



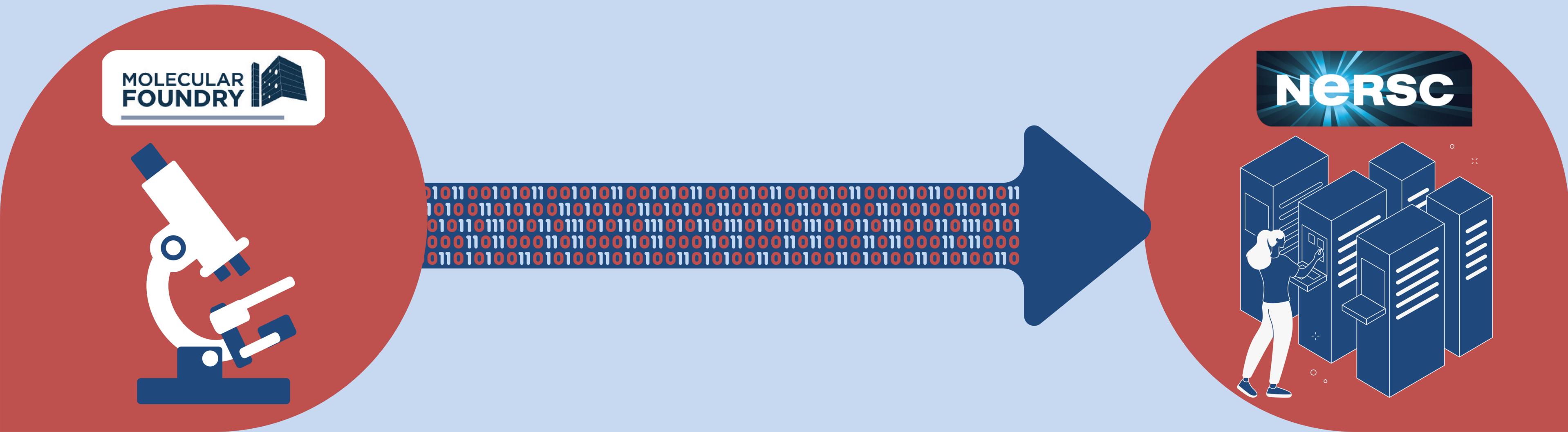
U.S. DEPARTMENT OF
ENERGY

Office of
Science



Live Streaming of Large Electron Microscope Data to NERSC

Sam Welborn, Bjoern Enders, Peter Ercius, Chris Harris, Deborah Bard



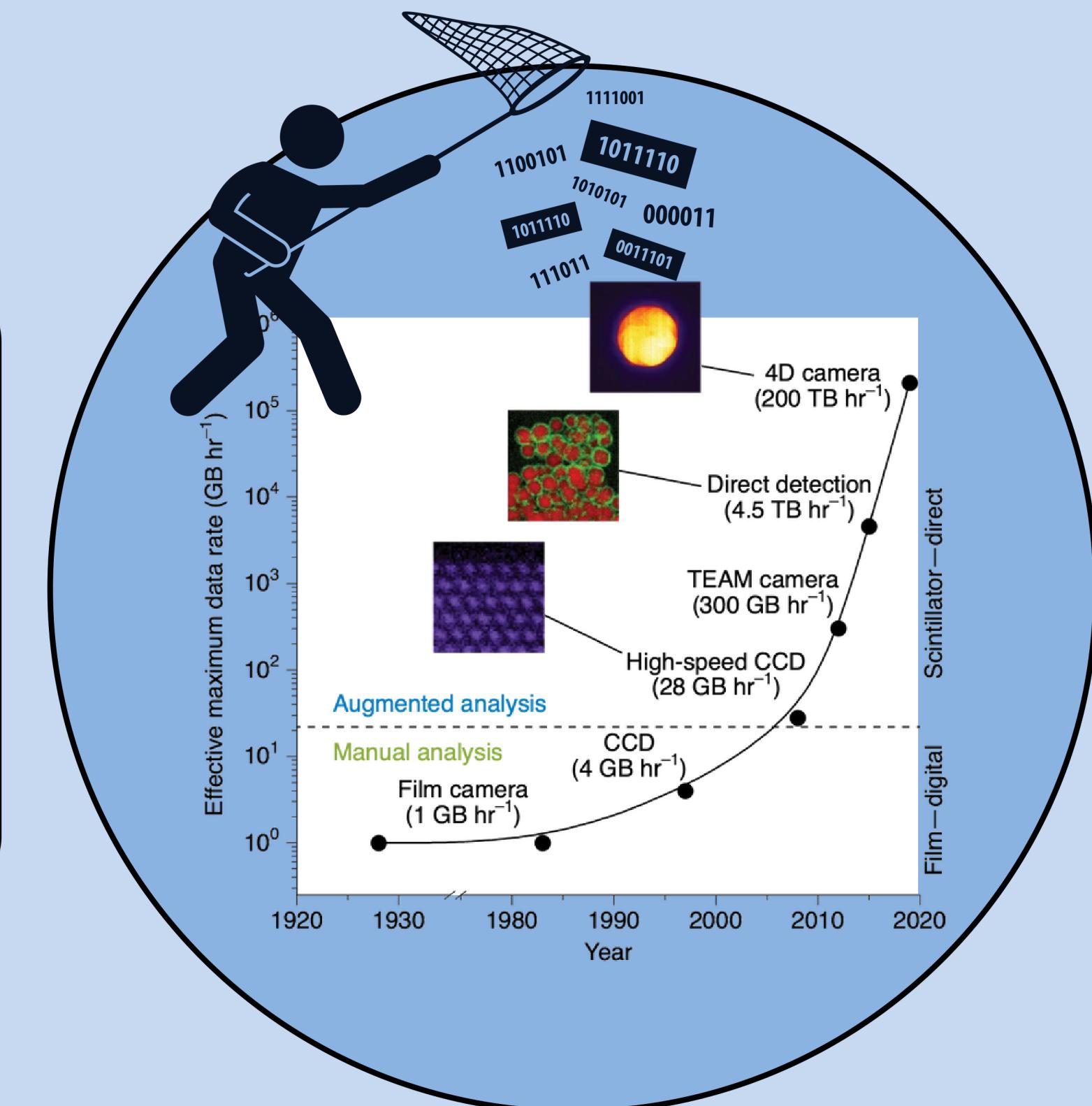


The data deluge

Faster detectors have led to unprecedented data generation rates

- Lightsources (e.g., ALS, NSLS-II, APS) will cumulatively generate an **exabyte** of data per year by 2028
- 10-1000 PFLOPs peak on-demand compute resources

Schwarz, N. et al. doi.org/10.1007/978-3-030-63393-6_10



Read more

Spurgeon et al. Nature Materials volume 20, pages 274–279 (2021).



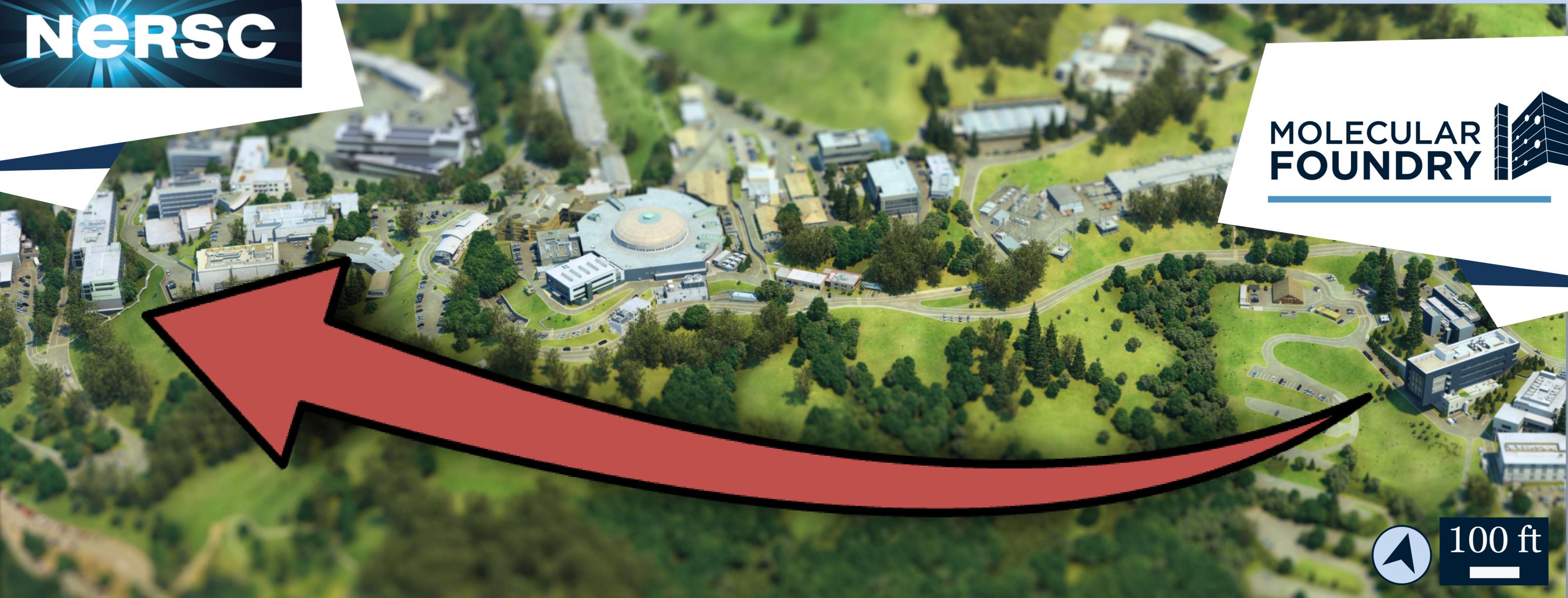
Berkeley Lab

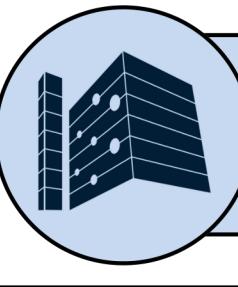
NERSC

**MOLECULAR
FOUNDRY**

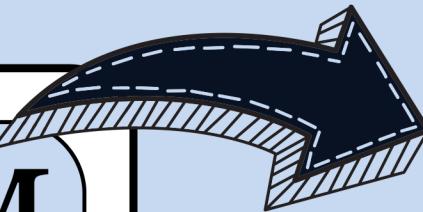


100 ft





The Molecular Foundry/NCEM



National Center for
Electron Microscopy
one of seven facilities in TMF

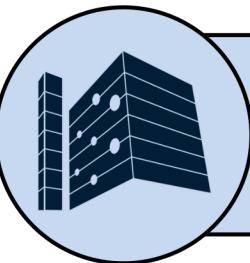
Instrumentation

- State-of-the-art methods and instrumentation in nanoscale science free of charge



