Surrogate-Enhanced Simulation Workflows for Fast and Efficient Neutronics Calculations

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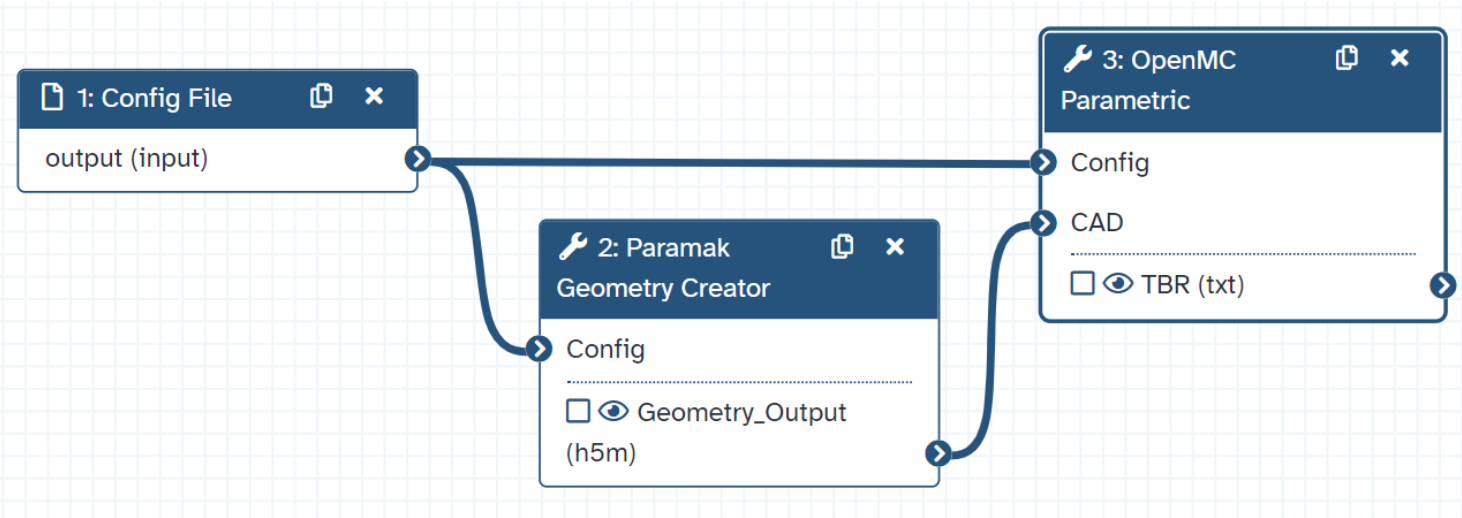
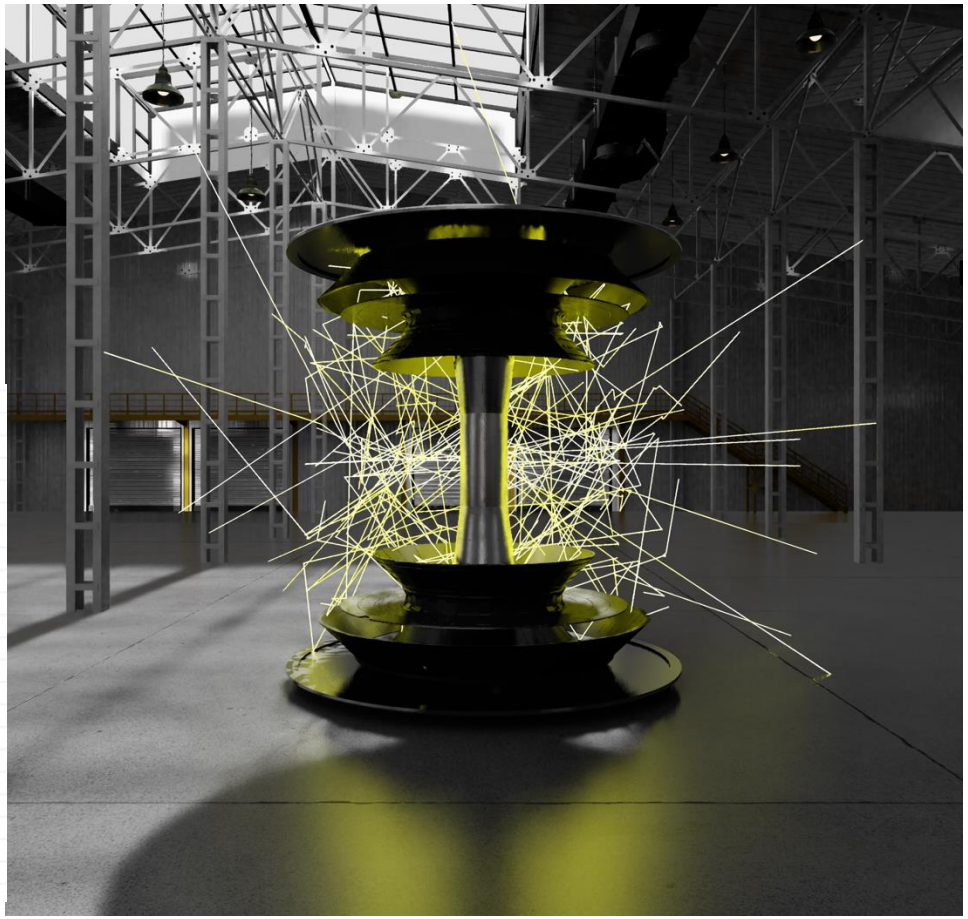
Introduction

- Motivation
- Uncertainty-Quantified ML
- Workflows
- Case Study
- Results & Discussion

