Cluster in the Cloud

Easy, Scalable, Heterogeneous

CLUSTER IN THE CLOUD

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The problem

- Researchers having cloud credits

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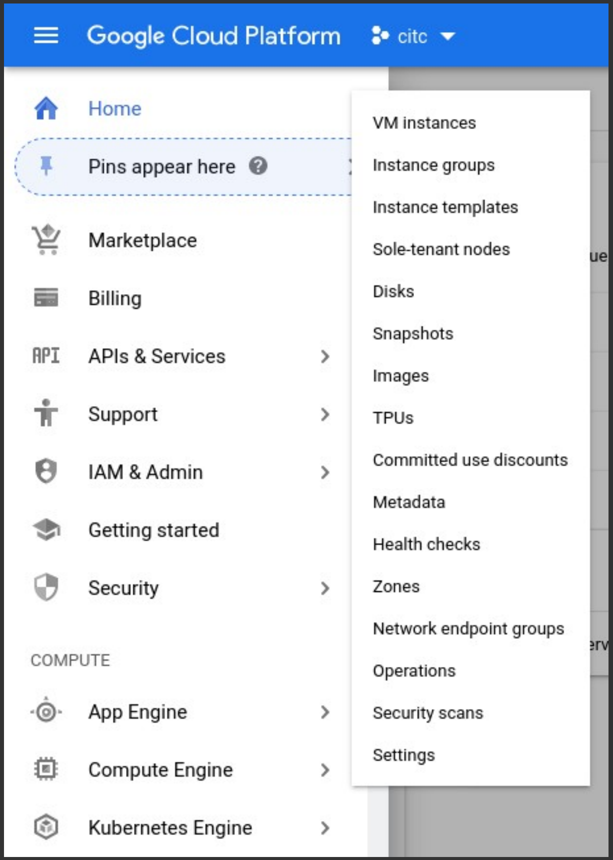
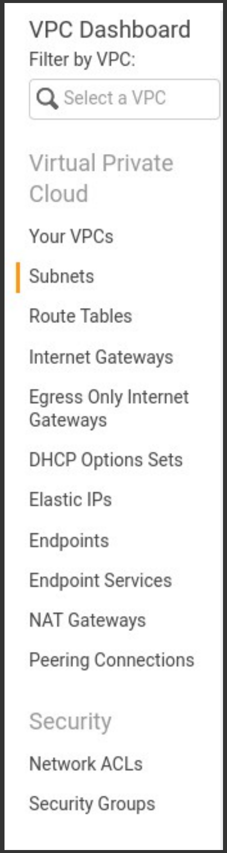
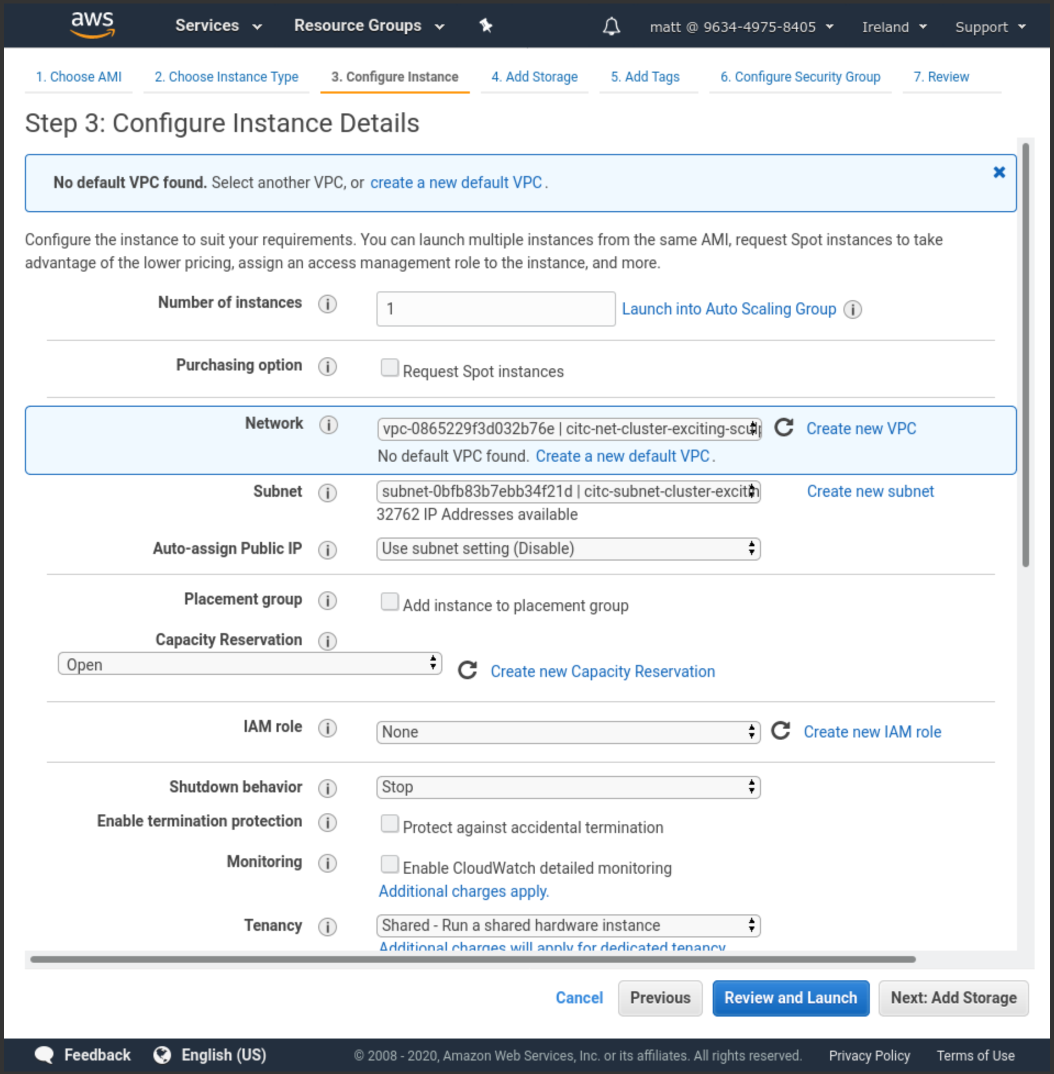
- Researchers having cloud credits
- Presented with:







