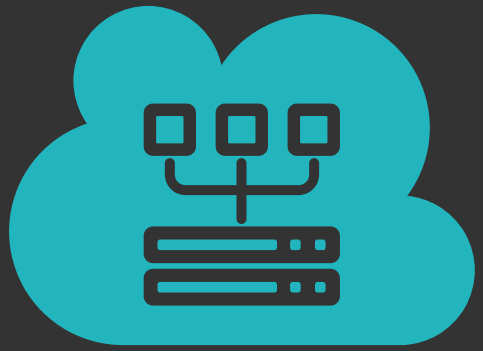
Cluster in the Cloud

Easy, Scalable, Heterogeneous



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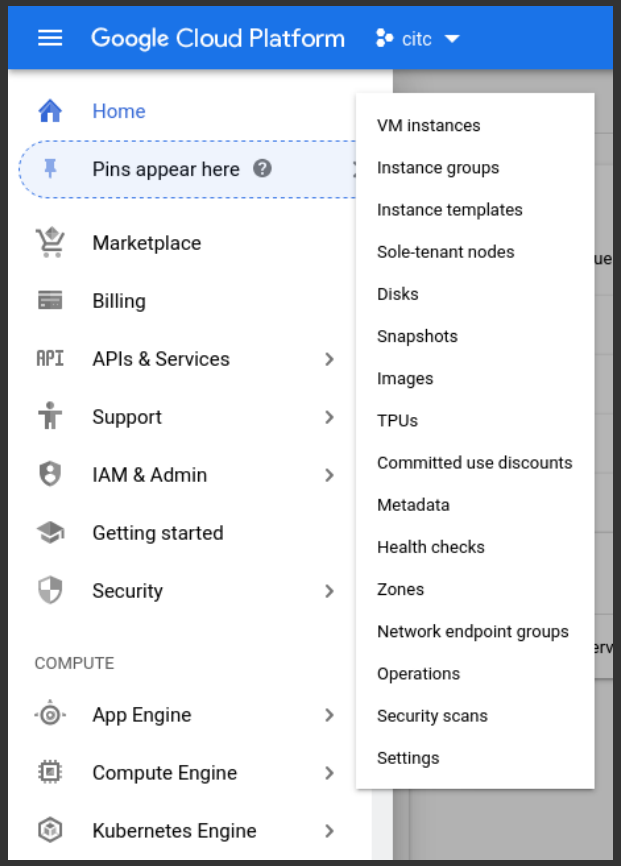
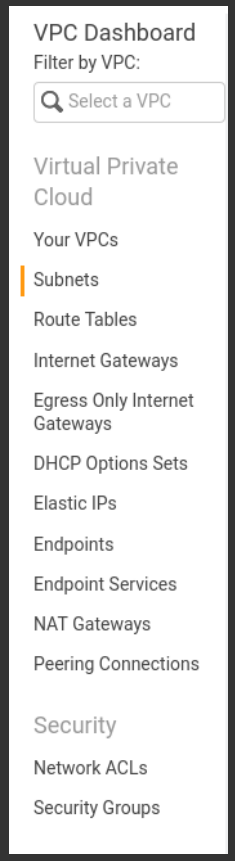
The problem

