

Workflows in the Cloud

MDI Biological Laboratory

2nd May, 2025

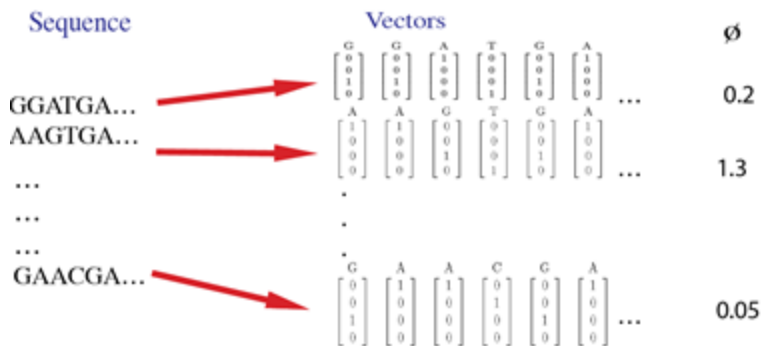
Saba Nafees, Ph.D.
MemVerge, Nextflow Ambassador



MDI Biological Laboratory
Computational Biology Core

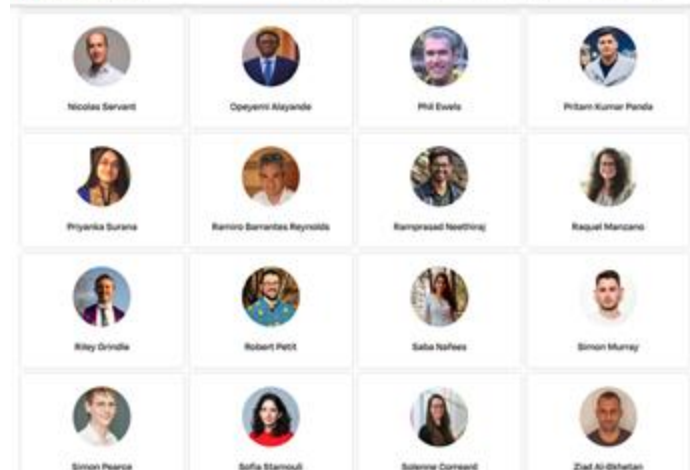
Background

- Research: Understanding sequence–phenotype relationships using novel analytical methods.
- Bioinformatics (analysis, pipeline development & optimization, etc.); computational biology problems (gene expression, immune/antibody analysis, etc.); methods development.
- community building (nf-core), training/teaching, and mentorship!



nextflow

Documentation Examples Training Resources Forums



Basis of ortho_seqs work



https://www.nextflow.io/our_ambassadors.html

Little bit about MemVerge...

Raised ~\$100M of investment

Headquarters in San Jose, CA



**Founders created
\$B product lines**



Software is used by genomics customers in four continents

Launched Memory Machine for AWS at re:Invent 2022



**Award winning solution helps automate & lower the cost of
running genomics workloads on AWS**



Europe



USA

Running pipelines at scale while optimizing resources

Running multiple pipelines at scale, given lots of sequence samples and limited resources can be a bottleneck for R&D.

Have you used EC2 Spot instances?

First the benefits...

Customers
have saved
over \$8B



EC2 Spot prices can
be 50-80% less vs.
On-Demand

Spot instances introduce unpredictability

Costs can end up being higher than just running with on-demand instances



Runtimes can be much longer when jobs are interrupted, 2-minute warning

Pain Point: Spot reclamations & long runtimes

Use case example:

Molecular diagnostics startup working on cell free mRNA assay for Alzheimer's

- running nf-core rnaseq pipeline on samples
- need fast turnaround times for bioinformatics analysis + results
- analysis informs further iterations of assay
- without results, subsequent experiments are delayed
- pipeline runs monitored on Seqera, spot reclamations led to increased runtimes
 - hybrid strategy of switching to OnDemand (Nextflow config) reduced failures.
- cost & time optimization was key

```
1  aws {
2    batch {
3      maxSpotAttempts = 2
4    }
5  }
6
7  process {
8    errorStrategy = { (task.attempt <= process.maxRetries) ? 'retry': 'ignore' }
9    maxRetries = 3
10   queue = { task.attempt == 1 ? 'TowerForge-spot instance TowerForge-ondemand }
11 }
```

Pain Point: Cloud Costs

“Stuck between a rock and a hard place”



“Savings vs. On-Demand vs. Interruption Frequency”

Instance Type ▾	vCPU ▾	Memory GiB ▲	Savings over On-Demand ▾	Frequency of interruption ▾
m6i.2xlarge	8	32	57%	>20% ■■■■■□
g5g.4xlarge	16	32	59%	>20% ■■■■■□
r7iz.xlarge	4	32	60%	<5% □□□□□
a1.metal	16	32	59%	<5% □□□□□
c6in.4xlarge	16	32	57%	<5% □□□□□
c6i.4xlarge	16	32	53%	5-10% ■■□□□□
c6gd.4xlarge	16	32	56%	>20% ■■■■■□
m7gd.2xlarge	8	32	57%	15-20% ■■■■■□
c6gn.4xlarge	16	32	55%	<5% □□□□□
r7i.xlarge	4	32	60%	>20% ■■■■■□

On-Demand		\$\$\$
no commitment		
Reserved Instances	\$\$	long term
commit		
Cloud Savings Plans	\$\$	long term
commit		

Spot Instances
no commitment

\$?