Step 3: Configure Instance Details

No default VPC found. Select another VPC, or create a new default VPC.

Configure the instance to suit your requirements. You can launch multiple instances from the same AMI, request Spot instances to take advantage of the lower pricing, assign an access management role to the instance, and more.

Number of instances: 1 Launch into Auto Scaling Group

Purchasing option: □ Request Spot instances

Network: vpc-0865229f3d032b76e | citc-net-cluster-exciting-sc Create new VPC
No default VPC found. Create a new default VPC.

Subnet: subnet-0bfb83b7ebb34f21d | citc-subnet-cluster-excit Create new subnet
32762 IP Addresses available

Auto-assign Public IP: Use subnet setting (Disable)

Placement group: □ Add instance to placement group

Capacity Reservation: Open Create new Capacity Reservation

IAM role: None Create new IAM role

Shutdown behavior: Stop

Enable termination protection: □ Protect against accidental termination

Monitoring: □ Enable CloudWatch detailed monitoring
Additional charges apply.

Tenancy: Shared - Run a shared hardware instance
Additional charges will apply for dedicated tenancy

The problem 😕

- What they already know:
  - Their field of research
  - Python/R/GROMACS/Relion
  - `sbatch/qsub`
- We can’t expect researchers to be professional sysadmins
  - The intersection is well handled by Research Software Engineers

The solution ✅

- Give them what they are used to, but in a cloud environment
- They don't have to know the difference
- Except:
  - No queuing
  - Only pay for what they use

Cluster in the Cloud

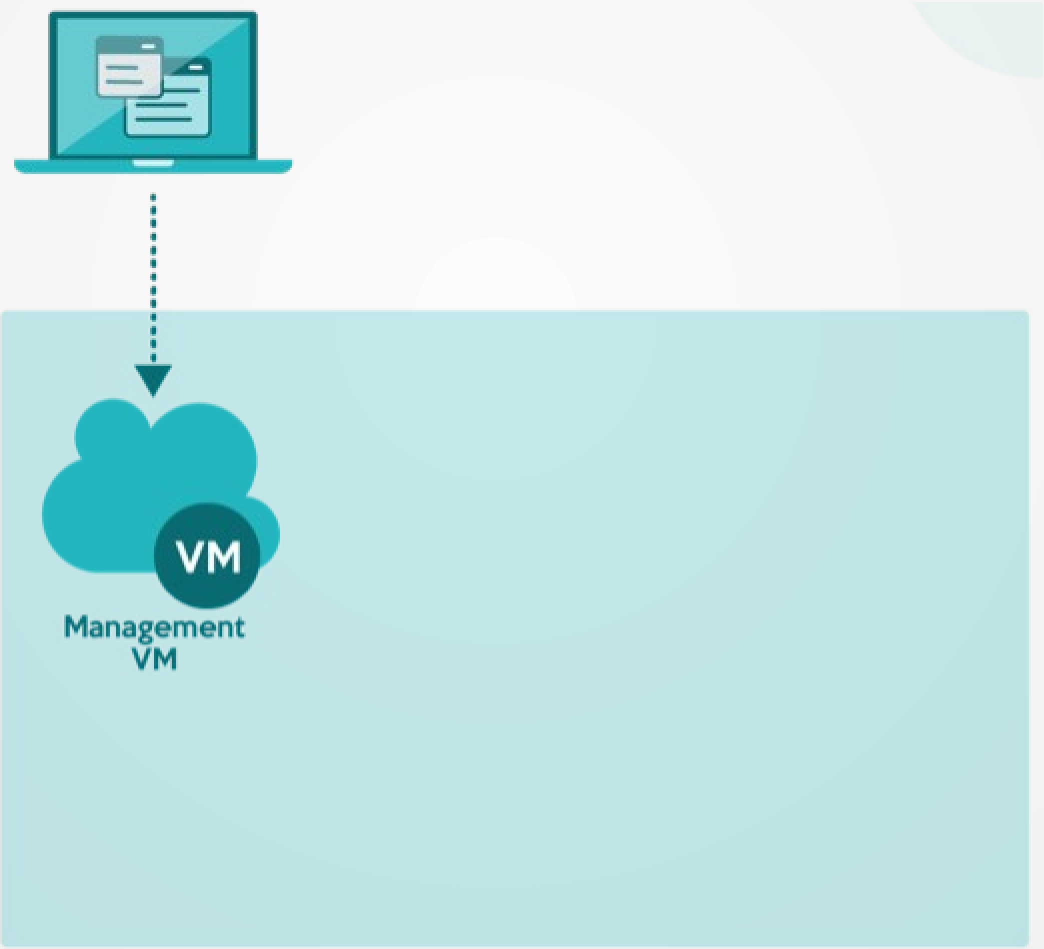
- An automatically-provisioned Slurm cluster
- Uses Terraform to create:
  - Networking
  - Shared file system (Elastic File System)
  - Management/login VM (`t3a.medium`)
- Uses Ansible to configure the management VM and compute image

