



Containerized Hybrid Cloud Environment for Research Computing

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Interns: Lim Zi Xuan Jeremy (FOE), Yang Zi Yun (CEG)

Supervisors: Yeo Eng Hee, Kumar Sambhav, Wang Jun Hong, Rikky Purbojati



NUS
National University
of Singapore

Information
Technology

What is High Performance Computing (HPC)?

- 1 HPC Cluster with accelerators (CPU, GPU)
- 2 Computational Science & Engineering Software
- 3 Data Analytics & AI Computing Platform (R, Matlab, Python, Tensorflow, PyTorch, etc)
- 4 Data Repository & Analytics System (Hadoop, Sparks)
- 5 On-demand Storage
- 6 High-speed Data Transfer (100Gbps research network)



How do users utilise HPC?

```
#!/bin/bash

#PBS -P Project_Name_of_Job
#PBS -j oe
#PBS -N Job_Name

###--- Setting for parallel8, parallel12, parallel24, parallel20 ----
###--- To activate the setting, change ###PBS to #PBS for the line. ----

#PBS -l select=16:ncpus=1:mem=12GB
#PBS -l place=pack

###--- Set different walltime/running time (max=720 hours) ----
###--- To activate the setting, change ###PBS to #PBS for the line. ----
###PBS -l walltime=720:00:00

cd $PBS_O_WORKDIR; ## this line is needed, do not delete and change.
np=$( cat ${PBS_NODEFILE} |wc -l ); ### get number of CPUs, do not change

##--- Put your exec/application commands below ---
###source openfoam 3.0.1
module load singularity
cd /[redacted]/ANSYS/fluent_benchmark1
singularity exec /[redacted]/ANSYS/Fluent.sif ./run_cmd.txt
echo $PWD
```

How do users utilise HPC?

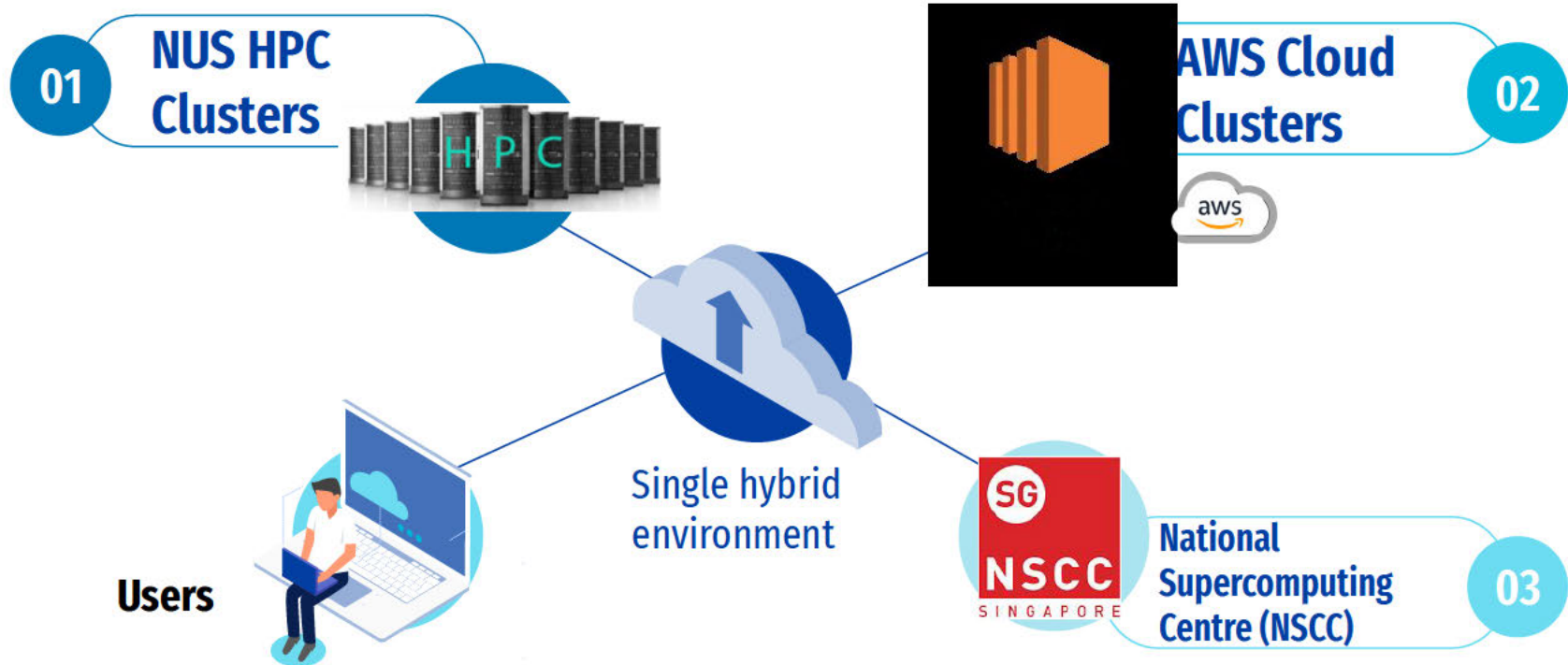
```
[ ]$ qsub jobscript.txt
```

```
3111323.venus01
```

```
[ ]$ qstat
```

