

# Explainable optimization by explainable AI

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Air Liquide

Fraunhofer ITWM

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KE-EN

# Air Liquide

## Leveraging the power of digital & data

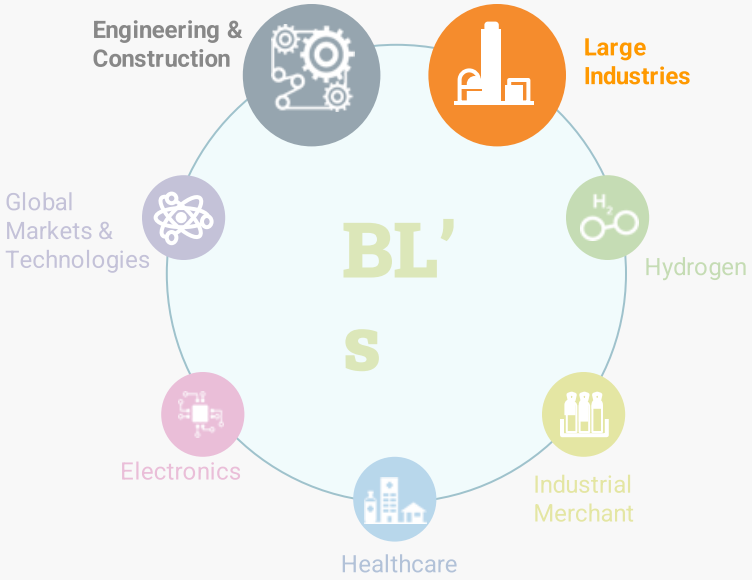
Air Liquide, we **leverage the power of digital …**

It involves harnessing data and **developing digital solutions** to

- better manage our **Assets**,
- interact with our **Customers** and patients,
- and leverage our **Ecosystems**
  -> **the ACE strategy**

### Key Assets

- People: Enabling talents to thrive
- Data: 1 B data points/day




https://www.airliquide.com/group/digital-transformation-strategy

# KEEN @ Air Liquide

*"AI-based Process Digital Twin"*

## Our approach:

### Focus to our main R&D strength

- Test advanced concepts
- Demonstrate - Generate experience
- Deliver new tools

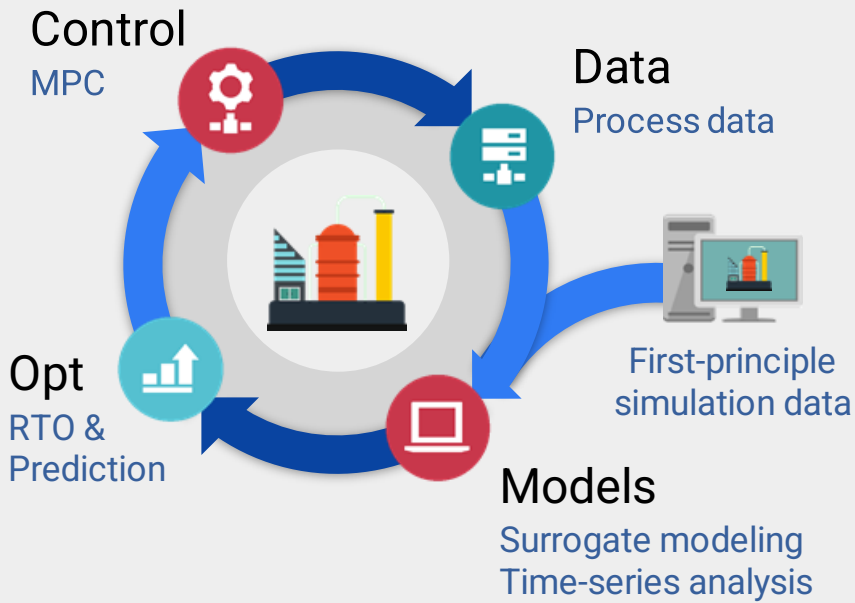
**Key for success: our partner**

### Covering the whole cycle

### Three main topics:

- Optimisation
- Performance prediction
- MPC & ML

**Paves the way for applications in our SIO centers**



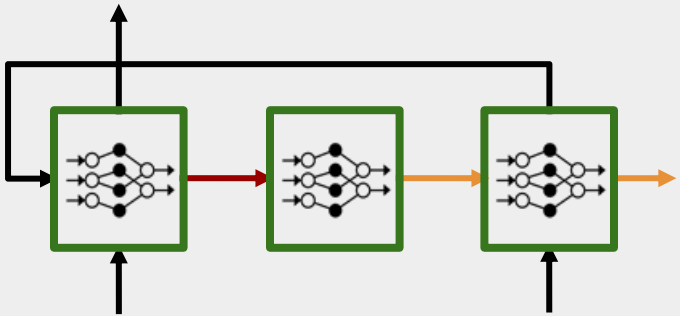
# Joint activities of Air Liquide and ITWM in KEEN

