

Workflow approaches in high throughput neuroscientific research.

Jake Carroll - Senior ICT Manager, Research
The Queensland Brain Institute, UQ, Australia
jake.carroll@uq.edu.au



Queensland Brain Institute

What is QBI?

- The Queensland Brain Institute is one of the largest (and probably the most computationally + storage intensive) neuroscience research focused institutes in the world.
- Labs are dedicated to understanding the fundamental mechanisms that regulate brain function.
- We're working to solve some of the greatest problems that humanity faces in terms of mental illness.
- QBI is an early adopter. *We are* the crazy ones.

Why am I here?

- I came to learn, primarily. A great audience, a great set of people speaking. A wealth of capability and experience in this crowd.
- I came to show you how workflows **matter** to my industry and the evolving nature of storage in this space.
- I came to discuss how we can revolutionise storage platforms of best fit, together, with workflows at the centre of the design principles.

What types of science drive our workloads?

- Basic biology.
- Computational neuroscience.
- Complex trait genomics (*you thought NGS was data-intensive? Check this stuff out!*)
- Electrophysiology.
- Cognitive neurosciences.
- Computational biology.

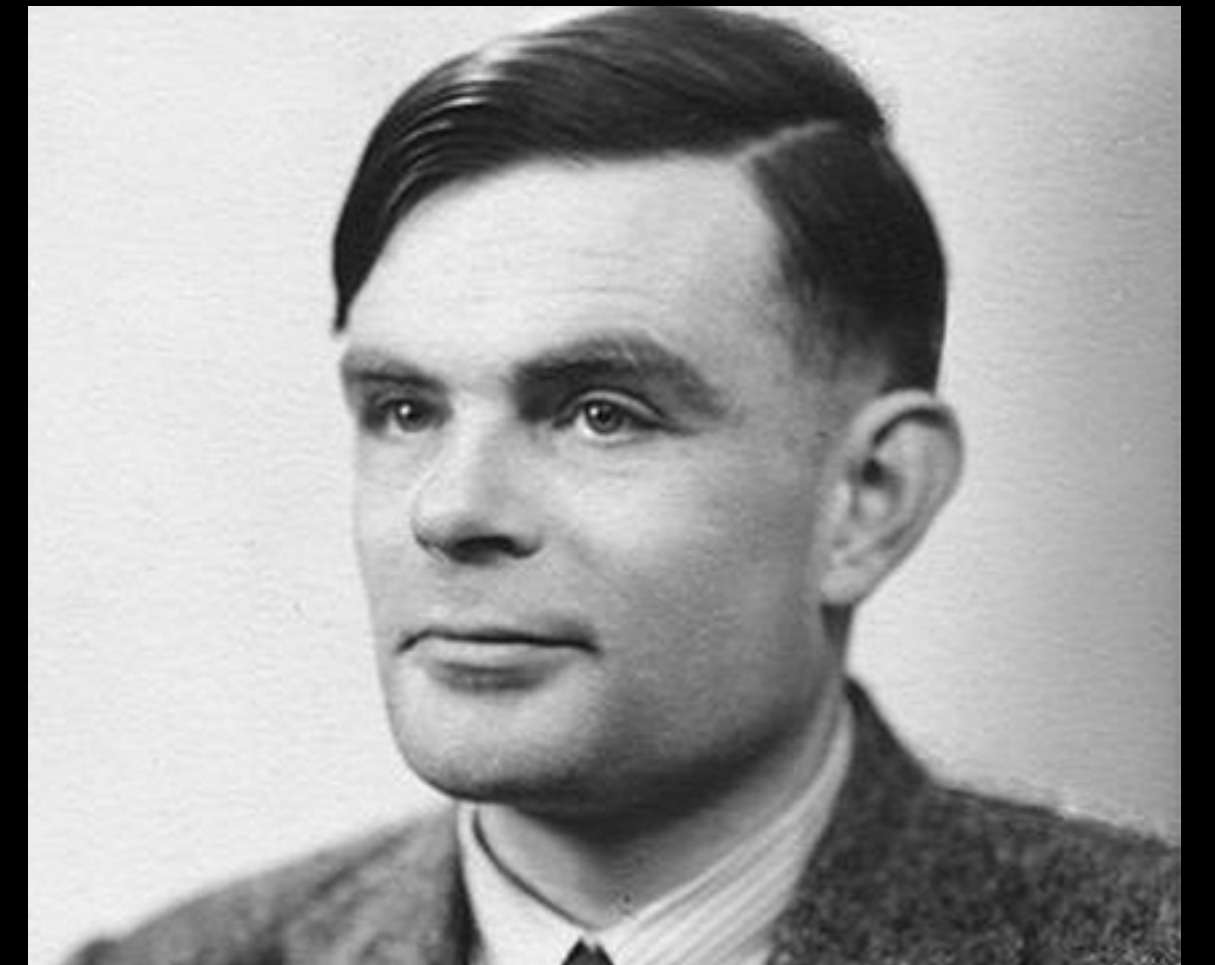
What does QBI want with workflows?

- Traditional beginnings:
 - Big supers, big storage, significant complexity. Clever people using clever things to find the clever answers to complex questions, in theory.
- Turns out, biologists don't have the time to learn the in's and out's of parallel filesystem semantics or computer scheduler eccentricities.
- They just want to get their work done, put it somewhere and publish, 99.95% of the time.
- Every aspect of the scientific "life" in the lab can be expressed 'in-silico' as a workflow, so we've found. This pays some homage to Ian Corners "birth, death and marriage" registration concept of data.

There are two user-types.



