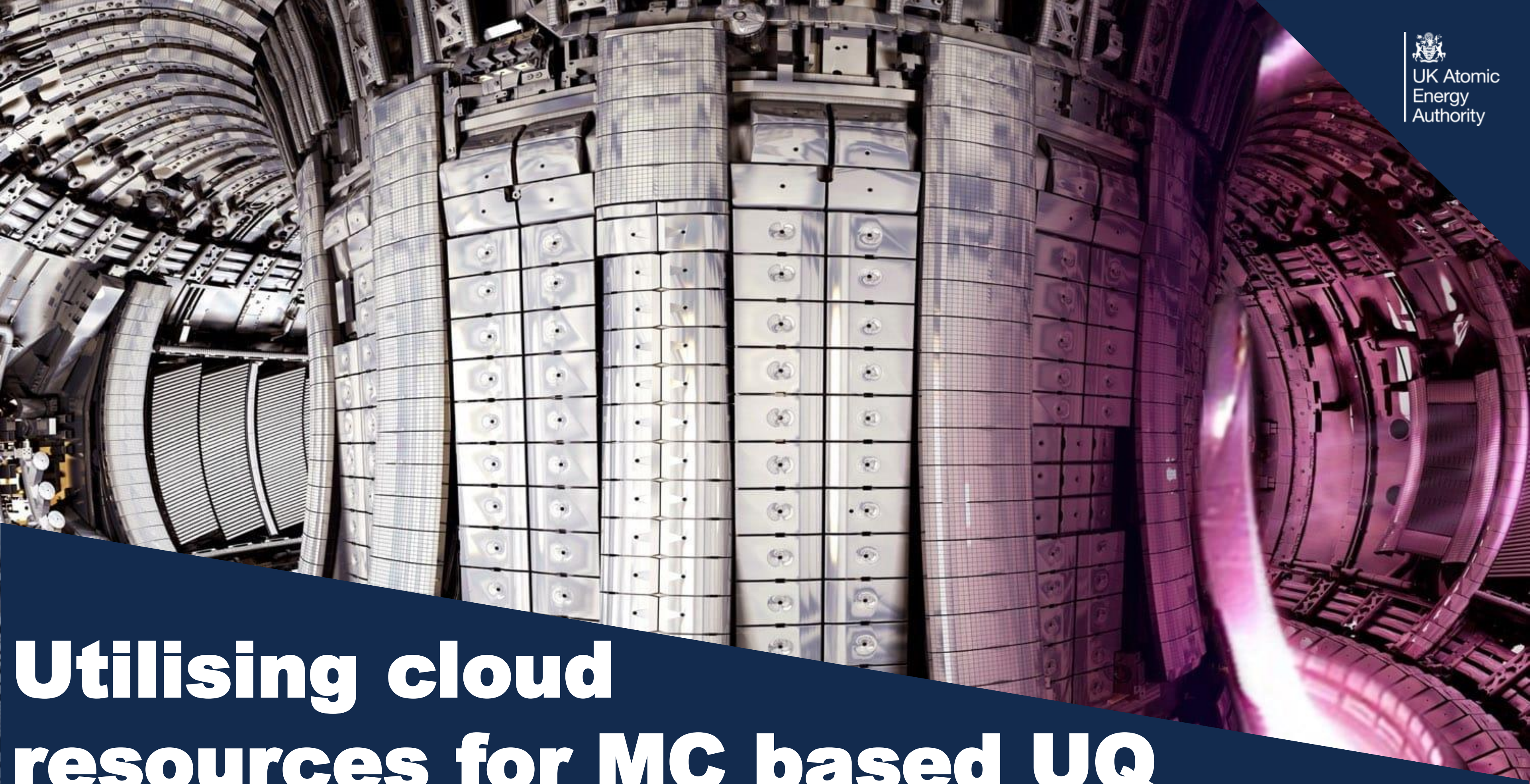
UK Atomic Energy Authority



Utilising cloud resources for MC based UQ

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Overview

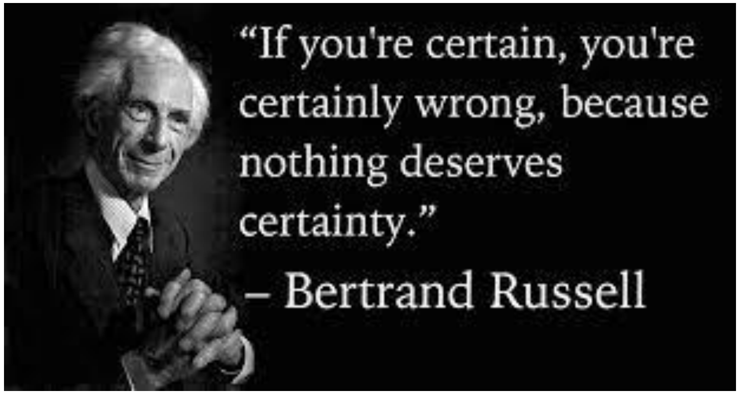
- **Brief introduction to uncertainty quantification**
  - Monte-Carlo sampling for uncertainty propagation
- **The VVeb.UQ framework**
  - Existing VVUQ frameworks
  - VVeb.UQ components
  - Web interface
- **Proof of concept examples**
  - EFIT + TRANSP
  - Data generation for NN training
- **Future work**

Uncertainty Quantification

- Quantifying uncertainty around a result is a fundamental aspect of scientific investigation, be it empirical or theoretical.
  - UQ enables more robust comparisons between theory and experiment.

- Uncertainty quantification is also important for making *informed decisions*, for instance around designing a fusion reactor.

- We want predictions from simulation to be equipped with uncertainties as only then can they be correctly interpreted and be considered *actionable*.



