Introduction to containers

for UM-Bridge models/benchmarks

Alan Correa[1]
Methods for Model-based Development in Computational Engineering, RWTH Aachen
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[1]correa@mbd.rwth-aachen.de

Agenda

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Aims: Introduce the main concepts behind 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

Why use docker?

- **Easy installation:** The installation process for any model or benchmark comes down to a single docker command.
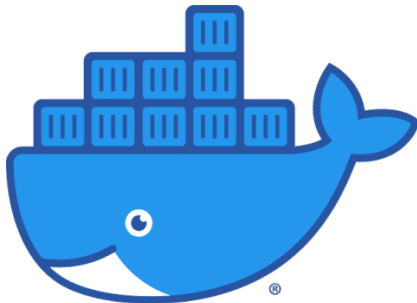
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- **Platform independent:** The installation/running of a model/benchmark no longer relies on assumptions on the users OS or installed packages/software or versions.
- **Scaling to HPC/Cloud:** UM-Bridge allows for easy access to HPC-scale performance in cloud computing environments or classical HPC systems.
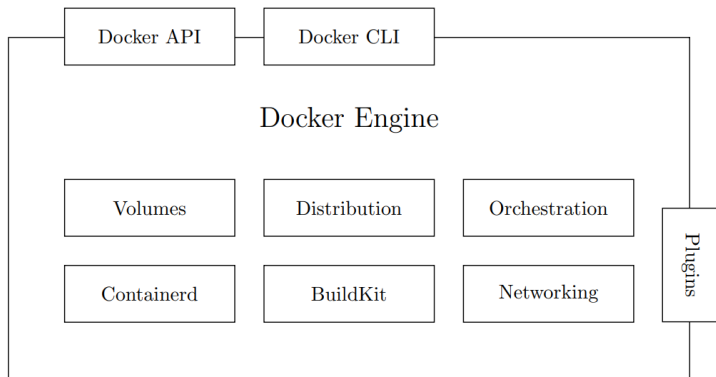
  UM-Bridge provides a reference kubernetes configuration and loadbalancers for SLURM, which take care of load balancing on large-scale clusters. $\rightarrow$ See session 3.

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

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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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- This is running new container, we are simply pulling the latest ubuntu image from dockerhub
- `-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 our "application" and the command to run that "application"

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- Copying the same commands into a Dockerfile will give us a docker container with our application

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

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```

Or to clean up all unused images/containers

```
docker system prune
```

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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For advanced usage get inspired and learn more:
https://github.com/UM-Bridge/benchmarks/tree/main/models

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What about MPI?
https://um-bridge-benchmarks.readthedocs.io/en/docs/mpi_container.html

UM-Bridge Workflow

To create an UM-Bridge server, we

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To test our new server

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

Connect to model

```python
import umbridge
model = umbridge.HTTPModel("http://localhost:4242", "forward")
```

UM-Bridge: Client

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Display input / output dimensions

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print(model.get_input_sizes())
print(model.get_output_sizes())
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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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print(model([[0.0, 10.0]]))
```

Optionally, pass configuration options

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

UM-Bridge: Server

Defining a model class

```python
class TestModel(umbridge.Model):
    def get_input_sizes(self):
        return [2] # Number and dimensions of input vectors
    def get_output_sizes(self):
        return [1] # Number and dimensions of output vectors
    def call(self, parameters, config = {}):
        # Do something with the input: y = 2 * x_0 + 3 * x_1
        output = parameters[0][0]*2 + parameters[0][1]*3
        return [[output]]
    def supports_evaluate(self):
        return True
```

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```

Serve model via HTTP

```python
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

Goal

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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- **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

L. Seelinger, A. Reinarz, et al, Democratizing uncertainty quantification, Journal of Computational Physics, 2025 (https://doi.org/10.1016/j.jcp.2024.113542).

UM-Bridge Models

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 infererence 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 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?

Tutorial

- We will continue where we left off with the tutorial
  https://um-bridge-benchmarks.readthedocs.io/en/docs/tutorial.html
- Option 1: Solve end-to-end UQ Problem (Section 2 & 3)
- Option 2: Setup your own Model Container (Section 4 & 5)