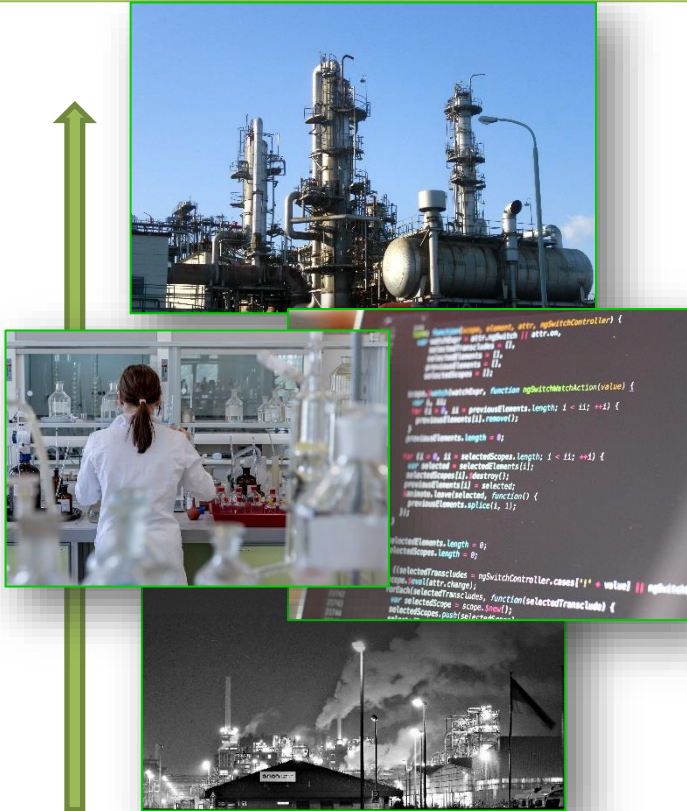# Surrogate-assisted Global Optimization of Chemical Process Flowsheets

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Motivation

- Design and rethink chemical processes
    - More cost efficient
    - More CO2 efficient
- Enhance the process design
    - Flowsheet is designed in a process simulator
    - Most commercial process simulator act as a black-box, i.e. the underlying mathematical model is not known

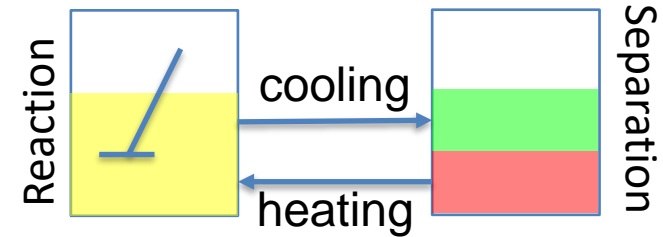# Overview: Process design

- Which process is more efficient?

