LIFE SCIENCES INSTITUTE
UNIVERSITY OF MICHIGAN

Software tools to deploy and manage cryo-EM jobs in the cloud

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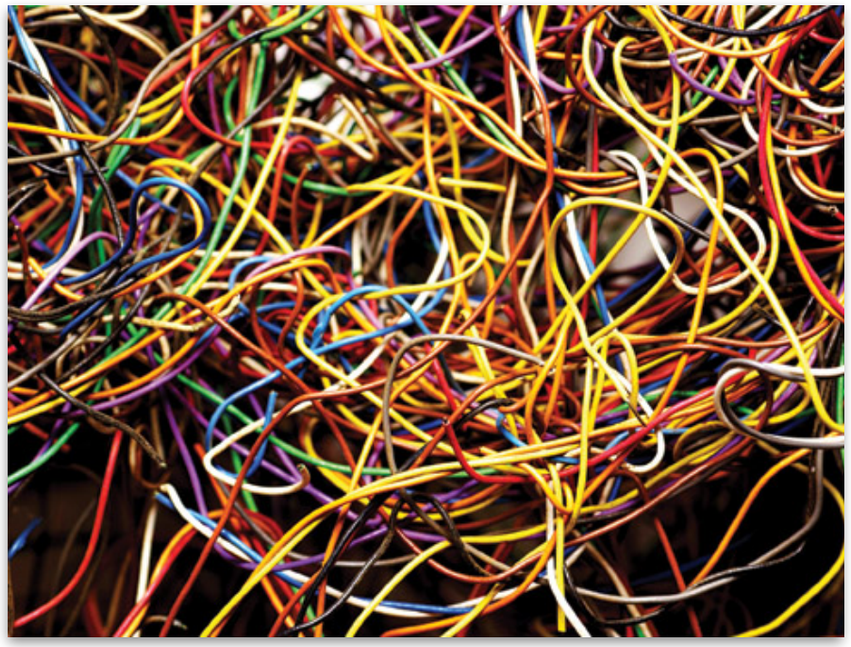
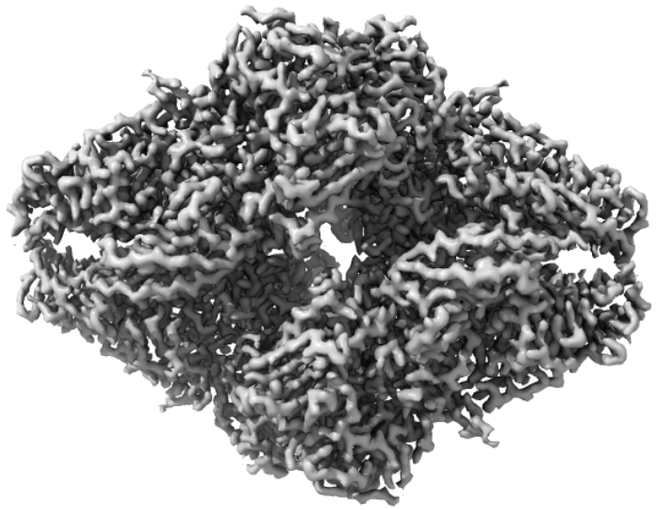
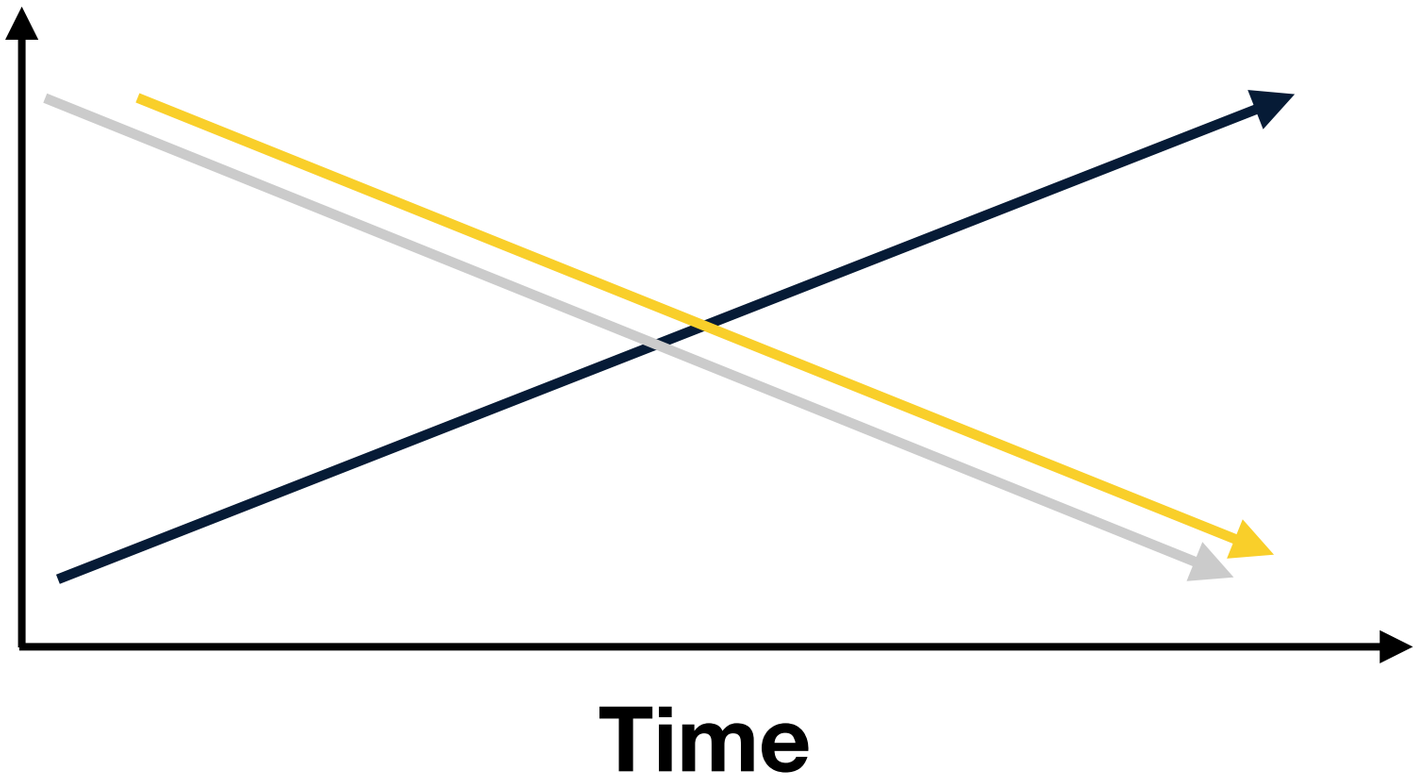
‘State of the art’ computing for cryo-EM





- Data processing occurring at a different site than data collection
- Data copying & moving; living at multiple locations
- New users left on their own to navigate the complex world of computing & storage

Current state of computing in cryo-EM



# of cryo-EM users

“Expert” level knowledge

Cyber-infrastructure available per user

How do we scale computing *and storage* for cryo-EM?