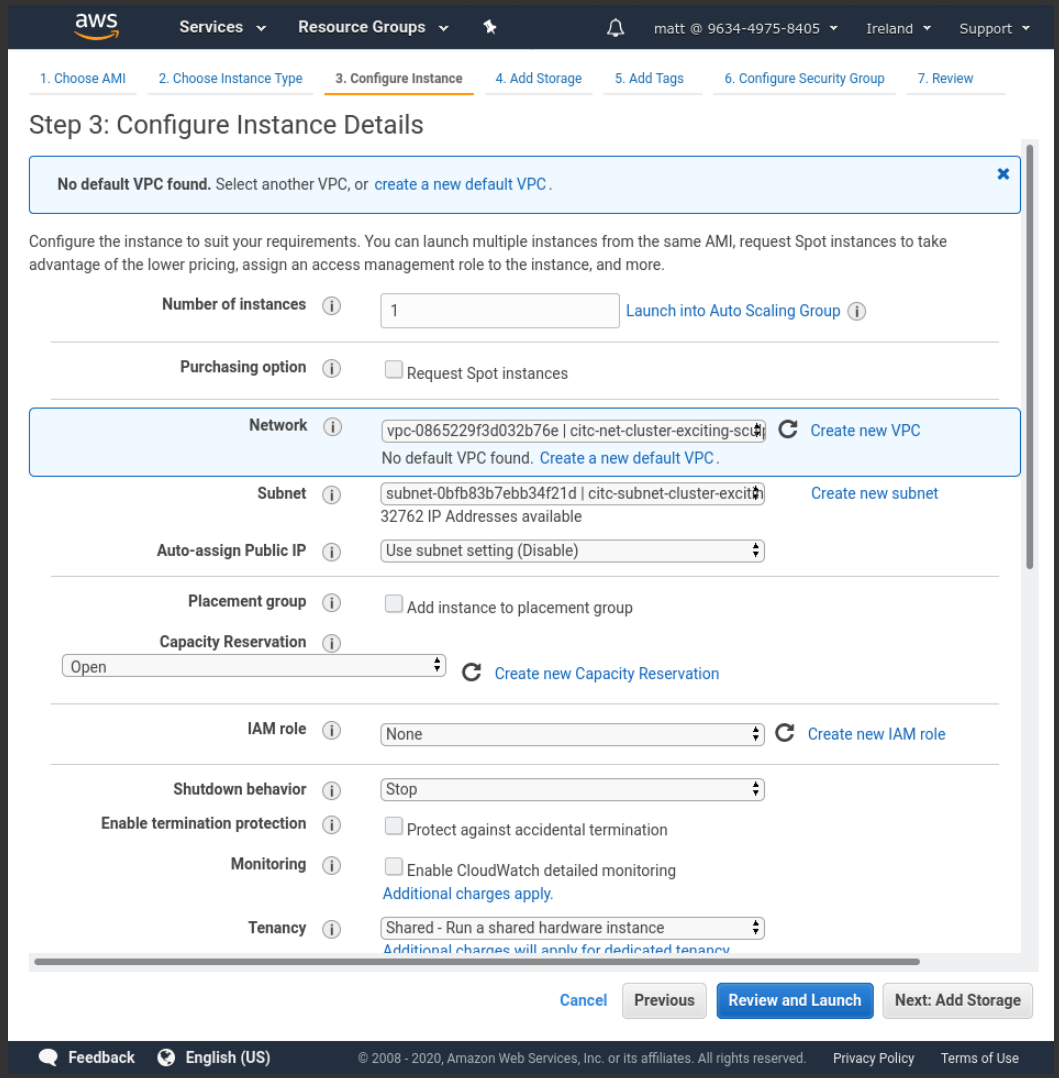
- Researchers having cloud credits

The problem 😕

- Researchers having cloud credits
- Presented with:







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*

Cluster in the Cloud

An automatically-provisioned Slurm cluster

Uses Terraform to create:

- Networking
- Shared file system
- Management/login VM (e.g. `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
6. **Open source**: Under the MIT license and is free to use.

