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RESEARCH TECHNOLOGIES

Jetstream2

Jetstream2:

Unidata's use and growth with Jetstream

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Lead of Scientific Computing Applications

DeSouza Award Seminar - November 2, 2023

About Jetstream2

- NSF-funded production cloud environment
- Ease-of-use focus, rapid on-ramp to ACCESS (allocated ONLY via ACCESS)
- On-demand interactive computing and persistent services for science gateways
- Enables configurable environments; *programmable cyberinfrastructure*
- Building on the success of Jetstream1
  - The 63 science gateways that utilized Jetstream indirectly supported over 183,197 people.
  - Six year of operations an overall availability of 98.54%, incl. planned and unplanned outages
  - An uptime of 99.9967% where the system was operating but at a reduced capacity

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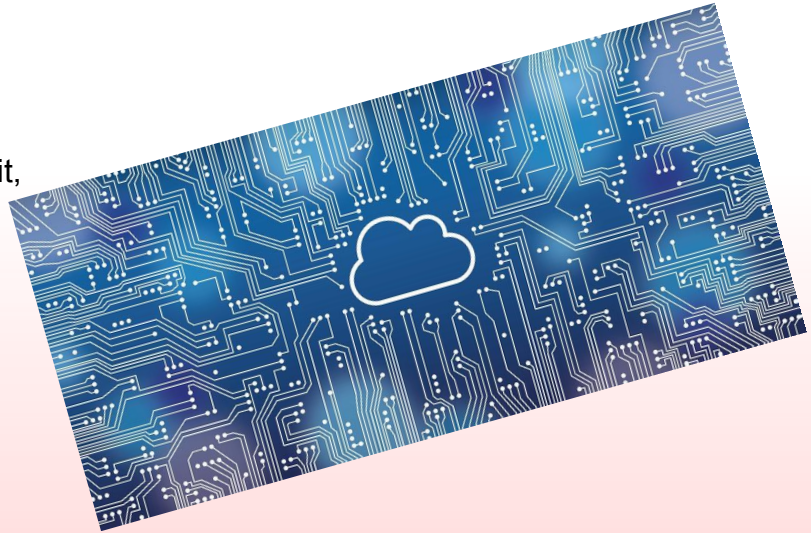
Jetstream2 Features

- Primary Cloud (IU)
  - 400 compute nodes -- AMD EPYC 3rd Generation Milan CPUs – 128 cores per node + 512gb RAM
  - 90 GPU nodes – 4 x NVIDIA A100 40gb per node
  - 32 Large Memory nodes with 1TB of RAM
- Regional Clouds available by invitation/request (Arizona State, Cornell, Hawaii, TACC)
- Shared application store with common applications (NVIDIA HPC Toolkit, multiple compilers, R/Rstudio, Matlab, Anaconda, etc)
- Federated JupyterHubs, Virtual Clusters, and orchestration are all available with features being added and refined
- Commitment to >99% uptime
  - 99.87% availability for 9-7-22 to 3-31-23 (last NSF reporting period)



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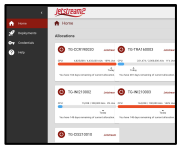
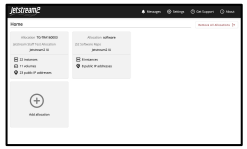
Platform Overview

Horizon

OpenStack CLI



CACAO



Exosphere

Science Gateways

Authentication Service

ACCESS Accounting

OpenStack | Ceph | OpenStack

Jetstream2 Core System

Some sample use cases

- Science gateways
- Research-supporting infrastructure / Infrastructure as a service
- Education support – compute and desktops for courses, workshops, tutorials
- Domain science interactive compute
- Domain science long running compute
  - Smaller core counts, ”pleasingly parallel”, etc
- Jupyter notebooks and Hubs
- Research software development
- Machine learning – training and workflow development and data analysis
- [Your use case here]

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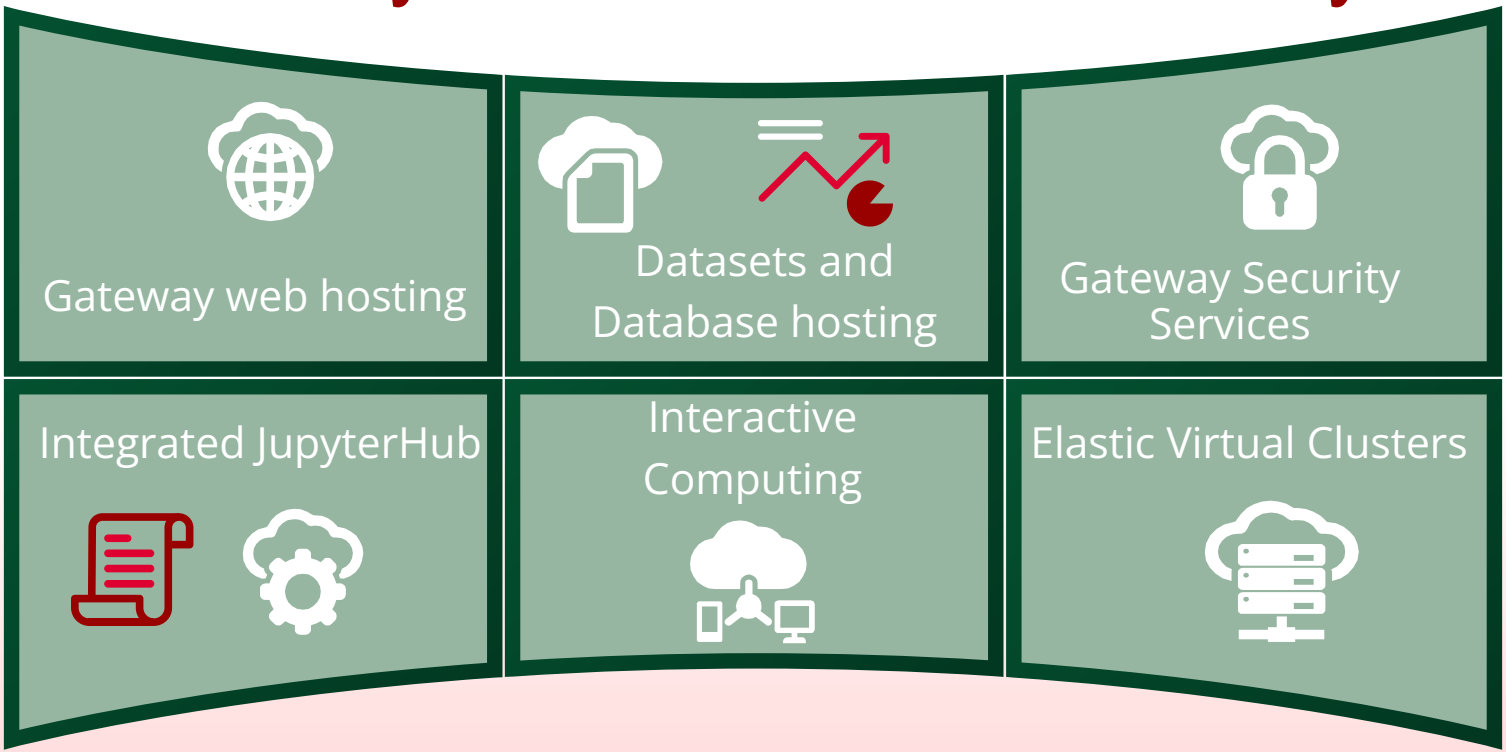
Gateways use JS2 in several ways



