

NVIDIA DGX BasePOD: Multi-cloud Architecture with Amazon Web Services

Deployment Guide

Featuring NVIDIA DGX BasePOD and NVIDIA GPUs through Amazon Web Services

Document History

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Abstract

As part of the NVIDIA DGX[™] platform, NVIDIA DGX BasePOD[™] provides on-premises infrastructure for artificial intelligence (AI) workloads. This infrastructure is an excellent fit for stable use cases and resource requirements.

However, demands can sometimes outstrip resource availability or users might need access to different resources than those provided by their DGX infrastructure.

Managing a separate pool of resources to support changing requirements typically involves the development of significant expertise in cloud management tools and interfaces. A separate pool of resources often requires user education to request the appropriate system or environment—leading to suboptimal resource utilization and user confusion.

Those scenarios are now resolved through the capabilities of NVIDIA Base Command™ Manager (BCM) software. Administrators can now integrate on-demand public cloud resources directly with an on-premises DGX BasePOD private cloud environment and make the combined resources available transparently in a multi-cloud architecture.

This document describes how to extend DGX BasePOD with additional NVIDIA GPUs from Amazon Web Services (AWS) and manage the entire infrastructure from a consolidated user interface. Given the breadth of instances offered by AWS for both general-purpose and accelerated computing with NVIDIA GPUs, it is a great option for use as the basis of cloud resource integration in BCM.

Providing concordant access to on-premises and public cloud resources through existing infrastructure drastically simplifies both the administrator and user experience and makes using the right tool for any job easy.

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Chapter 1. Introduction

Deployment of public cloud integration into DGX BasePOD should be done after on-premises components and services have been deployed, according to the <u>NVIDIA DGX</u> <u>BasePOD Deployment Guide</u>. The tool within BCM that enables this integration is Cluster Extension (cm-cluster-extension). It allows an administrator to integrate a public cloud provider account into an on-premises deployment and configure what resources will be provisioned using that public cloud provider and what regions those resources will be provisioned in. The public cloud resources appear side-by-side with on-premises resources in administrator tools, with access to public cloud-specific configuration capabilities when necessary.

Chapter 2. softwareimage and Category Creation

Before configuring AWS using cm-cluster-extension, create the software images and non-director node categories that are necessary for the target public cloud environment.

- ssh to the head node as root or a user capable of gaining root permissions.
 Specify the external network address or hostname of the head node to gain access.
 # ssh <head-node>
- 2. Enter the cmsh configuration shell.

cmsh



Note: This document uses # to indicate commands executed as the root user on a head node and % to indicate commands executed within cmsh. The prompt change is in the preceding block. If it is unclear where a command is being executed, check the prompt that precedes it.

3. Enter the softwareimage menu and create three additional software images as clones of the default-image—one for each of the node types to be provisioned in the public cloud.

```
% softwareimage
% clone default-image cloud-director-image
% clone default-image k8s-cloud-master-image
% clone default-image k8s-cloud-gpu-worker-image
% ..
% commit
```

4. Enter the category menu and create categories for k8s-cloud-master and k8s-cloud-gpu-worker.

The cm-cluster-extension tool automatically creates a category for the cloud-director (softwareimage is configured at a later step).

```
% category
% clone default k8s-cloud-master
% set softwareimage k8s-cloud-master-image
% commit
% clone default k8s-cloud-gpu-worker
% set softwareimage k8s-cloud-gpu-worker-image
% commit
```

5. Augment the disksetup of the new categories as well.

This guide was executed with a disk layout that maximized the root partition size to avoid scenarios where containers quickly fill a smaller partition. Save the following text to /tmp/big-cloud-disk.xml.

```
<diskSetup>
 <device>
    <blockdev>/dev/sda</blockdev>
    <blockdev>/dev/I</blockdev>
    <blockdev>/dev/vda</blockdev>
    <blockdev>/dev/xvda</blockdev>
    <blockdev>/dev/cciss/c0d0</blockdev>
    <blockdev>/dev/nvme0n1</plockdev>
    <blockdev mode="cloud">/dev/sdb</blockdev>
    <blockdev mode="cloud">/dev/hdb</blockdev>
    <blockdev mode="cloud">/dev/vdb</blockdev>
    <blockdev mode="cloud">/dev/xvdb</blockdev>
    <blockdev mode="cloud">/dev/xvdf</blockdev>
    <blockdev mode="cloud">/dev/nvme1n1</blockdev>
    <partition id="a0" partitiontype="esp">
     <size>100M</size>
     <type>linux</type>
     <filesystem>fat</filesystem>
      <mountpoint>/boot/efi</mountpoint>
      <mountOptions>defaults, noatime, nodiratime</mountOptions>
    </partition>
    <partition id="a1">
     <size>max</size>
      <type>linux</type>
     <filesystem>xfs</filesystem>
      <mountpoint>/</mountpoint>
      <mountOptions>defaults,noatime,nodiratime</mountOptions>
    </partition>
    <partition id="a2">
      <size>12G</size>
      <type>linux swap</type>
    </partition>
 </device>
</diskSetup>
```

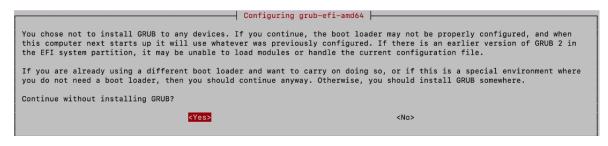
6. Assign the new disk layout file to the cloud categories in Step 4.

```
$ cmsh
% category
% use k8s-cloud-master
% set disksetup /tmp/big-cloud-disk.xml
% commit
% use k8s-cloud-gpu-worker
% set disksetup /tmp/big-cloud-disk.xml
% commit
```

7. Exit the cmsh configuration shell and update all three images.

```
# cm-chroot-sw-img /cm/images/k8s-cloud-master-image/
# apt update && apt -y upgrade
# exit
# cm-chroot-sw-img /cm/images/k8s-cloud-gpu-worker-image/
# apt update && apt -y upgrade
# exit
# cm-chroot-sw-img /cm/images/cloud-director-image/
# apt update && apt -y upgrade
# exit
```

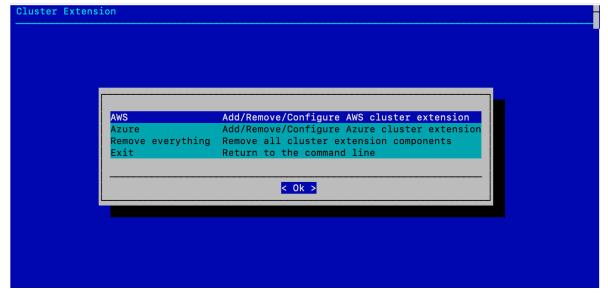
8. When a terminal menu is displayed to confirm that GRUB does not need to be installed, select Yes to continue.