- $\min f(x)$

    $$\text{s.t. } g_i(x) \leq 0$$

    $$h_j(x) = 0$$

- $DoFs \subset x$

- x in-accessible if simulation fails

- MINLP Problem with
  in-accessible derivatives
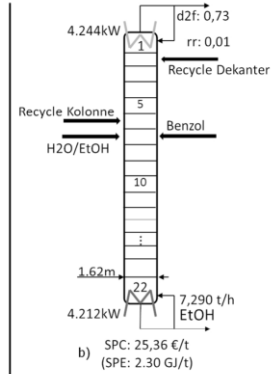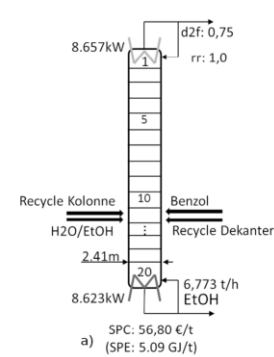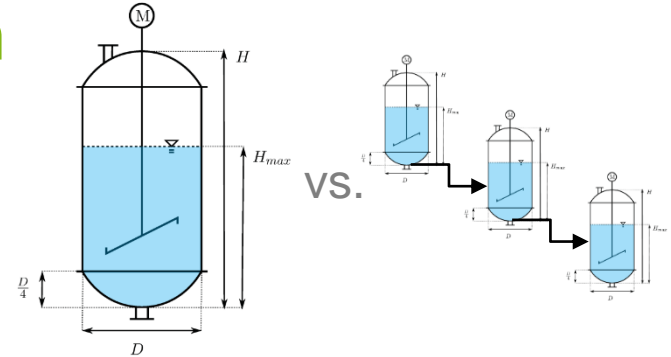
Case-Study: Hydroformylation of 1-dodecene in TMS
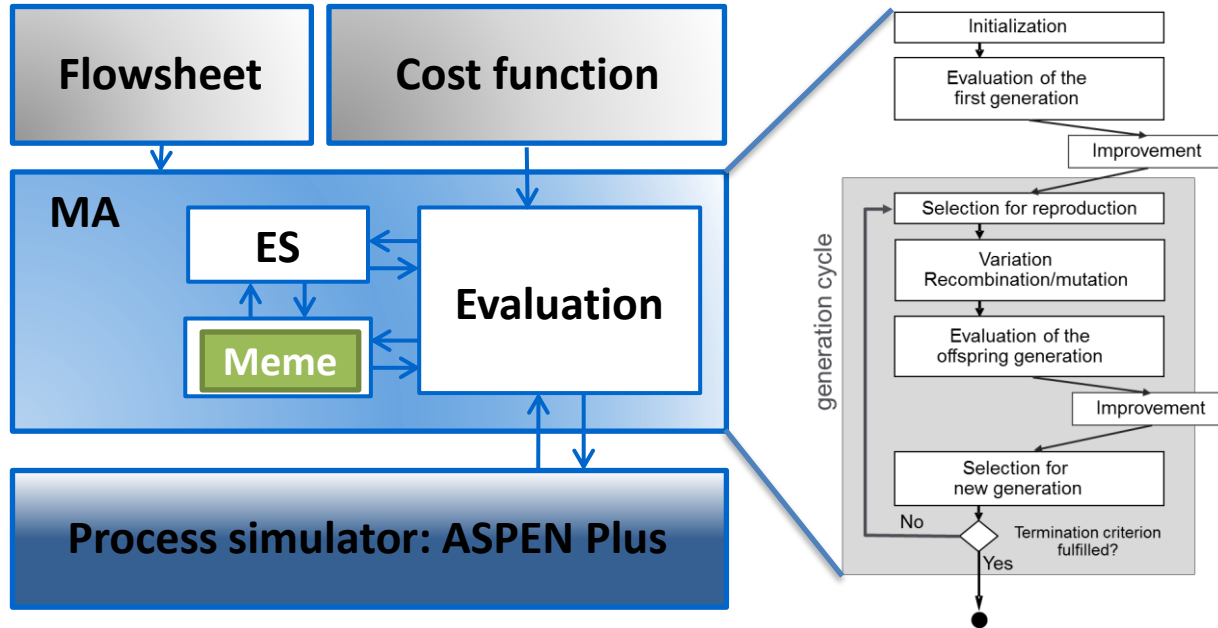
- Thermomorphic solvent system:
  - High temperature → one mixture
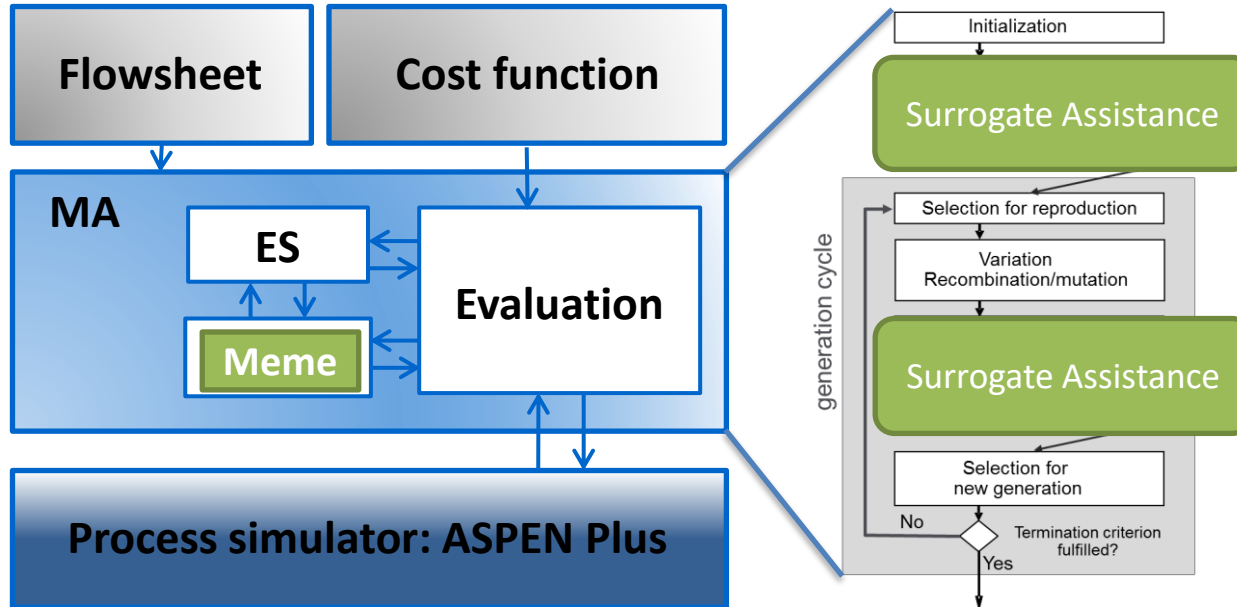 - low temperature → two liquid phases