University-wide

Computing -$$

Data storage - $$

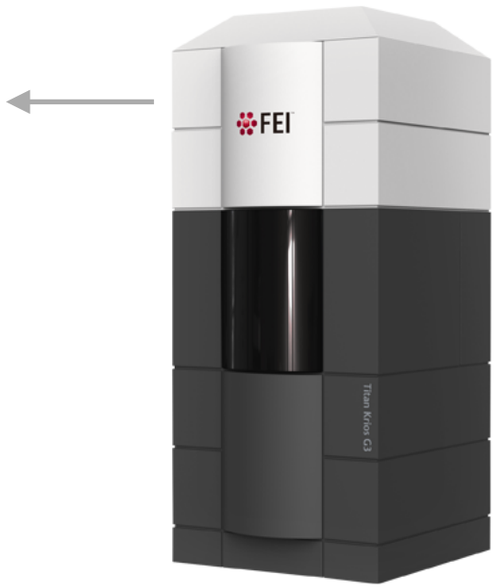
Scalable

Individual laboratory / facility

Capital investments - $$$

IT support required - $$$

Difficult to scale



National supercomputers

Free computing

Scalable

No data storage

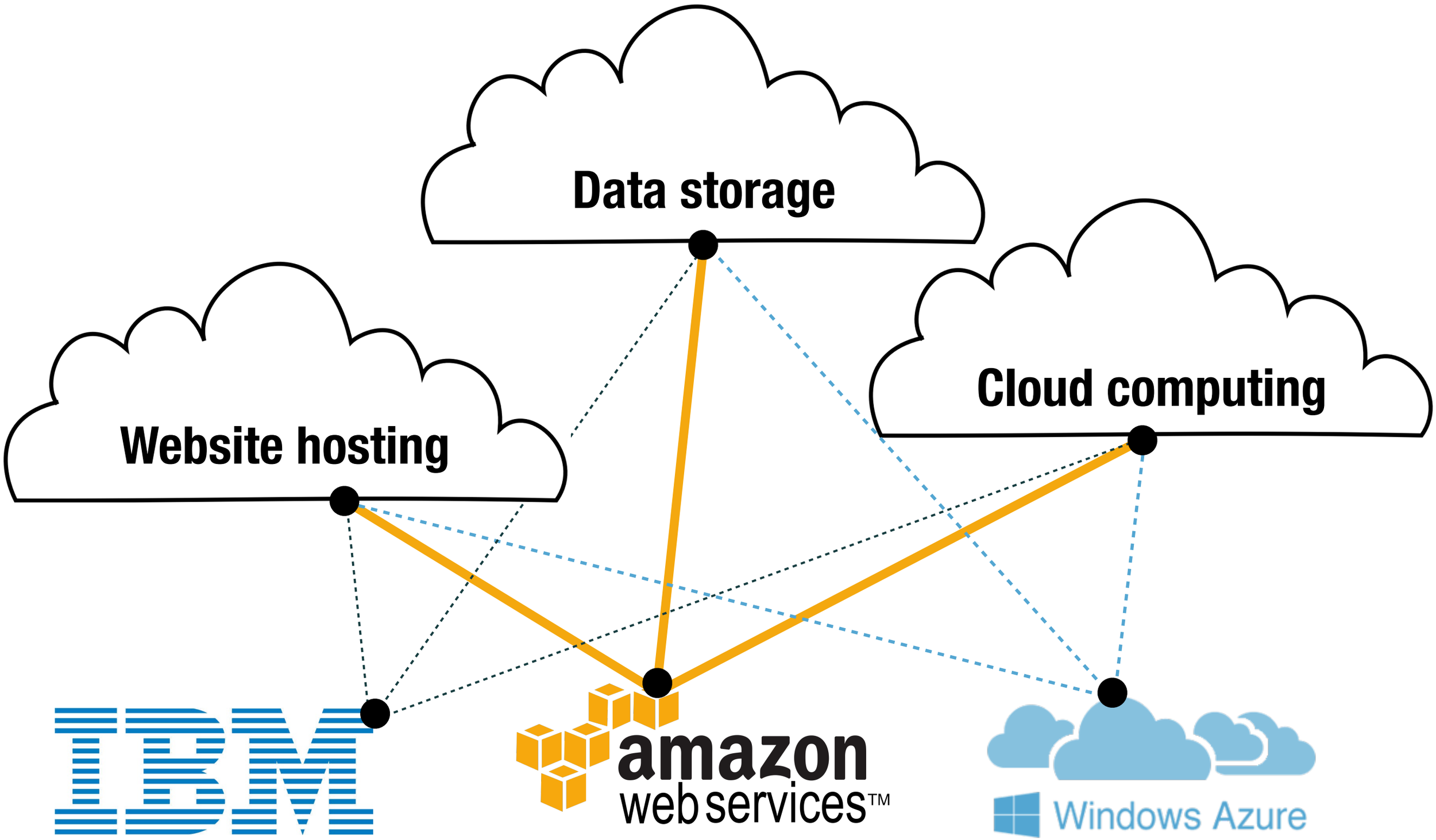
Cloud computing

Computing -$

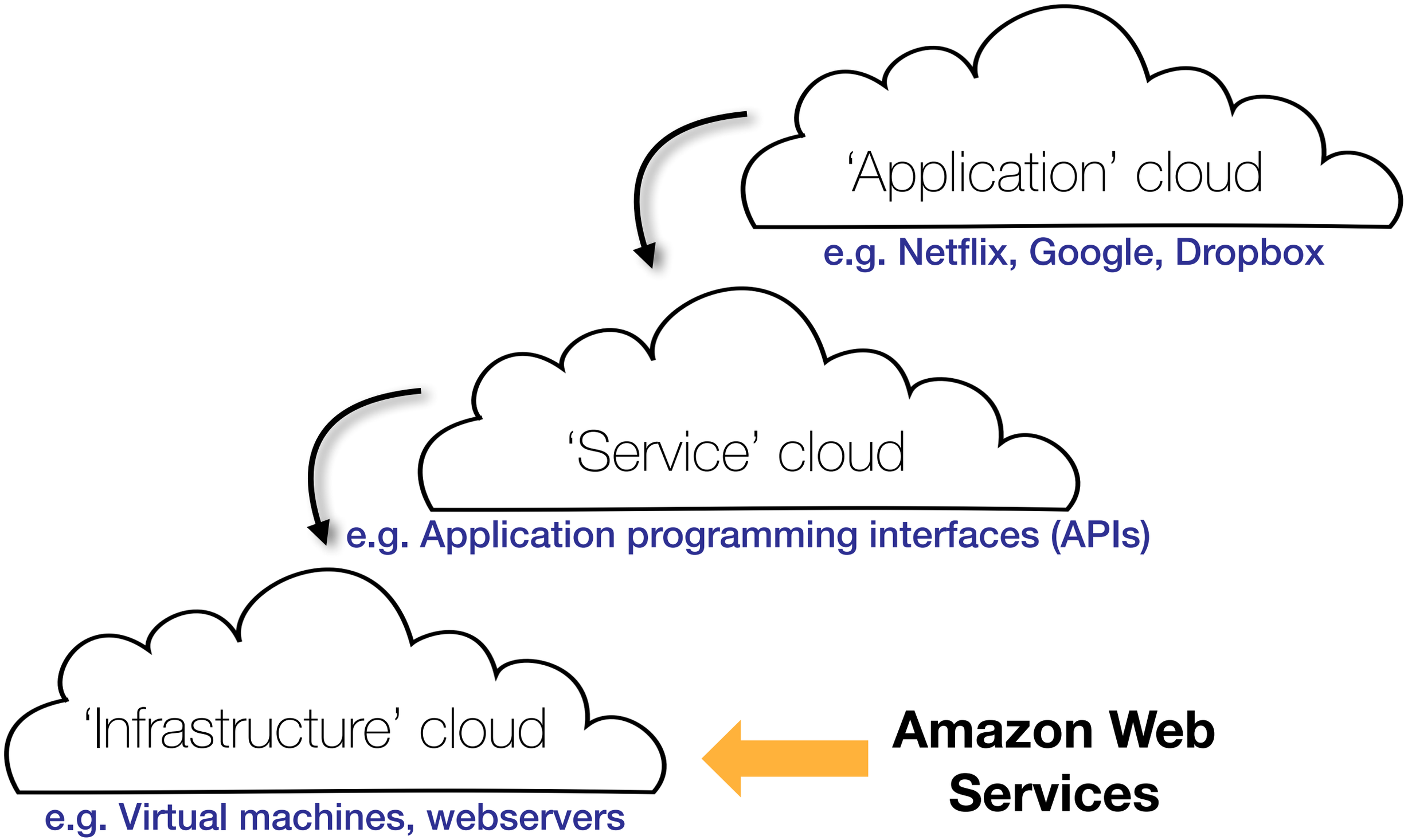
Scalable

Data storage - $

The cloud is a ubiquitous feature of our daily lives



The cloud is a ubiquitous feature of our daily lives



Key principles of cloud computing

1. Cost effective

- Economies of scale
- Someone else takes care of IT hardware support
- *Pay as you go (pro-rated to the minute)*

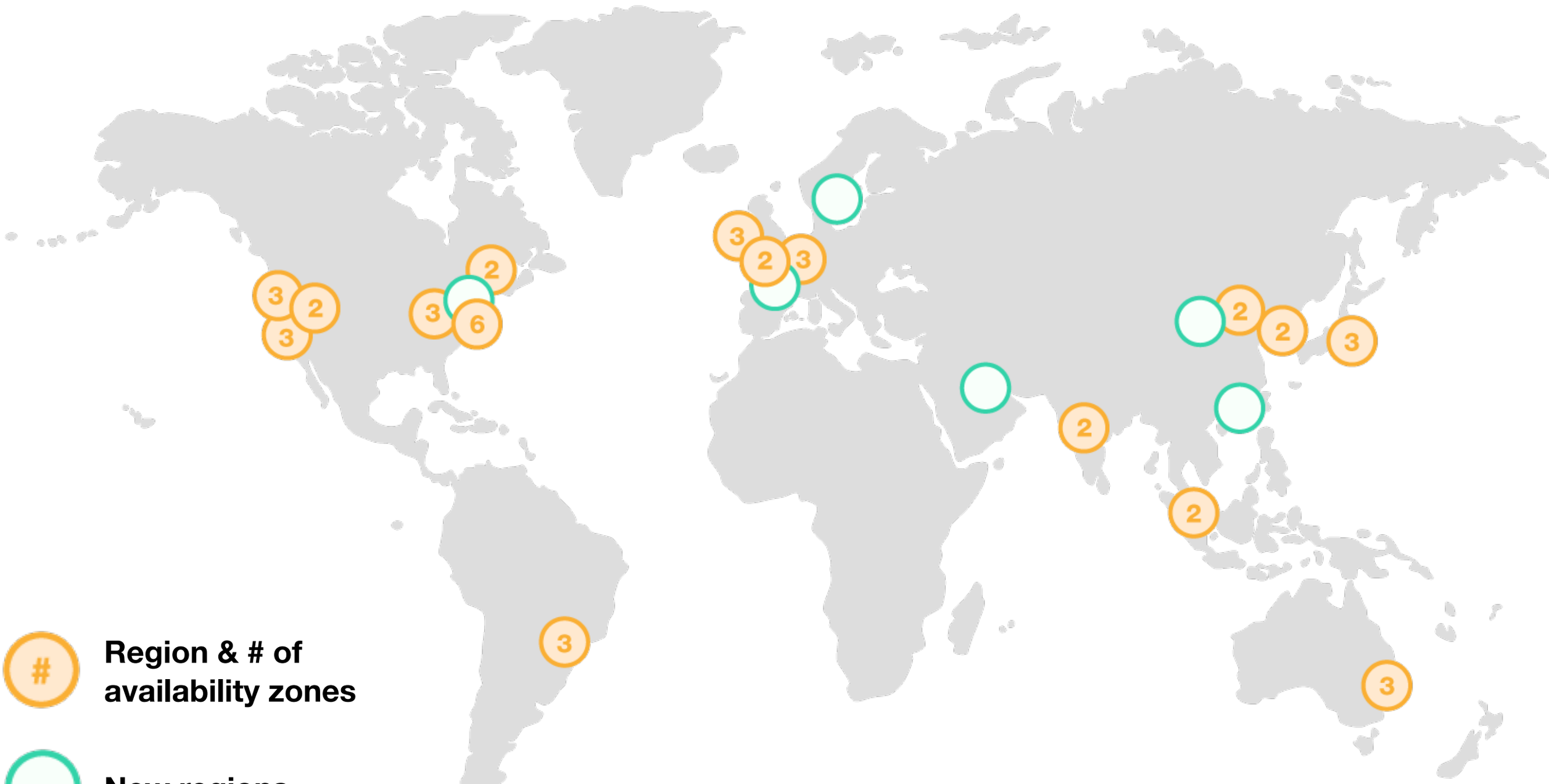
2. Reliable data storage

- Backed up offsite, multiple locations

3. Flexibility

- Global footprint
- As more computing power is needed, easy to add more
- No need to ‘choose’ between CPU vs GPU resources
- Instant access to hundreds of CPUs

Amazon Web Services (AWS) is the world's largest cloud provider



**Region & # of availability zones**

New regions

Region *= Data center*
Availability Zone *= Building within data center*

Computing options on AWS

Instance *= virtual machine on AWS*

vCPU *= hyper thread on CPU core*

Memory (GB RAM)

 # CPU/GPU

t2.nano
1 vCPU
0.5 GB RAM

c4.8xlarge
36 vCPU
60 GB RAM

g3.4xlarge
1 GPU / 16 vCPU
122 GB RAM

p2.xlarge
1 GPU / 4 vCPU
61 GB RAM

g3.8xlarge
2 GPU / 32 vCPU
244 GB RAM

m4.16xlarge
64 vCPU
256 GB RAM

p2.8xlarge
8 GPU / 32 vCPU
488 GB RAM

g3.16xlarge
4 GPU / 64 vCPU
488 GB RAM

r4.16xlarge
64 vCPU
488 GB RAM

p2.16xlarge
16 GPU / 64 vCPU
732 GB RAM

x1.32xlarge
128 vCPU
1952 GB RAM

…59 total instances (48 more than shown here)