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Elastic Virtual Clusters

One Click OnDemand Cluster Augmenting the cloud capabilities

- Bundled lightweight HPC Stack, including SLURM.
- Users deploy scientific software with complete OS control.
- Dedicated and Responsive scheduler for rapid testing and development like workloads.
- Mounted persistent storage.

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A few key stats…

3,200

Users using Jetstream2 directly since June 2022

198,000

Users using Jetstream2 via Science Gateway

74

Fields of science represented on Jetstream2

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Accessing Jetstream2

Go To https://jetstream-cloud.org/

Before you can use Jetstream2 you must first have an Access ID and be on an active Jetstream2 allocation!

What is Access?

Provides Access to National Advanced Computing Resources

https://access-ci.org/

The NSF's ACCESS (Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support) program builds upon the successes of the 11-year XSEDE project, while also expanding the ecosystem with capabilities for new modes of research and further democratizing participation.

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Getting Your Own Allocation

https://access-ci.org/

Applying for an allocation is like applying for a small grant that provides computational resources.

The first level of application “Explore ACCESS” is a single form and only takes a few minutes approval comes at the longest in a few days.
~$40,000 worth of cloud resources for a few minutes of effort.

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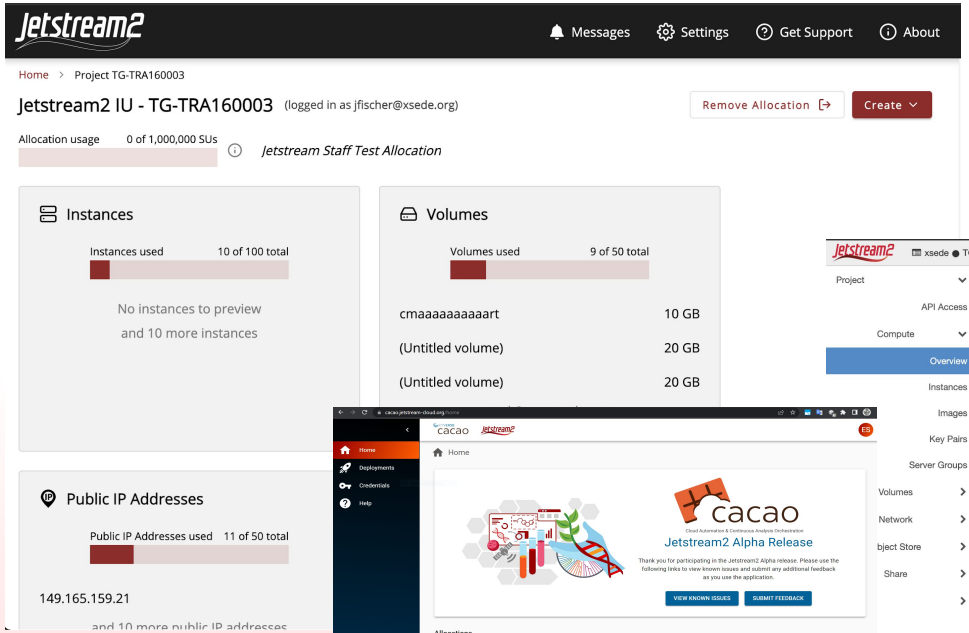
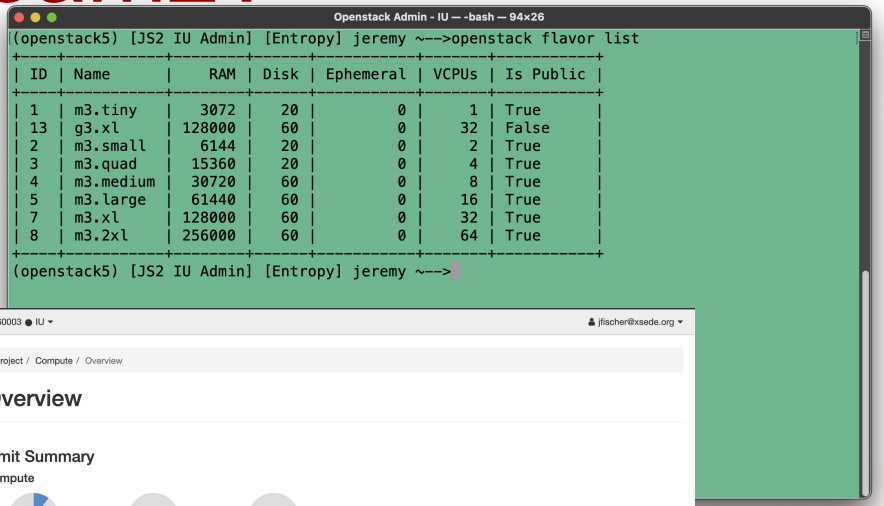
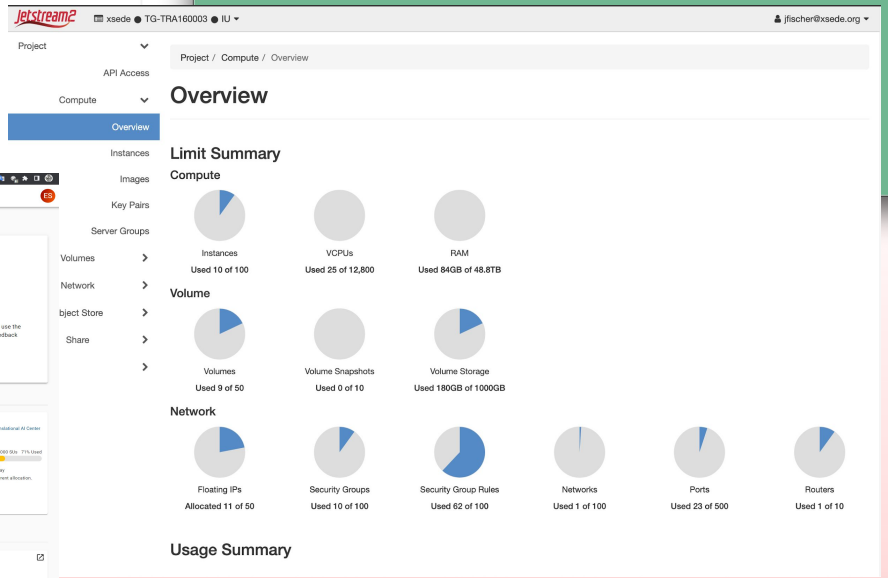
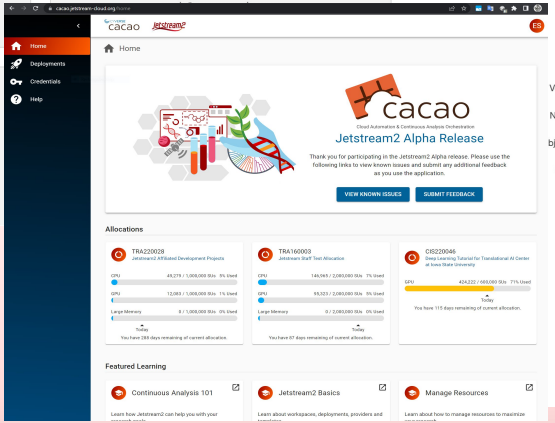
How do I access Jetstream2?









