Deep Gaussian Process-based Multi-fidelity Bayesian Optimization for Simulated Chemical Reactors

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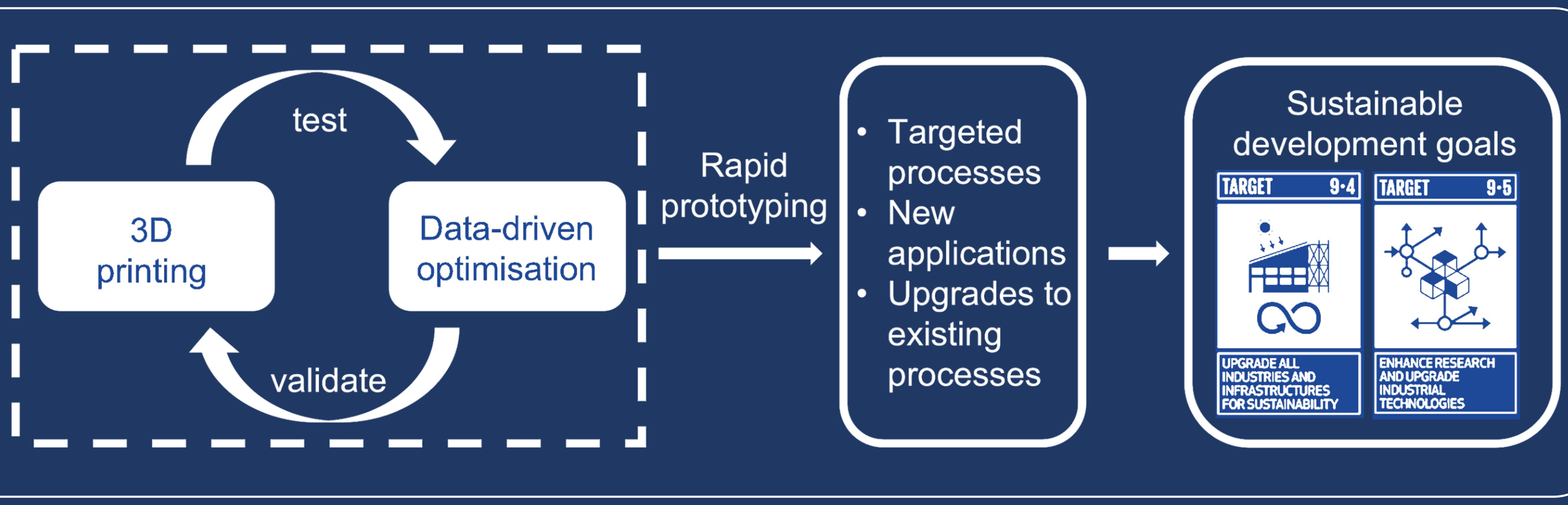
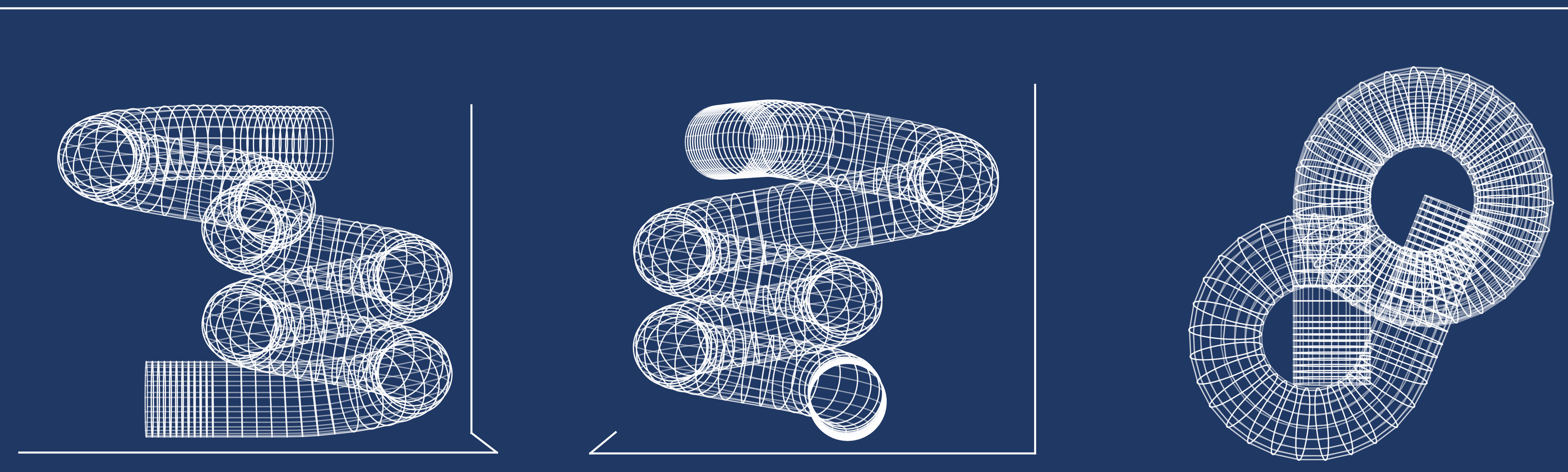
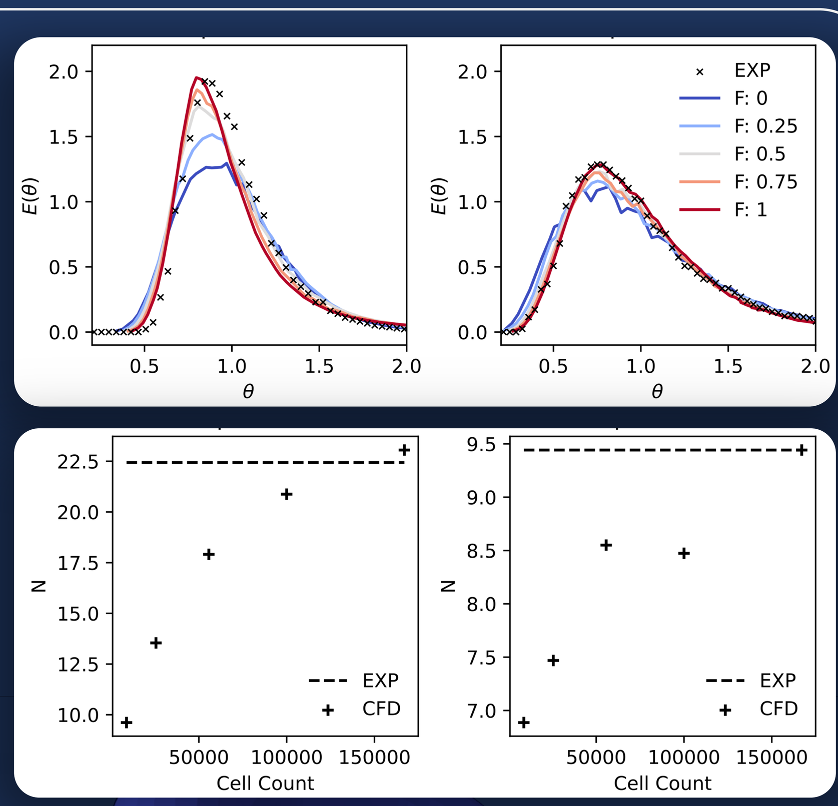
- The development of new manufacturing techniques such as 3D printing have enabled the creation of previously infeasible chemical reactor designs.
- Now able to manufacture and optimize reactors with highly parameterised geometries.
  - Vital to ensure enhanced mixing characteristics;
  - Satisfy feasible manufacturability.