Computing options on AWS

Instance *= virtual machine on AWS*

vCPU *= hyper thread on CPU core*

Memory (GB RAM)

 # CPU/GPU

Price per hour

$0.0058 1 vCPU 0.5 GB RAM			
$1.591 36 vCPU 60 GB RAM			
	$1.14 1 GPU / 16 vCPU 122 GB RAM	**$0.90** 1 GPU / 4 vCPU 61 GB RAM	**$3.20** 64 vCPU 256 GB RAM
		$2.28 2 GPU / 32 vCPU 244 GB RAM	**$7.20** 8 GPU / 32 vCPU 488 GB RAM
			$4.56 4 GPU / 64 vCPU 488 GB RAM

$4.256 64 vCPU 488 GB RAM	
	$14.40 16 GPU / 64 vCPU 732 GB RAM
	$13.338 128 vCPU 1952 GB RAM

Reserving instances on AWS

Pay-per-hour

On-demand

Pay ‘standard’ price
Instance is 100% yours

Cheaper

Reserved

Pay 1-3 yr upfront to reserve instance
Instance is 100% yours

Cheaper

Spot

Bid on marketplace
Instance is yours until somehow outbids you

Data storage on AWS

Local SSDs

Directly attached to instance — *No cost*

Elastic block storage (EBS)

SSDs that can be attached/detached — *$0.10/GB/mo.*

Object storage: Scalable storage (active & cold)

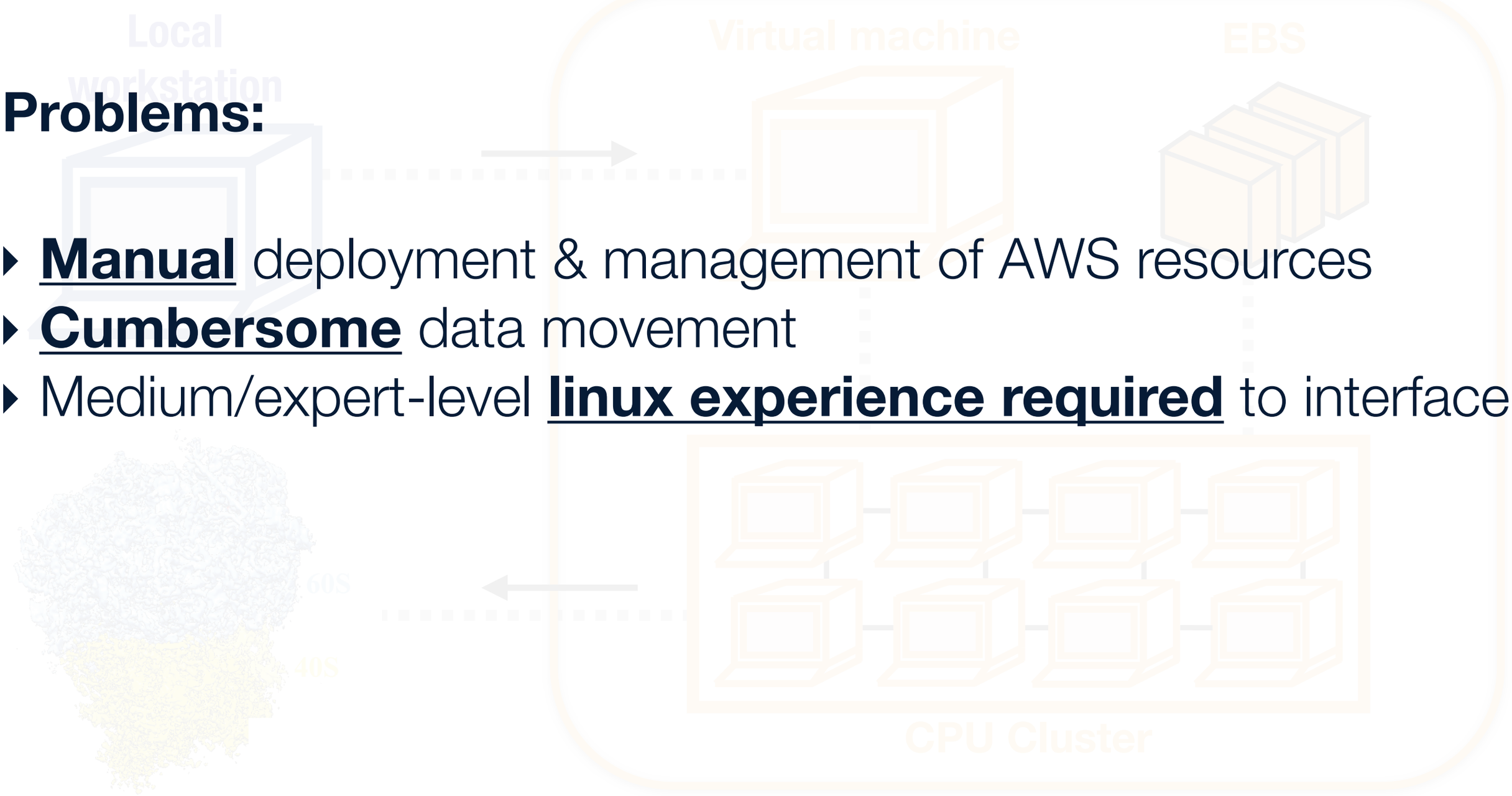
Simple storage service (S3) — *$0.023/GB/mo.*

Glacier — *$0.004/GB/mo.*

Previously…

Problems:

- **Manual** deployment & management of AWS resources
- **Cumbersome** data movement
- Medium/expert-level **linux experience required** to interface

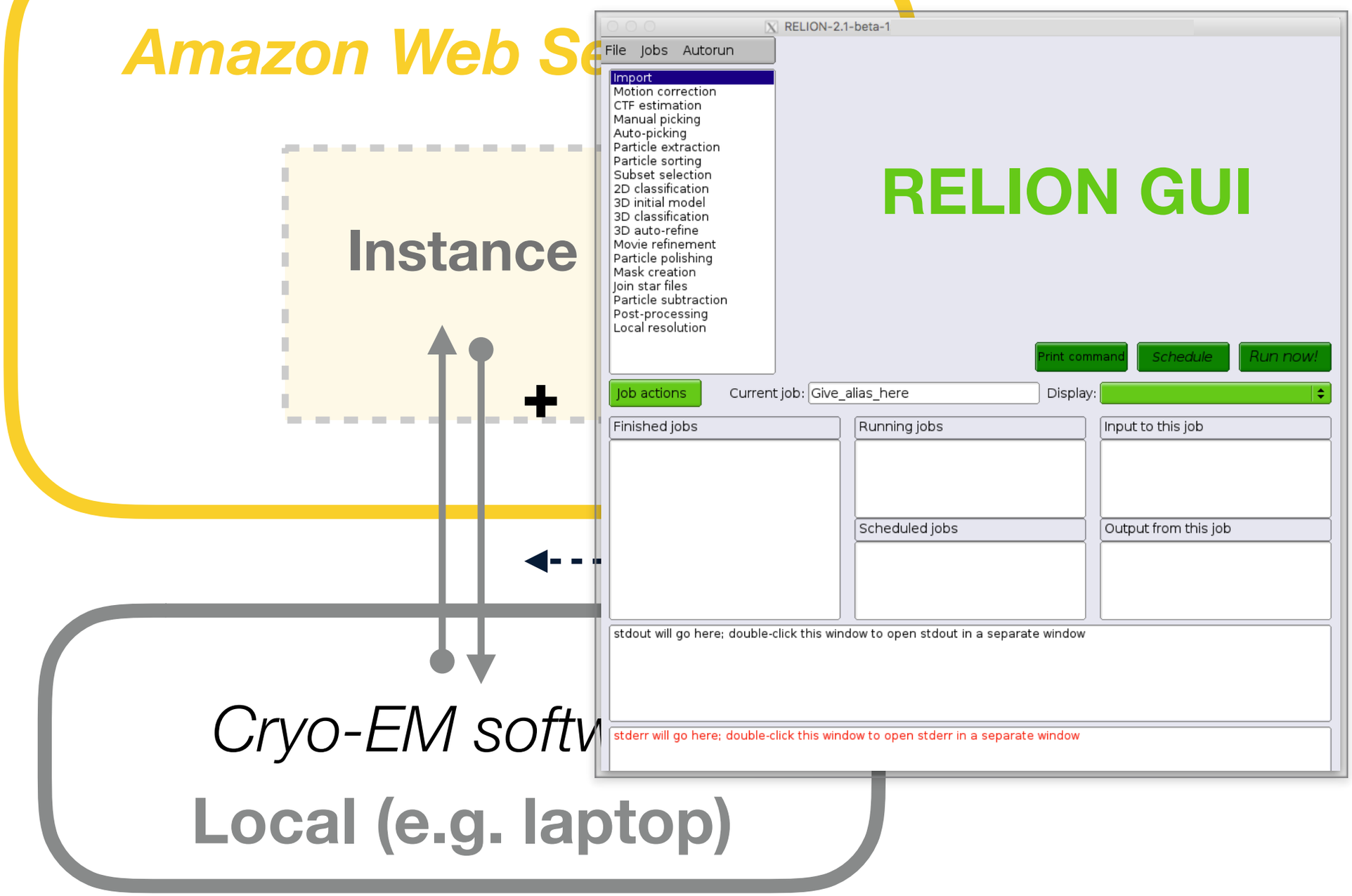


What is the best way to use the cloud?

"Hybrid cloud architecture is the integration of on-premises resources with cloud resources."

