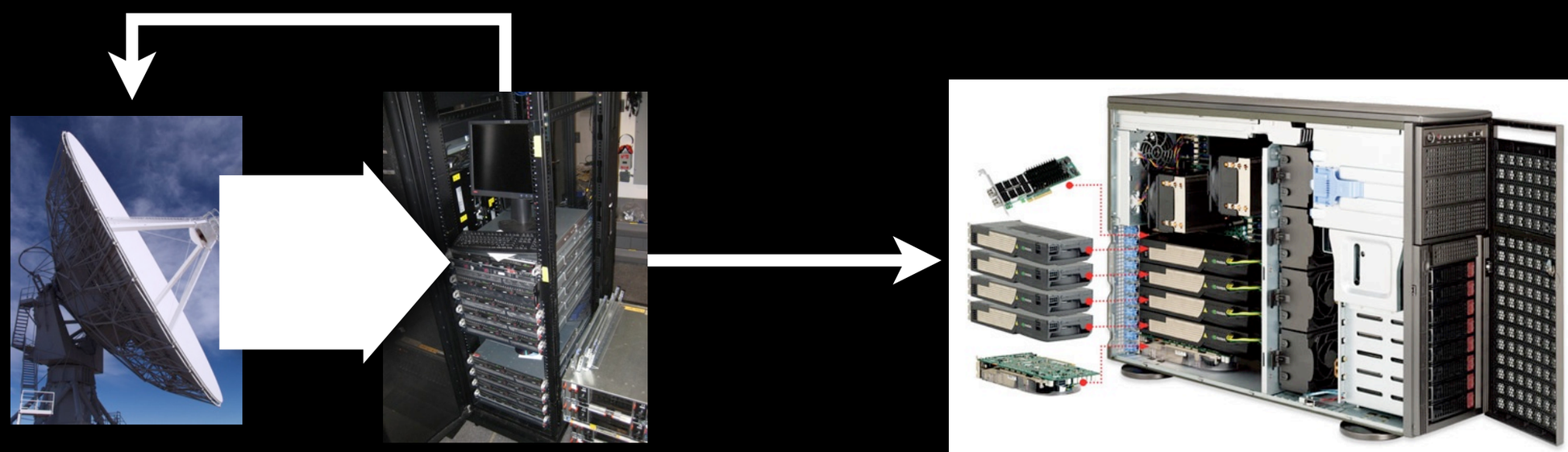

2 million fluid nodes (1000 iterations)
150.0
112.5
75.0
37.5
0
Speedup
10.0
17.0
29.8
53.0
82.8
120.5
1
2
4
8
16
28
Number of C1060 NVIDIA GPUs