"If you're certain, you're certainly wrong, because nothing deserves certainty."
– Bertrand Russell

Types of uncertainties

There are broadly 2 kinds of uncertainties:

Aleatory *or* ***Statistical Uncertainties****:*

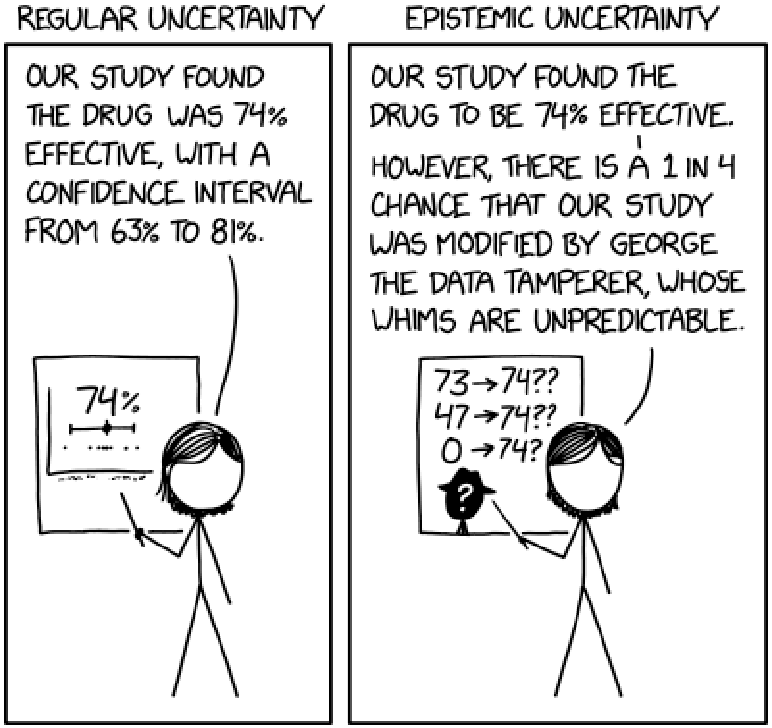
These typically correspond to randomness in a process.

Epistemic *or*
Systematic Uncertainties*:*

These are uncertainties which arise due to absence of knowledge, for instance missing physics in a model or the impact of assumptions.

They are typically harder to quantify.

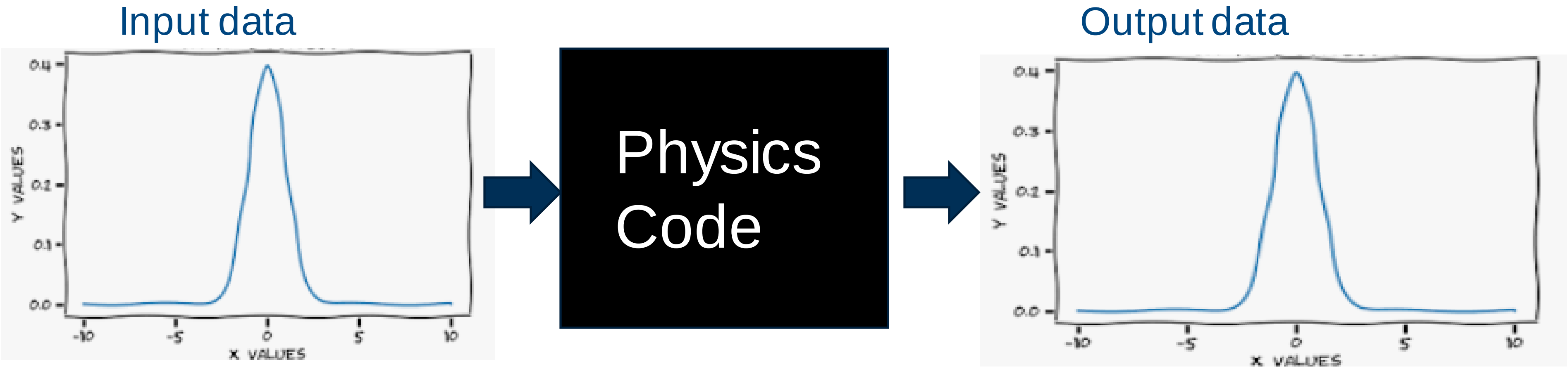
Epistemic Uncertainty


REGULAR UNCERTAINTY
EPISTEMIC UNCERTAINTY
OUR STUDY FOUND THE DRUG WAS 74% EFFECTIVE, WITH A CONFIDENCE INTERVAL FROM 63% TO 81%.
74%
OUR STUDY FOUND THE DRUG TO BE 74% EFFECTIVE. HOWEVER, THERE IS A 1 IN 4 CHANCE THAT OUR STUDY WAS MODIFIED BY GEORGE THE DATA TAMPERER, WHOSE WHIMS ARE UNPREDICTABLE.
73→74??
47→74??
0→74?
?

R. Munroe https://xkcd.com/2440

Uncertainty Propagation

- We will focus on the *propagation* of parameter uncertainties through simulation codes.
- These cases typically fall into the aleatory bracket, but one can treat epistemic uncertainties if one feels the uncertainty can be characterised by sampling from a distribution.