Job id	Name	User	Time Use	S	Queue
3111323.venus01	Job_Name		0	Q	short

Objective: Hybrid Cloud Environment



Containerization of applications



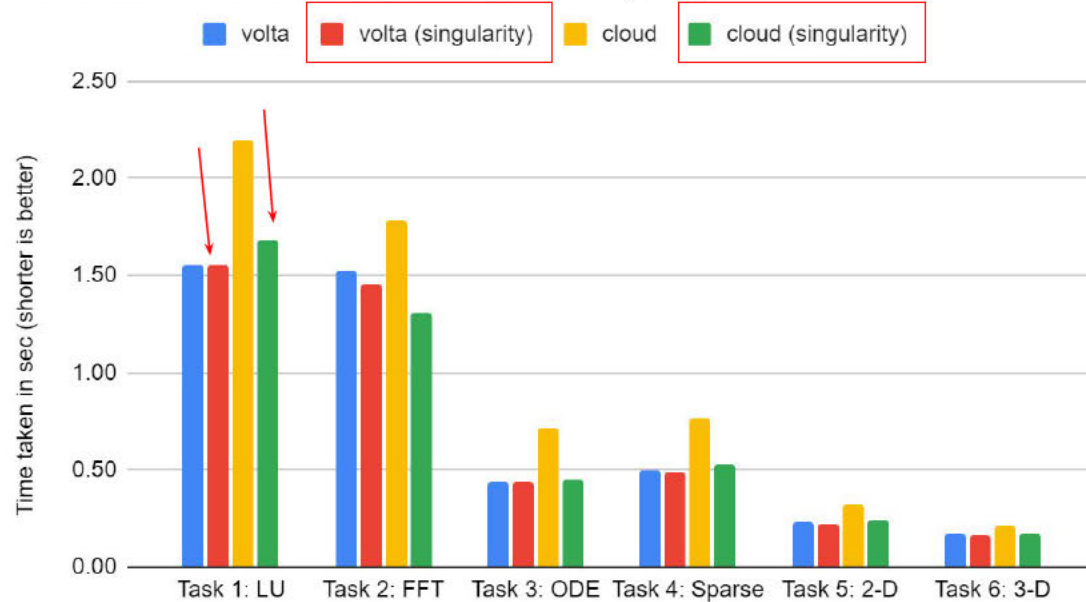
Singularity containers



Benchmarking of containers



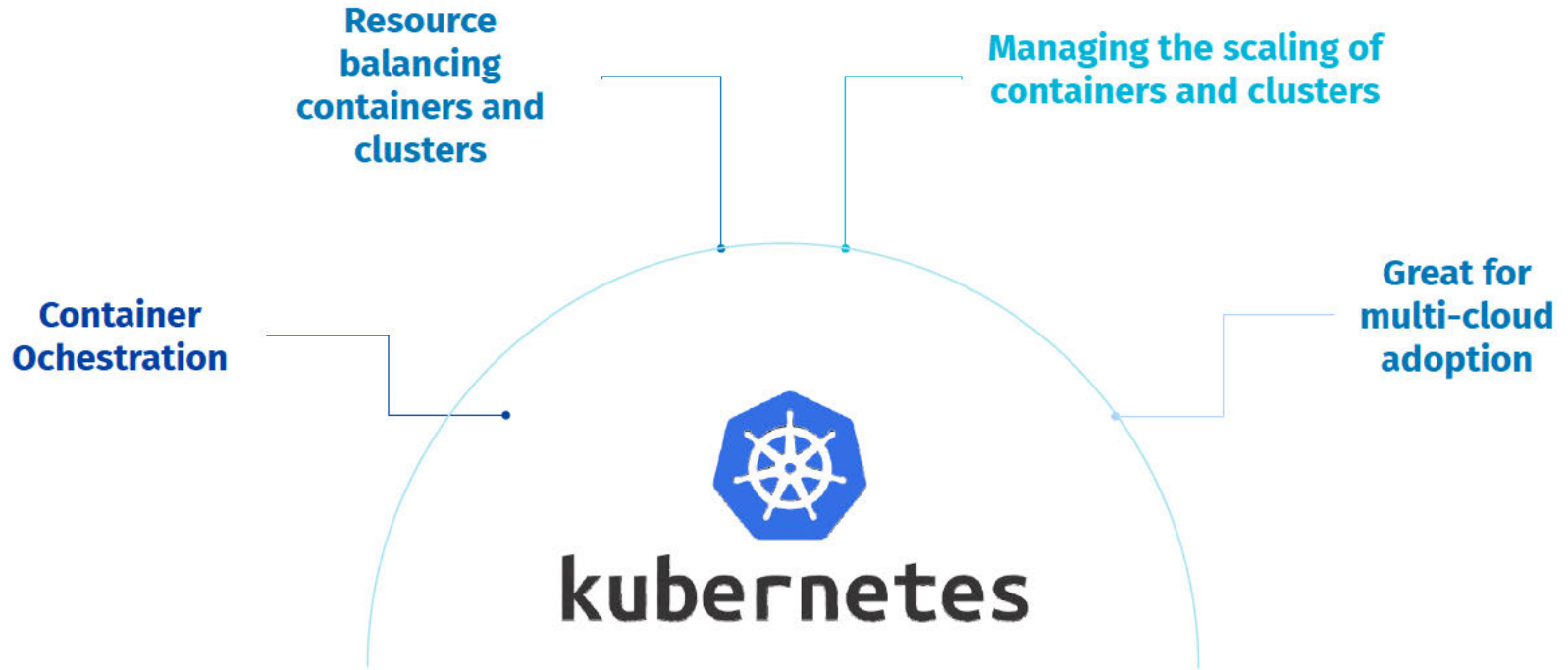
Time taken for benchmarking tasks (sec)



