EPFL

Generating configurations

Prof. François Marechal

IPESE
Industrial Process
and Energy Systems
Engineering

Generating ordered list of system configurations

- Integer cut constraint on the equipment set $\{y_u\}$
  - assuming that we know already the solution k
  - The problem k + 1 is defined by adding to the previous MILP problem the integer cut constraint

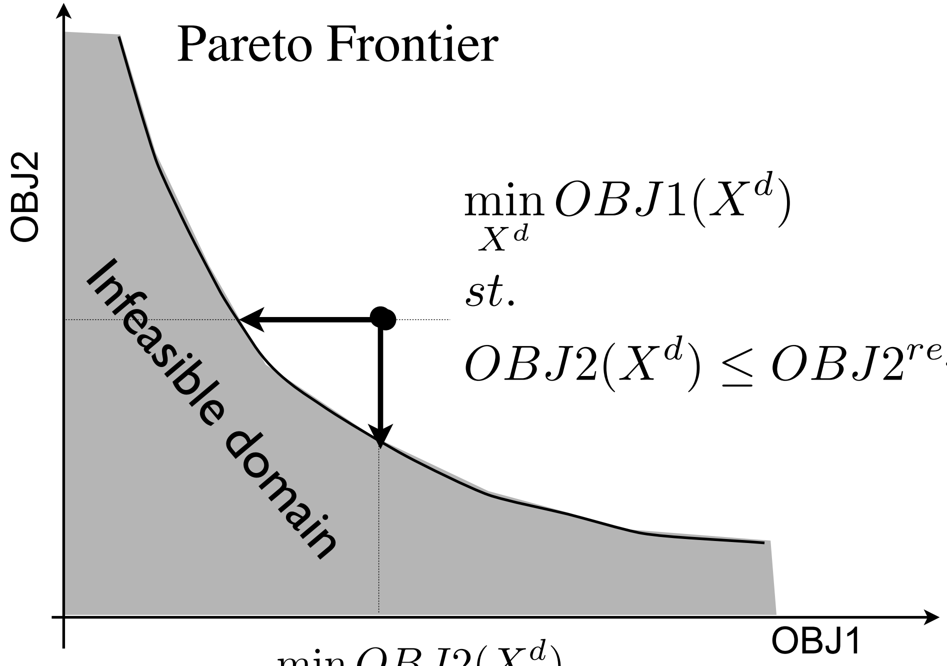
$$Problem^{k+1}:$$

$$Problem^{k}$$

$$\sum_{i=1}^{n_y}(2y_i^k - 1) * y_i \leq \sum_{i=1}^{n_y} y_i^k$$

where y_i^k value of y_i in solution of problem k

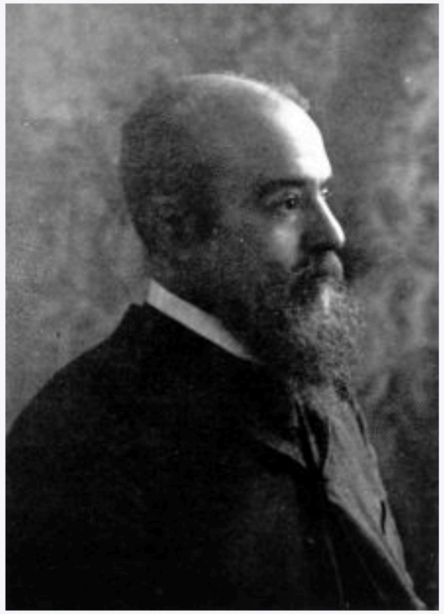
Multi objective optimization



$$\min_{X^d} OBJ1(X^d)$$
$$st.$$
$$OBJ2(X^d) \leq OBJ2^{ref}$$

$$\min_{X^d} OBJ2(X^d)$$
$$st.$$
$$OBJ1(X^d) \leq OBJ1^{ref}$$

Vilfredo Pareto



Born	15 July 1848 Paris, France
Died	19 August 1923 (aged 75) Céligny, Switzerland
Nationality	Italian
Institutions	University of Lausanne
Field	Microeconomics Socioeconomics

source : wikipedia

Muti-objective optimisation

- Single objective parametric
  - Weighting

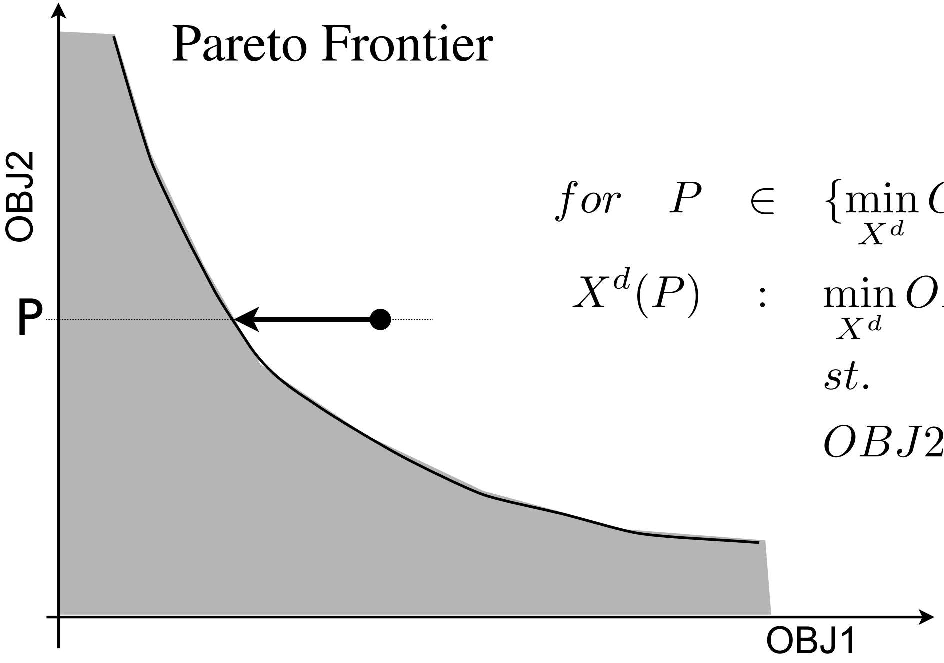
$$X_d(w) : min_{X_d}(1-w) \cdot OBJ_1(X_d) + w \cdot OBJ_2(X_d)$$

