MOSKopt — simulation-based stochastic black-box optimization under uncertainty

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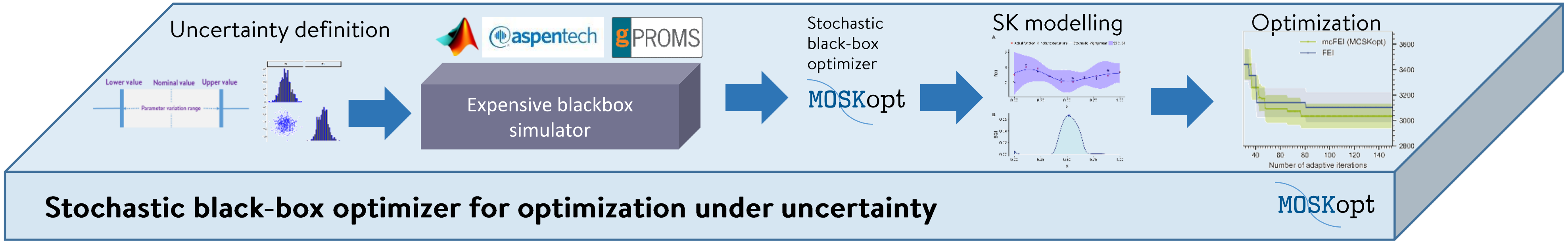
A simulation-based stochastic black-box optimizer

A new generic black-box solver: MCSKopt



introducing

MCSKopt

Stochastic black-box optimizer for optimization under uncertainty of complex systems, e.g. digital twins.

available on

GitHub

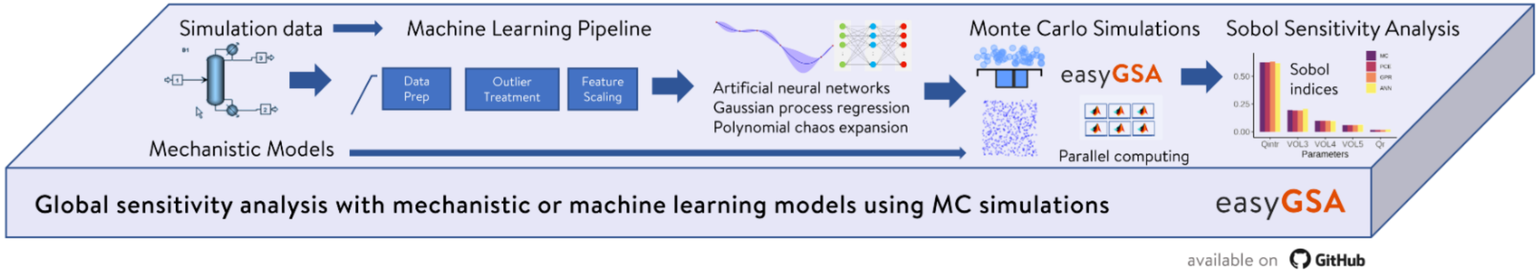
Download

- > Available from a GitHub repository, documentation in preparation.
- > A generic *stochastic black-box optimizer*, implements the workflow.
- > *Embedded* Monte Carlo simulations for uncertainty quantification.
- > Allows for multiple uncertainty *hedging* strategies.
- > Implements SK modelling, infill optimization, and provides the popular as well as the newly proposed infill (mcFEI) criteria.
- > Object-oriented programming → *user-extendable* infills.
- > Applications to other processes (e.g., *fermentation*) underway.

DTU

Chapter 5 > Outcomes

easyGSA



MATLAB® File Exchange MENDELEY DATA GitHub

introducing

easyGSA

Global sensitivity analysis framework using mechanistic or machine learning algorithms

available on GitHub

Download

> Easy-to-work syntax → plug in *any* model.
> GSA methods: the Sobol method and the SRC method.
> Sampling schemes: Sobol sequences, LHS.
> Statistical *inference* for distributions in user data.
> Support for *multiple outputs* → expensive simulations.
> Hyperparameter optimization → GPR models.
> Gridsearch optimization algorithm → ANN models.
> Allowing *user provided data* to fit surrogates and perform Sobol GSA.
> ML pipeline for automatic *data treatment*.
> Efficient use of available *parallelization* architecture.
> Inc. in course materials, already used by MSc and PhDs.

Input arguments overview

Required argument
Optional argument
Available options
Default setting in bold

‘Model’	‘N’	‘InputSpace’	
@ishigami @mymodel.m	**2e3** ..	‘LowerBounds’ ‘UpperBounds’	
‘SamplingMethod’	**‘Estimator’**	**‘UseSurrogate’**	**‘Method’**
‘Sobol’ ‘LHS’	**‘Jansen’** ‘Saltelli’	‘GPR’ ‘ANN’	**Sobol** SRC
‘UserData’	**‘UseParallel’**	**‘Verbose’**	
Data.X Data.Y	true **false**	**true** false	

Syntax

```
[Si,STi,results] = easyGSA(f,N,InputSpace{:},...
                    'SamplingMethod','LHS',...
                    'Estimator','Saltelli',...
                    'UseSurrogate','GPR',...
                    'UseParallel',true,...
                    'Verbose',false)
```

Use Latin hypercube sampling to sample the input space

Use ‘Saltelli’ estimator for Sobol indices calculation

Use Gaussian process models as a surrogate

Activate parallel computing

Suppress command line messages

More detailed results of the analysis containing all the models and simulation results.

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DTU Summer School on Uncertainty and Sensitivity Analysis

Chapter 6 > Introduction

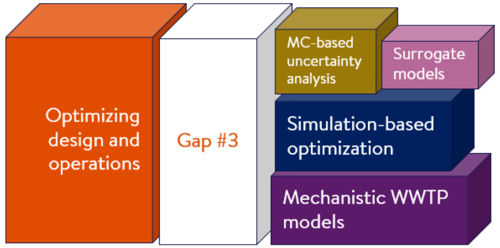
Optimization of WWTP networks under uncertainty

Chapter motivations

> WWTP design is subject to high uncertainty.
> Use the community's well-matured first principles simulation models to do design optimization (e.g., ADM1).
> Address Gap#3 identified in literature review.
> Further optimize WWTP layouts that are identified as *promising* in Chapter 4.
> Quantify and integrate the impacts of uncertainties (e.g., influent composition).

Gap #3

No applicable workflow for optimizing WWTPs using simulation models under uncertainty.



