Introduction to UM-Bridge

Linking UQ and Models from Prototype to HPC

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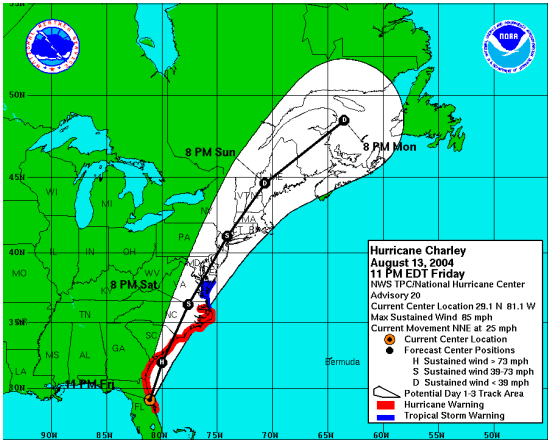
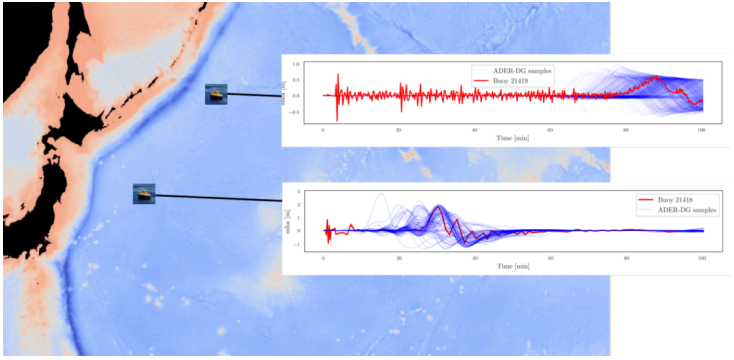
Why Uncertainty Quantification (UQ)?



- "Don't focus on the skinny black line"
  - US Hurricane Center
- Uncertain data $\Longrightarrow$ uncertain prediction / inferences.
  UQ: Quantify this!

Tsunami Problem



- Modelling Tohoku event (2011) using Shallow Water eq. and real bathymetry
- Forward model built on ExaHyPE PDE engine
- Data: Buoy measurements. Parameter: Tsunami source

How to solve UQ problems?

Many methods:

- MC / MCMC
- Stochastic Galerkin
- Optimization-based MAP point search
- Multilevel / Multiindex MC / MCMC
- ...

Large-scale problems need HPC!

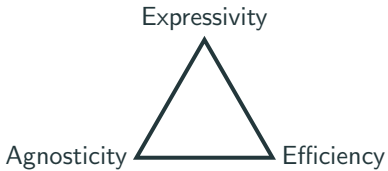
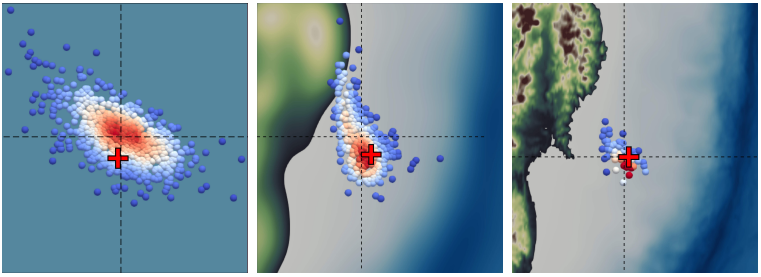


Figure 1: Main aspects of UQ methods

Example: Markov chain Monte Carlo (MCMC)

Online demo

Results



lvl l	t_l[s]	ρ_l	$\mathbb{V}[Q_0]$ or $\mathbb{V}[Q_l - Q_{l-1}]$		$\mathbb{E}[Q_0]+$ $\sum_{k=1}^{l} \mathbb{E}[Q_k - Q_{k-1}]$	
0	7.38	25	1984.09	1337.42	3.61	27.96
1	97.3	5	1592.17	1523.18	−12.29	23.39
2	438.1	0	340.56	938.53	−5.46	0.12

Run on 3456 cores (72 nodes of 48 cores)

UQ and Model in Math

Model in UQ: (Often) Just a function $F : \mathbb{R}^n \to \mathbb{R}^m$ with some of the following:

- Model evaluation $F(\theta)$,
- Gradient $v^\top J(\theta)$,
- Jacobian action $J(\theta)v$,
- Hessian action $H(\theta)v$.

$\to$ Simple, model-agnostic interface!

Linking model **software** and UQ **software**: Not that easy!

Complex software stack, conflicts (buildsystems, dependencies, languages, parallelization), need experts from both sides, ...

