



NUS Information Technology

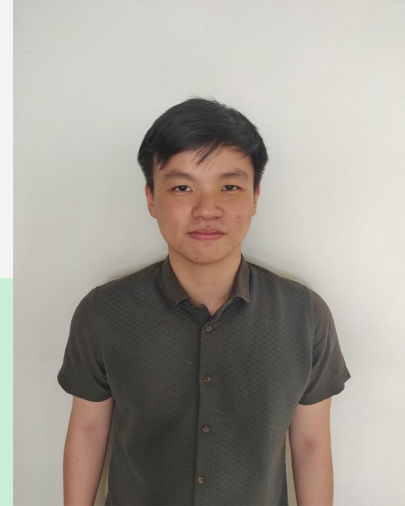
Research Computing Cloud
Development Internship

Yin YiRan
Ivan Andika Lie

Interns



Yin YiRan
Year 3 Information System
HPC Login Portal



Ivan Andika Lie
Year 2 Computer Engineering
Green Provisioning

HPC Login Portal

01

For users to register and check
their account status

02

For administrators to manage
HPC accounts, software
available, announcements

Project Overview

User interface

Improve the interface
of HPC login portal

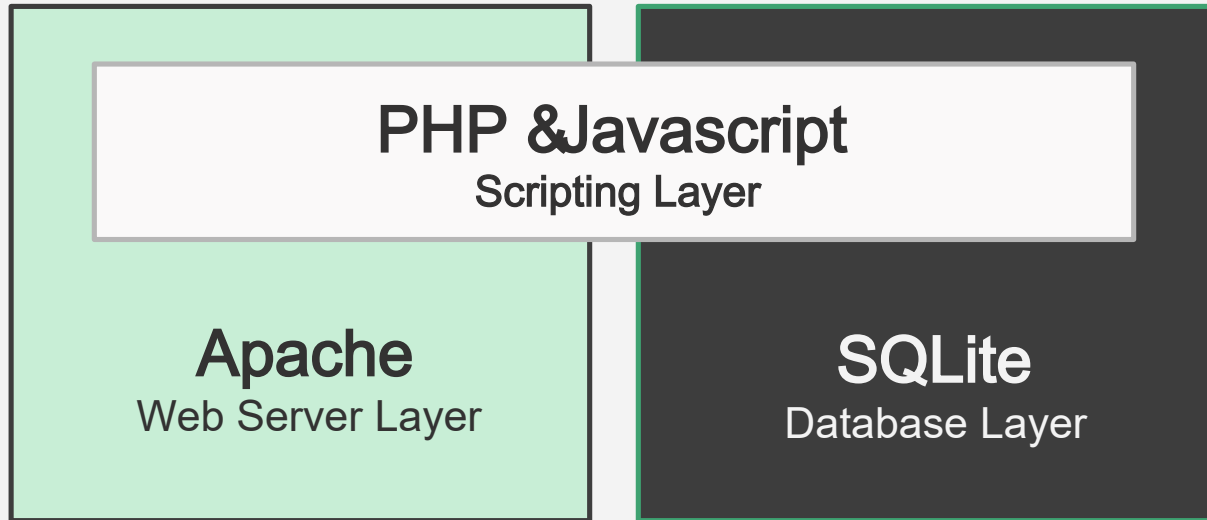
Security

Reduce portal's
vulnerabilities

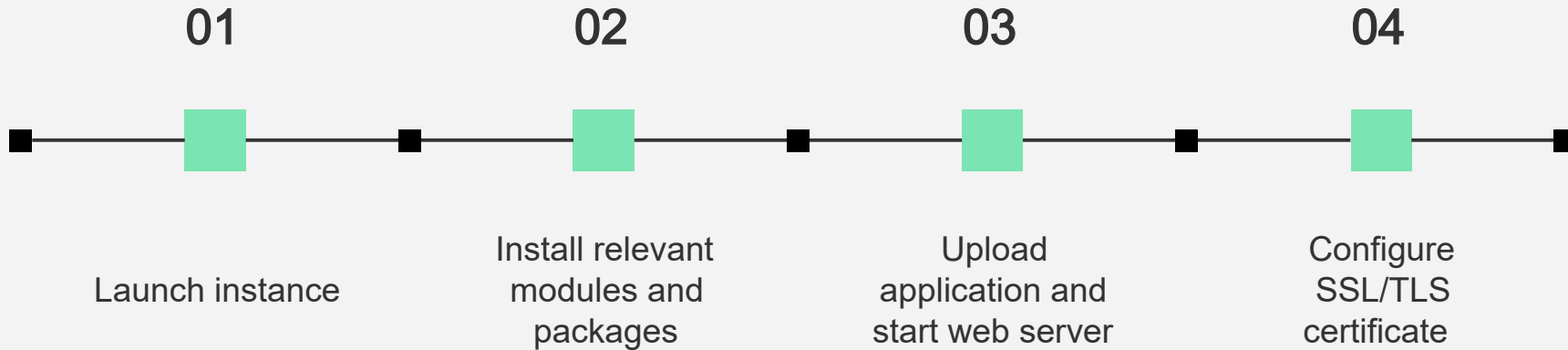
Deploy to cloud

From on-premise to
AWS cloud

Technology stack



Cloud deployment



Login page

- New announcement section
- Cleaner view

Register for HPC Services

Username	<input type="text" value="e02014"/>
Password	<input type="password" value="....."/>
Domain	<input type="text" value="NUSSTF"/>
<input type="button" value="Submit"/>	

Existing users, please skip.

Register for HPC Services

<input type="text" value="Username"/>
<input type="text" value="Password"/>
<input type="text" value="Domain"/>
<input type="button" value="Submit"/>

Useful Information/Announcement

HPC resources are open to all NUS staff and students who have a valid NUSNET id with the need to access high-performance computing resources.

Go to <https://nusit.nus.edu.sg/services/getting-started/registration-guide/> to read the procedure and start registration.
After registration, wait for about 1 hour, you will be able to use the userid and password to access all HPC resources. The NUSNET password is valid throughout all the hosts. As the access control and authentication of all HPC servers are through NUSNET account, change of NUSNET password will automatically take effect on all HPC servers. You are using your NUSNET account to access HPC services. You can change your password at exchange.nus.edu.sg.

Welcome page

Welcome e0201401! [[logout](#)]

Access to HPC Services

Access interactive & visual terminal, visualization, code compilation, batch job submission and other computation

Run biology-related applications

Name
Yin Yiran

Username
e0201401

Position
Undergraduate

Department
Information Systems

logout

Access to HPC Services

Access interactive & visual terminals - for modelling, visualization, code compilation, batch job submission and other computation

[HPC](#)
[Portal](#)

Project title/Course name*:
Research Computing Cloud Developments

Supervisor/Course instructor name*:
Yeo Eng Hee

Software used:

Reason for using HPC resources at SVU/Computer Centre*:
Student Internship for Research Computing Cloud Developments

Research objective*:
Research Computing Cloud Developments Internship

Update

- New profile, HPC account information section
- Option to edit HPC account details

Registration page

- Added more validation
- Word limit
- Special characters
- Sectioned the form to minimise scrolling

Register for HPC Services

Personal Information

Username*:
Domain*:
Name*:
Position*:
Department*:

Project Details

Project title/Course name*:
Supervisor/Course instructor name*:
NUS Internal collaborator name :
Internal collaborator position :
Internal collaborator department :
Industry partner name:
Industry partner

Register for HPC Services

Project Details

Project title/Course name*:

Research Computing Cloud Developments

Supervisor/Course instructor name*:

Please fill in this field

NUS Internal collaborator name :

\$

Please do not use special characters like \$, !, /, \.

Internal collaborator position :

Internal collaborator department :

Previous

Next



Admin page

- New announcement tab to edit or add announcements
- Menu bar for easier navigation
- Made buttons more visible

Welcome ! [\[logout\]](#) [\[open in new window\]](#)

Menu: [\[needs approval\]](#) [\[approved\]](#) [\[archived\]](#) [\[edit software\]](#) [\[edit departments\]](#)

Show entries

Username	Name	Position	Department	Project Title	Supervisor	Industry Contact	Industry Company	Software	Reason	Objective
a0088655	Dhruv Kumar Jaura	Undergraduate	Mechanical & Production Engineering	ME3101	Seeram Ramakrishna	Prof. Ramakrishna	Prof. Ramakrishna	Prof. Ramakrishna	Our Mechanical Engineering design project requires us to do	To model a water intake system at a sea basin and

a0097410	Tan Teck Wei	Undergraduate	Mechanical & Production Engineering	Me3101	Stanley
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a0102889	Wang Ting	Staff	Statistics & Applied Probability	Time Series Modeling of Individualized Heat Strain	Chen Ying
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chmv159	Shao Jiawei	Staff	Chemistry	Azuluene based PAH	CHI
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chmv310	Wu Qiong	Visiting Staff	Chemistry	Computational study of the mechanism of metal corrosion	Wonil Wah
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chmv347	Nan Zhihan	Visiting Student	Chemistry	Computational Chemistry	Wonil Wah
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HPC Accounts Software Department Announcement

Welcome !