A wet lab biologist



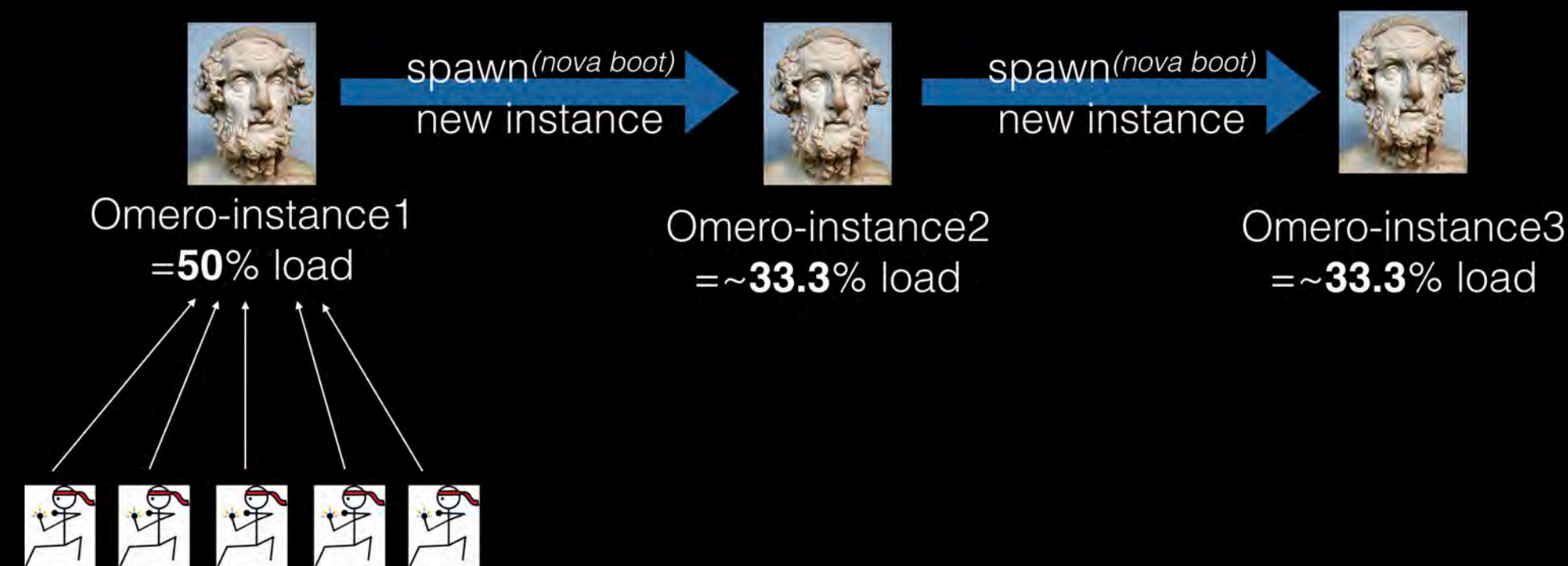
A computer scientist

Guess who has more sophisticated needs?

Hint: It isn't the computer scientist.

How are we helping our people?

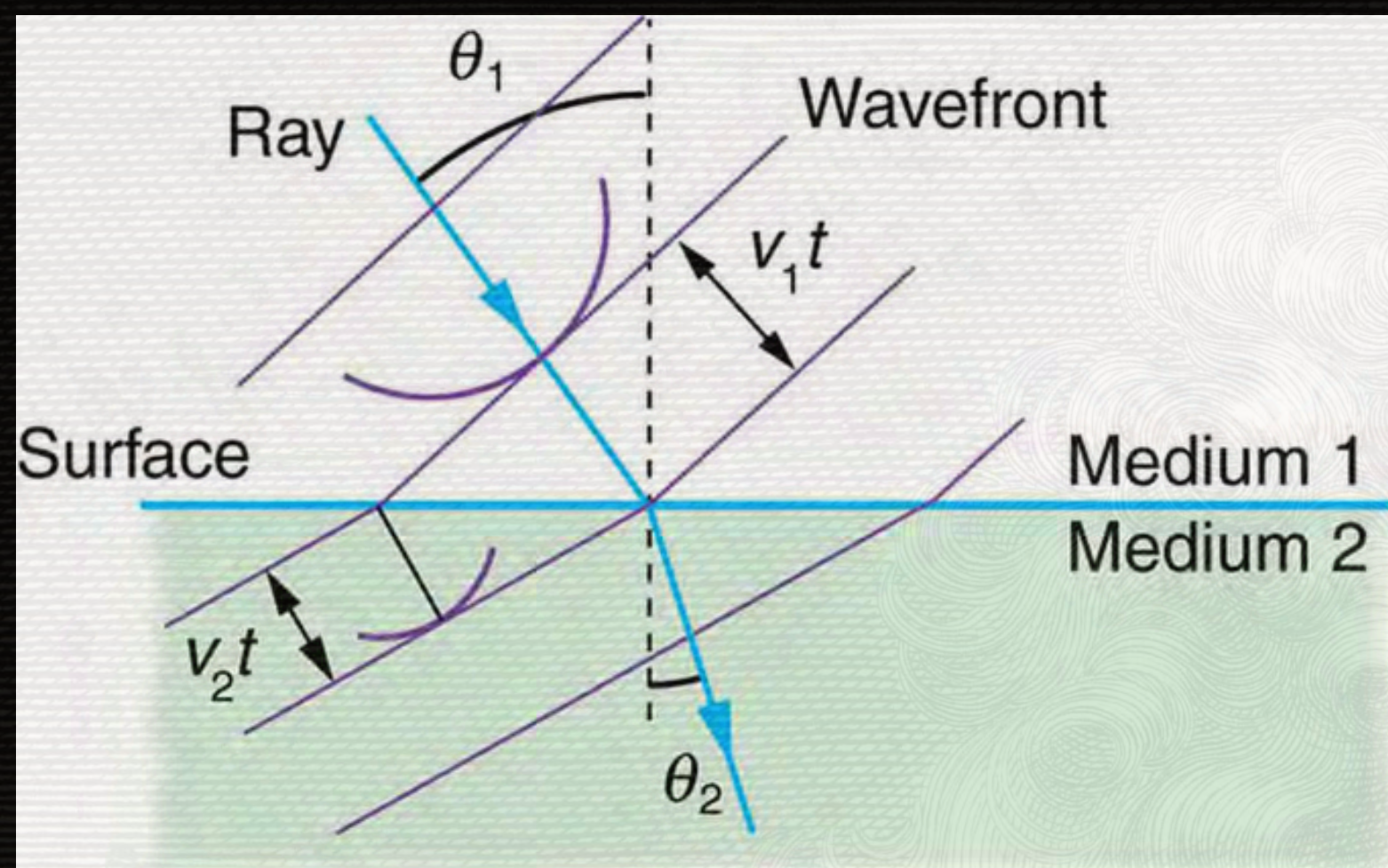
- We are in fact, building *pipelines* and *workflow engines*.