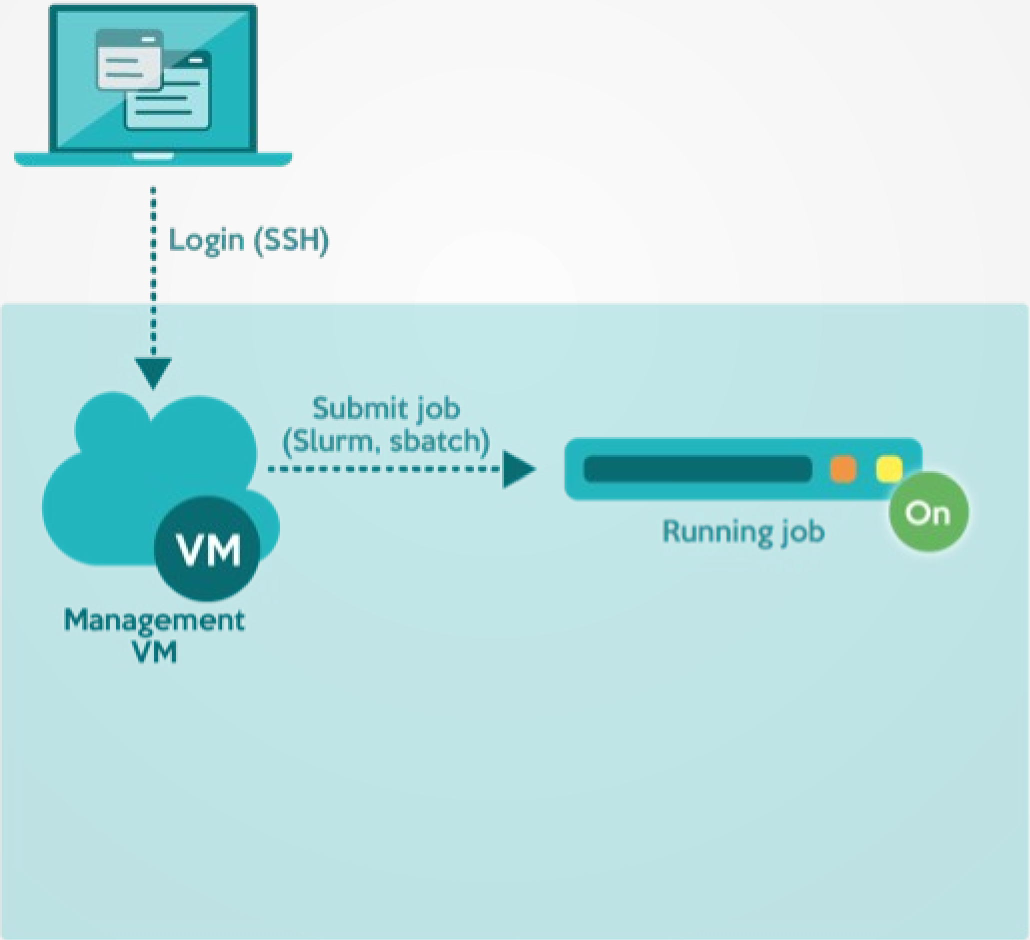
Key Features

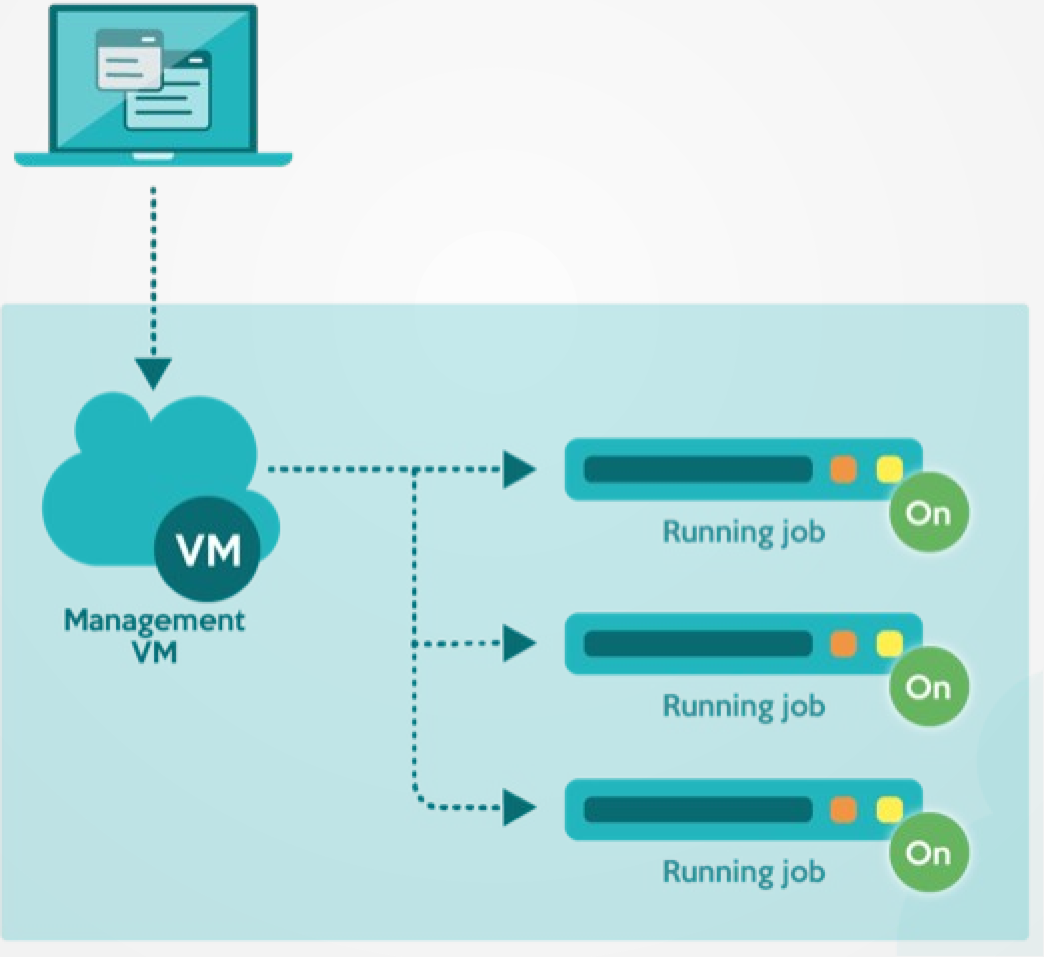
1. **Familiar**: known environment for researchers with Slurm, JupyterHub etc.
2. **Versatile**: Allows any number of any combination of instance types in a cluster
3. **Dynamic**: They are started only when needed
4. **Cheap**: Base cost is just one VM plus storage
5. **Cross-cloud**: Works on AWS, Google Cloud and Oracle

