Bayesian and Surrogate-Assisted Optimisation for CFD

CCP-WSI+ Focus Group Workshop 5 - ML for Floating Offshore Wind

Prof Gavin Tabor

2nd April 2025

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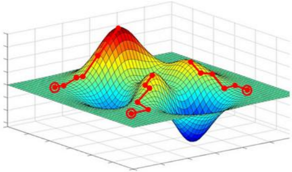
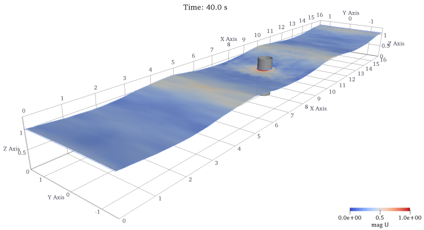
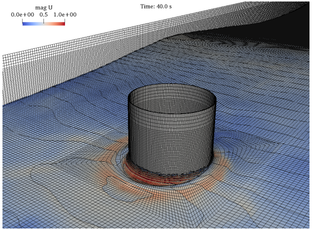
Automatic Design Optimisation

Multiple simulations – possibility of exploring design choices, design optimisation

Automated optimisation – remove human bias, save human time







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Surrogate-Assisted Evolutionary Optimisation

Gradient information difficult to evaluate – *adjoint optimisation*

Evolutionary/genetic optimisation :

- Good at exploring parameter space, finding global optimum
- Requires large number of function evaluations
- Can circumvent through use of *surrogate model*

Simple case : build surrogate model, apply GA

Sophisticated methodologies for expensive evaluations involve multiple optimisation strategies, ML

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Bayesian Optimisation

ML Methodology for optimisation based on *sparse data*

- Build *surrogate model* as basis for evolutionary optimisation
- Iteratively improve using further CFD simulations – acquisition function steers sampling to either explore parameter space or investigate global maximum
- Massively reduces required number of function evaluations

Applied to several engineering cases (simple problems $\rightarrow$ industrial test cases)

CFD simulations and Bayesian optimisation run on Isambard

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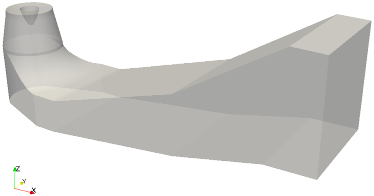
Hölleforsen Kaplan draft tube

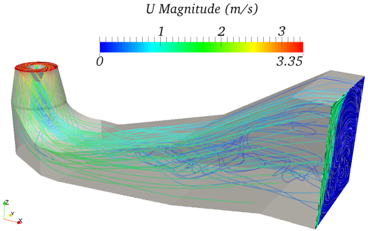
Geometry popularised by ERCOFTAC workshop series

3 parts; initial cone, elbow, end diffuser. Shape/velocity at inflow affects performance.

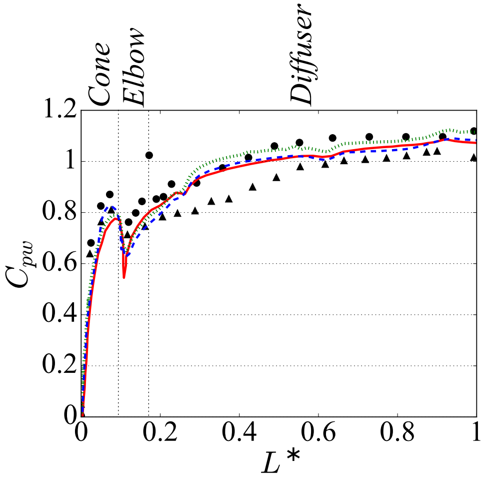
Design optimisation to date through empirical measurements. CFD applied focussing on :