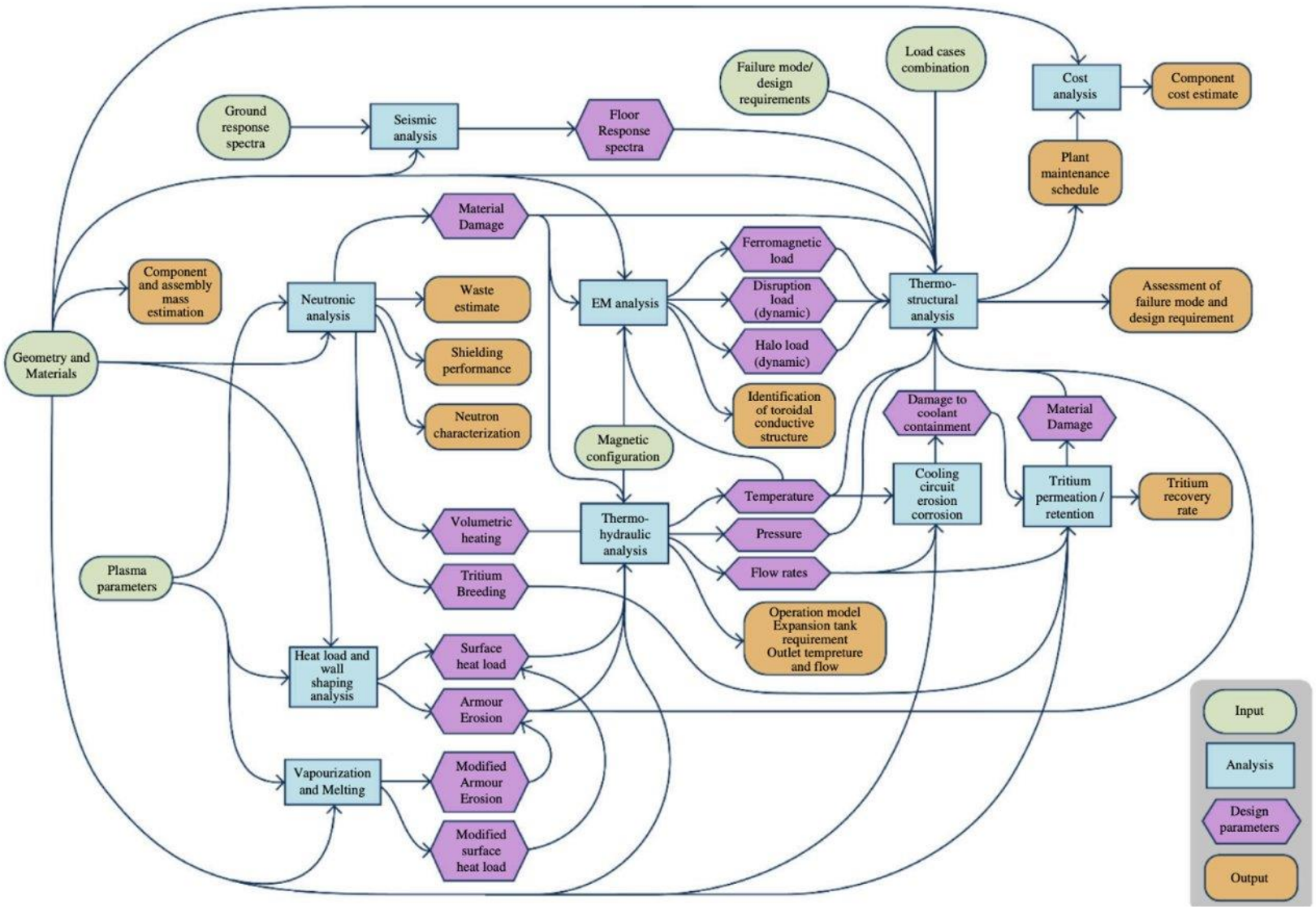




Fusion Power Plant Design is HARD

- Complex
- Highly coupled
- Iterative
- Computationally expensive
- Slow

How can we make design decisions quicker?



A. Davis et al. Digital: Accelerating the Pathway. The in-vessel system workflow for analysing design concepts.

Traditional Surrogates?

Yes, but…

- Usually require large initial datasets
  - Costly in time and resources
  - Might not need all the domain space well-mapped
- Effort intensive
  - Large time investment by users in generating data, training and refining models
  - Time spent learning how to use ML
- Unclear certainty of results

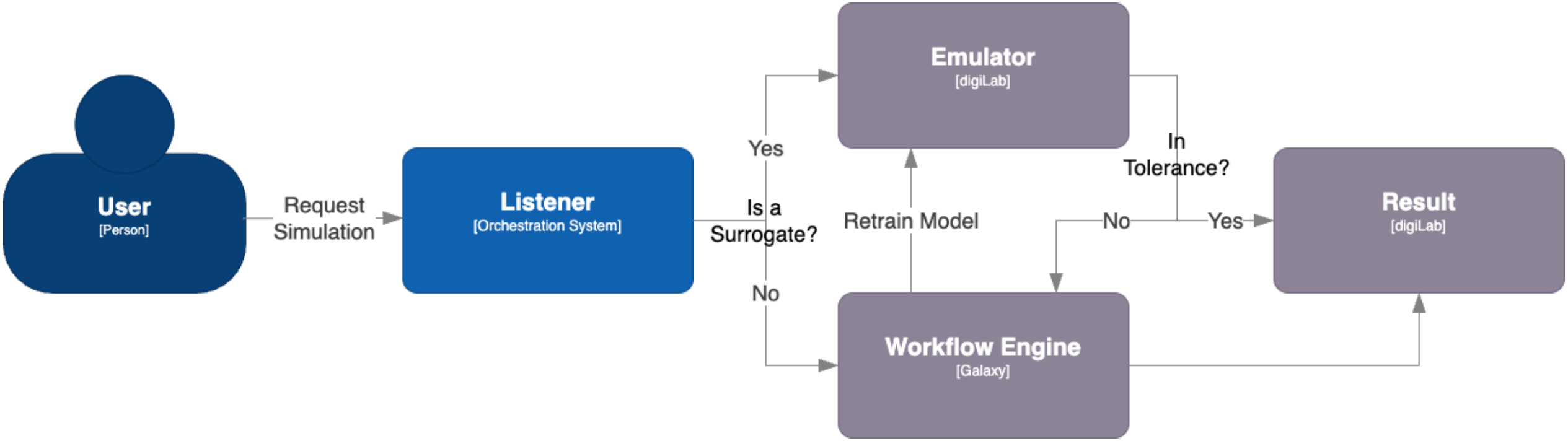
Proposed Solution

- Automate the production of uncertainty-quantified emulators without running unnecessary simulations
- No additional effort for the user
- Wrap around existing simulation workflows, allowing emulation of multiple tools while not adding large overheads

In short:

An automated surrogate caching layer

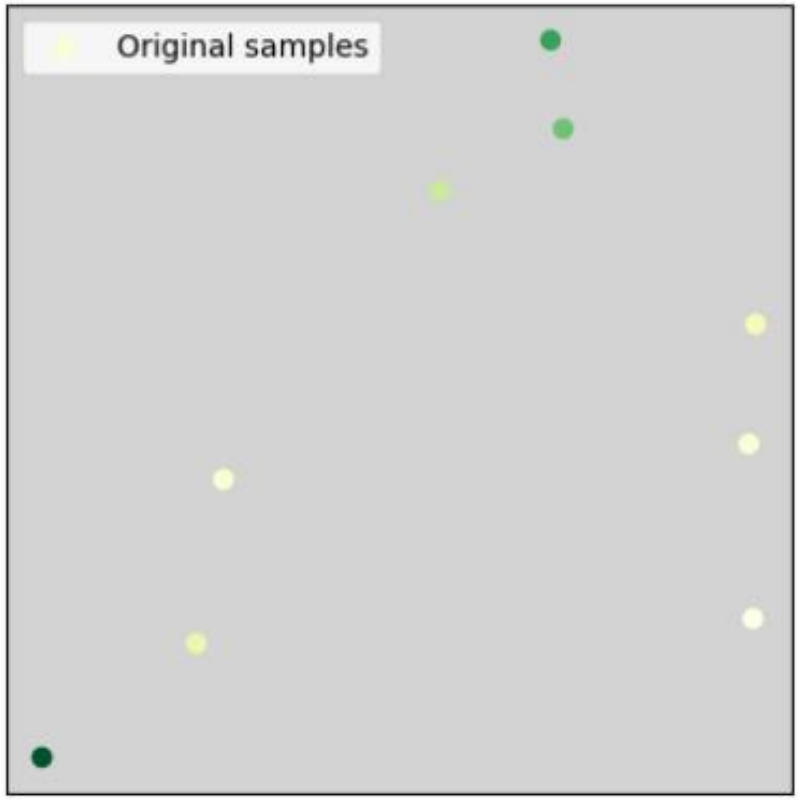
Concept


User
[Person]
Request Simulation
Listener
[Orchestration System]
Is a Surrogate?
Yes
No
Emulator
[digiLab]
Retrain Model
Workflow Engine
[Galaxy]
In Tolerance?
No
Yes
Result
[digiLab]