$$\forall w \in [0,1]$$

  - Note : if OBJ1 is a cost function

$$\frac{w}{1-w} \text{ is a tax on } OBJ_2(X_d)$$

Parametric programming



$$for \quad P \in \{\min_{X^d} OBJ1(X^d)..\min_{X^d} OBJ2(X^d)\}$$

$$X^d(P) : \min_{X^d} OBJ1(X^d)$$

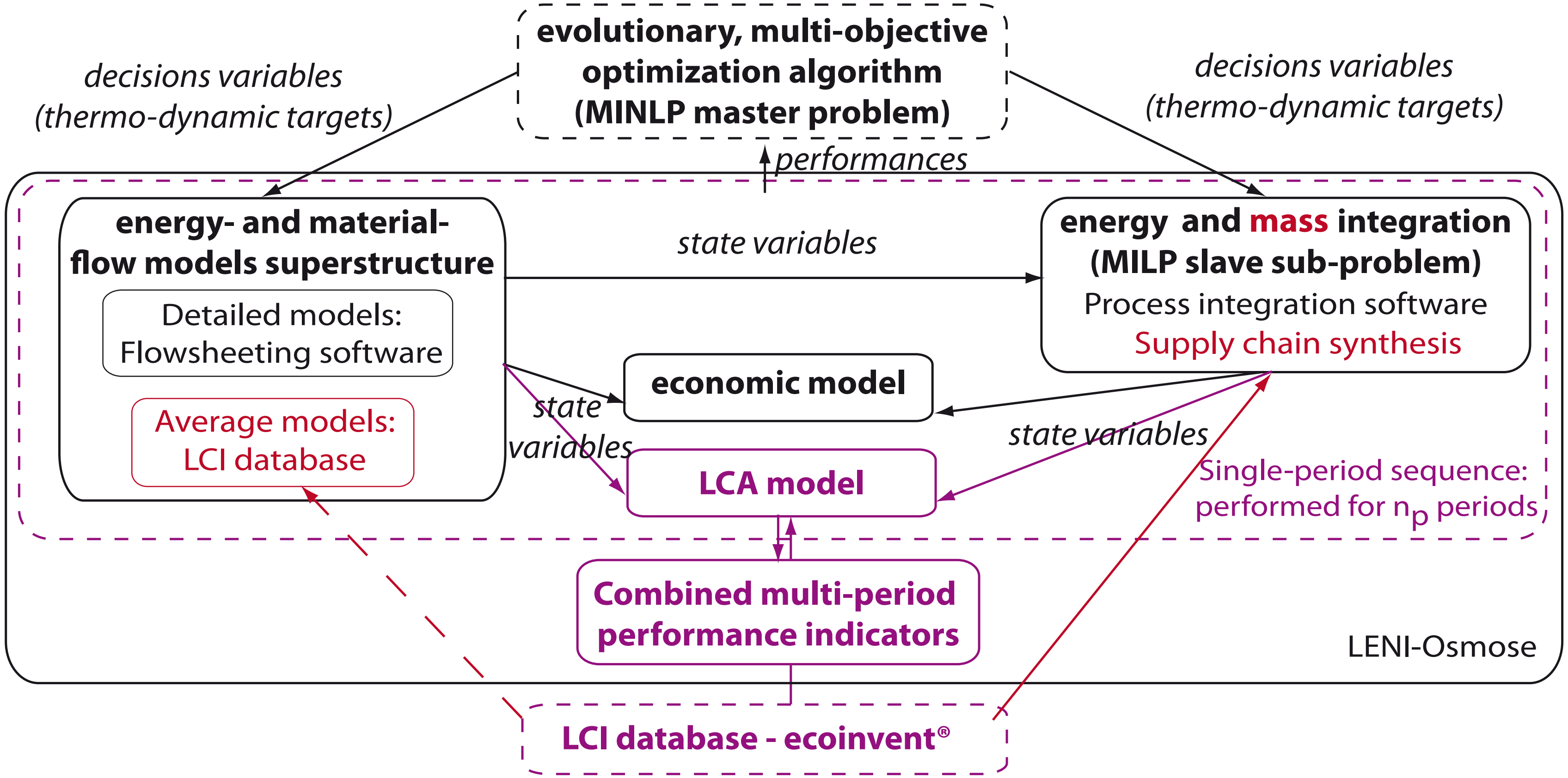
$$st.$$

$$OBJ2(X^d) \leq P$$

Note : the Lagrange multiplier of inequality gives the slope of the Pareto curve

Non linear optimisation

- Extension to supply chain synthesis and identification of recyclings



MINLP : decomposition problem

- Master (M) -Slave (S) decomposition

$$\min_{X_M} \quad Obj(X_M, X_S(X_M), \pi)$$ => partition variable

$$s.t. X_S(X_M) \quad \min_{X_S} Obj_S(X_S, X_M, \pi)$$ => Simple to solve

$$s.t. \quad H(X_S, X_M, \pi) = 0$$

$$H(X_S, X_M, \pi) \geq 0$$

X_M Master Variables

X_S Slave Variables

π Parameters

Master Level : Black Box strategy

$$\min_{X^*_{decision}} \quad TotalCost(X^*_{decision}, X(X^*_{decision}))$$

$$s.t. \quad G(X^*_{decision}, X(X^*_{decision})) \leq 0 \quad \text{inequality constraints}$$

$$where$$

$$X^*_{decision} = \{x_{decision}, y_{decision} \epsilon \{0,1\}\}$$

$X(X^*_{decision})$ Calculated by solving:

$$F(X_{state}) = 0 \Rightarrow \text{equipment model}$$

$$L(X_{state}) = 0 \Rightarrow \text{linking equations}$$

$$T(X_{state}) = 0 \Rightarrow \text{constitutive equations}$$

$$S(X_{state}) = 0 \Rightarrow \text{Specification equations}$$

$$X_{decision} - X^*_{decision} = 0 \Rightarrow \text{Specification of the value of decision variables}$$

$$where$$

$$X_{state} = \{x_{StateVariables}, x_{UnitParameters}, y_{decision} \epsilon \{0,1\}\}$$