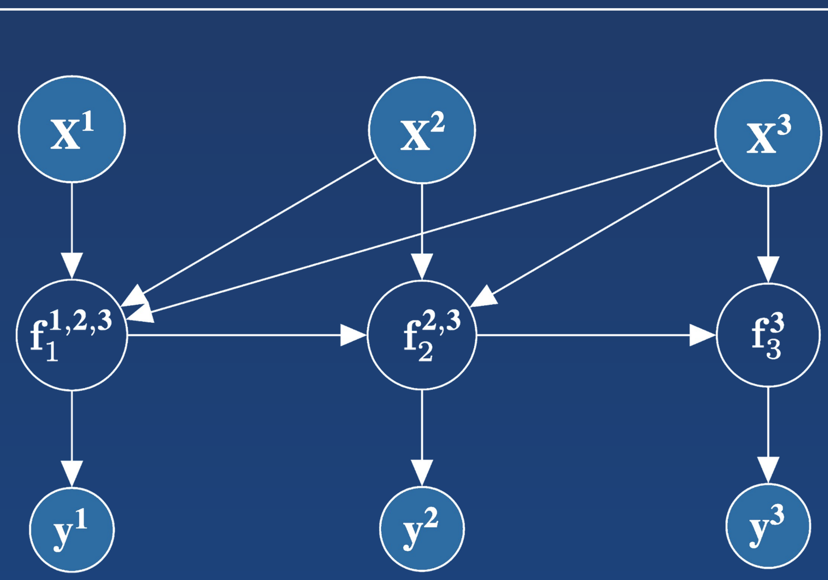
Objective: **maximise plug-flow characteristic**
Issues: Highly nonlinear, derivative-free, **expensive**

- Parameterize a pulsed-flow coiled tube reactor
  - Coil radius
  - Pitch
  - Inversion Location
  - Frequency
  - Amplitude
  - Reynolds Number
- Define discrete simulation fidelities
- Experimentally validate different fidelity simulations