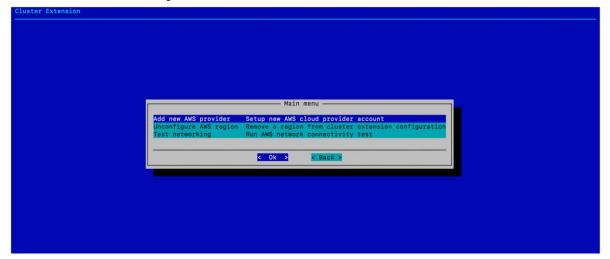
Chapter 3. Cluster Extension Configuration

With images and categories prepared, the environment is now ready for AWS integration and initial configuration. The AWS integration will be accomplished using the <code>cm-cluster-extension</code> command.

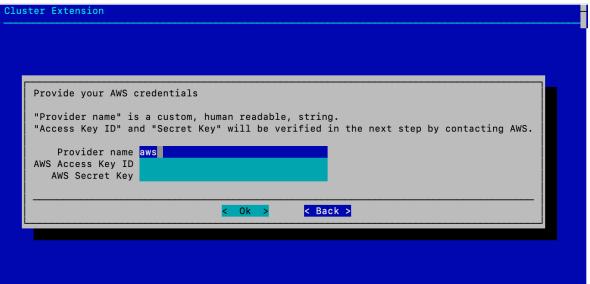
- 1. Create an AWS IAM group with an appropriate policy for a user account to integrate into the BCM on-premises head node.
 - To create a minimum viable policy set, refer to <u>this Bright Knowledge Base article</u>. Assign the policy to the target group and provision a new user in that group. Create a new access key and associated secret access key for that user for use with Bright. Securely document the access key and secret access key for use in this section.
- 2. Run the cm-cluster-extension command to get started. # cm-cluster-extension
- 3. Choose the AWS extension and then select Ok.



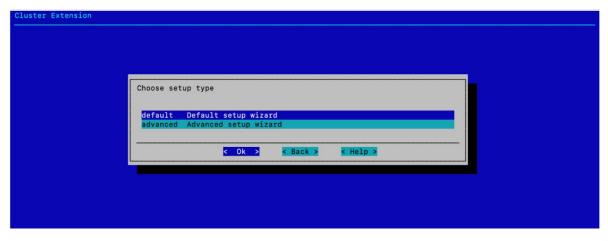
4. Choose Add new AWS provider and then select Ok.



5. Enter the required AWS credential information and then select ok.

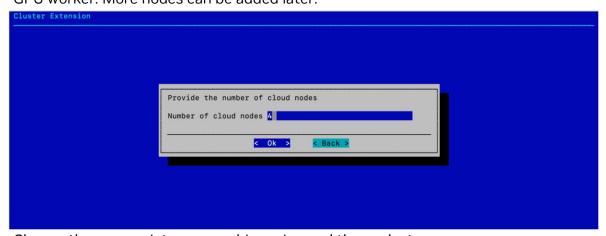


6. Add the provider to the new region by choosing the default setup type and then select Ok.



7. Enter 4 for the quantity of cloud nodes and then select Ok.

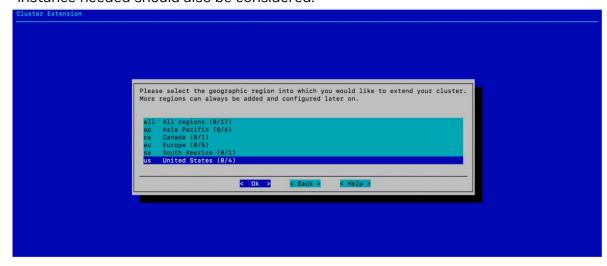
There will be three nodes for the Kubernetes (K8s) control plane and one node as a GPU worker. More nodes can be added later.



8. Choose the appropriate geographic region and then select ok.

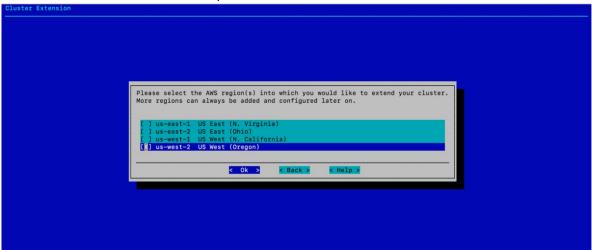
Choosing a region near the on-premises cluster typically increases network performance. If the configuration is designed for regional fault tolerance, choose a more distant region. Because not all instances are available in all regions, the type of

instance needed should also be considered.



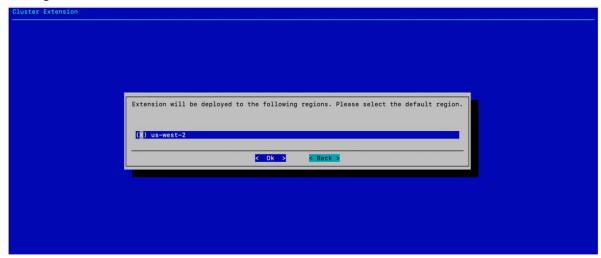
9. Choose a region in the subsequent screen and then select $\circ \mathtt{k}.$

us-west-2 is used in this example.



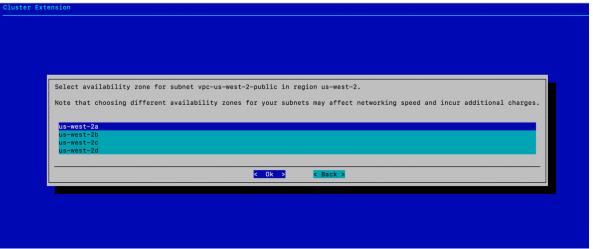
10. Choose a default region and then select Ok.