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https://docs.jetstream-cloud.org/overview/overview-doc/

Using and preserving VMs

- You can install just about anything*
  - But generally limited to Linux**
- Snapshots are fairly simple and easily shared with your allocation
- One general practice is often to pull from Git(hub/lab) or pull a container

* Standard warnings about licensed software here.

** Here there be dragons.

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Jetstream2 Allocation/Usage Considerations

- No scheduled downtime for upgrades
  - Upgrades are generally done while the system stays live overall
  - 99.87% availability for 9-7-22 to 3-31-23 (last NSF reporting period)
- Persistent IP addresses (for the life of an allocation if desired)
- No runtime limits – VMs can exist as long as there is an active allocation with SUs available
- No allocation limits for SUs – if you can justify it and we can provide it, we do
- Instance, core, and ram limits are flexible and extendable – if you can justify it and we can provide it, we do
- Storage allocations are reasonably generous – 1TB default up to 50TB in volume, shared, or object storage

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Where can I get help?

Jetstream2 docs: https://docs.jetstream-cloud.org/

ACCESS docs: https://support.access-ci.org/

ACCESS Support Form: https://support.access-ci.org/open-a-ticket

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A (very) brief history with Unidata on Jetstream1 and 2

- One of the first allocations on Jetstream1 in 2016 early operations
- Ran a combination of API side and Atmosphere instances on Jetstream1
- Evolved into all API side by the end of JS1 with a large auto-scaling JupyterHub deployment based on Dr. Andrea Zonca's tutorials
- Early operations allocation on Jetstream2 in 2022 under a new allocation
- Continuing the JupyterHub deployment and EDEX operations
- Presently over 100 running instances on JS2 (about 30 labeled test)

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DeSouza award

Honorees of this award are exemplars of an inclusive community that promotes the **sharing of data, software, and ideas through computing and networking technology**. While direct involvement in the Unidata community is one avenue by which such contributions may be made, this is not a requirement — the distinguishing ethos of awardees is their contribution and dedication to **accessible and reproducible science and education** within the geosciences.

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PyAOS JupyterHubs - slide from Julien Chastang

- 1,400 Users for semester classes and workshops since 2020
- 19 Universities
- 22 Workshops
- ~ 90 Hubs launched
- Tailored to objectives of instructor / professor

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Deploy Kubernetes and JupyterHub

- On Jetstream 2 Openstack deployment
- Kubernetes for orchestration/networking/logging/resiliency
- JupyterHub runs a pod for each user across the cluster

