Interactive distributed computing with Jupyter, Python and Dask on Jetstream2 for Science Gateways

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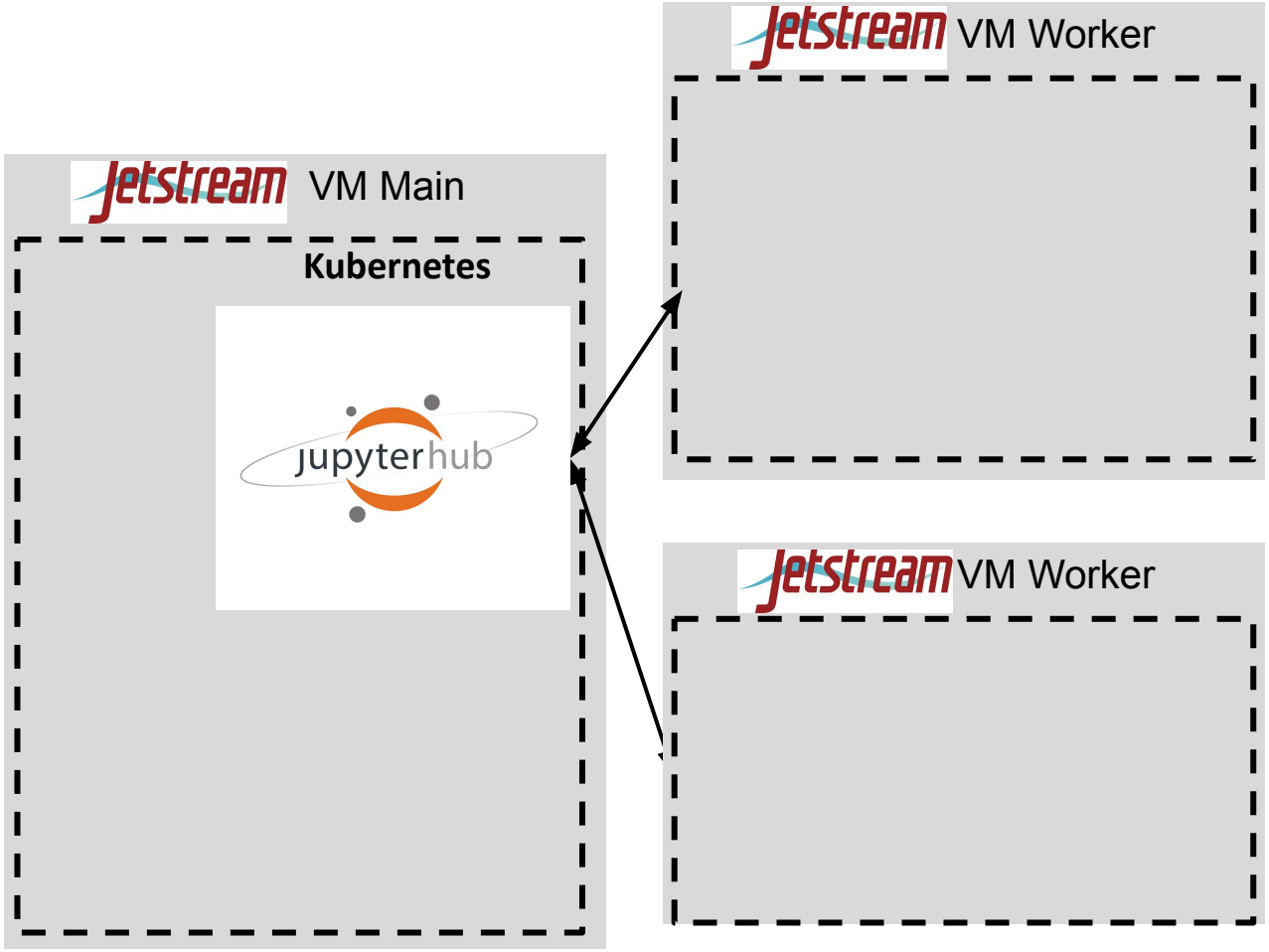
Deploy Kubernetes and JupyterHub