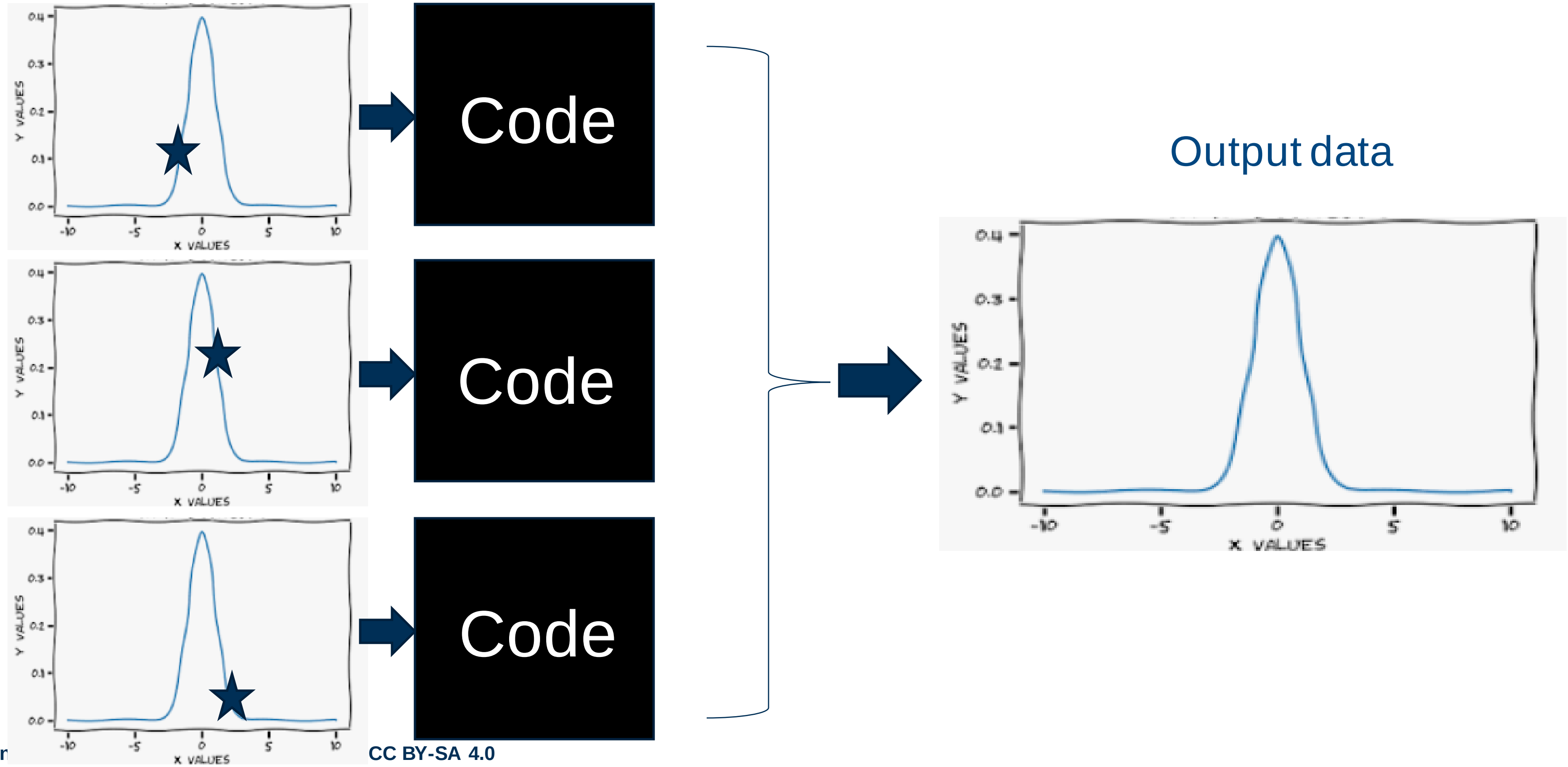
Input data

Physics Code

Output data

Uncertainty Propagation II

The simplest conceptual approach to propagating such uncertainties is to **sample** values from the input distributions and **run ensembles** of simulations with these data to build up distributions of output quantities.



Code

Code

Code

Output data

Cloud Computing

There are many good existing platforms for performing ensemble uncertainty quantification:

VECMAtk

VECMA

H2020 project - https://www.vecma.eu/

DAKOTA

Explore and predict with confidence.

+ several others...

Sandia Laboratories https://dakota.sandia.gov/

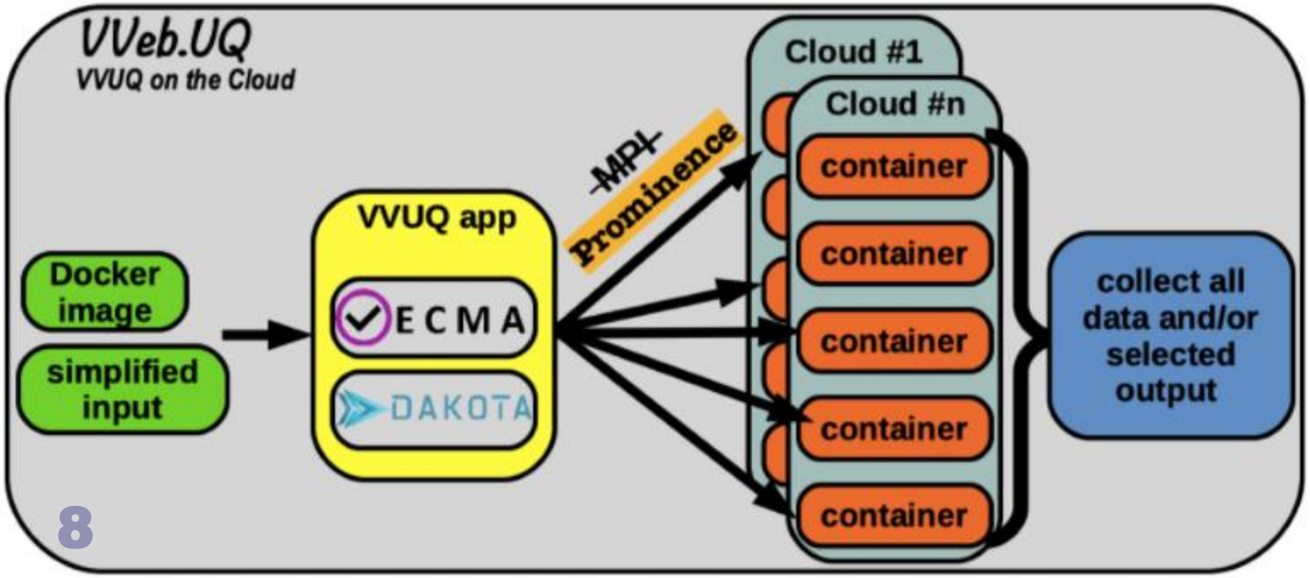
Most of these frameworks contain a plethora of well-developed, well tested UQ capabillities but are targetted towards running ensembles on traditional HPC resources.

Can we use these to build something oriented towards the increasing availability of **cloud resources**?