> The potential of simulation-based optimization is not investigated.
> Quantification and incorporation of uncertainties in optimization.

Primary goals:

> Develop/demonstrate an applicable simulation-based workflow for WWTP design *optimization under uncertainty (OUU)*.
> Automate the workflow in a generic tool.

Exhaustive sampling-based optimization

- Used as a benchmark method.
- Discretizes both the design and the uncertainty spaces using sampling.
- Allows for an exhaustive search for an optimum under uncertainty.
- Effective yet heavily suffers from the *curse of dimensionality*.
- $N_d \times N_u$ simulations needed.

Table 6.1: Pseudocode for the exhaustive sampling-based method for design space exploration.

Algorithm 1: **Design space exploration via exhaustive sampling**

1: **input**
$S_d = \{x_i \in X_d : i = 1,\ldots,N_d\}$, and $S_u = \{u_j \in X_u : j = 1,\ldots,N_u\}$
2: $DS \leftarrow U$
3: **for all** $x_i \in S_d$ **do**
4: $DS \leftarrow DS \cup \left\{x_i;\ \hat{\mathrm{P}}[G(x_i,\cdot) \leq 0 \mid S_u]\right\}$
5: **end for**
6: **return** DS

Hedging strategies against the uncertainties

- Tune the level of conservativeness.

Name	Explanation
Mean	The mean of constraint observations acquired from the Monte Carlo simulations is less than the constraint limit.
UCI95	The upper confidence interval for the mean of constraint observations acquired from the Monte Carlo simulations is less than the constraint limit.
PF80	The probability of the feasibility calculated from the Monte Carlo simulations is higher than 80 %.
MeanPlusSigma	The mean plus one standard deviation of constraint observations acquired from the Monte Carlo simulations is less than the constraint limit.

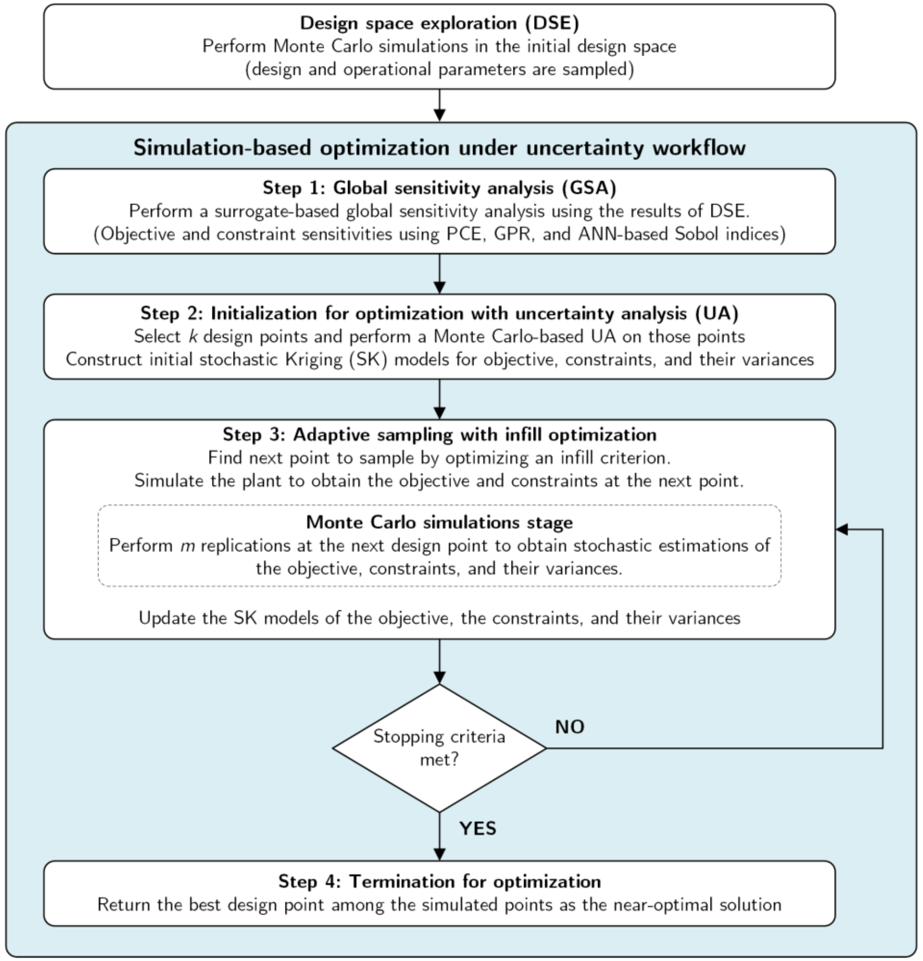
Chapter 6 > Methods

Simulation-based optimization under uncertainty

- Employs surrogate models for *a better-informed exploration* in the design space.
- Generic workflows have 3 stages: initialization, adaptive sampling, and termination.

- We integrate *2 more stages*: global sensitivity (prior to initialization) and uncertainty analysis (both in initialization and in adaptive sampling stages).

- Key to its success is the *infill criterion*,—an internal optimization of an expected improvement measure using surrogates.



Stochastic Kriging modeling

> An extension of *Kriging*,—an interpolation-based meta-model.

> Introduced by Ankenman *et al*. as a meta-modeling technique for stochastic simulations.

> Found *promising uses* in simulation optimization.

Wang and Ierapetritou, 2018. *Comput Chem Eng* 118. Picheny *et al*., 2013. *Technometrics* 55.