We make running on Spot simple...and...

Submit Job

Apply a Template | Start from Scratch

Load a Template: Select a Template

Basic | WaveRider | Environment Variables | Network | Misc.

☒ CPU and Memory ☐ Instance Type

vCPU (min) vCPU (max) Memory (min GB) Memory (max GB)

VM Policy
VM instance creation policy

☒ Spot First ☐ Spot Only ☐ On-Demand Only

Retry Limit: 3 | Retry Interval: 600 s | Price Limit:

Storage Volumes

Generated command line

```
float submit --vmPolicy  
[spotFirst=true,retryLimit=3,retryInterval=600  
s] --migratePolicy  
[cpu.disable=true,mem.disable=true,stepAuto=tr  
ue,evadeOOM=true] --dumpMode full
```

Cancel Submit

Memory Machine = Spot Reclaim Immunity

Sample: Axolotl Instances

Runtime: 38hrs, 49 secs

EC2 Instances: 37 Spot

Workflow: Nextflow **Process:** NECODE-ATACSEQ-ATACSEQ-EASTO-ALIGN-RWA-RWA-MEM

ID	Host	User	Submitted Time	Wall Time	Cost
lli9y794k1xov01t53cy1		sateesh	2024-02-21 21:43:11	38h0m49s (Queue Time: 0s)	33.1605 USD

Output
container state: exited (0)

Instances (37)

Storage Volumes (17)

Settings

Attachments

WaveWatcher

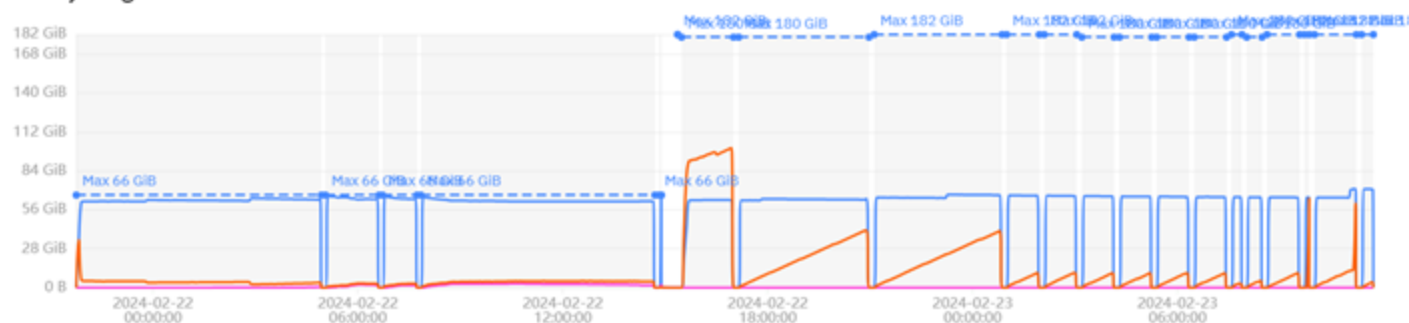
[Download Log Bundle](#)

Area Marking: ☒ Executing ☐ Migrating

2024-02-21 21:45:01 → 2024-02-23 11:44:01



● Memory Used
 ● Swap Used
 ● Buffer Cache



How is my Nextflow pipeline run going?

MMCloud OpCenter

+ Submit Job

Cost Summary

Jobs

Workflows

Job Templates

App Library

SERVICE

Gateways

ADMINISTRATION

SurfZone

Users and Groups

System Settings

Workflow Details - gigantic-wescoff

Refresh

Pipeline	User	Submitted	Updated	Wall Time	CPU Time	Cost
nf-core-rnaseq	sateesh	2024-03-05 13:14:41	2024-03-05 22:54:21	9h39m40s	792.02 Core Hours	\$ 25.9751

Jobs Success 276 Running 0 Pending 0 Failed 0 Migrations 9 Cloud Instances 8 On-Demand 277 Spot