Technical details: Terraform 

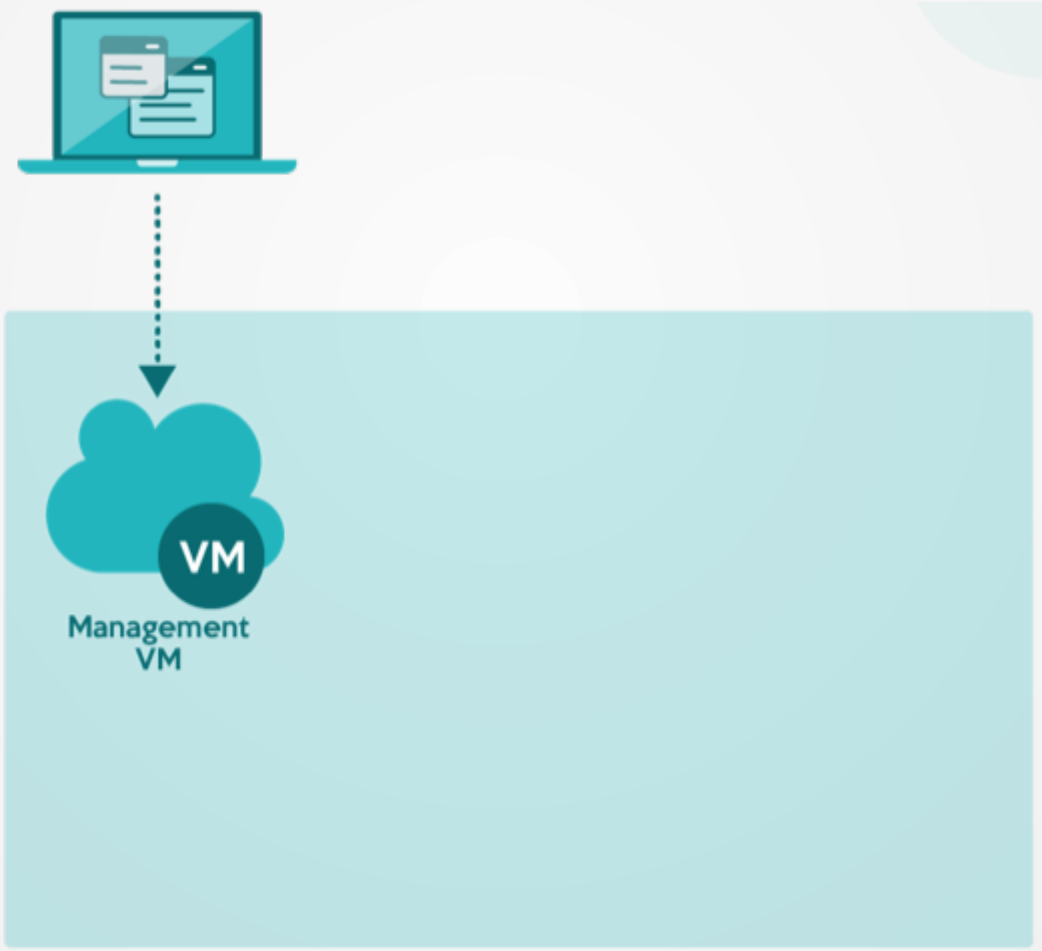
- Terraform is used to create the skeleton
- https://github.com/clusterinthecloud/terraform
  - AWS: ~500 LOC
  - Google: ~400 LOC
  - Oracle: ~450 LOC
- Written from scratch for each platform