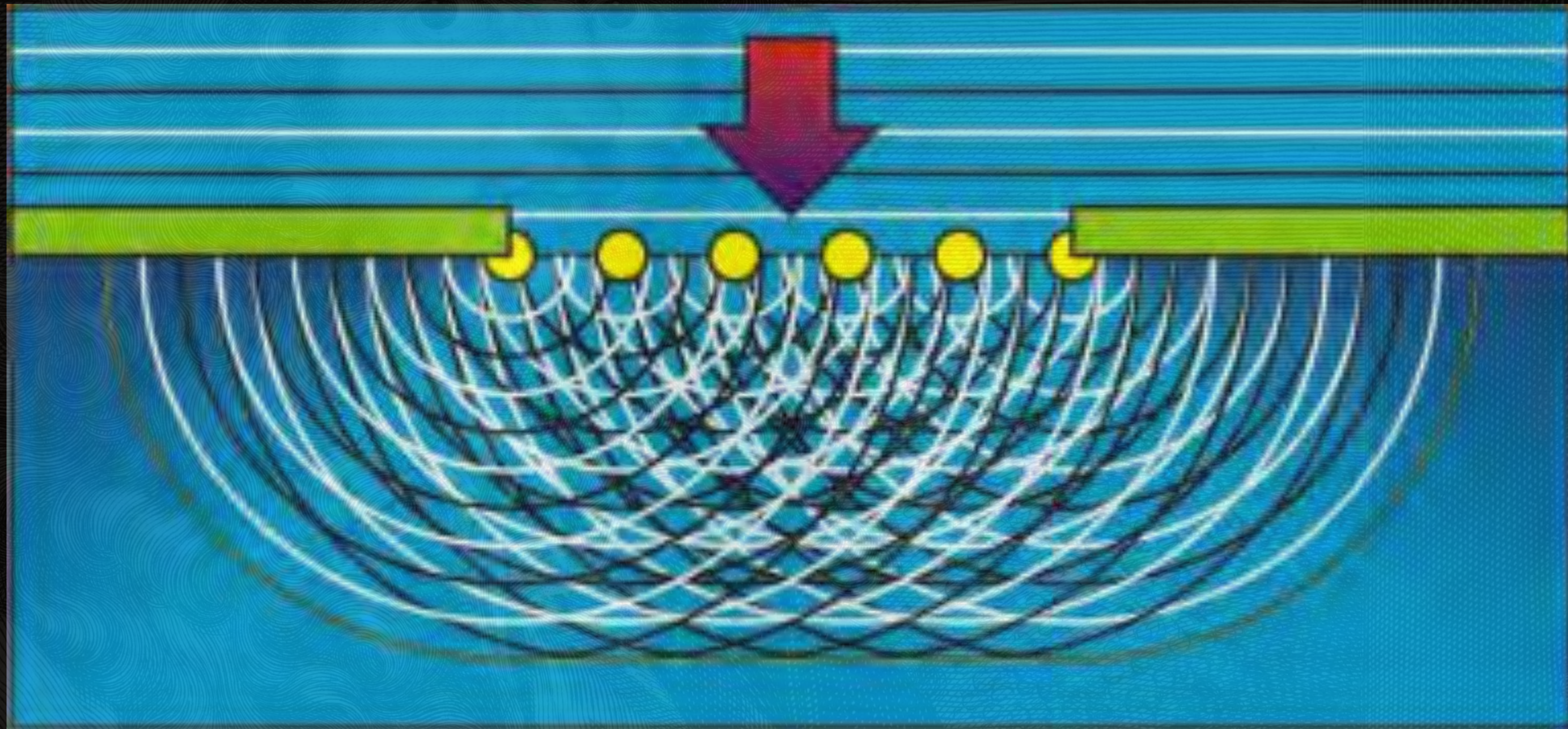
- Building tools to get data “up and out” and to the right locations, harvesting meta data along the way.
- People without backgrounds in HPC only peripherally appreciate the difference between scratch, campaign and archival storage. At the end of the day, they shouldn't need to care and the workflow should be smart enough to put their data where it best fits based upon workflow.
- When we build, we build for the workflow - **not** the IOPS or throughput of XYZ disk array.