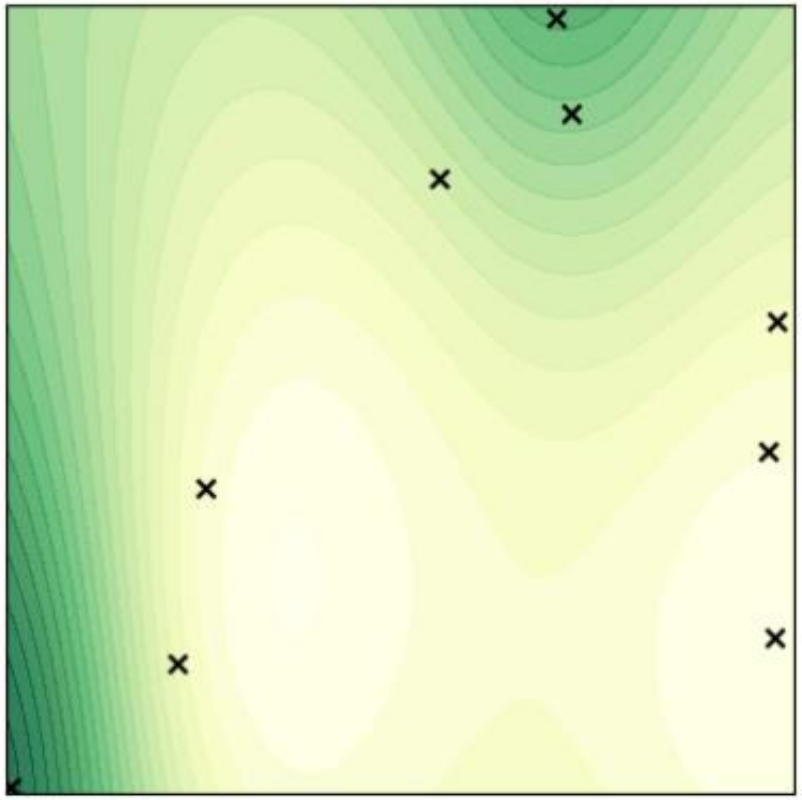
Emulation

digiLab

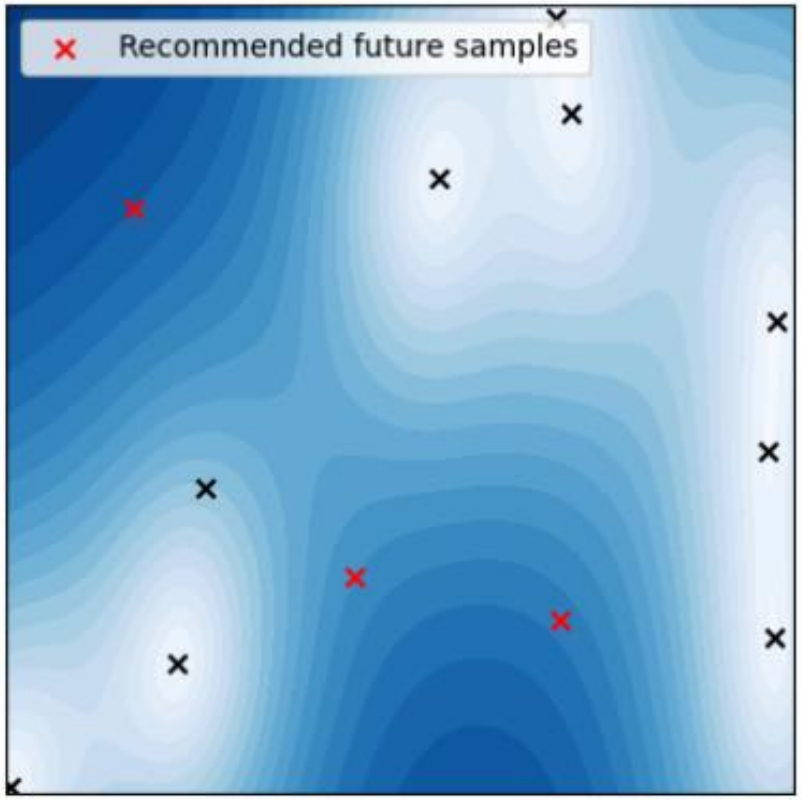
Data



Emulator Model



Emulator Uncertainty

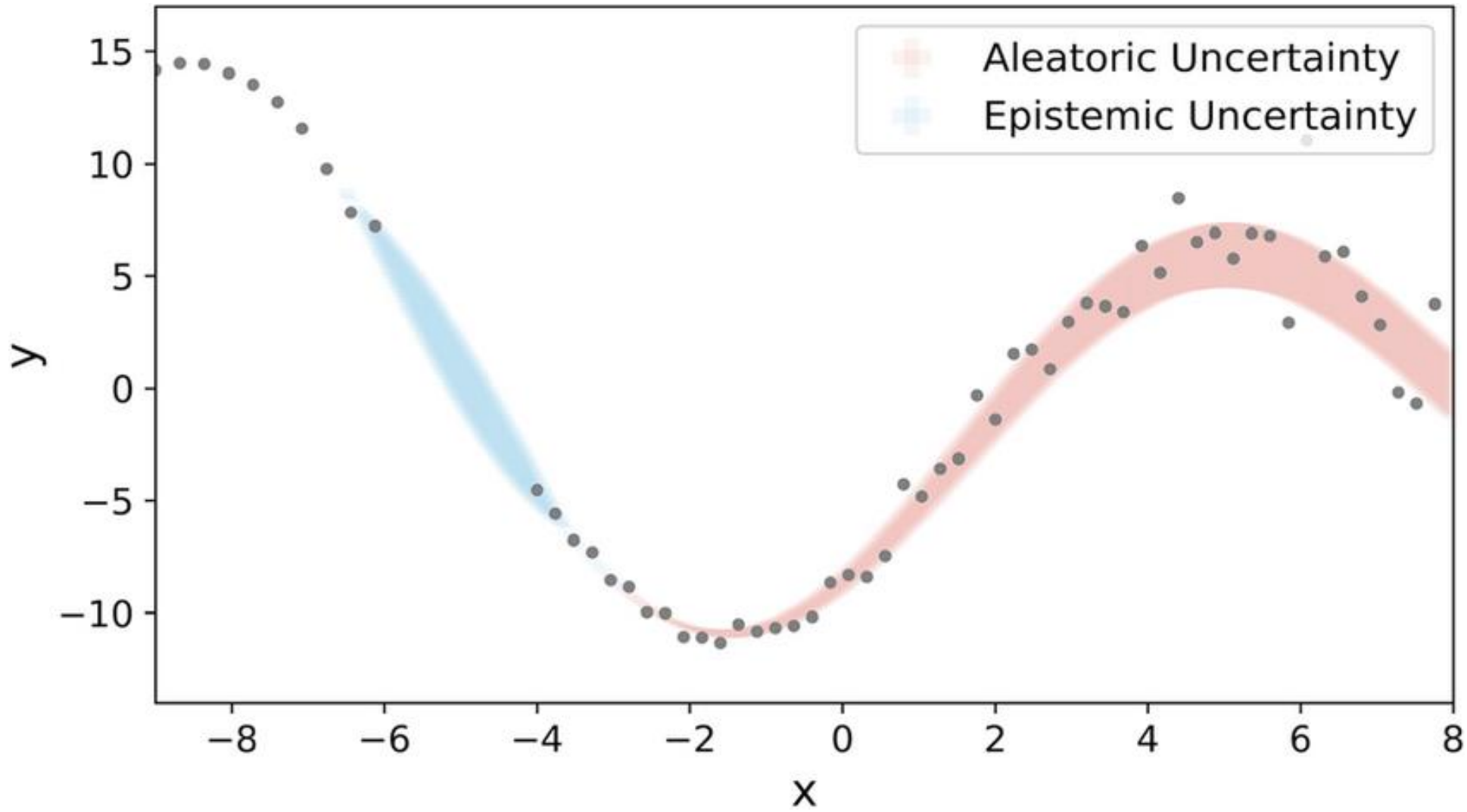


Uncertainty Engine

A. Mead, digiLab: Introducing Active Learning with twinLab

Uncertainty Quantification

digiLab



Yang & Li, Journal of Cheminformatics: Explainable uncertainty quantifications for deep learning-based molecular property prediction

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- Lightweight Python interface to Uncertainty Engine
- Using Gaussian Processes for UQ and good sparse data performance
- Active learning
  - Minimise computation with only necessary simulations
  - Train initial model on a small number of data points
  - Re-train on any new simulated data
- Recommendation learning
  - Simulations that give the largest uncertainty reduction
  - Optimised use of computation for model improvement

Workflows

Formalised chains of software tools, explicitly defining the flow of data between them

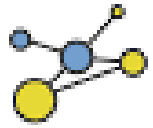
- **Abstract**: declarative process logic separated from data flow, input agnostic
- **Automated**: reusable, capture of metadata enabling qualification of processes and components
- **Scalable and Portable**: cross-platform, compatible with local, cloud HPC
- **Shareable and Citable**: platforms e.g. workflowhub.eu/ create DOIs