- Flowsheet modeled in process simulator Aspen Plus
  - 10 degrees of freedom
  - 25% Non converging simulations
  - Approximately 2200 equations
  - Approx. 6 seconds per simulation
  - Purity constraint on 99% mol on product stream
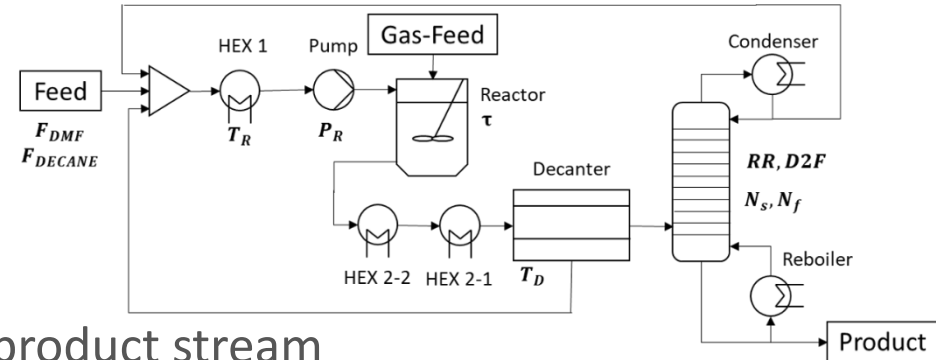
Memetic Algorithm for Flowsheet Optimization
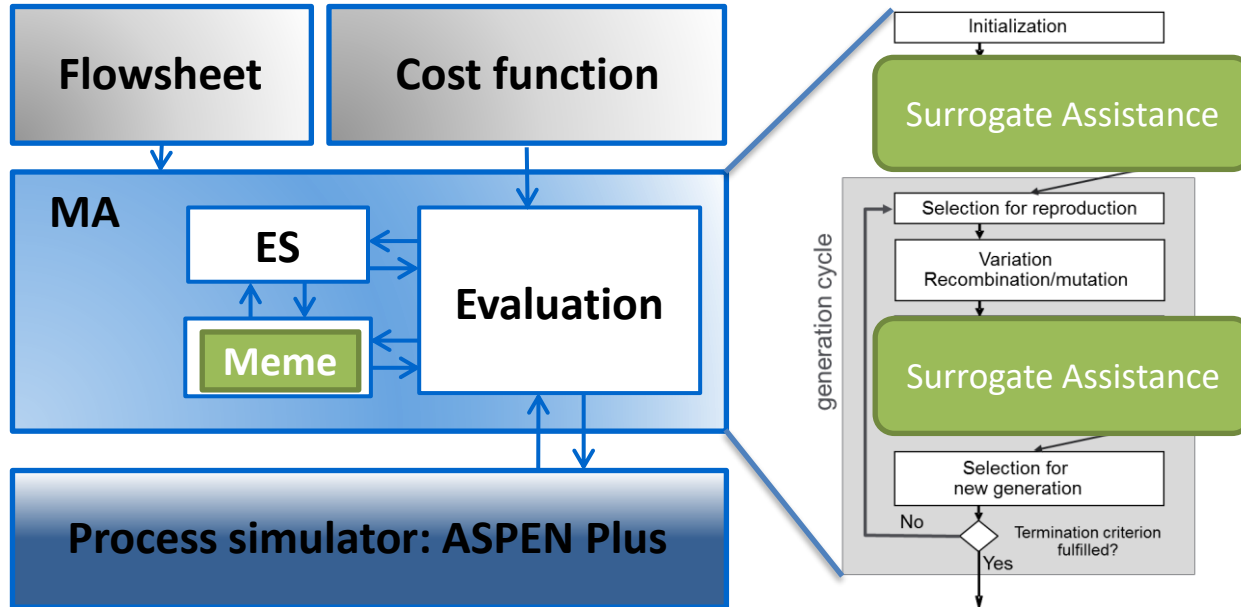
Memetic Algorithm for Flowsheet Optimization

- **Train** surrogate models (shallow neural networks) on the fly.