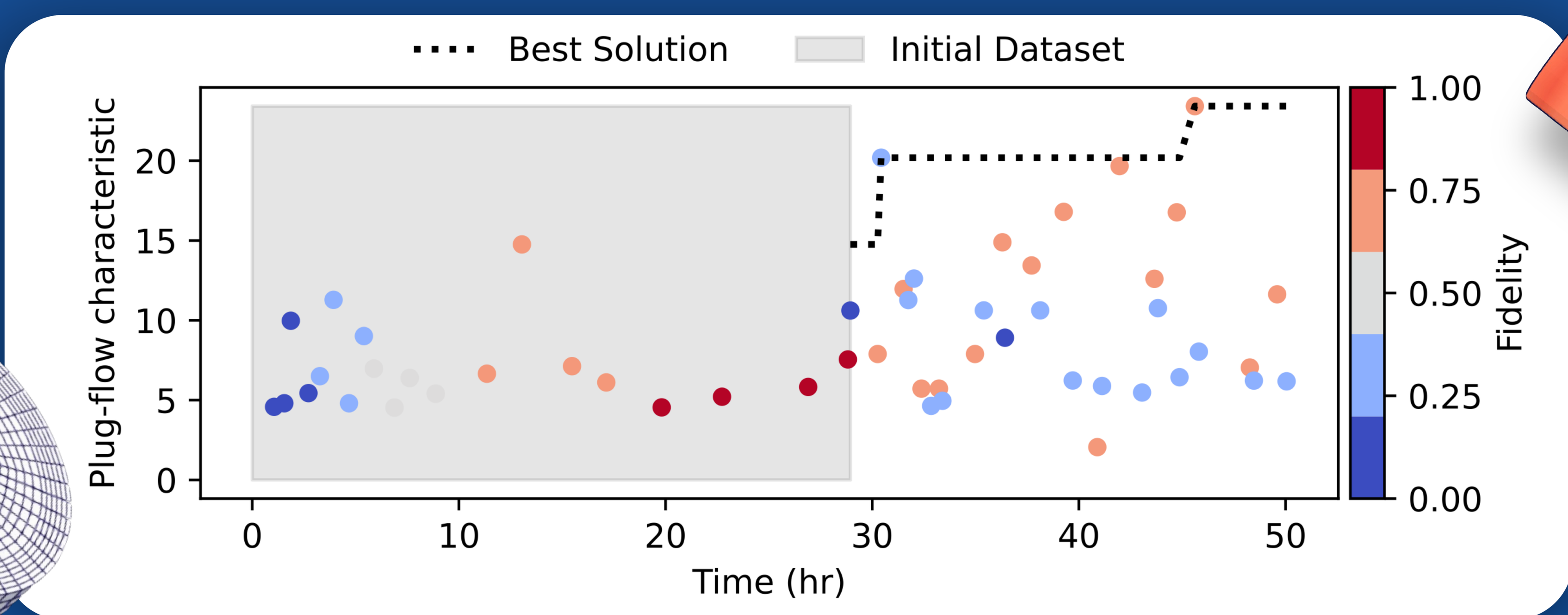
Multi-fidelity Deep Gaussian Processes

- $f_t(x) = \rho_t f_{t-1}(x) + \delta_t(x)$ [AR1]
  - Fails to capture nonlinear relationships between fidelities.
- $f_t(x) = \rho_t(f_{t-1}(x), x) + \delta_t(x)$ [NARGP]
  - Inaccurate uncertainty estimation.
- $f_t(x) = g_f(f^*_{t-1}(x), x)$ [MF-DGP]
  - End-to-end trained, higher fidelity data influences the prediction of lower fidelity functions.



Algorithm 1 Deep GP-based Multi-fidelity Bayesian Optimization

Require: $f_1(x) \dots f_T(x)$, $\mathcal{X}$, n
  for t in $1, \dots, T$ **do**
    Generate n samples, $\mathbf{x}_t$, and evaluate $f_t(\mathbf{x})$ resulting in $\mathbf{y}_t$.
    $\tau_t \leftarrow$ average simulation time
  end for
  while Budget not exhausted **do**
    Train DGP using $\mathbf{x}_1, \dots, \mathbf{x}_T$ and $\mathbf{y}_1, \dots, \mathbf{y}_T$
    Solve UCB for highest-fidelity: $x^* \leftarrow \arg\max_x \{\mu_T(x) + \beta^{1/2}\sigma_T(x) | x \in \mathcal{X}\}$
    Choose fidelity based on variance of DGP and simulation cost: $t^* \leftarrow \text{argmax}_t\{\gamma_t \beta^{1/2}\sigma_t(x^*)\}$
    where $\gamma_t = \max(\tau)/\tau_t$
    Evaluate $f_{t^*}(x^*)$, add x^* to $\mathbf{x}_{t^*}$ and $f_{t^*}(x^*)$ to $\mathbf{y}_{t^*}$
  end while



Conclusions

- Additive manufacturing → highly parameterised chemical reactors.
- Optimization of coiled-tube reactor geometry → expensive, multi-fidelity black-box problem.
- Multi-fidelity Bayesian optimization using Deep Gaussian processes → enables solution.
- Framework → extended to other problems involving highly-parameterized CFD simulations.

References

- Deep Gaussian Processes for Multi-fidelity Modeling: arXiv:1903.07320
- Multi-fidelity Gaussian Process Bandit Optimisation: arXiv:1603.06288
- Oscillatory fluid motion unlocks plug flow operation in helical tube reactors at lower Reynolds numbers ($Re \leq 10$): DOI:10.1016/j.cej.2018.10.054

- Tom Savage would like to thank the Imperial College President's Scholarship Fund
- PREMIERE (EP/T000414/1)
- Dr Jonathan McDonough, Newcastle University
- Ilya Sandoval for discussion