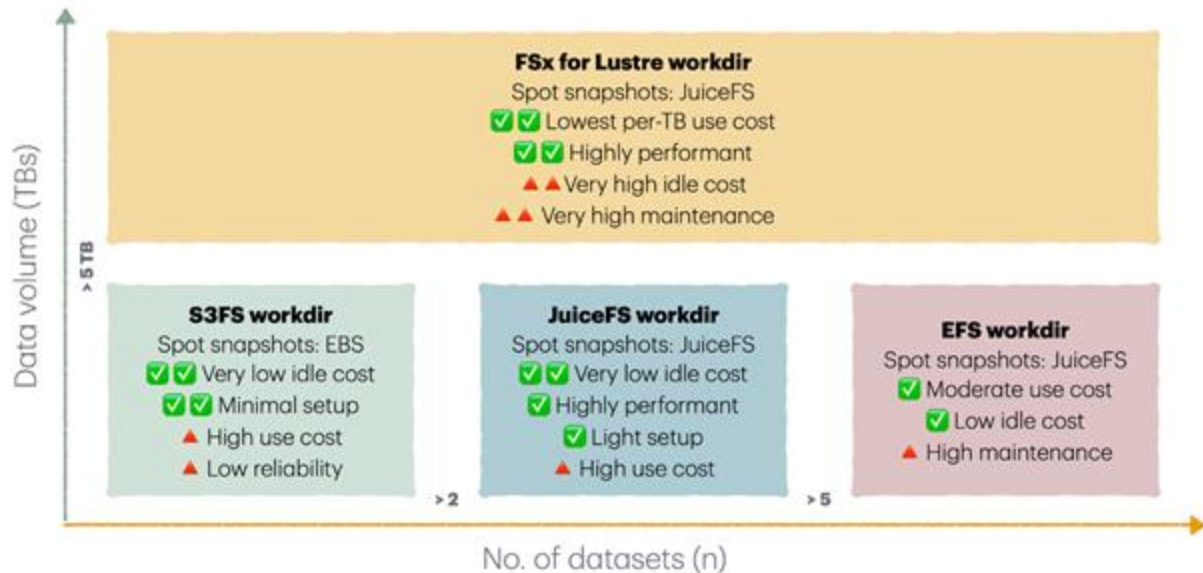
Jobs Timeline

ID	Name	Process	Host	Status	Submitted Time	Wall Time	Cost
jzprga5ga8u2s8x7ae-69m	multiqc-383tcl-r4.2xlarge	NFCORE-RNASEQ-RNASEQ-MULTIQC		Completed	2024-03-05 22:49:10	5m11s	0.0195 USD
cbz7g1214x08m9g7-rd6ko	ucsc-bedgraphtobigwig-wqpcvq-m5.large	NFCORE-RNASEQ-RNASEQ-BEDGRAPH-BEDCLIP-BEDGRAPHTOBIGWIG-FORWARD		Completed	2024-03-05 20:29:29	3m49s	0.0025 USD
fkjnjfg2sagn1onxd4bzj	ucsc-bedgraphtobigwig-wqpcvq-m5.large	NFCORE-RNASEQ-RNASEQ-BEDGRAPH-BEDCLIP-BEDGRAPHTOBIGWIG-FORWARD		Completed	2024-03-05 20:29:16	3m54s	0.0025 USD

Use the right file system for various workloads without getting vendor locked

Nextflow on MM Cloud

Design Matrix



Jupyter notebooks that can EC2 Spot-Surf

MMCloud OpCenter

< Jobs

📄 📁 ? 🗑️ 👤 jxie ▾

Submit Job

📄 Cost Summary

📄 Jobs

📄 Job Templates

📄 App Library

👤 Users and Groups

⚙️ System Settings

SERVICE

🔌 Gateways

Job Details - demo-jupyter-2023-09-26 Suspended

🔄 Refresh 📁 Migrate ⚙️ Modify More Actions ▾

[docker.io/memverge/jupyter_server:v3.5.0](#)

ID	Host	User	Submitted Time	Wall Time	Cost
Y1VxHHGCatIC Kh70a1IF		awir sch	2023-09-26 13:04:24	1728h47m15s (Queue Time: 1728h47m15s)	32.886 7 USD

Output

[I 2023-12-07 16:09:08.363 ServerApp] 302 GET / (@87.236.176.125) 0.48ms
[I 2023-12-07 16:09:08.808 LabApp] 302 GET /lab? (@87.236.176.125) 0.77ms

Instances (9)

Storage Volumes (3)

Settings

Attachments

WaveWatch

▼ Instance ID: i-00e77bd8cd09d64c2

Zone: us-east-1d

Spot t3.medium | 2 Core 4 GB

Address	Public IP	Status	Start Time	End Time	Cost
172.31.31.21:43	208.15.43	reclaim ed	2023-09-26 13:04:36	2023-09-26 13:21:14	0.0048 USD

72 days running continuously on AWS EC2 for less than your daily coffee

How does it work?

Memory Machine provides an automated checkpoint recovery service called **SpotSurfer** that enables long-running batch and even stateful apps to run on low-cost Spot instances