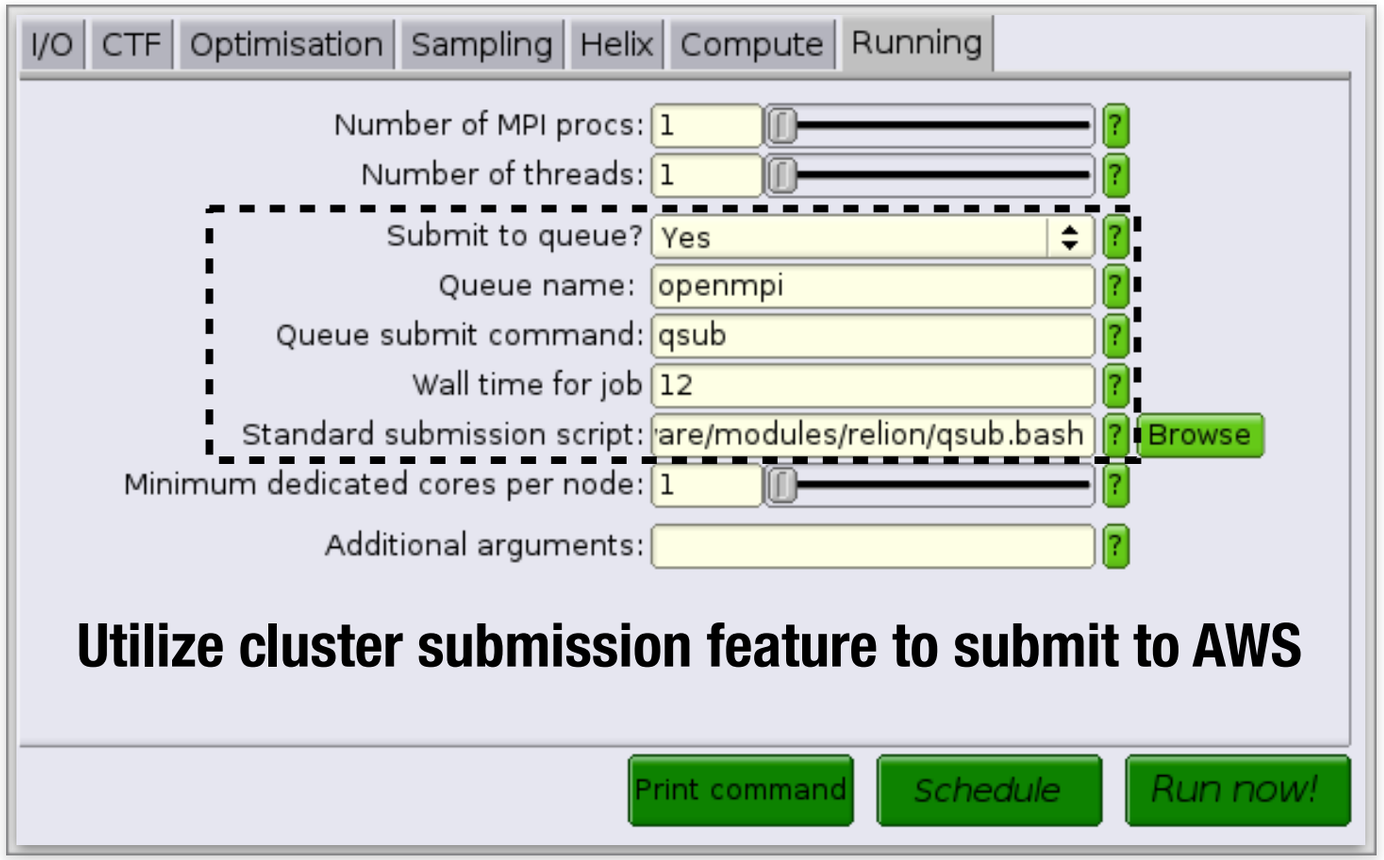
Building a hybrid cloud infrastructure for cryo-EM

RELION as a prototype



Building a hybrid cloud infrastructure for cryo-EM

RELION as a prototype

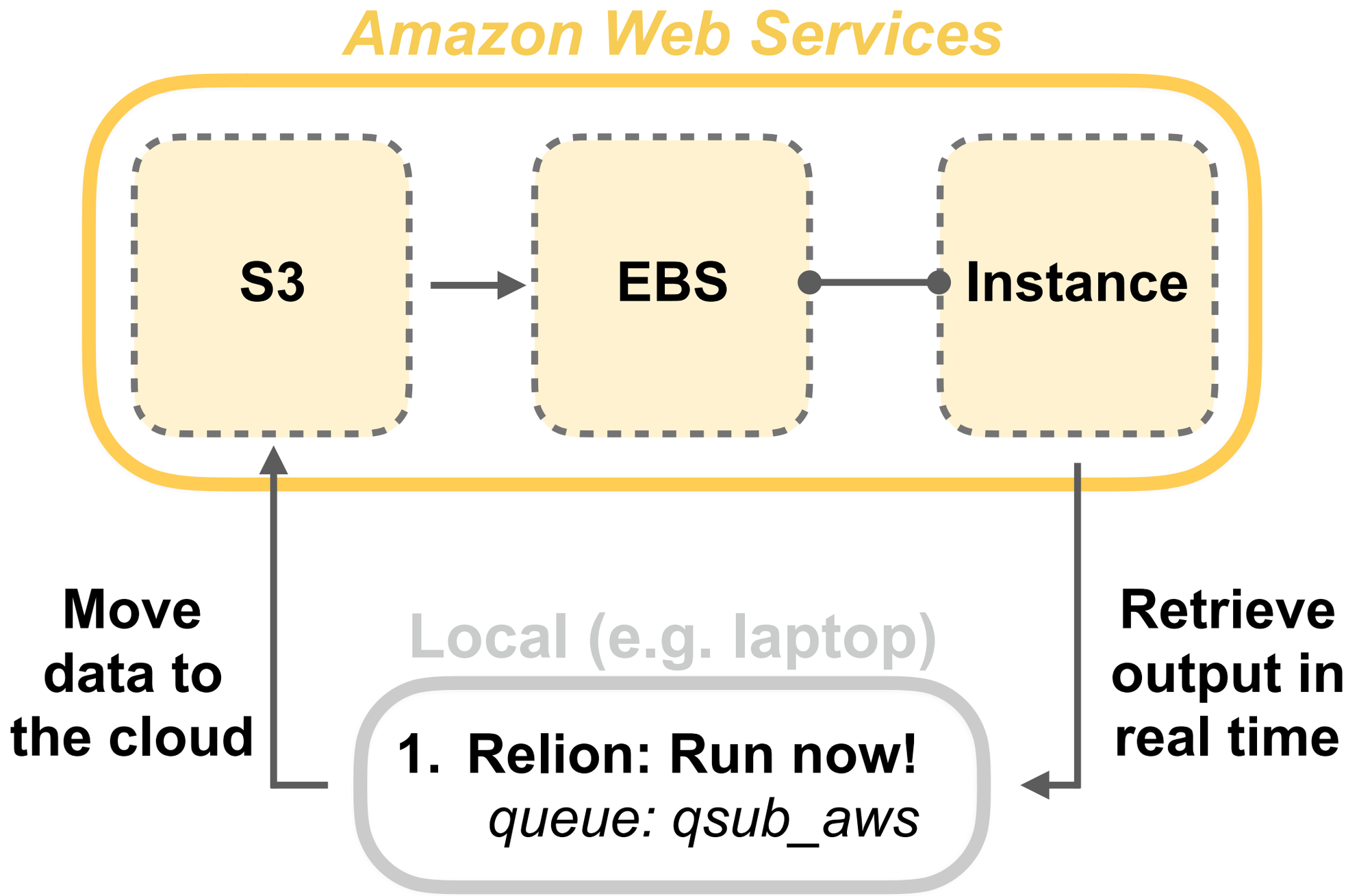


Building a hybrid cloud infrastructure for cryo-EM

RELION as a prototype

Implement for all jobtypes

cryoem-cloud-tools: software to run cryo-EM on the cloud



Amazon Web Services

AWS

Region (e.g. US-West-2)

Availability Zone (e.g. US-West-2a)

S3 Bucket

Aligned movies

Movie alignment

5 x 128 vCPUs

Micrographs

Micrograph particle extraction

1 x SSD

16 vCPUs

ed by Cloud Watch to

ninate instance if idle > 1hr.

Multi-file uploads:

150 MB/sec

movies = ~22TB in 15 hrs

128 vCPUs

‘Enhanced networking’ on AWS (10 or 20 Gigabit)

Input/output files transferring over the internet

Security group to restrict access to user’s IP address

Particles

RELION: Run now!

queue: qsub_aws

Amazon Web Services

AWS

Region (e.g. US-West-2)

Availability Zone (e.g. US-West-2a)

S3 Bucket

AutoPick, CTF estimation,
2D/3D classification, auto-refine

1 x SSD

1,2, 4, 8,16 GPUs

Averages,
3D models

GPU-accelerated processing

RELION: Run now!
queue: qsub_aws

Amazon Web Services

AWS

Region (e.g. US-West-2)

Availability Zone (e.g. US-West-2a)

S3 Bucket

Movie particle extraction

8 x 36 vCPUs
42 TB / instance

Movie refinement

1 x 128 vCPUs

Particle polishing

1 x 128 vCPUs

Particles

RELION: Run now!
queue: qsub_aws

Movie processing

Amazon Web Services

AWS

Region (e.g. US-West-2)

Availability Zone (e.g. US-West-2a)