- 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


Jetstream VM Worker
Jetstream VM Main
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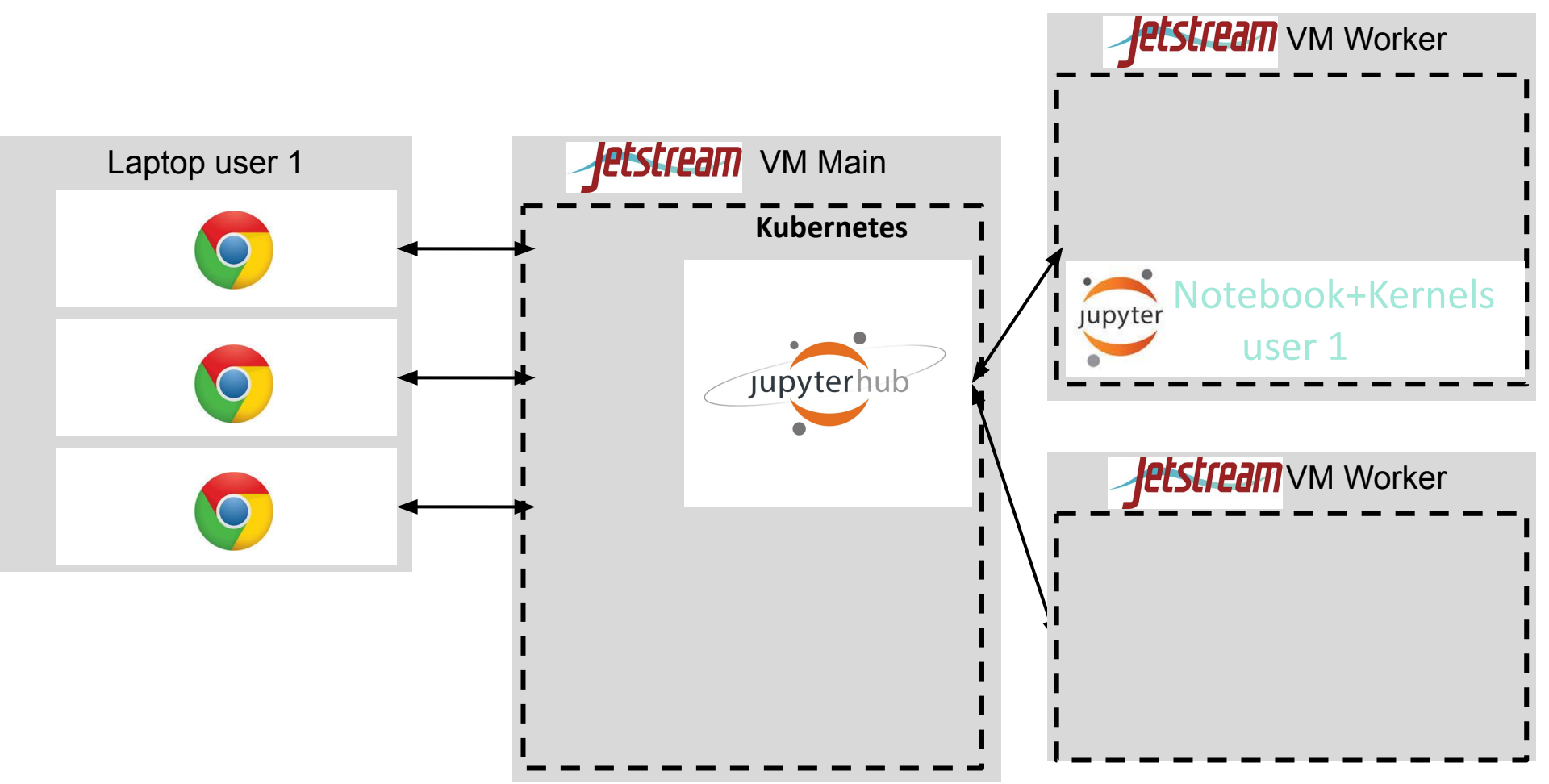
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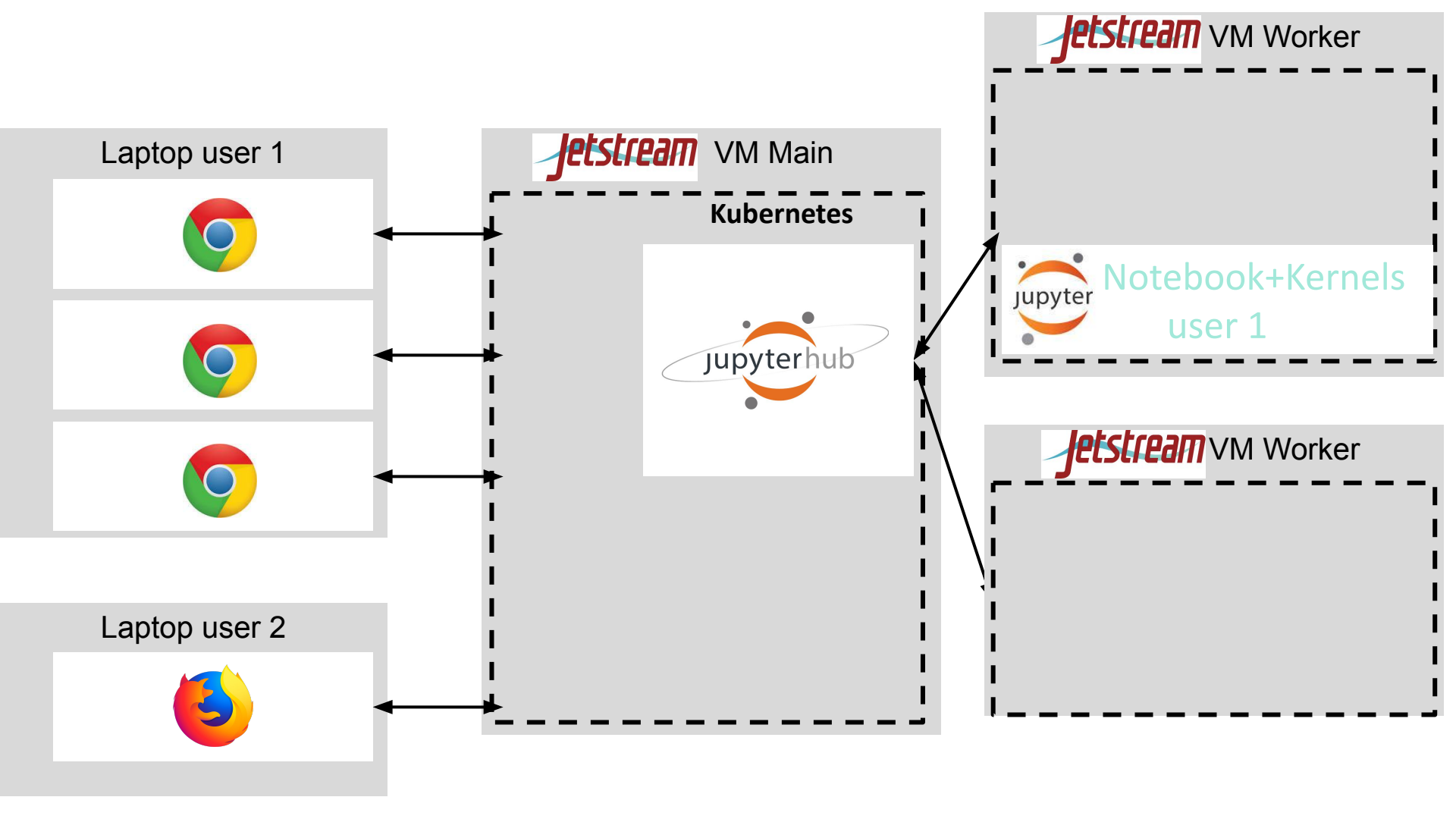