Our image deconvolution workflow

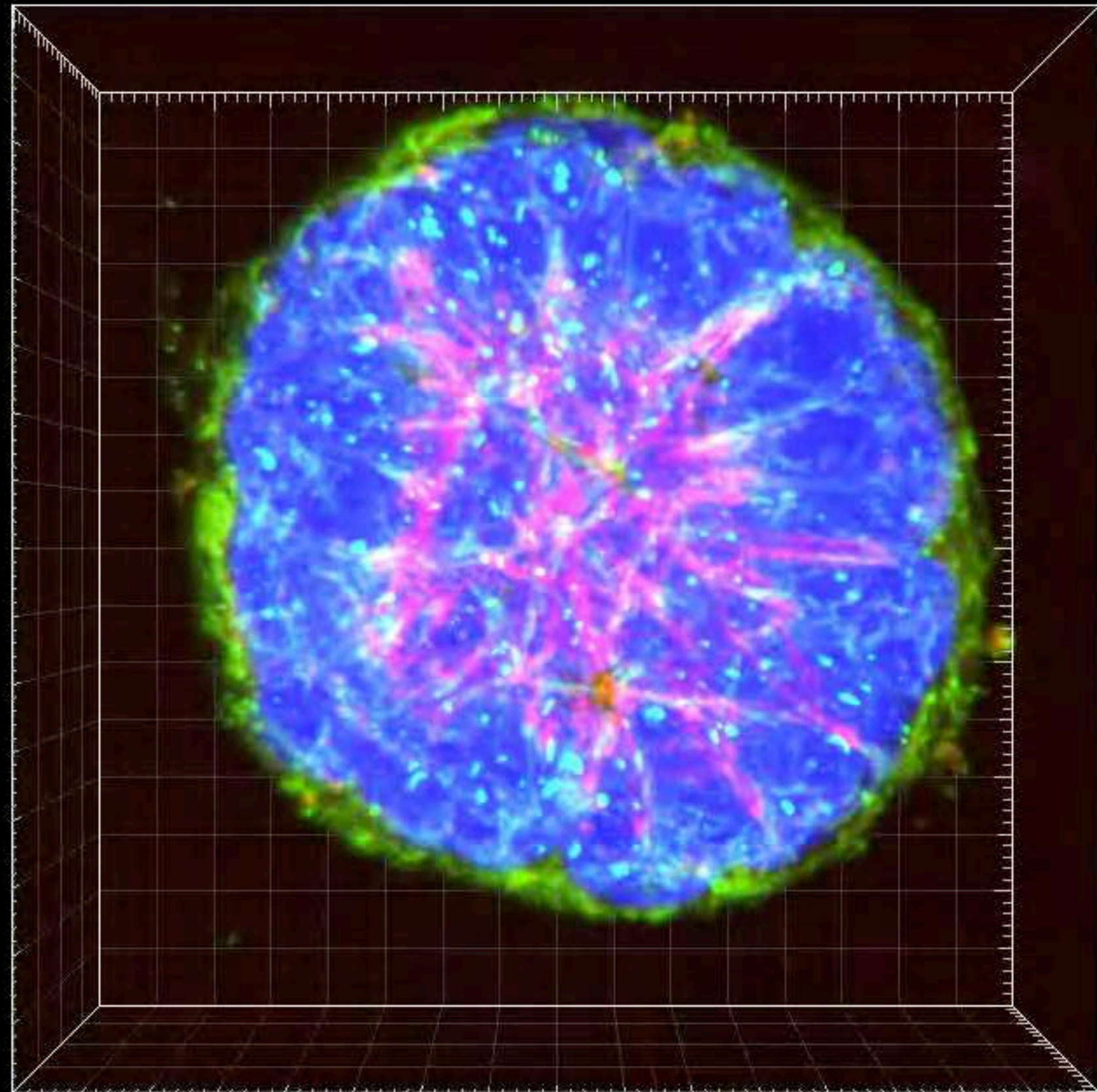
- First, what is deconvolution?
- Deconvolution is a mathematical operation used in image restoration to recover an object from an image that is degraded by blurring and noise. In fluorescence microscopy, the blurring is largely due to diffraction limited imaging by the instrument; the noise being mainly photonically induced.
- Our version of this runs on GPU's. [nVidia K80's]. P100's if nVidia will let me near them...



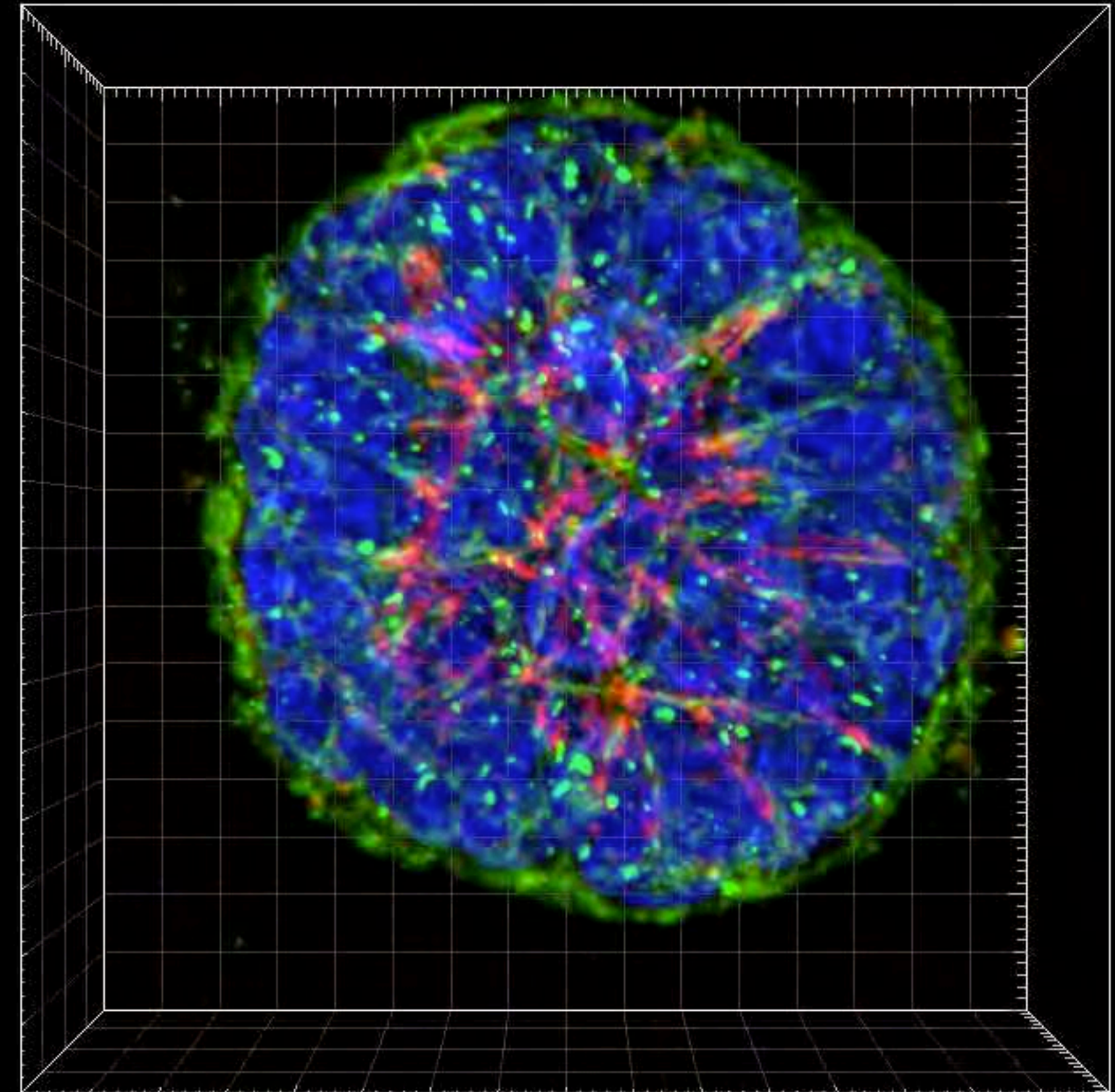
The **Huygens-Fresnel** principle states that every point on a wave-front is a source of wavelets. These wavelets spread out in the same forward direction, at the same speed as the source wave. The new wave-front is a line tangent to all of these wavelets.