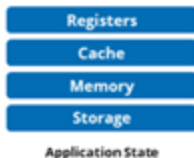
Deploy job on
Spot instance



Spot Reclaim
Notice



Create
AppCapsule



Provision a new
Spot instance



Restore on new
Spot instance

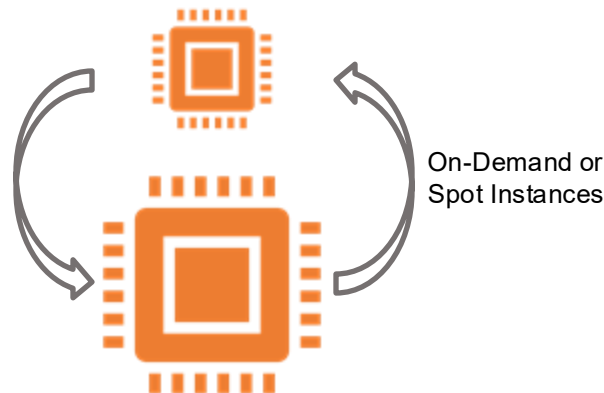
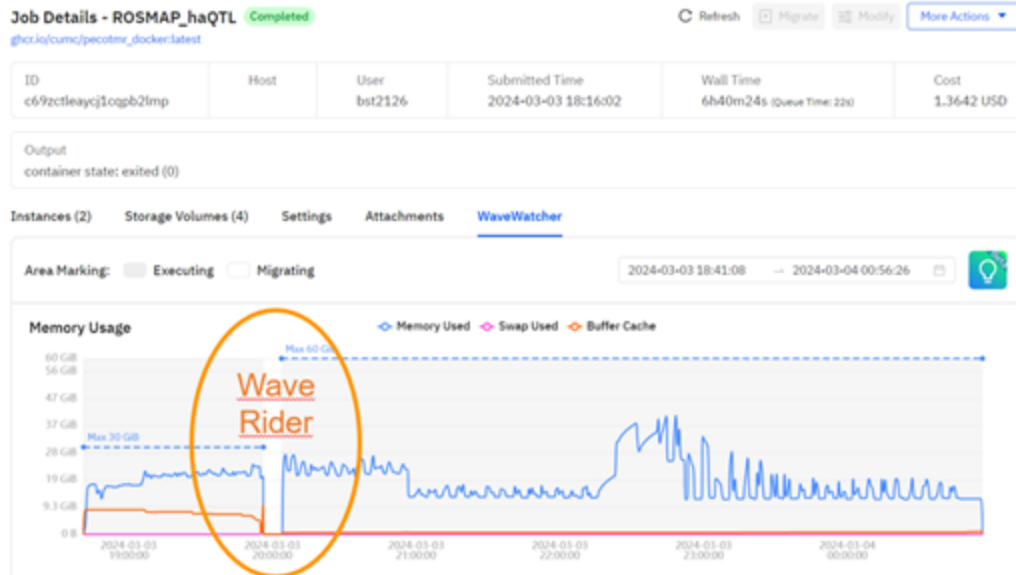


Automated

If no Spot instances are available SpotSurfer can recover using on-demand instances

Have you ever run out of memory?

Memory Machine provides an automated service called **WaveRider** that migrates workloads to larger or smaller instances based on real-time CPU & memory utilization



Running Alphafold on AWS for less than \$2

Alphafold is an open-source workflow developed by Google Deepmind. Its purpose is to predict protein structure base on the provided protein sequence. Alphafold can be considered as two parts: MSA search(rely on CPU) and inference prediction(heavily rely on GPU)

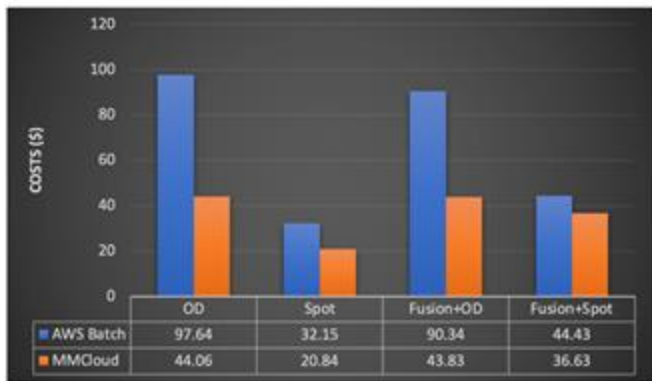
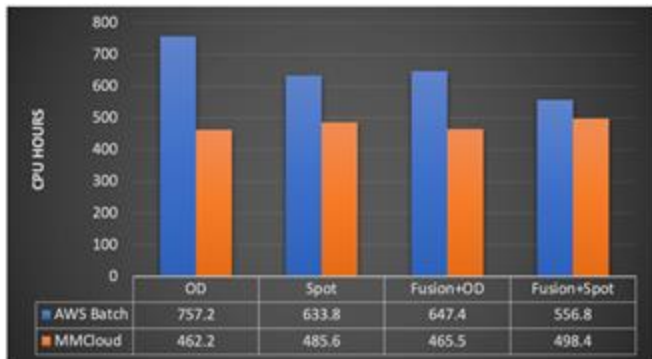
khgqgliqxuez42g7jl wiv	7ktt.fasta_inference _prediction	admin	Completed	2024-03-15 19:38:49	2024-03-15 22:47:30	3h8m41s	0.9439 USD	▶ 📄 ✕
35tb9c5crauyb5t3n rrdr	7ktt.fasta_msa_sea rch	admin	Completed	2024-03-15 18:27:30	2024-03-15 19:38:18	1h10m47s	0.2723 USD	▶ 📄 ✕
vn9ucfhrc2kjug8j8x w2r	7FC7.fasta_inferenc e_prediction	admin	Completed	2024-03-17 19:01:12	2024-03-17 19:26:55	25m43s	0.1288 USD	▶ 📄 ✕
1hae2l9fi2u09fvolp 9pi	7FC7.fasta_msa_se arch	admin	Completed	2024-03-17 18:08:57	2024-03-17 19:01:00	52m2s	0.2017 USD	▶ 📄 ✕

- 7ktt -- 1142 residues
- 7FC7 -- 96 residues

Cost per run = \$1.22 using MMCloud

85-90% less than alternative options...