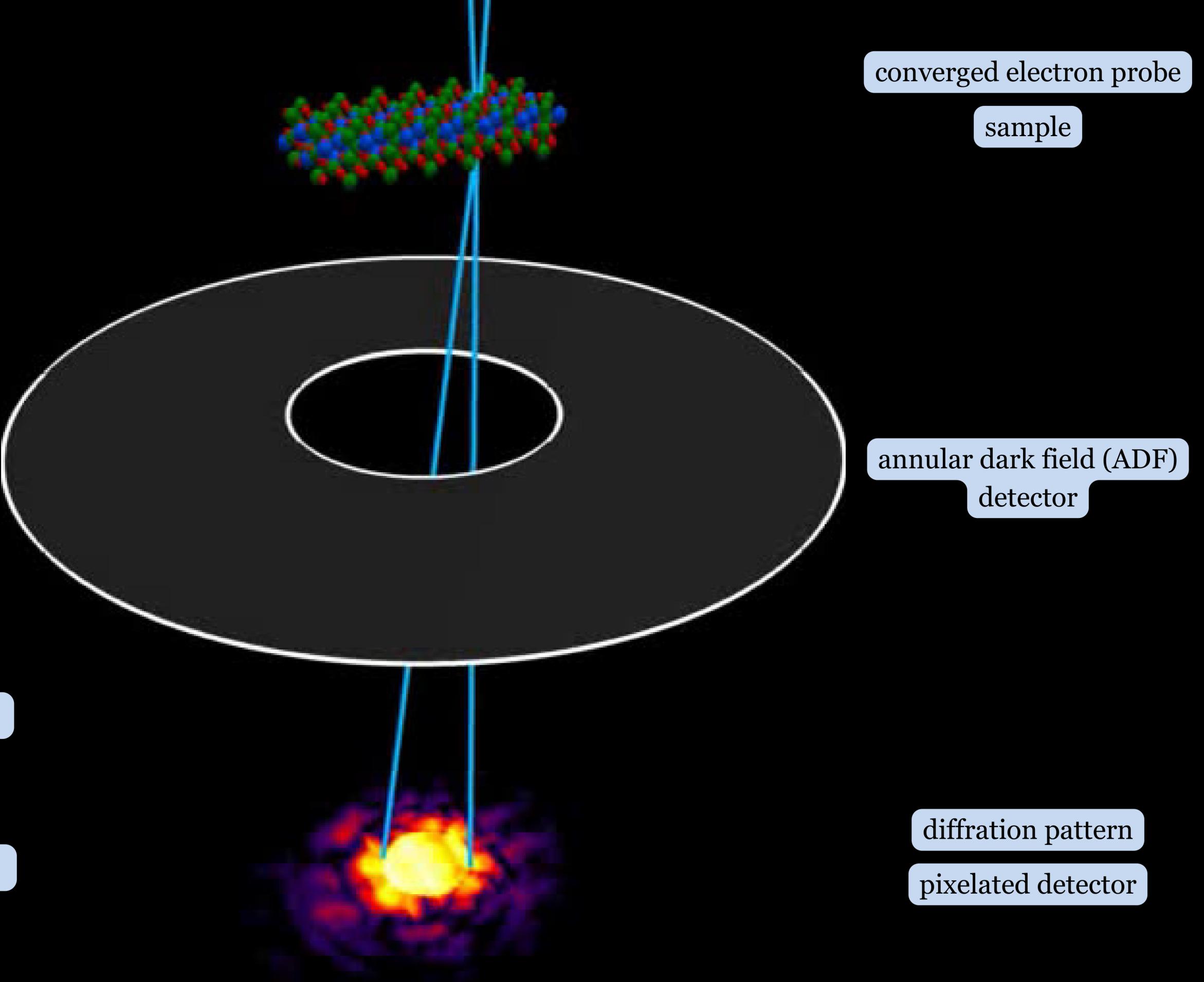
Expertise

- Leaders in:
4DSTEM,
image simulation,
electron detector in situ,
technology high resolution,
tomography,
in situ,
soft materials



STEM

Scanning Transmission
Electron Microscopy



2D images recorded over a 2D grid of probe positions:

Four dimensional scanning transmission electron microscopy
(4D-STEM)

converged electron probe

sample

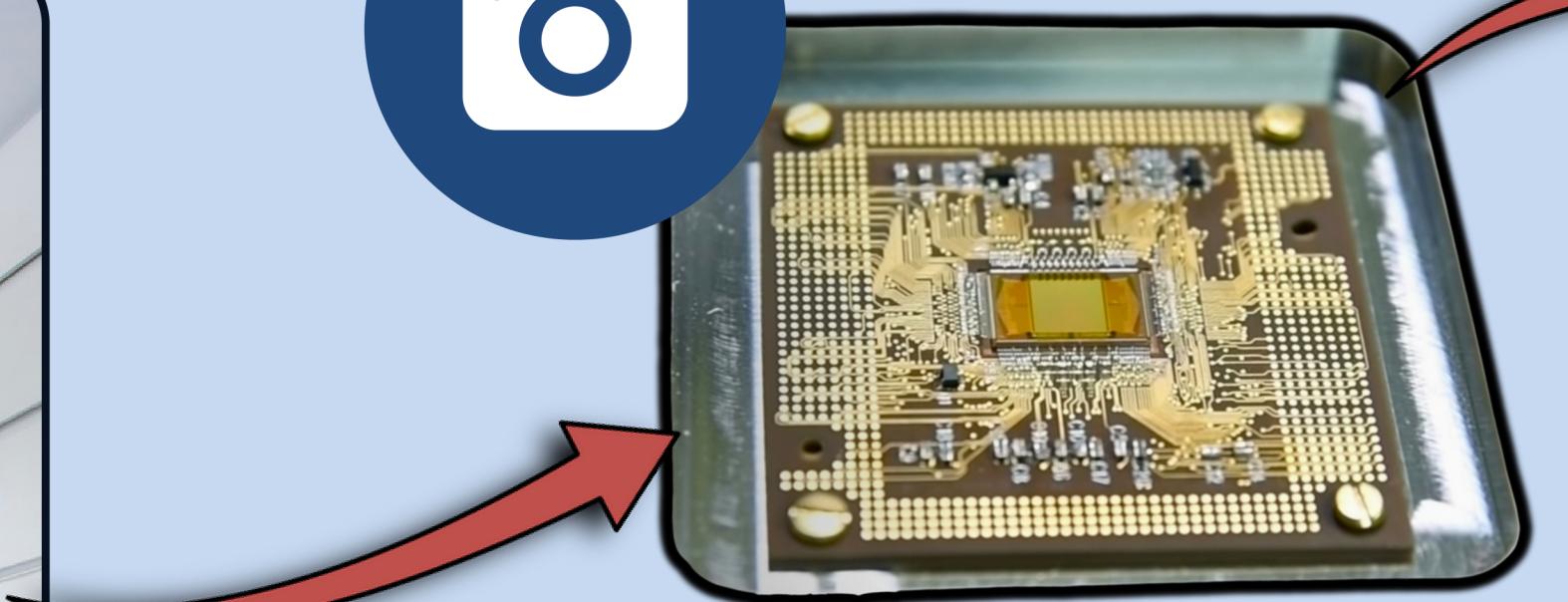
annular dark field (ADF)
detector

diffraction pattern

pixelated detector



The 4D Camera



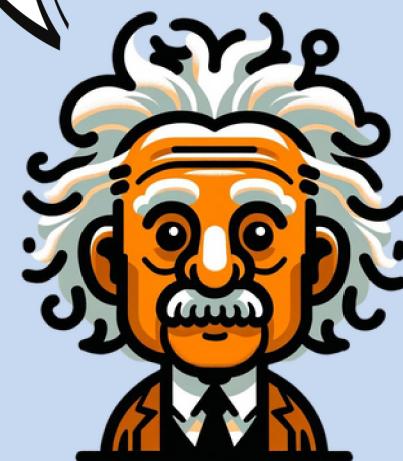
4D Camera



What is that?



Something your
models didn't
predict...