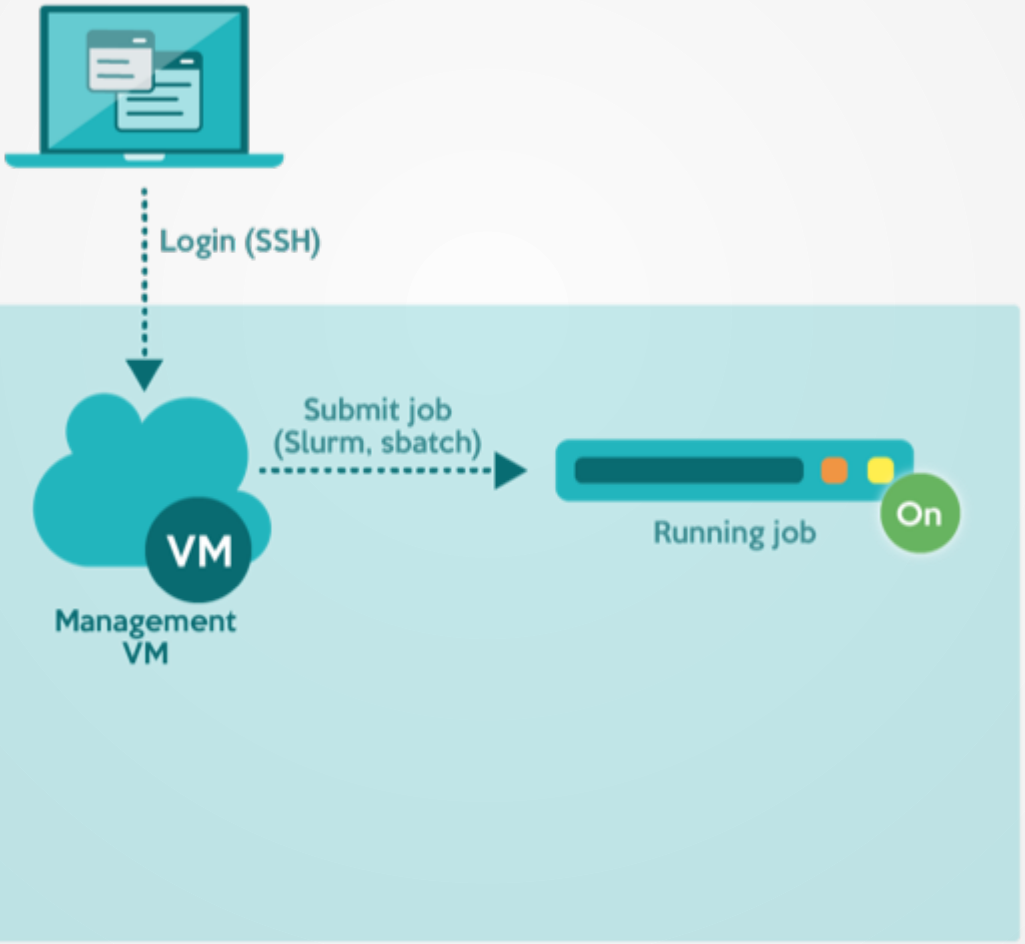
Technical details: Ansible

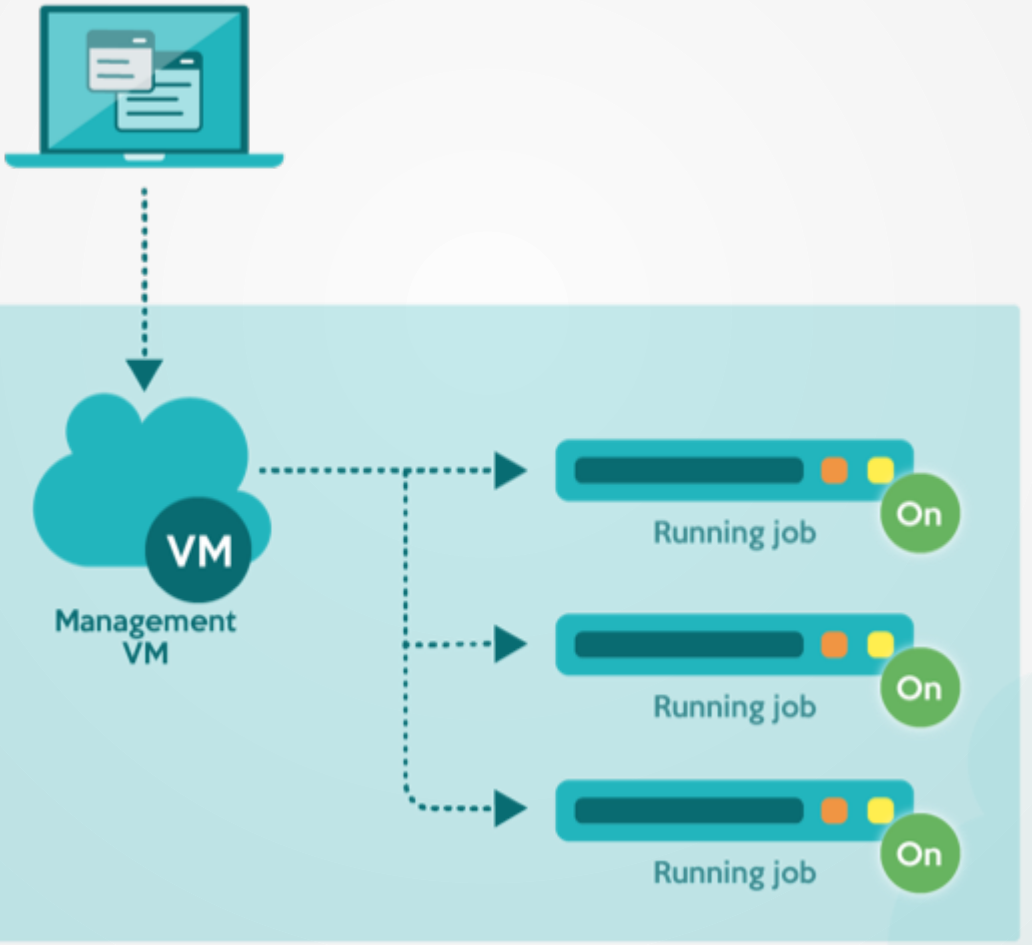
- ~1.5K lines of Ansible
- https://github.com/clusterinthecloud/ansible
- Configures:
  - Mounting shared filesystem
  - LDAP for user management
  - Slurm
    - Including node start/stop scripts
  - Monitoring (Grafana)
  - Base software set
  - And more...
- Covers both the management VM and compute image