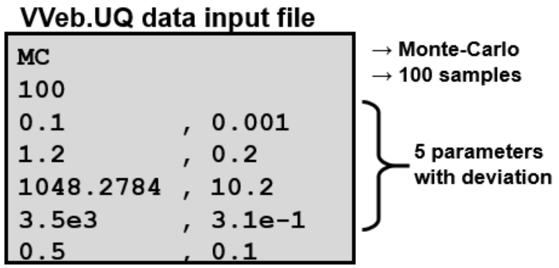
VVeb.UQ

We have developed an infrastructure built on these tools for running large numbers of instances of a code on cloud resources.

- The app is an apache2-php server in a docker container.
- Reads uncertain parameters in simple formats:
  - netCDF
  - csv
- Uses docker to run container instances of users' code.
- Uses **Prominence** for job submission and scheduling.



VVeb.UQ data input file

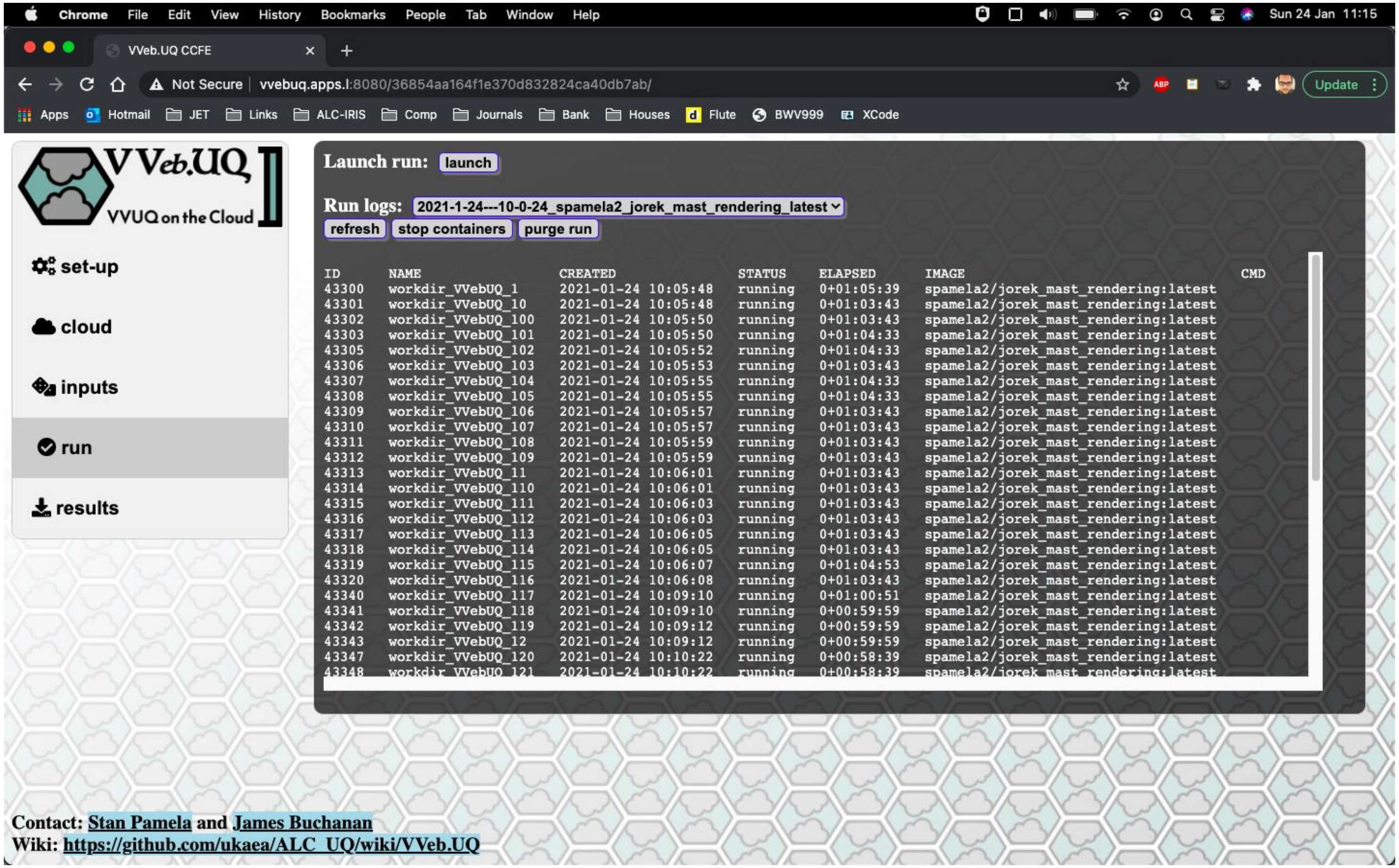


```
MC
100
0.1        , 0.001
1.2        , 0.2
1048.2784  , 10.2
3.5e3      , 3.1e-1
0.5        , 0.1
```

→ Monte-Carlo
→ 100 samples
5 parameters with deviation

Web Interface

A web interface allows users to specify inputs and code containers and handle submission and recovery of runs. Alternatively, a REST API can be used.


Chrome File Edit View History Bookmarks People Tab Window Help
Sun 24 Jan 11:15
VVeb.UQ CCFE
Not Secure | vvebuq.apps.l:8080/36854aa164f1e370d832824ca40db7ab/
Update
Apps Hotmail JET Links ALC-IRIS Comp Journals Bank Houses Flute BWV999 XCode
VVeb.UQ
VVUQ on the Cloud
set-up
cloud
inputs
run
results
launch
refresh
stop containers
purge run