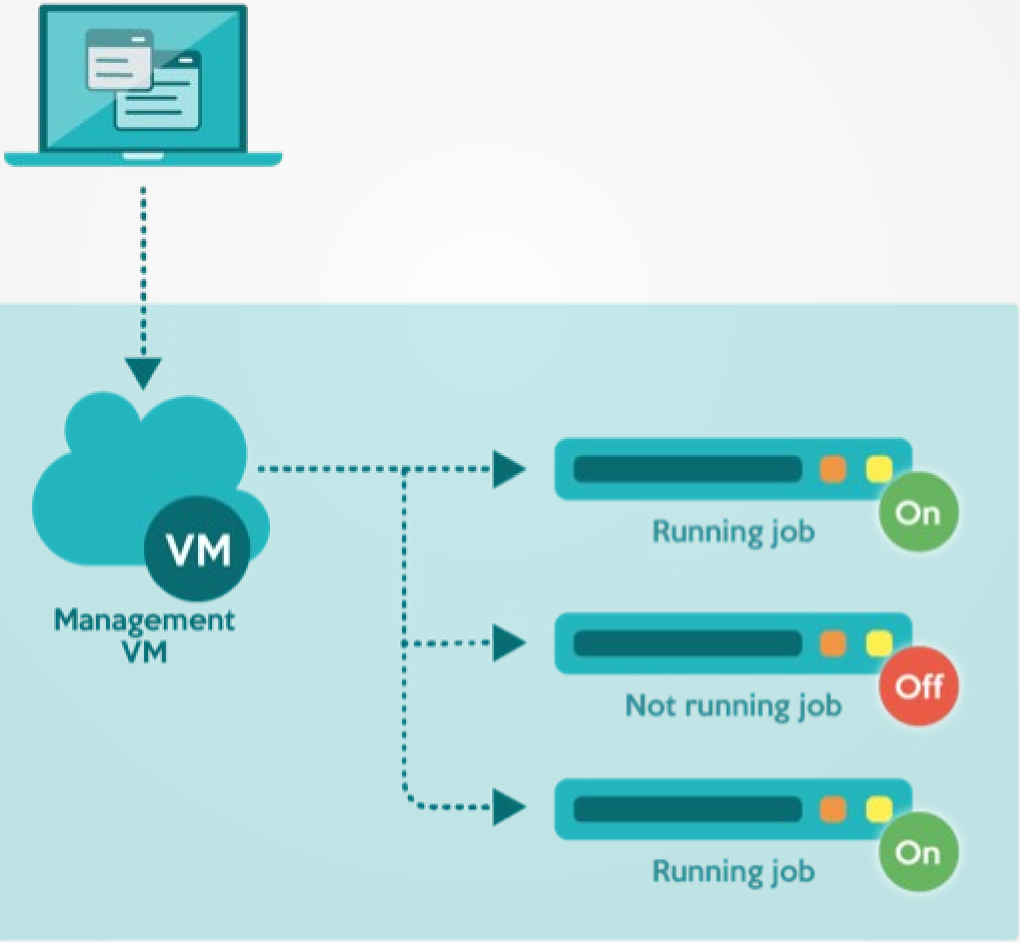
⚡ Slurm power management

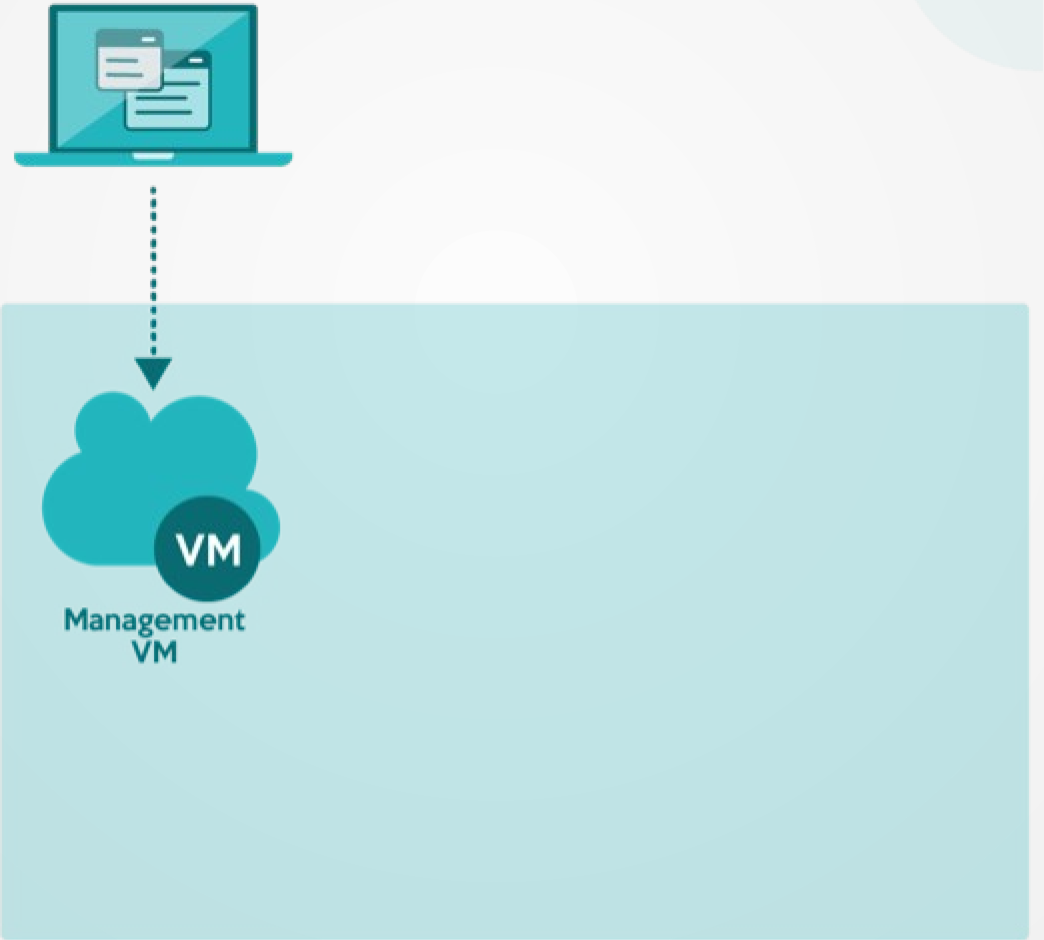
- Python plugin calls the AWS API
- Initial configuration creates any number of *potential* nodes of each desired type:
  - e.g. 1000 32-core, 1000 16-core, 1000 GPU etc.
- On job submission Slurm
  1. Chooses a node type
  2. Creates an instance from an image
  3. Runs the job
  4. Destroys it (after a timeout)