- Inflow velocity calibration
- Turbulence modelling validation

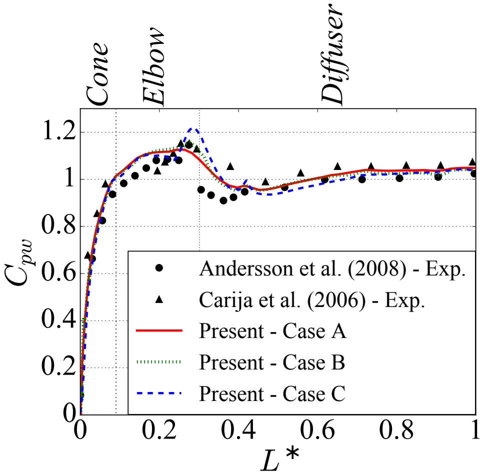




Validation

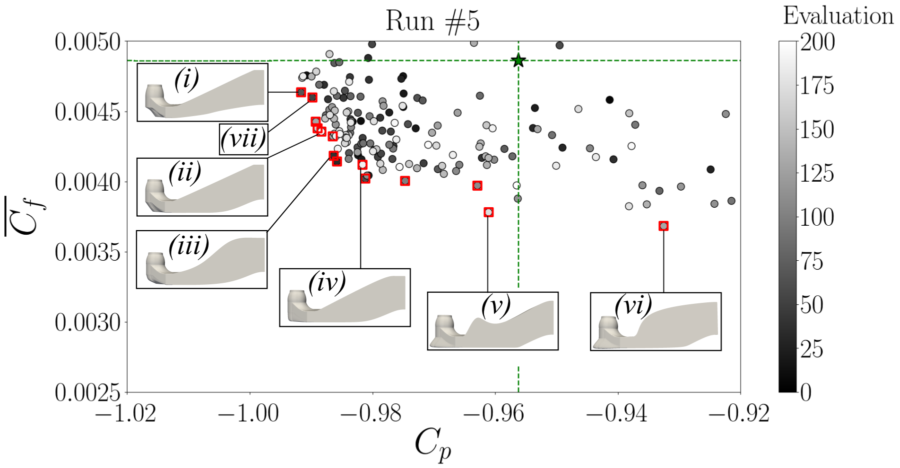


Upper surface



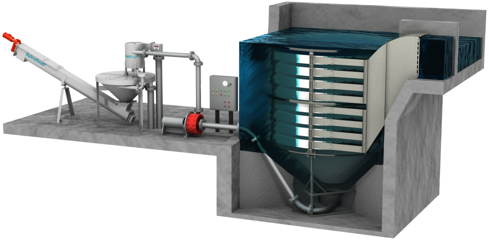
Lower surface

Optimisation



Applications : Vortex Separator

Case study from Hydro International Ltd (Headcell separator) : used for SUDS applications.



Induced vortex produces long residence times. Interaction with conical plates separates particulates from clean water.

Trays: Objectives

Tray components:

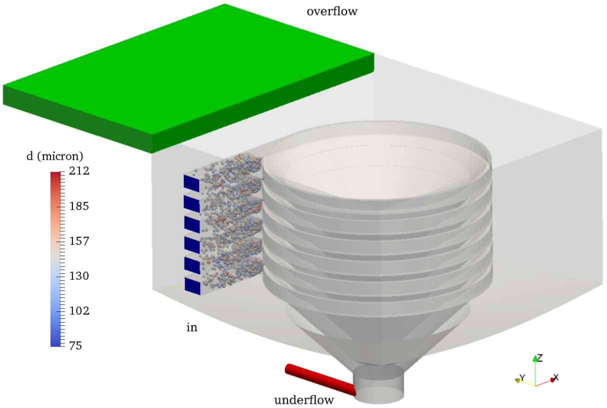
- Trays $\times$ 6
- Benching $\times$ 1

Objectives:

- $\eta_{under} = \frac{m_{underflow}}{m_{in}}$
- $\eta_{total} = \frac{m_{in} - m_{overflow}}{m_{in}}$

Dimensionless Numbers:

- $Re = \frac{U_{nozzle} D_{tray}}{\nu}$
- $Stk = \frac{\rho_p d^2_{p,median} U_{nozzle}}{18 \mu D_{tray}}$



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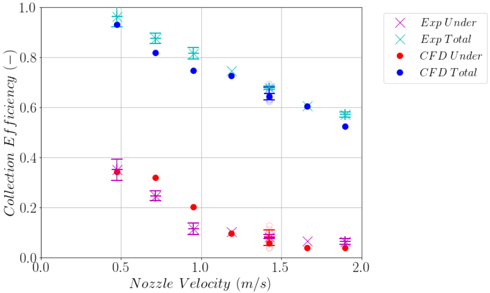
Validation

Flow patterns and particle tracking unsteady (stochastic) – however full transient CFD prohibitive

`simpleFoam` + parcel tracking – need to understand level of accuracy and reliability

Track $\sim 10k$ particles – continue SIMPLE iterations to estimate CFD error bars