Generates data at 480 Gb/s

700 GB dataset collected in 15 seconds

TEAM 0.5



File transfer workflow

User





File transfer workflow

User



TEAM 0.5

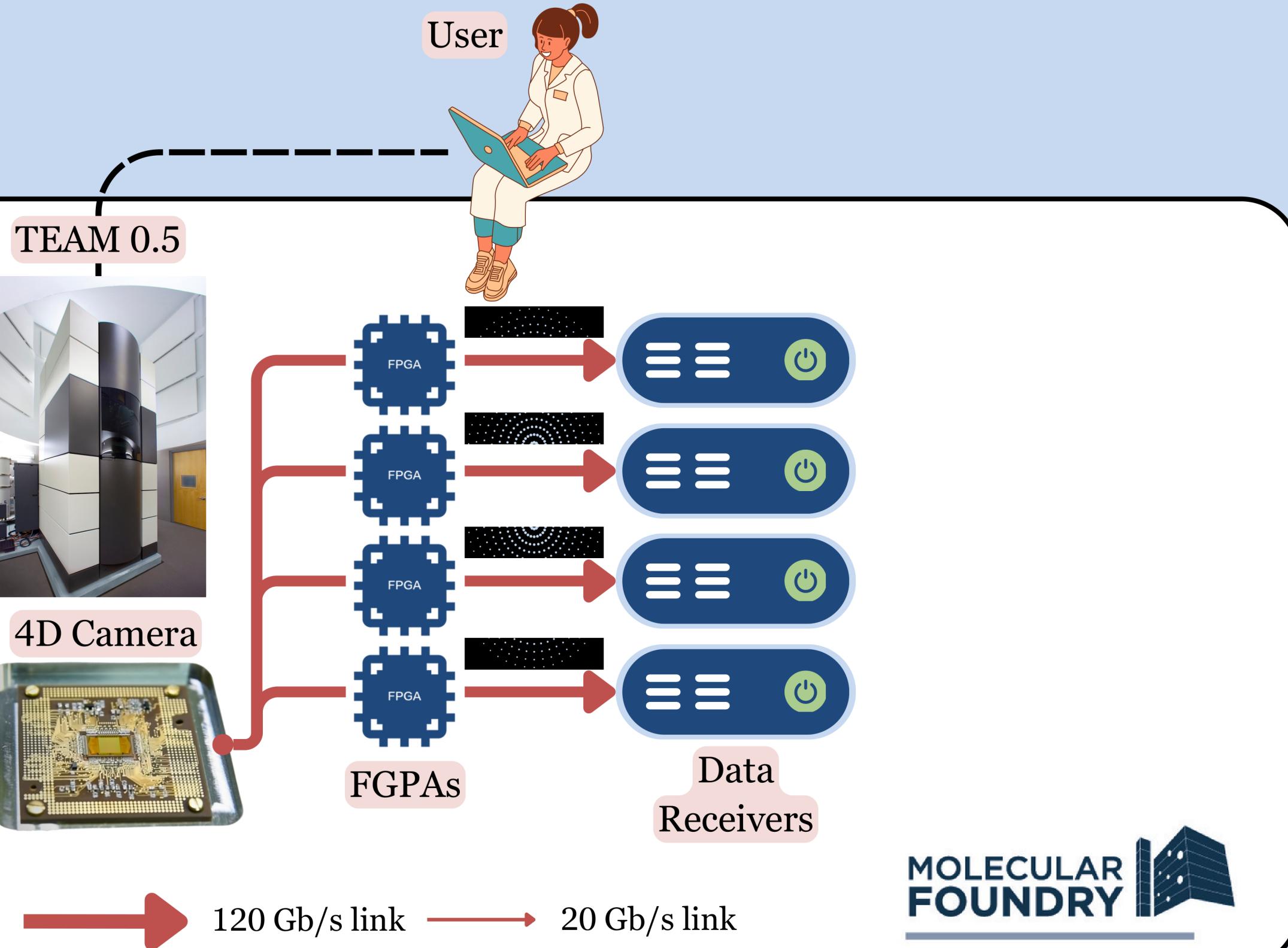


4D Camera





File transfer workflow





File transfer workflow

User



TEAM 0.5



4D Camera

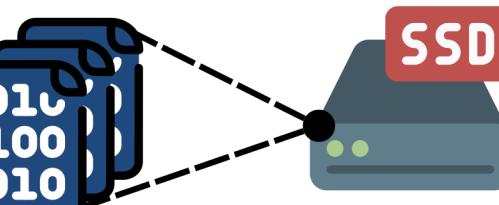
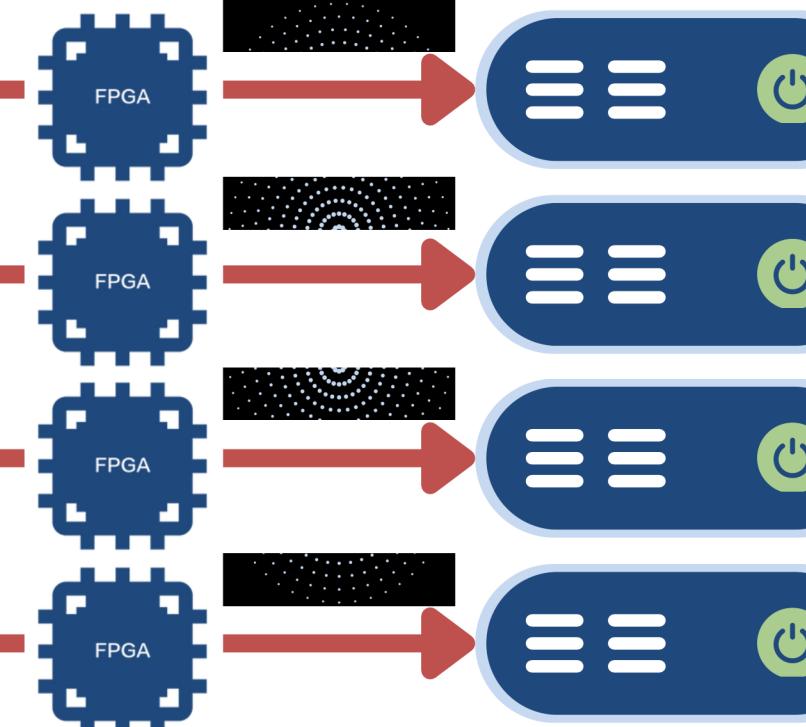


FGPAs

Data
Receivers

120 Gb/s link

20 Gb/s link

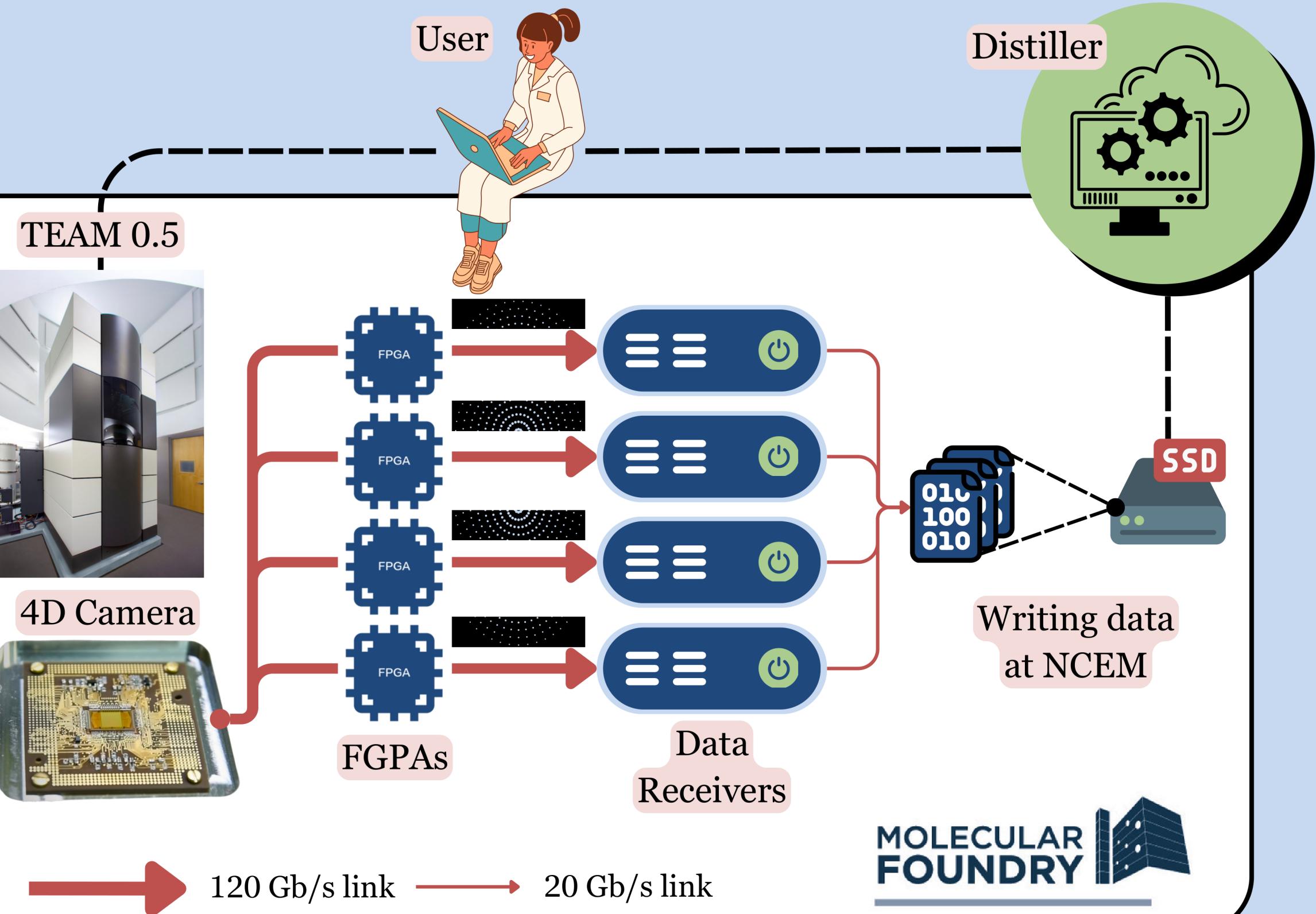


Writing data
at NCEM

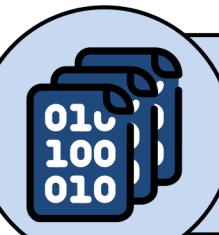
MOLECULAR
FOUNDRY



File transfer workflow



File transfer workflow



TEAM 0.5



4D Camera



FGPAs

Data
Receivers

120 Gb/s link

20 Gb/s link

User



Distiller



Spin

kubernetes

Frontend:
React

Redux

docker

Backend:
FastAPI
Superfacility API

SQLAlchemy
kafka

SQL

MOLECULAR
FOUNDRY

Writing data
at NCEM

File transfer workflow



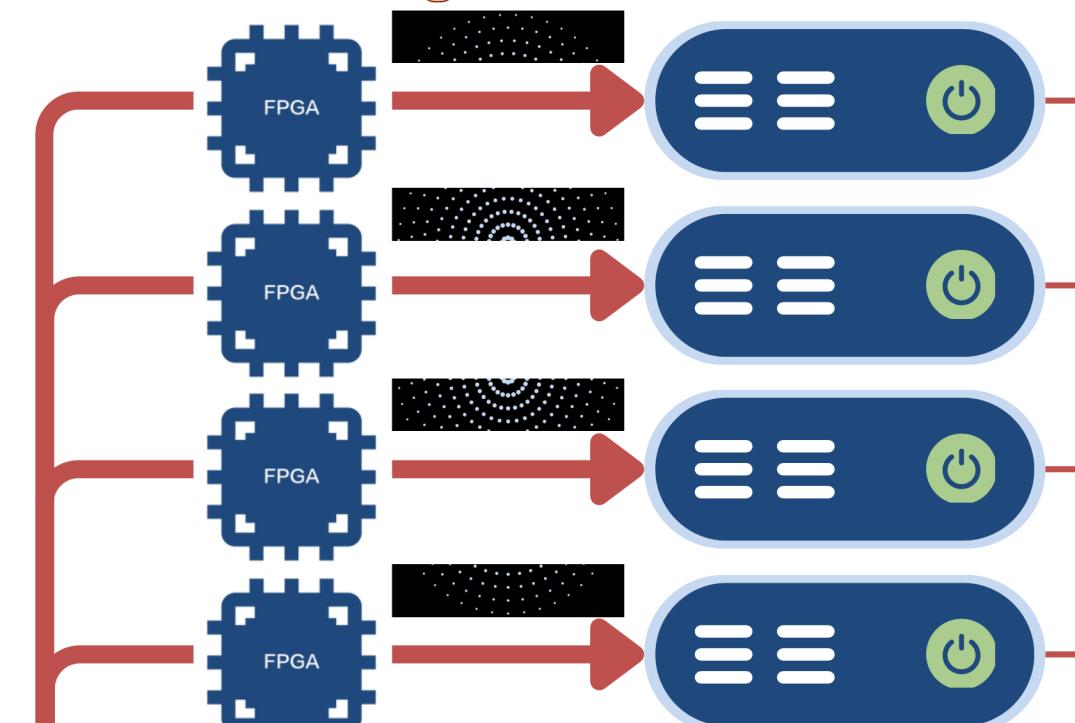
TEAM 0.5



4D Camera



FPGAs



Data
Receivers

MOLECULAR
FOUNDRY

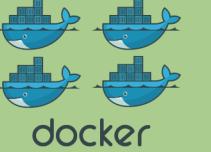
120 Gb/s link → 20 Gb/s link

Distiller

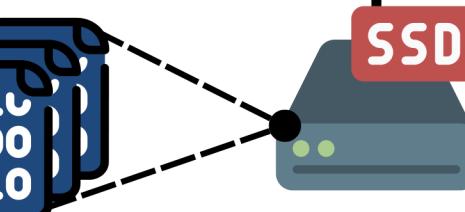
Spin

kubernetes

Frontend:



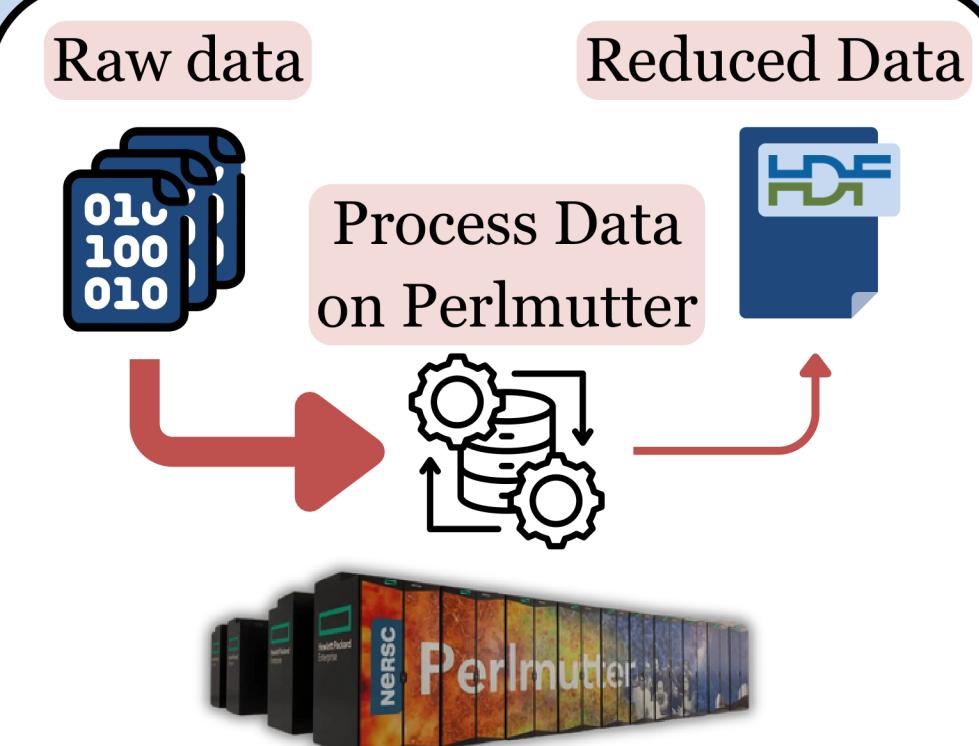
Backend:
FastAPI
Superfacility API



Writing data
at NCEM

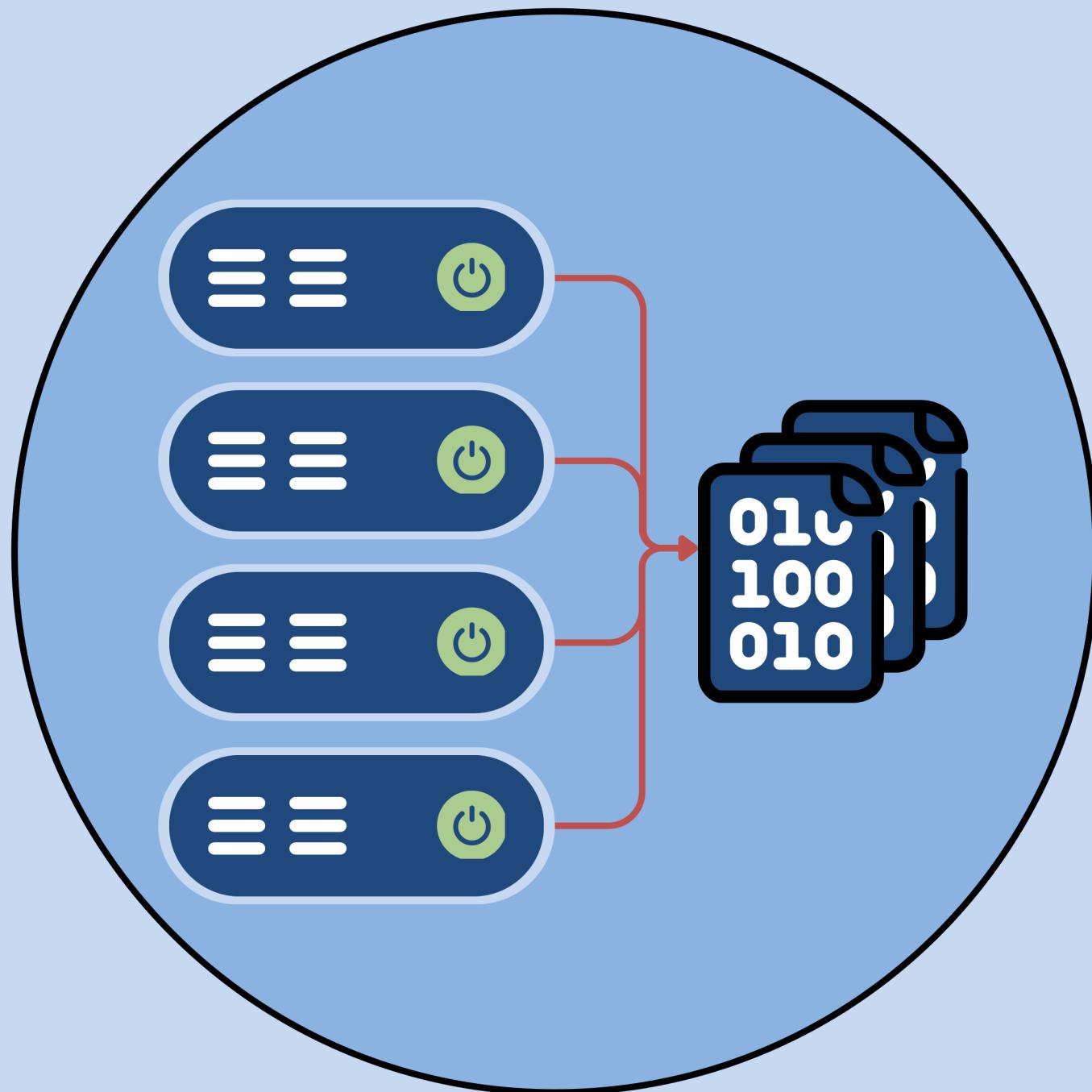
010
100
010
0110
101001
01101110101101
0110