Spinning Disk Z-stack
no deconvolution



Spinning Disk Z-stack
with deconvolution

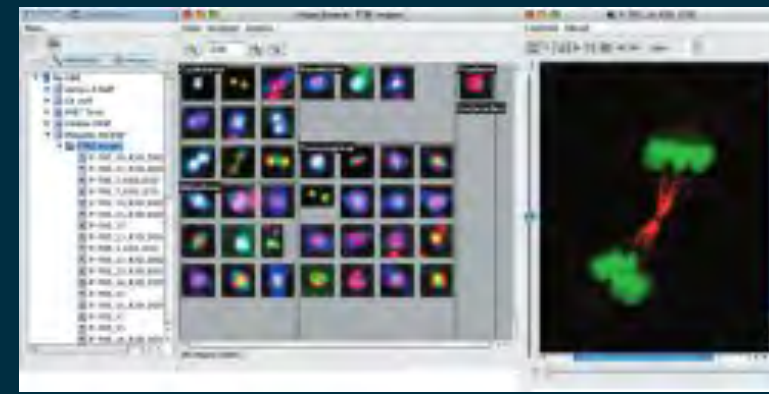


5GB/sec of PCI-E bandwidth for one hour.
86,000,000,000 neurons in a human brain.

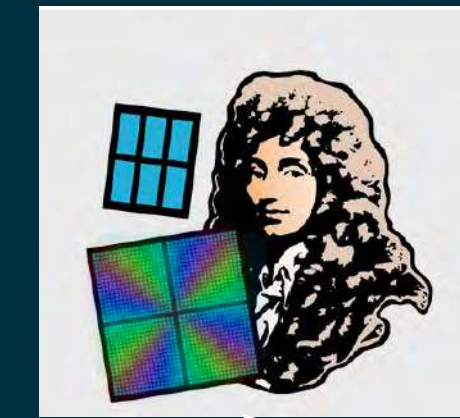
1. Acquire data at the scope



2. Uploader gathers meta data, dumps into object storage or POSIX depending upon workload



3. Automatic deconvolution on GPU infrastructure



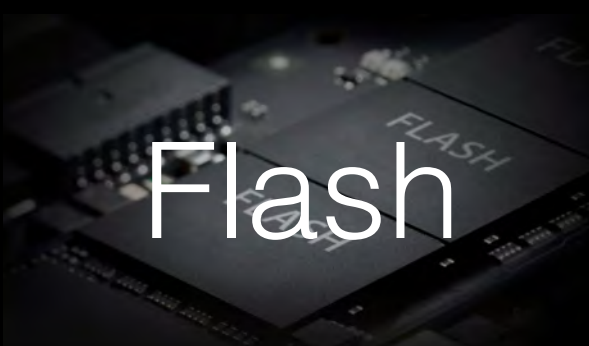
Then all the meta data about all of this runs off to “the repository” so it searchable, indexable reusable and discoverable. That’s an immutable, fixity-assured experiment in-silico, right there.



Ceph
(volume store as XFS)

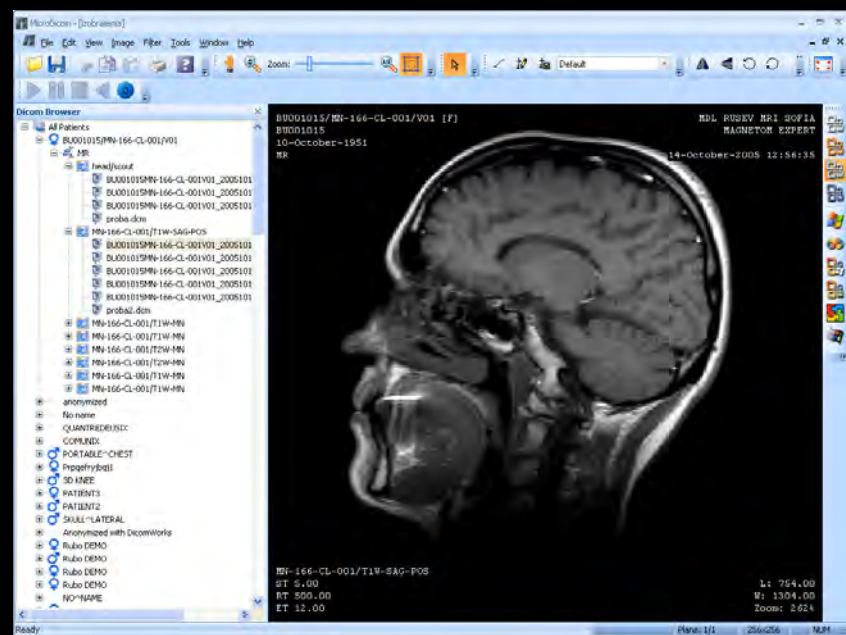


Deconvolved data back from GPU array



What does the repository look like?