## Data generation:

- Interface Python ↔ Aspen
- Test of sampling strategies on Air Liquide Pre-Reformer model

## Surrogate model generation

- Training of surrogates for flowsheet models and combining them to a surrogate of the complete process



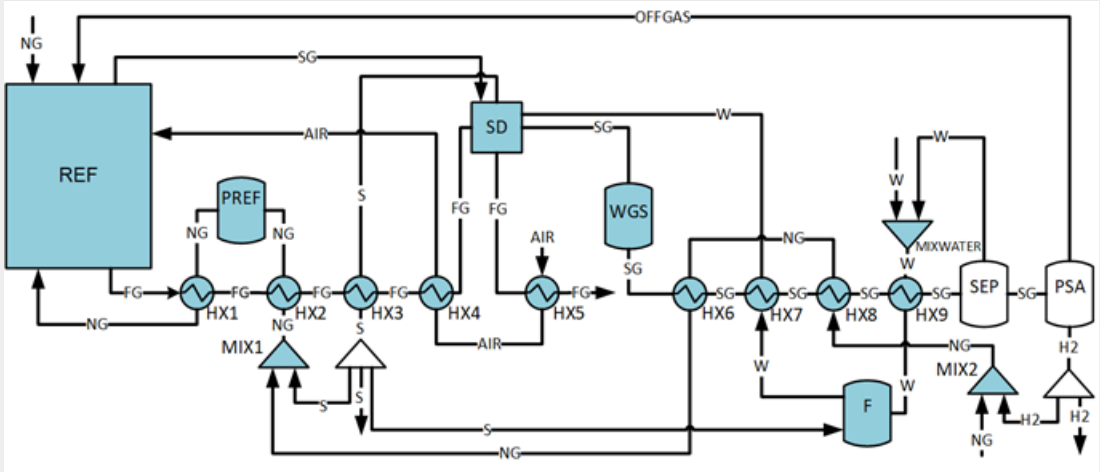
# Surrogate Based Flowsheet Simulation

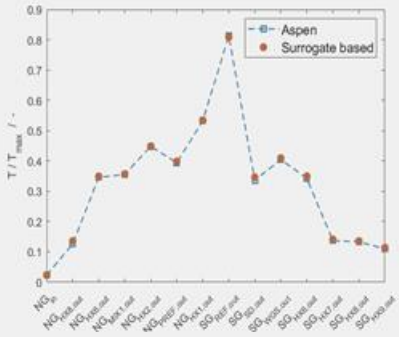
## Flowsheet Simulation Based on Single Surrogates

Fraunhofer ITWM

Fraunhofer Institute for Industrial Mathematics ITWM

- Use Case: Steam Methane Reforming (**SMR**)
- **Surrogate unit models** for key units
- Connection of single unit models by ***Pyomo***




**AI model** builder and usage of **surrogates** in recent versions of commercial flowsheet simulators, e.g. **Chemcad**, **Aspen Plus**