Log out

Pending Approval Approved Archived

Search: Show entries

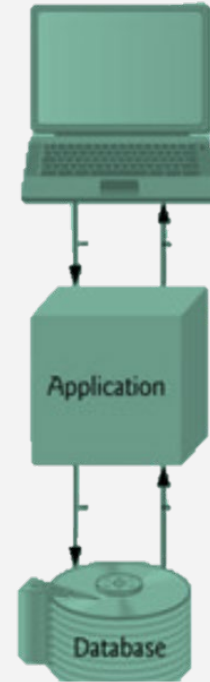
Approval	Username	Name	Position	Department	Project Title	Supervisor
<button>APPROVE</button>	a0102889	Wang Ting	Staff	Statistics & Applied Probability	Time Series Modeling of Individualized Heat Strain	Chen Ying
<button>APPROVE</button>	a0097410	Tan Teck Wei	Undergraduate	Mechanical & Production Engineering	Me3101	Stanley
<button>APPROVE</button>	a0088655	Dhruv Kumar Jaura	Undergraduate	Mechanical & Production Engineering	ME3101	Seeram Ramakrishna
<button>APPROVE</button>	intern01-5	Shreyas Rajesh, INTERN01-5	Visiting Student	Division of Bioengineering	blood flow in avian embryonic heart with 4D ultrasound model	Dr Yap Choon Hwai
<button>APPROVE</button>	intern01-4	Daniel Anojan Atputharuban, INTERN01-4	Visiting Student	Division of Bioengineering	Ultrasound needle tracking	Dr.Hongliang REN
<button>APPROVE</button>	matv94	Yi Wenfan	Visiting Staff	Mathematics	Numerical methods for highly oscillatory PDEs	Zhenning Cai
<button>APPROVE</button>	mpev415	Song Fenhong	Staff	Mechanical & Production Engineering	Cold thermal energy storage	Lee Poh Seng
<button>APPROVE</button>	chmv159	Shao Jiawei	Staff	Chemistry	Azuluene based PAH	CHI Chunyan
<button>APPROVE</button>	smrvyh	Wong Yit Han	Staff	Singapore-MIT Alliance	Future Urban Mobility	Kakali Basak
<button>APPROVE</button>	nniv120	Tara Prasad Mishra	Visiting Student	Materials Science & Engineering	Three Dimensional Reconstruction from SingleProjection EM image	Prof. Stephen John Pennycook

Showing 1 to 10 of 19 entries

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Improvements



Lessons Learnt

01

AWS Cloud

02

Basic Linux system
administration

03

Apache server and PHP
Programming



**Thank
you!**



Green Provisioning in NUS HPC Cloud Environment

NUS Information Technology

Ivan Andika Lie

Objectives

1. Optimize the use of the cloud resources and to minimize costs
2. Customize the automatic scaling of cloud resources to our requirements
3. Help provision cloud resources to NUS departments, when required