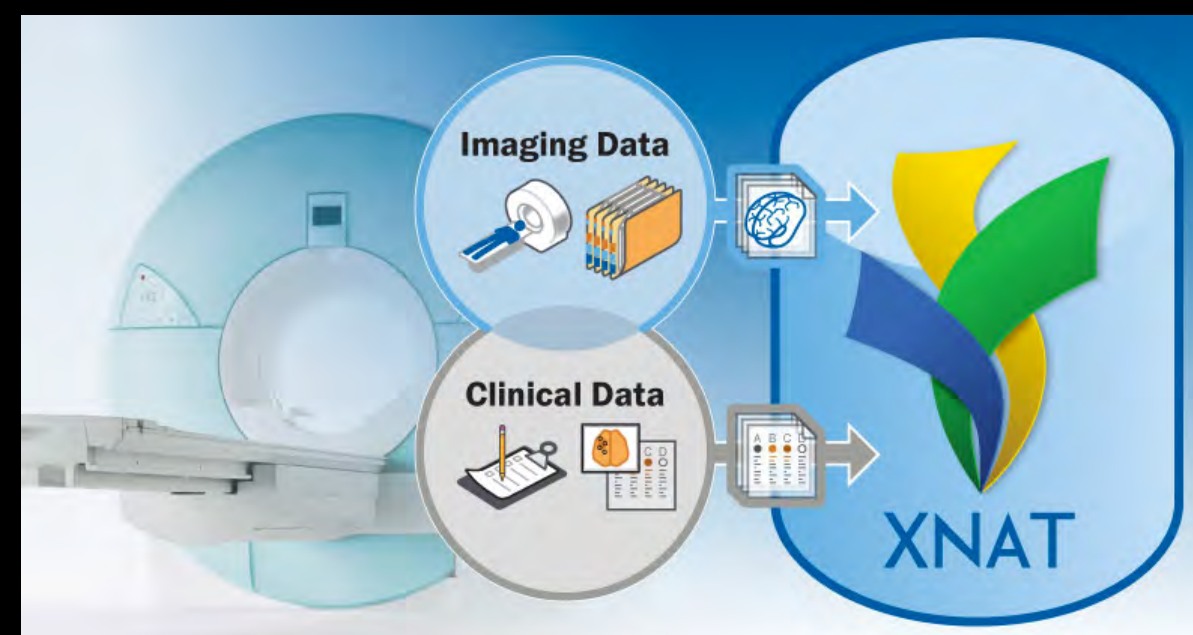
Massive multi-domain aware workflow and workload metadata consolidation in an object DB