Allow wrapping of existing applications

Galaxy PROJECT

Findable

Accessible

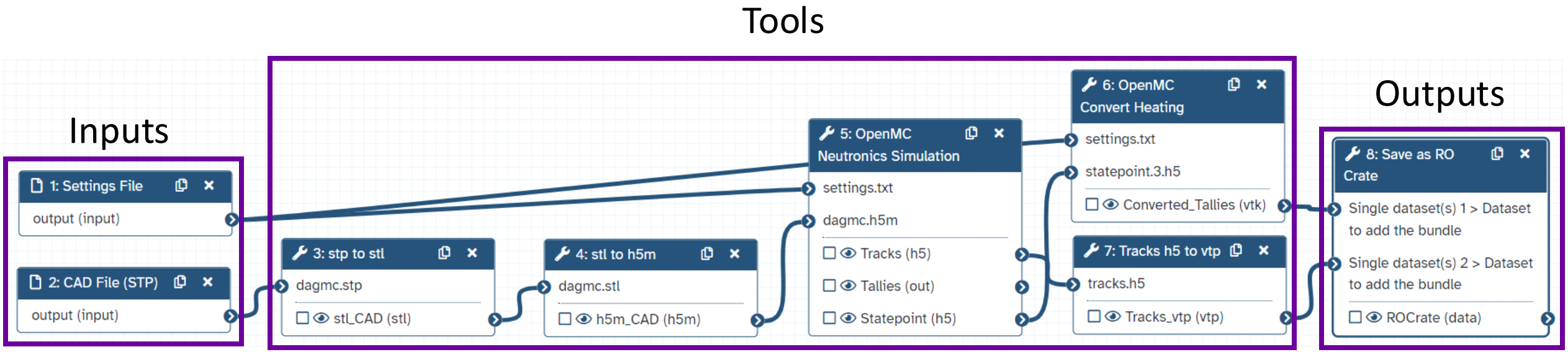


Interoperable

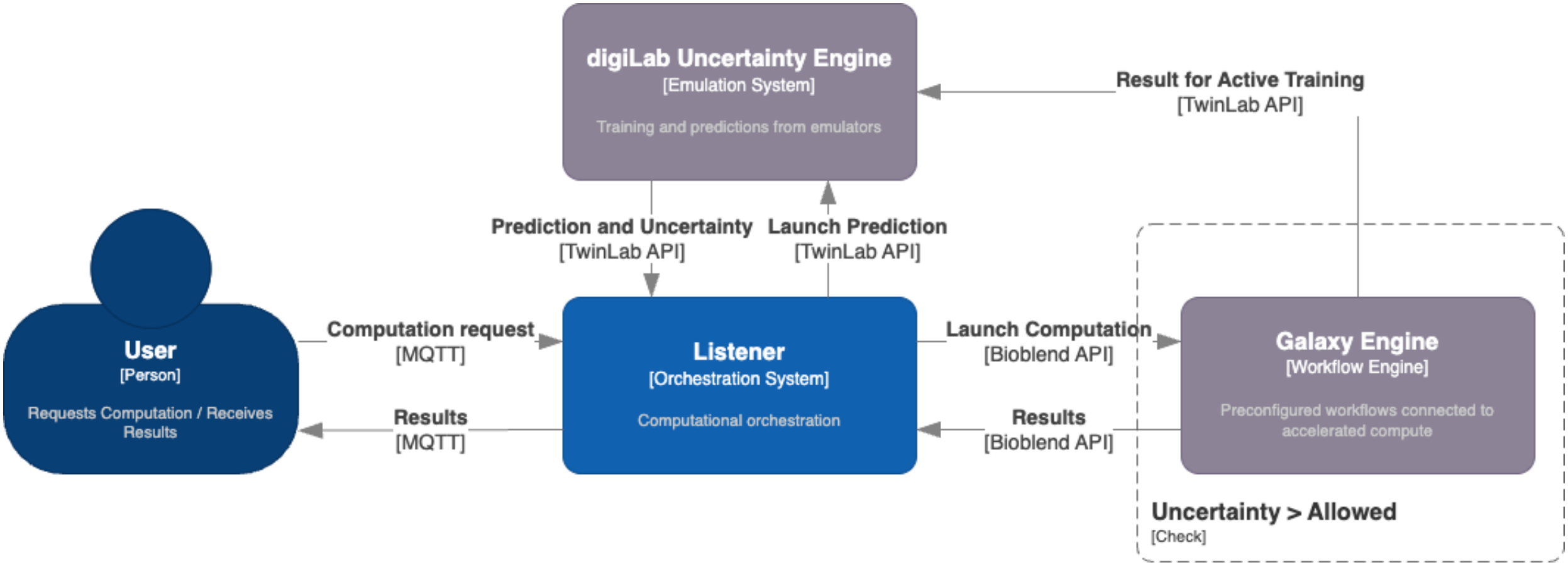
Reusable

Workflows

- Tools wrap existing packages (simulation codes, processing steps)
- Workflows define the flow of data between tools
- Simple and intuitive web UI
- Set-up once, then reuse tools in different configurations
- Simple Python API, allowing integration with external packages

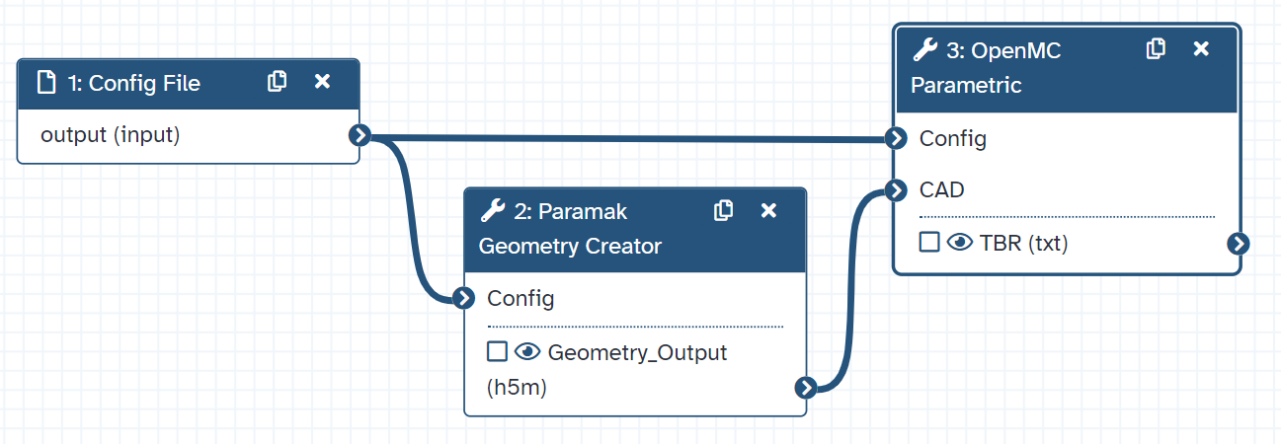