Benchmarking nf-core/rnaseq

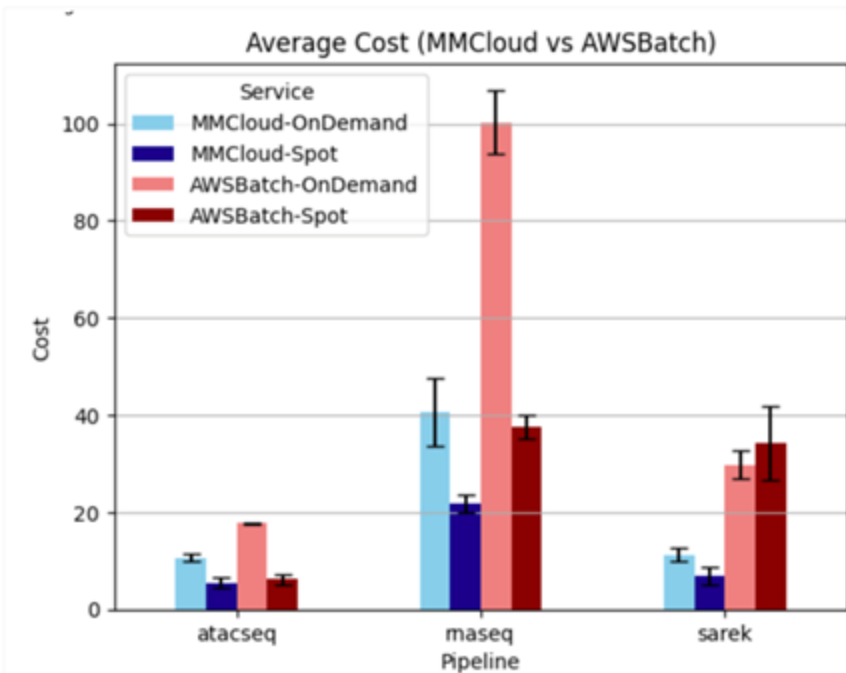


- ✓ MemVerge delivered equal or better rnaseq performance and cost without the use of a commercial file system called Fusion from Seqera
- ✓ MemVerge's superior EC2 automation and selection logic outperformed AWS Batch when comparing both "OD" On-Demand runs and Spot runs
- ✓ The cost of using MemVerge managed Spot instances for rnaseq was 78.7% lower than using AWS Batch managed On-Demand instances
- ✓ MemVerge SpotSurfer can guarantee consistent CPU hours and cost per run on Spot instances at scale while AWS Batch cannot (see next slide)

78.7% Savings

Benchmarking nf-core cont'd...

Pipeline	MMCloud-OnDemand	MMCloud-Spot	AWSBatch-OnDemand	AWSBatch-Spot
atacseq	10.70	5.45	17.70	6.20
maseq	40.66	21.77	100.34	37.60
sarek	11.21	6.94	29.73	34.33



- ✓ MemVerge's superior EC2 automation and selection logic outperformed AWS Batch when comparing both "OD" On-Demand runs and Spot runs
- ✓ The cost of using MemVerge managed Spot instances for ranged from 69% to 78% lower vs AWS Batch managed On-Demand instances
- ✓ MemVerge SpotSurfer can guarantee consistent CPU hours and cost per run on Spot instances at scale while AWS Batch cannot (see Sarek data)

69-78% Savings

Have you ever had AWS billing surprises?

Memory Machine **SurfZone** is a service that minimizes the risk of runaway compute spend by cancelling or suspending jobs when a user's "quota" is exceeded

The screenshot displays the MMCloud OpCenter interface for managing SurfZones. A modal dialog titled "Edit SurfZone" is open, showing the configuration for a SurfZone named "JingZone".

Edit SurfZone Configuration:

- Name:** JingZone
- Quota Type:** Cost
- Quota Amount:** \$ 100 USD
- Usage Notification Threshold:** 80 %
- Quota Exceeded Action:** Suspend (selected over Cancel)
- Auto resume jobs after quota refreshed:** ☒

The background interface shows a list of SurfZones with columns for Name, Quota Exceeded Action, and Actions. The list includes entries like "JingZone", "surfzone-1", "vince", and several "yt-surfzone-1-suspend" entries.

Name	Quota Exceeded Action	Actions
JingZone	Suspend (Auto Resume)	Edit Delete
surfzone-1	Suspend	Edit Delete
vince	Suspend (Auto Resume)	Edit Delete
yt-surfzone-1-suspend	Suspend (Auto Resume)	Edit Delete
yt-surfzone-100-cancel	Cancel	Edit Delete
yt-surfzone-100-suspend	Suspend (Auto Resume)	Edit Delete

Thank you!

If you have questions or want to collaborate, problem solve, etc., please reach out!