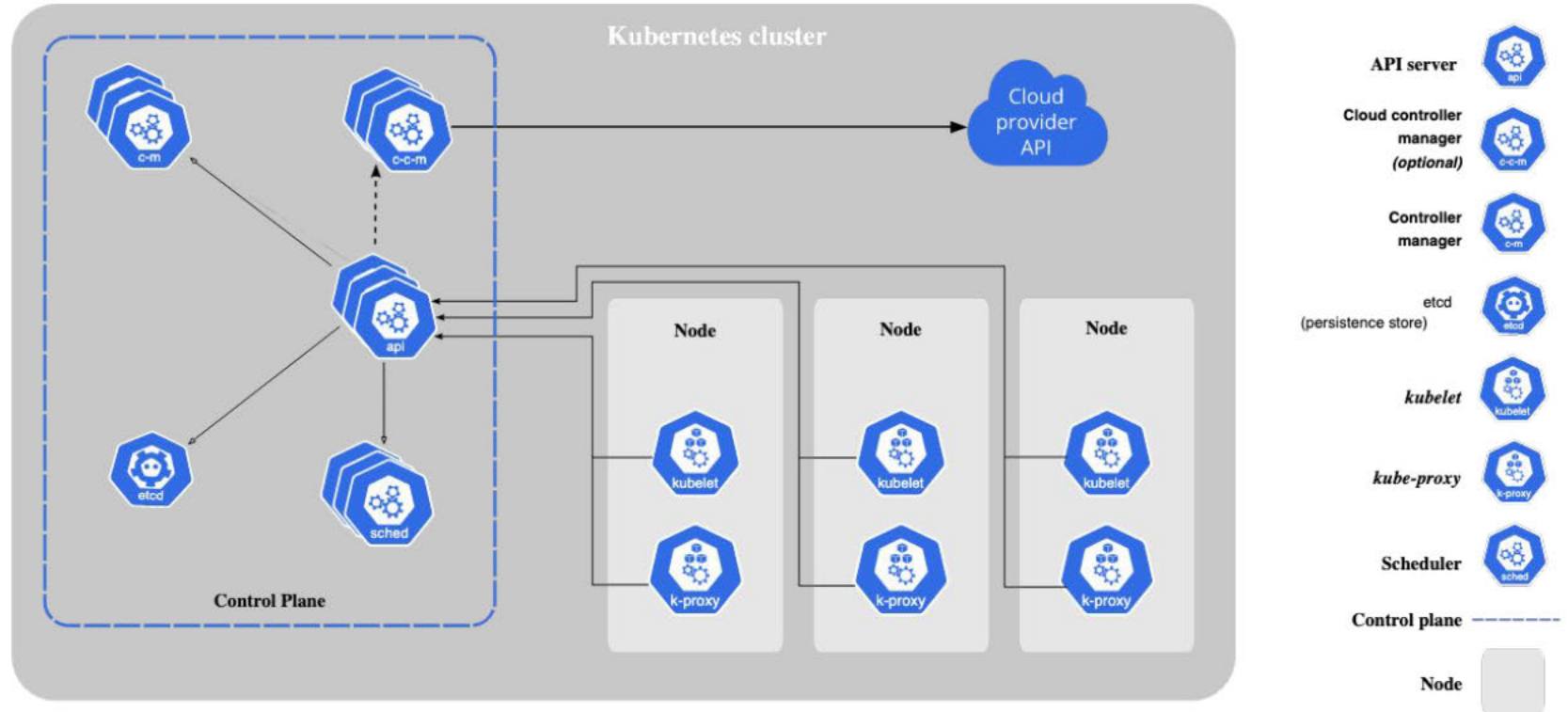
Singularity containers



Kubernetes



Kubernetes Architecture Overview



Kubernetes

```
apiVersion: batch/v1
kind: Job
metadata:
  name: simplematlab
spec:
  template:
    spec:
      nodeName: appserv-80
      containers:
      - name: simplematlab # Job Name
        image: local.file/shared_file/containers/matlab-full-2021.sif # Desired Container
        command: ["/bin/bash"]
        args:
        - -c
        - cd /[REDACTED]/hpccStreamBenchmark && matlab -r new # Command to run
      volumeMounts:
      - name: nfs-home-pv
        mountPath: /home/svu
      - name: nfs-hpctmp-pv
        mountPath: /hpctmp
      restartPolicy: Never
      volumes:
      - name: nfs-home-pv
        persistentVolumeClaim:
          claimName: nfs-home-pvc
      - name: nfs-hpctmp-pv
        persistentVolumeClaim:
          claimName: nfs-hpctmp-pvc
      backoffLimit: 4
```

Kubernetes

```
[centos@appserv-118 yaml]$ kubectl apply -f example.yaml
job.batch/simplematlab created
[centos@appserv-118 yaml]$ kubectl get job
```

NAME	COMPLETIONS	DURATION	AGE
simplematlab	0/1	7s	7s

Kubernetes

```
[centos@appserv-118 yaml]$ kubectl get job
NAME                COMPLETIONS  DURATION  AGE
simplematlab         1/1           79s       2m6s