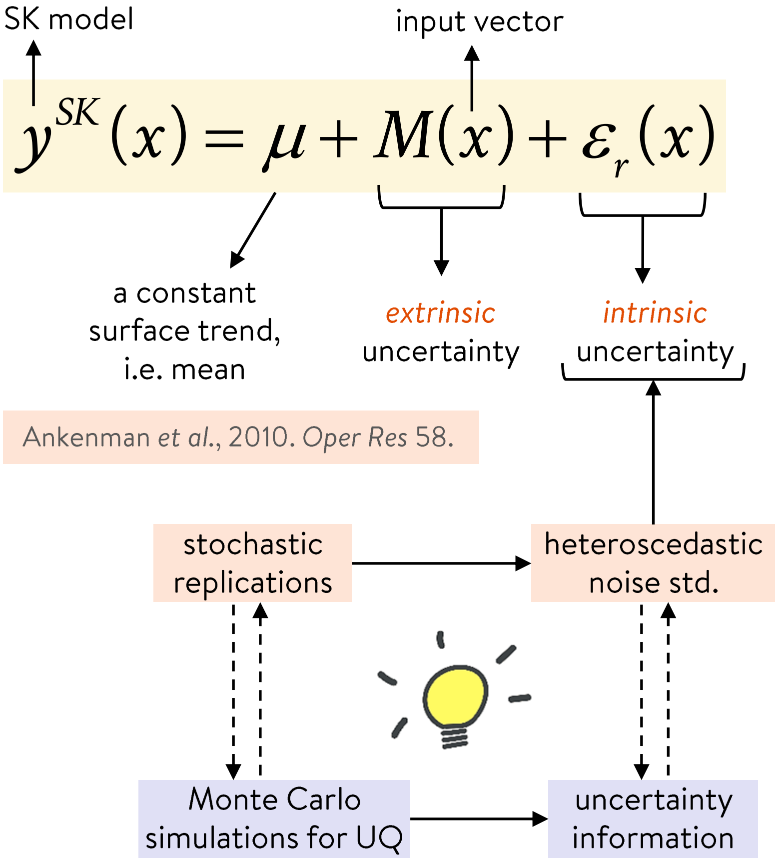
Extrinsic uncertainty

> The lack of certainty of the meta-model about the simulation model's behavior at regions where no observations are obtained.

Intrinsic uncertainty

> The lack of certainty in the original simulation model's responses.

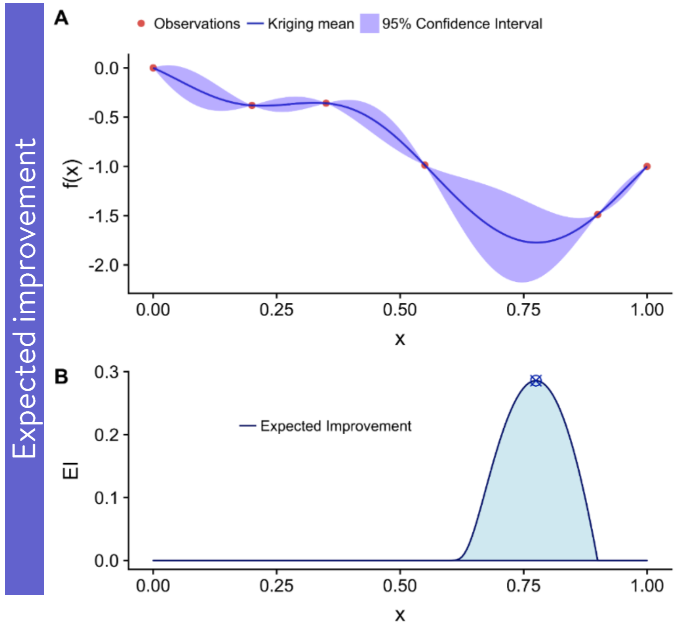
Stochastic Kriging model structure

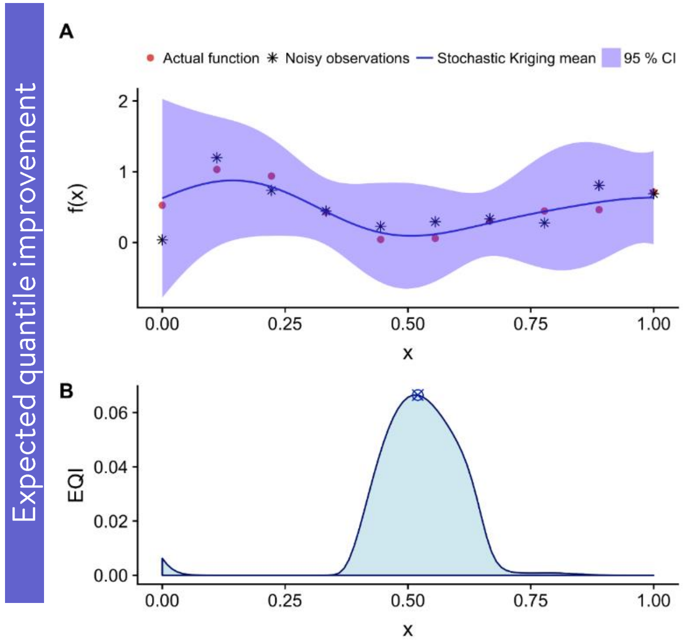


Chapter 6 > Methods

Infill criteria for optimization

Understanding infill optimization





Expected Improvement

Mockus, J., 1975. *Opt Techniques* → Jones *et al.*, 1998. *J Glob Optim* 13.

$$E\left[I(x) \mid f^{n}\right] = \left(f_{\min} - \mu_f(x)\right)\Phi\left(\frac{f_{\min} - \mu_f(x)}{\hat{s}_f(x)}\right) + s(x)\phi\left(\frac{f_{\min} - \mu_f(x)}{\hat{s}_f(x)}\right)$$

Unconstrained deterministic

Expected Quantile Improvement

Picheny *et al.*, 2013. *Technometrics* 55.

$$EQI_n(x) = \left(q_{\min} - m_Q(x)\right)\Phi\left(\frac{q_{\min} - m_Q(x)}{s_Q(x)}\right) + s_Q(x)\phi\left(\frac{q_{\min} - m_Q(x)}{s_Q(x)}\right)$$

Unconstrained stochastic

Constrained Expected Improvement

Wang and Ierapetritou, 2018. *Comput Chem Eng* 118.

$$cAEI_f(x) = \underbrace{E\left[I_f(x)\right]}_{\text{improve objective}} \cdot \underbrace{P\left(G_i(x) \le 0\right)}_{\text{prioritize feasible regions}} \cdot \underbrace{\left(1 - \tau_f \,/\, \sqrt{\tau_f^2 + \hat{s}_f^2}\right)}_{\text{balance between explore \& exploit}}$$

Feasibility Enhanced Expected Imp. (FEI)

Wang and Ierapetritou, 2018. *Comput Chem Eng* 118.

$$FEI(x) = cAEI_f(x) + \underbrace{P(Y_f(x) \le f^{***})}_{\text{focus on areas where f is small}} \cdot \underbrace{EQI_g(x)}_{\text{handle stochasticity in the constraint}}$$

Multiple-constrained FEI (mcFEI)

Al *et al.*, 2020. *Comput Chem Eng* (under review).

$$mcFEI(x) = mcAEI(x) + P(Y_f(x) \le f^{***}) \cdot \prod_{i=1}^{c} EQI_{g_i}(x)$$

$$mcAEI(x) = E[I_f(x)] \cdot \left(1 - \tau_f \,/\, \sqrt{\tau_f^2 + \hat{s}_f^2}\right) \cdot \prod_{i=1}^{c} P[G_i(x) \le 0]$$

handle stochasticity in multiple constraints

Sasena: An illustrative example

Sasena test problem

- Mathematical formulation (*modified*).