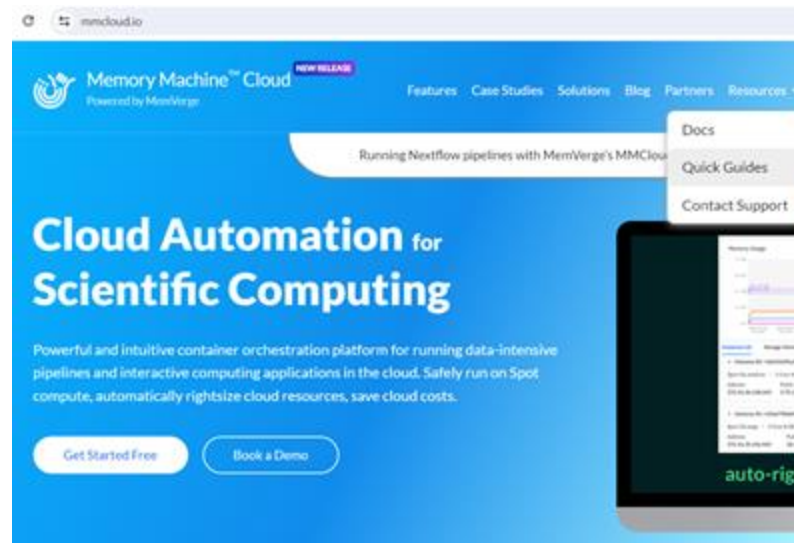
saba.nafees@memverge.com

Interested? Here's how to get started!

Email Jing for more info:

jing.xie@memverge.com

Quick start guides: www.mmcloud.io



Sign up for a free trial

Slack support is available to all users

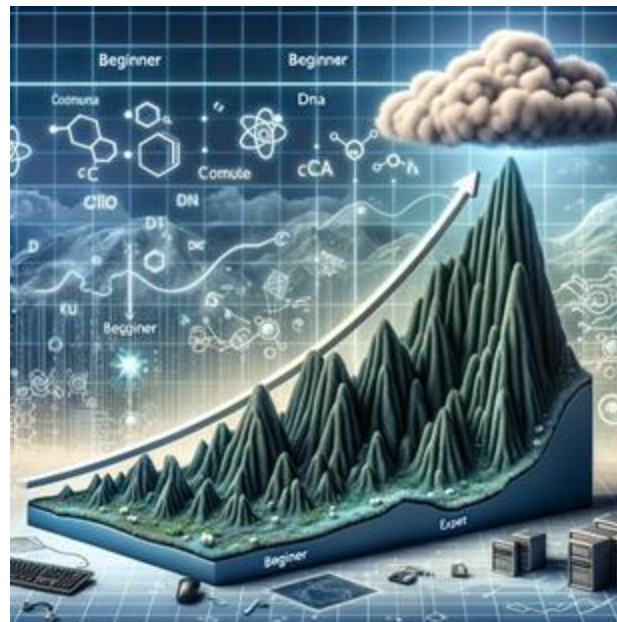
<https://www.mmcloud.io/customer/register>