100 Gb/s
link

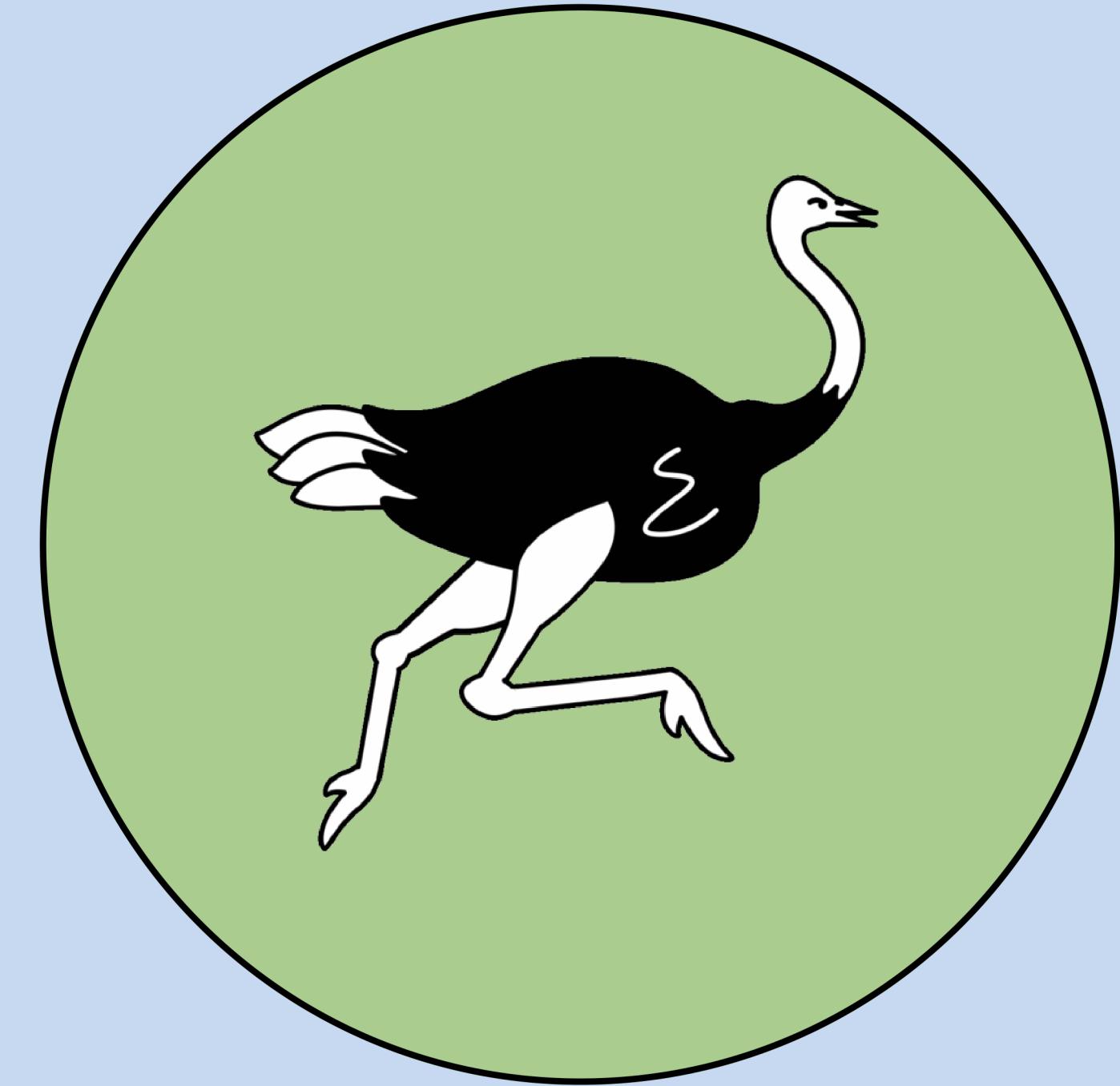
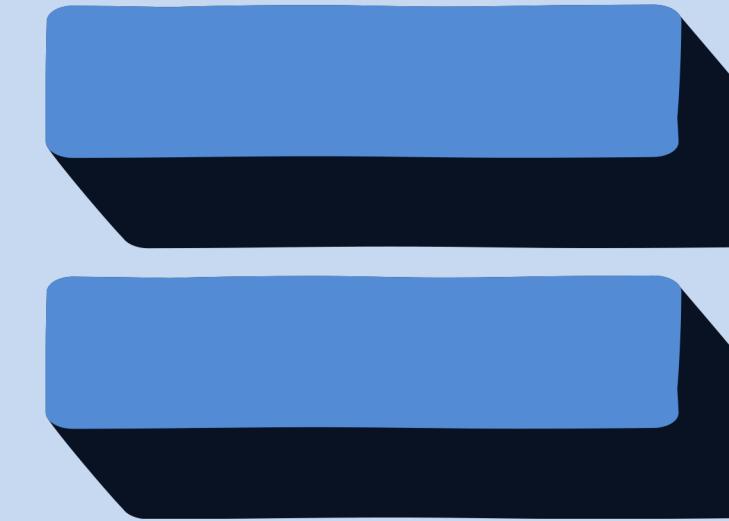
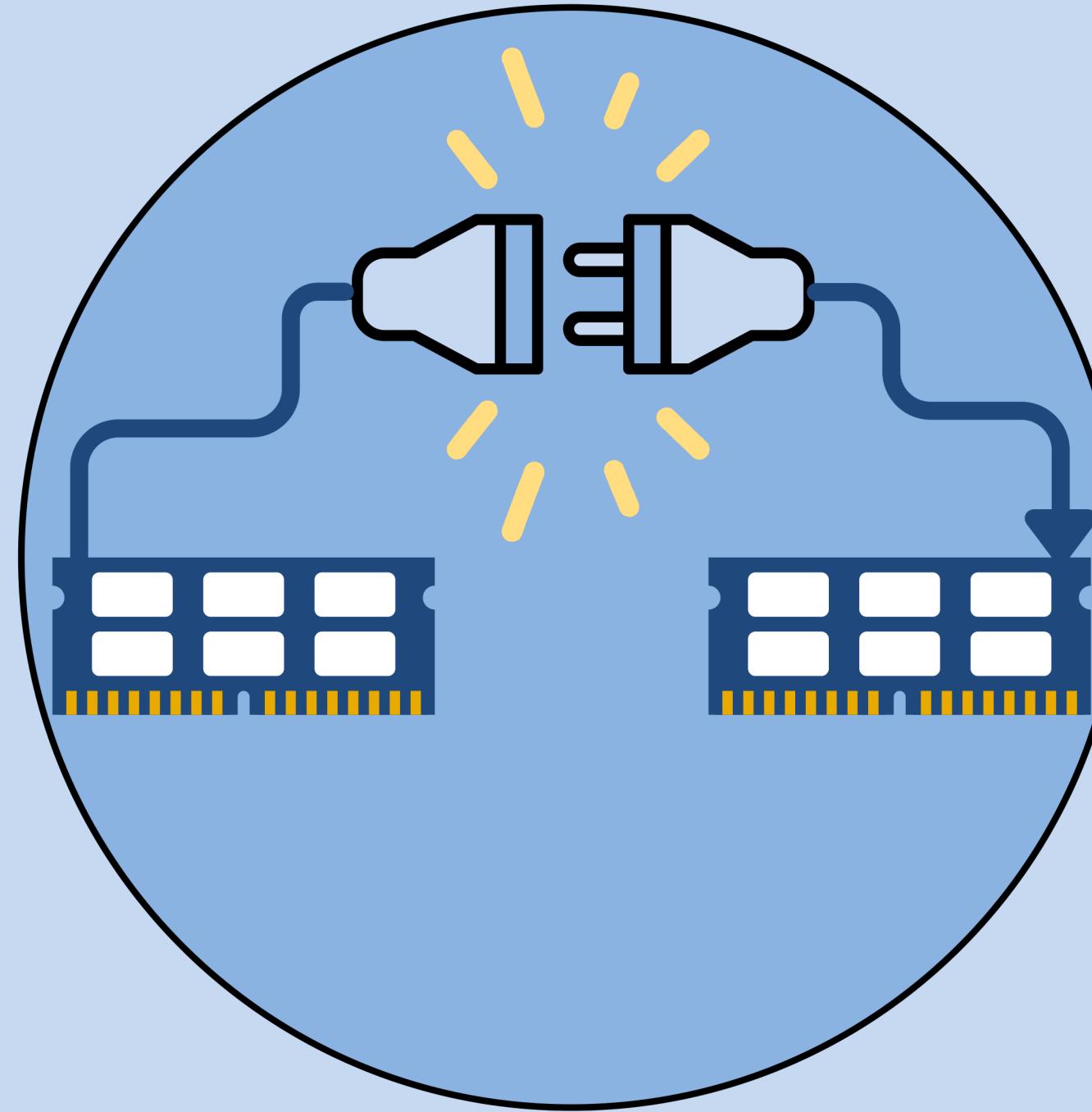