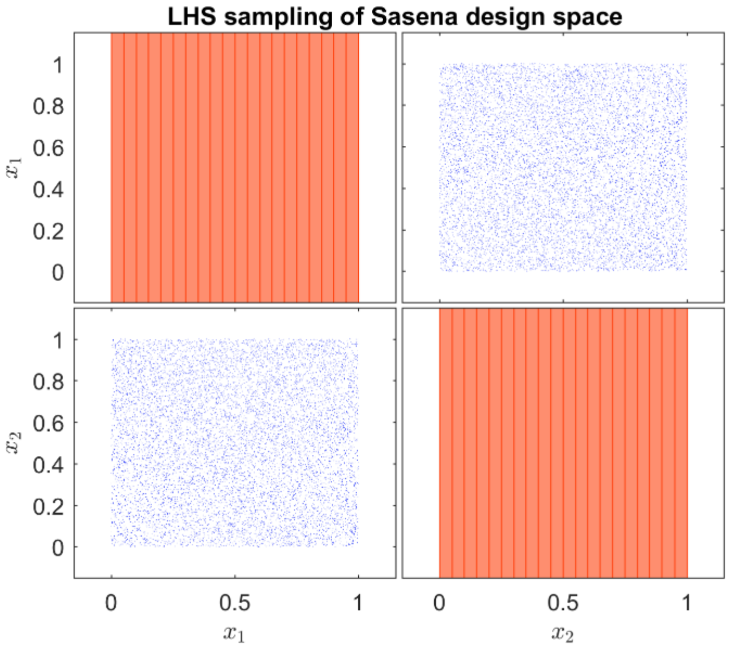
$$
\begin{aligned}
\min_{x} \quad & f(x) = -u_1(x_1-1)^2-(x_2-0.5)^2 \\
s.t. \quad & g(x) = [g_1(x),\ g_2(x),\ g_3(x)] \le 0 \\
& g_1(x) = (u_2(x_1-3)^2+(x_2+2)^2)e^{-x_2^7}-12 \\
& g_2(x) = 10u_3x_1+x_2-7 \\
& g_3(x) = (x_1-0.5)^2+u_4(x_2-0.5)^2-0.2 \\
& 0 \le x_i \le 1 \ \text{ for } i=1,\ 2 \\
& \ln(u_j) \approx \mathcal{N}(\mu,\sigma) \text{ for j}=1,..,4
\end{aligned}
$$

- 2 decision variables,—visualize the design space.
- 4 uncertain parameters,—following normal and lognormal distributions.

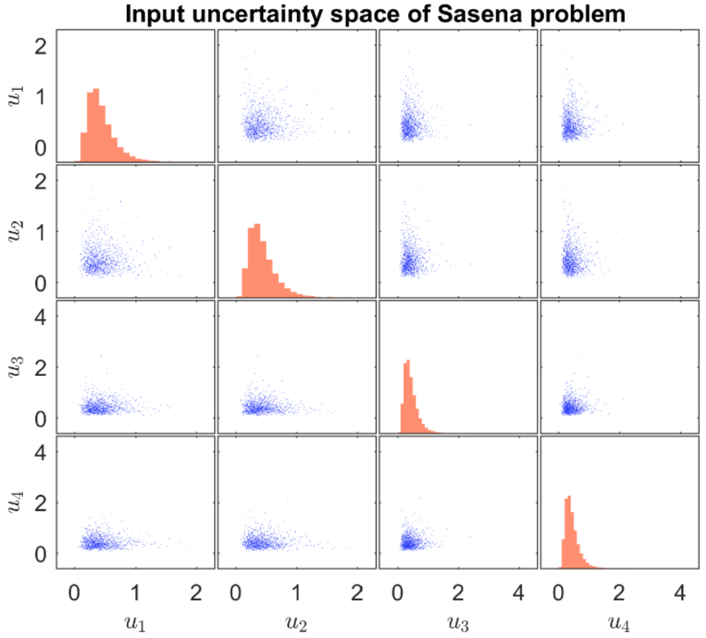
Solution via Exhaustive sampling

- From 10 to 10^5 LHS design samples x 10^3 LHS uncertainty samples.
- *Vectorized* Monte Carlo simulations → simultaneous exploration in both spaces.