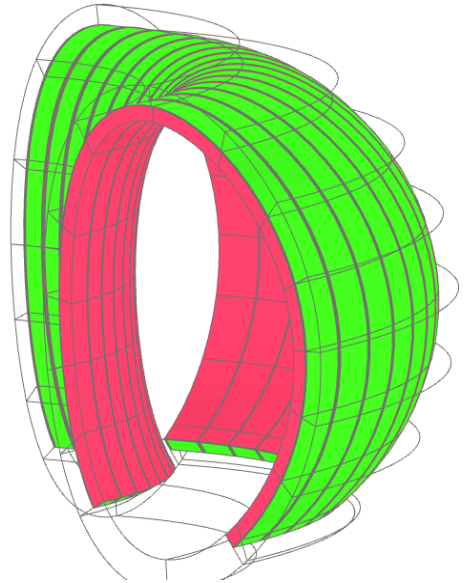
Integration

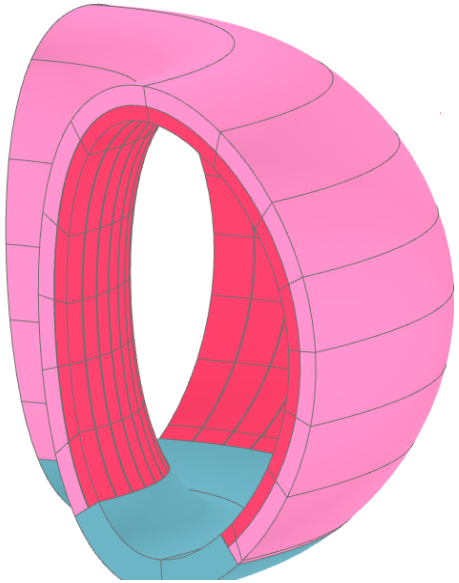


Case Study

- Optimisation problem for TBR
- Parametric CAD (Paramak)
- Neutronics simulation (OpenMC)
- Pre/Post Processing







Case Study Setup

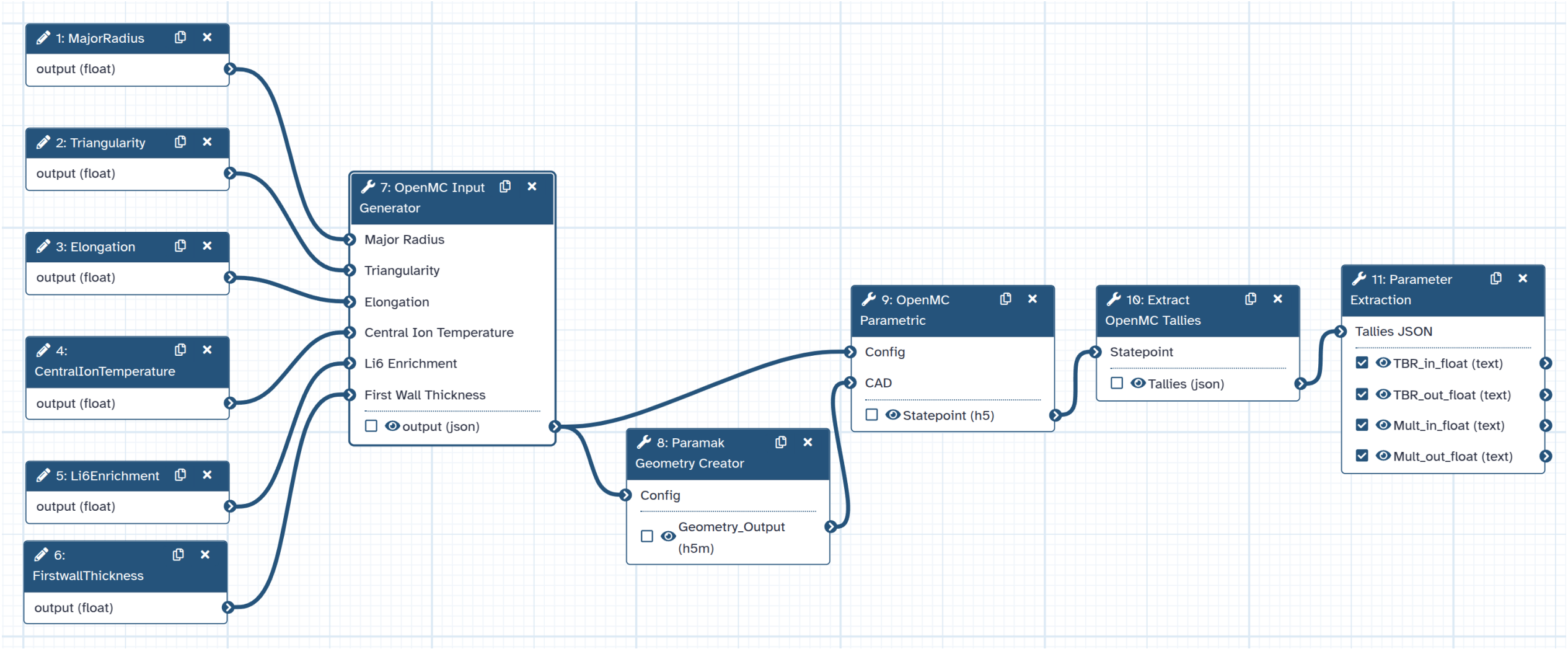
- Uniform distribution over parameter space
- Test at multiple uncertainty thresholds
- ‘Dumb’ testing configuration
  - Run pointwise & no tasks in parallel
  - No targeted uncertainty reduction (recommendation learning)