- **Train first** surrogate after 500 simulations

- **Retrain** every 200 simulations

[1] Janus, T., Lübbers, A., & Engell, S. (July 2020). Neural Networks for Surrogate-assisted Evolutionary Optimization of Chemical Processes. In Press: WCCI IEEE CEC 2020.

Memetic Algorithm for Flowsheet Optimization

Flowsheet

Cost function

MA

ES

Meme

Evaluation

Process simulator: ASPEN Plus

Initialization

Surrogate Assistance

generation cycle

Selection for reproduction

Variation Recombination/mutation

Surrogate Assistance

Selection for new generation

No — Termination criterion fulfilled?

Yes

- **Prescreen** simulation candidates **based on potential**

- **Classifier:** Will the simulation converge?

- **Rule on Purity:**
  $$p_e < 0.99 - p_t$$

[1] Janus, T., Lübbers, A., & Engell, S. (July 2020). Neural Networks for Surrogate-assisted Evolutionary Optimization of Chemical Processes. In Press: WCCI IEEE CEC 2020.

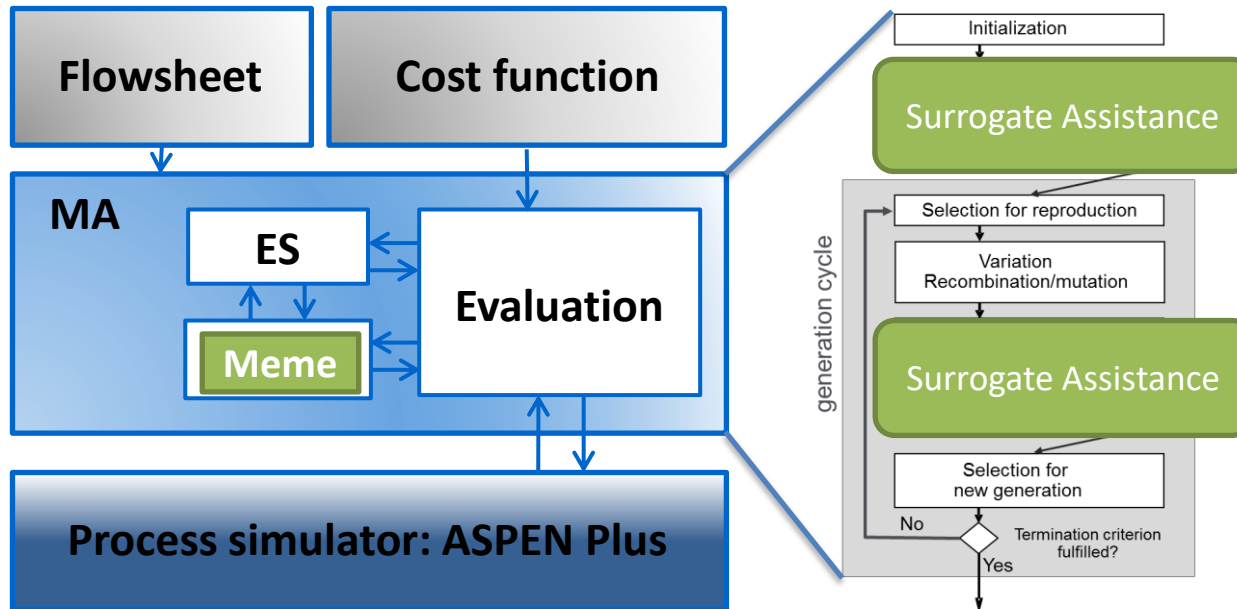# Memetic Algorithm for Flowsheet Optimization