Launch run: launch

Run logs: 2021-1-24---10-0-24_spamela2_jorek_mast_rendering_latest

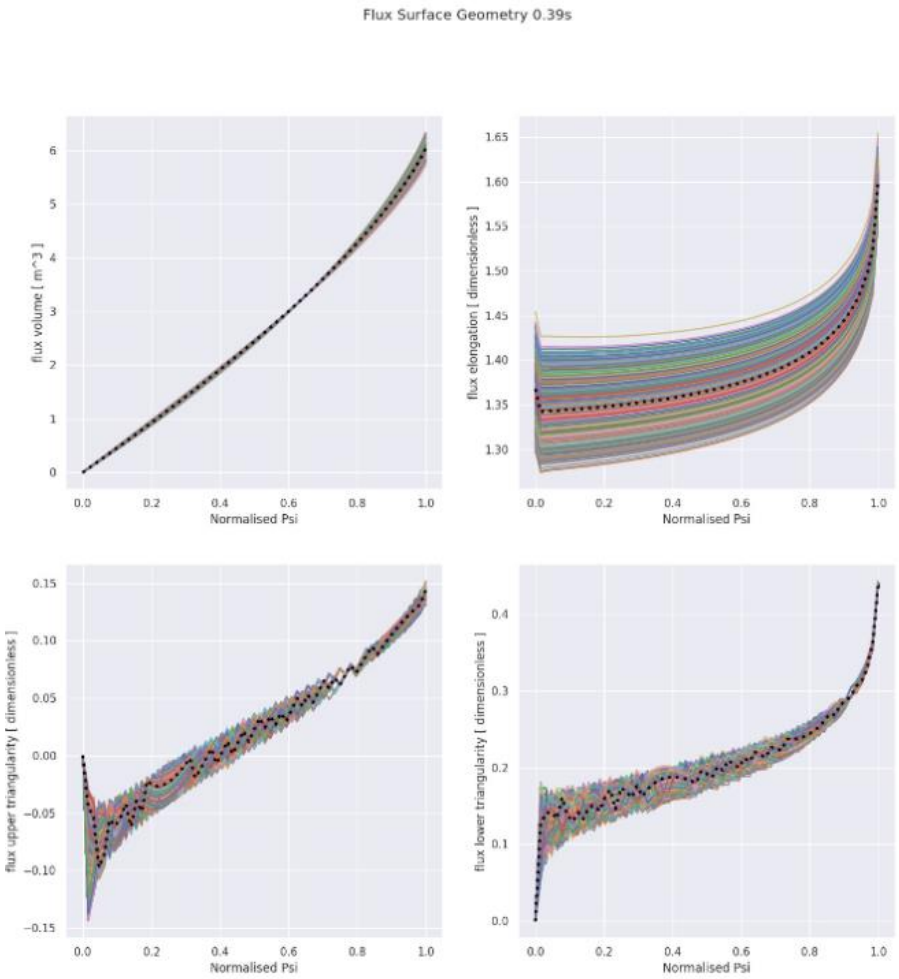
```
ID      NAME                 CREATED               STATUS     ELAPSED      IMAGE                                  CMD
43300   workdir_VVebUQ_1     2021-01-24 10:05:48   running    0+01:05:39   spamela2/jorek_mast_rendering:latest
43301   workdir_VVebUQ_10    2021-01-24 10:05:48   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43302   workdir_VVebUQ_100   2021-01-24 10:05:50   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43303   workdir_VVebUQ_101   2021-01-24 10:05:50   running    0+01:04:33   spamela2/jorek_mast_rendering:latest
43305   workdir_VVebUQ_102   2021-01-24 10:05:52   running    0+01:04:33   spamela2/jorek_mast_rendering:latest
43306   workdir_VVebUQ_103   2021-01-24 10:05:53   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43307   workdir_VVebUQ_104   2021-01-24 10:05:55   running    0+01:04:33   spamela2/jorek_mast_rendering:latest
43308   workdir_VVebUQ_105   2021-01-24 10:05:55   running    0+01:04:33   spamela2/jorek_mast_rendering:latest
43309   workdir_VVebUQ_106   2021-01-24 10:05:57   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43310   workdir_VVebUQ_107   2021-01-24 10:05:57   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43311   workdir_VVebUQ_108   2021-01-24 10:05:59   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43312   workdir_VVebUQ_109   2021-01-24 10:05:59   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43313   workdir_VVebUQ_11    2021-01-24 10:06:01   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43314   workdir_VVebUQ_110   2021-01-24 10:06:01   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43315   workdir_VVebUQ_111   2021-01-24 10:06:03   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43316   workdir_VVebUQ_112   2021-01-24 10:06:03   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43317   workdir_VVebUQ_113   2021-01-24 10:06:05   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43318   workdir_VVebUQ_114   2021-01-24 10:06:05   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43319   workdir_VVebUQ_115   2021-01-24 10:06:07   running    0+01:04:53   spamela2/jorek_mast_rendering:latest
43320   workdir_VVebUQ_116   2021-01-24 10:06:08   running    0+01:03:43   spamela2/jorek_mast_rendering:latest
43340   workdir_VVebUQ_117   2021-01-24 10:09:10   running    0+01:00:51   spamela2/jorek_mast_rendering:latest
43341   workdir_VVebUQ_118   2021-01-24 10:09:10   running    0+00:59:59   spamela2/jorek_mast_rendering:latest
43342   workdir_VVebUQ_119   2021-01-24 10:09:12   running    0+00:59:59   spamela2/jorek_mast_rendering:latest
43343   workdir_VVebUQ_12    2021-01-24 10:09:12   running    0+00:59:59   spamela2/jorek_mast_rendering:latest
43347   workdir_VVebUQ_120   2021-01-24 10:10:22   running    0+00:58:39   spamela2/jorek_mast_rendering:latest
43348   workdir_VVebUQ_121   2021-01-24 10:10:22   running    0+00:58:39   spamela2/jorek_mast_rendering:latest
```