jupyter
Notebook+Kernels
user 1
Jetstream VM Worker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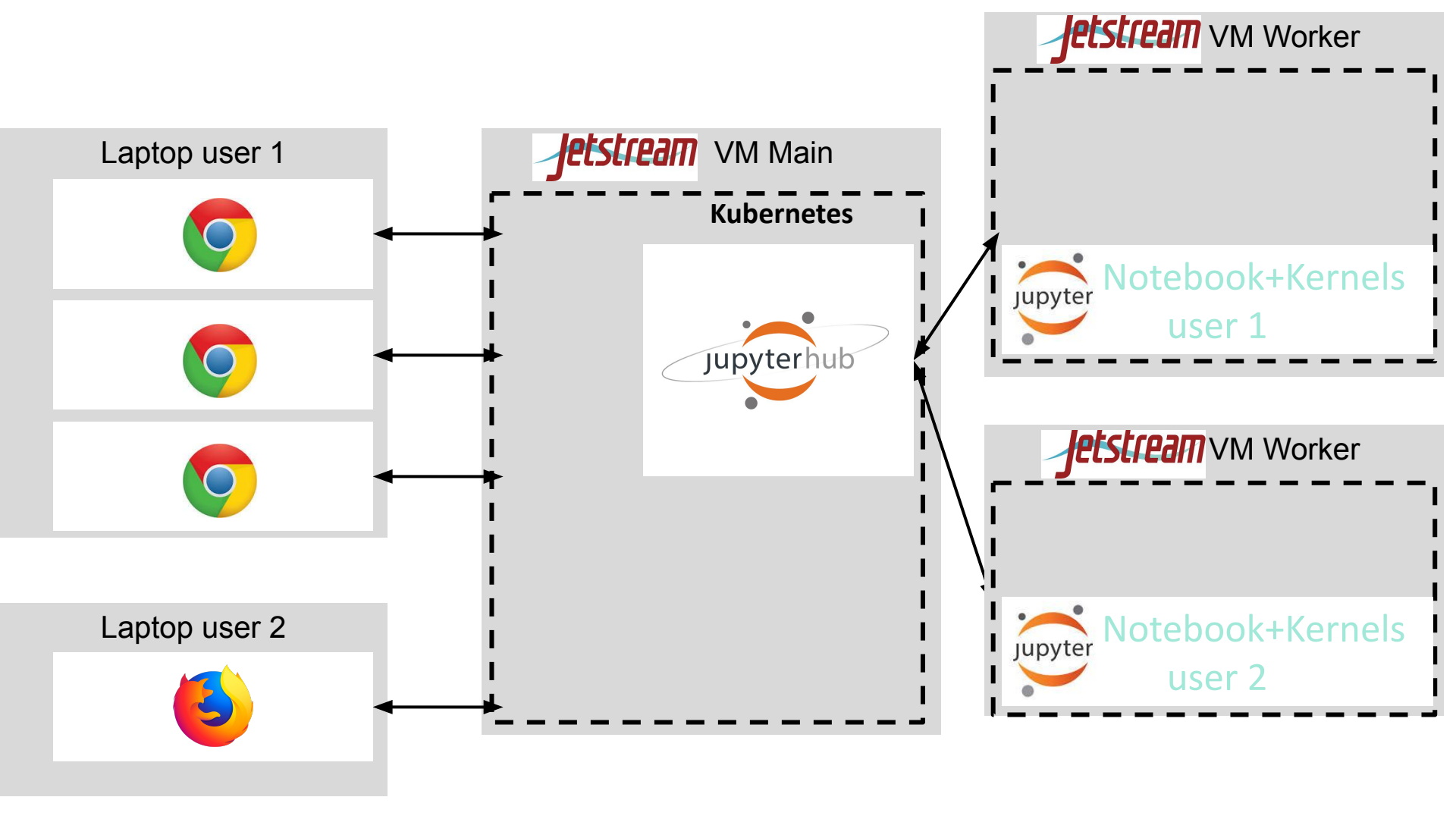
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Jetstream VM Worker
jupyter
Notebook+Kernels
user 2