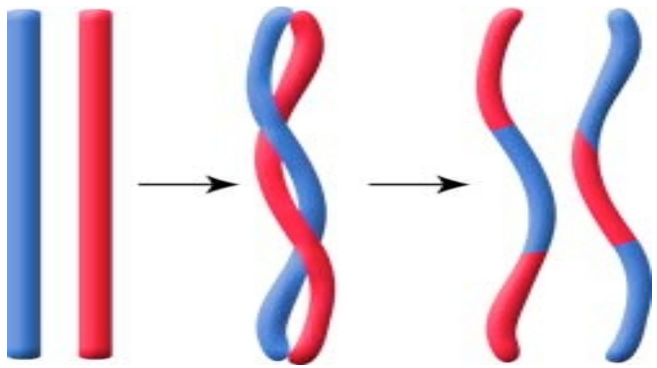
Heuristic methods to systematically generate optimal configurations

- Applies only on black box strategy
- Exploring the search domain
  - systematically
  - based on some analogy
- Simulated annealing
  - based on the analogy with metallurgy
    - heating/cooling of metal to minimize the energy content
- Evolutionary algorithm
  - genetic algorithms
    - based on the analogy of the evolution
      - Best fitted individuals have a higher probability to survive and reproduce
      - Reproduction based on sharing gene info
- Particle swarm
  - initial speed + communication between agents
- Ants colony

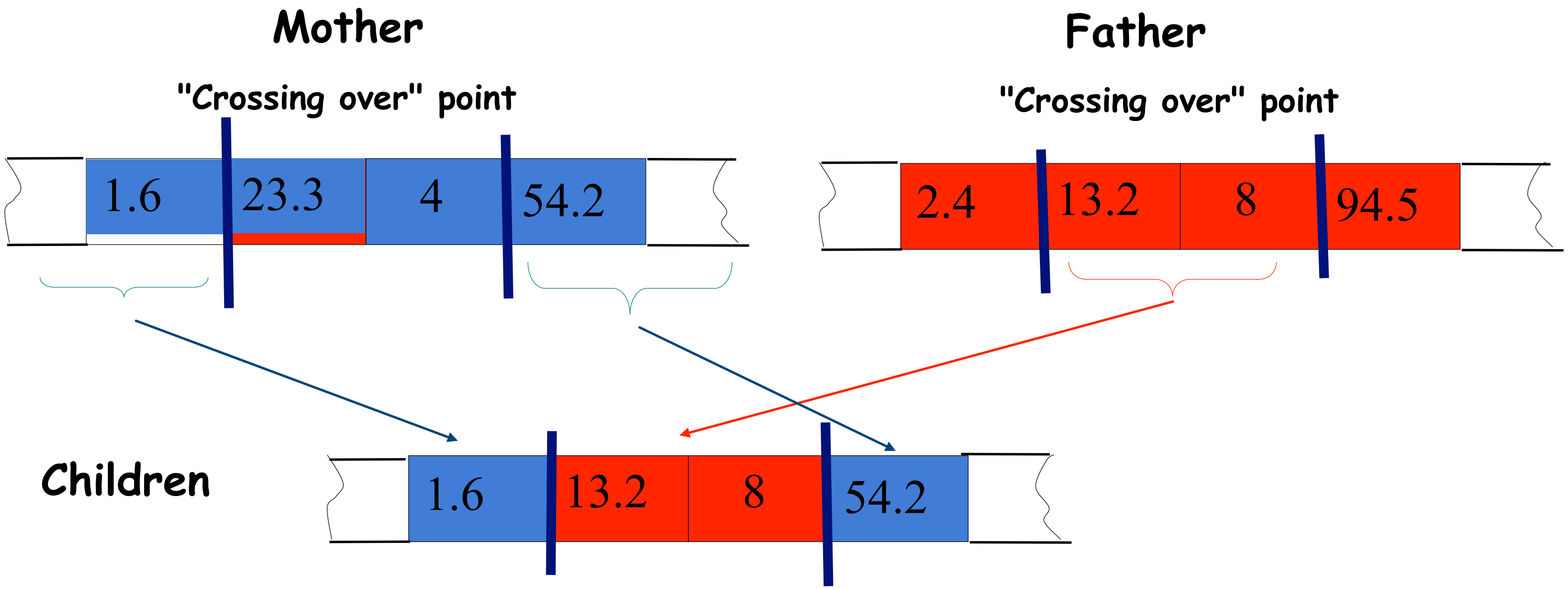
Evolutionary algorithms

- Characteristics
  – Population (X)
  – Objective Function(s) : Performances Y=F(X)
  – No direction (No derivatives - No “iteration”)
  – Heavy duty : Computing time !
  – Problem definition is free
  – Random nature : explore the search space
  – Inequality constraints ?
- Principle
  – Initialization (random population generation (e.g. 100 sets))
  – Reproduction => select parents & reproduce
  – New individual
    - Cross-over (random)
    - Mutation
  – Update population (maintain population)
    – eliminate the worst individuals
    – re-group by types to preserve diversity

reproduction by "Crossing over"



Random selection of parents in the population
Random selection of the genes to share