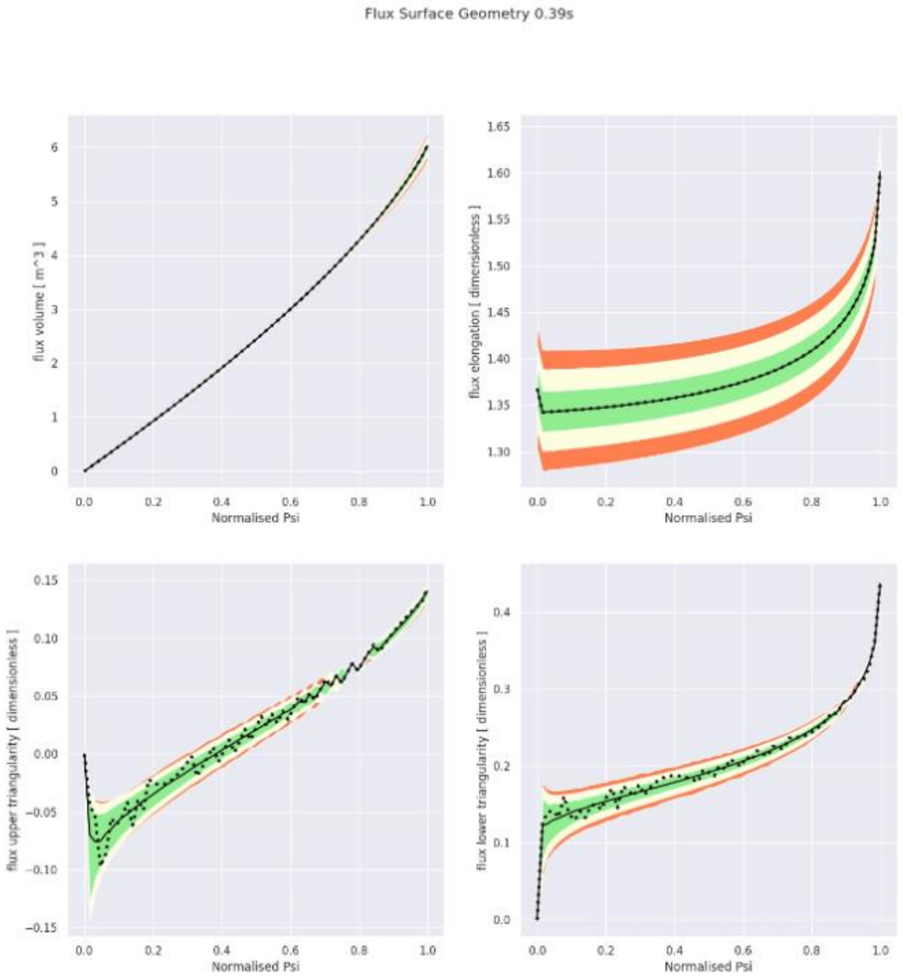
Contact: Stan Pamela and James Buchanan
Wiki: https://github.com/ukaea/ALC_UQ/wiki/VVeb.UQ

UKAEA instance at http://vvebuq.apps.l:8080

Example cases

Using the output data statistical quantities like confidence intervals can be constructed.





The flux volume, elongation, upper and lower triangularities at 0.39s for MAST shot 29827 calculated with EFIT++

Example cases

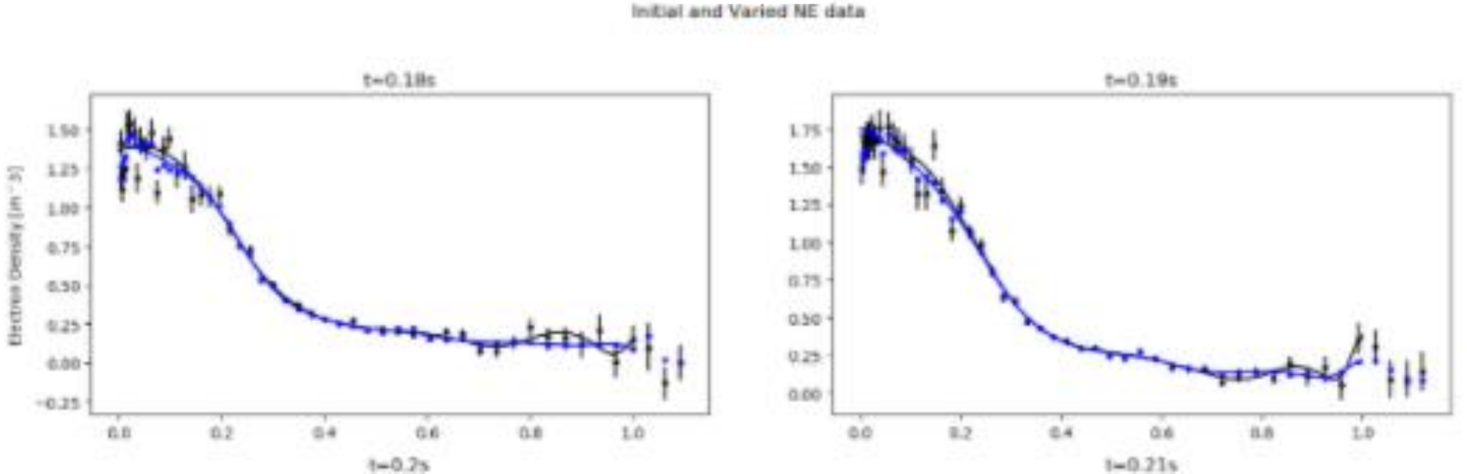
Both EFIT and TRANSP have been containerised and built into a workflow which can be executed using the app for shots on MAST and MAST-U. The following sources of uncertainty were considered:

EFIT++:

- Magnetic Probe Uncertainties
- Flux Loop Uncertainties
- Plasma Current Uncertainty
- Plasma Boundary Uncertainty
- MSE Uncertainties

TRANSP:

- Equilibrium Uncertainties
- Profile Uncertainties
- Bolometry Uncertainty
- Z effective Uncertainty