Two cases:

- ‘Simple’ – Just TBR output
- ‘Complex’ – TBR in/outboard & multiplication factor in/outboard

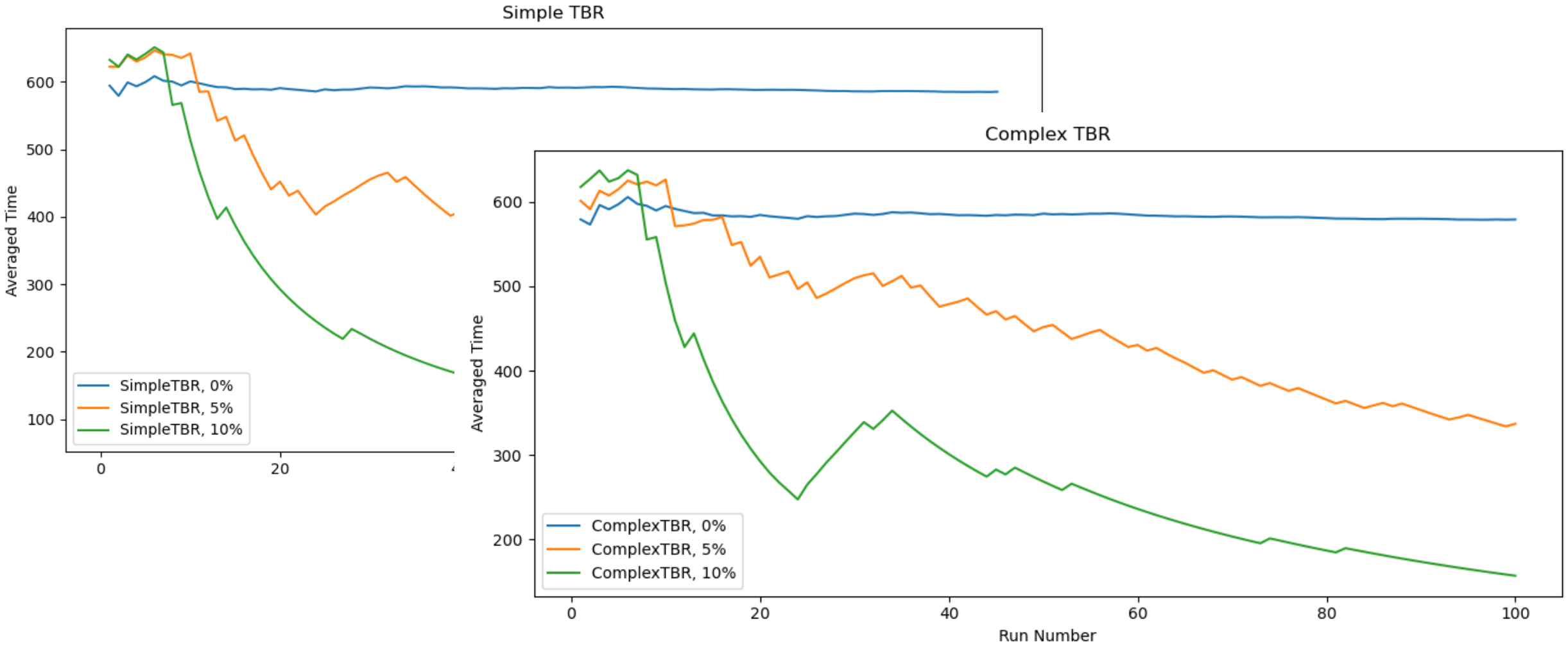
Parameter	Range
Major Radius (cm)	850-950
Triangularity	0.4-0.6
Elongation	1.7-1.95
Central Ion Temp (eV)	40-50
Li6 Enrichment (%)	0-30
First Wall Thickness (cm)	1-3