Hands-on: Login to JupyterHub

Point browser to:

bit.ly/gw23jhub

Authenticate with any Github account

Open terminal:

```
git clone https://github.com/zonca/dask-jetstream-tutorial
```

Execute `01_enviroment.ipynb`

Hands-on: Dask tutorial with local threads

Point browser to:

bit.ly/gw23jhub

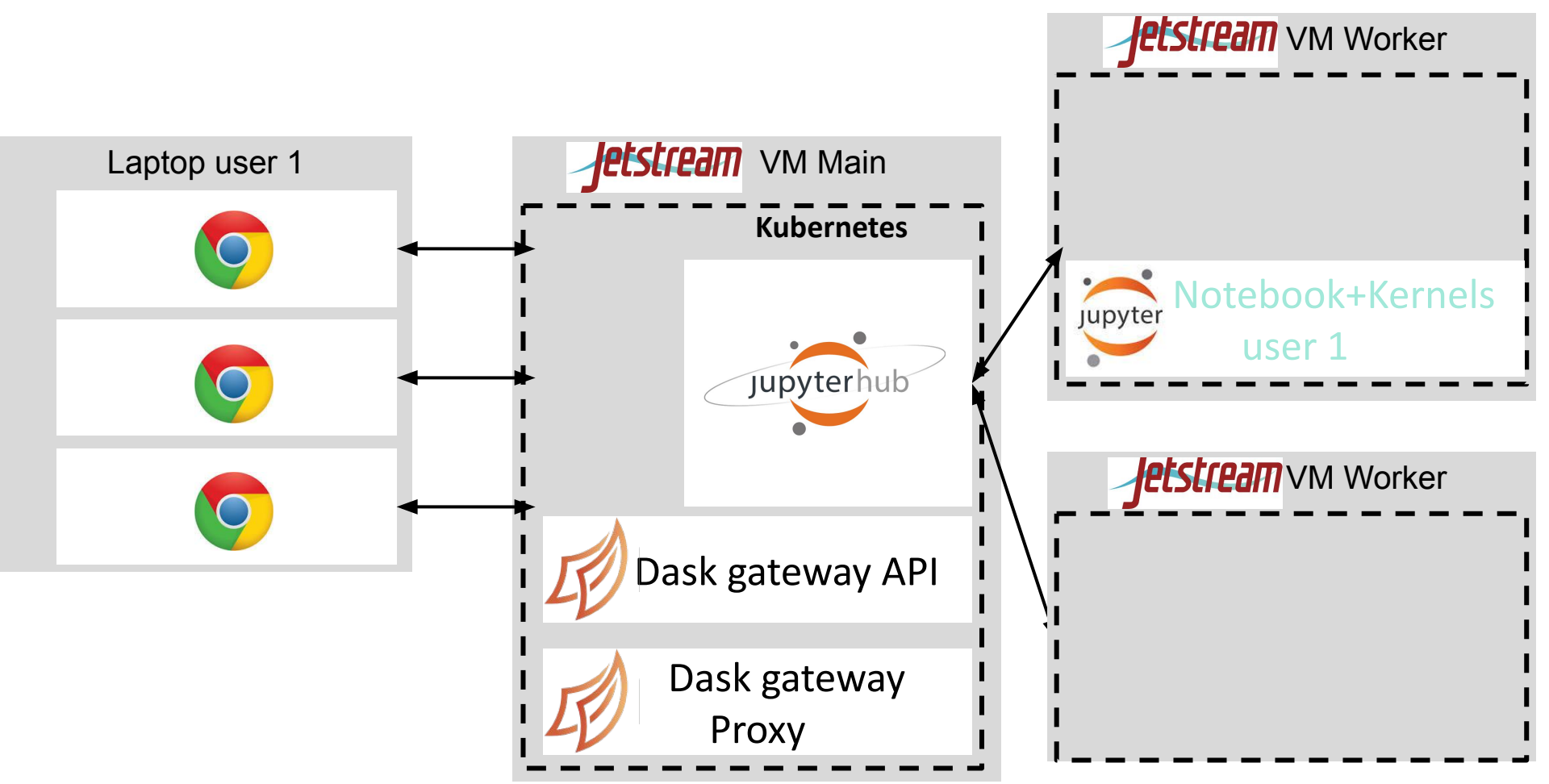
Dask - single machine - local threads scheduler

- **`00_install_dot.ipynb`**
- **`02_dataframe.ipynb`**
- **`03_array.ipynb`**
- **`04_delayed.ipynb`**