VM
Management VM


Login (SSH)
Submit job
(Slurm, sbatch)
VM
Management
VM
On
Running job

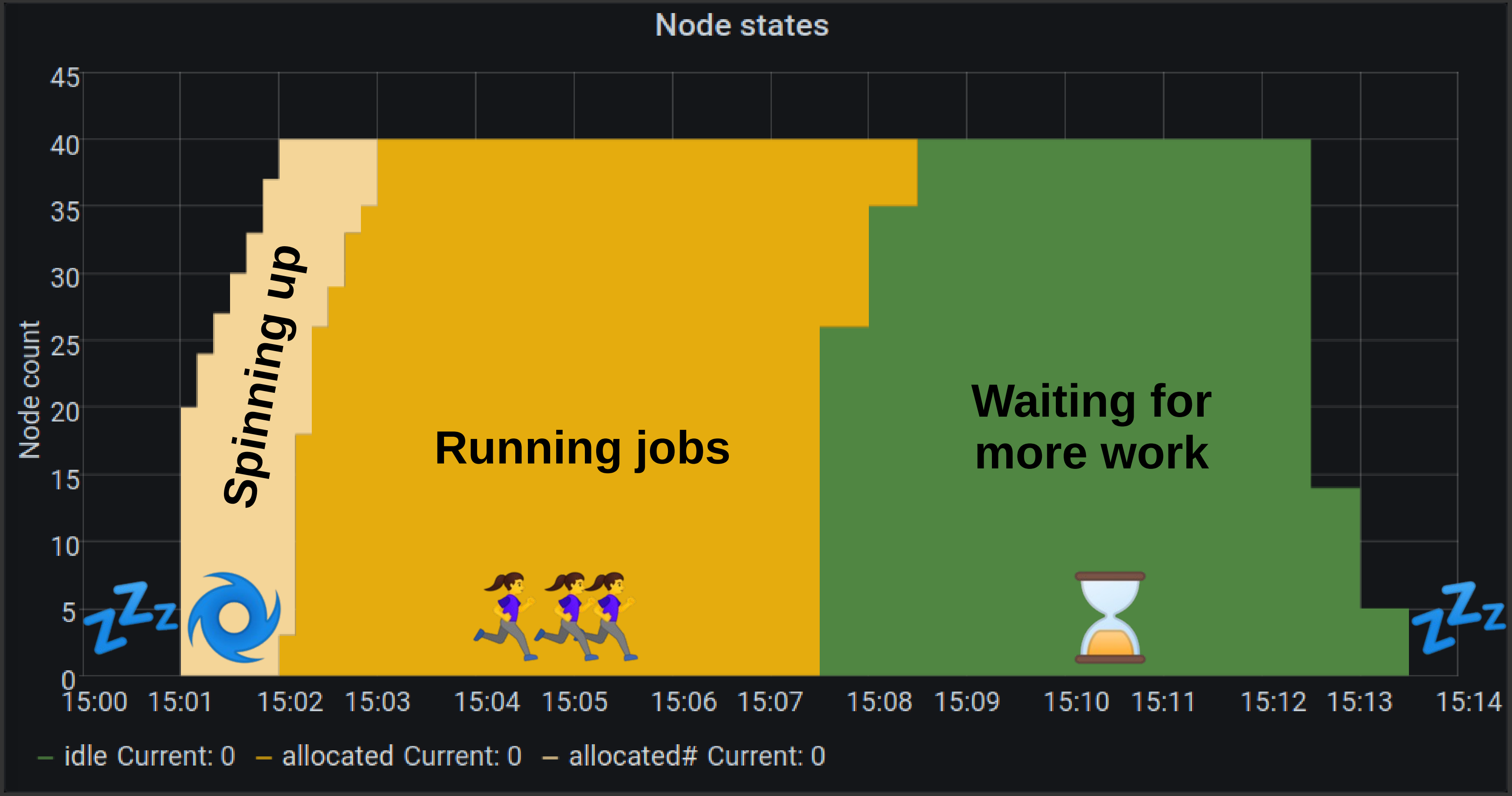

VM
Management VM
On
Running job
On
Running job
On
Running job


VM
Management VM
Running job
On
Not running job
Off
Running job
On


VM
Management VM

Node states

- 40-node array job, 5 minute runtime



Timings ⏱️

- Full system test ~17 minutes on AWS
  1. Create cluster from scratch, including node images
  2. Run test job
  3. Check other system statuses
  4. Tear down whole cluster
- Job submit → job start: 1 minute

Performance characteristics 🏎️

- ✓ Best-suited to heterogeneous high-throughput tasks
  - Pipelines needing different node type for different parts
  - Can be much more specific than the average on-premise cluster
  - Always access to latest hardware, e.g Graviton 2
- ✗ At present is not optimised for multi-node workloads
  - No fast interconnect support
  - Future work will rectify this, e.g. EFA
- ✓ Great for teaching clusters and benchmarking
- ✓ Suitable for Dask, Spark, Singularity

Users

- **Smoking cessation**: A General Mechanism for Signal Propagation in the Nicotinic Acetylcholine Receptor Family
  10.1021/jacs.9b09055
- **Vaccine delivery**: Synthetic self-assembling ADDomer platform for highly efficient vaccination by genetically encoded multiepitope display
  10.1126/sciadv.aaw2853
- **Other projects**:
  - COVID research
  - Molecular dynamics
  - Carbon sequestration
  - Radiotherapy research

Graviton

- CitC supports all Graviton 1 and 2 instance types, including all A1, M6g, C6g , R6g; virtual and BM
- Enable in `limits.yaml` with, e.g.:

```
c6g.4xlarge: 100
r6g.metal: 40
c6g.xlarge: 300
```

- Launch job with:

```
sbatch --constraint="arch=aarch64" job.slm
```

Elastic Fabric Adapter (EFA)