Supplementary

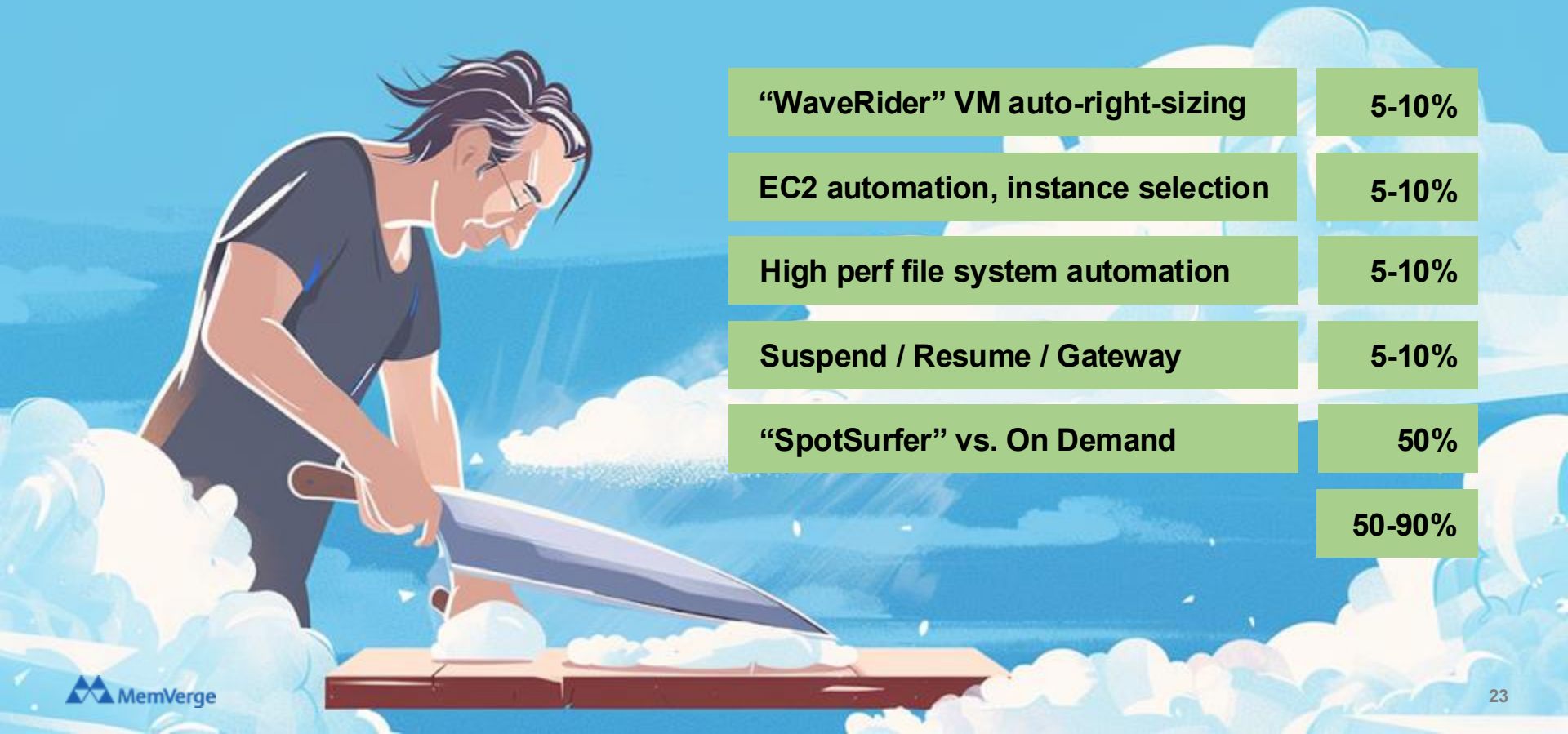
Pain Point: Cloud Skills

Cloud Computing comes with a learning curve

- How do I “submit a job” on AWS, GCP?
- How do I know I’m using the right compute?
- How can I optimize and run this job for less?
- How do I monitor my lab’s job(s) and user(s)?
- How can I do the above in a more automated way?



How MemVerge MMCloud Cuts Cloud Costs



“WaveRider” VM auto-right-sizing

5-10%

EC2 automation, instance selection

5-10%

High perf file system automation

5-10%

Suspend / Resume / Gateway

5-10%

“SpotSurfer” vs. On Demand

50%

50-90%

Easily run containerized apps, tools on AWS

The screenshot displays the MMCloud OpCenter App Library interface. On the left is a sidebar with navigation options: Cost Summary, Jobs, Workflows, Job Templates, App Library (selected), SERVICE (Gateways), and ADMINISTRATION (SurfZone, Users and Groups, System Settings). The main area is titled 'App Library' and shows a list of applications under the 'Built-in (21)' tab. The 'Data Science' category is selected, showing a list of apps: blast, bwa, cactus, cellranger, gateway, gatk, jfs, jupyter, megahit, monocle, nextflow, pantools, sentieon, seurat, spades, supernova, trinity, jupyter_server, and rstudio. The right pane displays details for three selected apps: blast, bwa, and cactus. Each app card shows its URI, version, status (Available or Ready), size, and path.

App	URI	Version	Status	Size	Path
blast	docker.io/memverge/blast	2.14.0	Available	319.76 MB	s3://opcenter-bucket-48b761c0-890a-11ee-9763-0e1e99d868ff/images/xcf7tyhu3.tar
bwa	docker.io/memverge/bwa	0.7.17	Available	119.27 MB	
cactus	docker.io/memverge/cactus	2.5.1	Ready	913.18 MB	

Customer testimonials

“MMCloud has helped our team in the Computational Biology Core at MDI Biological Laboratory better utilize AWS Spot EC2 instances to save cloud computing costs. In addition, the WaveWatcher tool has let us observe resource usage in real time, providing new insights into optimizing resource allocations for our work with Nextflow pipelines”



-Joel Graber, Director of the Computational Biology and Bioinformatics Core

“We have been impressed by the performance of the WaveRider for Sentieon solution. Early testing shows 4-5x speed-ups out-of-the-box and we expect to improve the results as we fine tune the solution. Faster processing coupled with leveraging Spot instances is dramatically lowering our cloud costs too. This solution enables us to complete our NGS more efficiently than ever and will help elevate our research to a new level.”