DICOM/Human model data

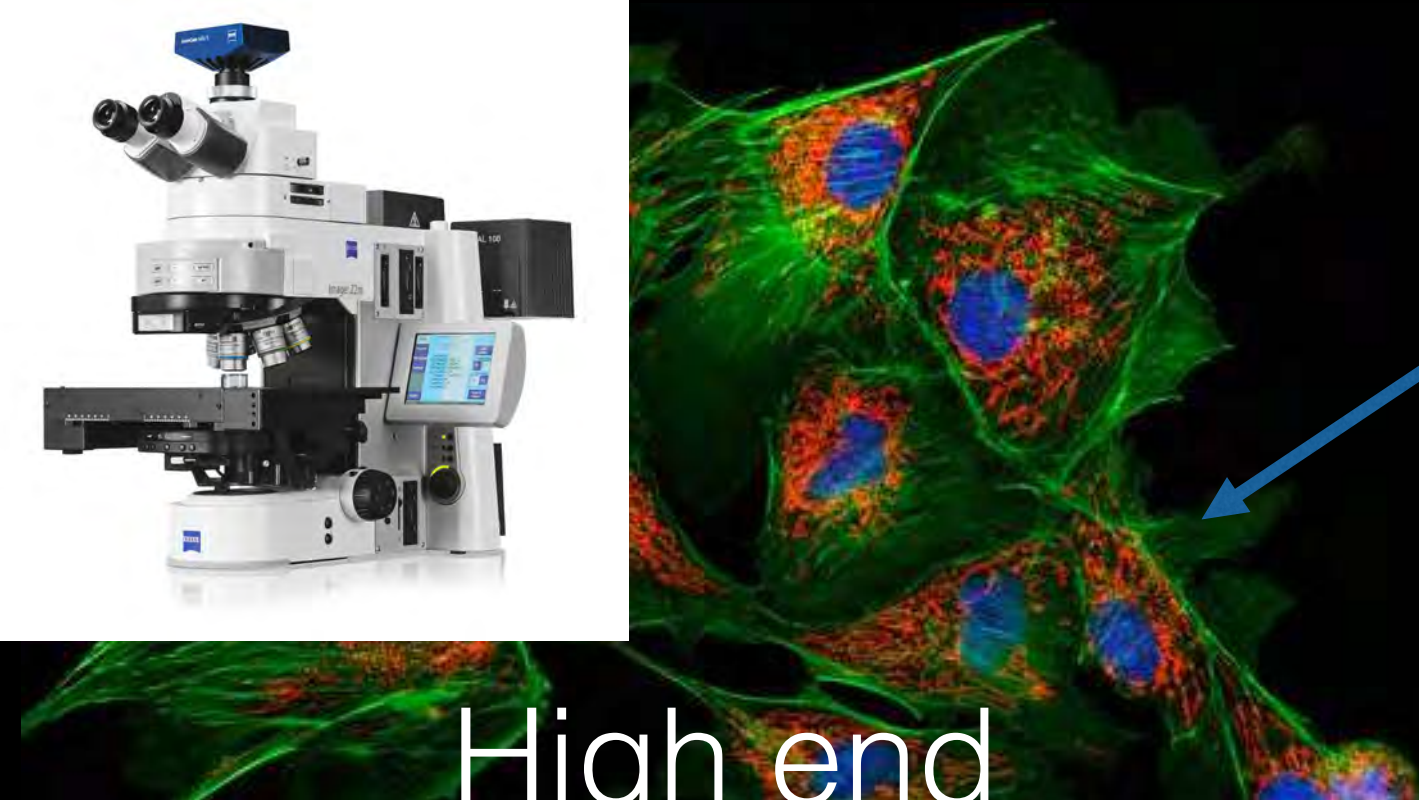


NGS/Genomics sequencers

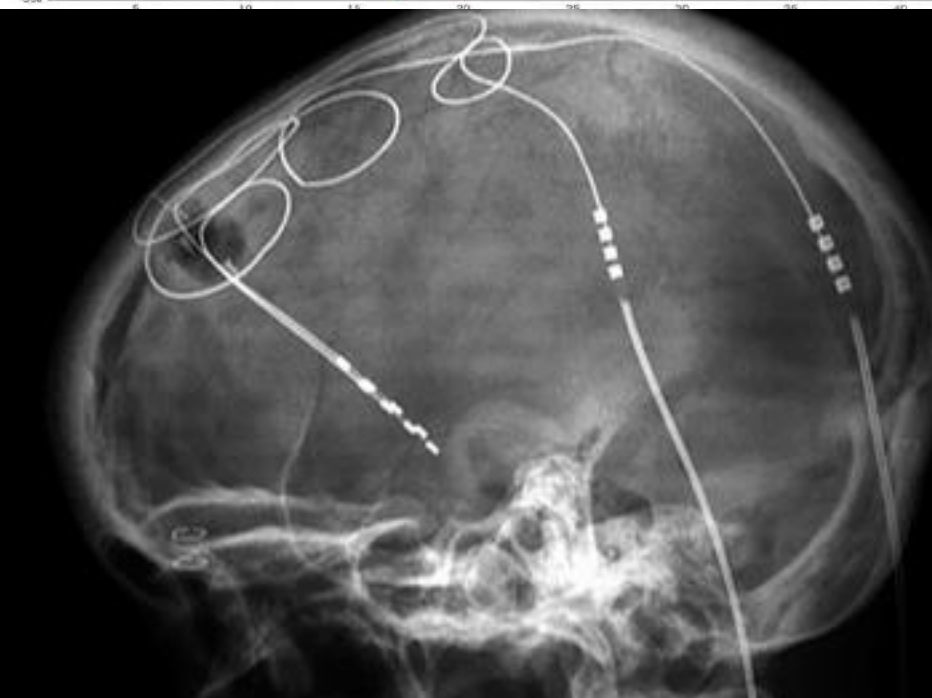
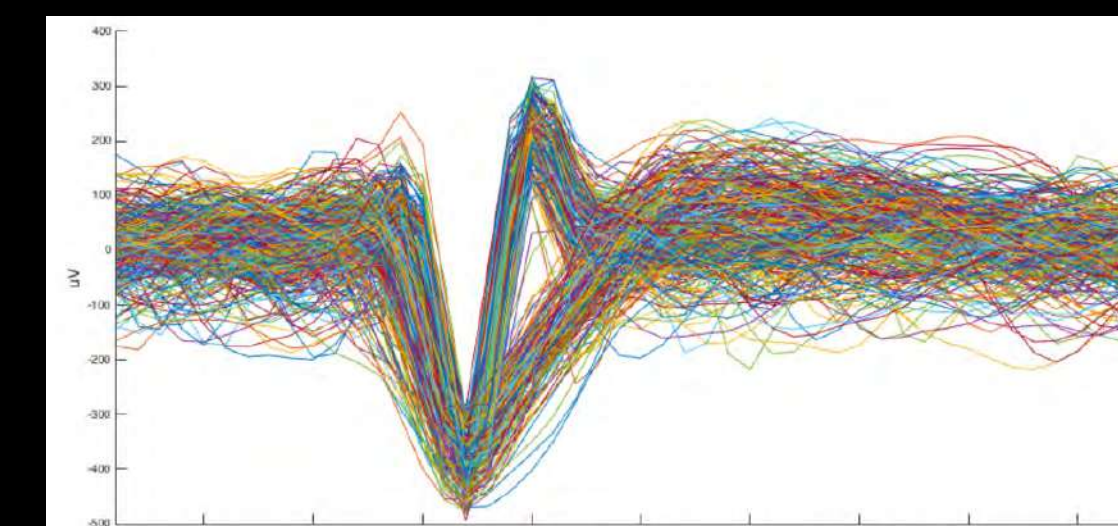