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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Notebook+Kernels user 1
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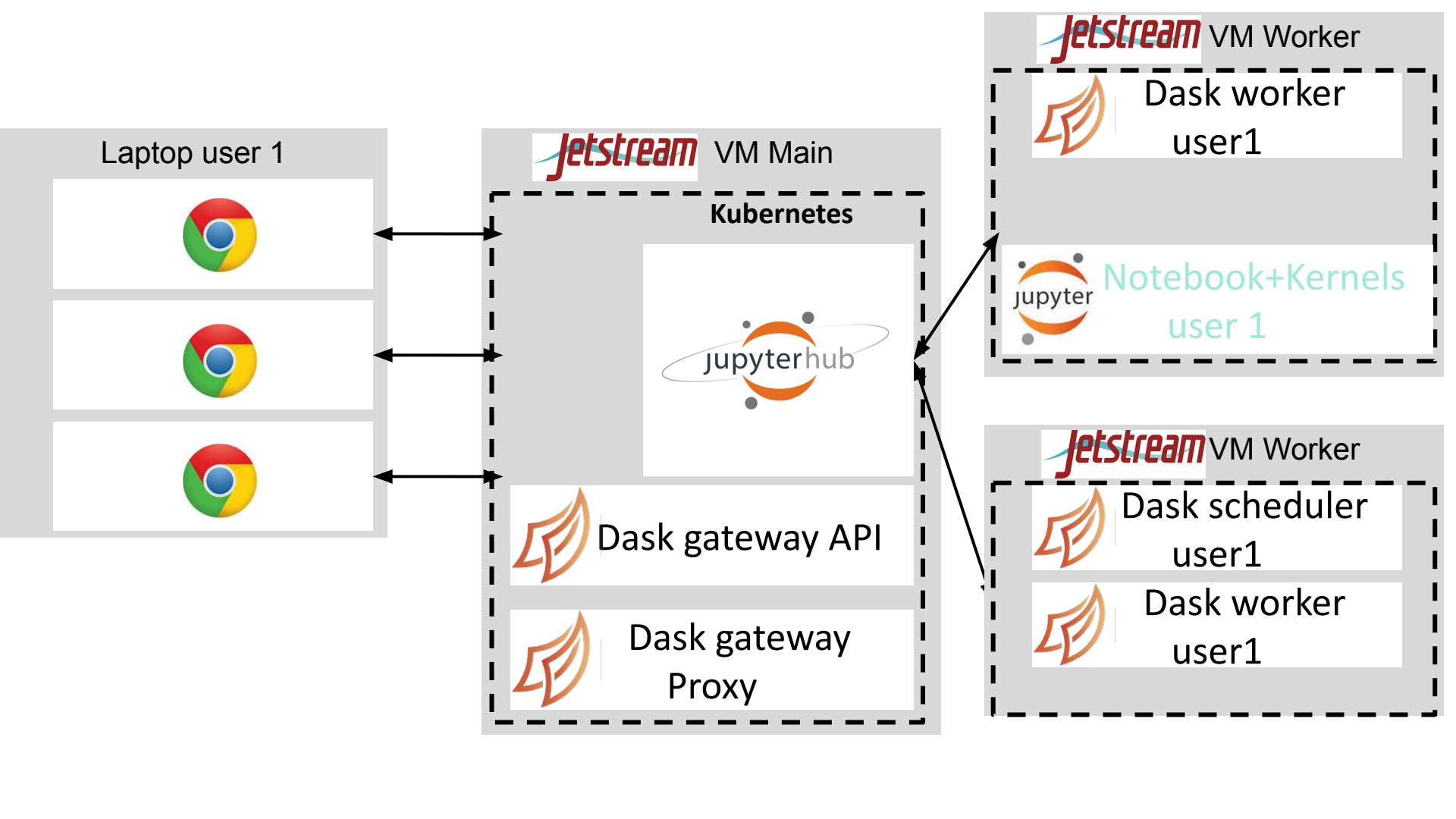
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Dask worker user1
jupyter
Notebook+Kernels user 1
Jetstream VM Worker
Dask scheduler user1
Dask worker user1

Hands-on: Dask tutorial with Dask gateway workers

Point browser to:

bit.ly/gw23jhub

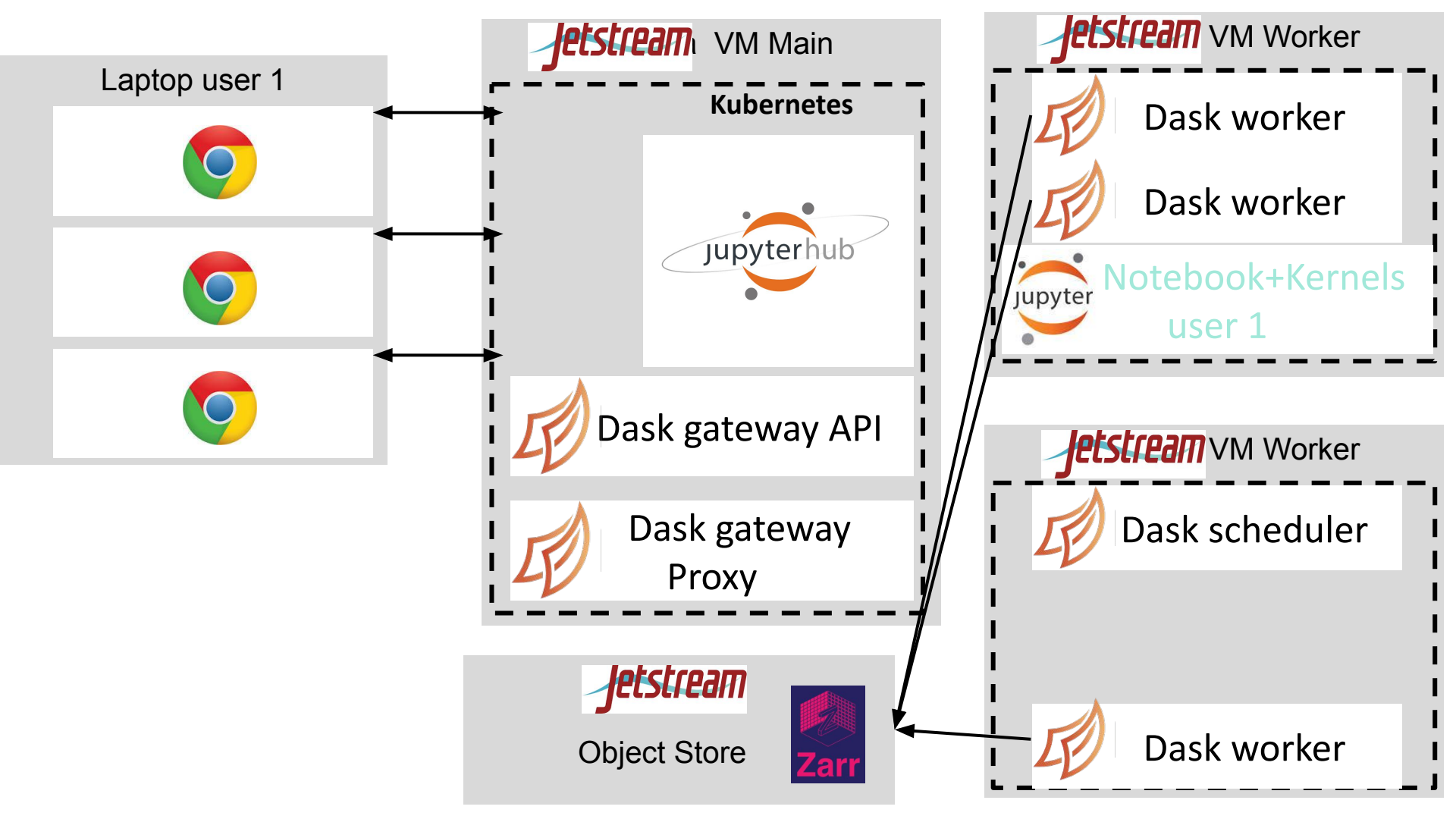
Dask - 2 workers - distributed scheduler

- **`05_dask_gateway.ipynb`**
- **`06_array_distributed.ipynb`**

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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Dask worker
Dask worker
jupyter
Notebook+Kernels user 1
Jetstream VM Worker
Dask scheduler
Dask worker
Jetstream
Object Store
Zarr

Hands-on: Write data to Object Store in Zarr format

Point browser to:

bit.ly/gw23jhub

Dask - write to object store with Zarr

- **`07_zarr_object_store.ipynb`**

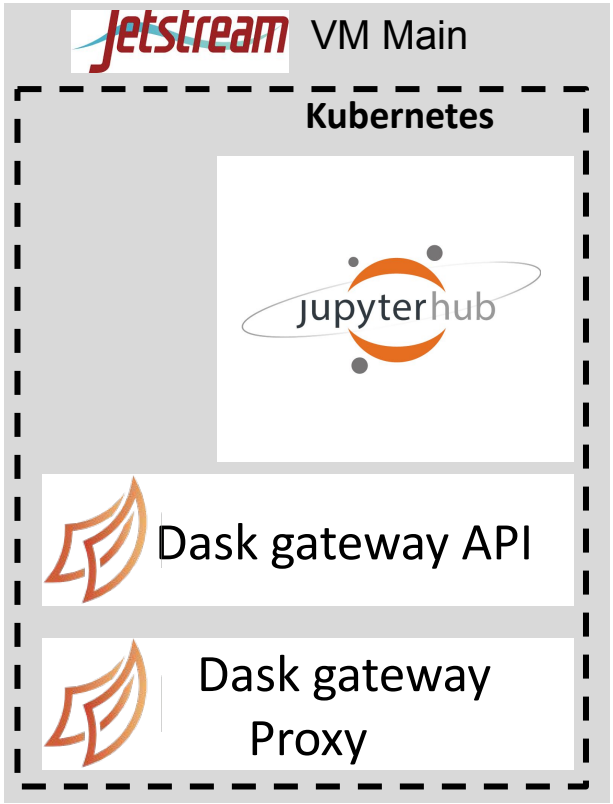
The end

Links, slides, tutorials: zonca.dev/posts/gw23

Email Andrea Zonca (zonca@ucsd.edu), or let's meet in Pittsburgh!