The Future

- Minimally invasive early detection

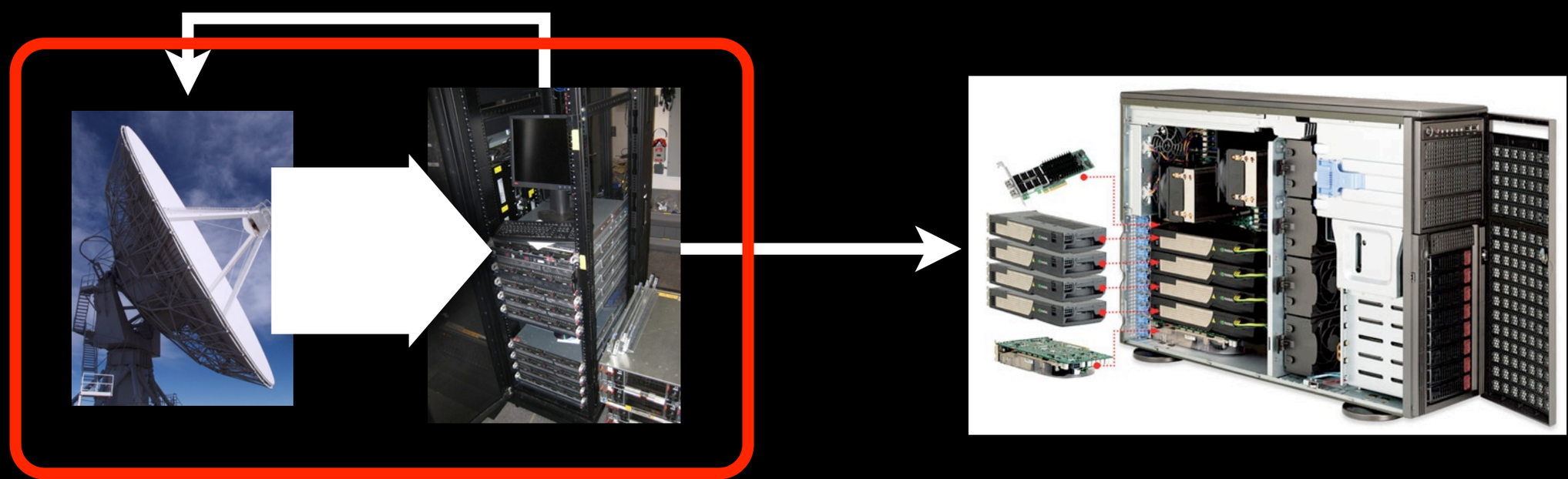
UCLA Medical Center Newsletter

HTC Lessons



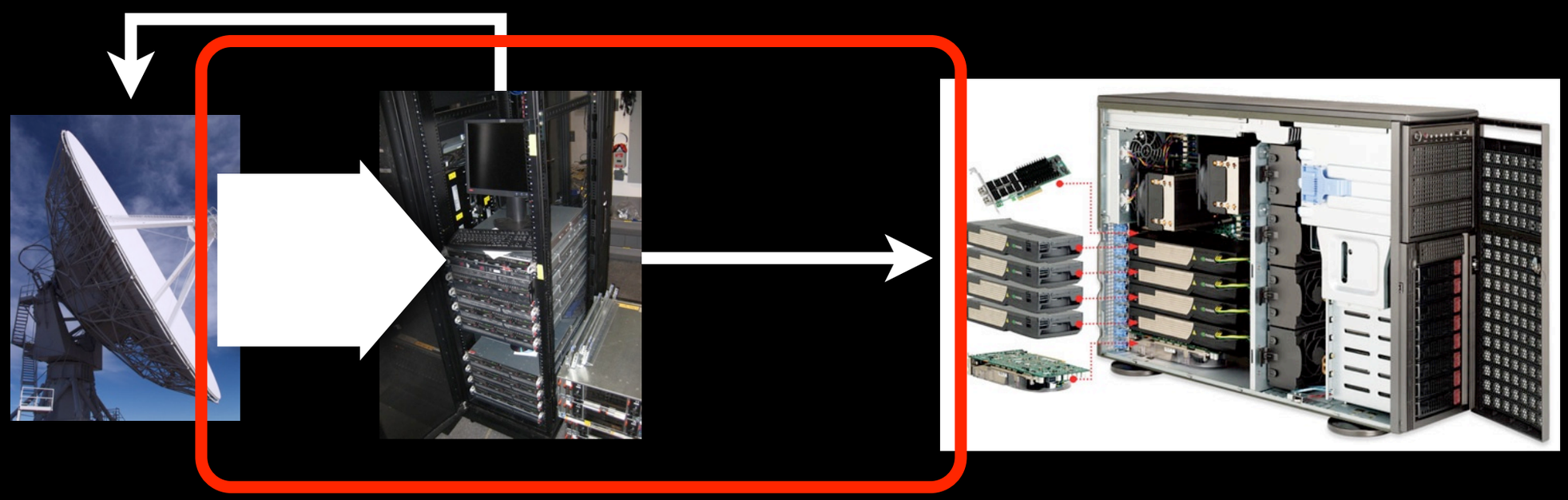
HTC Lessons

- Move the computation to the source