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UM-Bridge:
Universal interface in software

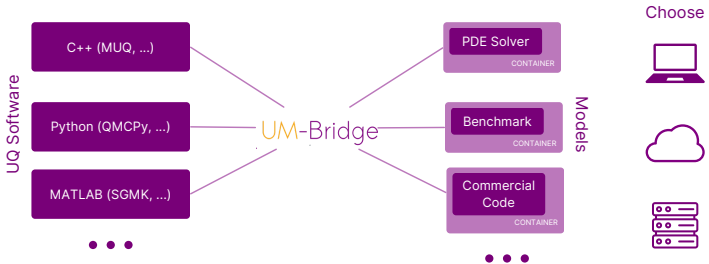
UM-Bridge: Model Abstraction in Software

Interface mimics math: Model provides pointwise

- evaluation $F(\theta)$,
- Gradient $v^\top J(\theta)$ (optional),
- Jacobian action $J(\theta)v$ (optional),
- Hessian action $H(\theta)v$ (optional).

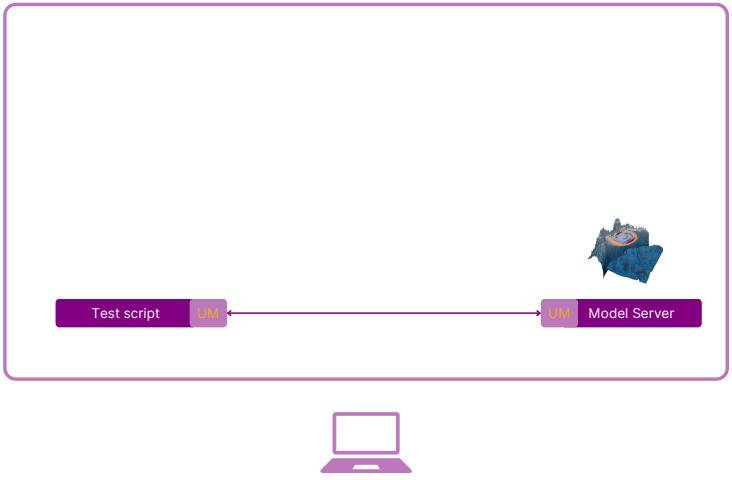
Inspired by microservices (established in software industry)

UM-Bridge: Enabling UQ from Prototype to HPC

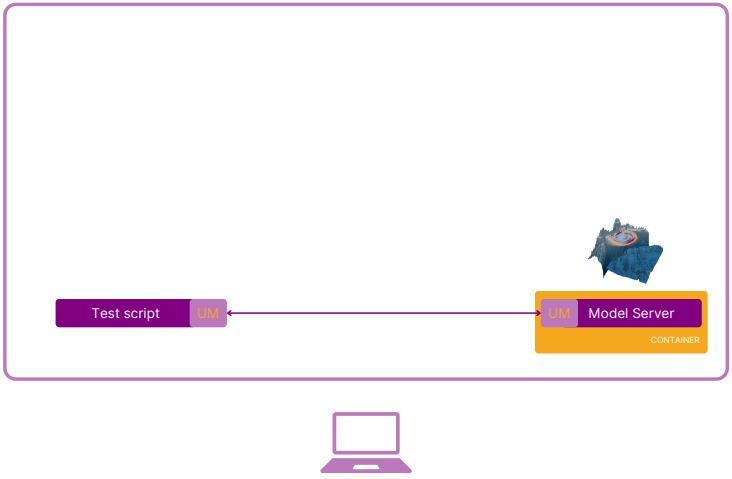


- Single point of entry for UQ and Models
- Separation of concerns
- Straightforward scalability