https://docs.jetstream-cloud.org/general/k8skubespray/

https://zonca.dev/2022/03/jetstream2-jupyterhub.html

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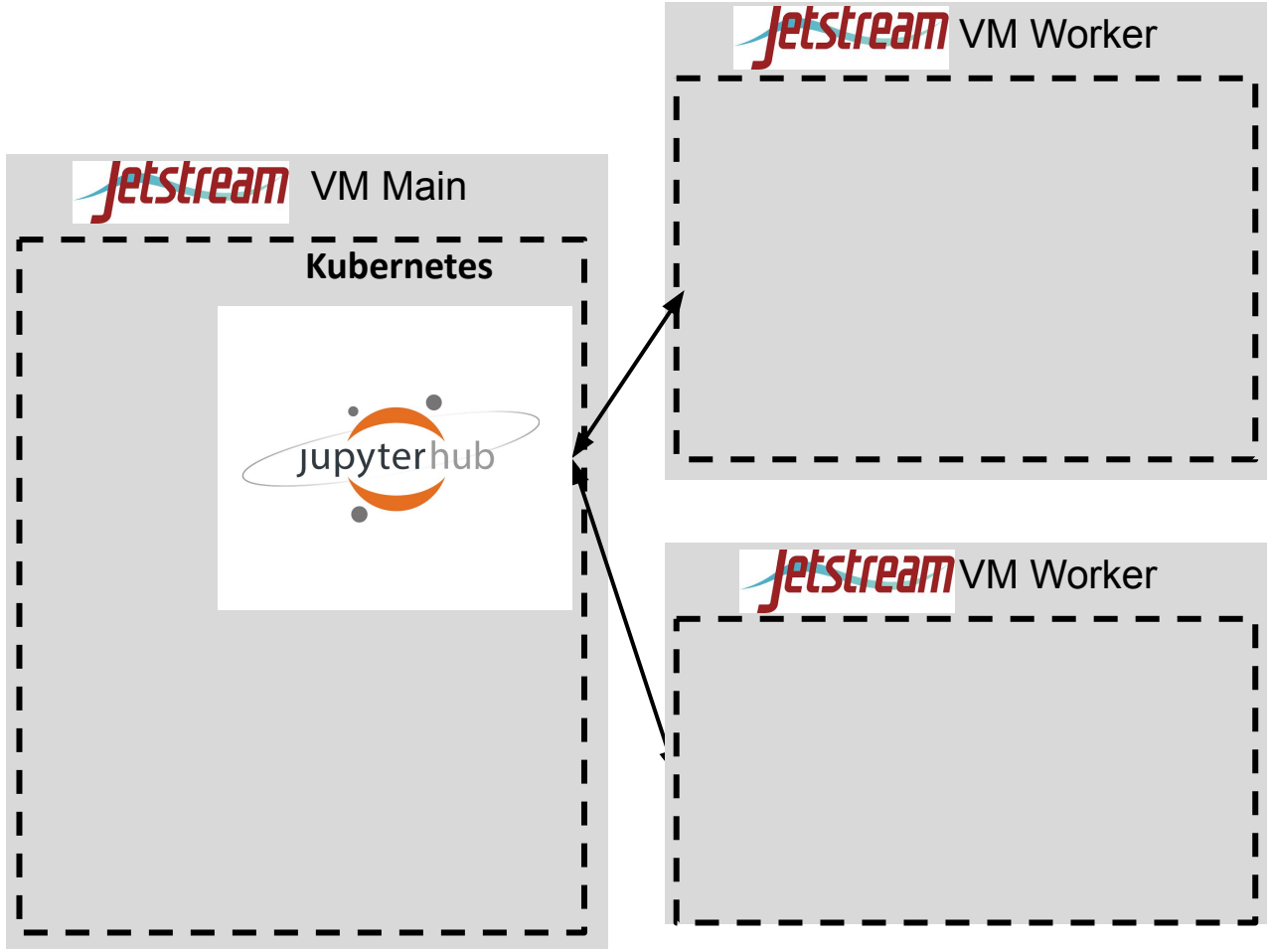
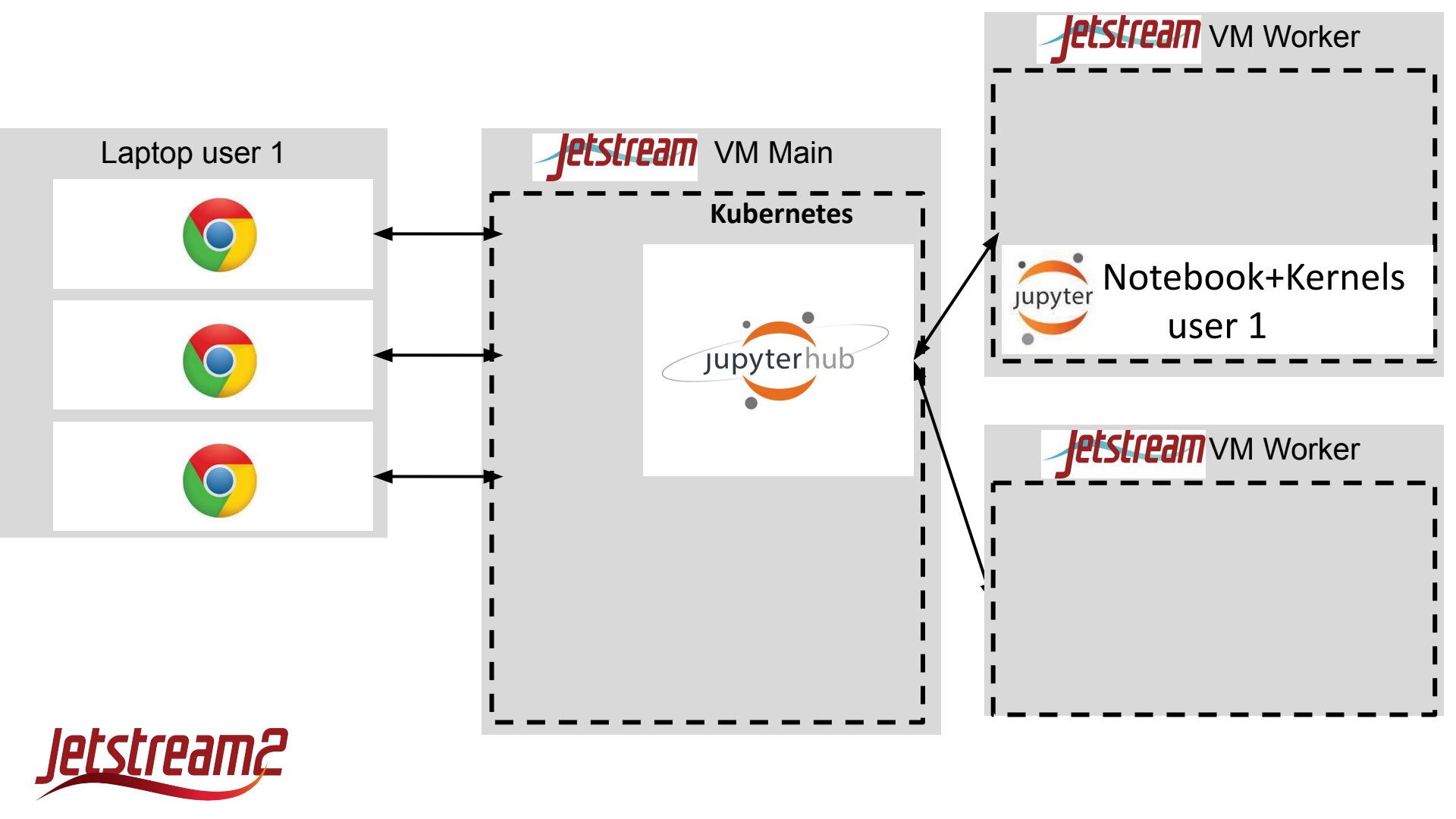
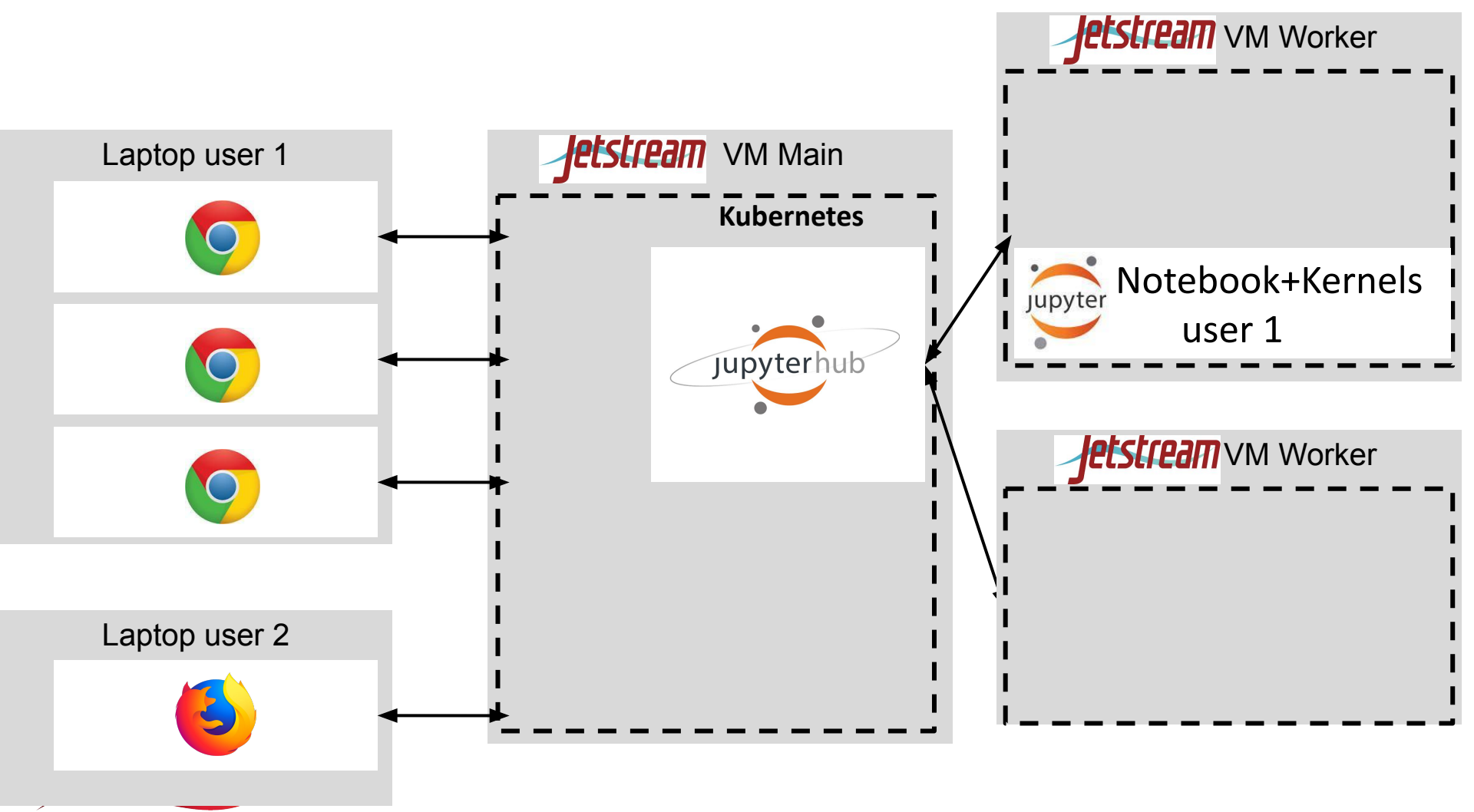
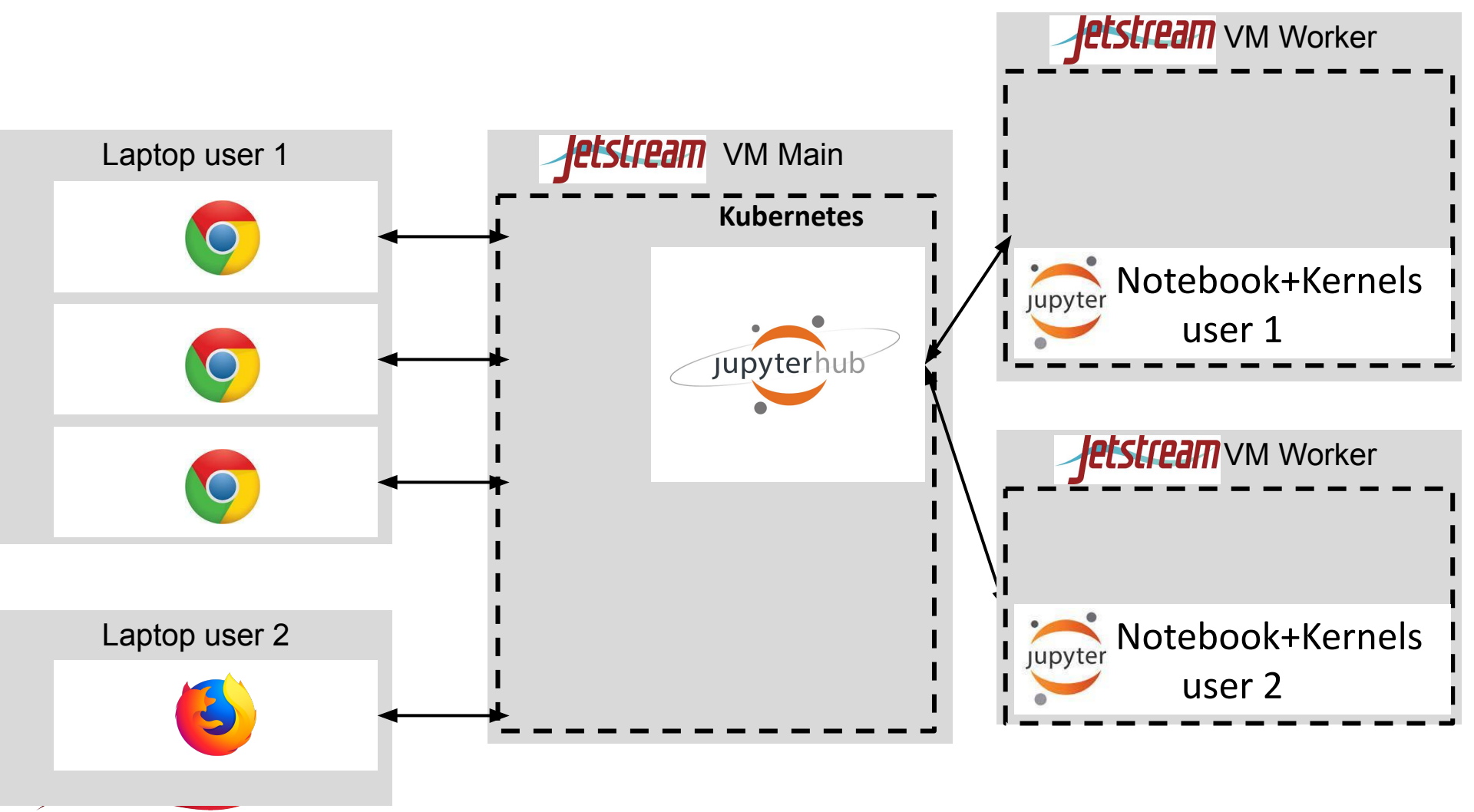