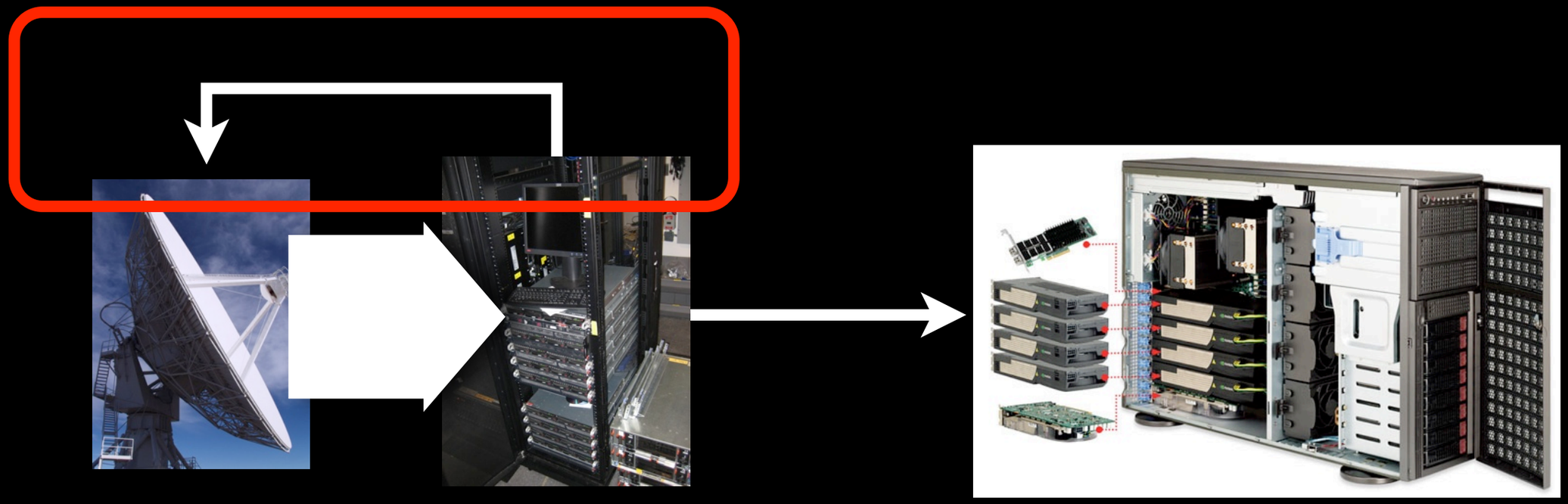
HTC Lessons

- Quickly reduce the data to its essentials



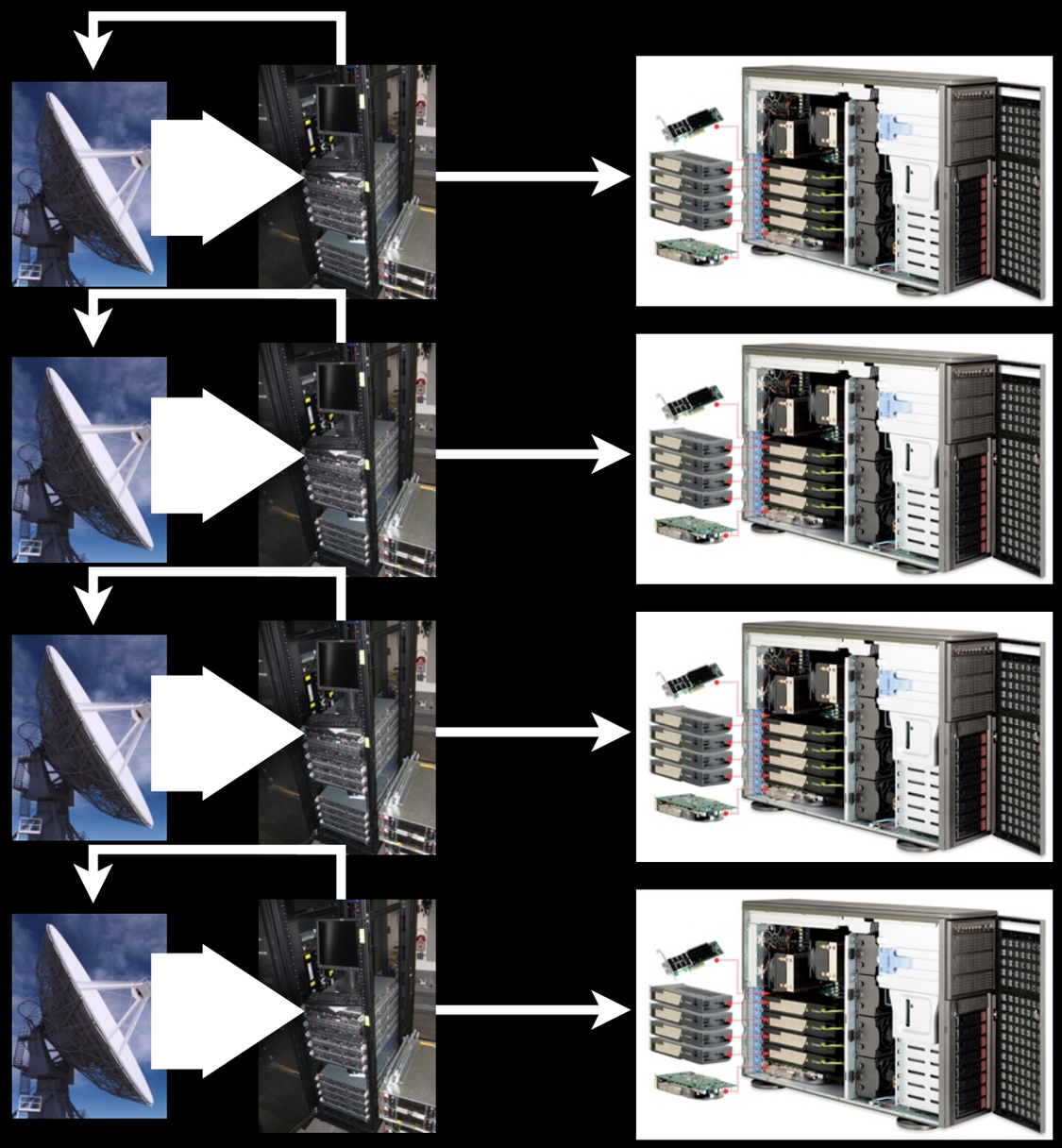
HTC Lessons

- Use feedback to optimize the acquisition



HTC Lessons

