"Computational Infrastructure: What Do You Need?"
Based on People/Microscopes/Projects

Personnel
(Example)

1-2 Cryo-EM Labs
Users:
5-10 PD/students
Room to Grow.

IT Staff

Institute or Lab
Supported

Cryo-EM Facility

1 FT Res. Staff
2 Labs, 4 TEMs

Microscope
Service Support

Data Acquisition
(Example)

Titan Krios or F20

Summit Processor
(FPGA)

K2 Controlling PC
1.3 TB SSD for Storage
During Acquisition

Processing →

~0.5-1 GB
per stack
(more for sup. res.)
X
~1200 stacks
per day

= ~1-2 TB per day
(but could reach ~5 TB)

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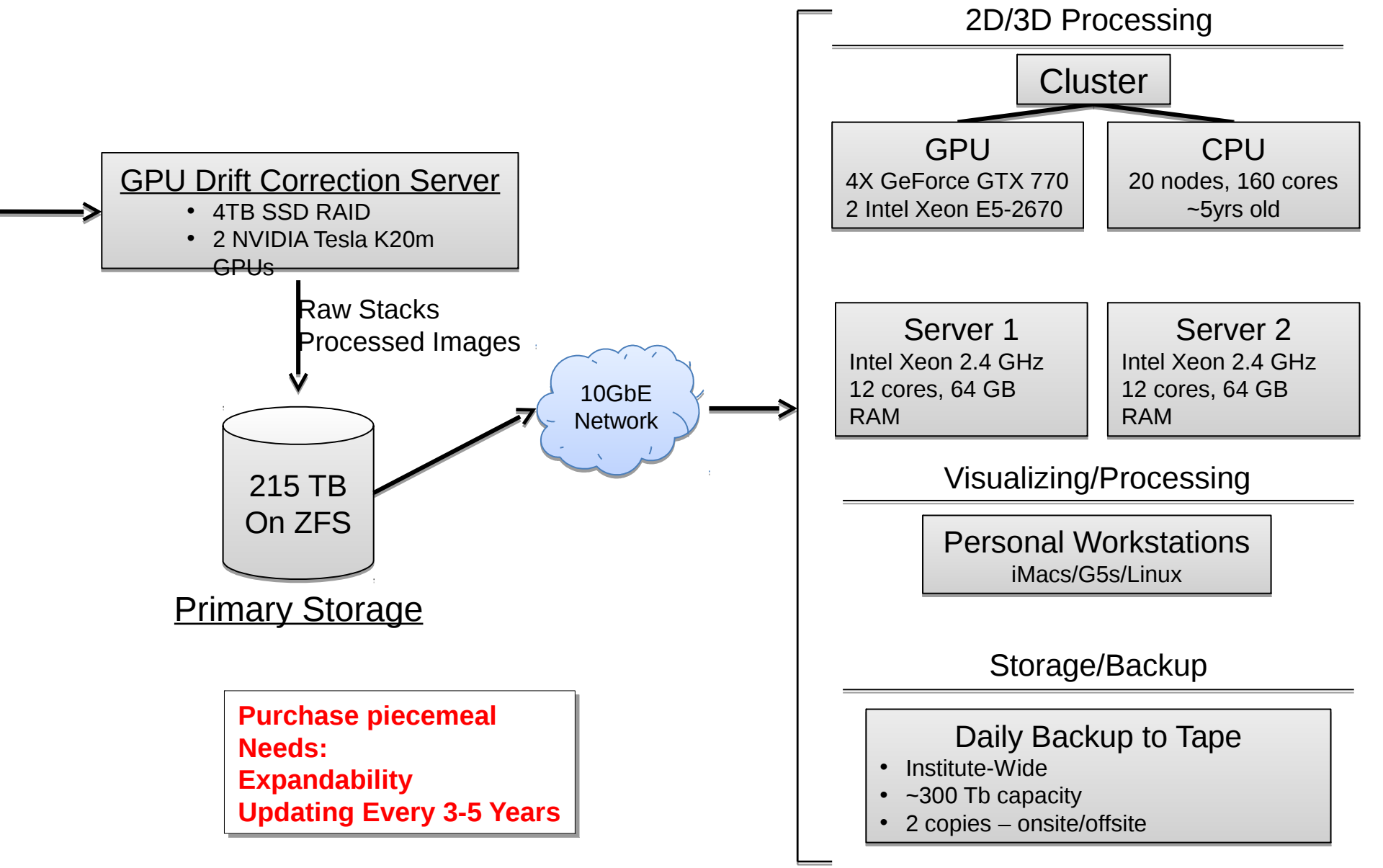
"Computational Infrastructure: What Do You Need/Buy?"

(Example)



“Are so called supercomputer centers of value?”

Depends on:

- Data Transfer Rate – Can be to slow for back-and-forth requirements from local storage source (main bottleneck).
- Storage Availability – Ideally need reasonably large, long-term storage (length of a project) to access data to avoid transferring from local storage drives .
- Cost – Often pricing structure is not optimized for cryo-EM needs. Ex. $6/cpu/month ‘rental’ use with ~1TB storage is very expensive long-term.
- Architecture – May not be ideal for RAM-intensive cryo-EM processing needs.

-Possible Advantage: Buy-in with local/university resource – purchase own CPU’s , storage that are maintained offsite.

-Still need investment in local computation resources.

“What about cloud computing?”

- Not an option - transfer rates too slow.
- Perhaps for archiving, but cost may be high

“What software do you need up and running?”

Data Acquisition
-Digital Micrograph
-FEI EPU
-UCSF Image
-Leginon
-In-house scripts for data transfer

Drift Correction
-Digital Micrograph
-UCSF MOTION_CORR
-RELION, and others

Particle Picking
-E2 Boxer semi-automated
-RELION, others

2D Classification/Analysis
-SPIDER
-ISAC, EMAN
-RELION, jothers

CTF Cor./3D Class./Refinement
-SPIDER, EMAN, FREALIGN, RELION

Many Others for:
Validation, Modeling, Visualizing

“How do you support the hardware and software?”

- Leginon/Appion
  -Automation, many options for processing, requires good IT/cryo-EM staff support, training.
- SBGrid, Harvard
  -Good for smaller labs, limited IT time, but costly
- Excellent local/dedicated IT support
- Departmental/Institute support.

How do you validate the software

- Use everything and compare results.
- Validation of the reconstruction steps.
- Talk to people, go to meetings.

Our Current Bottlenecks

Transfer Rates
- -During Acquisition
- -For Processing
- -Backups after Acquisition

Drift-correction on the fly

Storage
- -Short-term during acquisition
- -long-term (TB per person?)
- -Archive, backup

Processing
- -CPUs, availability, age
- -RAM per CPU
- -Head node, allocation
- -Optimal utilization by software