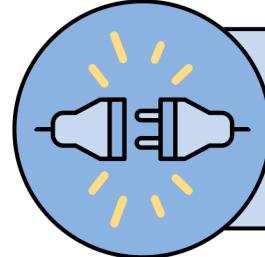
NERSC

File I/O is slow



RAM-to-RAM transfer is fast



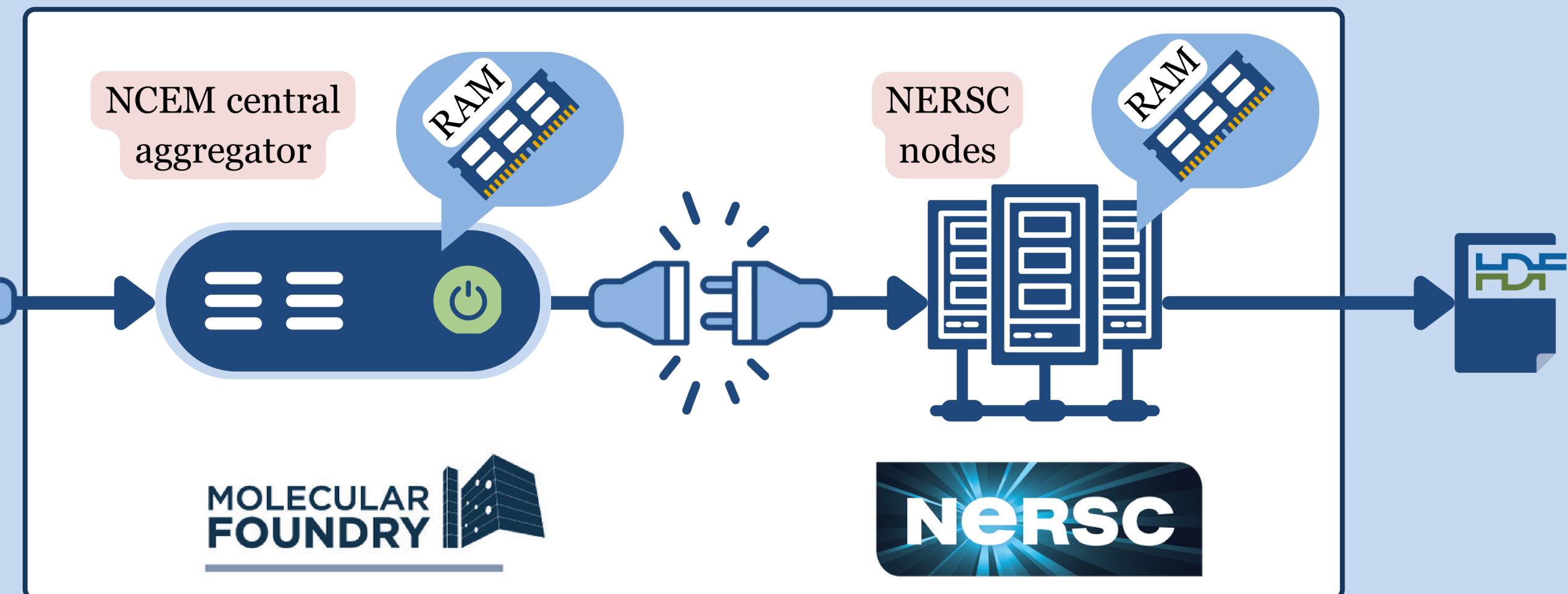


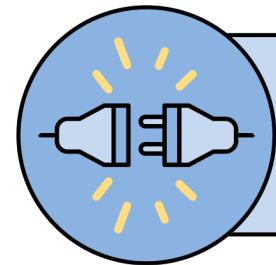
Streaming workflow

Data Receivers

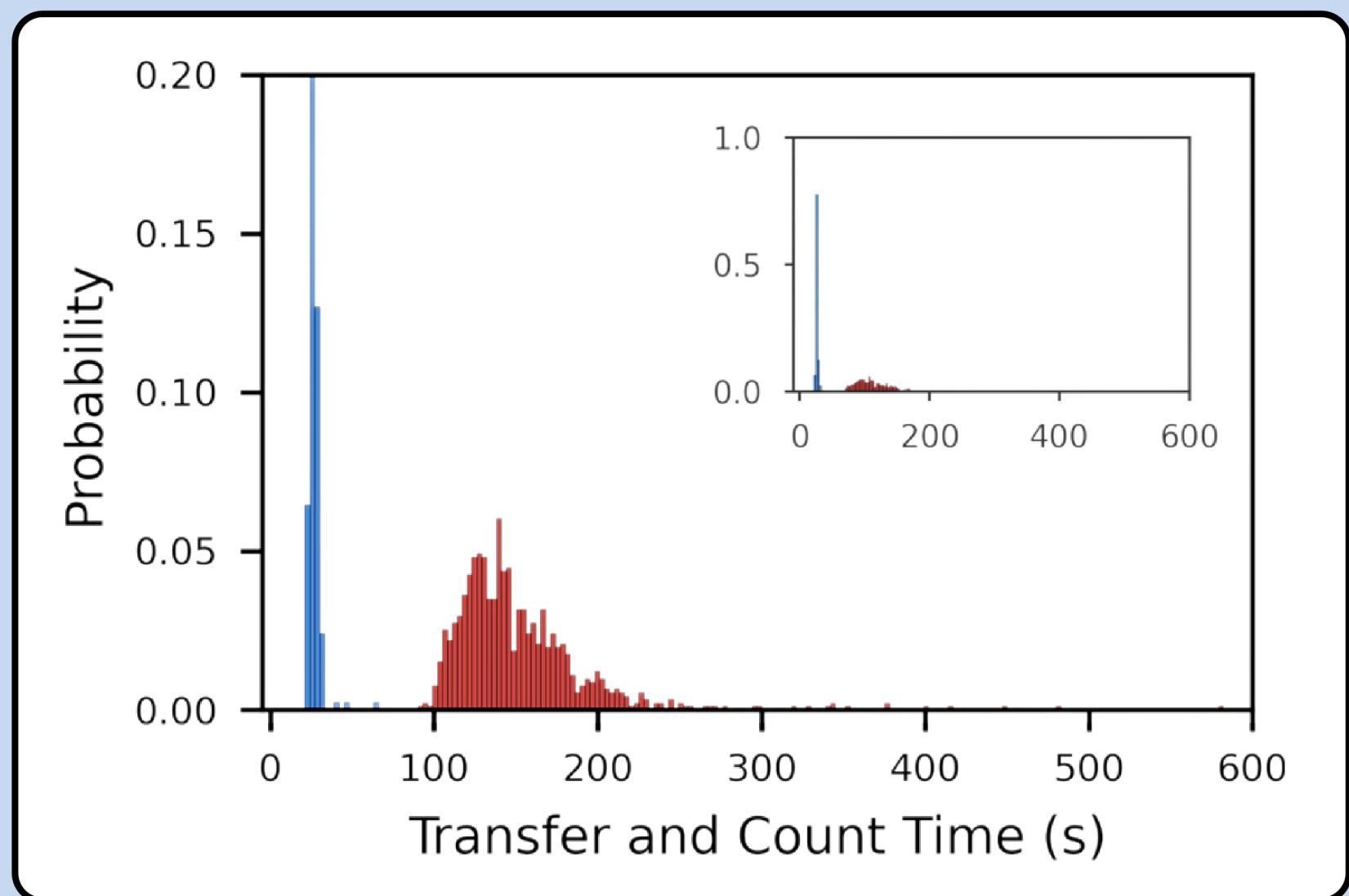


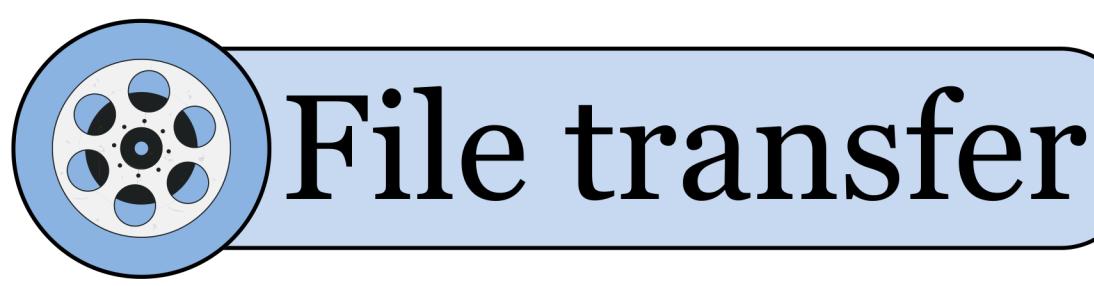
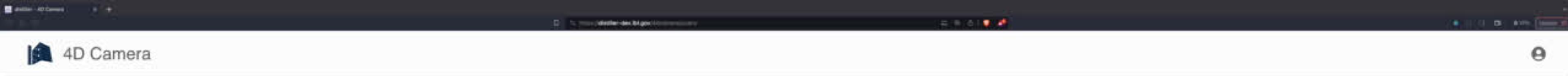
ØMQ sockets
connect our network

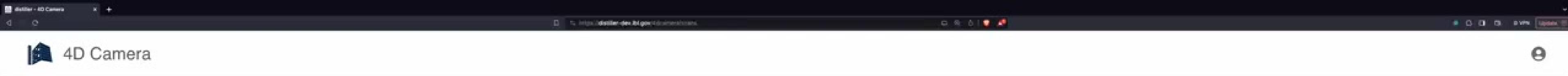




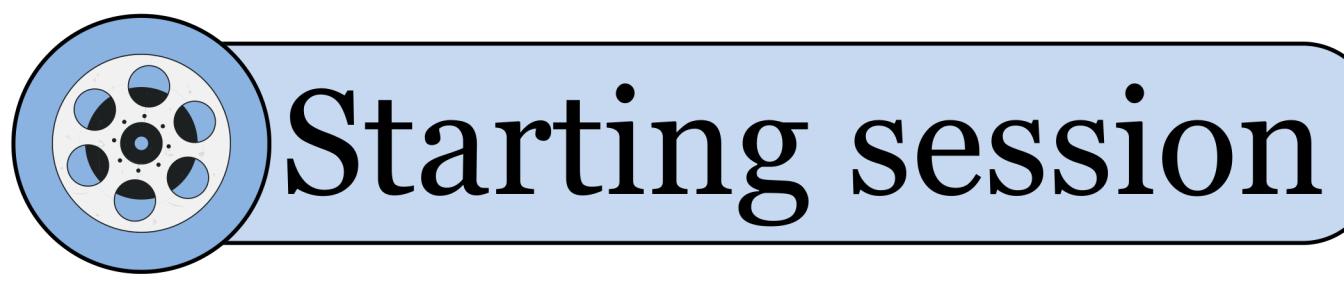
Streaming workflow: results







	ID	Scan ID	Notes	Location	Created	Progress
<input type="checkbox"/>	4680	5439	not streaming	 128.55.132.192 X	11/8/2023	
<input type="checkbox"/>	4677	5436		 128.55.132.192 X permuter	11/7/2023	
<input type="checkbox"/>	4676	5435		 128.55.132.192 X permuter	11/7/2023	
<input type="checkbox"/>	4675	5434		 128.55.132.192 X permuter	11/7/2023	
<input type="checkbox"/>	4674	5433		 128.55.132.192 X	11/7/2023	
<input type="checkbox"/>	4673	5432		 128.55.132.192 X permuter	11/7/2023	
<input type="checkbox"/>	4672	5431		 128.55.132.192 X permuter	11/7/2023	
<input type="checkbox"/>	4671	5430		 128.55.132.192 X permuter	11/7/2023	
<input type="checkbox"/>	4670	5429		 128.55.132.192 X permuter	11/7/2023	
				 128.55.132.192 X permuter	11/7/2023	



4D Camera

Storage Usage 5.8 TB Free

EXPORT FILTER

ID	Scan ID	Notes	Location	Created	Progress
4660	5419		128.55.132.192	perlmutter	11/7/2023
4659	5418		128.55.132.192	perlmutter	11/7/2023
4658	5417		128.55.132.192	perlmutter	11/7/2023
4657	5416		128.55.132.192	perlmutter	11/7/2023
4656	5415		128.55.132.192	perlmutter	11/7/2023
4655	5414		128.55.132.192	perlmutter	11/7/2023
4654	5413		128.55.132.192	perlmutter	11/7/2023
4653	5412		128.55.132.192	perlmutter	11/7/2023
4652	5411		128.55.132.192	perlmutter	11/7/2023

DigitalMicrograph - Overlay Image

Scanning 100 kV Mag x 12M CL: 14 nm

Scanning 100 kV Mag x 12M CL: 14 nm

5 nm

Scan

OneView Camera

4D Camera Control

Interpolate: Average

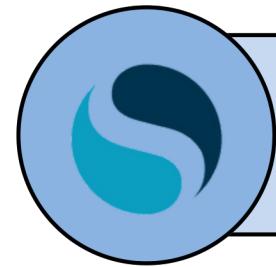
Auto scale

Reset Dark: Take Dark

Scan selector

1 // Acquire a set of 4D Camera scans.
2 // Set the sleep_time to account for offload time.
3
4 string command, ipAddressHost, reply
5 TagGroup Old, OldItems
6
7 // Gatan user variables
8 number rotation = 0 // degrees, it matches FEI software
9 number width = 256 // pixel, final 4D scan image is width + 1
10 number height = 256 // pixel
11
12 // 4D Camera user variables
13 number nread = 1 // frames per scan position
14 number nskip = 0 // number to skip between probe positions
15 number nflyback = 100 // typically this is set to 100 (# frames for flyback time)
16
17 // Multi-scan variables
18 number num_scans = 15
19 number sleep_time = 20 // seconds (55 seconds is good for 41600)

Streaming



What does starting a session mean?

User (client)