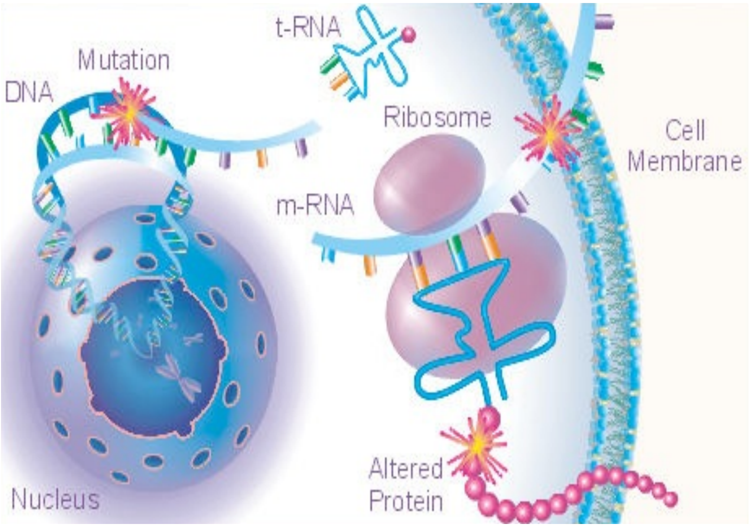


Cross over

- Cross-over can use interpolation techniques
  - e.g. quadratic approximation based on a subset of the population
  - select randomly and/or take the bests
- Preserve the random nature !
  - e.g. random relaxation

Mutation

Mutation allows to ensure that the system will not be trapped in a local optimum and that the whole space will be observed



Random Mutation

5

before mutation

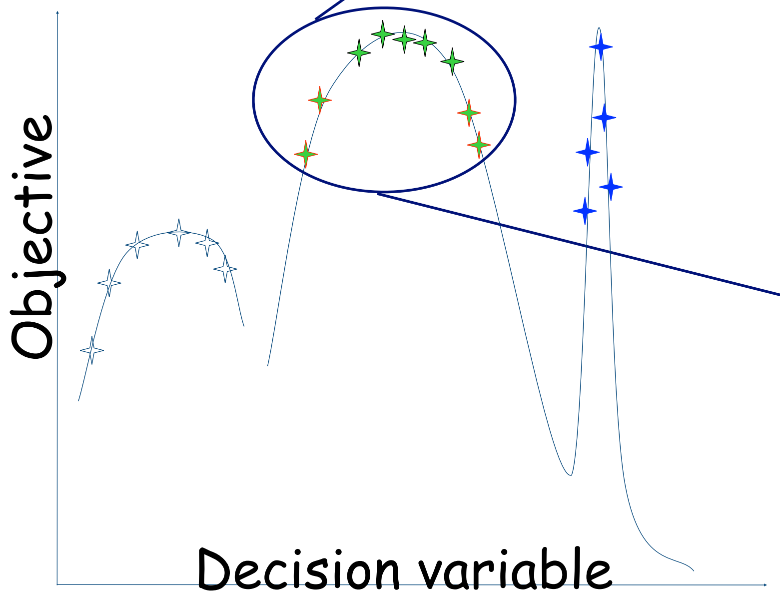
1.6	23.3	~~8~~	94.5

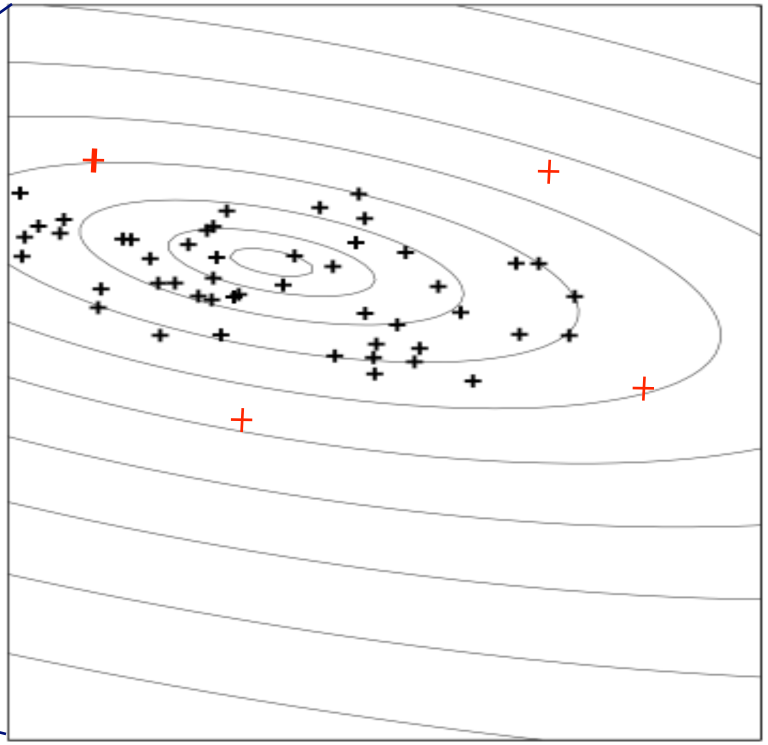
after mutation

1.6	23.3	5	94.5

Elimination

Elitism : preserve the best candidates





Elitism is defining the population in which the good candidates are selected : this allows multi-objective optimisation and the search for local and global optimum.

Evolutionary algorithms : conditions

- Black box approach
  - Equality constraints are solved explicitly
  - Inequality constraints transformed into decision variables bounds
- Fast F(X) calculation
  - Search space exploration => huge number of evaluation
- Robust F(X) calculation
  - search space response
- No efficient mathematical programming methods
  - Non differentiable problems
  - MINLP
- Limited number of degrees of freedom

Evolutionary algorithm : advantages

- Global optimisation
  - Exploration of the search space
- Black Box
  - Accepts different type of objective function
    - incl. observations
- Non differentiable problems
  - The objective function can have jumps or steps
- Easy to parallelise
- Freedom in the choice of decision variables
  - x1*x2*x3 is not a problem
- Multi-objective problem
  - Efficient use of the computing time
  - Dominancy criteria

Evolutionary algorithm : drawbacks

- Speed of resolution of F(X)
  - Requires a large number of F(X) evaluation
  - Use of surrogate models
- Number of decision variables
  - Convergence properties is a combinatorial function of the number of variables
- Limited Feasible domain
  - Probability of finding feasible F(X) is low
  - Choice of the decision variables
- Constraints handling
  - Equality or inequality

Evolutionary algorithm

- Handling inequality constraints

$$\min_{X} OBJ(X)$$
$$st.$$
$$F(X) = 0$$
$$G(X) \leq 0$$

$$\min_{X^d} OBJ(X^d, Y(X^d)) + P(X^d)$$
$$st.$$
$$Y(X^d) = F(X^d)$$
$$P(X^d) = \sum (max(G(X^d, Y(X^d)), 0))^2$$
$$X^d_{max} \leq X^d \leq X^d_{max}$$