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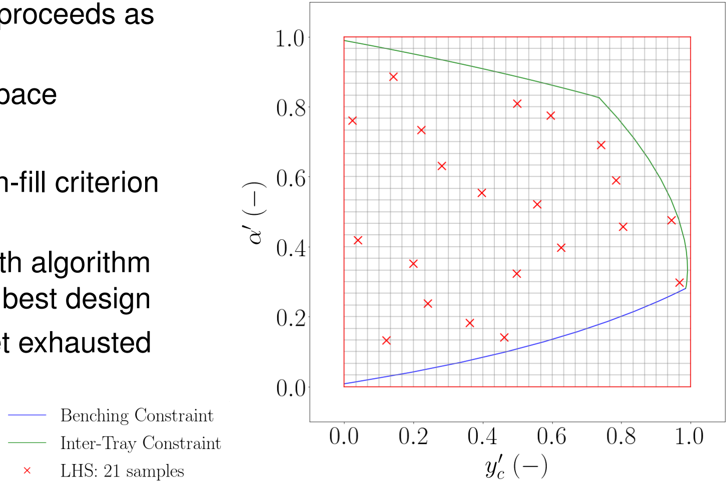
Trays: Bayesian Optimisation

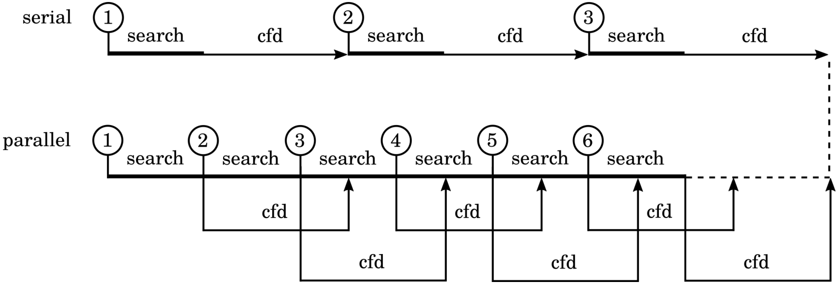
Bayesian Optimisation proceeds as follows:

- Sample decision space
- Train GP Models
- Determine scalar in-fill criterion (MPoI)
- Search criterion with algorithm (CMA-ES) for next best design
- Repeat until budget exhausted



Trays: Parallelisation

- CFD wall clock time is around 21 hours (128 cores per simulation)
- 100 samples $\rightarrow$ 3.5 months in serial
- Run batches of 5 in parallel
- 100 samples $\rightarrow$ 18 days in parallel



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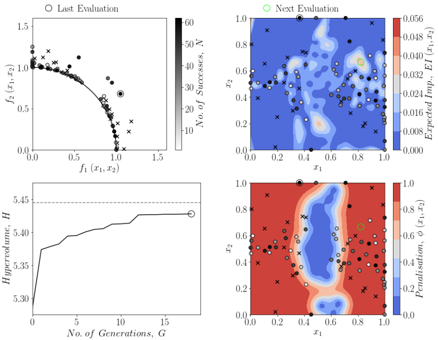
Meshing – Failure handling

CFD can fail in a number of ways, often mesh-related. Two ways to detect :

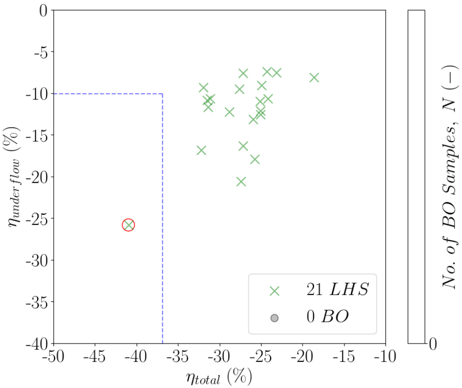
- `checkMesh` (cheap)
- non-convergence (expensive)

Can the algorithm "learn" what works?

Introduce penalisation function and (permanently/temporarily) penalise Expected Improvement (EI)



Optimisation



Initial surrogate – LHC comprising 21 samples

Pareto Front:

- Improvement in $\eta_{underflow} > 20\%$
- Improvement in $\eta_{total} > 5\%$

Pareto solutions share similar characteristics – new IP

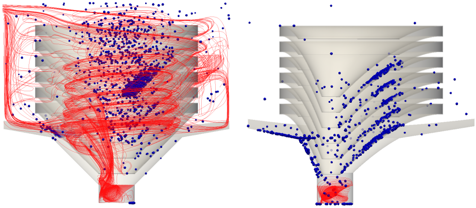
Trays: Physical Explanation

Streamlines and Particles:

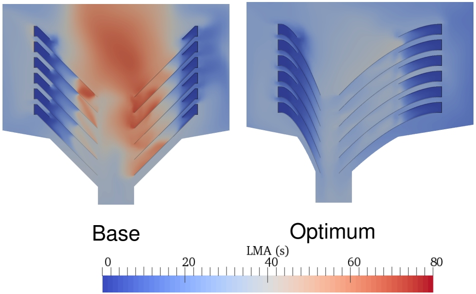
- Backflow cloud removed
- Particles in trays

Local Mean Age of Fluid

- More uniform
- Residence time lowered



Base Optimum



Base Optimum

Surrogate-Assisted Evolutionary Algorithms

Based on single-objective benchmarking, examined 3 SAEAs : Lipschitz Surrogate-Assisted Differential Evolution (LSADE), Two-Stage Data-Driven Evolutionary Optimisation (TS-DDEO), Evolutionary Sampling Agent (ESA)

LSADE

- DE pre-screening on RBF/Lipschitz surrogates
- Greedy acquisition on best-data local surrogate

TS-DDEO

- Early exploration using surrogate-assisted PSO
- Switches to data-driven methods

ESA

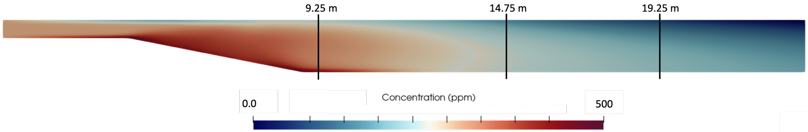
- 4 independent sampling strategies
- Includes reinforcement learning for problem-specific strategies

Applied to DTLZ Test functions, Sand-Trap test case

Conference presentation : “Performance benchmarking of Surrogate-Assisted Evolutionary Algorithms”, Ben Moore, Andrew Roberts, Daniel Jarman, Alma Rahat, Jonathan Fieldsend, Gavin Tabor. Euromech/ERCOFTAC Colloquium on Data-Driven Fluid Mechanics, London, April 2nd - 4th 2025

Sand-Trap Problem

Hyperparameter optimisation of long diffuser for sediment removal

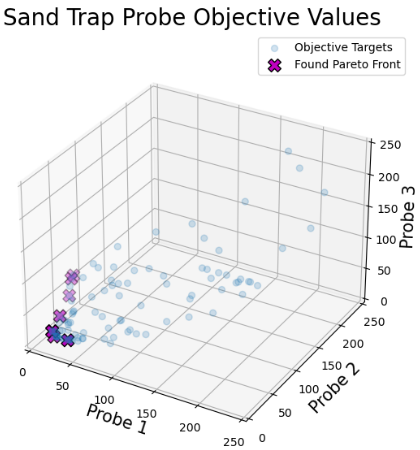


Physical study measured sand concentration at 3 locations

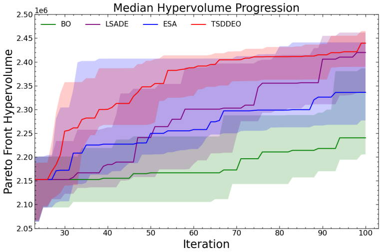
Solvers `simpleFoam/sediDriftFoam` used for calculation

3-objective, 6 parameter optimisation – 4 bin particle categorisation

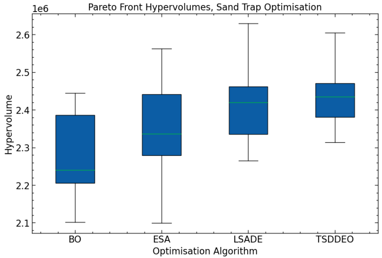
Results



Sand Trap Probe Objective Values
Objective Targets
Found Pareto Front
Probe 1
Probe 2
Probe 3



Median Hypervolume Progression
1e6
BO
LSADE
ESA
TSDDEO
Pareto Front Hypervolume
Iteration



Pareto Front Hypervolumes, Sand Trap Optimisation
1e6
Hypervolume
BO
ESA
LSADE
TSDDEO
Optimisation Algorithm

PINNs

Various AI/ML algorithms (particularly data-driven, neural networks) being applied to CFD, including for :

- Solution techniques
- Turbulence (and other) models
- Enhancing existing models
- Case setup/coding (ChatGPT)

Source : "Enhancing computational fluid dynamics with machine learning", R. Vinuesa and S. L. Brunton, Nature Computational Science V2, pp.358 – 366 (2022)

Physics Informed Neural Networks (PINNs) introduce actual physics into the NN. Pure PINN $\equiv$ solving EOM; hybrid PINN $\equiv$ supplement with (numerical) data.