- Provides scalable and power efficient systems



Higher-Level Programming Models

- 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
```

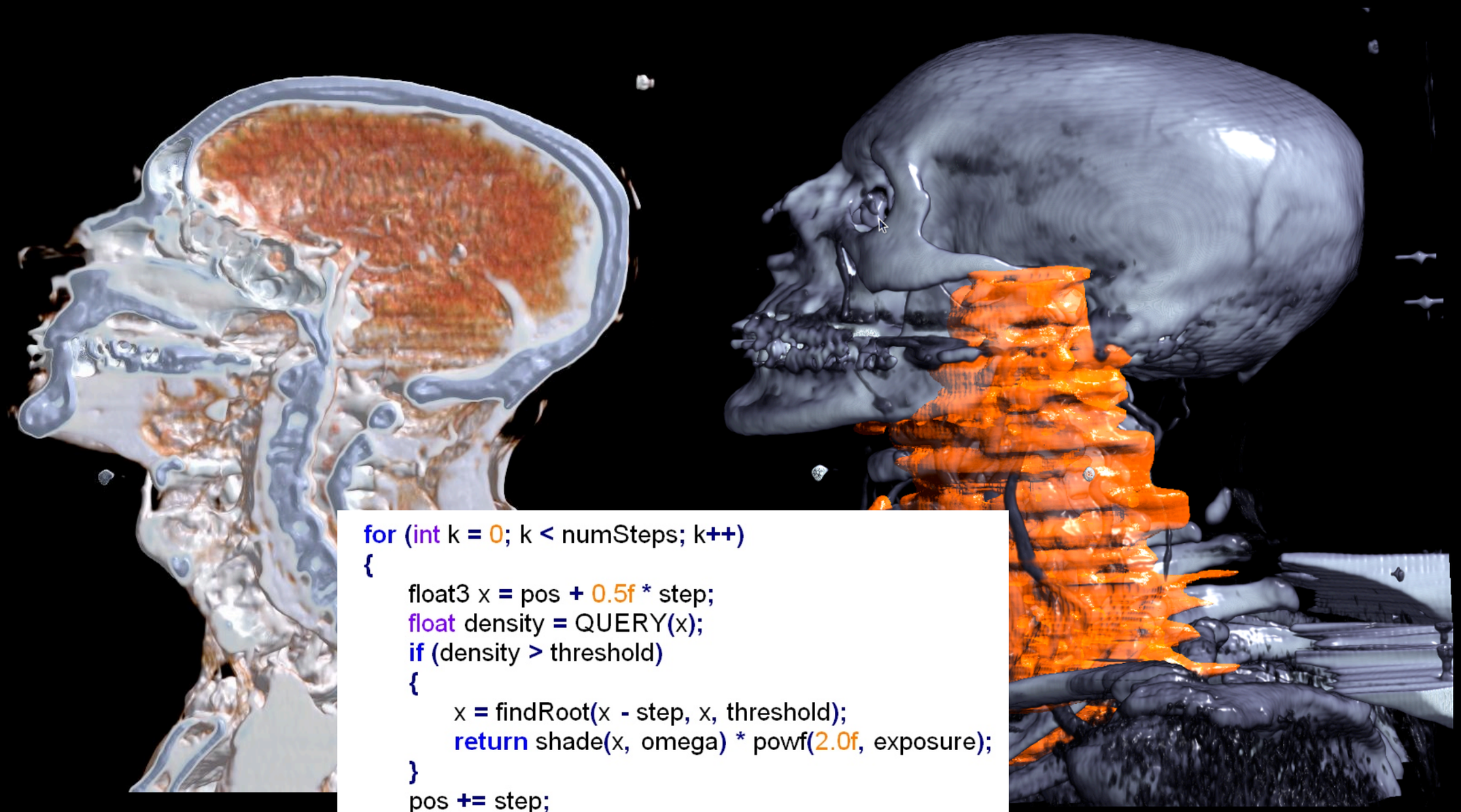
(b) Direct implementation (unfused code)