Jetstream VM Worker
Jetstream VM Main
Kubernetes
jupyterhub
Jetstream VM Worker

Jetstream2


Laptop user 1
Jetstream VM Main
Kubernetes
jupyterhub
Jetstream VM Worker
jupyter
Notebook+Kernels
user 1
Jetstream VM Worker
Jetstream2


Laptop user 1
Laptop user 2
Jetstream VM Main
Kubernetes
jupyterhub
Jetstream VM Worker
jupyter
Notebook+Kernels
user 1
Jetstream VM Worker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Laptop user 2
Jetstream VM Main
Kubernetes
jupyterhub
Jetstream VM Worker
jupyter
Notebook+Kernels
user 1
Jetstream VM Worker
jupyter
Notebook+Kernels
user 2

Deploy Dask Gateway

- Give more computational resources to users
- Use dask for high-level distributed computing

https://www.zonca.dev/posts/2023-09-28-dask-gateway-jupyterhub

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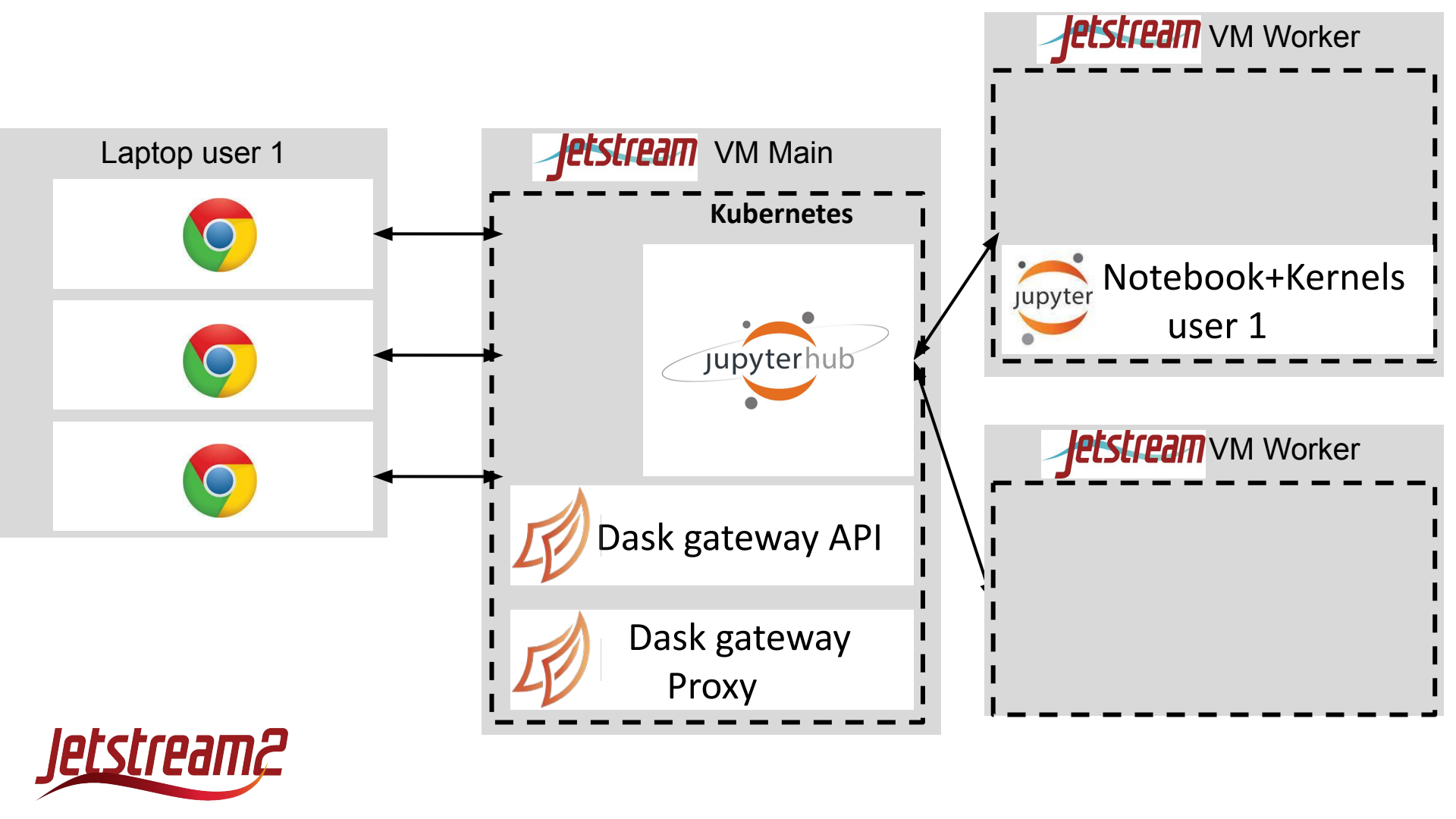
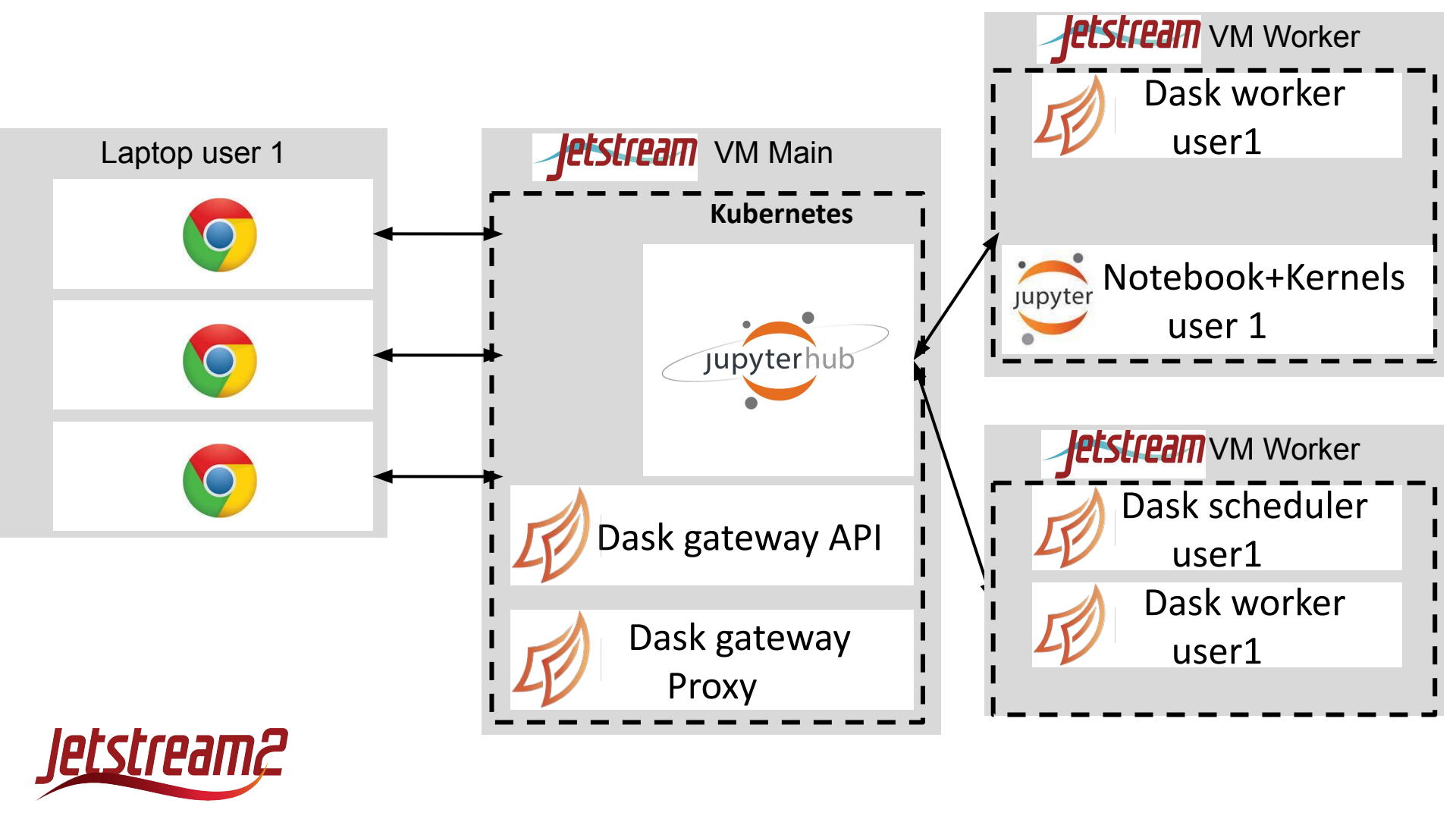

Laptop user 1
Jetstream VM Main
Kubernetes
jupyterhub
Dask gateway API
Dask gateway Proxy
Jetstream VM Worker
jupyter
Notebook+Kernels user 1
Jetstream VM Worker
Jetstream2


Laptop user 1
Jetstream VM Main
Kubernetes
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Dask gateway API
Dask gateway Proxy
Jetstream VM Worker
Dask worker user1
jupyter
Notebook+Kernels user 1
Jetstream VM Worker
Dask scheduler user1
Dask worker user1
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Parallel data storage with Object Store and Zarr

- Read/write data in parallel to Object Store with dask in Zarr format
- Zarr is a cloud-native file format for chunked/compressed/multi-dimensional arrays