- Choosing the appropriate decision variables

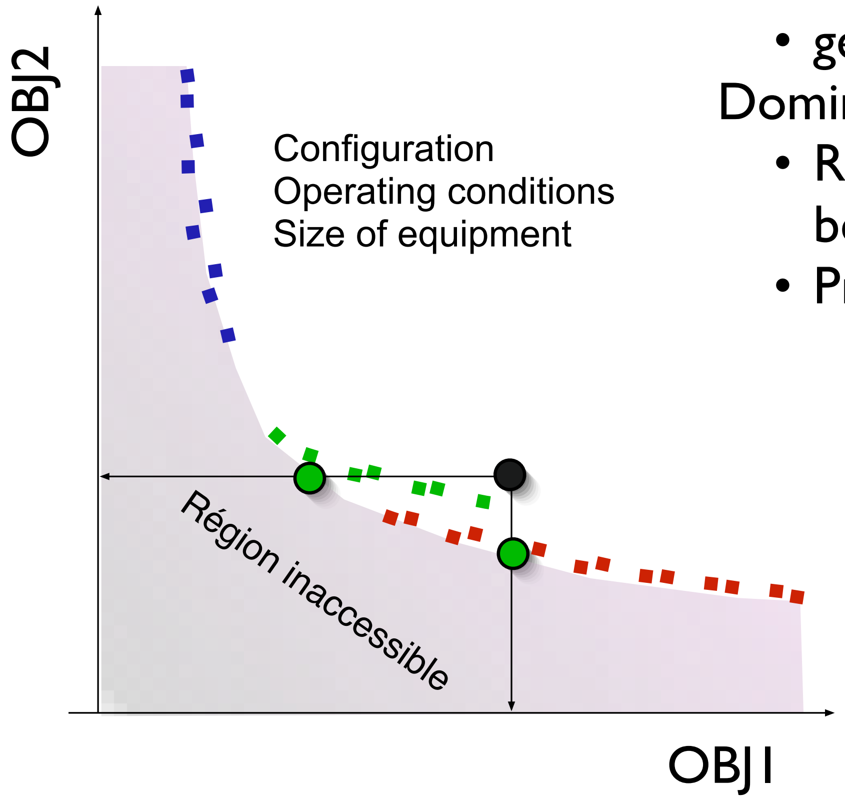
$$\min_{x_1,x_2} f(x_1,x_2)$$
$$st.$$
$$x_1 \leq x_2$$
$$x_1^{min} \leq x_1 \leq x_1^{max}$$
$$x_2^{min} \leq x_2 \leq x_2^{max}$$

Becomes

$$\min_{x_1^*,x_2} f(x_1 = x_1^{min} + (min(x_2, x_1^{max}) - (min(x_2, x_1^{max}) - x_1^{min})) \cdot x_1^*, x_2)$$
$$st.$$
$$0 \leq x_1^* \leq 1$$
$$x_2^{min} \leq x_2 \leq x_2^{max}$$

Works well for Evolutionary algorithm
do not use for mathematical programming

Multi-objective optimisation



Clustering techniques (big data)

- identify decision variable sub-spaces
- generate multiple Pareto curves

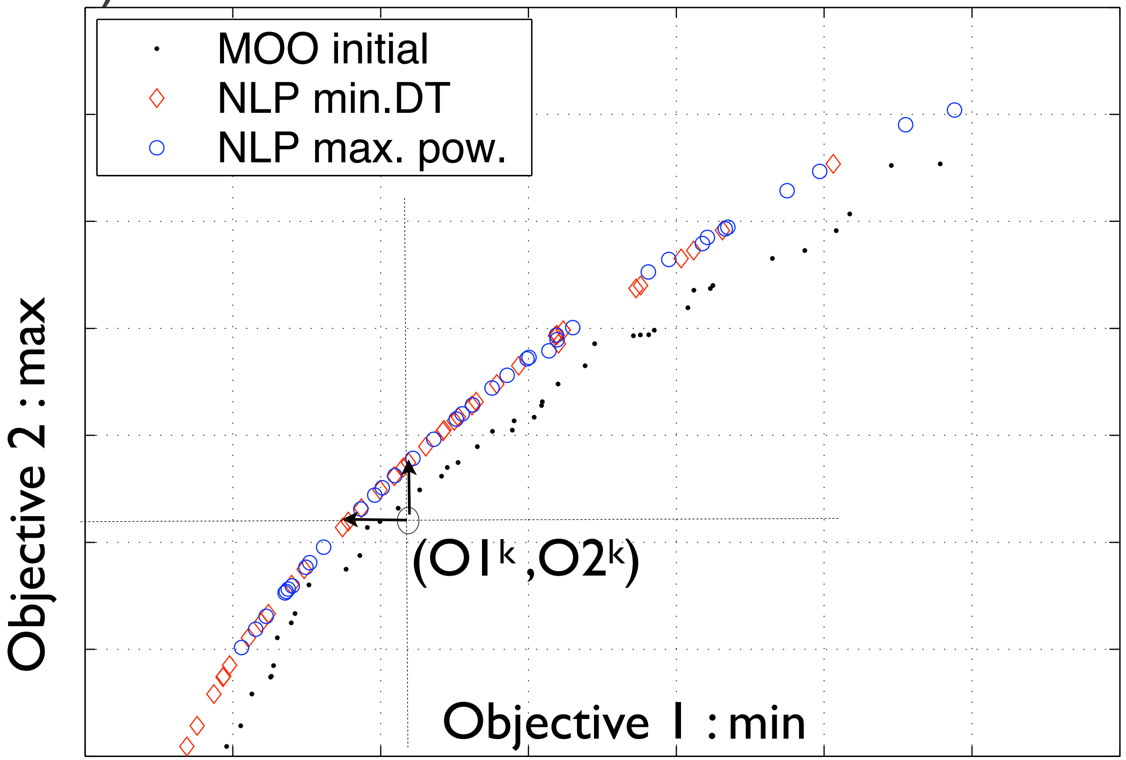
Dominancy

- Remains in the population if at least better than others for 1 objective
- Preserve sub-optimal population