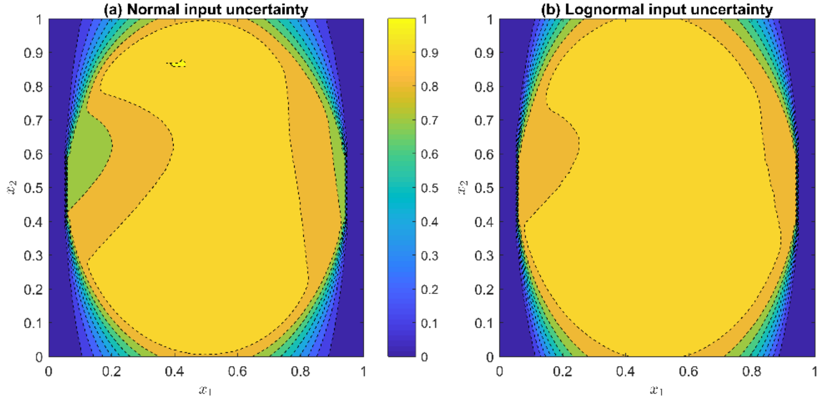
Design space



Uncertainty space



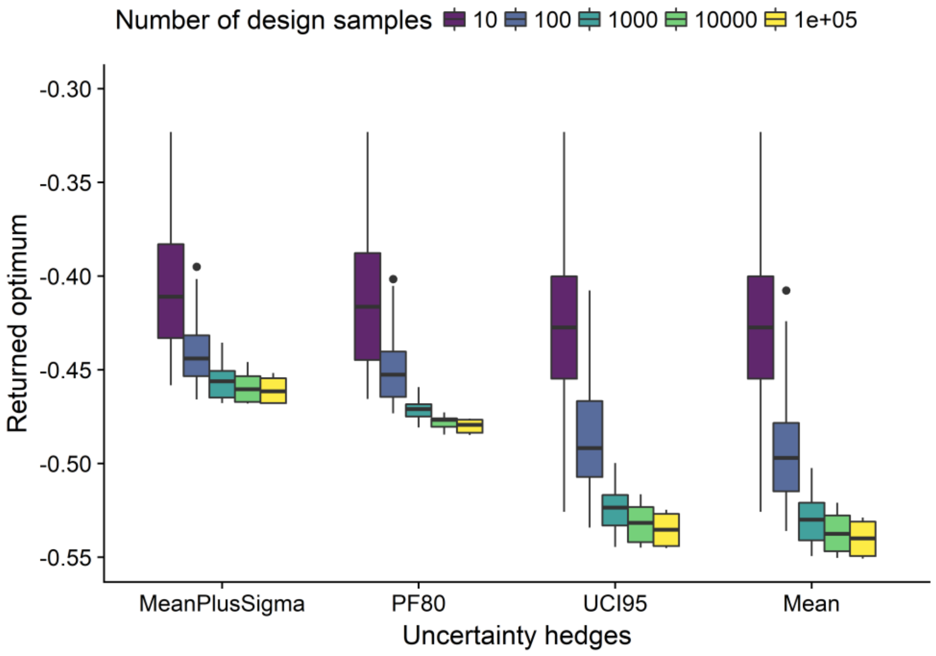
Probabilistic design spaces



Sasena results

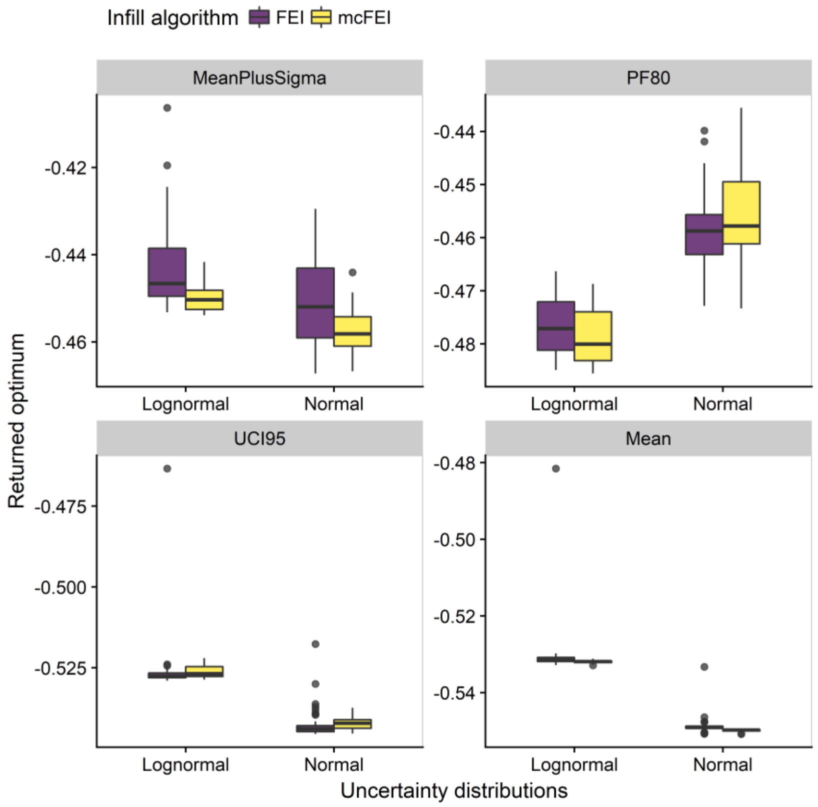
Solutions via Exhaustive sampling

> Competitive solutions already at 10^3 samples.



Solutions via simulation-based optimization

> 100 design samples, 50 independent repetitions.



Rosen Suzuki: A higher dimensional example

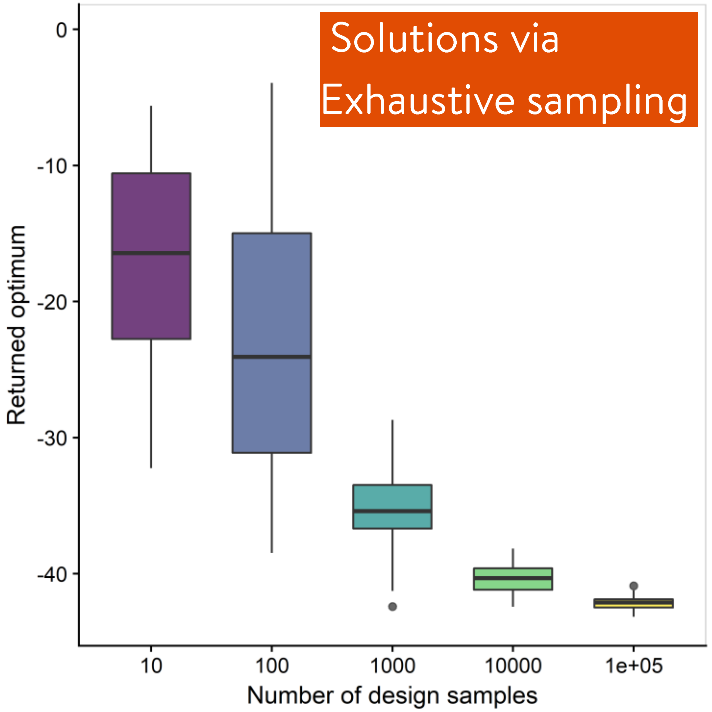
Rosen Suzuki test problem

> Mathematical formulation (*modified*).

$$
\begin{aligned}
\min_{x} \quad & f(x) = x_1^2 + x_2^2 + 2u_1 x_3^2 + x_4^2 - 5x_1 - 5x_2 - 21x_3 + 7x_4 \\
s.t. \quad & g(x) = [g_1(x),\ 100 g_2(x),\ 1000 g_3(x)] \le 0 \\
& g_1(x) = x_1^2 + u_2 x_2^2 + x_3^2 + x_4^2 + x_1 - x_2 + x_3 - x_4 - 8 \\
& g_2(x) = x_1^2 + 2x_2^2 + x_3^2 + 2u_3 x_4^2 - x_1 - x_4 - 10 \\
& g_3(x) = 2x_1^2 + u_4 x_2^2 + x_3^2 + 2x_1 - x_2 - x_4 - 5 \\
& -3 \le x_i \le 3 \ \text{for } i = 1,..,4 \\
& u_j \approx \mathcal{N}(\mu,\sigma) \text{ for j} = 1,..,4 \text{ and } \mu = 1,\ \sigma = 0.25
\end{aligned}
$$

> 4 decision variables.