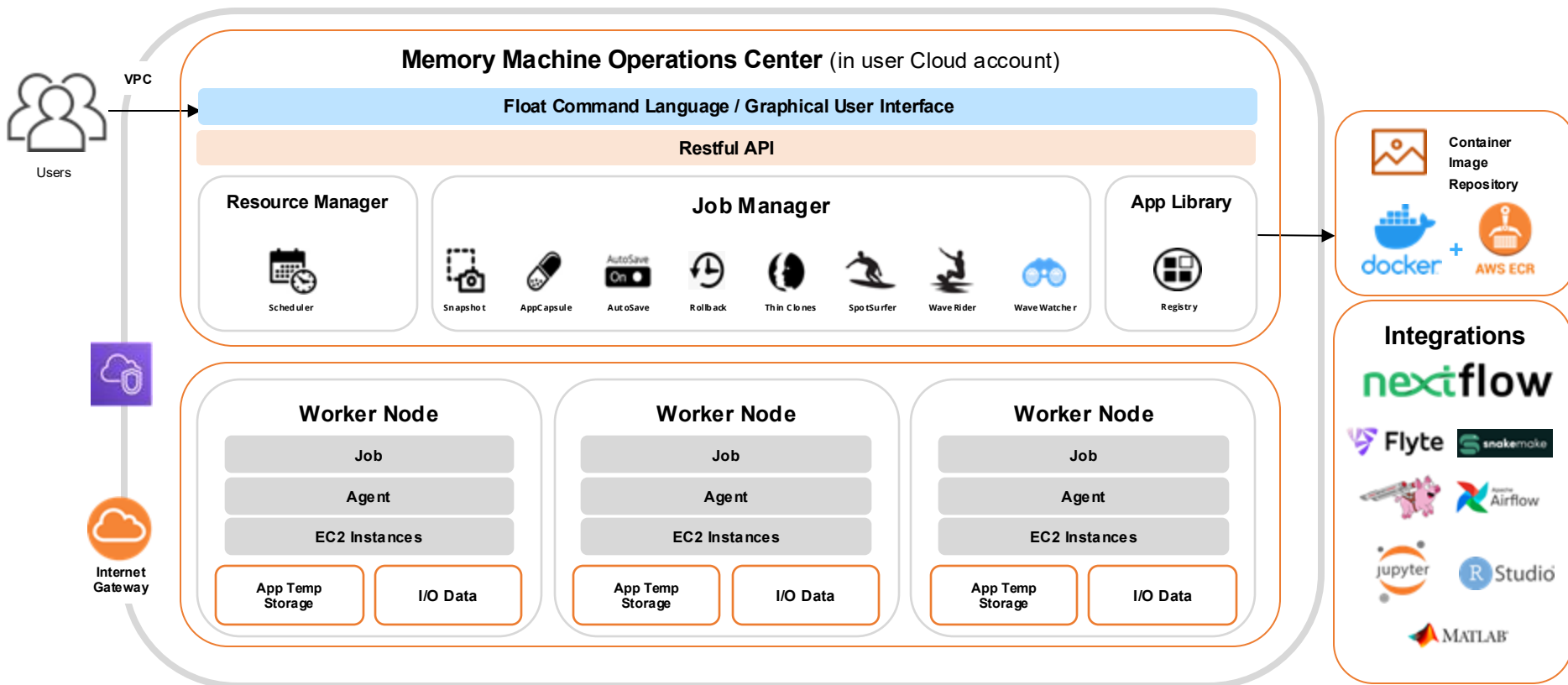
-Remco Ursem, Program Leader of Bioinformatics

“I was getting up to 80% batch failure rates with Spot EC2, now with SpotSurfer we have already brought failure rates due to Spot reclaims to below 1%, and we are just getting started. WaveRider picks the most appropriate VM for each of the thousands of jobs launched by Nextflow. That is giving me more efficiency than ever. Very cool.”



-Vince Pagano, Senior Scientific Programmer

Full Stack Solution or Embeddable



Case Study: Leading Genomics Research Institute (TGen)

Background:

Large 501(c)(3) research institution focused on accelerating genetic research was struggling to cost-effectively run Nextflow on AWS

Pain Points:

- Huge # of worker nodes, > 20K+ VMs per workflow
- ~75% failure rate using when using Spot EC2



Solution:

Memory Machine Cloud on AWS

Results:

70% EC2 savings

Reduced Failure Rate to Zero

Real-time automated EC2 optimization

nextflow Integration



SpotSurfer
Spot Protection



WaveRider
Resource Rightsizing

**Memory Machine
Differentiators**

Current implementation supports scaling to 1,000 concurrent worker nodes per Memory Machine Op Center, larger solutions can be supported via multiple Memory Machine Op Centers.

Case Study: Leading Genomic Medicines Company

Background:

Large biotech pioneering the future of genomic medicine with multiple clinical and pre-clinical product pipelines

Pain Points:

- Limited IT budget, multiple days to get compute spun up for researchers
- No easy way to refactor pipelines and cost-optimize for running in the cloud

Solution:

Memory Machine Cloud on AWS

Results:

>35% cost savings w/ On-Demand EC2

>80% cost savings w/ Spot EC2

AWS resource provisioning in seconds vs. days

Leading Genomics Company	BAU On-Demand	Memory Machine CE WaveRider Spot	Memory Machine CE WaveRider On-Demand
Total Compute Time (Hours)	7.5	7.72	7.72
Instance(s)	r5.24xlarge	r5.large to r5.24xlarge (multiple)	r5.large to r5.24xlarge (multiple)
EC2 Cost / Hour	\$6.048	\$0.126 to \$6.048	\$0.126 to \$6.048
Cost Per Job	\$45.36	\$8.32	\$28.45
% Savings vs. BAU		-82%	-37%
EC2 Instance(s) WaveRider Managed			
			Duration
r5.large			0:06:49
r5.xlarge			0:08:25
r5.large			0:07:27
r5.xlarge			0:12:41
r5.2xlarge			0:10:57
r5.4xlarge			0:13:47
r5.12xlarge			3:18:18
r5.24xlarge			2:32:29
r5.12xlarge			0:52:24

Optimizing AWS resources

- Reduce the # of spot attempts under the hood
- Error strategy
 - Retry
 - Ignore
- Tell nextflow to go from spot to ondemand after 1 attempt so that resource consuming tasks can be done via ondemand

```
1  aws {
2      batch {
3          maxSpotAttempts = 2
4      }
5  }
6
7  process {
8      errorStrategy = { (task.attempt <= process.maxRetries) ? 'retry': 'ignore' }
9      maxRetries = 3
10     queue = { task.attempt == 1 ? 'TowerForge-[redacted] spot instance' : 'TowerForge-[redacted] ondemand [redacted] }
11 }
```