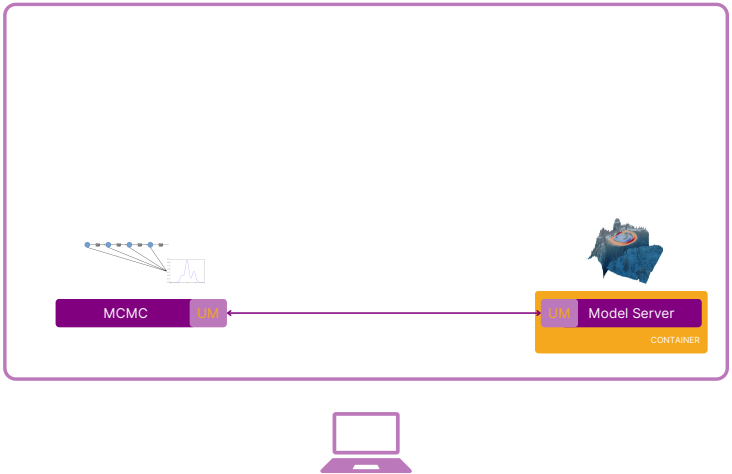
Workflow



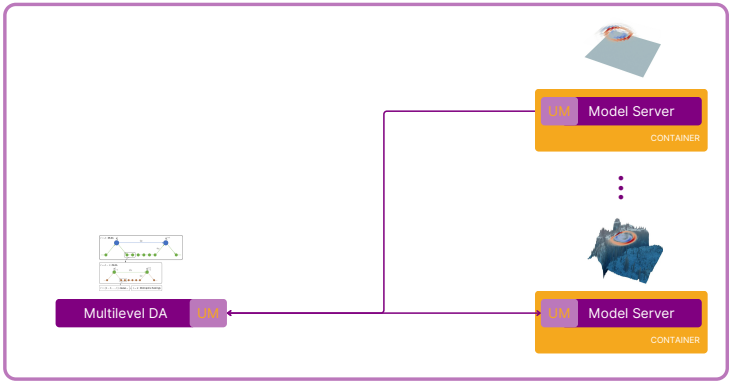
Workflow



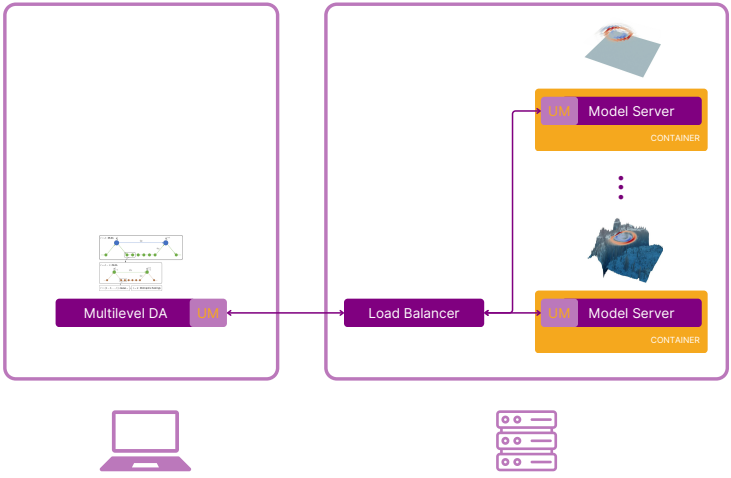
Workflow



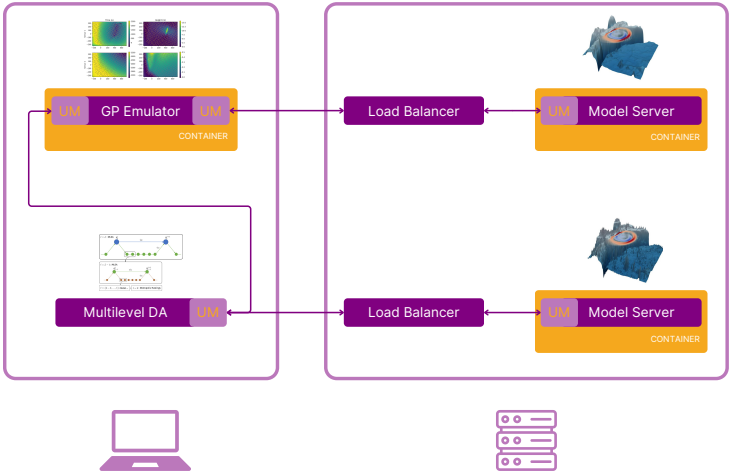
Workflow


UM
Model Server
CONTAINER
UM
Model Server
CONTAINER
Multilevel DA
UM

Workflow


UM
Model Server
CONTAINER
Multilevel DA
UM
Load Balancer
UM
Model Server
CONTAINER

Workflow



Successfully run on 2800 core Google Kubernetes Engine cluster

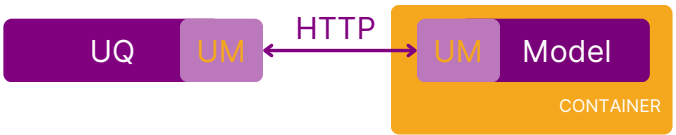
Demo

Demo

UM-Bridge Demo

Upcoming topics

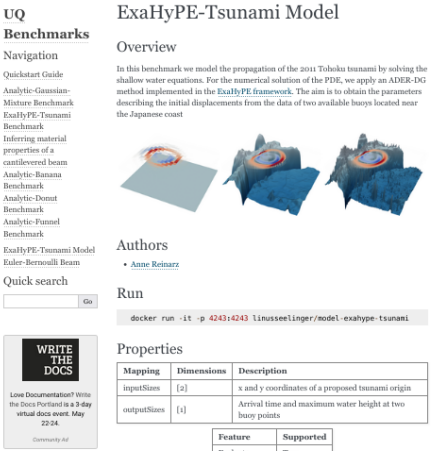
UM-Bridge: Containerization - Portable Models



- 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]])
  ```

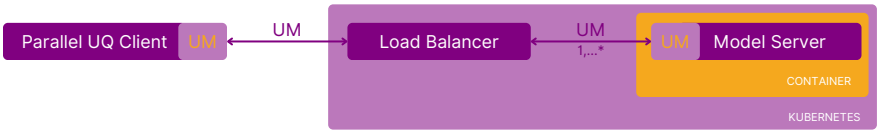
→ Separation of concerns!

UQ Benchmarks



- Community project:
  $>$ 20 models and benchmarks,
  $>$ 15 contributors from
  $>$ 10 institutions
- Ready-to-run containers
- Automated builds, testing etc.

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!

Conclusions

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- Universal UQ / model interface, following maths
- Easy to use in various languages and frameworks
- Opens up new possibilities for UQ:
  - Portable models, separation of concerns
  - Library of reproducible UQ benchmark problems
  - Easy scaling to Cloud / HPC

Practical

Tutorial sections 1-3