In this example, the only option is us-west-2 because no other regions were configured.



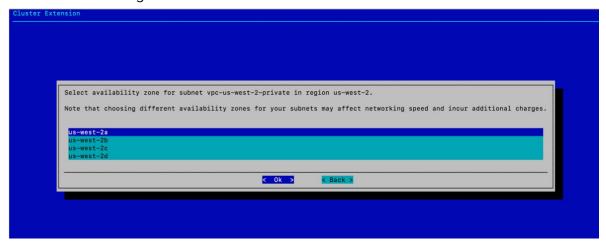
11. Choose an availability zone for the public subnet that Cluster Extension will create and then select ok.

us-west-2a was selected in this example.

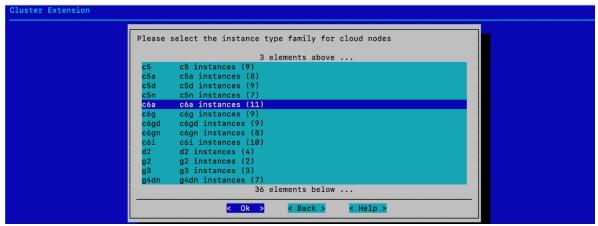


12. Choose an availability zone for the private subnet that Cluster Extension will create and then select ok.

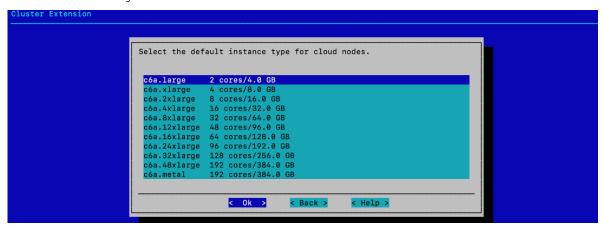
us-west-2a was again selected.



13. Choose c6a for instance type family for cloud nodes and then select Ok. c6a instances are widely available and provide good performance and value for this use case. At a later step, one of the preallocated public cloud nodes will be configured to use an instance type with NVIDIA GPUs.

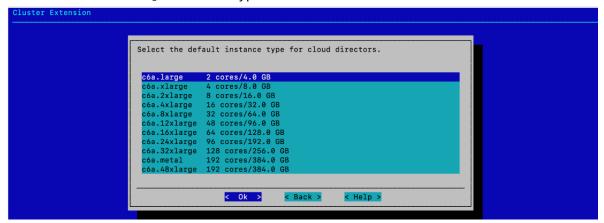


14. Choose c6a.large instances and then select Ok.



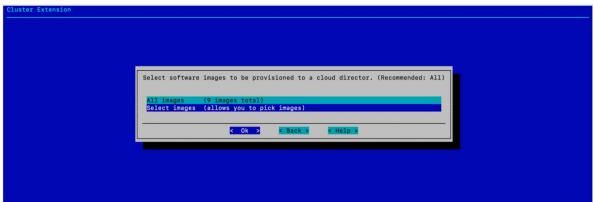
15. Choose the c6a instance type family for cloud directors and then select Ok.

16. Choose the c6a.large instance type and then select Ok.



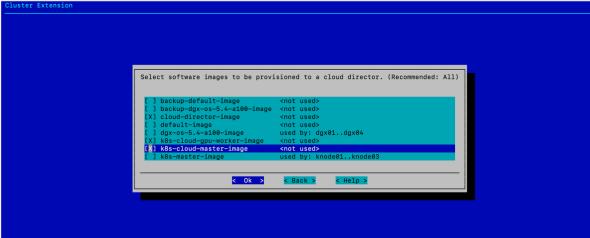
17. Choose Select images and then select Ok.

This selects the subset of images that can be used in the public cloud and eliminates those that cannot be used (such as DGX OS).

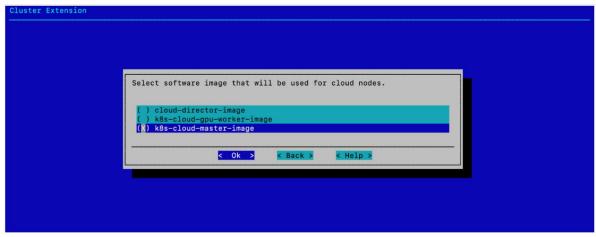


18. Choose the images that were created for this deployment and then select Ok.

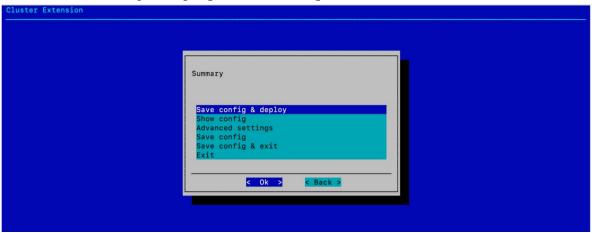
cloud-director-image, k8s-cloud-gpu-worker-image, and k8s-cloud-master-image should be checked. Additional images can be added later if necessary.



19. Choose k8s-cloud-master-image for the default cloud node image and then select Ok.



20. Choose Save config & deploy on the Summary screen and then select Ok.



21. Specify the filepath and then select Ok.

A default filepath is displayed. A region name or other identifying information should be added to the file name to allow multiple configuration files.