**+ high accuracy and flexibility achievable**

**- high manual effort required**

# Surrogate Based Flowsheet Simulation

## Overall Process Surrogate

Fraunhofer ITWM

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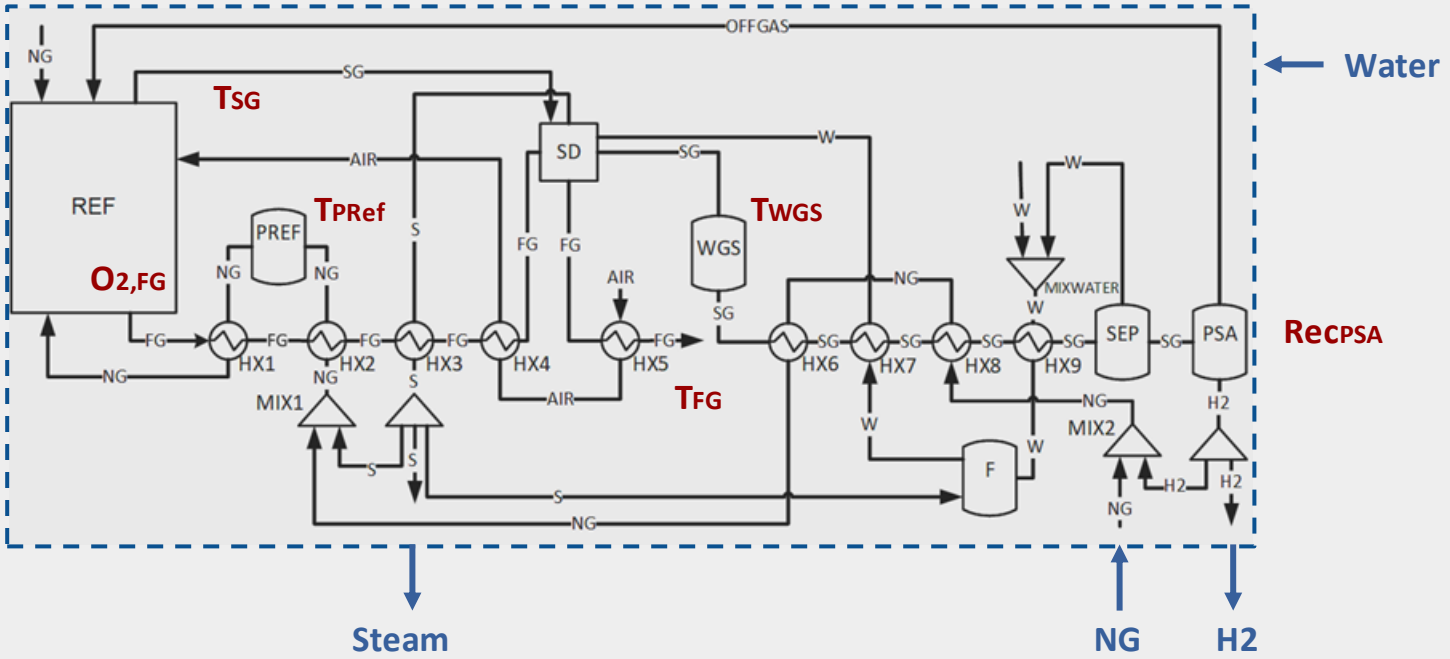


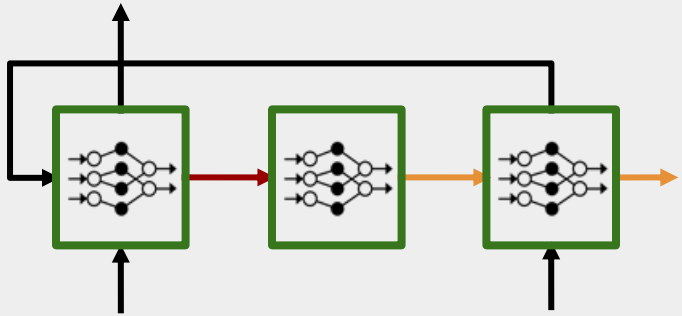
# Use of surrogates

## “What-if“ scenarios:

- If inputs changed → How do the outputs change?
- If the outputs should meet a target → How to change the inputs to achieve this?