No support yet but is planned

Needs support for CentOS 8

Will automatically attach to supported instance types

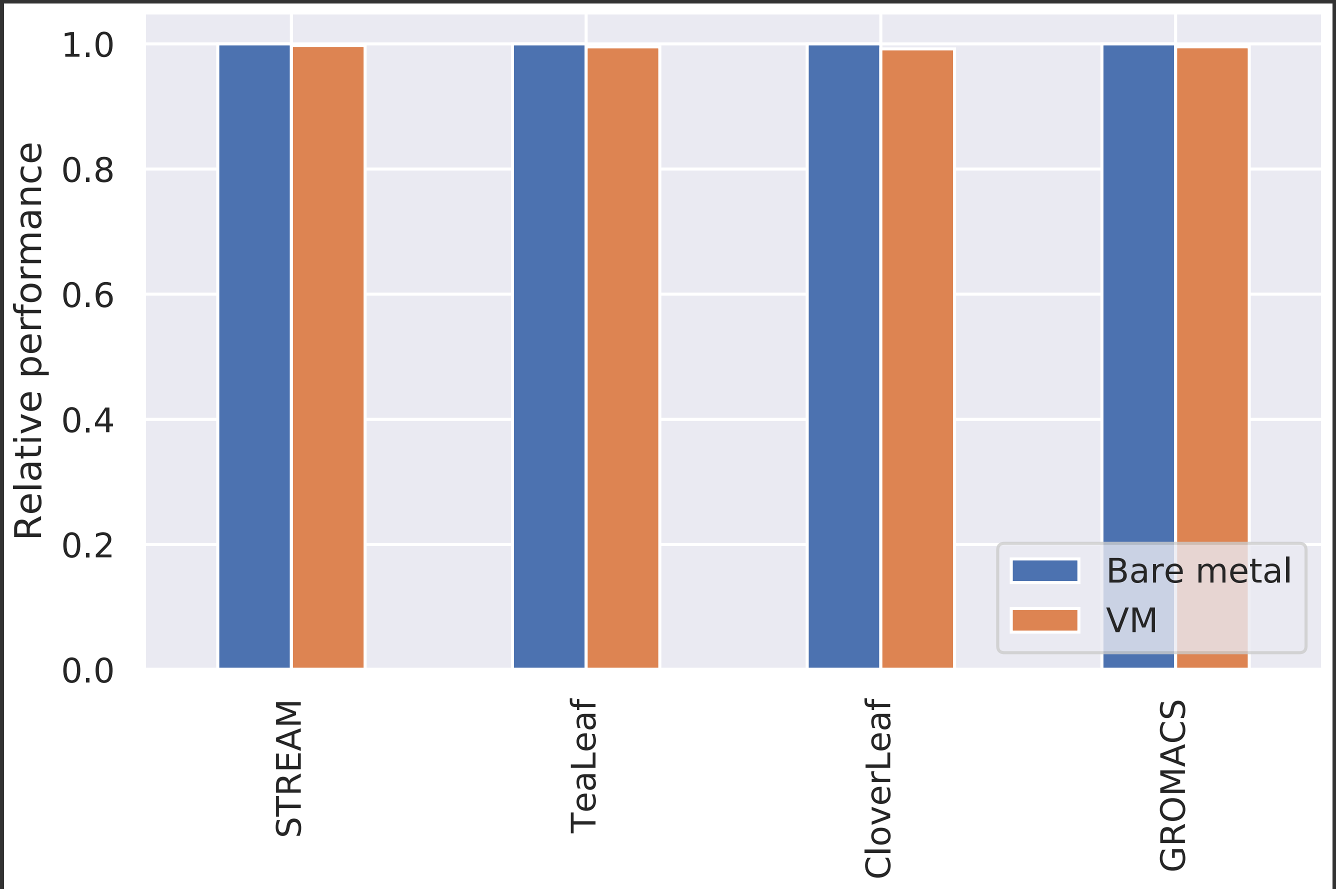
Benchmarks

- Single core Python benchmarks
  - On a C6g, Graviton 2 gets 1.9 times the performance per dollar than Graviton 1
  - Even R6g are 1.3 better value than Graviton 1
- UoB-HPC Benchmarks
  - Repo: https://github.com/UoB-HPC/benchmarks
  - Synthetic: STREAM
  - MiniApps: CloverLeaf, TeaLeaf
  - Full apps: GROMACS, VASP, UM etc.
  - Thanks to Chris Edsall for running these over the weekend!