22. The configuration begins executing on the BCM head node.

When completed, output like the following should be displayed.

```
## Progress: 100

Took: 04:09 min.
Progress: 100/100
################# Finished execution for 'Cluster Extension', status: completed

Cluster Extension finished!
```

23. Verify that the initial setup was successful.

Run list -f in cmsh as shown in the screenshot and compare it to the output provided—it should be similar (additional listed systems are redacted, and the exact IP subnet may be slightly different).

| [hybridbasepod-b-primary->device]% list -f Type,Hostname,Category,Ip,Network,Status | | | | | | | | | | |
|---|--------------------|----------------|----------------------|----------------|-----------|--------|------|---|--|--|
| Type | Hostname (key) | MAC | Category | Ip | Network | Status | | | | |
| | | | | | | | | | | |
| CloudNode | us-west-2-cnode001 | 00:00:00:00:00 | us-west-2-cloud-node | 172.17.0.1 | us-west-2 |] | DOWN |] | | |
| CloudNode | us-west-2-cnode002 | 00:00:00:00:00 | us-west-2-cloud-node | 172.17.0.2 | us-west-2 | [| DOWN |] | | |
| CloudNode | us-west-2-cnode003 | 00:00:00:00:00 | us-west-2-cloud-node | 172.17.0.3 | us-west-2 | [| DOWN |] | | |
| CloudNode | us-west-2-cnode004 | 00:00:00:00:00 | us-west-2-cloud-node | 172.17.0.4 | us-west-2 | [| DOWN |] | | |
| CloudNode | us-west-2-director | 00:00:00:00:00 | aws-cloud-director | 172.17.255.251 | us-west-2 | [| DOWN |] | | |

24. Augment the OpenVPN port if needed.

The Cluster Extension functionality relies on OpenVPN to run a VPN tunnel between the on-premises head node and the targeted public cloud environment. The default configuration uses UDP port 1194. To configure a different protocol or port, refer to this Bright Knowledge Base article.

Chapter 4. Host Preparation After Cluster Extension Configuration

With AWS cloud resource access configured, the next step is to modify the device entries created using the <code>cm-cluster-extension</code> to leverage the correct categories and make changes when necessary to public cloud settings.

1. Rename the nodes according to their expected usage as follows from the device sub-menu.

```
# cmsh
% device
% rename us-west-2-cnode001 us-west-2-knode001
% rename us-west-2-cnode002 us-west-2-knode002
% rename us-west-2-cnode003 us-west-2-knode003
% rename us-west-2-cnode004 us-west-2-gpu-node001
% commit
```

2. Update the categories for all four public cloud nodes.

```
% set us-west-2-knode001 category k8s-cloud-master
% set us-west-2-knode002 category k8s-cloud-master
% set us-west-2-knode003 category k8s-cloud-master
% set us-west-2-gpu-node001 category k8s-cloud-gpu-worker
% commit
```

3. Increase the EBS volume size to 100 GiB on the knode systems.

```
% cloudsettings us-west-2-knode001
% storage
% set ebs size 100GiB
commit
% ..
% ..
% cloudsettings us-west-2-knode002
% storage
% set ebs size 100GiB
commit
% ..
% ..
% cloudsettings us-west-2-knode003
% storage
% set ebs size 100GiB
commit
% ..
% ..
% cloudsettings us-west-2-knode003
% storage
% set ebs size 100GiB
commit
% ..
% ..
% ..
% ..
```

4. Increase the EBS volume size of us-west-2-gpu-node001 to 100 GiB and change the instancetype for us-west-2-gpu-node001 to g4dn.xlarge (a lower-cost GPU instance with a single T4 GPU).

If requirements justify a higher instance spec, use the appropriate instance type—any NVIDIA GPU instance should work.

```
% cloudsettings us-west-2-gpu-node001
% set instancetype g4dn.xlarge
% commit
% storage
% set ebs size 100GiB
% commit
```

5. Increase the EBS volume size to 200 GiB on the director system.

```
% ..
% ..
% cloudsettings us-west-2-director
% storage
% set ebs size 200GiB
% commit
```

6. Update the softwareimage for the aws-cloud-director category.

```
% category
% use aws-cloud-director
% set softwareimage cloud-director-image
```

7. Update disksetup for the cloud director to use the same partitioning scheme set for the other public cloud nodes.

```
% set disksetup /tmp/big-cloud-disk.xml
% commit
```

Chapter 5. Power On and Provision the Cloud Nodes

Now that the required post-installation configuration has been completed, it is time to power on and provision the public cloud nodes. Public cloud node behavior is slightly different from on-premises equipment—the systems will not be provisioned in the target public cloud until they are first powered on. Additionally, the director node must be powered on and provisioned first—until it is fully provisioned, it is not possible to deploy the public cloud nodes it manages in a region. Just as with on-premises deployments, the public cloud nodes can be accessed through ssh during the installation process.

Watch the /var/log/messages and /var/log/node-installer log files to verify that everything is proceeding smoothly if you are unsure of a given node's deployment state.

1. Power on the cloud director.

It will enter a [PENDING] state, then transition to [DOWN] (Instance has started).

```
# cmsh
% power on us-west-2-director
```

The provisioning of the cloud director may take two or more hours due to the tens of gigabytes of software image data that must be synchronized to the public cloud. The process is complete when the cloud director moves to an $[\ UP\]$ state.

2. Power on the four public cloud nodes concurrently.

Once the cloud director is fully provisioned, bringing up the other four public cloud nodes is much faster because their base images are already stored in the target region with the cloud director.

```
% power on -n us-west-2-knode00[1-3],us-west-2-gpu-node001
```

3. Run device then list to ensure all public cloud nodes are in an [UP] state. Disregard any trailing Status output.

| % device % list Type | Hostname (key) | MAC | Category | Ip | Network | Sta | tus | |
|----------------------------|-----------------------|-------------------|----------------------|----------------|-----------|-----|-----|---|
| CloudNode | us-west-2-director | 00:00:00:00:00:00 | aws-cloud-director | 172.17.255.251 | us-west-2 | [| UP | 1 |
| CloudNode | us-west-2-qpu-node001 | 00:00:00:00:00:00 | k8s-cloud-qpu-worker | 172.17.0.4 | us-west-2 | Ī | UP | 1 |
| CloudNode | us-west-2-knode001 | 00:00:00:00:00:00 | k8s-cloud-master | 172.17.0.1 | us-west-2 | Ī | UP | ĵ |
| CloudNode | us-west-2-knode002 | 00:00:00:00:00:00 | k8s-cloud-master | 172.17.0.2 | us-west-2 | [| UP | 1 |
| CloudNode | us-west-2-knode003 | 00:00:00:00:00:00 | k8s-cloud-master | 172.17.0.3 | us-west-2 | [| UP | 1 |

4. Install the NVIDIA driver on us-west-2-gpu-node001. ssh to it as root and run all subsequent commands from the node in AWS.

```
# ssh us-west-2-gpu-node001
# apt install linux-headers-$(uname -r)
# distribution=$(. /etc/os-release;echo $ID$VERSION_ID | sed -e 's/\.//g')
# wget
https://developer.download.nvidia.com/compute/cuda/repos/$distribution/x86_64/cud
a-keyring_1.0-1_all.deb
# dpkg -I cuda-keyring_1.0-1_all.deb
# apt update
# apt install -y cuda-drivers -no-install-recommends
# rm cuda-keyring_1.0-1_all.deb
# nvidia-smi
```

5. Look for output from nvidia-smi, which like this, shows a successful installation. Expect possible variations in software versions and device utilization.