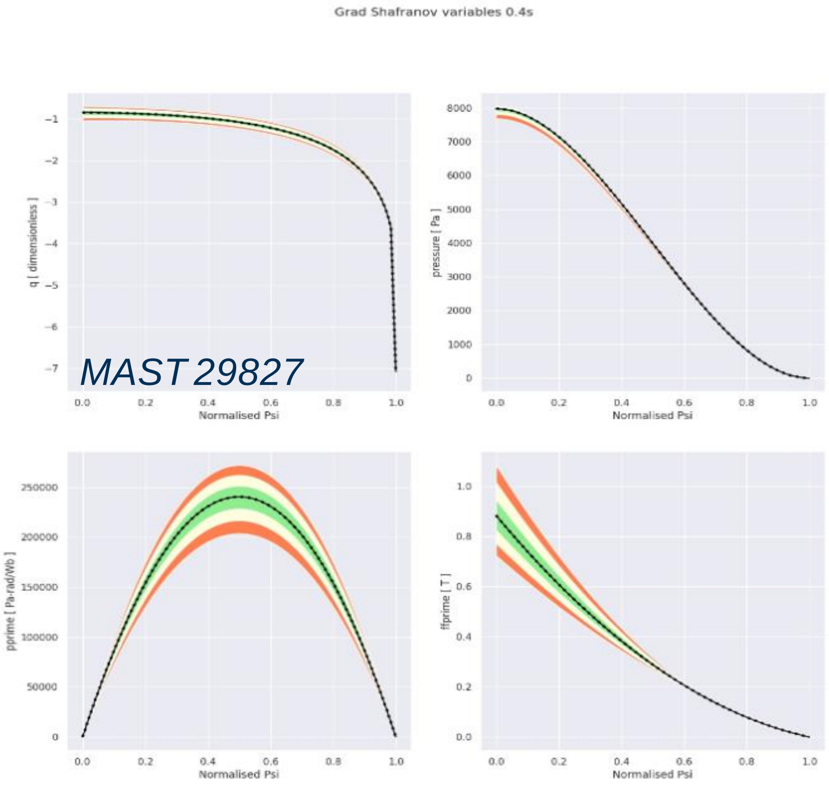


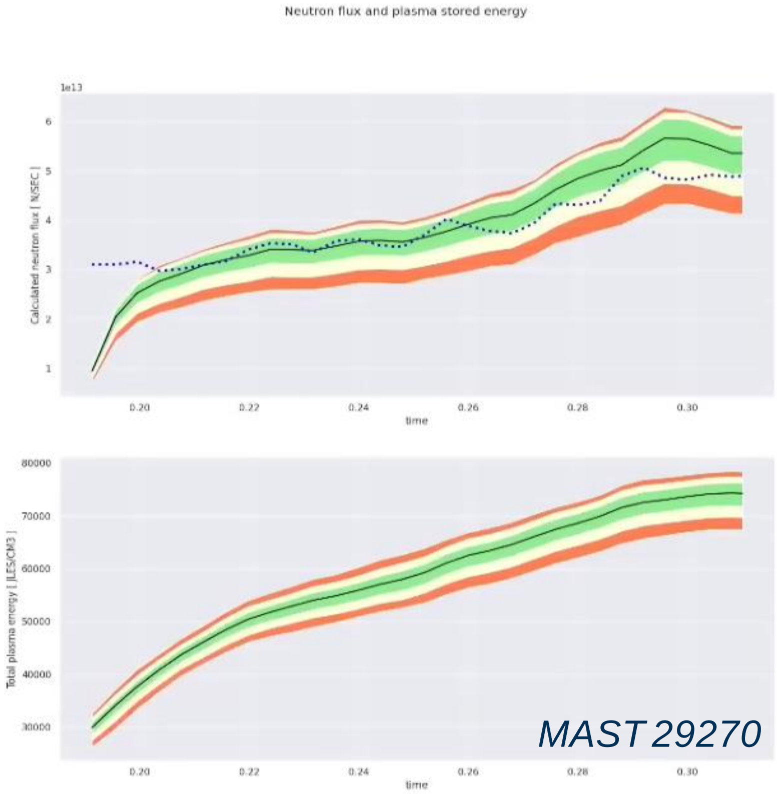
Variation of the electron density profiles for MAST shot 29231

Example cases

Just a proof-of-concept study...

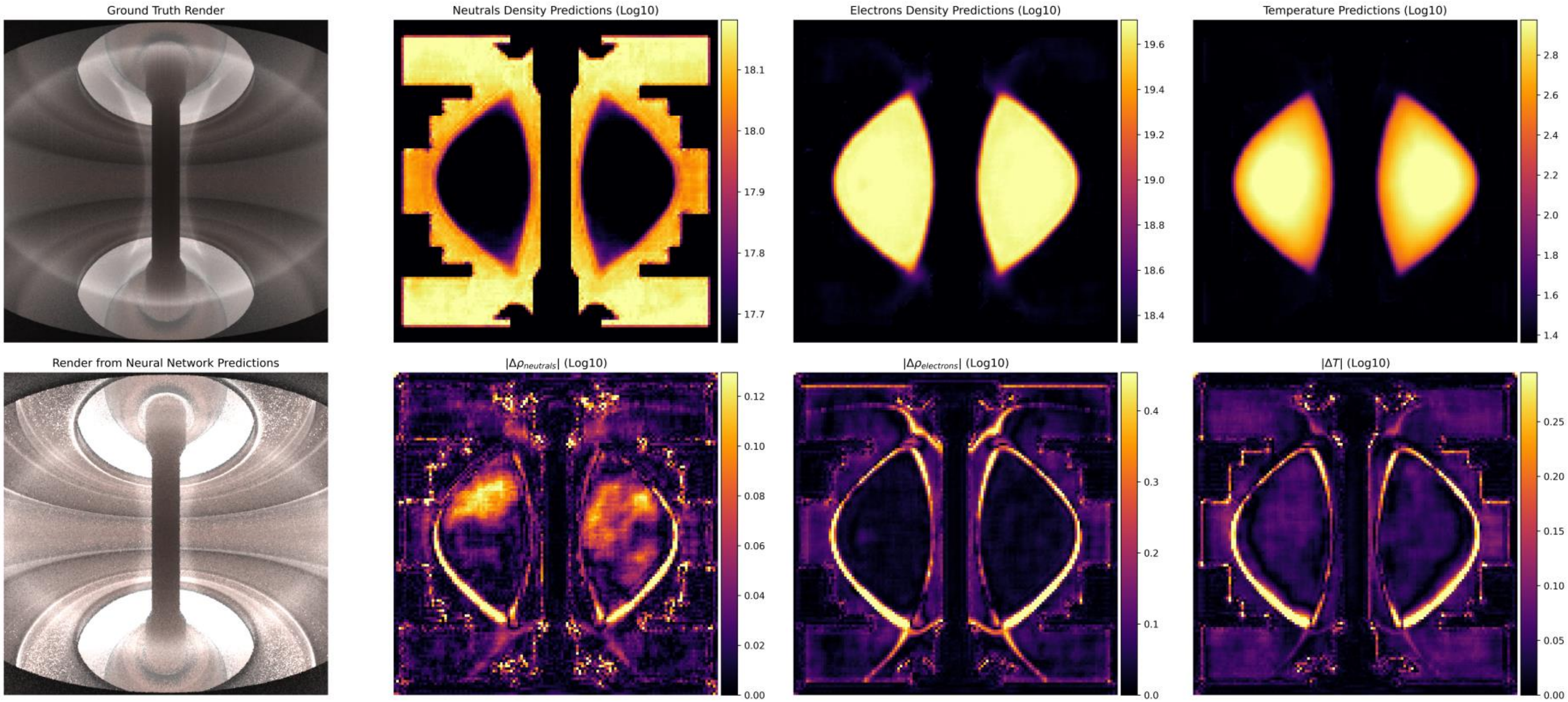
Executing ensembles of simulations with these data treated as uncertain allows characterisation of the uncertainties on the resulting equilibrium quantities (e.g. q,p,p',ff') as well as calculated neutron rates.