S3 Bucket

Movie alignment

5 x 128 vCPUs

Micrographs

Micrograph particle extraction

1 x gp2 SSD

16 vCPUs

AutoPick, CTF estimation,
2D/3D classification, auto-refine

1 x gp2 SSD

1,8,16 GPUs

Averages,
3D models

Movie particle extraction

8 x 36 vCPUs
42 TB / instance

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1 x 128 vCPUs

Particle polishing

1 x 128 vCPUs

Particles

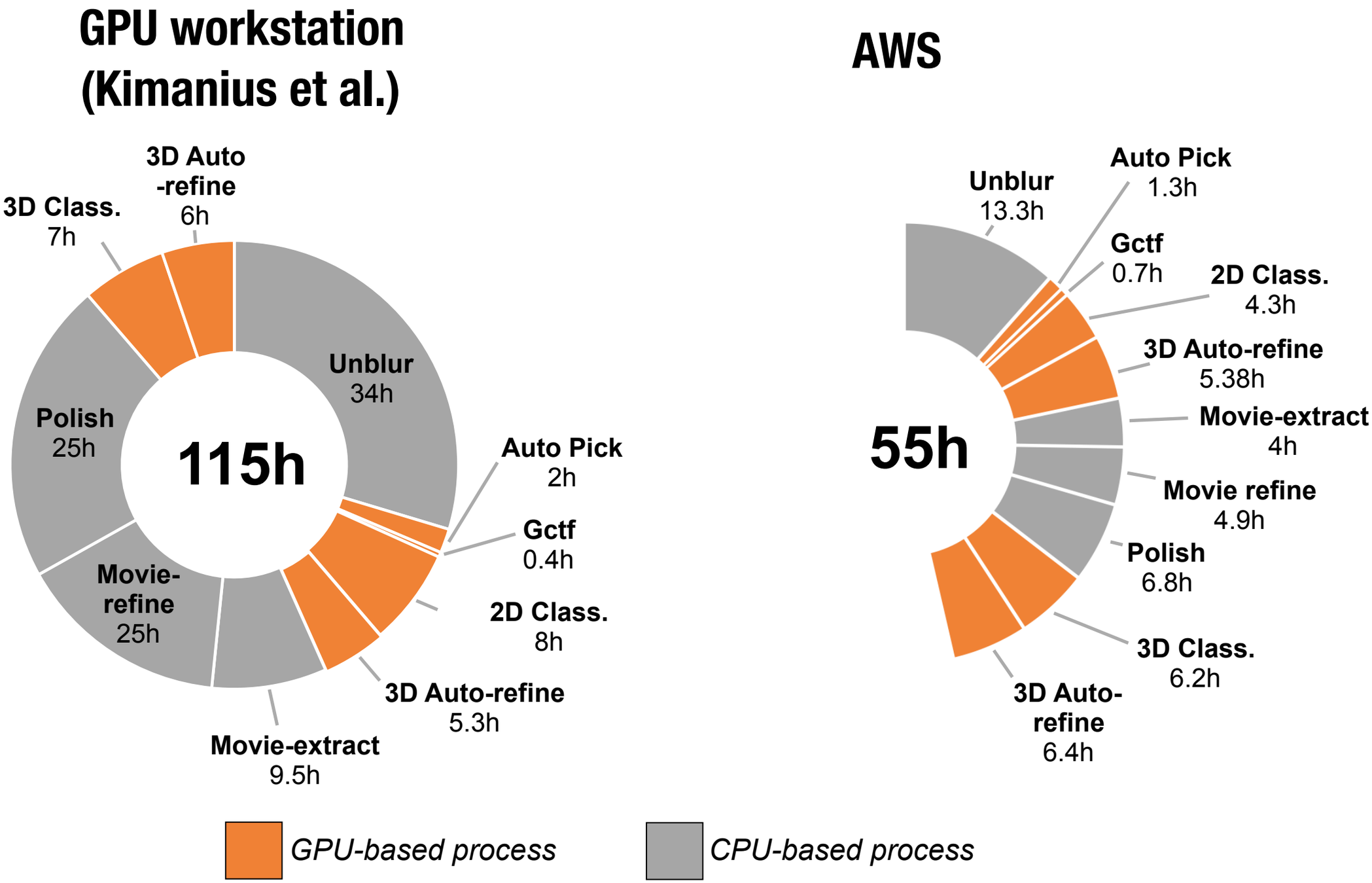
Particles

RELION: Run now!

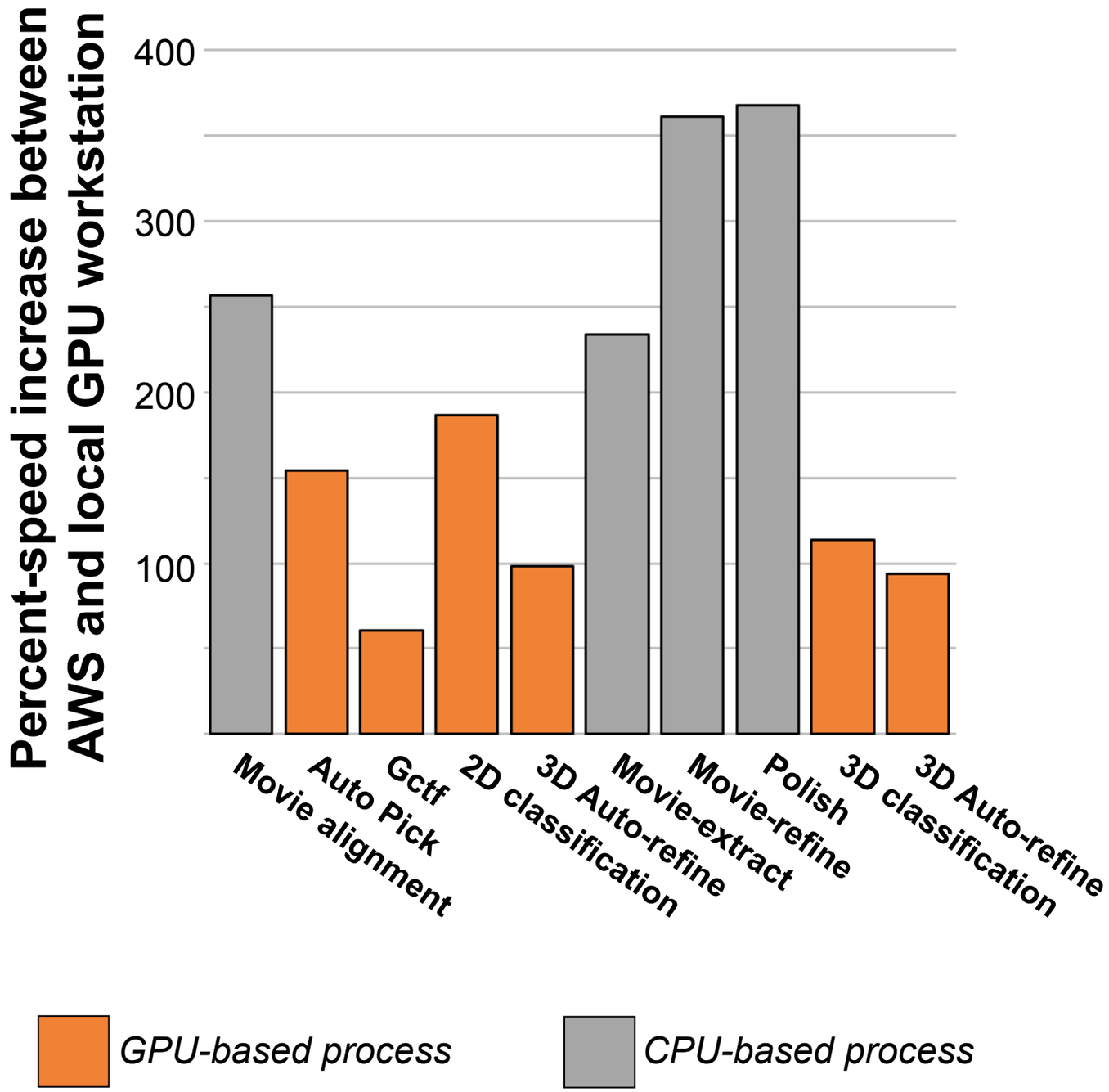
queue: qsub_aws

Comparison of AWS vs. local GPU workstation for RELION2

Comparing 2.2 Å beta-galactosidase dataset (EMPIAR 10061)