```
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]

Volume Rendering with Procedural Shaders

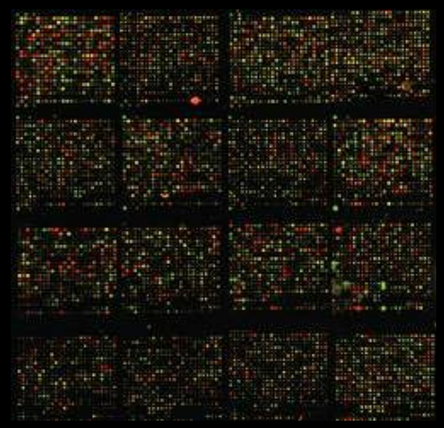


```
for (int k = 0; k < numSteps; k++)
{
    float3 x = pos + 0.5f * step;
    float density = QUERY(x);
    if (density > threshold)
    {
        x = findRoot(x - step, x, threshold);
        return shade(x, omega) * powf(2.0f, exposure);
    }
    pos += step;
}
```

Scalable Runtime Environments

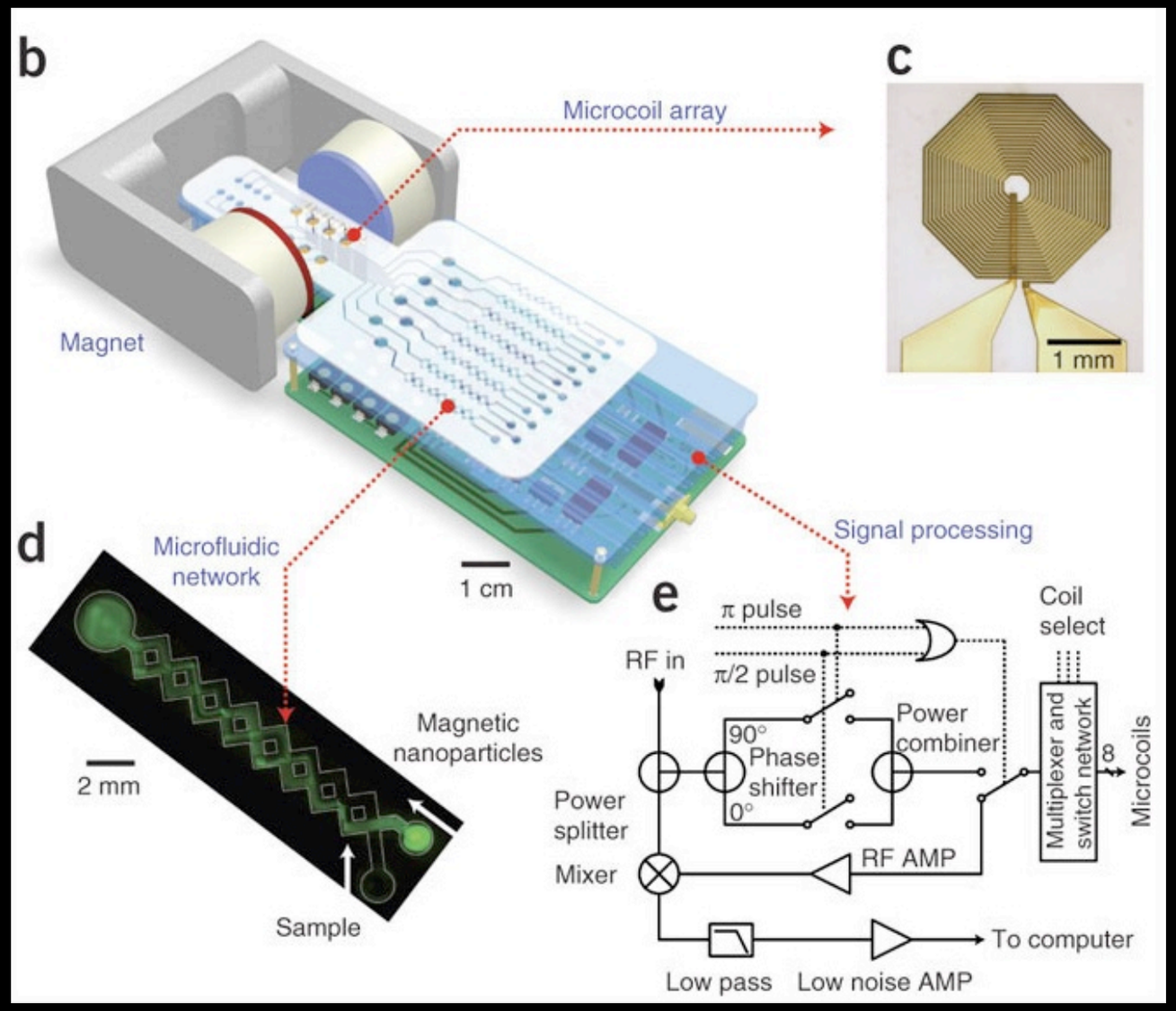
Chip Sensors

Gene Array Chips



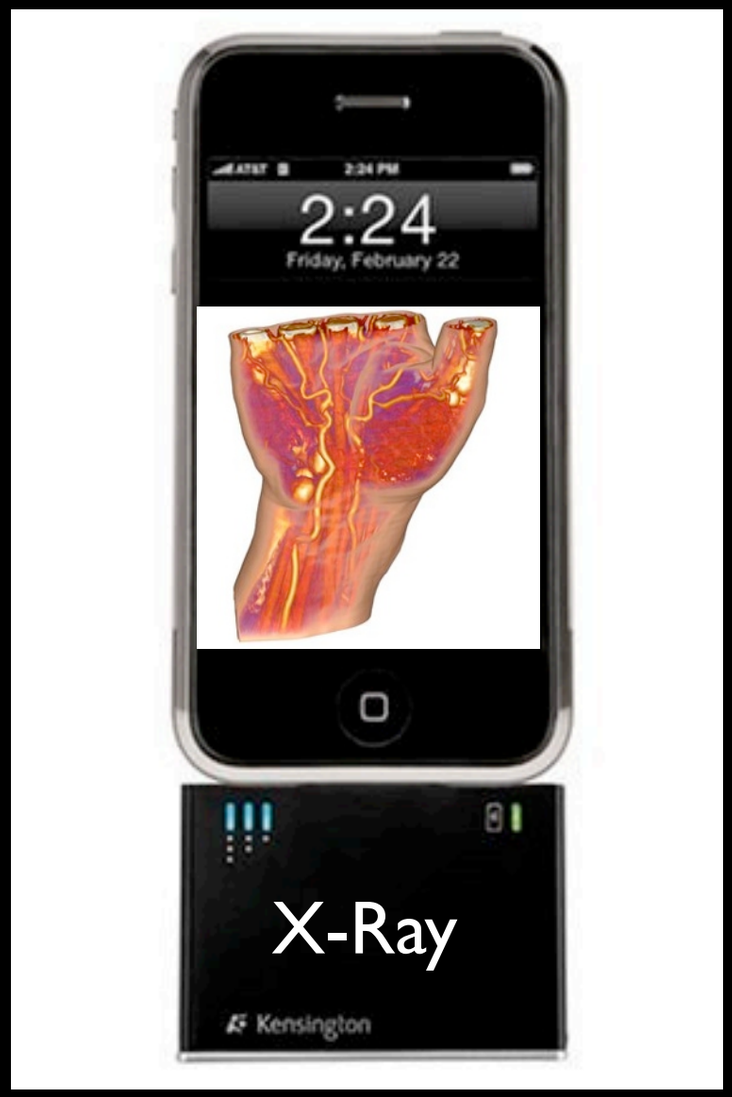
George Whitesides

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

Shameless Plugs

- cs264.org - Massively Parallel Computing course (spring 2011, Harvard Extension)