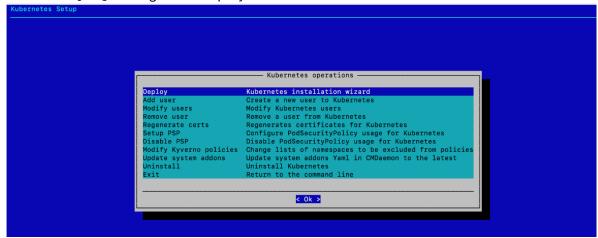
- 6. Log out of the public cloud GPU node and back into the on-premises head node.
- 7. Execute the following to capture the modifications made to the public cloud GPU node, which will then be present in the image of any additional public cloud GPU nodes provisioned in this environment.

```
$ cmsh
# device
# use us-west-2-gpu-node001
# grabimage -w
```

Chapter 6. Deploy Kubernetes

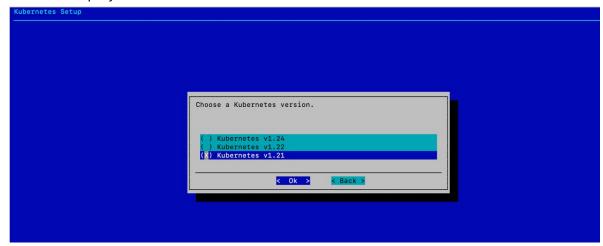
With all required public cloud instances deployed and configured for general use, the environment is ready for K8s deployment. In a hybrid environment, the same tool used to deploy on-premises K8s is used to deploy K8s in the public cloud as well.

- 1. Run the cm-kubernetes-setup CLI wizard as the root user on the head node. # cm-kubernetes-setup
- 2. Choose Deploy to begin the deployment and then select Ok.

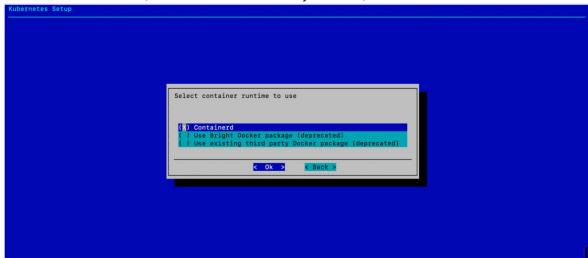


3. Choose Kubernetes v1.21 and then select Ok.

K8s version 1.21 was selected to match the version deployed in the on-premises DGX BasePOD deployment.

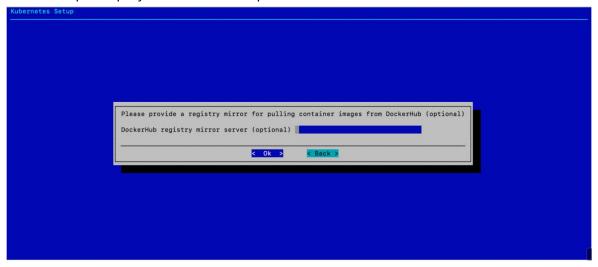


4. Choose Containerd (it should be selected by default) and then select Ok.



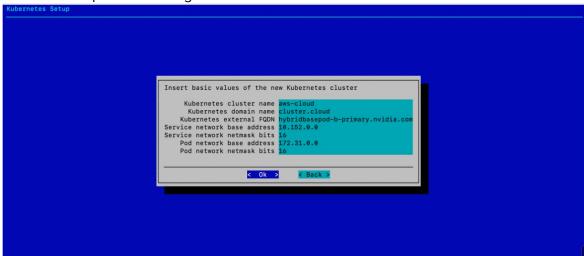
5. Optionally, provide a registry mirror and then select $\mathtt{o}\mathtt{k}$.

This example deployment did not require one.

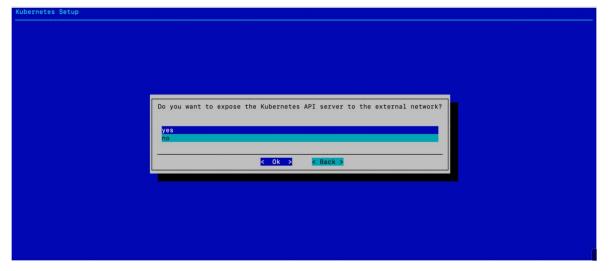


6. Configure the basic values of the K8s cluster and select Ok.

Choose names that make it easy to understand that the K8s deployment is using public cloud resources. In addition, ensure that the service and pod network subnets do not overlap with existing subnets in the cluster.

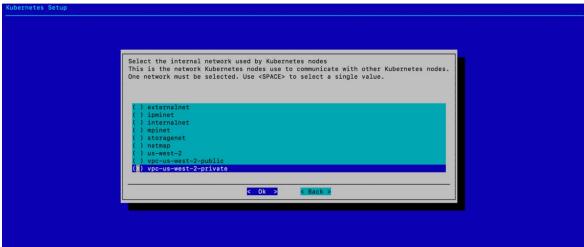


7. Choose yes to expose the K8s API server to the external network and then select ok. This allows users to use the K8s cluster from the head node.