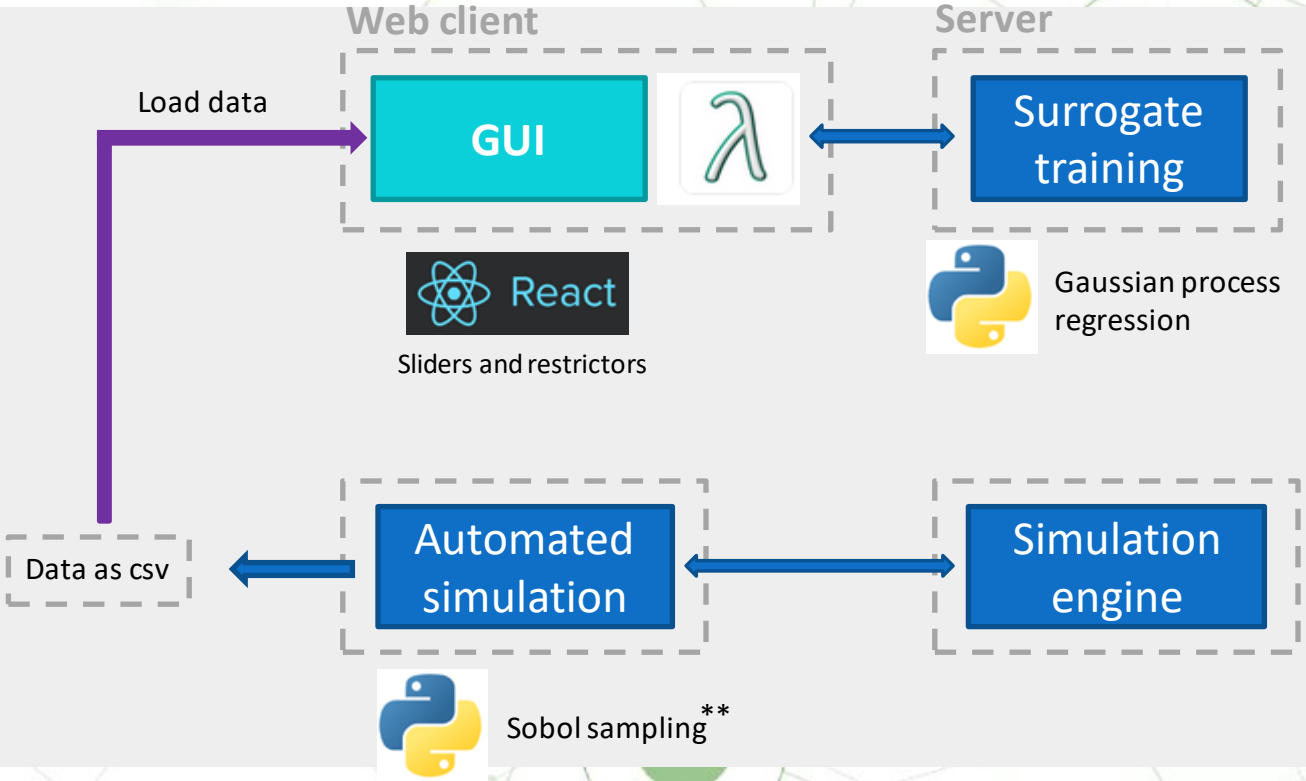
**User interaction with the surrogate model is important!**

**→ Graphical user interface to the surrogate**



# Architecture to surrogate models: Interactive what-ifs

Lovely analyser for models and data






** Laurens Lueg, Dominik Schack, Evrim Ös, Robin Schmidt, Patricia Bickert, Martin von Kumatowski, Patrick Otto Ludl, Michael Bortz, „Data-driven Process Design exemplified on the Steam Methane Reforming Process", Proceedings of the 31st European Symposium on Computer Aided Process Engineering June 6th to 9th, 2021, Istanbul, Turkey.