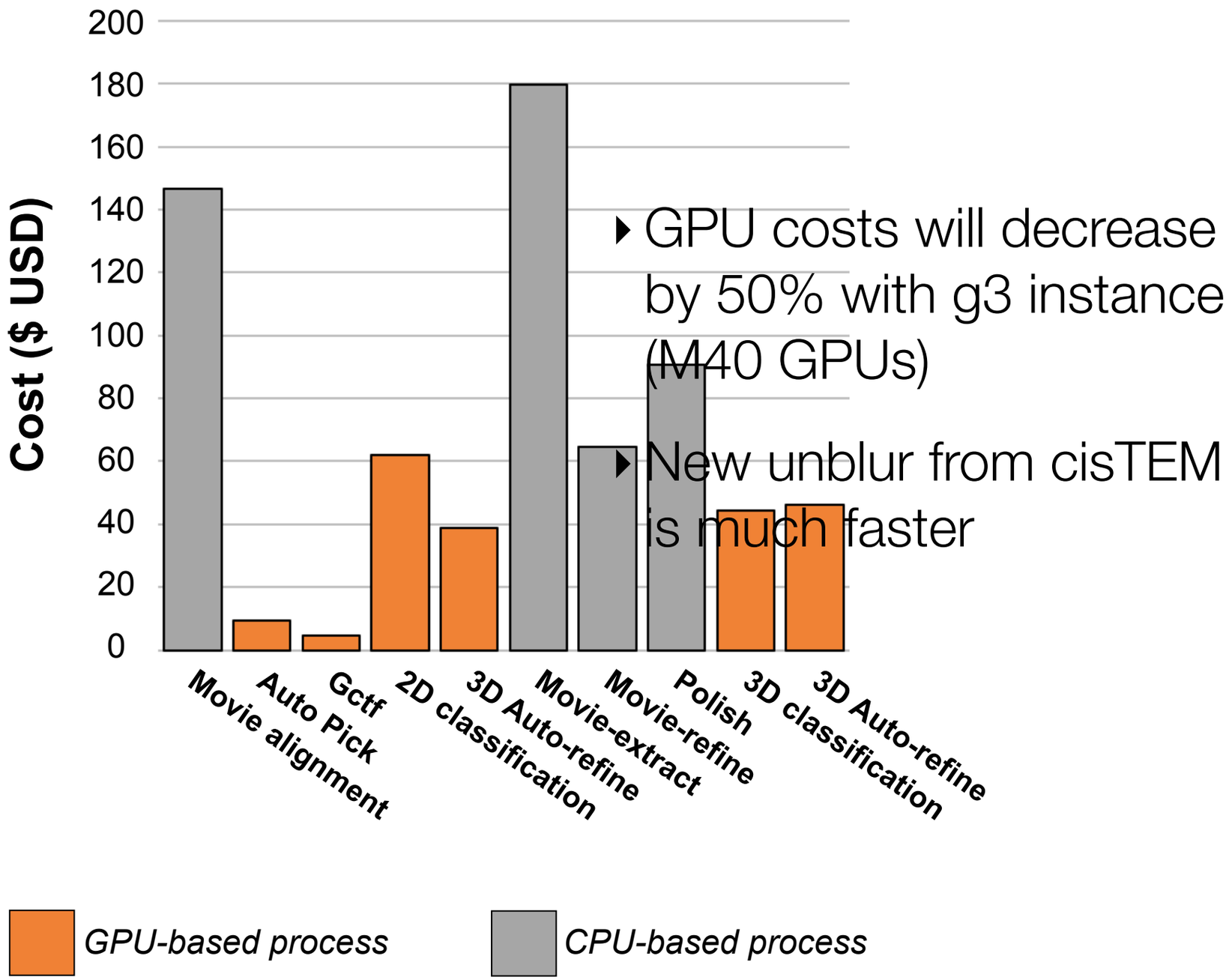


Comparison of AWS vs. local GPU workstation for RELION2



Cost breakdown of AWS

Total computing cost: $688.15

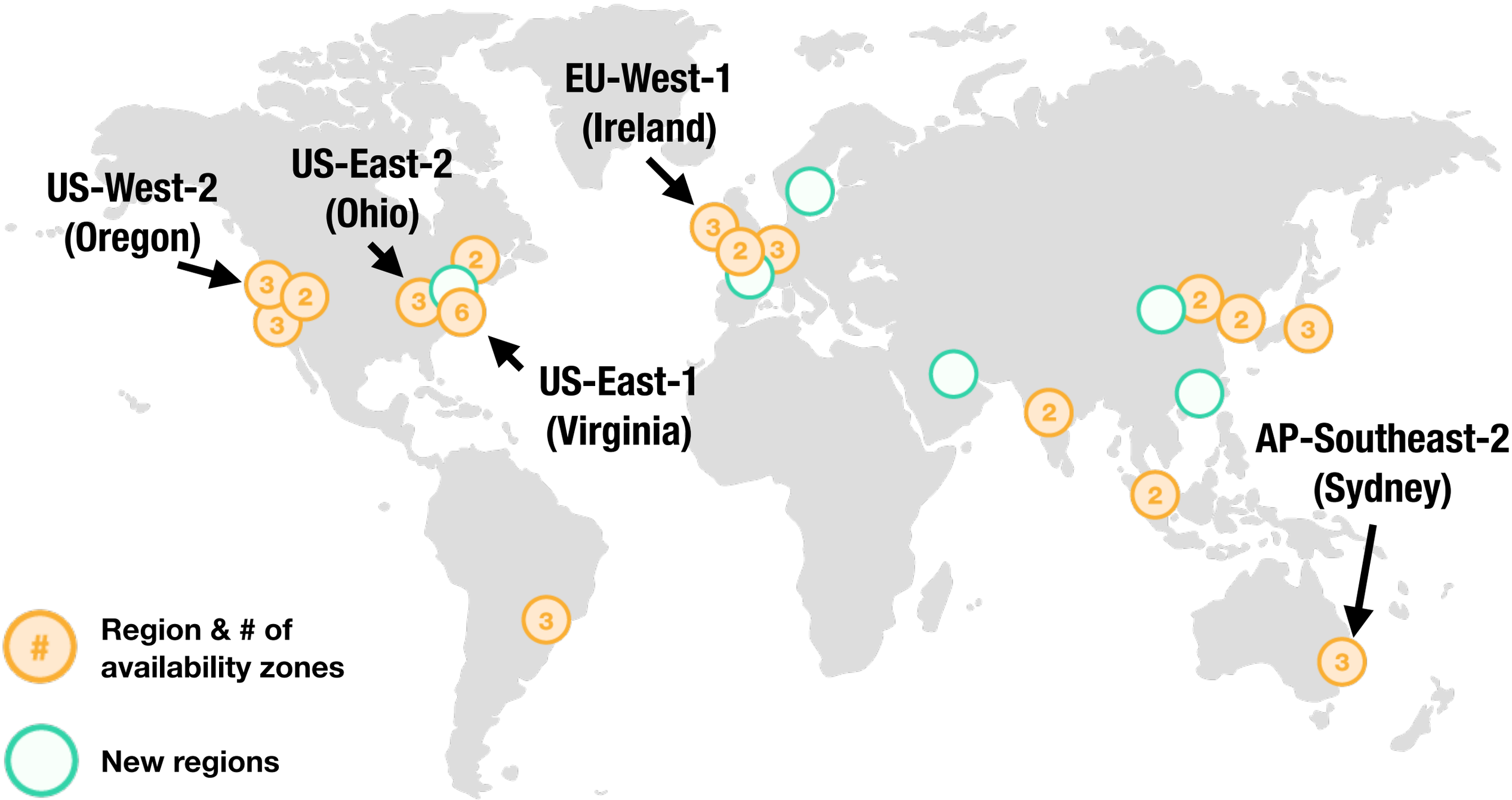


Cost comparison between AWS and local GPU workstation

	AWS	Local GPU workstation
Computing costs*	$688.17	$72.45
Processing time (h)	55	115
Number of working days	5	10

**For local GPU workstation, $10,000 workstation cost = $0.63/hr (60% utilization).*

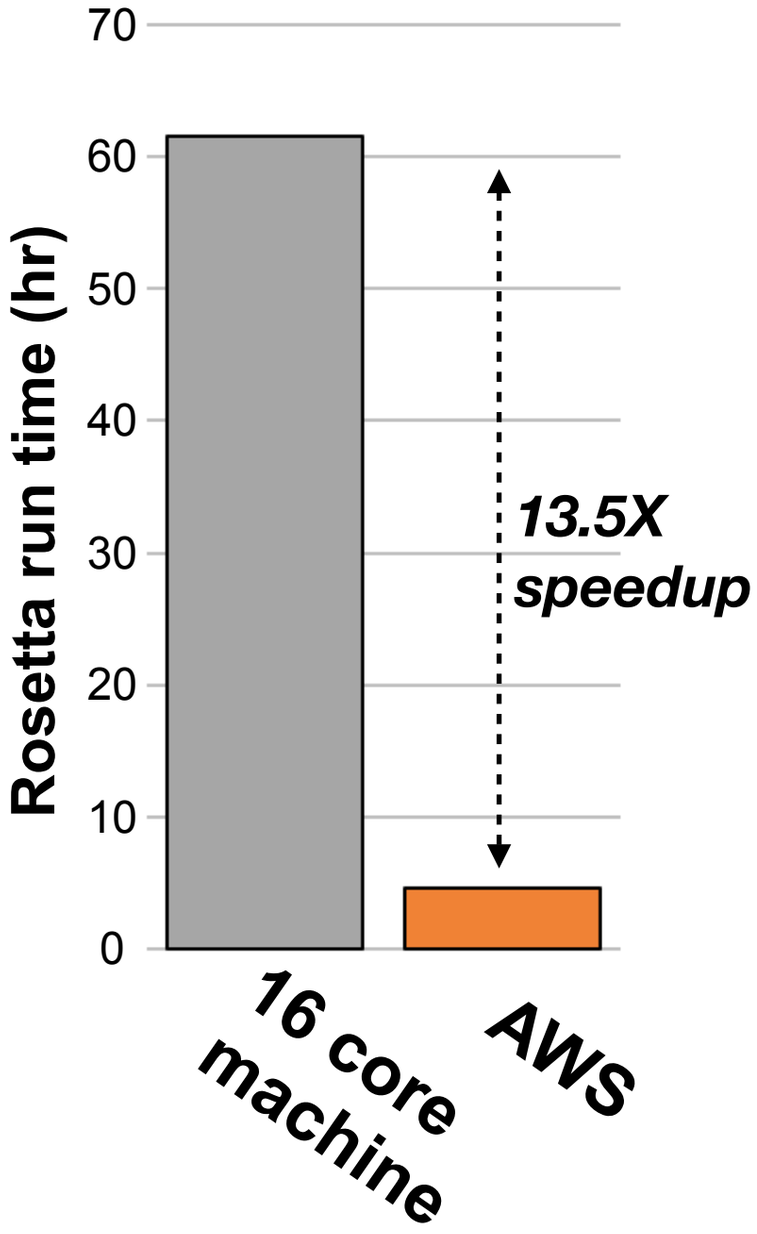
Global footprint of *cryoem-cloud-tools*