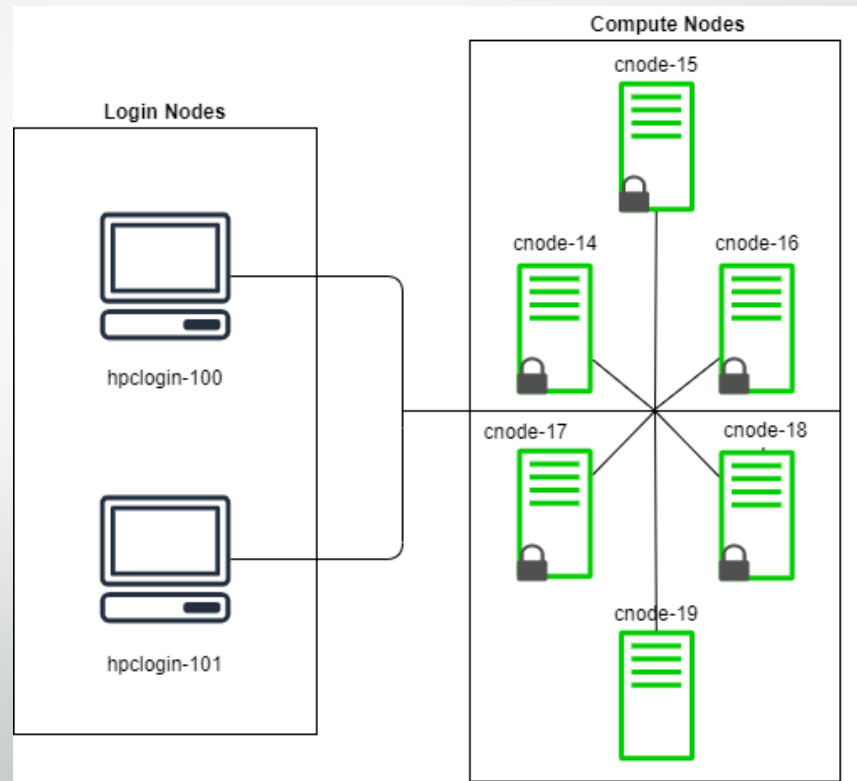
NUS HPC Cloud Environment

- Uses PBS (Portable Batch System) Pro
- Distributed workload management system which manages and monitors the computation workload on a set of one or more computers
- Hosted on Amazon Web Services (AWS) – Cloud Provider
- Uses EC2 (Elastic Compute Cloud) in an isolated Virtual Private Cloud (VPC) for security



Initial HPC Complex

- 2 Login Nodes (Scheduler and Server)
- 6 Static Compute Nodes (MoM)
 - Powered on all the time

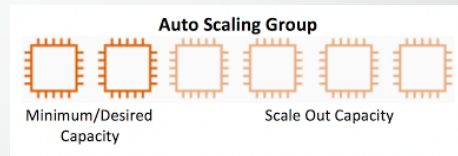


Project Outline – Green Provisioning

- Making use of PBS Pro Green Provisioning Package to achieve the following:
 - Reduce costs by intelligently scheduling power management based on predicted and actual utilization
 - Provide the ability to schedule jobs to minimize the use of compute nodes, and provides a shut-down service when computing resources are not in use
- To customize this package for the HPC cloud environment

Comparison with Alternative Solutions

- EC2 Auto Scaling
 - AWS native tool to automatically scale the compute nodes
 - Incompatible with PBS Scheduler resource management
 - Doesn't scale based on the HPC workload in the job scheduler
- PBS Pro Proprietary Solution
 - Commercial solution by PBS Pro
 - Not available in our PBS license package – additional cost required
- Green Provisioning is the free customizable package offered by PBS Pro to meet our needs



Project Timeline

Familiarisation

- PBS Pro and AWS Services

Development and Testing

- Green Provisioning in Test Environment: 1 login node and 6 test compute nodes (3 static, 3 dynamic)

Deployment to the PBS Production Complex

- 4 Statics Compute Nodes, 8 Dynamic Compute Nodes

Provisioning Cloud Resources to NUS Departments

- Assist the Data Analytics Consultancy Centre under the Department of Statistics and Applied Probability to have their own **dedicated** and **secure** AWS Cloud Environment to create instances tailored to run Deep Learning Tasks
- Prepare presentations and troubleshoot any problems encountered by the users
- Ensure smooth transitions and handover of the cloud environment to their administrators

Lesson Learnt

- Cloud SysOps Administration Skills
 - Understand the AWS Cloud Environment
 - Able to make cost and benefit consideration about a service
 - Good AWS Practices
- Practical Unix/Linux system administration
 - System admins knowledge
 - Write Linux service, scripts, general OS, and networking knowledge
- HPC job management and optimisation in Cloud Environment
- Web portal and web services development in the Cloud