Case Study Workflow



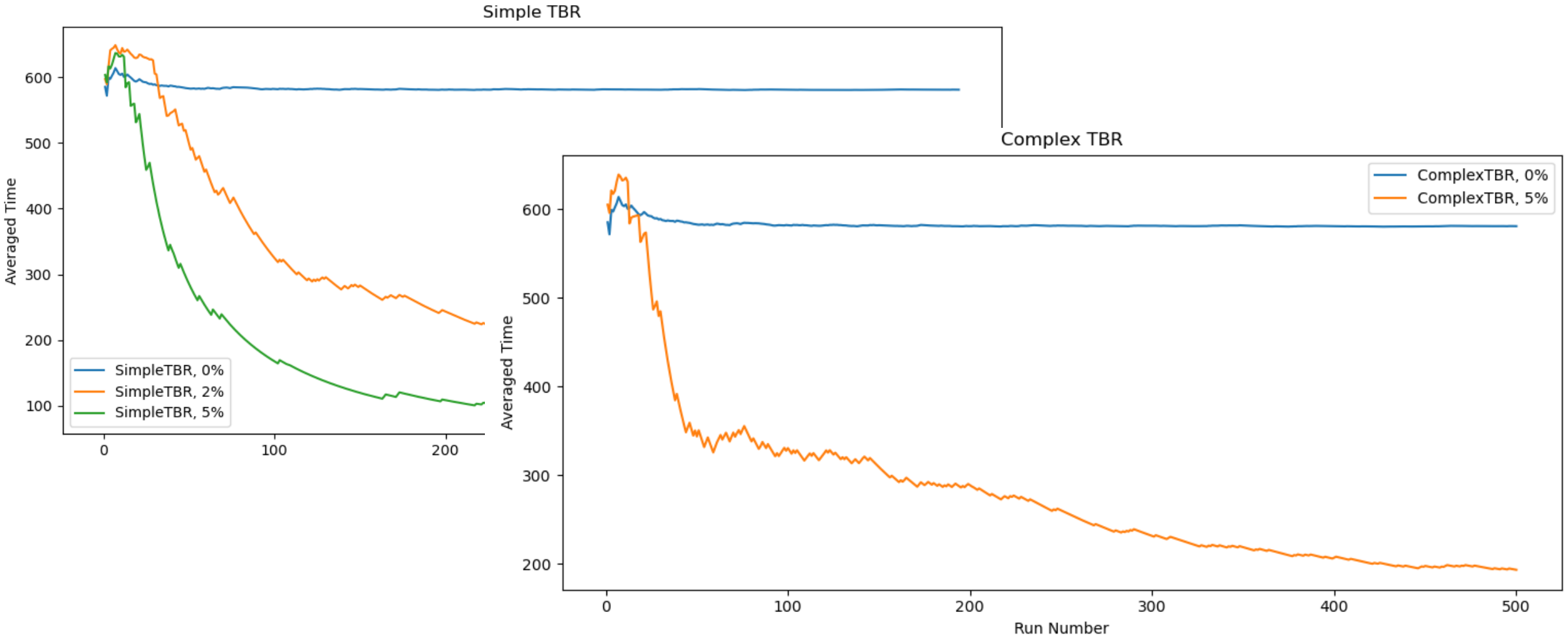
Initial Results

100 Runs



Initial Results

500 Runs



Summary

- Good speed up observed
- Minimal additional work on top of the existing system
- Small overheads – working on improving
- Save time, make better use of computation and re-use data
- Automated emulation layer as fast, uncertainty quantified option

Next Steps:

- Further testing with other cases
- 2D/3D Field emulation

Questions?

MANCHESTER 1824

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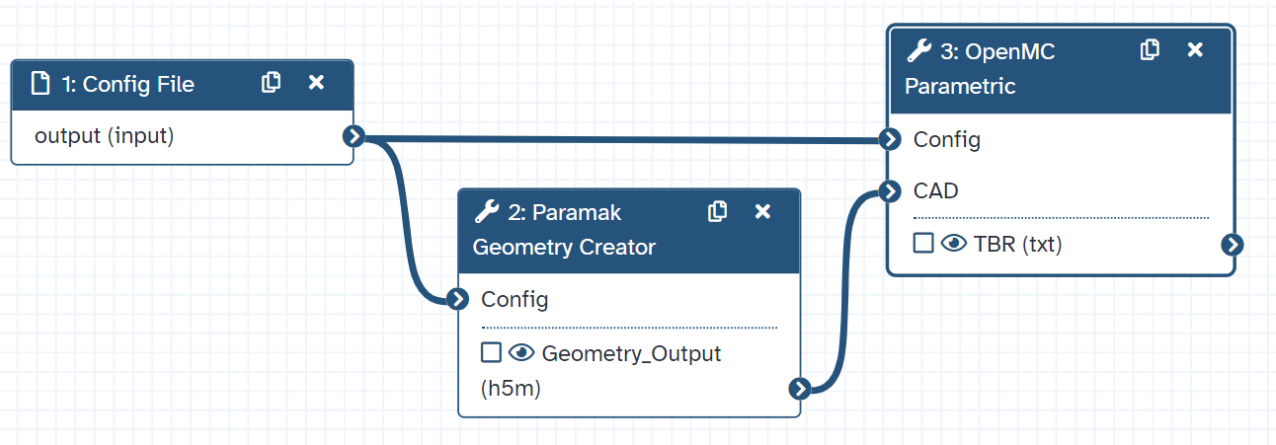
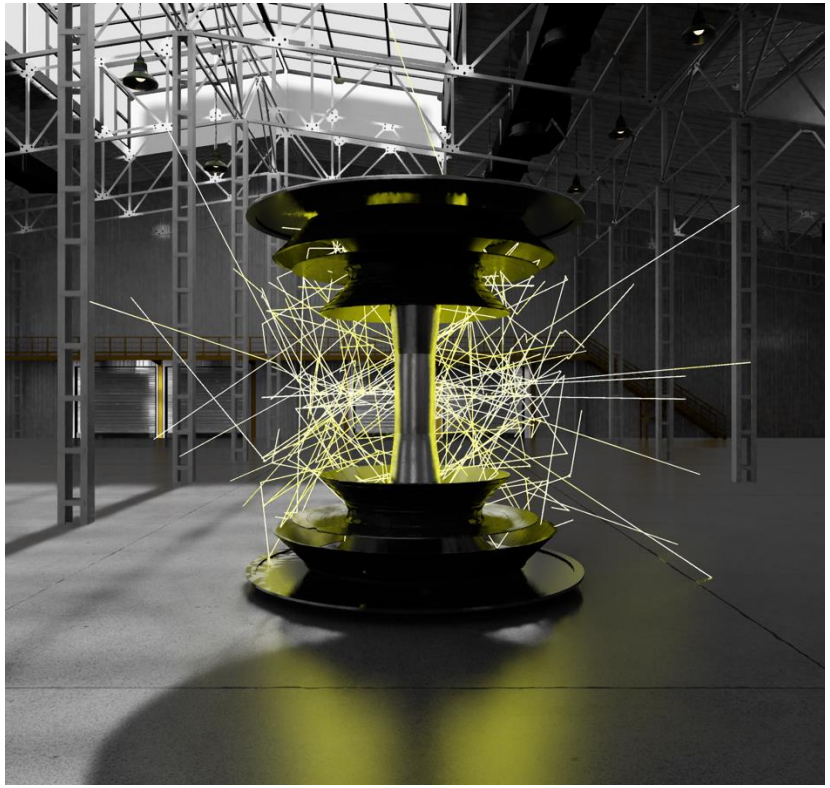
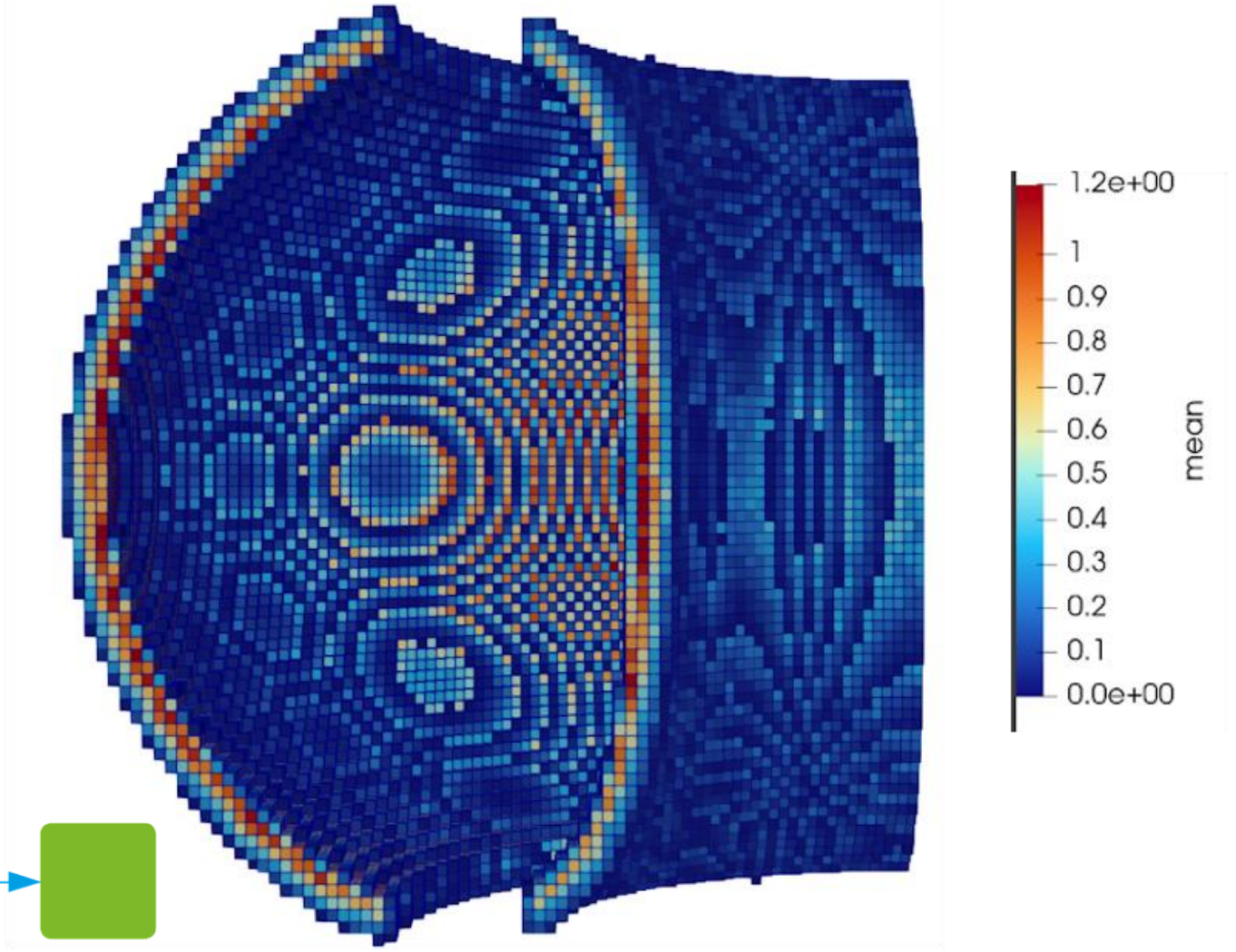