The goal is indeed to take decisions : being informed about the collection of good solutions allows to have a better knowledge of what is building a solution and for which reason the filan solution will be selected

Evolutionary solving strategies

- Hybrid methods
  - Use Evolutionary algorithm to find initial point for mathematical programming
  - Global optimization (find min of min)
  - Limited number of NLP
  - Do it in 2 directions
    - min obj1
    - min obj2



Multi-objective optimisation : Evolutionary algorithm

Clustering techniques
- identify decision variable sub-spaces

Dominancy
- in the population if at least better for 1 objective
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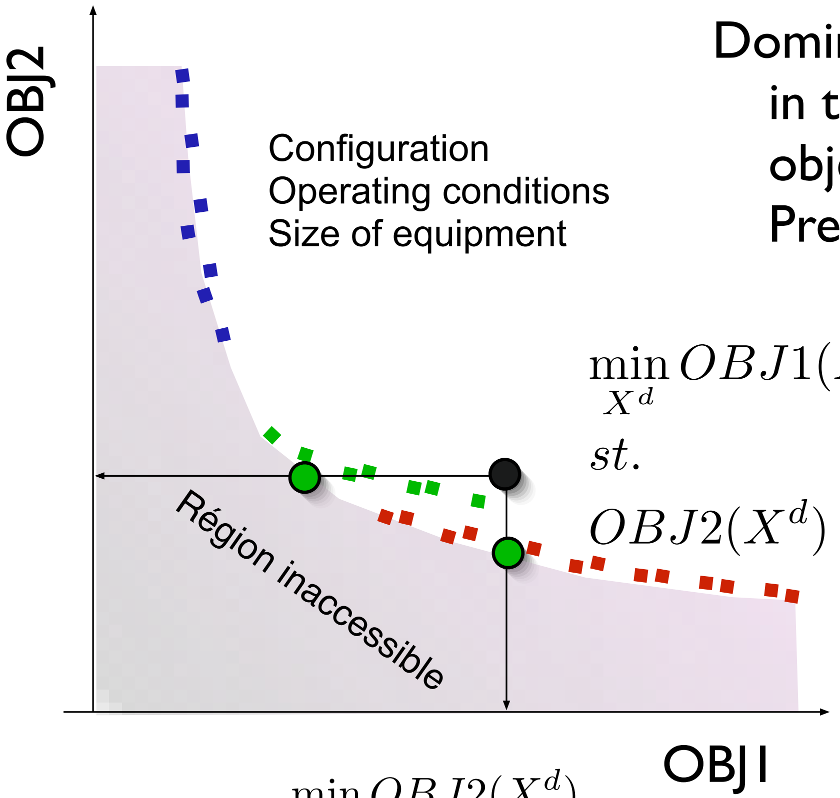

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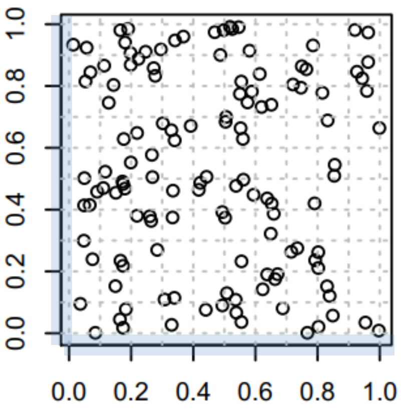
Interactive optimisation

Multi-parametric optimisation

$$
\begin{aligned}
\min_{x} \quad & f_{TC}(x,\theta) & & \text{Objective}\\
\text{subject to} \quad & f_{FAR}(x,\theta) \le \varepsilon_{n,FAR}, \qquad & \varepsilon_{FAR}^{min} \le \varepsilon_{n,FAR} \le \varepsilon_{FAR}^{max}, & \quad \text{KPI 1}\\
& f_{RES}(x,\theta) \le \varepsilon_{n,RES}, \qquad & \varepsilon_{RES}^{min} \le \varepsilon_{n,RES} \le \varepsilon_{RES}^{max}, & \quad \text{KPI 2}\\
& g(x,\theta) \le 0, & &\\
& h(x,\theta) = 0, & &
\end{aligned}
$$

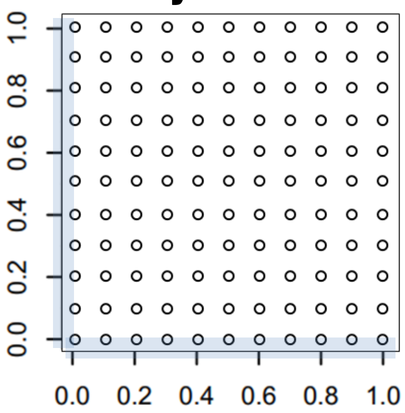
with $\epsilon_{en,FAR}$, $\epsilon_{en,RES}$ selected by a random sampling method

Random



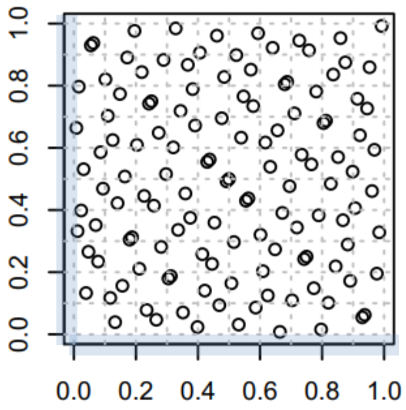
(Burhenne, 2011)

Systematic



(Gilbert, 1987)