Data generation for ML

Aside from the main UQ use case, VVeb.UQ has been used to generate input data for training NNs to predict plasma properties. The following used training data generated using JOREK.



Ekin Ozturk

Limitations

- Currently **no handling of correlations** between input uncertainties. Could be added but these correlations are often unknown.

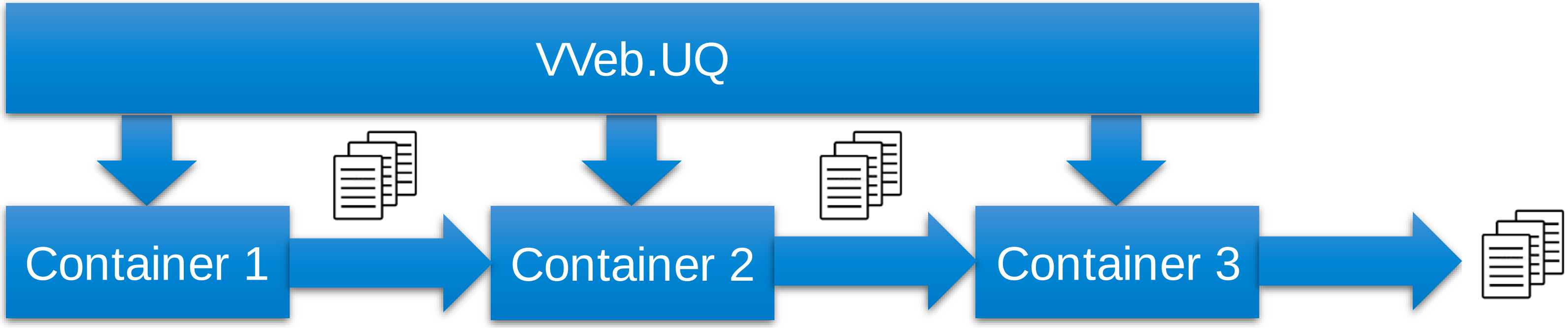
- Many codes are **systematically dominated** and so these uncertainties represent a lower limit on the true uncertainty.

- **No automatic post-processing of data**. At present results are accumulated in a directory which is returned. Some post-processing functionality could be added.

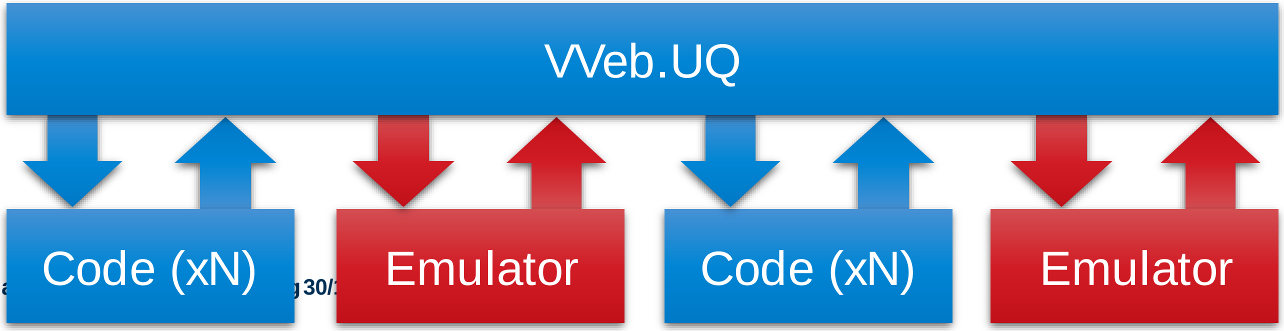
- Limited to codes which can viably be run in reasonably sized ensembles on available resources.

Future work

- At present the framework executes a single user code container per parameter set. We could explore extending this to handle workflows involving sequentially running sets of containerised codes.



- We wish to explore dynamic workflows where the results of runs are used by the framework. An example is training a surrogate model and using sequential design to orchestrate new simulations.



Summary

- The **VVeb.UQ** tool is built on top of existing UQ frameworks like **DAKOTA** and **VECMA** and provides a simplified way of exploiting cloud resources for simple sample-based propagation of uncertainties.
- VVeb.UQ utilises the **PROMINENCE** cloud deployment system for job management.
- Simple proof-of-principle demonstrations have been performed using **EFIT++** and **TRANSP**.
- Future extensions will involve the construction of more complex workflows consisting of chains of codes or dynamic tasks like **training surrogate models**.

https://github.com/ukaea/ALC_UQ