- **Generate candidates** by optimization **on surrogate models**
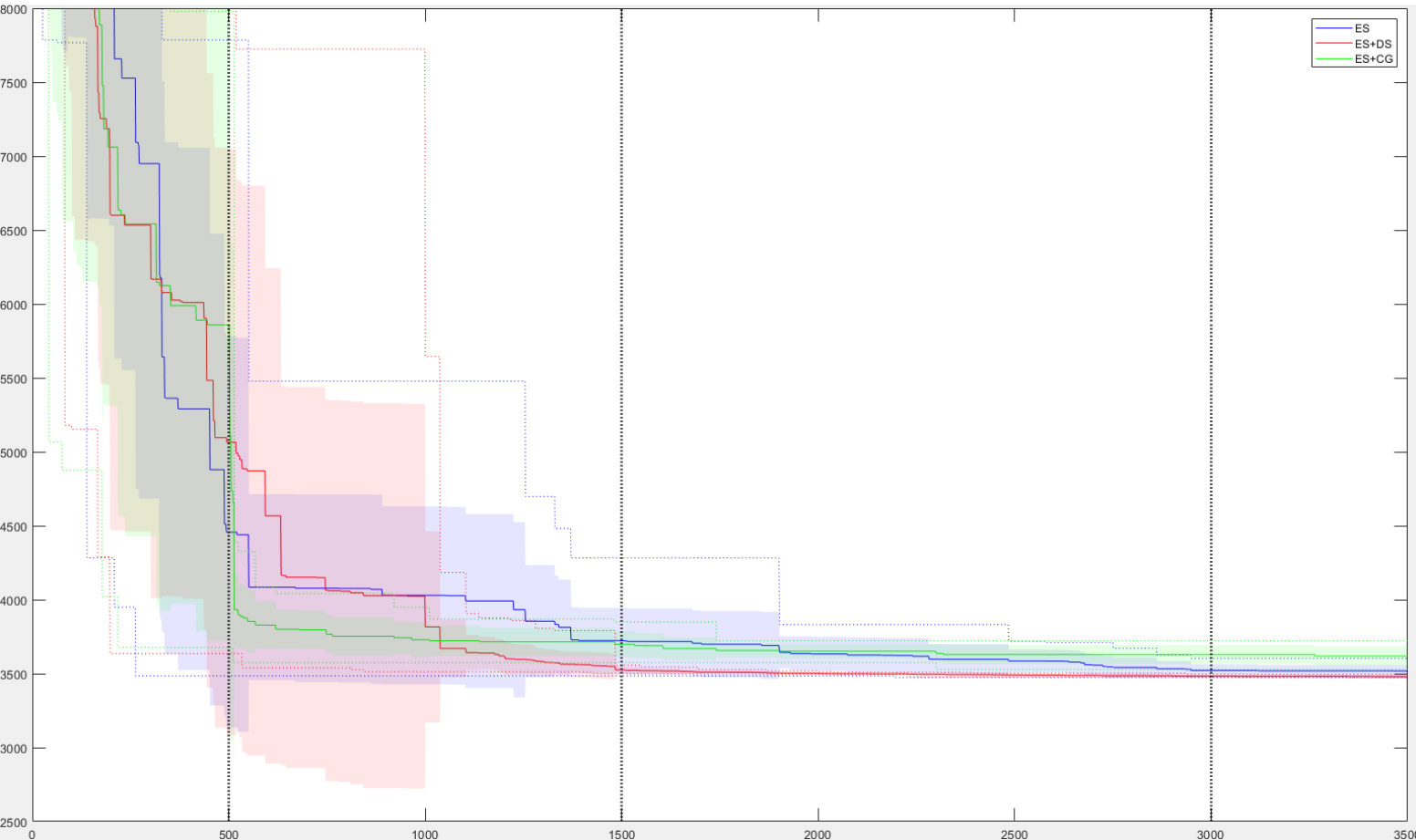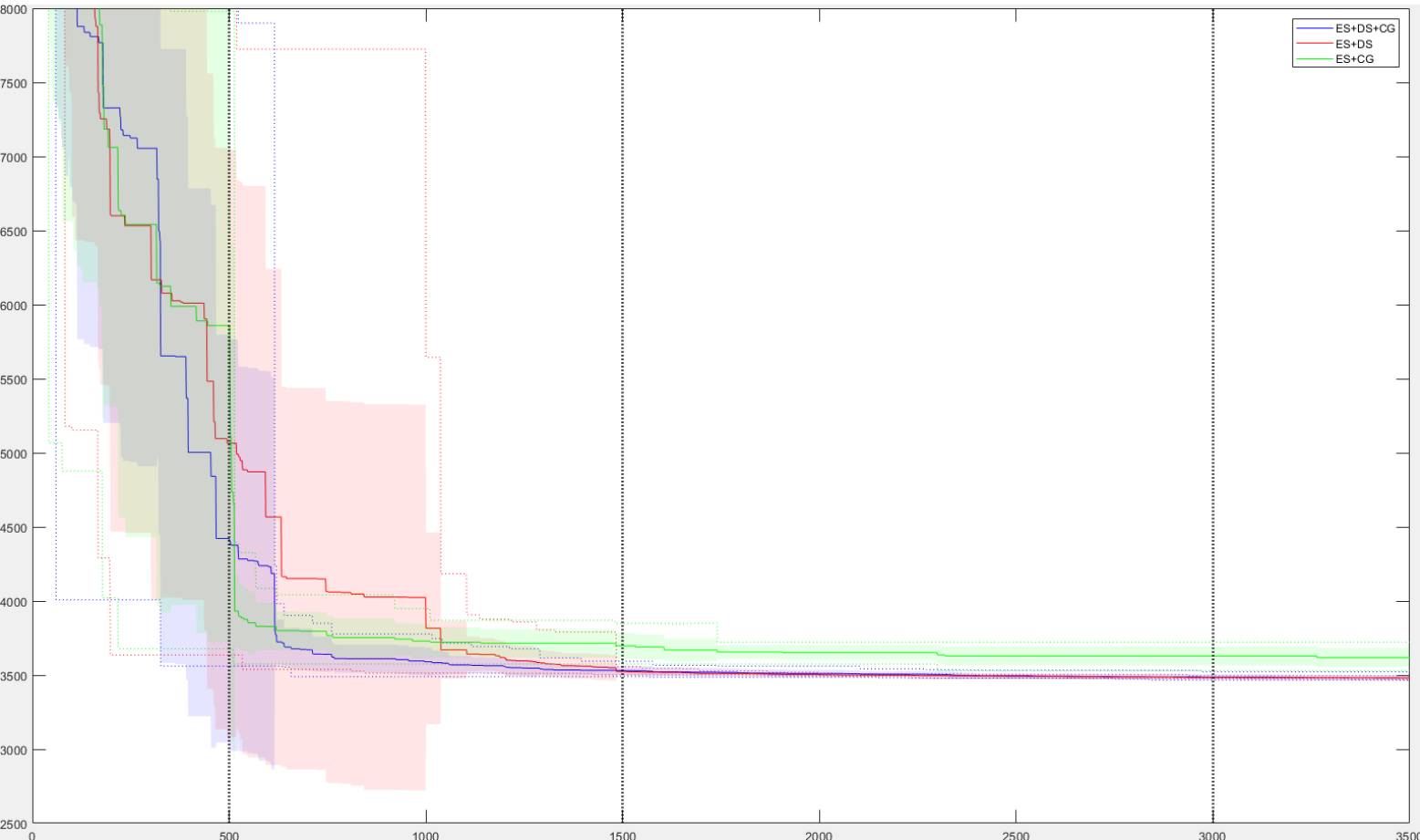 - Use **derivative-based** algorithms
  - fmincon

[1] Janus, T., Lübbers, A., & Engell, S. (July 2020). Neural Networks for Surrogate-assisted Evolutionary Optimization of Chemical Processes. In Press: WCCI IEEE CEC 2020.

Blue: Reference Algorithm (ES)
Red: ES and prescreening
Green: ES and candidate-generation

- #Sim over costs

- Ten repeats

- Solid mean value

- Area is variance

- Dotted is min/max

9

Blue: ES and both
Red: ES and prescreening
Green: ES and candidate-generation

- #Sim over costs

- Ten repeats

- Solid mean value

- Area is variance

- Dotted is min/max

~~Problems~~ Challenges

- Industrial-size case-study:
  - 30 or more DoFs
  - Simulation times in order of minutes
  - High number of simulations due to derivative-free optimization
  - Results for an European Congress of Chemical Engineering (ECCE) contribution was based on 100.000 simulations
  - Computational time in magnitude of weeks
- Divide and conquer

Thank you! To get in touch scan the QR Code!