Challenges Faced and Innovation Opportunities

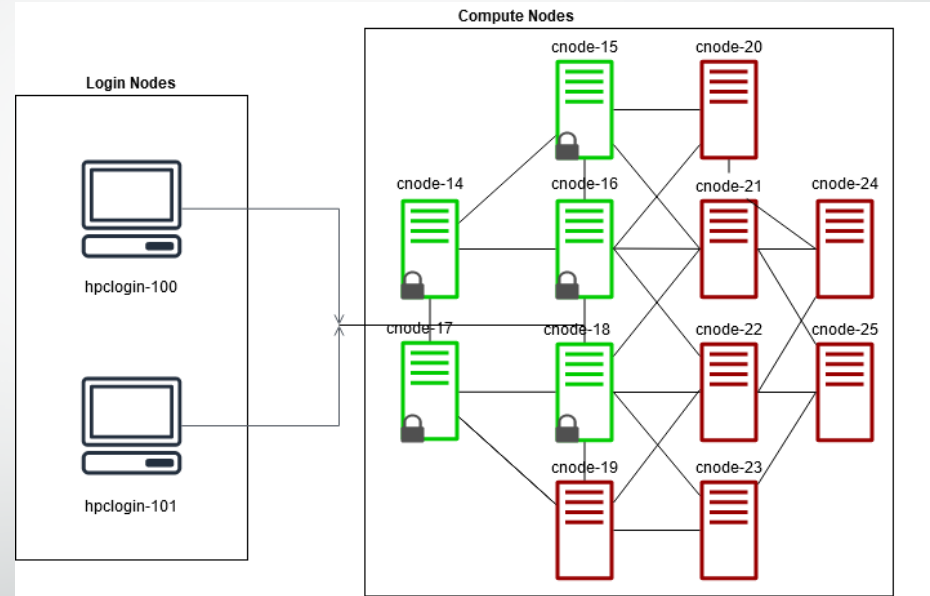
- Green Provisioning Package lacks Documentation
 - Have to dive into the implementation (codes and logs)
- Green Provisioning Package are not updated extensively by Altair
 - Have some bugs which need to be squashed
 - Need to write scripts tailored to suit our needs
- Green Provisioning Package are designed for on-premise use
 - Need to write scripts that uses AWS Cloud SDK to boot nodes, shutdown nodes, and get the status of the nodes.

A decorative graphic in the top-left corner consisting of two parallel lines, one blue and one black, forming an L-shape.

Demo

Upgraded HPC Complex

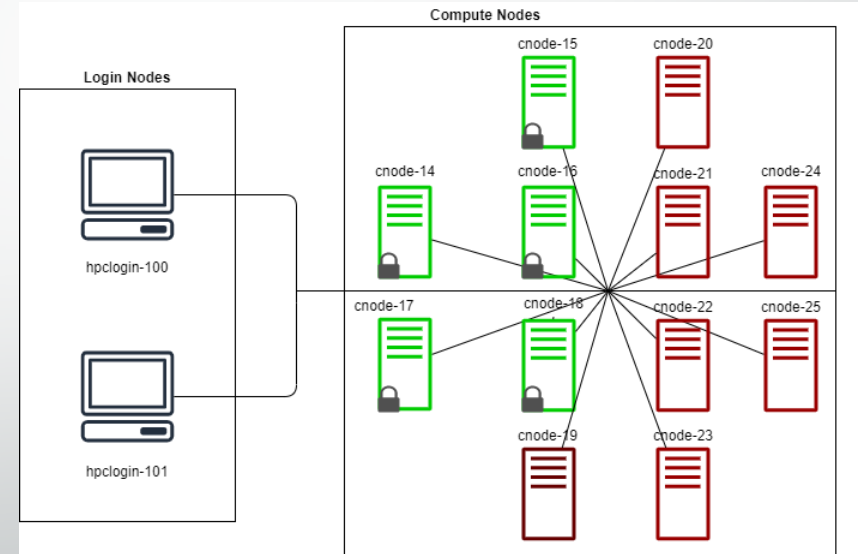
- 2 Login Nodes (Scheduler and Server)
- 5 **Static** Compute Nodes
 - Powered on all the time
- 6 **Dynamic** Compute Nodes
 - Only powered on when needed