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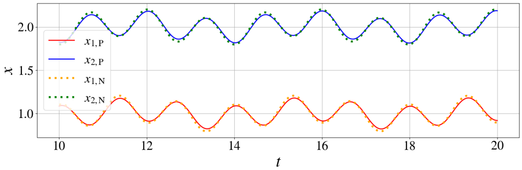
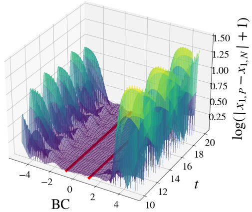
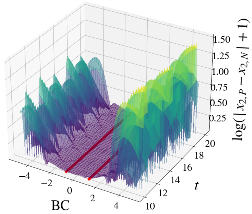
PINNs for Coupled Oscillators

Looking at PINNs for Boltzmann Transport Equation (iCASE with OI) and draft tube simulation (co-funded with IIT-Delhi)

Coupled oscillator case – plane wave PINN with trained BC (generalised PINN).







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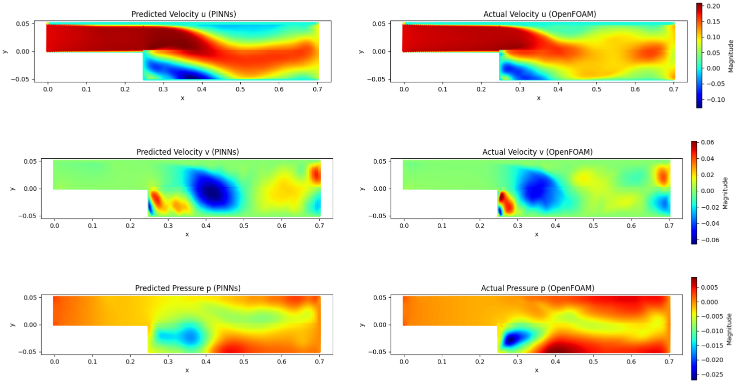
Draft tube – train NN to suppliment RANS model (LES data)

Investigating BFS case to solve NSE : Fourier-based NN – decomposition based on plane waves



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Conclusions

CFD can be used as a predictive tool in Engineering design

Coupled with Machine Learning (Bayesian/SAEA Optimisation) to provide automated optimisation

Real world applications of this – new IP for Hydro International

Next step(s) – Robust Optimisation, Uncertainty Quantification

New ML/AI tools adding to capability in CFD

Acknowledgements

Bayesian/SAEA Optimisation :

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PINNs :

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EPSRC Grant EP/M017915/1 *Data-Driven Surrogate-Assisted Evolutionary Fluid Dynamic Optimisation*, KTP 11477 *To develop and embed a toolset utilising Bayesian Optimisation and CFD techniques into Hydro*

Publications

Performance benchmarking of Surrogate-Assisted Evolutionary Algorithms, Ben Moore, Andrew Roberts, Daniel Jarman, Alma Rahat, Jonathan Fieldsend, Gavin Tabor. Euromech/ERCOFTAC Colloquium on Data-Driven Fluid Mechanics, London, April 2nd - 4th 2025

Plane wave decomposition and randomised training: a novel path to generalised PINNs for SHM. R. Clements, J. Ellis, Geoff Hassall, S. Horsley, G. Tabor. In preparation for :*Phys.Rev.E*

Multi-objective Bayesian shape optimization of an industrial hydrodynamic separator using unsteady Eulerian-Lagrangian simulations A.P. Roberts, A.A.M. Rahat, D.S. Jarman, J.E. Fieldsend and G.R. Tabor *Optim. Eng.* https://doi.org/10.1007/s11081-024-09907-2 (2024)

Application of multi-objective Bayesian shape optimisation to a sharp-heeled Kaplan draft tube S. J. Daniels, A. A. M. Rahat, G. Tabor, J. Fieldsend, and R. M. Everson. *Optimization and Engineering* **23** pp. 687 – 716 (2021)

Shape optimisation of the sharp-heeled Kaplan draft tube: Performance evaluation using Computational Fluid Dynamics, S. J. Daniels, A. A. M. Rahat, G. Tabor, J. Fieldsend, and R. M. Everson. *Renewable Energy* **160** pp.112 - 126 (2020).

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