Bare metal vs VM

Graviton 1 `a1.metal` vs `a1.4xlarge`

Less than 1% performance difference

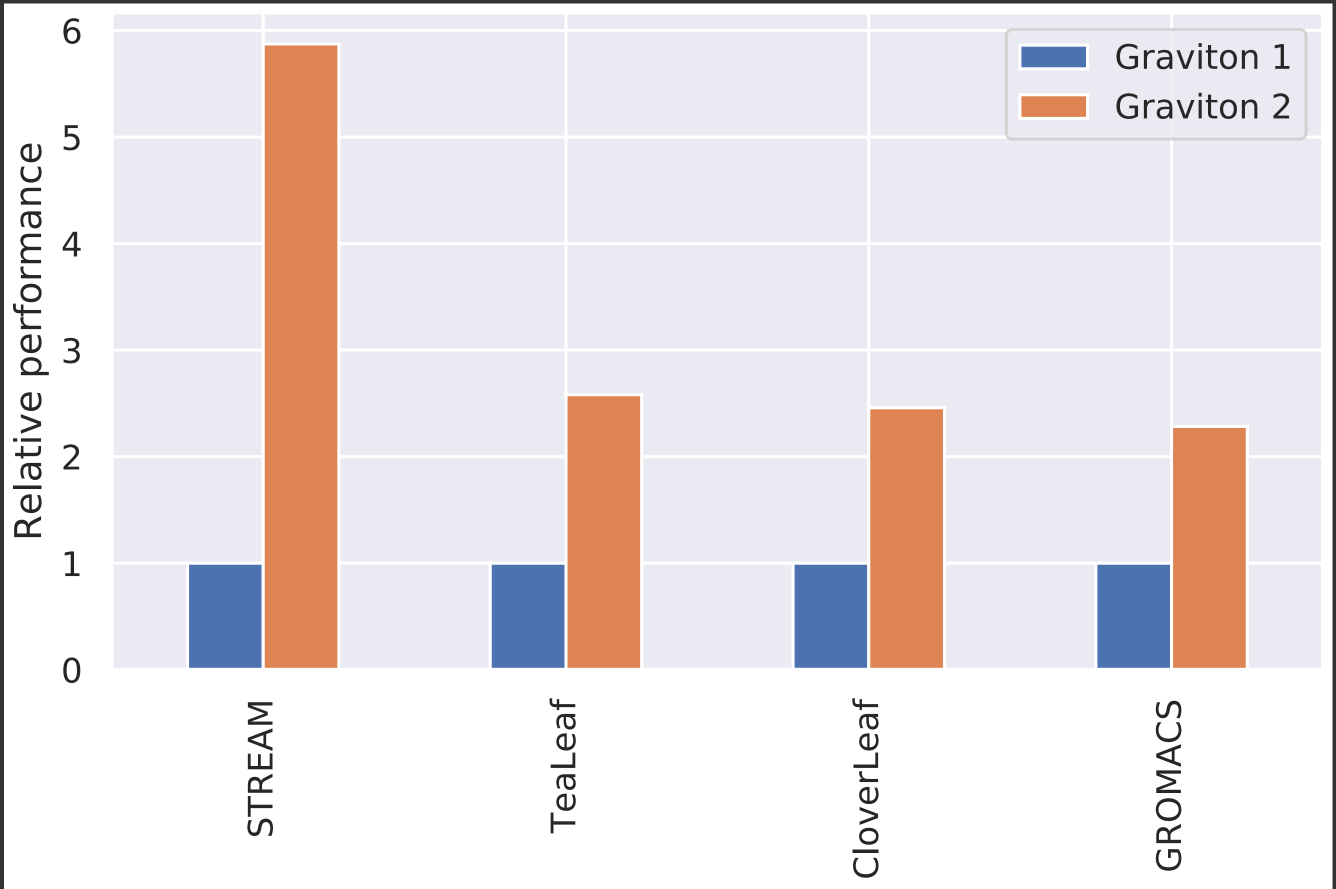


Provisional results, not publication quality!

Graviton 1 vs Graviton 2

Graviton 1 `a1.4xlarge` vs Graviton 2 `c6g.4xlarge`

Up to 6x performance improvement



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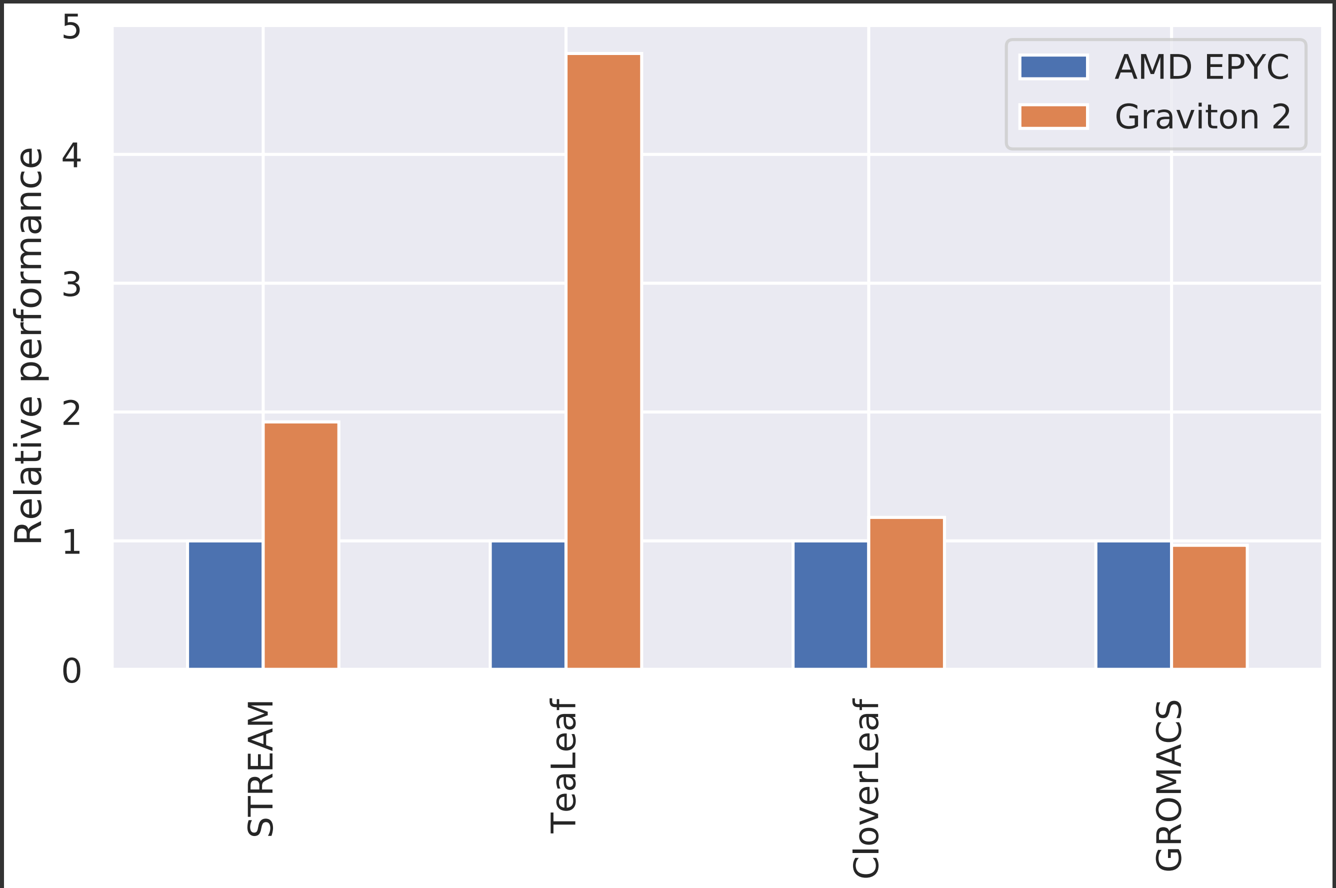
Graviton 2 vs AMD EPYC

AMD EPYC `c5a.16xlarge` vs Graviton 2 `c6g.16xlarge`

Up to 2x performance improvement



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Thank you

Find out more at
cluster-in-the-cloud.readthedocs.io

Thanks to AWS, Google and Oracle for supporting development and to the Bristol RSE team