Quasi-random



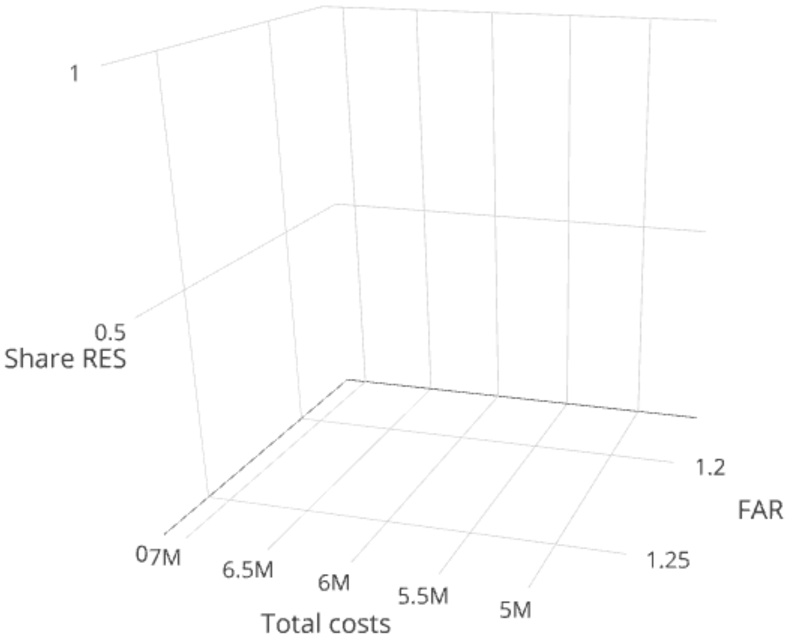
(Burhenne, 2011)

Latin hypercube

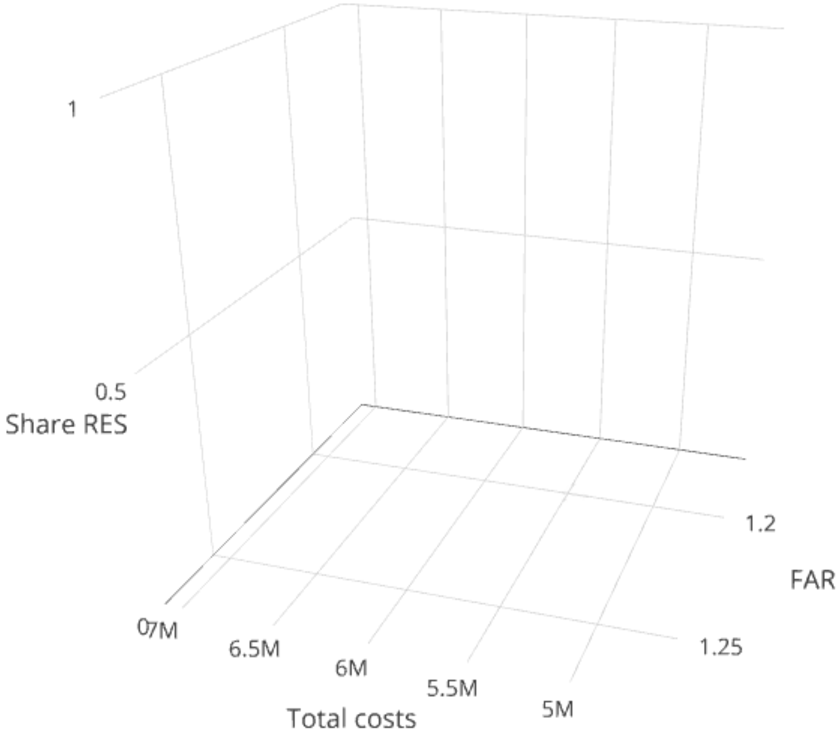
Sobol

Sobol sampling

Systematic



VS Sobol



Sobol sampling equations

$$
\begin{aligned}
\min_{x} \quad & f_l(x,\theta) \\
\text{subject to} \quad & f_j(x,\theta) \leq \varepsilon_{n,j}, && j = 1,\ldots,k, \quad j \neq l, \\
& \theta_t = \varepsilon_{n,t}, && t = 1,\ldots,u, \quad u \leq m, \\
& g(x,\theta) \leq 0, \\
& h(x,\theta) = 0,
\end{aligned}
$$

$$
E_{N\times P} = (\varepsilon_{n,p}) = \begin{pmatrix} \varepsilon_{1,1} & \varepsilon_{1,2} & \cdots & \varepsilon_{1,P} \\ \varepsilon_{2,1} & \varepsilon_{2,2} & & \varepsilon_{2,P} \\ \vdots & & \ddots & \vdots \\ \varepsilon_{N,1} & \varepsilon_{N,2} & \cdots & \varepsilon_{N,P} \end{pmatrix}, \quad \varepsilon_p^{min} \leq \varepsilon_{n,p} \leq \varepsilon_p^{max}
$$