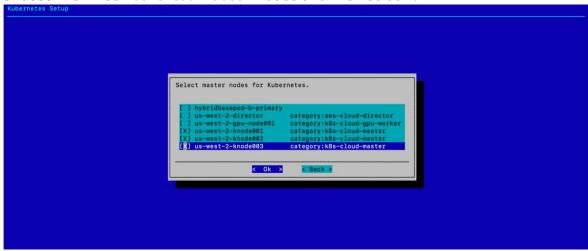


8. Choose vpc-us-west-2-private for the public cloud-based K8s environment and then select ok.

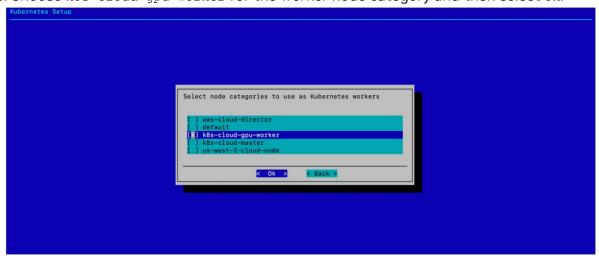
This keeps internal K8s traffic entirely in the public cloud.



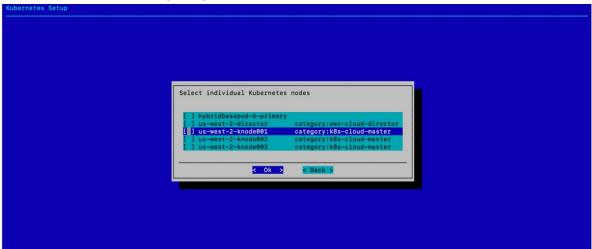
9. Choose the three k8s-cloud-master nodes and then select Ok.



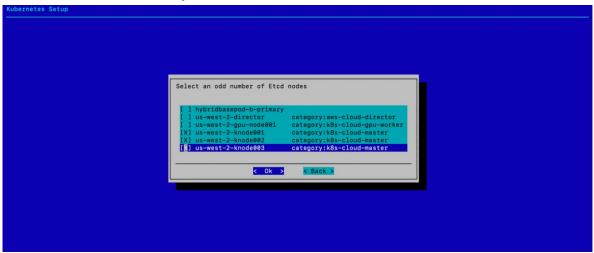
10. Choose k8s-cloud-gpu-worker for the worker node category and then select Ok.



11. Select Ok without configuring any individual K8s nodes.

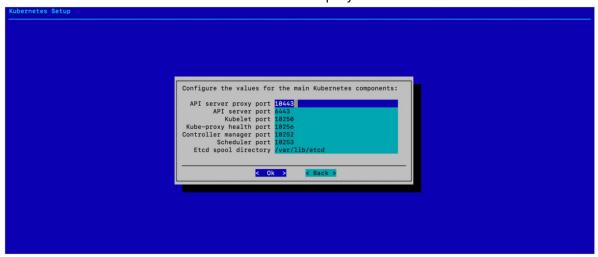


12. Choose the three knode systems for Etcd nodes and then select Ok.

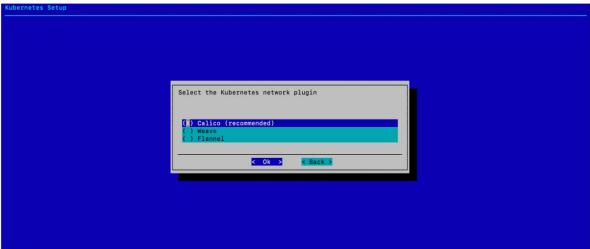


13. Configure the K8s main components and then select Ok.

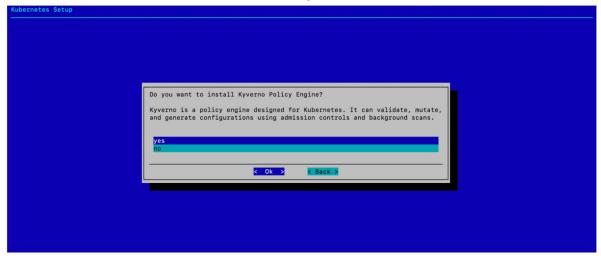
Use the default ports and path here unless the environment requires different values. The default values were used in this deployment.



14. Choose the Calico network plugin and then select Ok.

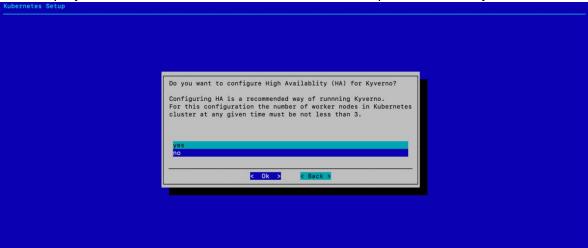


15. Choose yes to install the Kyverno policy engine and then select Ok.

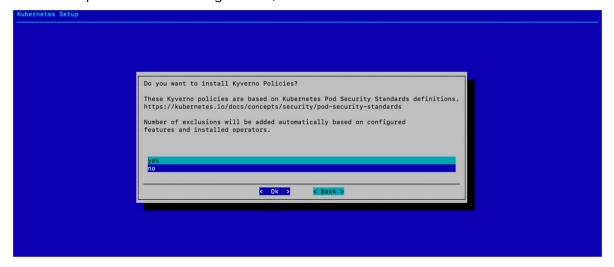


16. Choose no to decline to configure HA for Kyverno and then select ok.

This deployment does not meet the minimum node requirement for Kyverno HA.



17. Choose whether to install Kyverno Policies and then select ok. Unless required for the configuration, choose no.

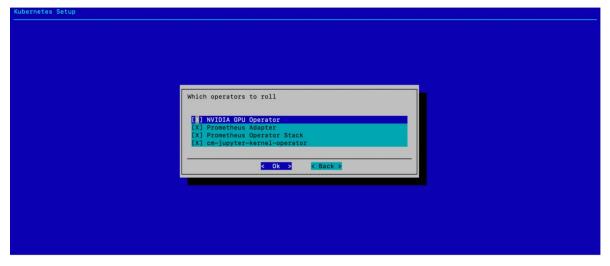


18. Choose the operator packages to install and then select ok.

As shown in the screenshot, choose NVIDIA GPU Operator, Prometheus Adapter, Prometheus Adapter Stack, and the cm-jupyter-kernel-operator.