[centos@appserv-118 yaml]$ kubectl logs job/simplematlab
MATLAB is selecting SOFTWARE OPENGL rendering.
```

```

                                < M A T L A B (R) >
                                Copyright 1984-2021 The MathWorks, Inc.
                                R2021a (9.10.0.1602886) 64-bit (glnxa64)
                                February 17, 2021
```

```
To get started, type doc.
For product information, visit www.mathworks.com.
```

```
a =
```

```
148.4132
```

```
a =
```

```
148.4132
```

```
[root@appserv-118 centos]# kubectl get nodes,pods --all-namespaces -o wide
```

NAME	STATUS	ROLES	AGE	VERSION	INTERNAL-IP	EXTERNAL-IP	OS-IMAGE	KERNEL-VERSION	CONTAINER-RUNTIME
node/appserv-118	Ready	control-plane,master	25d	v1.21.2	10.33.43.118	<none>	CentOS Linux 7 (Core)	3.10.0-1160.31.1.el7.x86_64	singularity://3.7.3
node/appserv-46	Ready	<none>	19d	v1.21.1	10.33.43.46	<none>	CentOS Linux 7 (Core)	3.10.0-1062.12.1.el7.x86_64	singularity://3.7.3
node/appserv-80	Ready	<none>	25d	v1.21.2	10.33.43.80	<none>	CentOS Linux 7 (Core)	3.10.0-1160.31.1.el7.x86_64	singularity://3.7.3
node/appserv-97	Ready	<none>	4d13h	v1.21.1	10.33.43.97	<none>	CentOS Linux 7 (Core)	3.10.0-1062.12.1.el7.x86_64	singularity://3.7.3