> 4 uncertain parameters,—following normal distributions.



Benchmark solution

Number of LHS design samples	Total number of calls to the model	Optimum value of the objective	Location of the optimum (x)
10^5	10^8	-42.152	[-0.026, 0.841, 1.951, -0.914]

Chapter 6 > Results > Case study 2

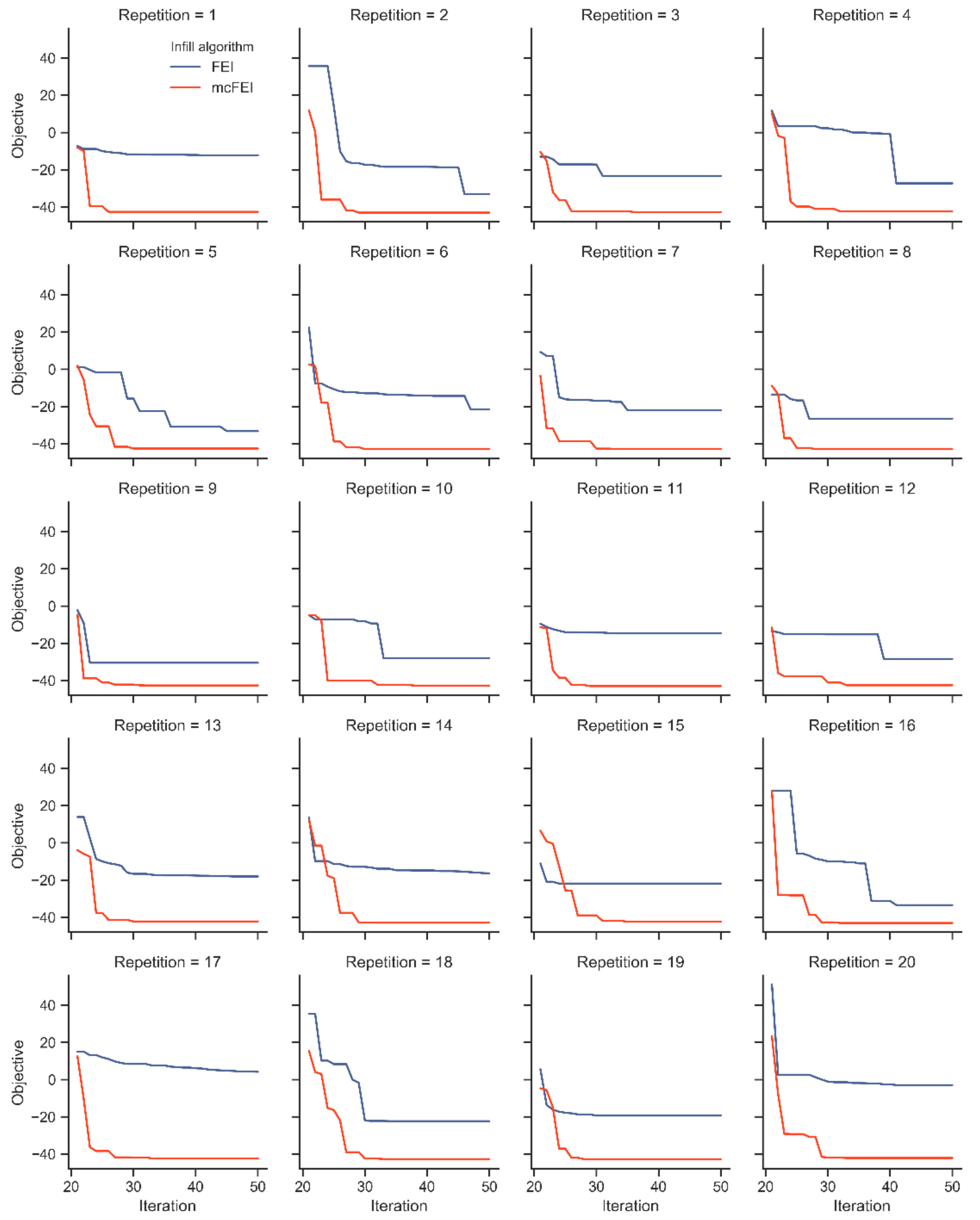
Rosen Suzuki

Solution via simulation-based optimization

- MCSKopt is called with two infills: FEI and mcFEI.
- 50 design samples with 50 independent runs.
- The mcFEI visibly *outperforms* FEI.
- The mcFEI solution (cost=50) is *even better* than the benchmark solution (cost=10^5). Why? → the *curse of dimensionality*.
- SK-based approach → a *better-informed* exploration.

Infill algorithm	Number of LHS design samples	Total # of calls to the model	Optimum value of the objective	Location of the optimum (x)
FEI	50	50×10^3	-24.915	[-0.368, 0.607, 1.468, 0.128]
mcFEI	50	50×10^3	-42.701	[0.028, 0.608, 1.996, -0.996]
Exhaustive	10^5	10^8	-42.152	[-0.026, 0.841, 1.951, -0.914]

Optimization progress: FEI (blue) vs mcFEI (orange)

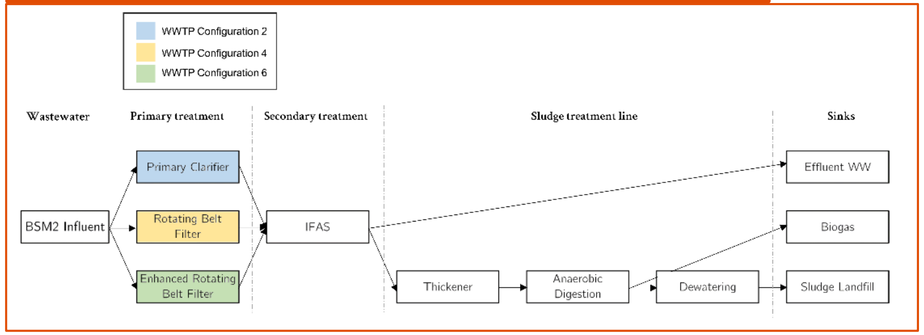


Chapter 6 > Results > Case study 3

WWTP design optimization

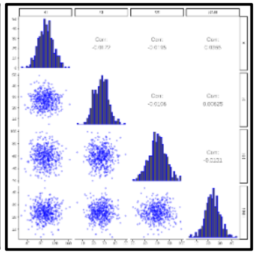
> Simulation-based optimization of the 3 layouts.