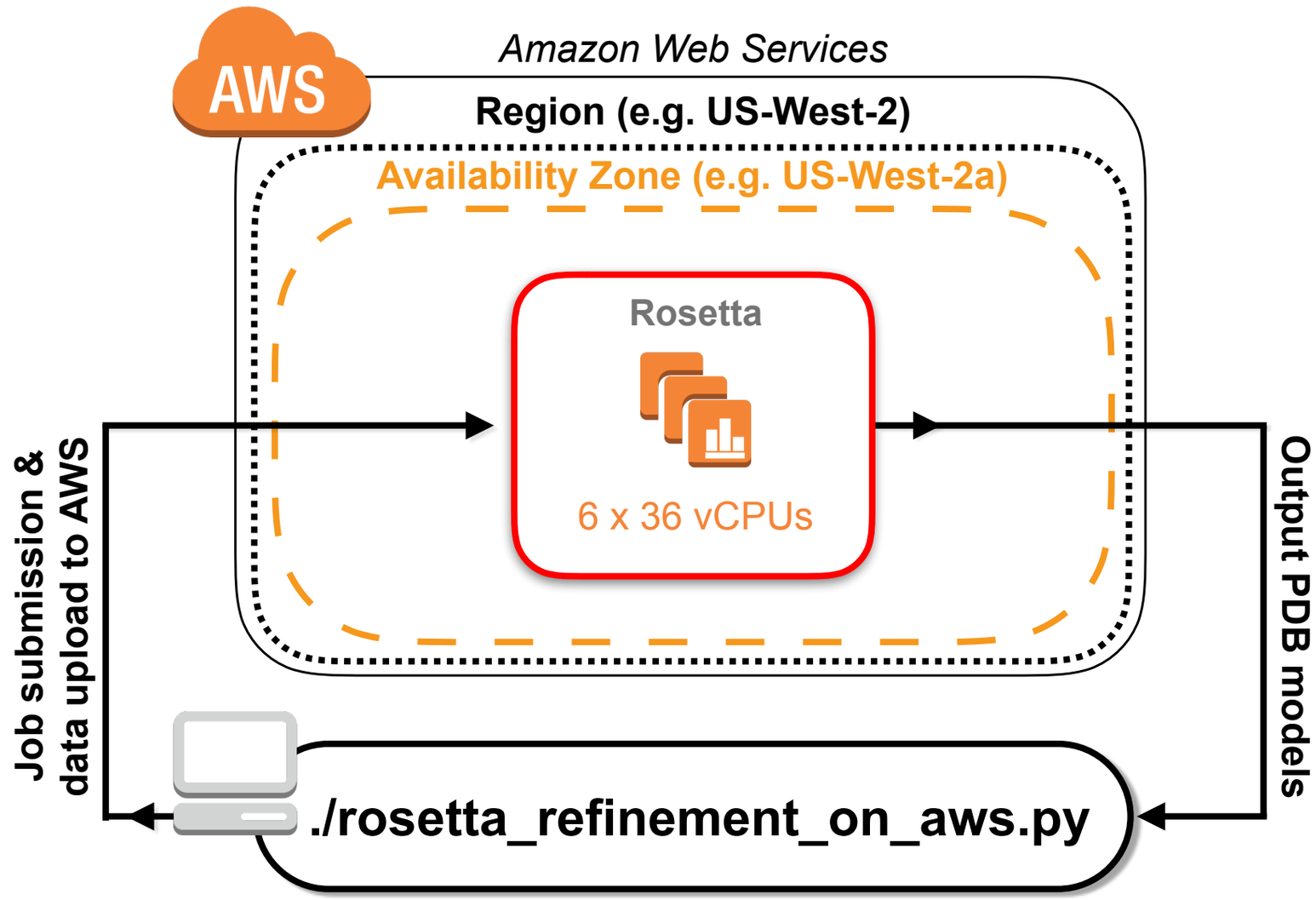


Tracking with expanding GPU availability on AWS

Extending *cryoem-cloud-tools*: Rosetta on AWS

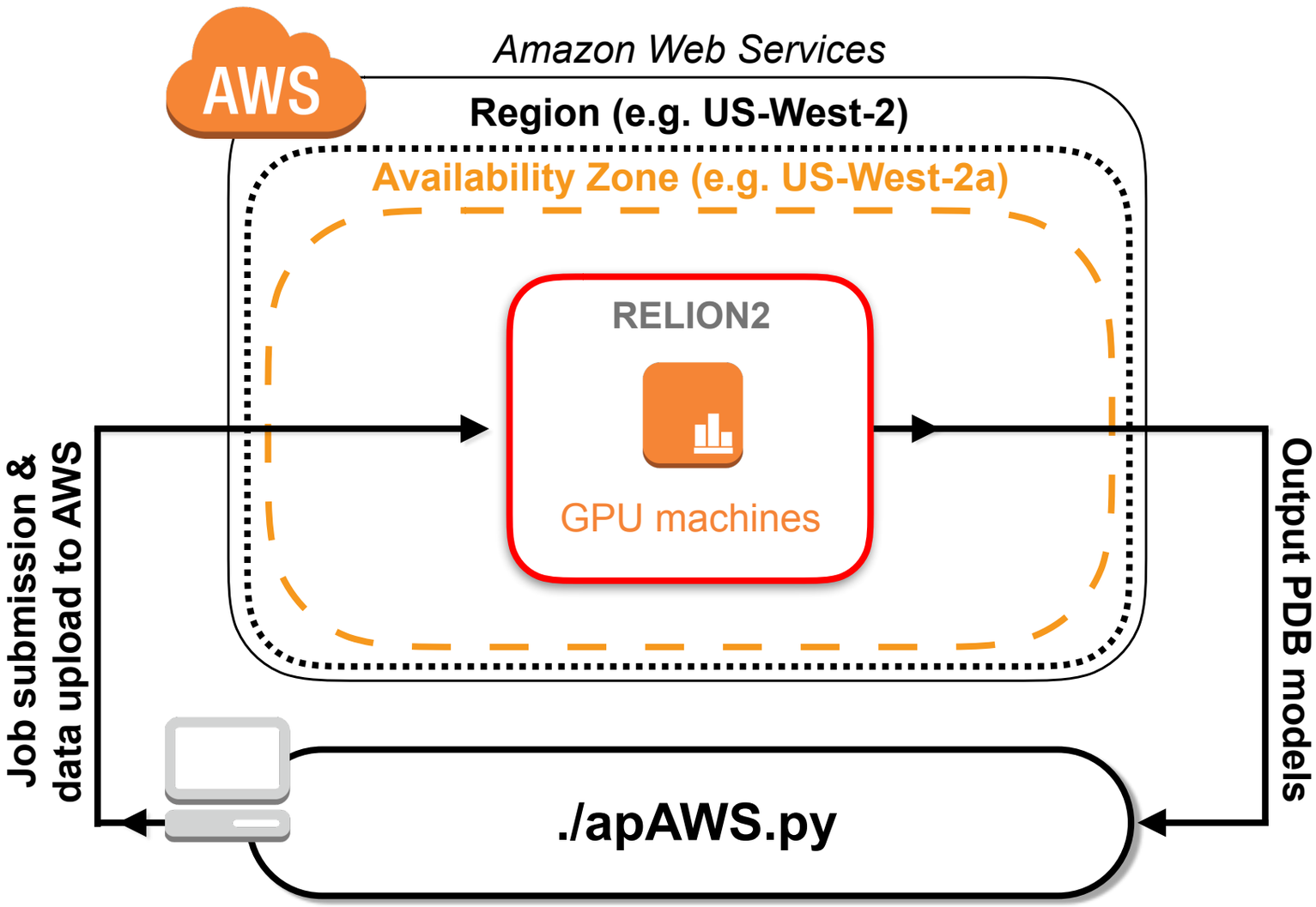
216 structures for each CM & Relax into 2.2 Å beta-galactosidase