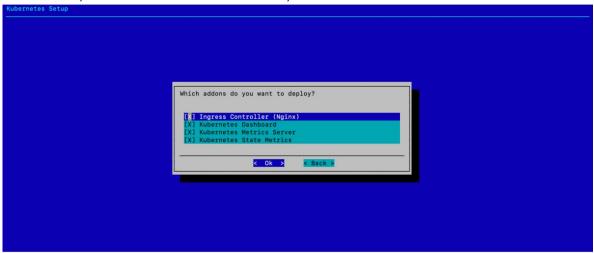


19. Choose the same four operators to be rolled up with the defaults and then select Ok.

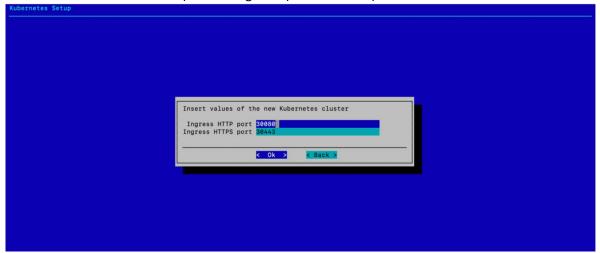


20. Choose the addons to deploy and then select Ok.

As shown in the screenshot, choose Ingress Controller (Nginx), Kubernetes Dashboard, Kubernetes Metrics Server, and Kubernetes State Metrics.



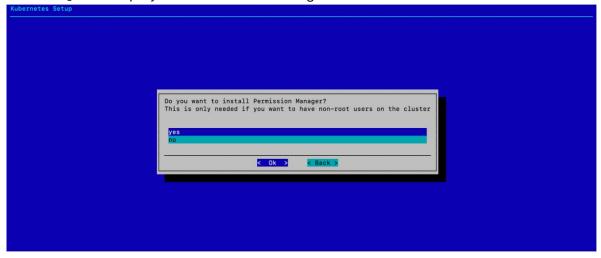
21. Choose the Ingress ports for the cluster and then select ok. Use the defaults unless specific ingress ports are required.



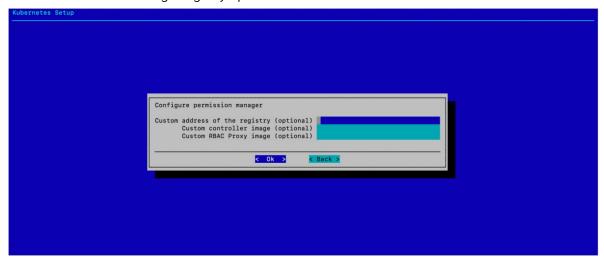
22. Choose no when asked to install the Bright NVIDIA packages and then select ok. Since the K8s control plane nodes do not have GPUs, the GPU Operator manages NVIDIA OS components.



23. Choose yes to deploy the Permission Manager and then select Ok.



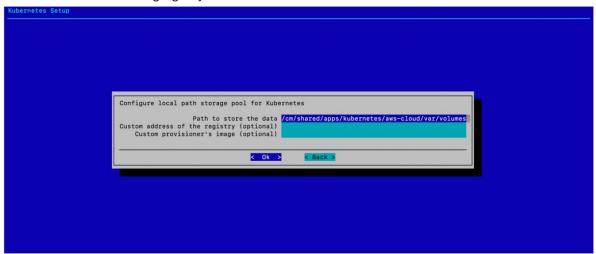
24. Select Ok without configuring any optional values.



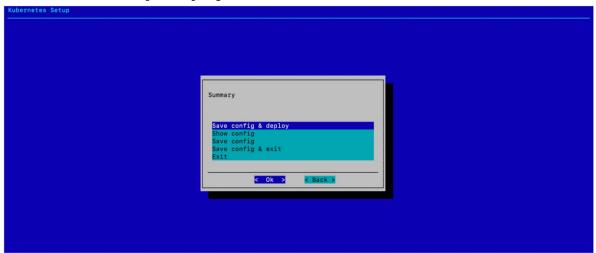
25. Choose both enabled and default for the Local path storage class and then select Ok.



26. Select $\bigcirc \Bbbk$ without changing any of the default values.

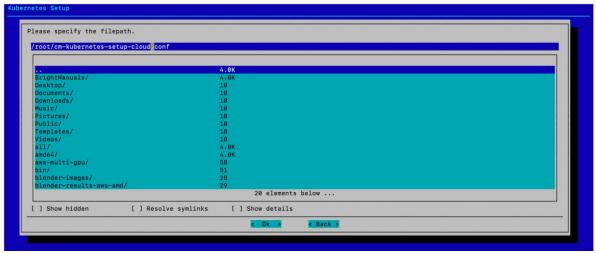


27. Choose Save config & deploy and then select Ok.



28. Change the filepath to /root/cm-kubernetes-setup-cloud.conf and then select Ok.

The filepath was changed to avoid name conflicts with the existing K8s configuration file from the initial on-premises deployment. Wait for the installation to finish.



29. Verify the K8s cluster is installed properly.

The K8s module may need to be unloaded for the on-premises deployment if already loaded or use the switch command as a shortcut to unload on-premises and load the public cloud module.

```
# module load kubernetes/aws-cloud/
# kubectl cluster-info
Kubernetes control plane is running at https://localhost:10443
CoreDNS is running at https://localhost:10443/api/v1/namespaces/kube-
system/services/kube-dns:dns/proxy
To further debug and diagnose cluster problems, use 'kubectl cluster-info dump'.
# kubectl get nodes
NAME
                      STATUS ROLES
                                                     AGE VERSION
us-west-2-gpu-node001 Ready worker
                                                    6m48s v1.21.4
us-west-2-knode001
                      Ready
                              control-plane, master 6m48s v1.21.4
                              control-plane, master 6m48s v1.21.4
us-west-2-knode002
                      Ready
                      Ready control-plane, master 6m48s v1.21.4
us-west-2-knode003
```

30. Verify that a GPU job can be run on the K8s cluster.

a. Save the following text to a file named gpu.yaml.

- b. Execute the code using kubectl apply.
 - # kubectl apply -f gpu.yaml
- c. Use kubectl logs to check the result.

The output should be like the following.

Chapter 7. Create Additional Worker Nodes

The steps in this section cover how to extend the pool of worker nodes.