# Interactive what-if exploration with λ

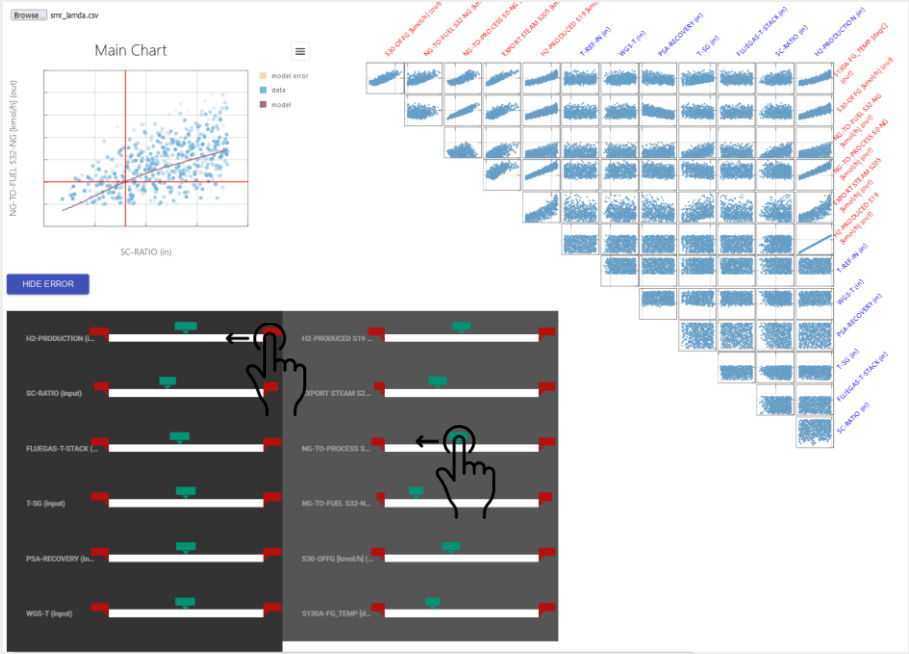
**Interactive (real-time) exploration**

**Direct/inverse navigation** + **Restriction**

More than a model evaluation

↓

**(NLP) Optimization**: find closest feasible solution in input space



# Navigation with λ

## Direct navigation

$$\min_{x} \|x - x^0\|_2 \quad \text{s.t.}$$

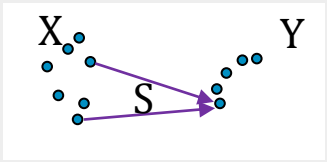
$$\begin{cases} x_k(x) = x_k^* \\ lbx \le x \le ubx \\ lby \le S(x) \le uby \\ Ax \le b \end{cases}$$

## Inverse navigation

$$\min_{x} \|x - x^0\|_2 + M\left\|S_{h\neq k}(x) - y^0_{h\neq k}\right\|_2 \quad \text{s.t.}$$

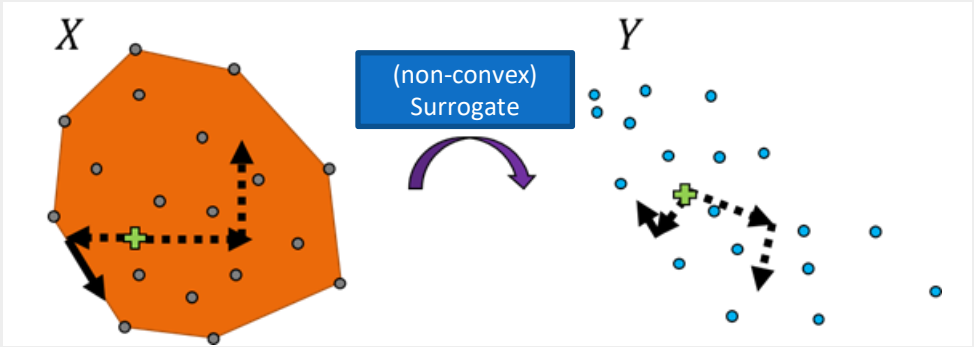
$$\begin{cases} S_k(x) = y_k^* \\ lbx \le x \le ubx \\ lby \le S(x) \le uby \\ Ax \le b \end{cases}$$


**No inverse surrogate**




M. Baldan et al., Chem. Ing. Tech. 2023, 95(7), 1–14

# Supporting a reliable surrogate




How to improve the **reliability** of the **surrogate**?

By **constraining** input sliders inside the **convex hull** spanned by the input data

Why a **convex hull**?

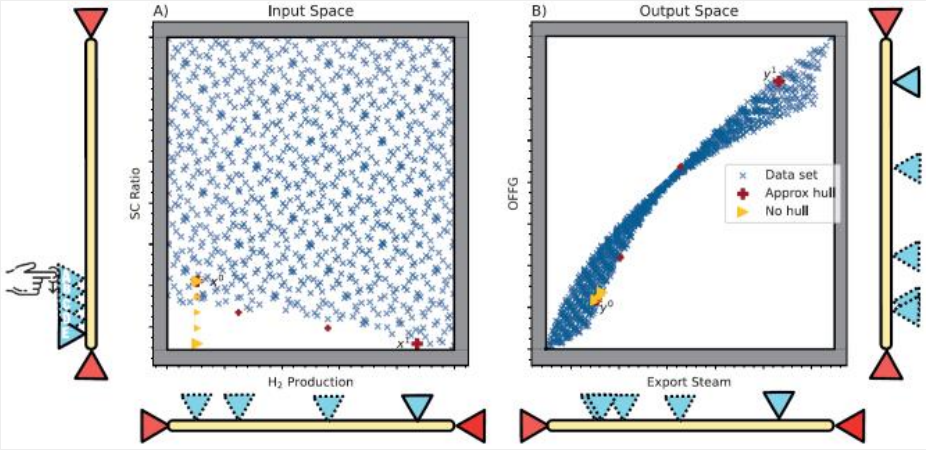
✓ Linear constraints
✓ Cheap to compute
✓ /✗ Convex space