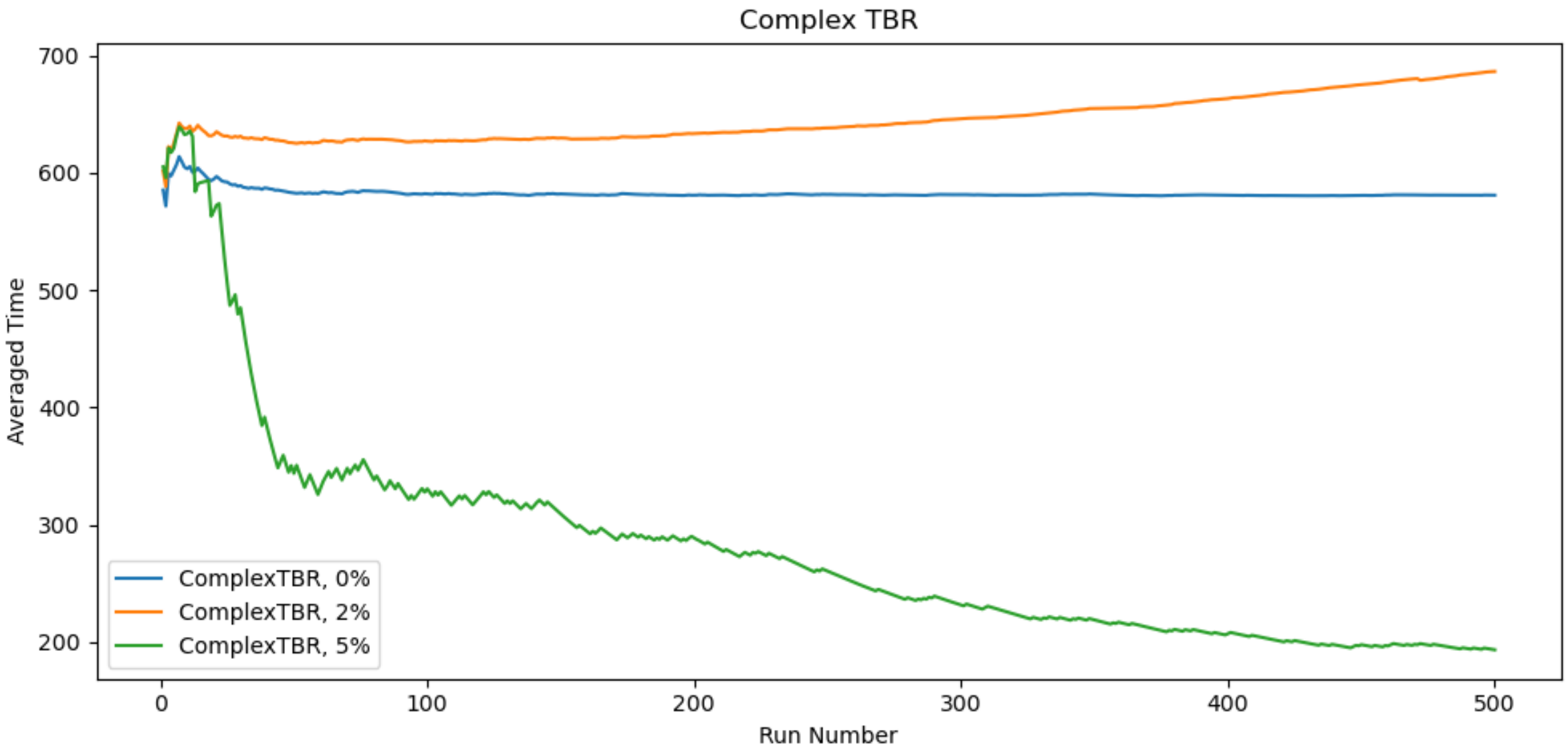


Backup Slides

- High dimensional emulation (full-field)
- ‘Model-update’ for quicker training
- Lower latency of predictions



Backup Slides



Backup Slides