1. Access cmsh and enter the device sub-menu.

```
# cmsh
% device
```

2. Clone the single worker node.

Maintaining the naming convention will automate the IP address increment.

```
% clone us-west-2-gpu-node001 us-west-2-gpu-node002 % commit
```

3. Power the additional worker node on and wait until it enters the $[\ \ UP\]$ state.

```
% power on us-west-2-gpu-node002
```

4. Verify the worker nodes are ready by using kubectl.

The worker node should automatically be available as part of the public cloud Kubernetes worker pool because the entire category is marked as worker nodes. The resources should be ready to use immediately.

```
# kubectl get nodes

NAME STATUS ROLES AGE VERSION

us-west-2-gpu-node001 Ready worker 25h v1.21.4

us-west-2-gpu-node002 Ready worker 10m v1.21.4

us-west-2-knode001 Ready control-plane, master 25h v1.21.4

us-west-2-knode002 Ready control-plane, master 25h v1.21.4

us-west-2-knode003 Ready control-plane, master 25h v1.21.4
```

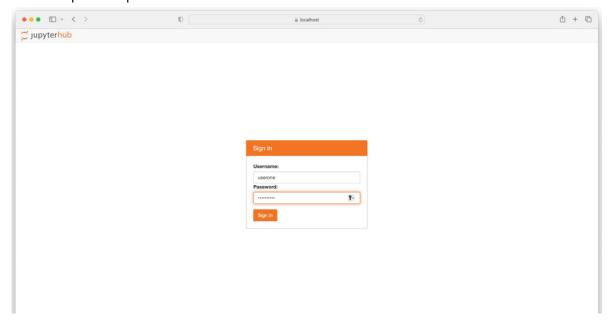
Chapter 8. (Optional) Enable Jupyter Operator Use in Cloud K8s Cluster

In the on-premises DGX BasePOD deployment guide, <code>cm-jupyter-setup</code> can be optionally configured and integrated into K8s. The same service, running from the head node, can be used to provide Jupyter access to the public cloud-based K8s cluster as well.

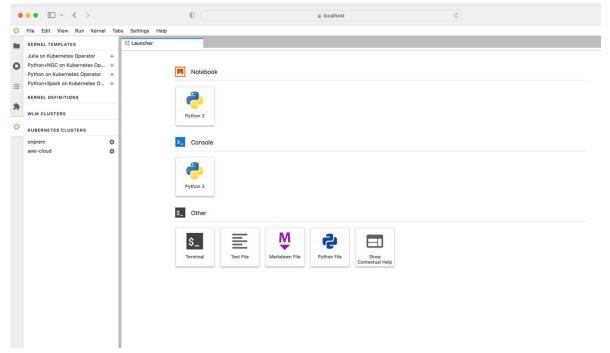
- 1. Validate cm-jupyterhub is set up and running correctly.
 - # service cm-jupyterhub status
- 2. Configure a user and provide access to the appropriate K8s cluster.
 - # cmsh -c "user; add userone; set password useronepwd; commit"
- 3. When using K8s via Jupyter, users must be added separately using K8s with the following commands. Users must have permission to access the Jupyter kernel operator in both K8s clusters to use the kernel templates.

```
# apt install cm-python39
# cm-kubernetes-setup --add-user userone --cluster aws-cloud --operators cm-
jupyter-kernel-operator
# cm-kubernetes-setup --add-user userone --cluster onprem --operators cm-jupyter-
kernel-operator
```

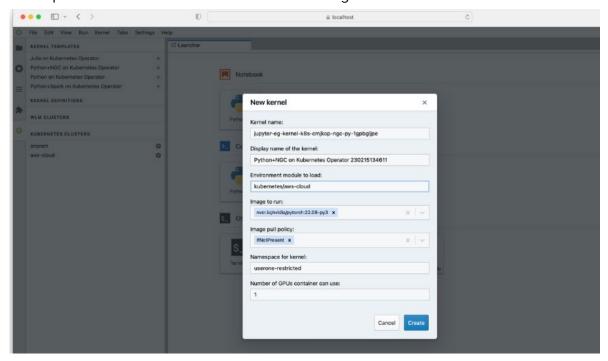
4. Sign in to the Jupyter web interface using the account configured with Jupyter kernel operator permissions.



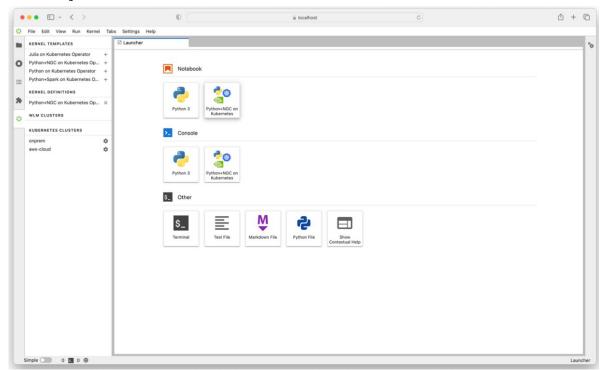
5. Navigate to the Bright tab, choose the Python+NGC on Kubernetes Operator kernel template, and then select Ok.



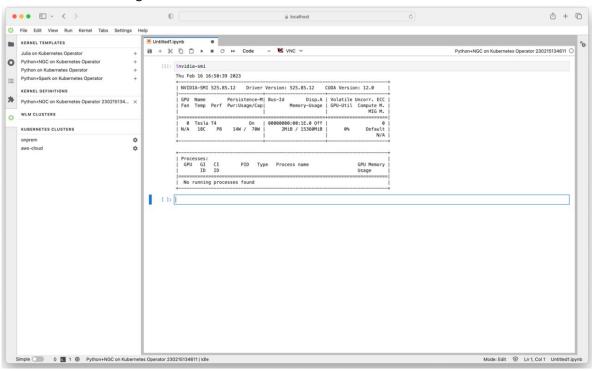
6. Fill in the required fields on the resulting New kernel window and then select Create. In this example, the public cloud-based K8s deployment was targeted by adding the cluster name (aws-cloud) as a path extension to the K8s environment module, and it was specified that the container could use a single GPU.



7. Select Python+NGC on Kubernetes in the Notebook section.



8. Once the state of the operator becomes Idle, run nvidia-smi to confirm the notebook is running on a T4 GPU instance.



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