Streaming Session

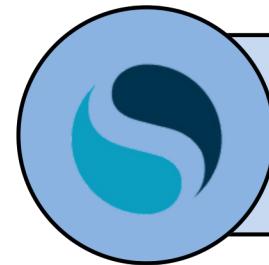
Start a new streaming session

Machine
perlmutter active ▾

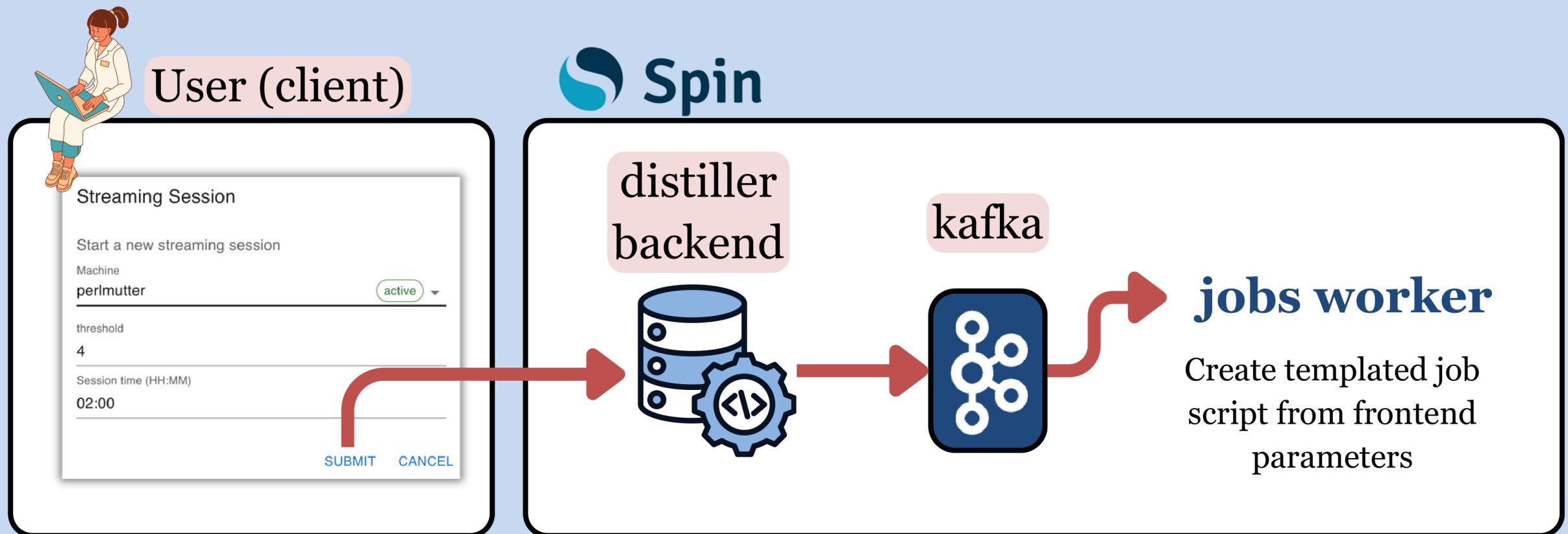
threshold
4

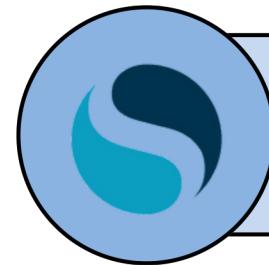
Session time (HH:MM)
02:00

SUBMIT CANCEL

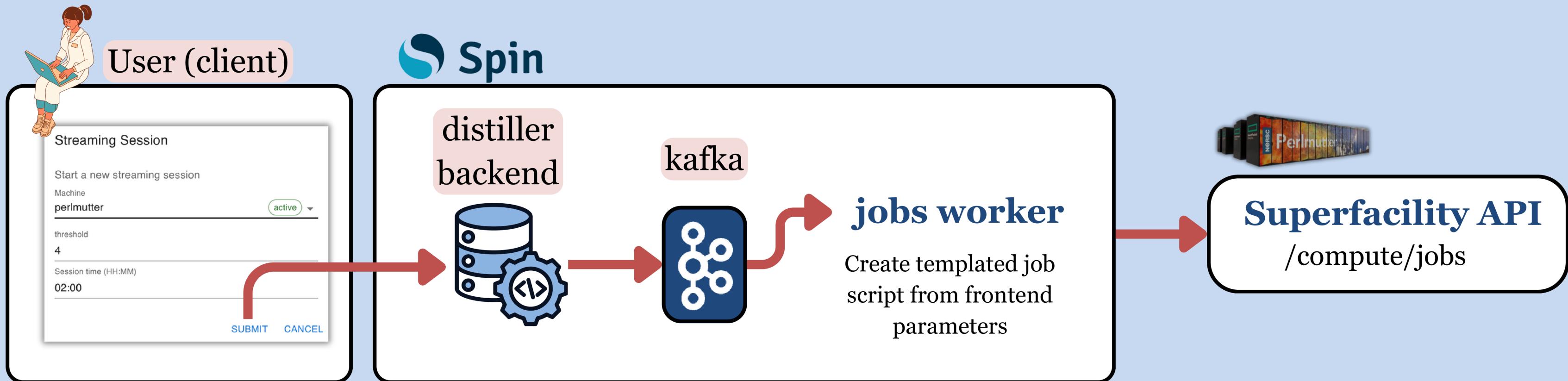


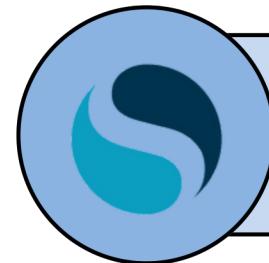
What does starting a session mean?



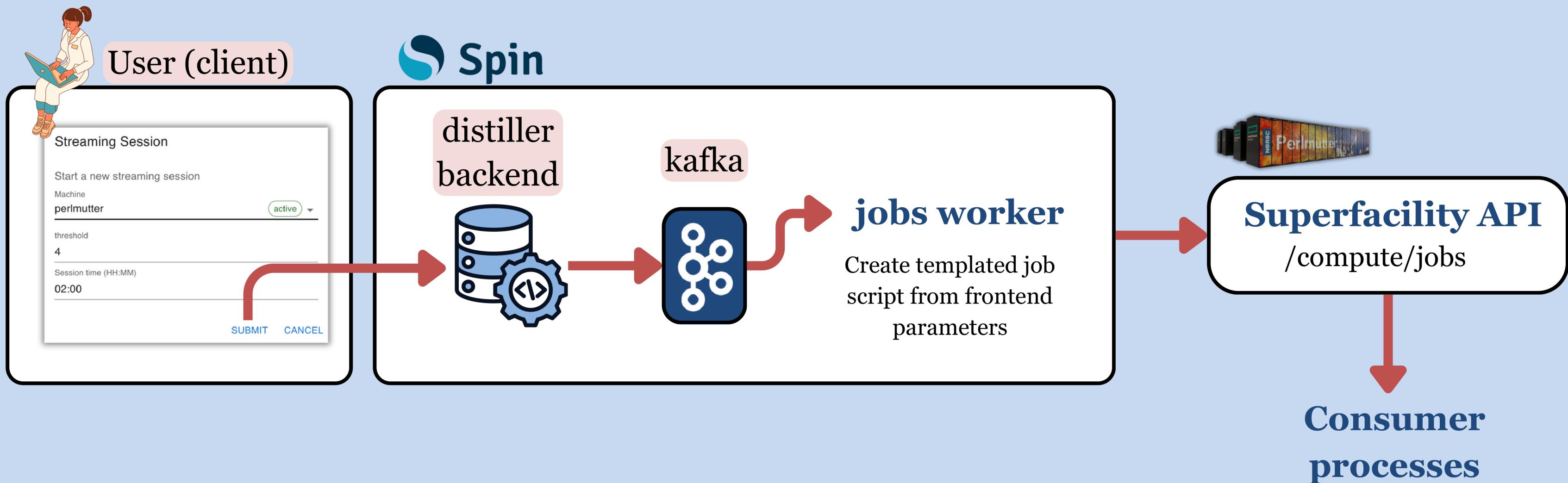


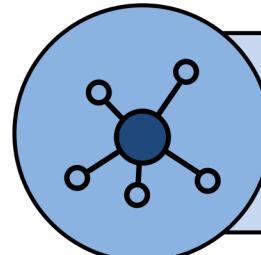
What does starting a session mean?





What does starting a session mean?





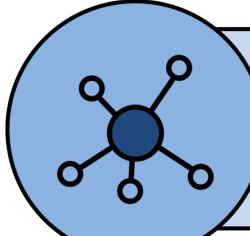
How do we connect the network of processes?



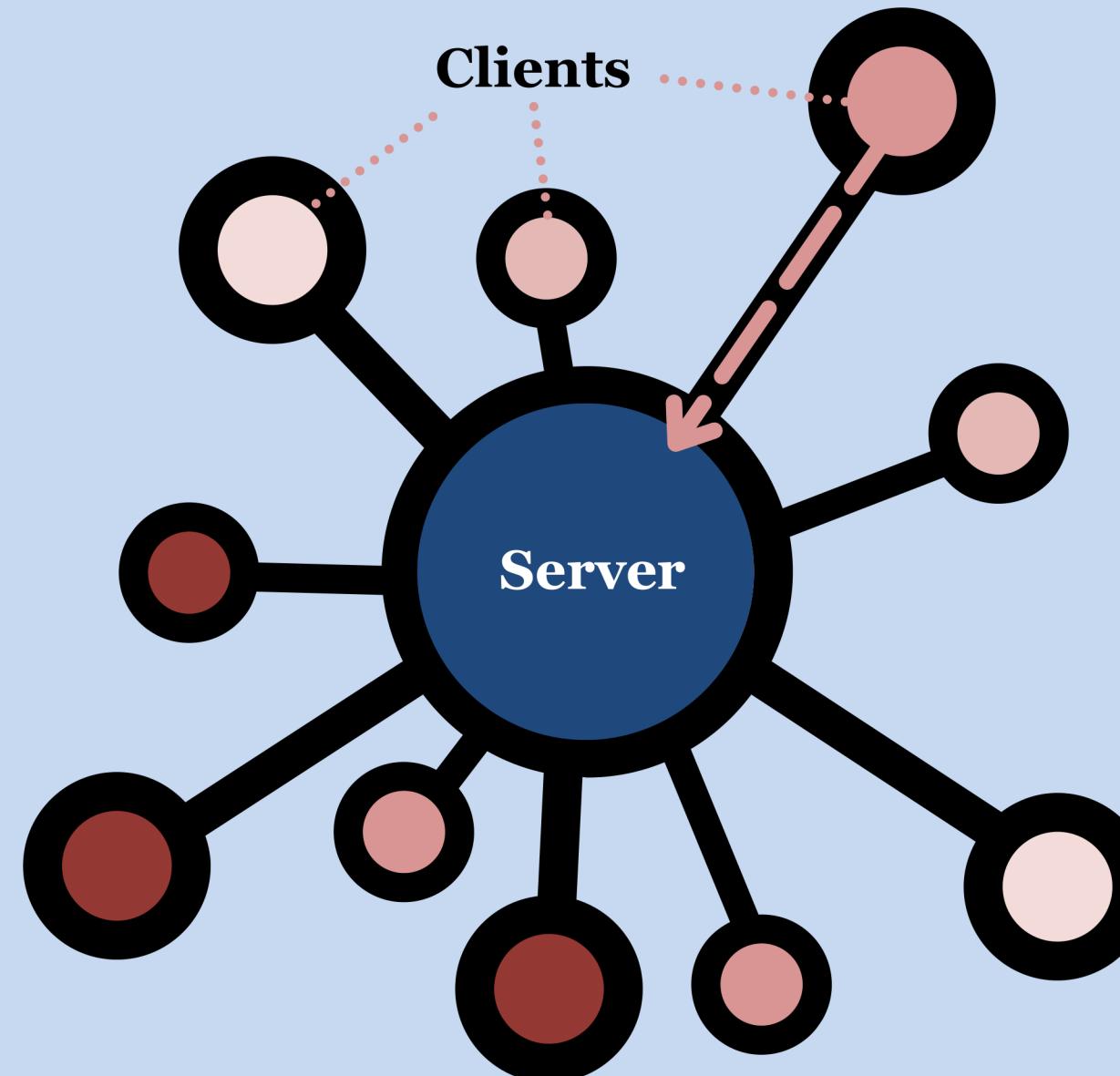
Every process is a client in a distributed key-value store

Clients

- Unique ID
- No. messages
- Current scan no.
- Status
- Ports/IP addresses



How do we connect the network of processes?