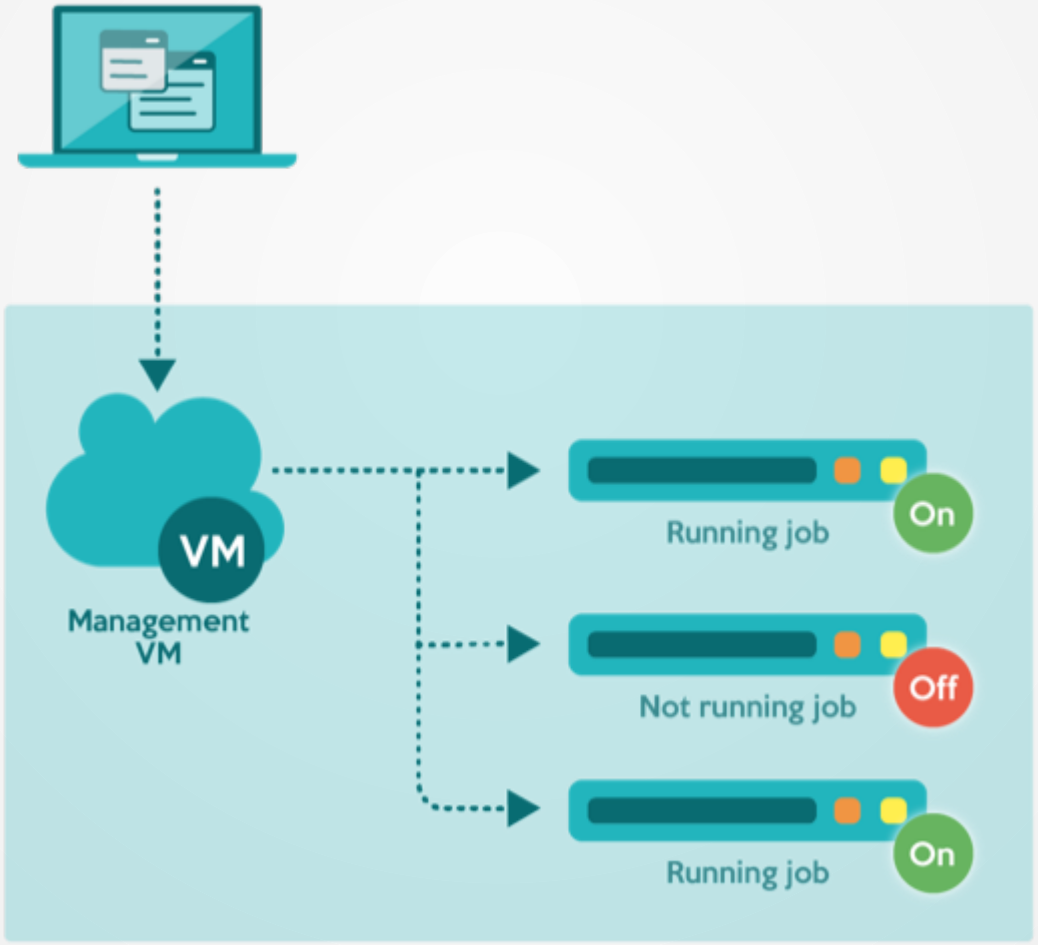
⚡ Scaleable

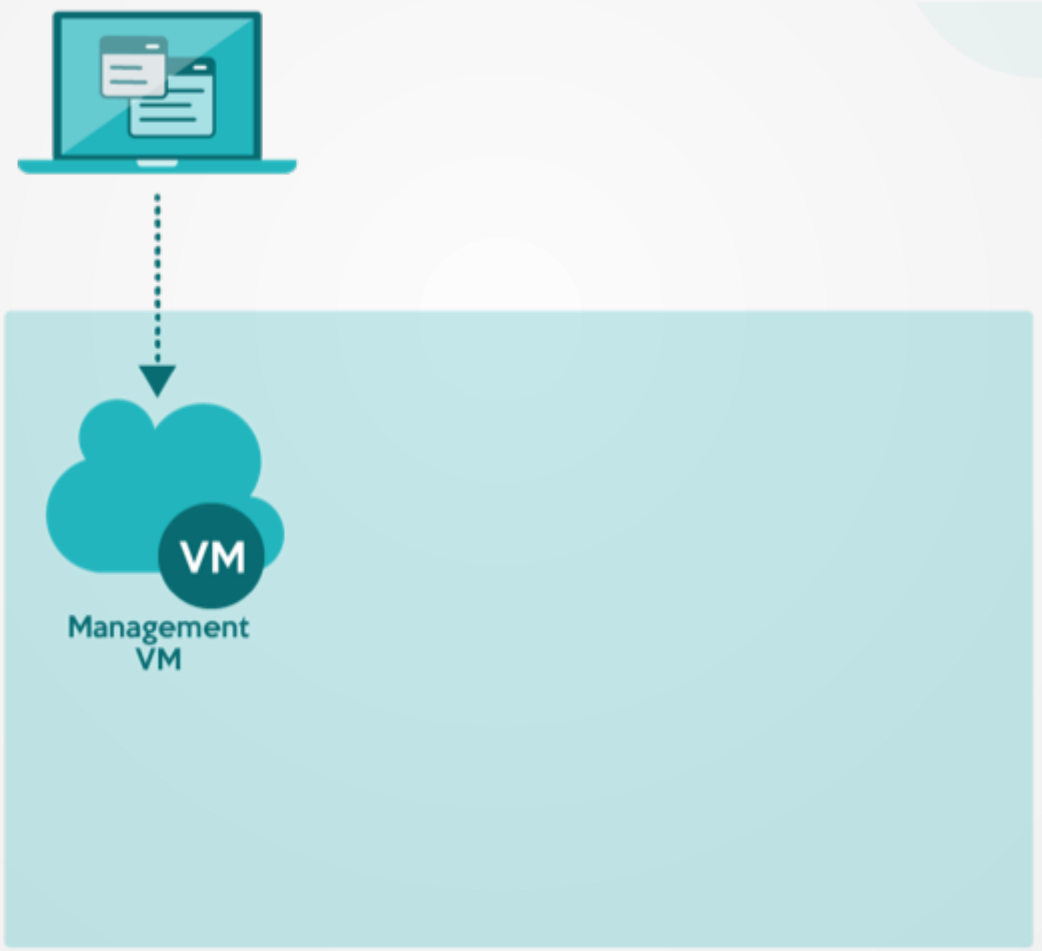
- At initial configuration you create any number of *potential* nodes of each desired type:
  - e.g. 1000 32-core, 1000 16-core, 1000 GPU etc.
- On job submission Slurm
  1. Chooses a node type
  2. Creates an appropriate instance from an image (via a Python script calling the cloud API)
  3. Runs the job
  4. Destroys it (after a timeout)