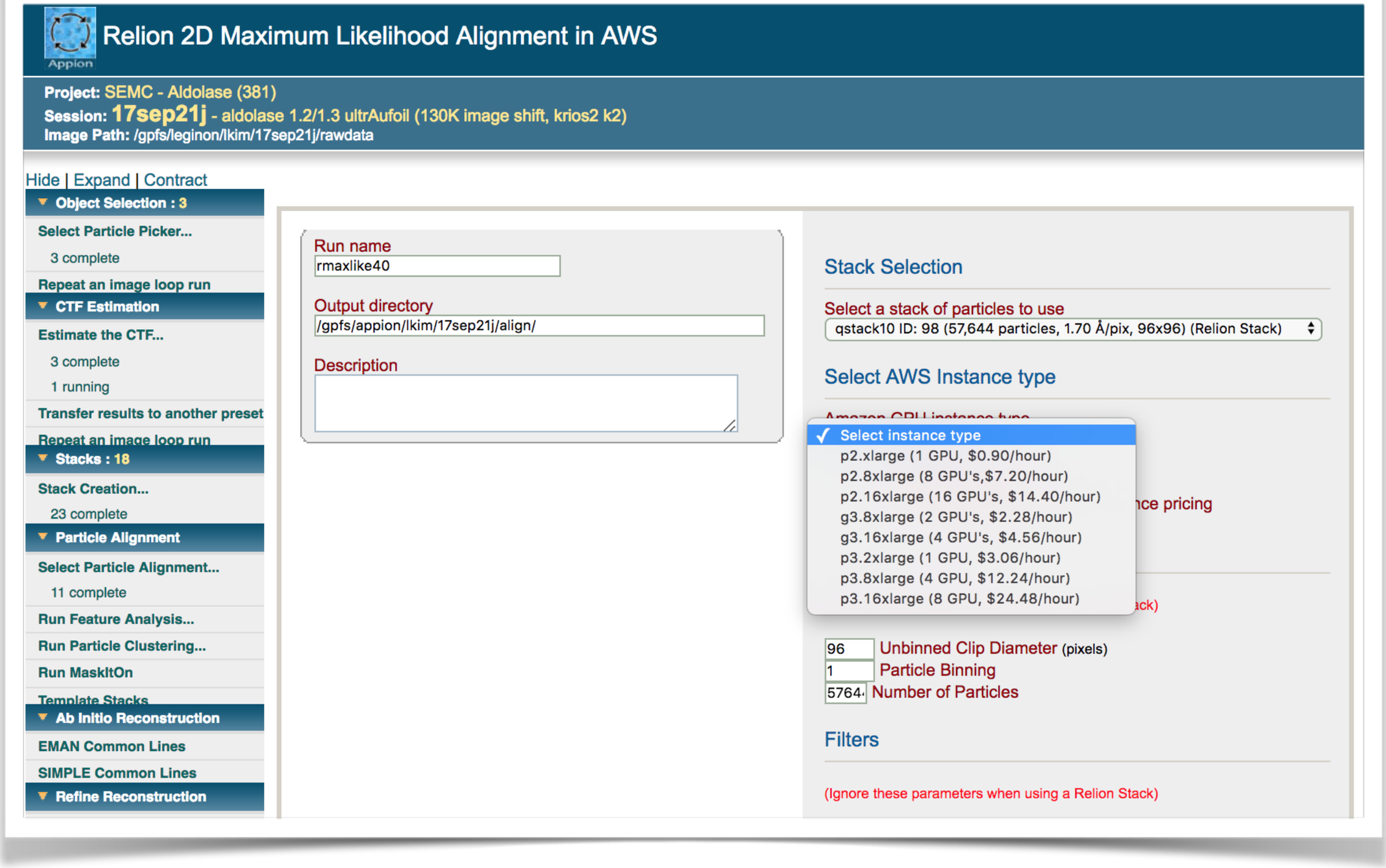


Total AWS Cost: $43.60

Extending *cryoem-cloud-tools*: Appion on AWS



Extending *cryoem-cloud-tools*: Appion on AWS



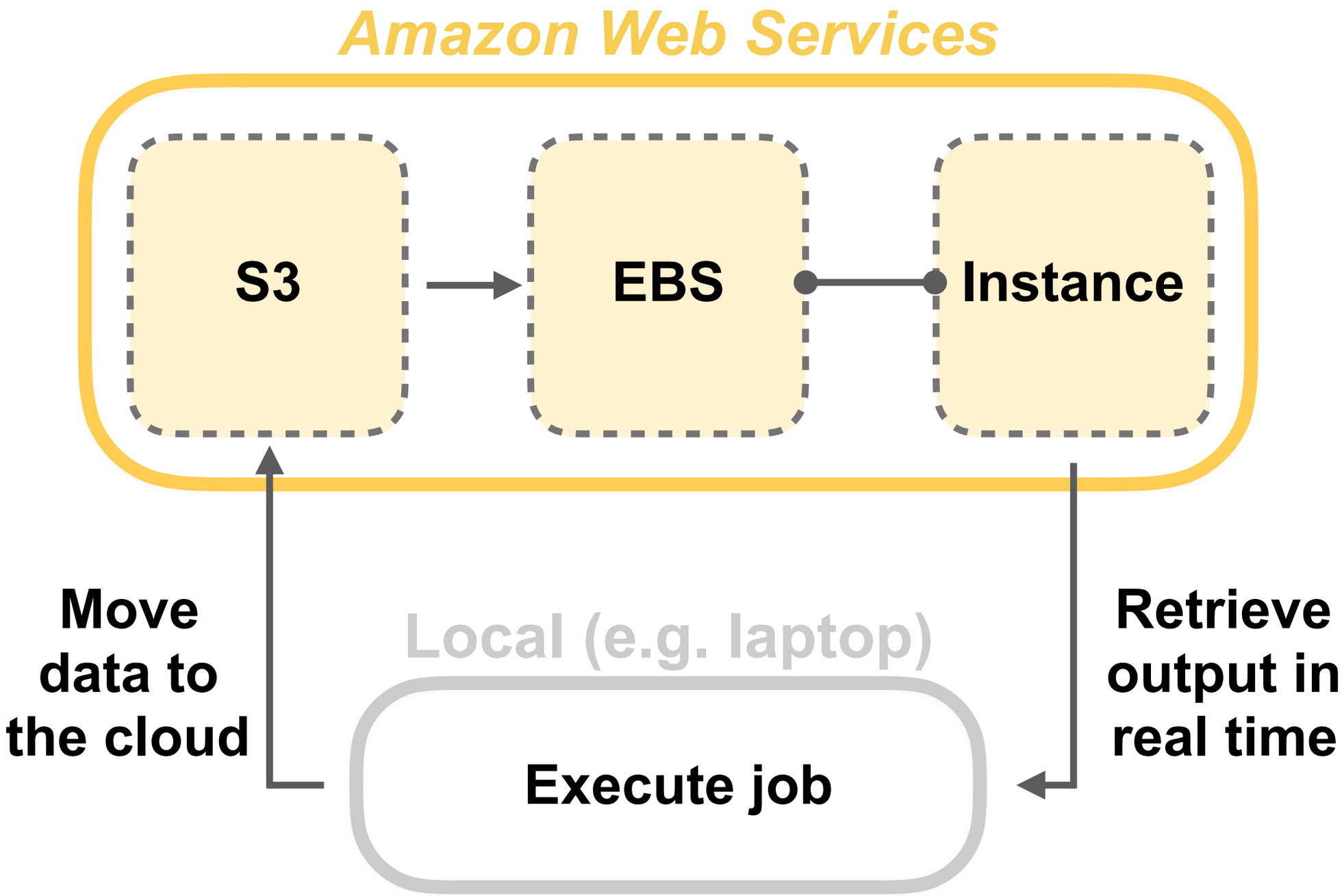
Extending *cryoem-cloud-tools*: Future directions

cisTEM

cryoSPARC

SPHIRE

….



Take-home points

Is the cloud useful for cryo-EM?

Yes - the cloud offers the following features:

1) Outsourcing of IT administration
2) Large choice of computing configurations
3) Active & cold data storage options

What types of resources are at the disposal of users?

Small to large CPU/GPU systems.

What are the appropriate workflows and benchmark comparisons?

Benchmarking can be found online at cryoem-tools.cloud under the RELION2 section of AWS

Punchline: There are many types of GPU machines to satisfy all types of RELION2 computing tasks

Take-home points

How does the cost compare to local infrastructure?

Per hour - these machines are more expensive than simply buying a standalone workstation. But, standalone workstations don’t come with back up storage.

Example storage quote:
$200/TB/year -> $0.0167/GB/mo. (S3: $0.023/GB/mo.) WITHOUT IT support

When should someone use the cloud?

1) Whenever someone is waiting for computing time. For RELION, 4xGPU machines cost $4.56/hr to run, which is much less than the hour wage of individuals working in the lab
2) Large facilities - the cloud lets users launch jobs from a single point of contact and can expand (seemingly) indefinitely
3) Need to solve successive structures under time limit

Questions?

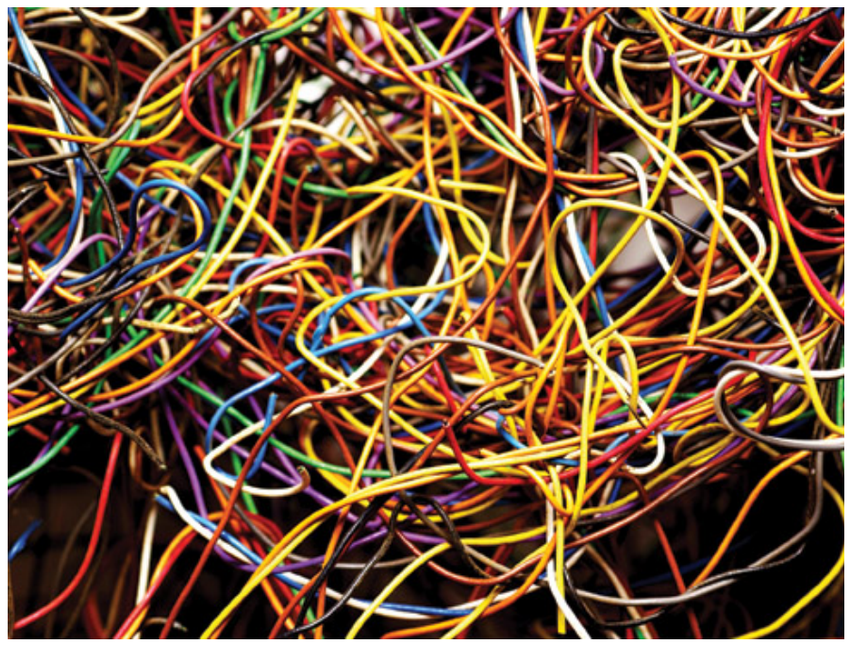
cryoem-tools.cloud

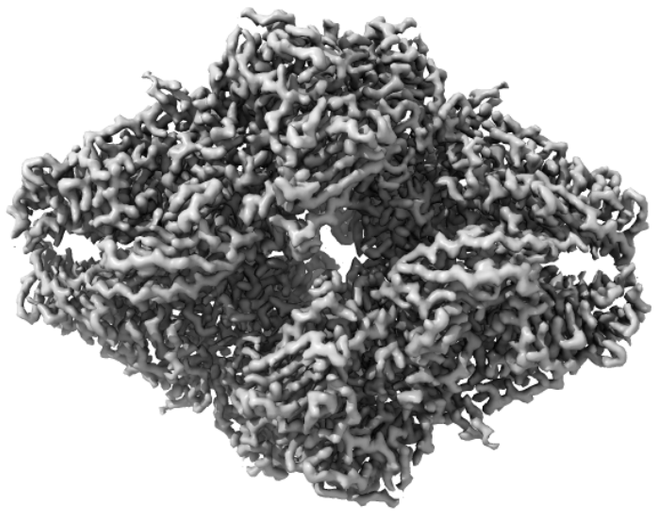
Demo of cryoem-cloud-tools @ Thursday breakout session

Take-home points

Cloud for software dissemination
No need to be pigeon-holed into a single setup
‘Hybrid’ architectures will have the biggest impact on the field - end users don't need to see the backend of AWS
Platform for plugging in new analysis (e.g. ML)
Undlerying data movement tools > agnostic to cloud; could be adapted for anywhere

What do we need?





On-the-fly data movement, analysis, and storage as movies are collected

✓ For *all* users who use facility

Computing options on AWS

Instance *= virtual machine on AWS*

vCPU *= hyper thread on CPU core*

Memory (GB RAM)

 # CPU/GPU

Price per vCPU per hour

$0.0058
1 vCPU
0.5 GB RAM

$0.044
36 vCPU
60 GB RAM

$1.14
1 GPU / 16 vCPU
122 GB RAM

$0.90
1 GPU / 4 vCPU
61 GB RAM

$0.050
64 vCPU
256 GB RAM

$0.067
64 vCPU
488 GB RAM

$2.28
2 GPU / 32 vCPU
244 GB RAM

$7.20
8 GPU / 32 vCPU
488 GB RAM

$4.56
4 GPU / 64 vCPU
488 GB RAM

$14.40
16 GPU / 64 vCPU
732 GB RAM

$0.104
128 vCPU
1952 GB RAM

Computing options on AWS

Instance *= virtual machine on AWS*

vCPU *= hyper thread on CPU core*

Memory (GB RAM)

 # CPU/GPU

Price per GPU per hour

$0.0058
1 vCPU
0.5 GB RAM

$1.591
36 vCPU
60 GB RAM

$1.14
1 GPU / 16 vCPU
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$0.90
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2 GPU / 32 vCPU
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488 GB RAM

$1.14
4 GPU / 64 vCPU
488 GB RAM

$0.90
16 GPU / 64 vCPU
732 GB RAM

x1.32xlarge
128 vCPU
1952 GB RAM

	GPU Workstation					Amazon Web Services							
	Total processing time (hr)	*Estimated elapsed time (working days)^*	*Number of GPUs*	*Number of CPU cores*	*Amount of RAM (GB)*	*Total processing time (hr)*	*Estimated elapsed time (working days)^*	*Data moving time (hr)*	*Job running time (hr)*	*EC2 Cost (USD)**	*Number of VMs*	*VM type*	*VM cost per hour (USD)*
Movie alignment	34.0	1	4	8	64	13.26	1	11.06	2.20	$146.72	5	x1.32xlarge	$13.34
Autopick	2.0	3	4	8	64	1.30	2	1.10	0.20	$9.36	1	p2.8xlarge	$7.20
CTF Estimation	0.4	3	4	8	64	0.66	2	0.55	0.11	$4.75	1	p2.8xlarge	$7.20
Extract	-	3	4	8	64	1.30	2	0.68	0.62	$1.04	1	m4.4xlarge	$0.80
2D classification	8.0	3	4	8	64	4.30	2	0.17	4.13	$61.92	1	p2.16xlarge	$14.40
3D autorefine	5.3	4	4	8	64	5.38	2	0.08	5.30	$38.74	1	p2.8xlarge	$7.20
Movie extract	9.5	4	4	8	64	4.07	3	3.35	0.72	$179.73	8	d2.8xlarge	$5.52
Movie-refine	17.5	5	4	8	64	4.85	3	0.75	4.10	$64.69	1	x1.32xlarge	$13.34
Polish	25.0	7	4	8	64	6.80	3	1.40	5.40	$90.70	1	x1.32xlarge	$13.34
3D classification	7.0	8	4	8	64	6.17	4	0.17	6.00	$44.42	1	p2.8xlarge	$7.20
3D autorefine	6.0	8	4	8	64	6.40	4	0.10	6.30	$46.08	1	p2.8xlarge	$7.20
Rosetta	N/A	9	4	8	64		5				6	c4.8xlarge	$1.59
S3 storage cost#	-	-	-	-	-	-	-	-	-	$690.00	-	-	-
Totals	114.7	10	-	-	-	54.5	5	19.4	35.1	$1,378.15	-	-	-