Every process is a client in a distributed key-value store

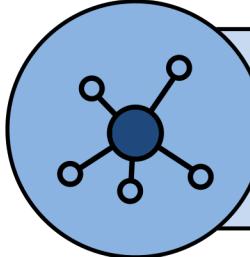
Clients

- Unique ID
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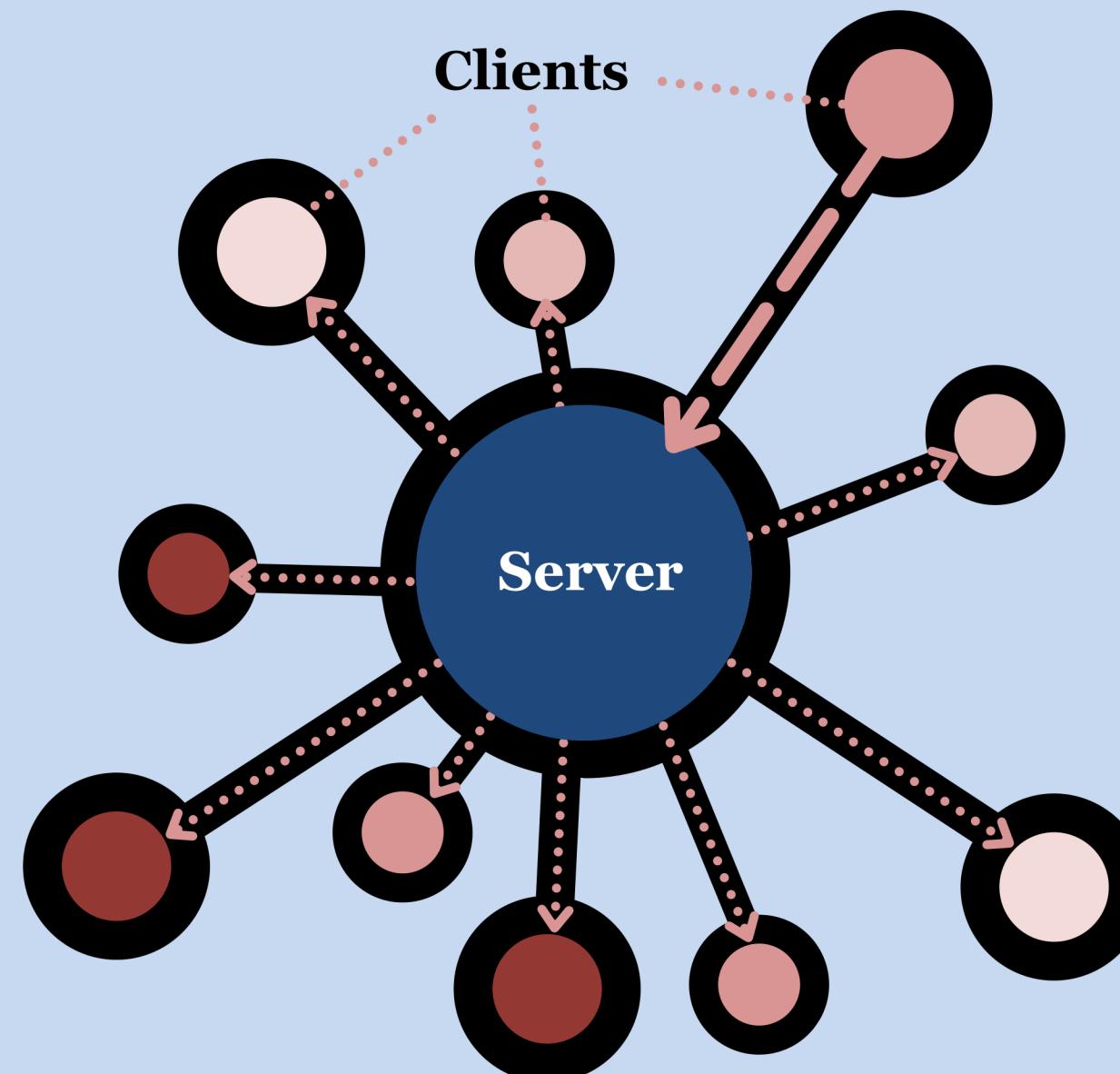
Server

- Check sequence
- Publish update
- Log full state

*different colors represent different clients
(producers, consumers, aggregators)



How do we connect the network of processes?



Every process is a client in a distributed key-value store

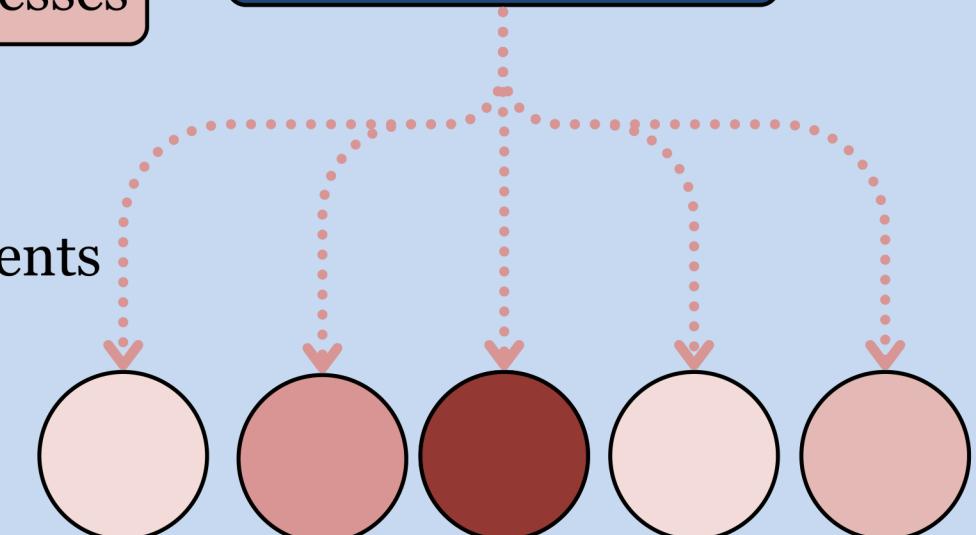
Clients

- Unique ID
- No. messages
- Current scan no.
- Status
- Ports/IP addresses

Server

- Check sequence
- Publish update
- Log full state

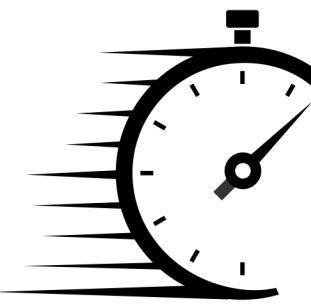
Update other clients



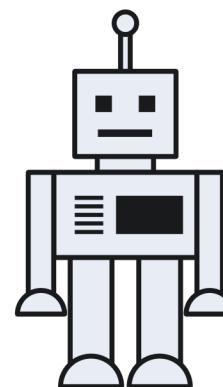
*different colors represent different clients
(producers, consumers, aggregators)



Implications



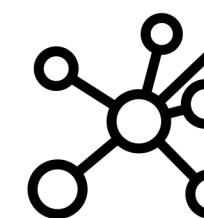
5x faster turnaround time.



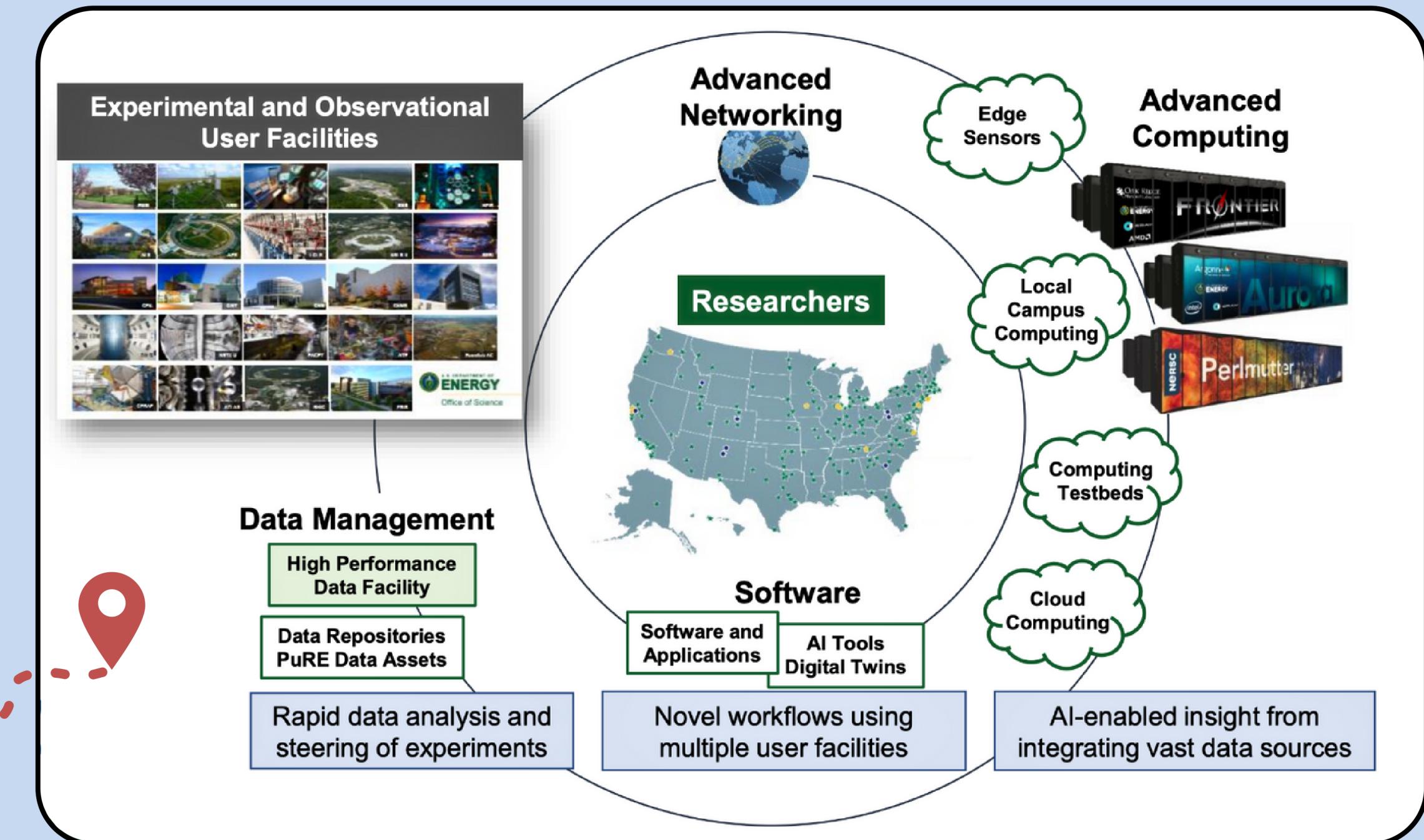
automated processing removes human in the loop.

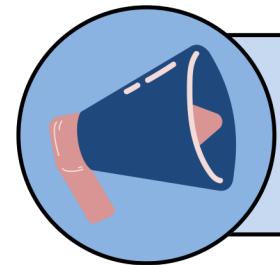


happier experimentalists.



new pathway for integrated research infrastructure.





Acknowledgements



Debbie Bard
(DSEG)



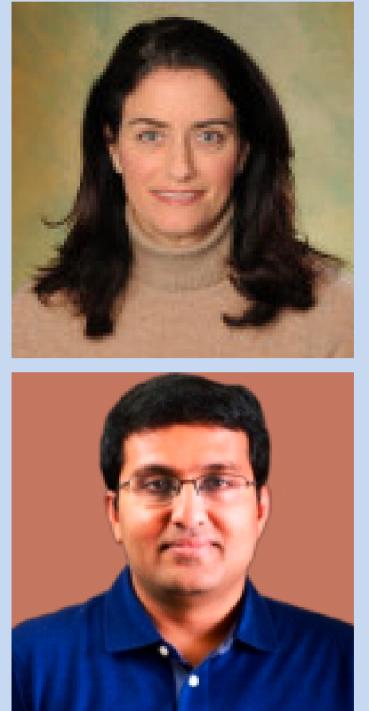
Bjoern Enders
(DSEG)



Peter Ercius
(NCEM)



Chris Harris Tavia Stone Gibbons,
(DAS) (SNG)
 Ashwin Selvarajan



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Office of
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