https://www.zonca.dev/posts/2022-04-04-zarr_jetstream2

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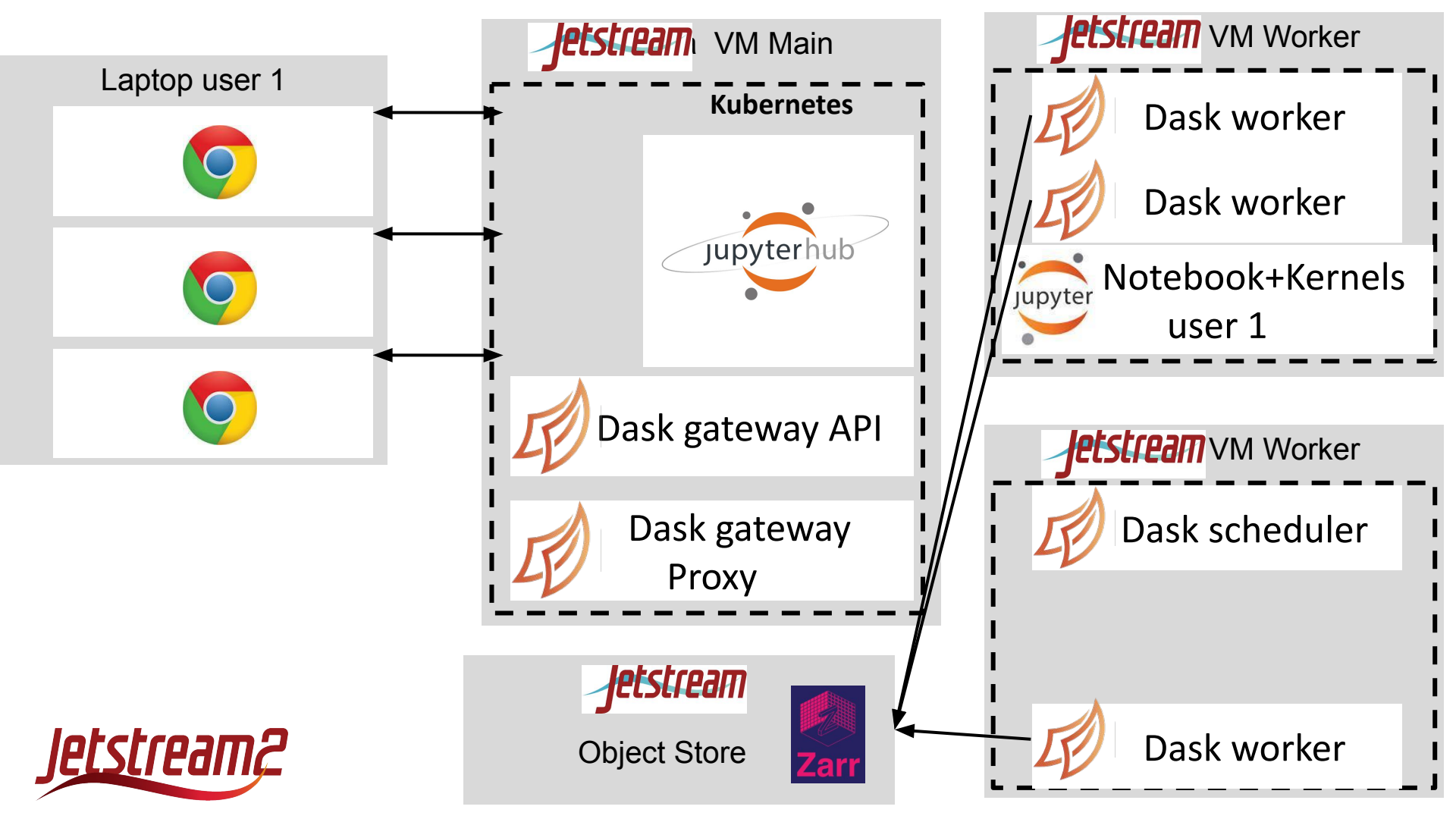
Laptop user 1
Jetstream VM Main
Kubernetes
jupyterhub
Dask gateway API
Dask gateway Proxy
Jetstream VM Worker
Dask worker
Dask worker
jupyter
Notebook+Kernels user 1
Jetstream VM Worker
Dask scheduler
Dask worker
Jetstream
Object Store
Zarr
Jetstream2

Deploy on GPU nodes

- Make GPUs available to containers running in Kubernetes
- Ideal for ML/AI applications

https://docs.jetstream-cloud.org/general/k8sgpu/

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Share volume across all JupyterHub users

- In case object storage is not suitable for a specific use-case
- Set read-only or read-write permissions by folder
- NFS service provided by Jetstream 2 via Manila

https://www.zonca.dev/posts/2022-12-05-jetstream2-kubernetes-manila

- Runs as a container in Kubernetes
- Saves data to persistent volume
- Expose SSH port externally for terminal access

https://www.zonca.dev/posts/2023-02-06-nfs-server-kubernetes-jetstream

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Shared persistent dask cluster

- Alternative to Dask Gateway
- 1 persistent cluster
- Multiple users accessing the same cluster

https://www.zonca.dev/posts/2018-05-04-shared-dask-kubernetes-jetstream.html#install-dask

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Load software stack from CVMFS

- CernVM File System software distribution service
- Used in High Energy Physics
- Runs in docker container managed by Kubernetes
- Caches software in a persistent volume
- Mounted through NFS in all users' JupyterHub containers
- Provides Jupyter Kernels

https://www.zonca.dev/posts/2020-02-26-kubernetes_cvmfs

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Deploy MariaDB database

- Runs as a container in Kubernetes
- Run separate pod for terminal access, e.g. ingest/dump data
- Either accessible from the web or just internally within the Kubernetes deployment

https://www.zonca.dev/posts/2022-06-06-mariadb

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Deploy BinderHub

- Instead of JupterHub, deploy BinderHub
- No persistent user data
- Builds containers on the fly based on Github repo

https://www.zonca.dev/posts/2022-11-15-binderhub-jetstream2

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Nightly backup of user data

- Automated volume backup system
- Saves offsite to Open Science Network object store
- Notifies admin if backup fails to notify completion

https://www.zonca.dev/posts/2021-04-19-jetstream-backup-kubernetes-volumes-object-store

https://www.zonca.dev/posts/2022-04-27-monitor-restic-backups-kubernetes

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Experimental autoscaling

- Adds and removes Virtual Machines based on load
- Runs as a service inside Kubernetes

https://www.zonca.dev/posts/2021-01-20-autoscaling_script_kubespray_jupyterhub

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In progress: Run Singularity containers inside Kubernetes

- Tutorial I'm currently working on
- Execute Singularity containers commands inside Docker
- Use Singularity containers as kernel providers for Jupyter

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In progress: Load balancer for High Availability Kubernetes

- Single point of failure in current setup is we the master node
- Use a load balancer provided by Jetstream 2
- Support multiple master nodes

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Conclusion

Interest in deploying services on Jetstream 2? Contact us

See the in-depth tutorial video about Distributed Computing with Dask on Jetstream 2 at the Gateways 2023 conference:

zonca.dev/posts/gw23

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Award #ACI-2005506

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