Acknowledgments: thanks to Indiana University and the Jetstream team for funding this work.

Backup slides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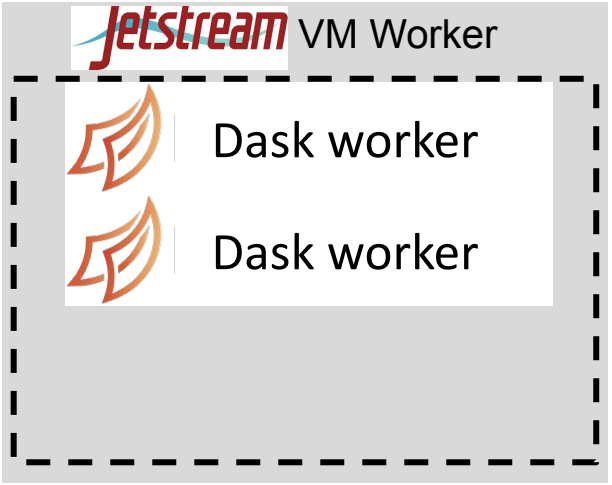
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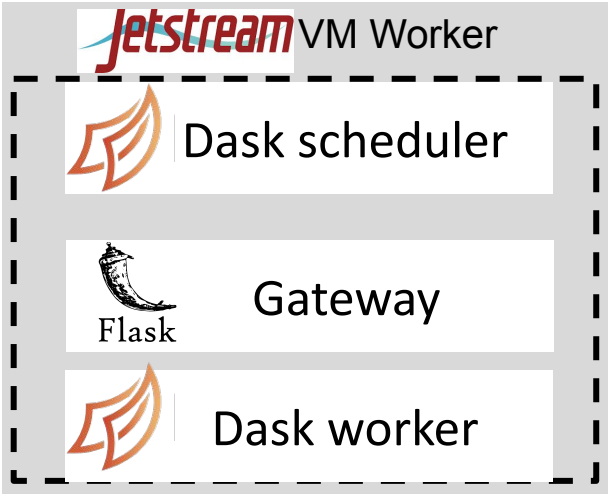
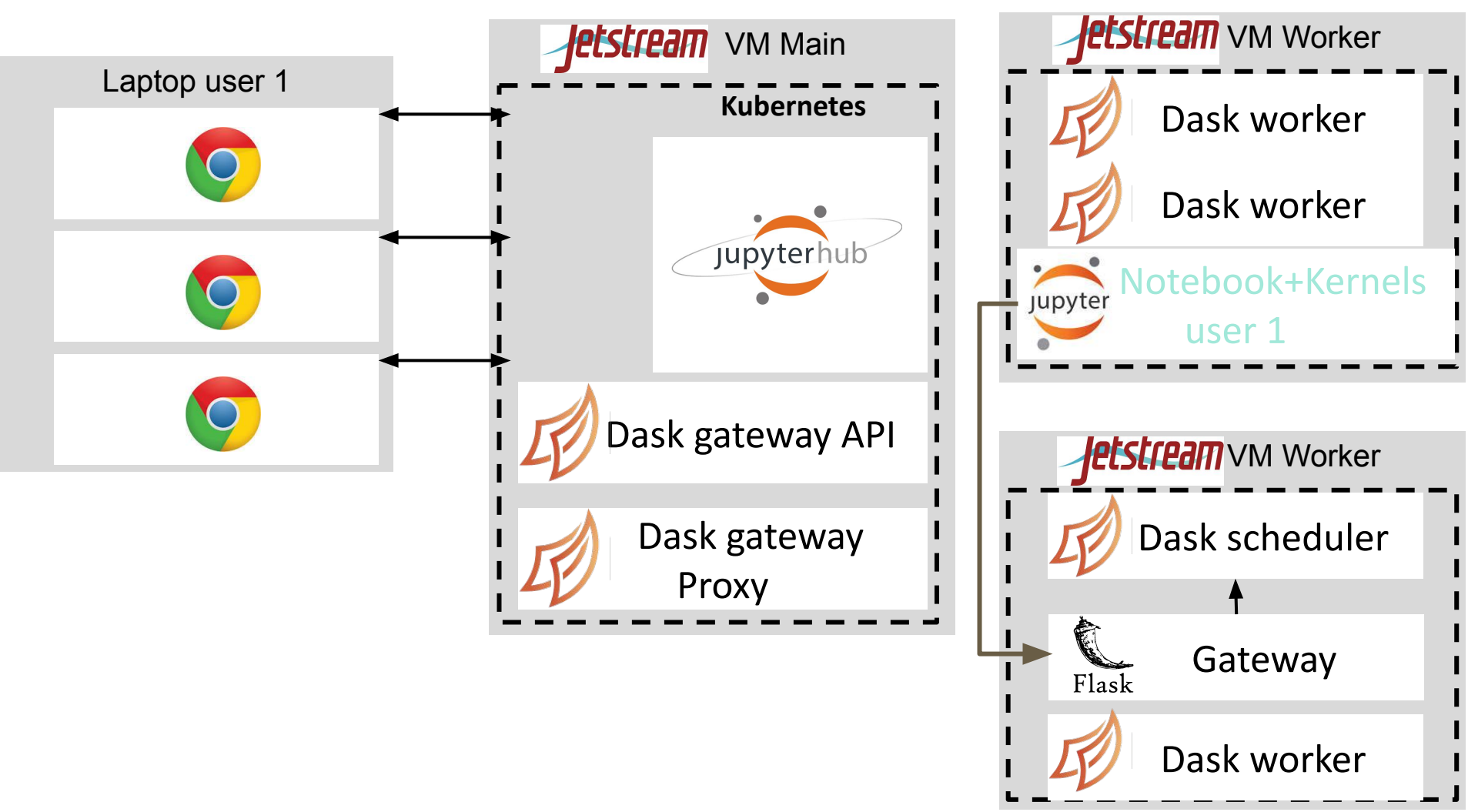
Dask worker
Dask worker


