Cloud HPC for UM-Bridge Models

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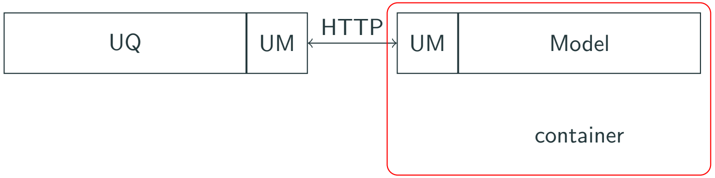
UM-Bridge and HPC

Goal: "Automagically" scale up UM-Bridge models for challenging UQ problems; keep UQ client simple

Wish list:

- Avoid machine specific model setup
- Many instances of (in turn parallel) UM-Bridge models
- Single point of entry for UQ, load balancing

UM-Bridge: Containerization - Portable Models



- Run tsunami model as easy as

```
docker run -p 4242:4242 linusseelinger/model-exahype-tsunami
```

- Evaluate model in python:

```
model = umbridge.HTTPModel('localhost:4242', 'forward')
model([[0.1,0.4]])
```

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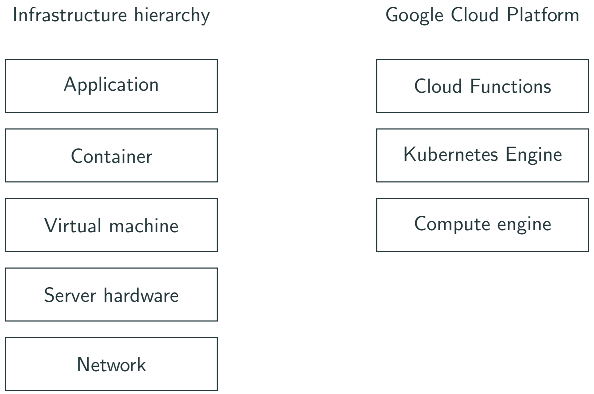
HPC and Cloud Convergence

- HPC systems moving towards containers for portability
- Cloud systems moving towards HPC support

$\Longrightarrow$ HPC and cloud are (somewhat) converging

We go with cloud systems for excellent container support

Overview: Cloud Infrastructure



Servers for rent, (very) different levels of abstraction possible

Kubernetes: "Container orchestration" - fully reproducible HPC setups

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Kubernetes

kubernetes

"Kubernetes, also known as K8s, is an open-source system for automating deployment, scaling, and management of containerized applications."

K8s setup defined through config files

$\rightarrow$ Reusable configuration of UM-Bridge models, load balancers etc.

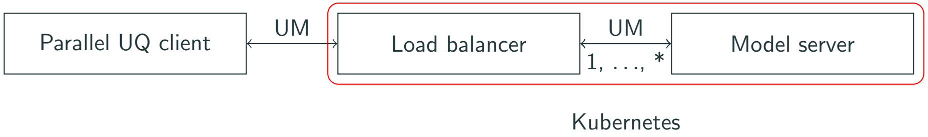
UM-Bridge Kubernetes Support

UM-Bridge currently provides two kubernetes configurations:

Parallel model instances,

- single node models
- multinode MPI parallel models

Kubernetes Configuration - Sequential Model



Pre-built configuration, simply plug in your own model container

UQ client only sees an UM-Bridge server. But may make parallel requests!

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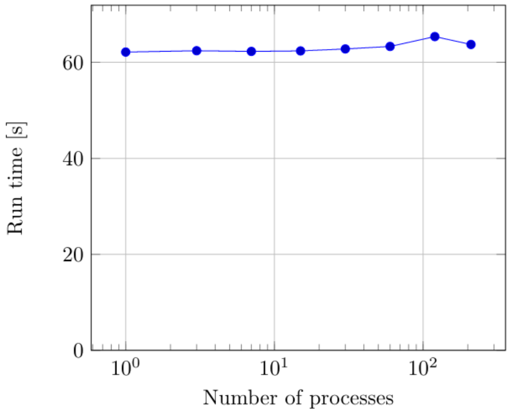
- Single point of entry for UQ, load balancing
  $\rightarrow$ UM-Bridge kubernetes config! ✓

Model Configuration: `model.yaml`

```yaml
apiVersion: apps/v1
kind: Deployment
metadata:
  name: model-deployment
spec:
  selector:
    matchLabels:
      app: model
  replicas: 4
  template:
    metadata:
      labels:
        app: model
    spec:
      containers:
      - name: model
        image: linusseelinger/model-l2-
             sea
        resources:
          requests:
            cpu: 1
            memory: 1Gi
          limits:
            cpu: 1
            memory: 1Gi
```

- `image`: Docker image with UM-Bridge model server (e.g. from Docker Hub)
- `replicas`: Number of model instances
- `requests` / `limits`: CPU and memory resources

Scalability (Preliminary)



- Model: L2-Sea
- Client: QMCPy with (unmodified!) thread parallelism
- Good weak scalability to 210 instances

Demo

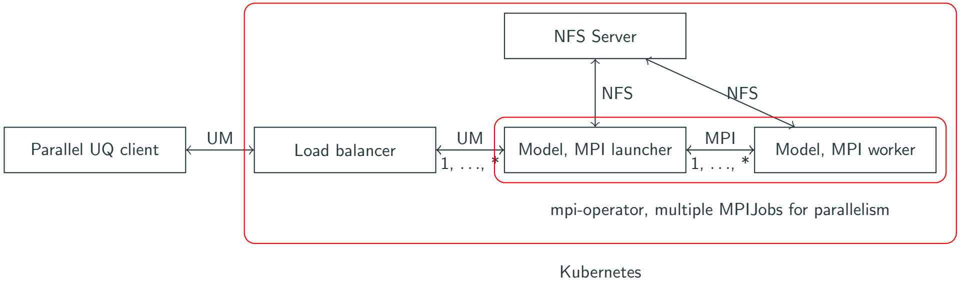
Demo: UM-Bridge Models on Google Kubernetes Engine

MPI Parallel Models

MPI Parallel Models

- MPI *within* containers trivial, but restricted to one hardware node
- MPI *across* containers/nodes: Separate kubernetes configuration
  Requires `mpioperator` base image for model container

Kubernetes Configuration - MPI Parallel Model



Pre-built reference configuration

Shared filesystem between nodes via NFS

Support for OpenMPI, Intel MPI, MPICH in the future

Minor restrictions on model container

Conclusions

Conclusions

- No model setup (due to containers)
- Reusable kubernetes configurations provided by UM-Bridge
- Simple UQ client can control HPC scale model