The DC Spears

Cloud infrastructure deployment using IBM and DigitalOcean

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NICIS CHPC STUDENT CLUSTER COMPETITION

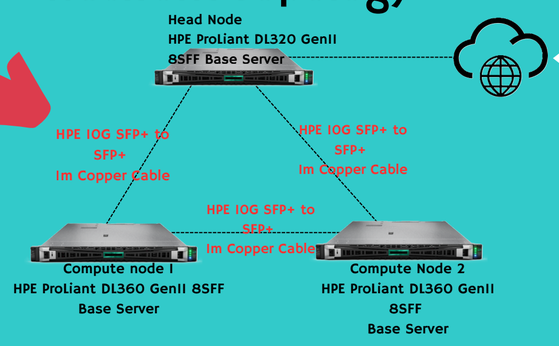
The Team

1. Introduction

The SCC required teams to design a multi-node HPC cluster, selecting appropriate CPUs, RAM, power budgets, and other server components from a provided range of HPE hardware.

The DC Spears worked on a cloud-deployment project using IBM Cloud and DigitalOcean, focusing on automating instance creation, configuration, and management through Terraform, Ansible, and CI/CD pipelines

Network Topology



2. Cluster design

- Rocky Linux based
- Intel Xeon CPUs
- 32 core head node & compute nodes
- 800W power supply
- 2.4TB head node storage +300GB compute nodes storage

3. Software Tools

- Terraform—Infrastructure as Code
- Ansible - Configuration Management
- GitHub Actions & CircleCI
- MobaXTerm - SSH access

4. Process flow

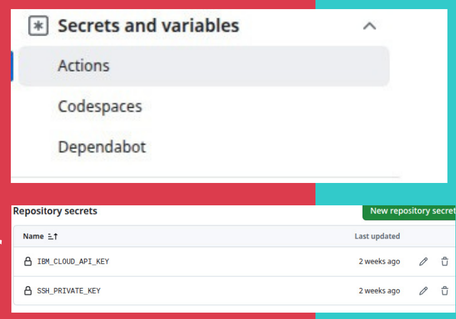
1. Created VM instances (Head & com nodes)
2. Configured networking and SSH
3. automated deployement with teraform
4. Linked pipelines with github actions
5. Tested NFS and user setup & intergrations

5. CI/CD Pipelines

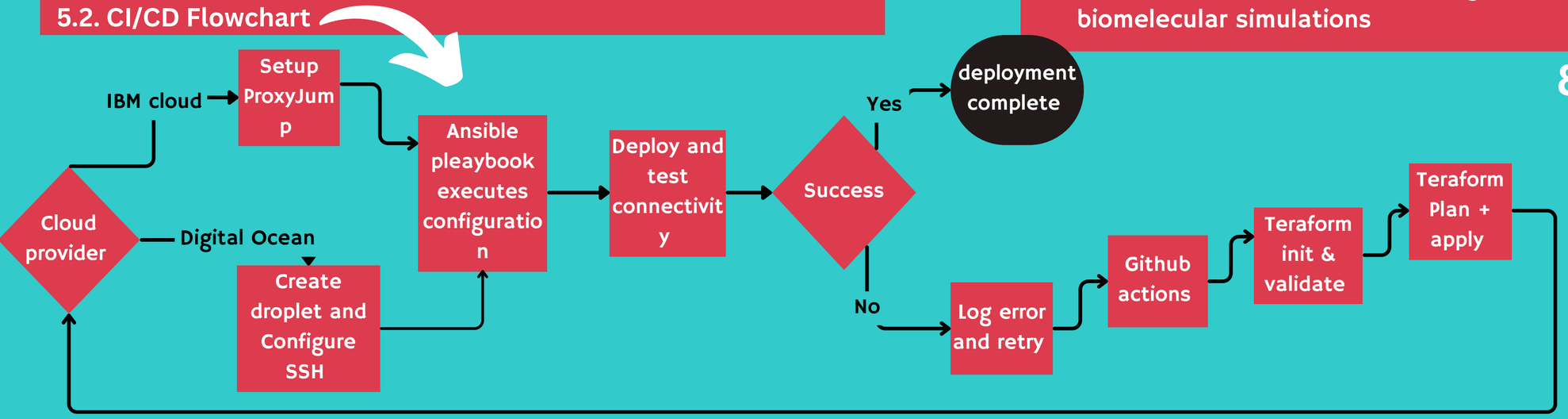
We automated the deployment and configuration of the HPC cluster using github Actions and ansible.

5.2. GitHub repository Setup

- separate GitHub repos for IBM cloud and DigitalOcean
- Repository secrets and private keys for cluster access added in Github secrets



5.2. CI/CD Flowchart



6. Cluster considerations

- Runs AmberMD, ASCOT5, DFTB+ & Mathworks applications
- Multicore CPUs per node (32cores) for parallel execution (Matlab) and matrix operations for quantum simulations
- Fast interconnects for MPI scaling for fusion orbit simulations
- 300GB RAM per com node for large biomelecular simulations

7. Findings

- The automated deployment pipeline cut setup from hours to just minutes.
- Tasks like VM creation, node configuration and NFS setup, once manual and time-consuming, are now completed with a few clicks.
- see our Github Repo for more

8. Challenges

Navigating complex hardware choices and optimizing benchmarks was daunting for a group with limited prior experience. We combined our strength, learned rapidly and managed to push through.