Jetstream
VM Worker
Dask scheduler
Flask
Gateway
Dask worker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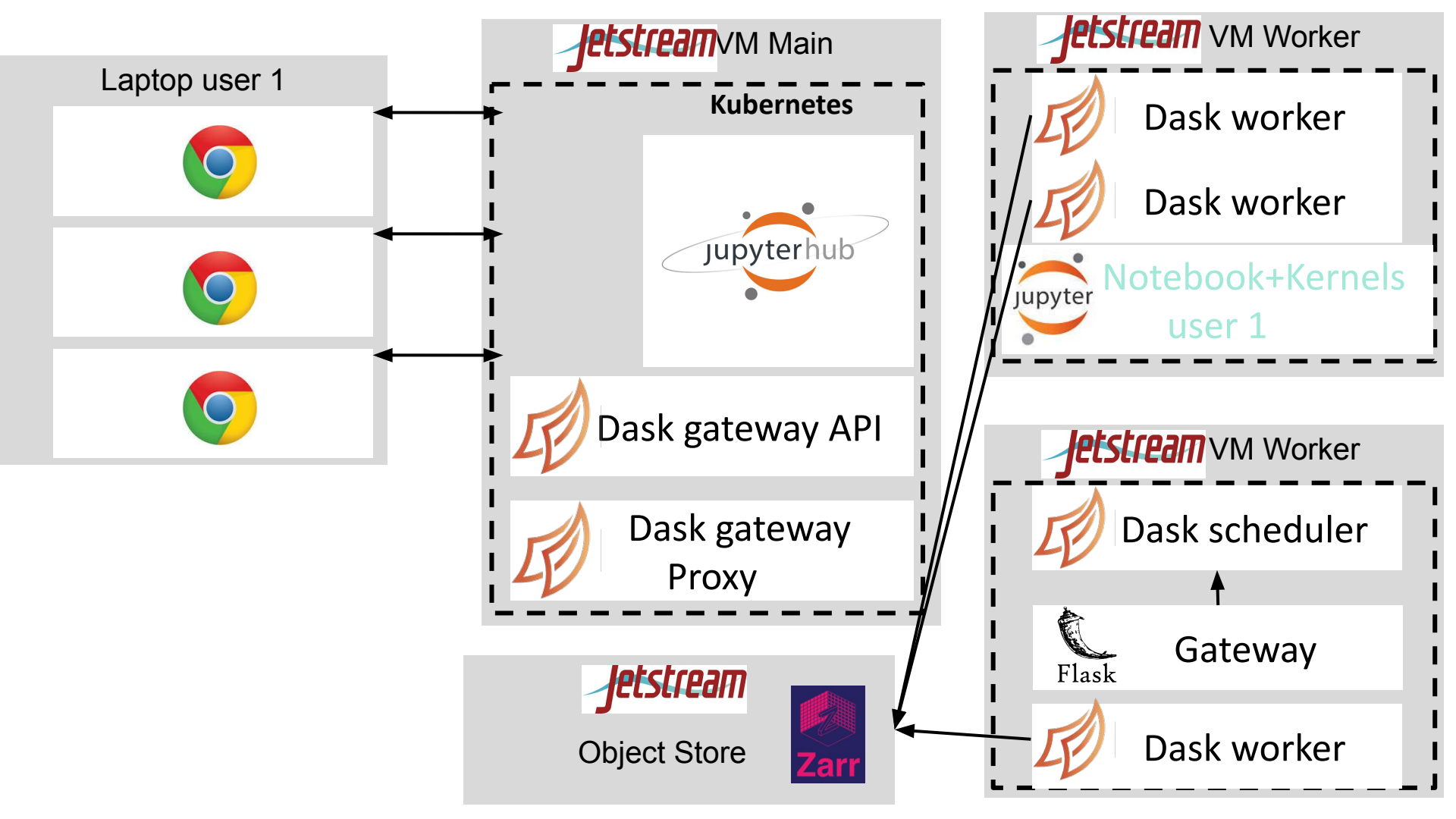
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