The 3 promising layouts from Chapter 4



Influent uncertainty

BSM2 influent states	Nominal value (μ) g COD/m^3	Variation (σ)
SI_{inf}	27.22	25 %
SS_{inf}	58.17	25 %
XI_{inf}	92.49	25 %
XBH_{inf}	50.68	25 %



influent

$$under \quad \left.\begin{matrix} SI_{inf} \\ SS_{inf} \\ XI_{inf} \\ XBH_{inf} \end{matrix}\right\} \approx \mathcal{N}(\mu,\sigma)$$

Uncertain influent fractions

Objective KPI

Decision variables

Aeration energy

Sludge production

External carbon

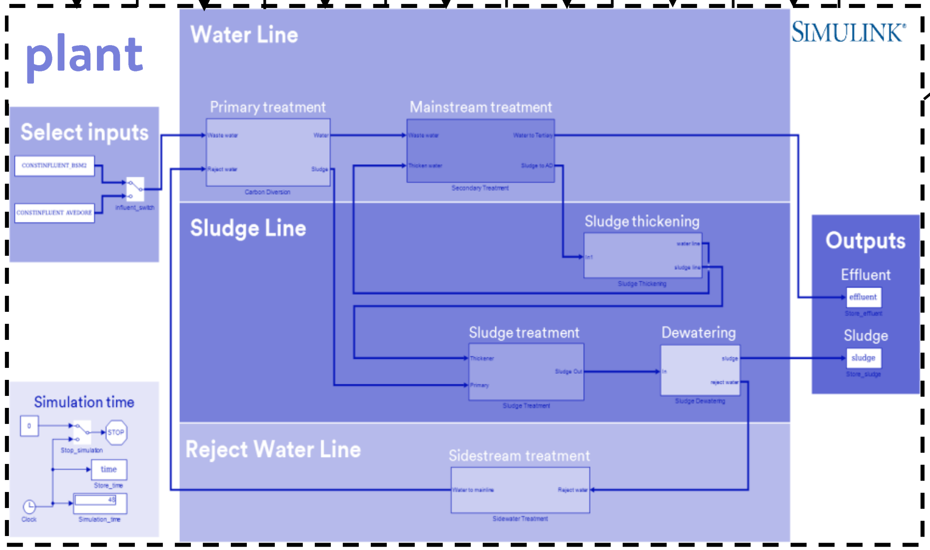
Mixing energy

Methane production

$$\min_{x} \quad OCI(x) = AE + 3\cdot SP + 3\cdot EC + ME - 6\cdot MP + HE^{net}$$

Heating energy

Plant-wide simulation-based objective function



Envelope for optimization

Quality limits

effluent

$$s.t. \quad E(COD_{eff}) + std(COD_{eff}) \le 100$$
$$E(SNH_{eff}) + std(SNH_{eff}) \le 5$$
$$E(TN_{eff}) + std(TN_{eff}) \le 15$$

Effluent quality KPIs

The impact of uncertainties

Chapter 6 > Results > Case study 3

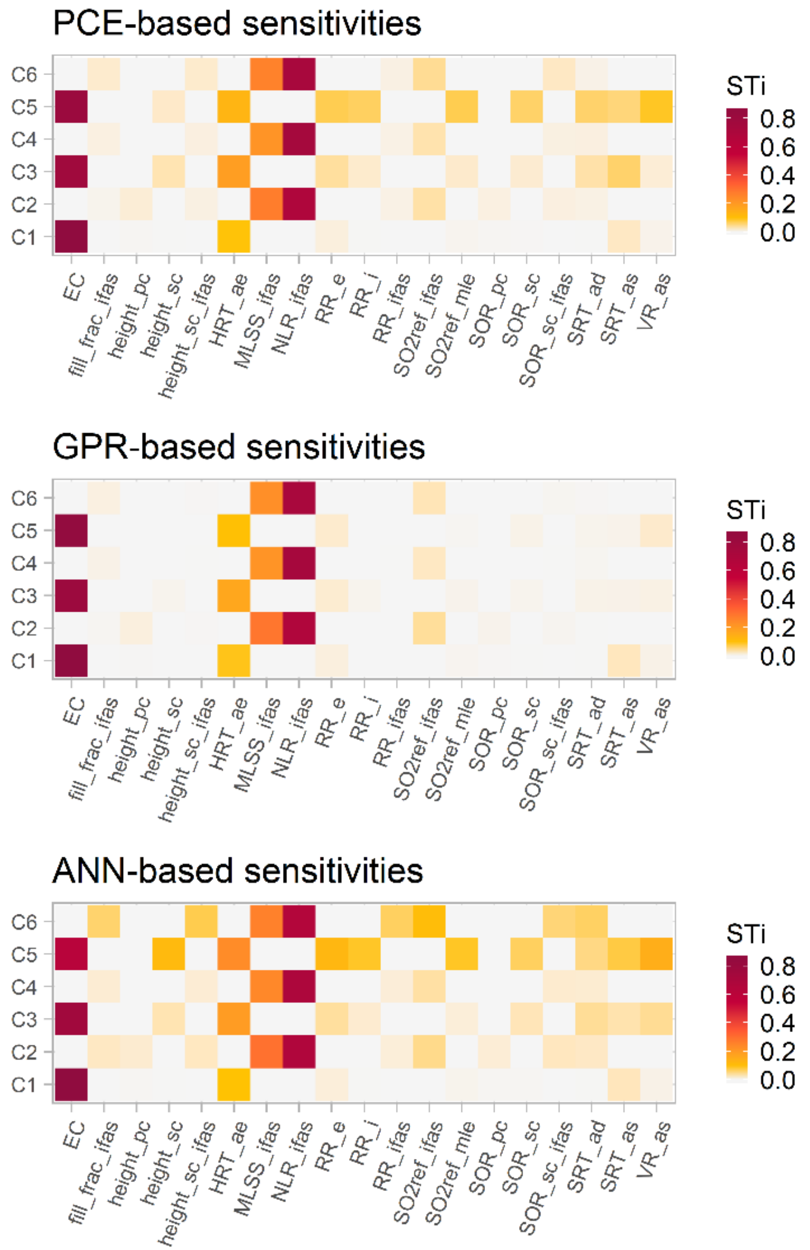
WWTP design optimization

- The results of MCS (from Chapter 4) → GSA with surrogates → further *refined design spaces* in C2, C4, and C6.
- Total impacts (as quantified by STi) of design/operational decisions quantified using 3 surrogates → ensemble approach.

