

Introduction to Docker containers

containerized UM-Bridge models/benchmarks

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Agenda

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Introduce Docker containers and how they are used in UM-Bridge to provide access to models and benchmarks.

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This Talk covers:

- Introduction to Docker Containers
- How docker containers are used in UM-Bridge
- How to set them up
- How to run them
- Overview of UM-Bridge models and benchmarks library

Docker containers

Brief Summary

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UM-Bridge benchmark library

Models and benchmark implementations support the UM-Bridge interface and are provided as containers for portability and ease of use.

Why use docker?

- **Easy installation:** The installation process for any model or benchmark comes down to a single docker command.

Why use docker?

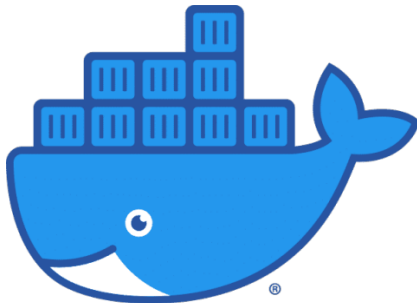
- **Easy installation:** The installation process for any model or benchmark comes down to a single docker command.
- **System independent:** The installation/running of a model/benchmark no longer relies on assumptions on the users OS or installed packages/software or versions.

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- **System independent:** The installation/running of a model/benchmark no longer relies on assumptions on the users OS or installed packages/software or versions.
- **Easy access to HPC resources:** UM-Bridge allows for easy access to HPC-scale performance in cloud computing environments. Model containers can be run on any kubernetes cluster without modification.

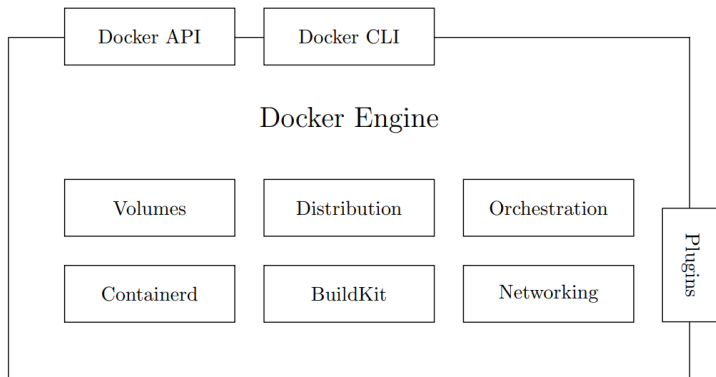
UM-Bridge provides a reference kubernetes configuration which takes care of load balancing on large-scale clusters. The UQ software can then make use of parallel model instances simply by making concurrent model calls.

What is docker?



- A Docker container image is a lightweight, standalone, executable package of software.
- The container packages code, runtime, system tools, system libraries and settings.

What is docker?



Useful Links

- For installation guidelines for most operating system look at:
<https://docs.docker.com/engine/install/ubuntu/>
- Docker has an extensive documentation at: <https://docs.docker.com/get-started/>
- The tutorials at <https://diveintodocker.com/> may also be interesting

Hello World

Let's test it

```
docker run hello-world
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- If the `hello-world` image does not exist locally it will be pulled from `dockerhub`
- Allows you to test your `docker` installation

A simple container

Let's try it for another simple example

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- `-i` or `--interactive` starts an interactive docker container. We connect to the container's `stdin`.

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- `-it` is shorthand for `-i -t`
- `-i` or `--interactive` starts an interactive docker container. We connect to the container's `stdin`.
- `-t` gives us access to the terminal in the docker container

A simple container

Inside the container we can run ubuntu commands:

```
apt update && apt install -y figlet  
figlet hello world
```

- We have installed the package necessary to run the hello world command from the previous container and

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- run the same command ourselves

The Dockerfile

The corresponding Dockerfile would look like this:

Dockerfile

```
FROM ubuntu
```

```
RUN apt update && apt install -y figlet
```

```
CMD figlet hello world
```

Running the new container

To build an image from a Dockerfile running

```
docker build -t image-name .
```

- `-t` means tag and gives the image a name rather than meaning terminal as in the run command

Other basic Docker CLI commands

To see current images

```
docker image ls
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To remove specific images

```
docker image rm name
```

Creating your own Dockerfile

Some commonly used docker commands:

- FROM sets the base image
- RUN executes linux commands while building
- CMD executes linux commands while running
- WORKDIR sets the working directory
- ENV sets environment variables
- COPY copies data into the image

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To run our new server

- Run the container with that image (we will need to specify ports)
- Send requests for model evaluations via UM-Bridge
- If we need to tweak the model, update the Dockerfile and rebuild

UM-Bridge: Client

Connect to model

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Evaluate model

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print(model([[0.0, 10.0]]))
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Evaluate model

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```

Optionally, pass configuration options

```
print(model([[0.0, 10.0 ]], {"level": 0}))
```

Defining a model class

```
TestModel(umbridge.Model):  
    def getinputsizes(self):  
        # Number and dimensions of input vectors  
        return [1]  
    def getoutputsizes(self):  
        # Number and dimensions of output vectors  
        return [1]  
    def call(self, parameters, config ={}):  
        output = parameters[0][0]*2 # Do something with the input  
        return [[output]]  
    def supportsevaluate(self):  
        return True
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Serve model via HTTP:

```
testmodel = TestModel()  
umbridge.servemodel(testmodel , 4242)
```

Simple Example with UM-Bridge

- Grab the minimal server and copy it into the Dockerfile

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Simple Example with UM-Bridge

- Grab the minimal server and copy it into the Dockerfile
- Run the UM-Bridge server instead of our figlet command
- When running we need to specify the ports with `-p 4242:4242`
- Try this yourself in the tutorial

UM-Bridge Models/benchmarks

UM-Bridge Models & Benchmarks Library

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Maintain a curated set of ready-to-run benchmark problems and models which can be used to reproducibly compare UQ methods.

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Maintain a curated set of ready-to-run benchmark problems and models which can be used to reproducibly compare UQ methods.

- **Automated testing** and building via Github actions.
- Partially-automated **documentation**.
- **Ease of use:** Each model or benchmark can be accessed from any supported language through a simple function call

Mathematically, an UM-Bridge model is a function mapping parameter vectors onto model output vectors, supporting some of the following: evaluation, gradient evaluation, Jacobian action, or Hessian action.

UM-Bridge models may be used in multiple benchmarks, e.g. there may be an inference problem and a propagation problem in the benchmarks library using the same model.

UM-Bridge Models

Name	Short description
Euler-Bernoulli beam	Deformation of an Euler-Bernoulli beam with a spatially variable stiffness parameter
L2-Sea	Total resistance estimation of the DTMB 5415 destroyer-type vessel at model scale by potential flow
Tsunami	Propagation of the 2011 Tohoku tsunami modeled by solving the shallow water equations.
Composite material	Elastic deformation of an L-shaped composite part with random wrinkles.
Tritium Desorption	Microscopic transport of tritium through fusion reactor materials using the Foster-McNabb equations.
Agent based disease transmission	Transmission of disease in a heterogenous population using EMOD, a stochastic agent based disease transmission model.
Membrane model	Determines the deformation of a membrane for a fixed right hand side given the stiffness values on an 8×8 grid that makes up the membrane.

UM-Bridge Benchmarks

Uncertainty quantification benchmarks are identical to models regarding implementation of both server and client. They only differ in that they fully define a UQ problem rather than just a forward model.

They are based on forward models of the previous section.

- The inference benchmarks define a complete Bayesian posterior density, including prior, likelihood and observations. The goal is then to determine the posterior distribution or quantities derived from it.
- The propagation benchmarks that are defined by a model and a specific distribution probability distribution. The goal is then to find the corresponding distribution of the model output, or a quantity derived therefrom.
- The optimization benchmark defines an optimization problem with a range of parameters under certain constraints.

UM-Bridge Inference Benchmarks

Name	Short description
Analytic densities	Infers the PDF of various analytic function.
Membrane model	Infers the PDF of stiffness values of a membrane from measured deformation data.
Tritium Diffusion Posterior	Computes the (unnormalised) posterior density of the input parameters given by experimental data.
Disease transmission model	Agent based model of disease transmission in an entirely susceptible population with correlation between disease acquisition and transmission. Provided problem is to infer the disease parameters that result in 40% of the population infected at the end of the outbreak.
Deconvolution problem	Defines a posterior distribution for a 1D deconvolution problem, with a Gaussian likelihood and four different choices of prior distributions with configurable parameter.
Computed Tomography	Defines a posterior distribution for a 2D X-ray CT image reconstruction problem, with a Gaussian noise distribution.

UM-Bridge Inference Benchmarks

Name	Short description
Heat inverse problem	defines a posterior distribution for a 1D heat inverse problem, with a Gaussian likelihood and Karhunen–Loève (KL) parameterization of the uncertain parameters.
Beam Inference	Bayesian inverse problem for characterizing the stiffness in an Euler-Bernoulli beam given observations of the beam displacement with a prescribed load.
Tsunami Source	Infer parameters describing the initial displacements leading to the tsunami from the data of two available buoys located near the Japanese coast
Poisson	Estimates a spatially varying diffusion coefficient in an elliptic PDE given limited noisy observations of the PDE solution.
p-Poisson	Estimates a two dimensional flux boundary condition on the bottom of a three dimensional domain with nonlinear p-Poisson PDE.

UM-Bridge Propagation Benchmarks

Name	Short description
Euler-Bernoulli beam	Models the effect of uncertain material parameters on the displacement of an Euler-Bernoulli beam with a prescribed load.
Genz	Multi-dimensional functions for testing integration and surrogate methods.
L2-Sea UQ	Forward UQ of the total resistance in calm-water conditional to operational and geometrical uncertain parameters.

UM-Bridge Optimisation Benchmarks

Name	Short description
L2-Sea UQ	Constraint deterministic optimization problem for the total resistance reduction in calm-water at fixed speed.

Contributing to the benchmark library

- The benchmark library should not be a static resource, it is a community building project and we welcome contributions!
- If you have a model/benchmark with features not found in existing benchmarks please add it
- We're happy to discuss/help
- Finally, to add it simply make a pull request on the repository

Contributing to the benchmark library

Models consist of at least:

- A Dockerfile containing the UM-Bridge server
- A README following a pre-defined structure (we provide a script that auto-generates this file so that you only need to fill in the description)
- A corresponding benchmark which uses this forward model

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They may also have

- Additional required files, e.g. code, input data
- More than one benchmark, e.g. a corresponding inference and propagation benchmark have been defined

Questions?

- We will continue where we left off with the tutorial
<https://um-bridge-benchmarks.readthedocs.io/en/docs/tutorial.html>
- Go to Section 5 and try to create your own model server
- If you don't have any application you want to wrap in a container you can use the minimal server you created in the earlier session.