VM
Management
VM


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

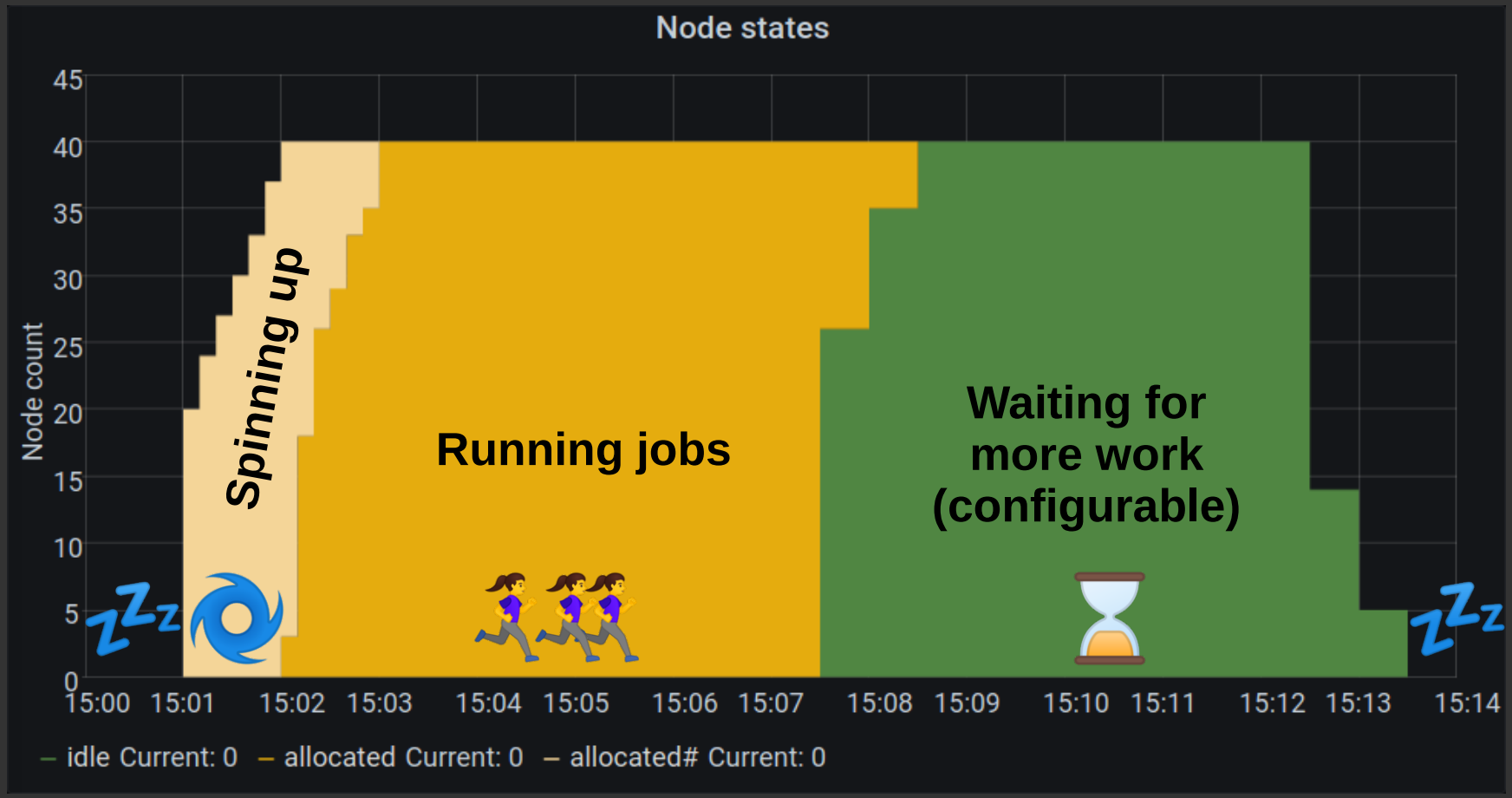

VM
Management
VM
Running job
On
Running job
On
Running job
On


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


VM
Management
VM

Node states

- Example 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 (work underway)
  - Only cheap shared storage
- ✔ 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
- **COVID-19**: Free fatty acid binding pocket in the locked structure of SARS-CoV-2 spike protein 10.1126/science.abd3255
- **Molecular dynamics**: Molecular Simulations suggest Vitamins, Retinoids and Steroids as Ligands binding the Free Fatty Acid Pocket of SARS-CoV-2 Spike Protein (under review)
- **Other projects**:
  - Carbon sequestration
  - Radiotherapy research

Future plans

- Improved web UI for managing users, node types, apps, benchmarking results etc.
- High-performance networking
- Pluggable storage solutions
- Easy backups to cloud storage
- Support for other clouds (Azure, OpenStack)

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