Refined design spaces in C2, C4, and C6

Configuration ID	Decision variable	Lower bound	Upper bound	Unit
2	$MLSS_{IFAS}$	1000	5000	g TSS/m^3
	NLR_{IFAS}	0.05	0.5	kg N/m^3d
	DO_{IFAS}	0.1	0.5	g/m^3
4	$MLSS_{IFAS}$	1000	5000	g TSS/m^3
	NLR_{IFAS}	0.05	0.5	kg N/m^3d
	DO_{IFAS}	0.1	0.5	g/m^3
	FF_{IFAS}	30	60	%
6	$MLSS_{IFAS}$	1000	5000	g TSS/m^3
	NLR_{IFAS}	0.05	0.5	kg N/m^3d
	DO_{IFAS}	0.1	0.5	g/m^3

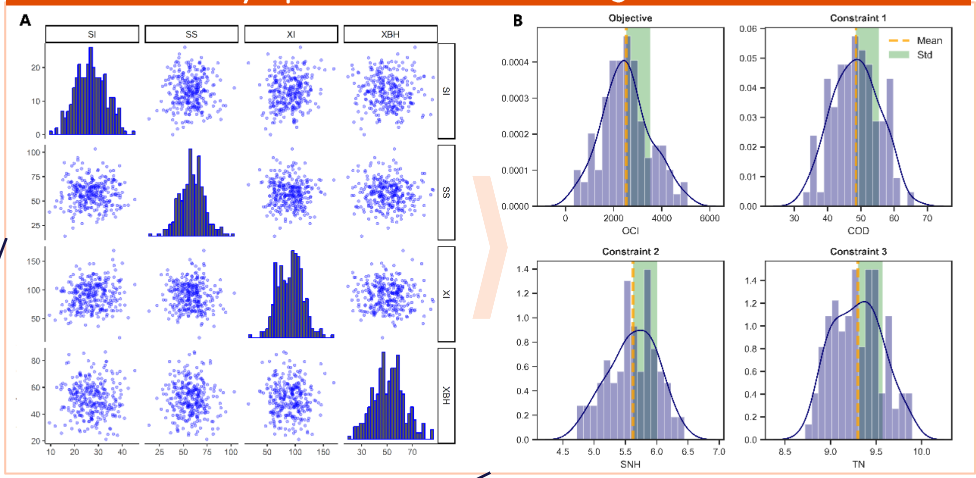
Global sensitivity analysis from MCS results



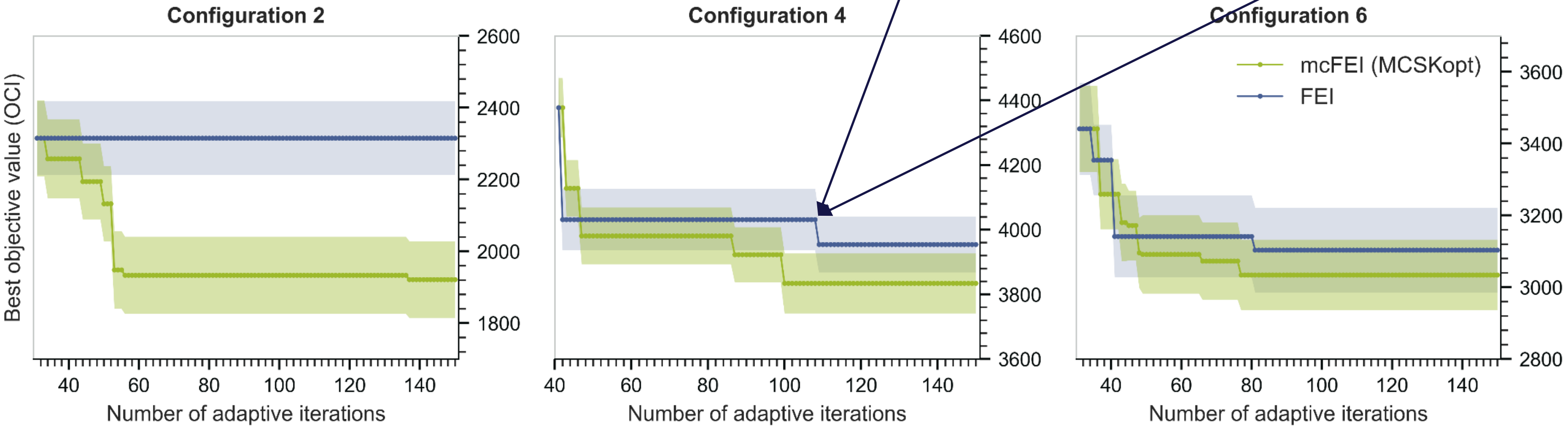
WWTP design optimization

- Continued from where Chapter 4 left off.
- 150 design samples in total (10*d* initial + adaptive).
- Parallelized MCS for uncertainty quantification.
- Hedging strategy for satisfying effluent quality constraints: MeanPlusSigma.
- Comparison of two infills: mcFEI *outperforms* FEI.

Uncertainty quantification using embedded MCS



Optimization progress: FEI (blue) vs mcFEI (green)



Summary and conclusions

- The developed workflow *enables using plant-wide WWTP models* for effectively formulating/solving rigorous design optimization problems under uncertainty.
- GSA using surrogates can help *identify decision variables* worth optimizing.
- Monte Carlo based uncertainty management can be effectively and *non-intrusively integrated* into simulation-based optimization workflows.
- Stochastic Kriging model provides *a means to model output uncertainties* in optimization objectives and constraints, hence making it suitable for simulation-based optimization under uncertainty problems.
- Maintaining feasibility while improving objective poses a significant challenge in systems subject to multiple stochastic constraints. The proposed *mcFEI infill criterion outperforms the FEI criterion* in returning near-optimal solutions for such systems.
- MCSKopt: an initial step towards making the developed workflow *applicable to design under uncertainty problems* arising in other domains.

Related publications

R. Al, C.R. Behera, K. V. Gernaey, G. Sin, **Stochastic simulation-based superstructure optimization framework for process synthesis and design under uncertainty**, Comput. Chem. Eng. (Under review).