✗ ~~Many~~ constraints (reduced hull)

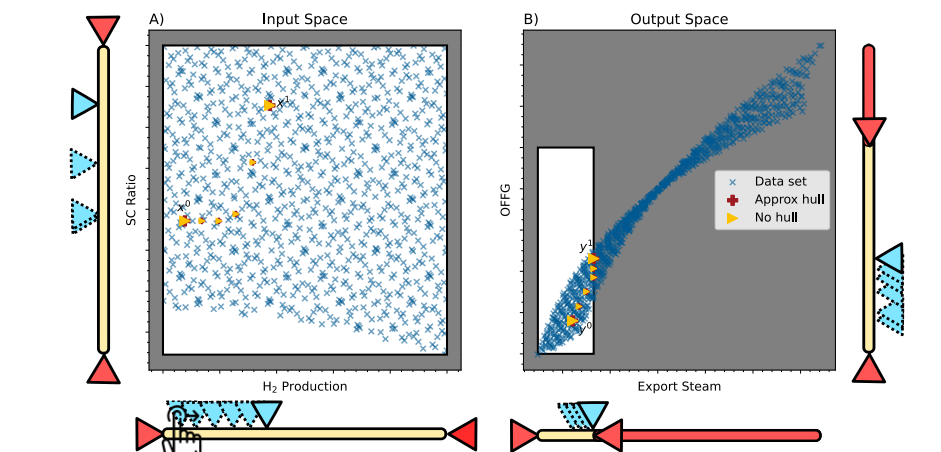
M. Baldan et al., Chem. Ing. Tech. 2023, 95(7), 1–14

# Navigation with λ

## Use Case: Steam Methane Reforming (SMR)




Effect of **convex hull**



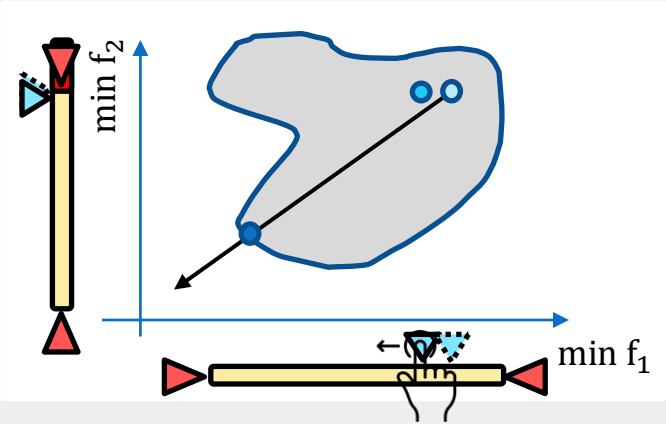

Effect of **restriction**

M. Baldan et al., Chem. Ing. Tech. 2023, 95(7), 1–14

# Multi-criteria optimization with λ navigation

$$\min_{x} S_1(x), \ldots, S_M(x)$$
$$\text{s.t.}$$
$$Ax \leq b$$
$$\ldots$$

**Inverse navigation**

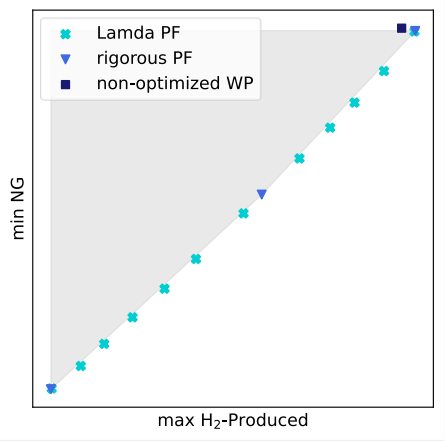



λ

Selection
Restriction

Pascoletti
Serafini
scalarization

SMR




✓ User friendly
✓ No (additional) optimizer
✓ Non-convex fronts

# Summary

- Software architecture to surrogates
- Real-time interactive exploraton supporting reliable surrogates
- Multi-criteria optimization via navigation
- Application to an industrial process

# Air Liquide, ITWM

- Contact:
  - Air Liquide: Robin Schmidt, Dominik Schack, Vanessa Gepert
  - ITWM: Patrick Ludl, Marco Baldan, Michael Bortz

**Thank you for your attention!**