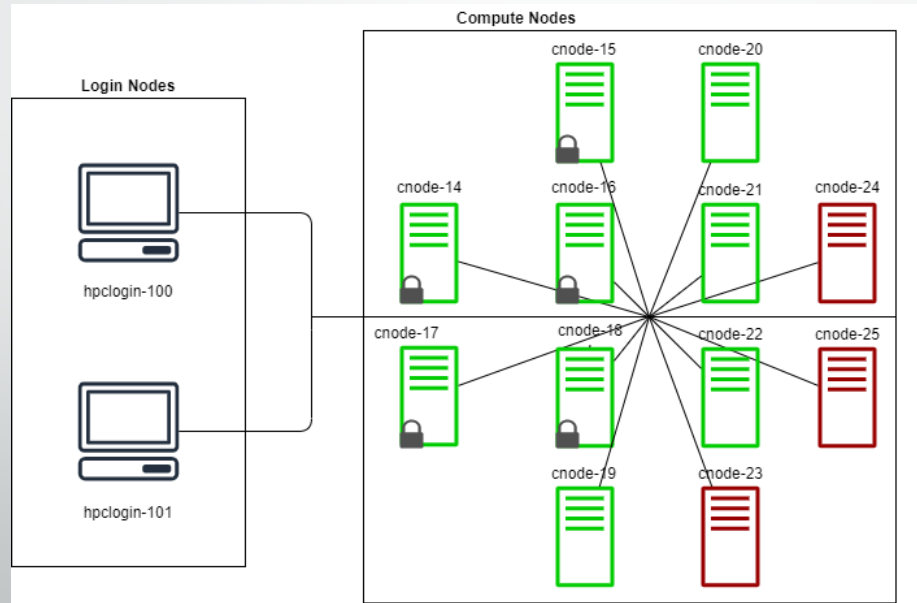
Initially all the nodes are off

```
[root@hpclogin-100 ~]# pstat
```

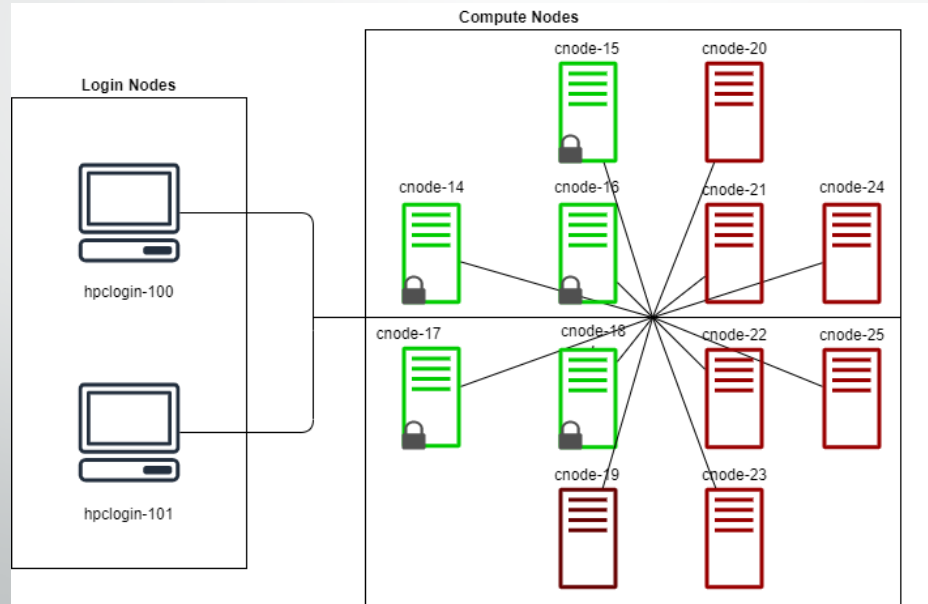
Name	Power State	Marked idle/Powered off at	PBS State
cnode-33-43-19	powered-off	OFF: Wed Jul 29 19:54:01 2020	state-unknown
cnode-33-43-20	powered-off	OFF: Fri Jul 24 16:34:00 2020	state-unknown
cnode-33-43-21	powered-off	OFF: Fri Jul 24 16:28:01 2020	state-unknown
cnode-33-43-22	powered-off	OFF: Fri Jul 24 16:07:23 2020	state-unknown
cnode-33-43-23	powered-off	OFF: Fri Jul 24 16:28:01 2020	state-unknown
cnode-33-43-24	powered-off	OFF: Fri Jul 24 18:04:01 2020	state-unknown
cnode-33-43-25	powered-off	OFF: Fri Jul 24 16:07:23 2020	state-unknown



When jobs exceed the capacity of the static nodes, Green Provisioning Package will boot the dynamic nodes



After the jobs finished running, the dynamic nodes will check if there are any jobs queued for them. If not, they will shut down after a short idle period



Further Improvements

- Using Spot instances for a more cost effective use of the dynamic nodes
 - Spot instances are heavily discounted cloud instances (up to 90% discount) for short interruptible workloads
- Configure to work for more than one queue and more instances based on workload requirements



Thank you!

Any question?