Multi-PB
object databases
for translational
workload correlation

**Bioinformatic analytics
effectively**

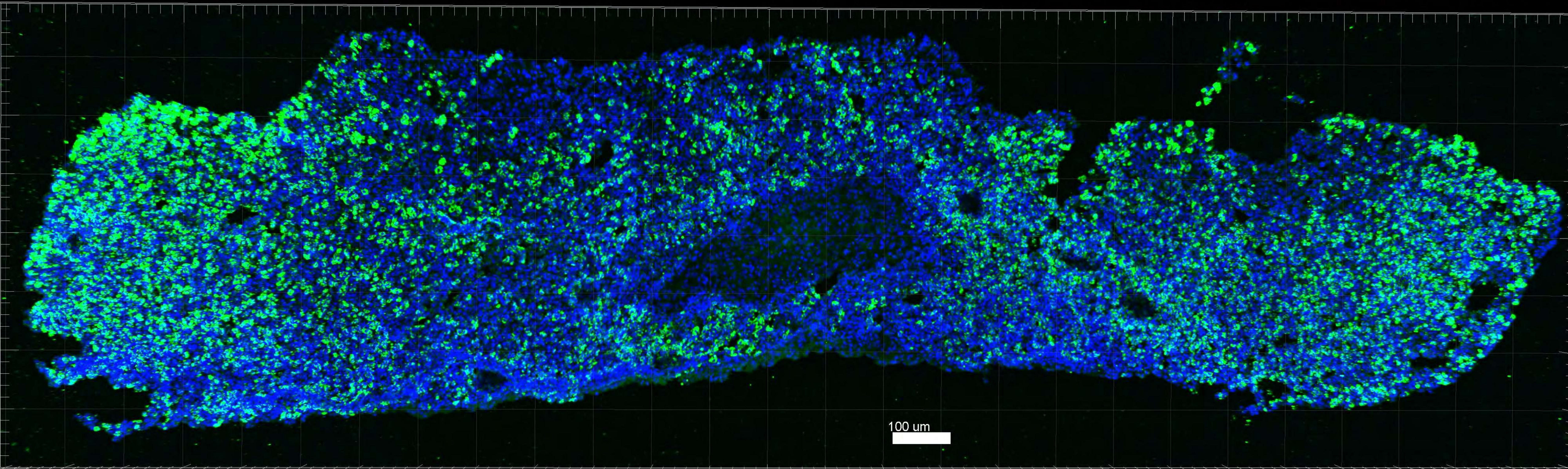


High end
super-res + confocal
microscopy



Ephys + DBS

And it is getting worse.



A 100,000 x 100,000 pixel cyst in a 3D deconvolved reconstruction of around 4TB of image data per sample.

Life is getting harder, in the life sciences - so we need to work smarter...

No better time than now
to start embedding *hints*
in your filesystem design.

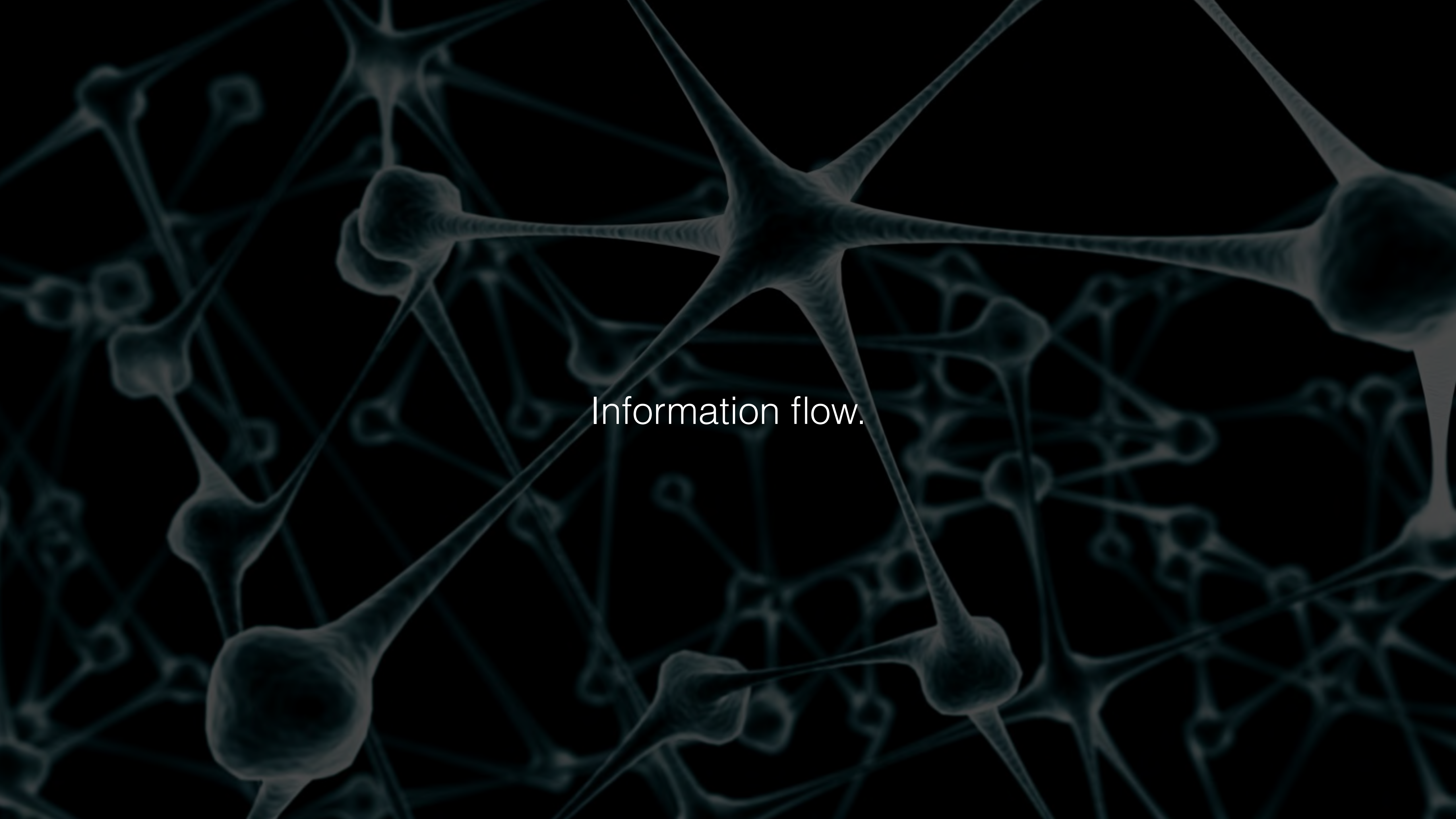
Build me storage subsystems that
are aware of locality, compute workloads
IO *patterns* and IO *personas*.

**(Please) stop thinking monolithically. Think about
patterns and use-case modularity.**

How cool would a fresh, reasonable, data locality
language or interface definition technology be that
proliferates compute, storage, the network and software?
And no, I don't mean DMAPI...

The take aways....

- Cross domain scientific research generates rich metadata for indexability, discoverability and reuse.
- Don't lose the lessons.
- Correlation and re-analysis,



Information flow.

CHANGE

STARTS HERE.

CAN WE COUNT YOU IN?