NAMESPACE	NAME	READY	STATUS	RESTARTS	AGE	IP	NODE	NOMINATED	NODE	READINESS	GATES
hpcuser	pod/nginx-deployment-7b77db5999-6rfjv	1/1	Running	0	35h	192.168.160.7	appserv-80	<none>		<none>	
hpcuser	pod/nginx-deployment-7b77db5999-8l2sf	1/1	Running	0	35h	192.168.160.9	appserv-80	<none>		<none>	
hpcuser	pod/nginx-deployment-7b77db5999-pbxtr	1/1	Running	0	35h	192.168.160.10	appserv-80	<none>		<none>	
hpcuser	pod/nginx-deployment-7b77db5999-r9mdr	1/1	Running	0	35h	192.168.160.8	appserv-80	<none>		<none>	
kube-system	pod/coredns-88d6f6b77-cx1br	1/1	Running	5	25d	192.168.96.6	appserv-118	<none>		<none>	
kube-system	pod/coredns-88d6f6b77-mnkt	1/1	Running	6	25d	192.168.96.7	appserv-118	<none>		<none>	
kube-system	pod/etcd-appserv-118	1/1	Running	3	25d	10.33.43.118	appserv-118	<none>		<none>	
kube-system	pod/kube-apiserver-appserv-118	1/1	Running	8	25d	10.33.43.118	appserv-118	<none>		<none>	
kube-system	pod/kube-controller-manager-appserv-118	1/1	Running	20	25d	10.33.43.118	appserv-118	<none>		<none>	
kube-system	pod/kube-proxy-fdmsq	1/1	Running	0	4d13h	10.33.43.97	appserv-97	<none>		<none>	
kube-system	pod/kube-proxy-gnvsg	1/1	Running	0	25d	10.33.43.80	appserv-80	<none>		<none>	
kube-system	pod/kube-proxy-jjllg	1/1	Running	0	19d	10.33.43.46	appserv-46	<none>		<none>	
kube-system	pod/kube-proxy-zx56q	1/1	Running	0	25d	10.33.43.118	appserv-118	<none>		<none>	
kube-system	pod/kube-scheduler-appserv-118	1/1	Running	22	25d	10.33.43.118	appserv-118	<none>		<none>	
kube-system	pod/weave-net-c7ql6	2/2	Running	0	6h17m	10.33.43.118	appserv-118	<none>		<none>	
kube-system	pod/weave-net-hdvr6	2/2	Running	0	6h17m	10.33.43.97	appserv-97	<none>		<none>	
kube-system	pod/weave-net-jk4cp	2/2	Running	0	6h17m	10.33.43.80	appserv-80	<none>		<none>	
kube-system	pod/weave-net-xz2q7	2/2	Running	0	6h17m	10.33.43.46	appserv-46	<none>		<none>	



kubernetes

Other Related Technologies

01

User Authentication



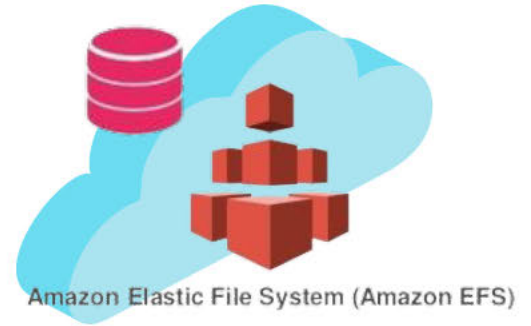
02

Job scheduling

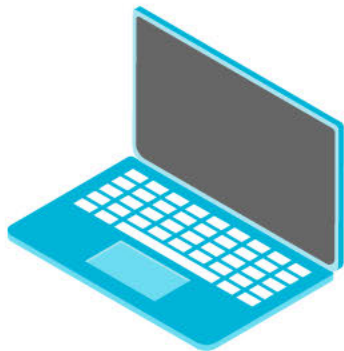


03

Data Storage



Future Works



**Set up proper
clusters on AWS**

**Integrate with
NSCC's
resources**



**Additional
Role-Based Access
Control (RBAC) for
better management**



**Streamline
proper logging**



Conclusion



**Practical Linux system
administration skills**



**Linux containers and
Kubernetes**



**In depth knowledge of
HPC environment**



**Learning
Outcome**

**Network and
intercommunications**



**Cloud SysOps
administration skills**



**Data
management**





Thank you