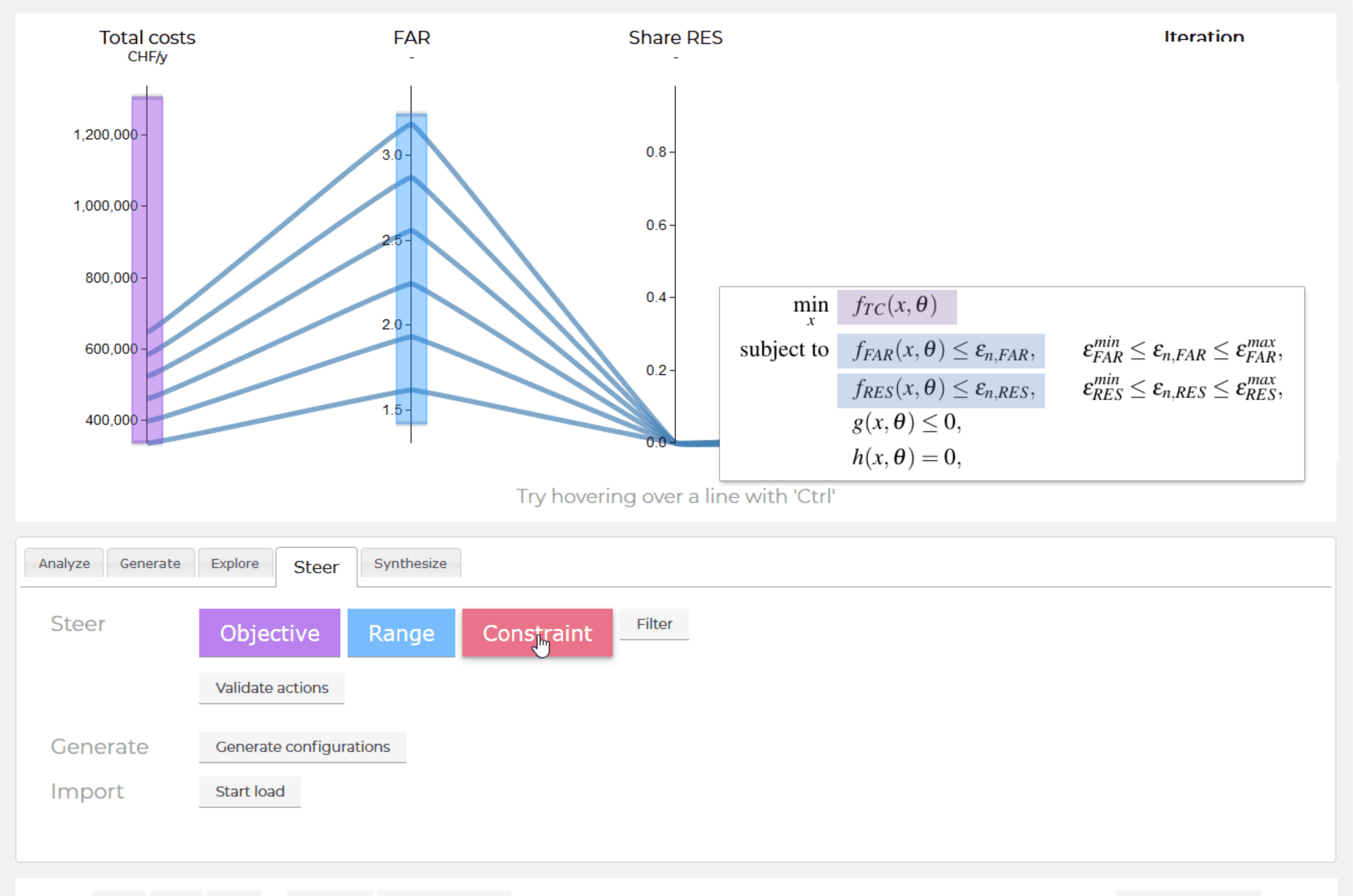
With the Sobol sampling approach, the user specifies a number of solutions N, and the corresponding parameters in E are computed as:

$$
\varepsilon_{n,p} = \varepsilon_p^{min} + s_{n,p} \cdot (\varepsilon_p^{max} - \varepsilon_p^{min}), \qquad n = 1,\ldots,N, \quad p = 1,\ldots,P, \tag{3.6}
$$

where $s_{n,p}$ is an element in the matrix $S_{N\times P}$, whose rows contain the Sobol sequence of N coordinates in a P-dimensional unit hypercube. Various computer-based Sobol sequence generators have been

$$
E^{sob}_{5\times 3} = S_{5\times 3} = \begin{pmatrix} 0.5 & 0.5 & 0.5 \\ 0.75 & 0.25 & 0.75 \\ 0.75 & 0.25 & 0.25 \\ 0.375 & 0.375 & 0.625 \\ 0.875 & 0.875 & 0.125 \end{pmatrix}
$$

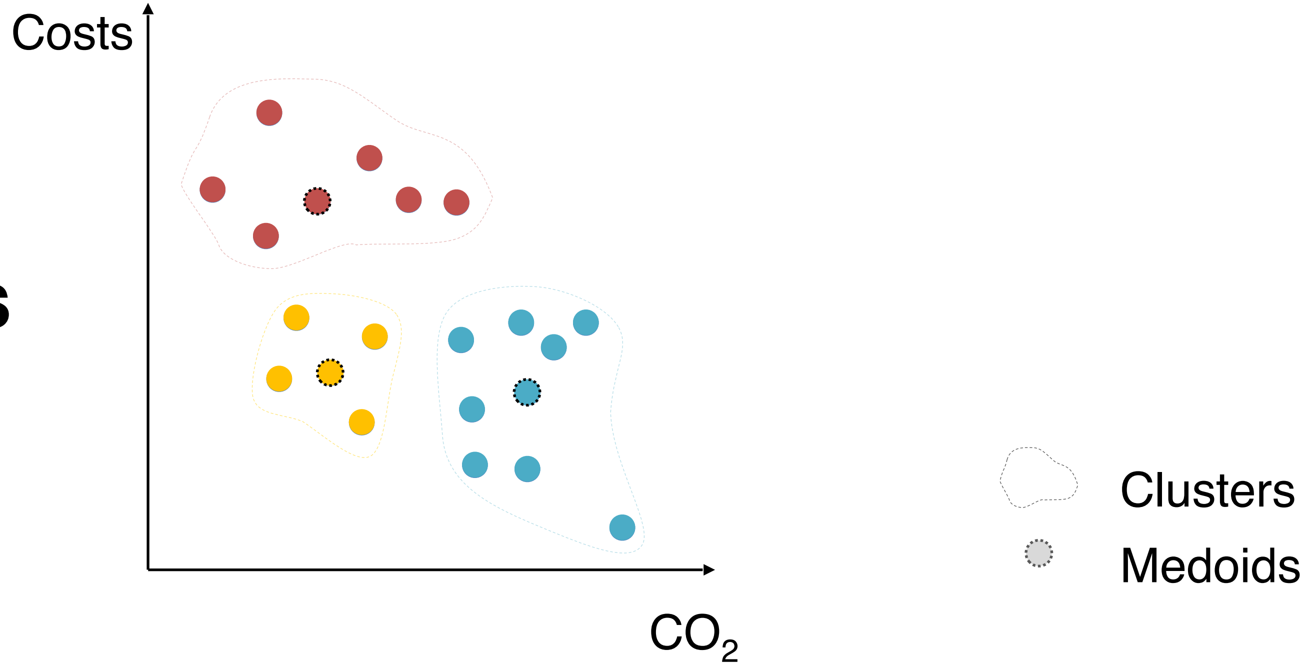
Interactive optimisation



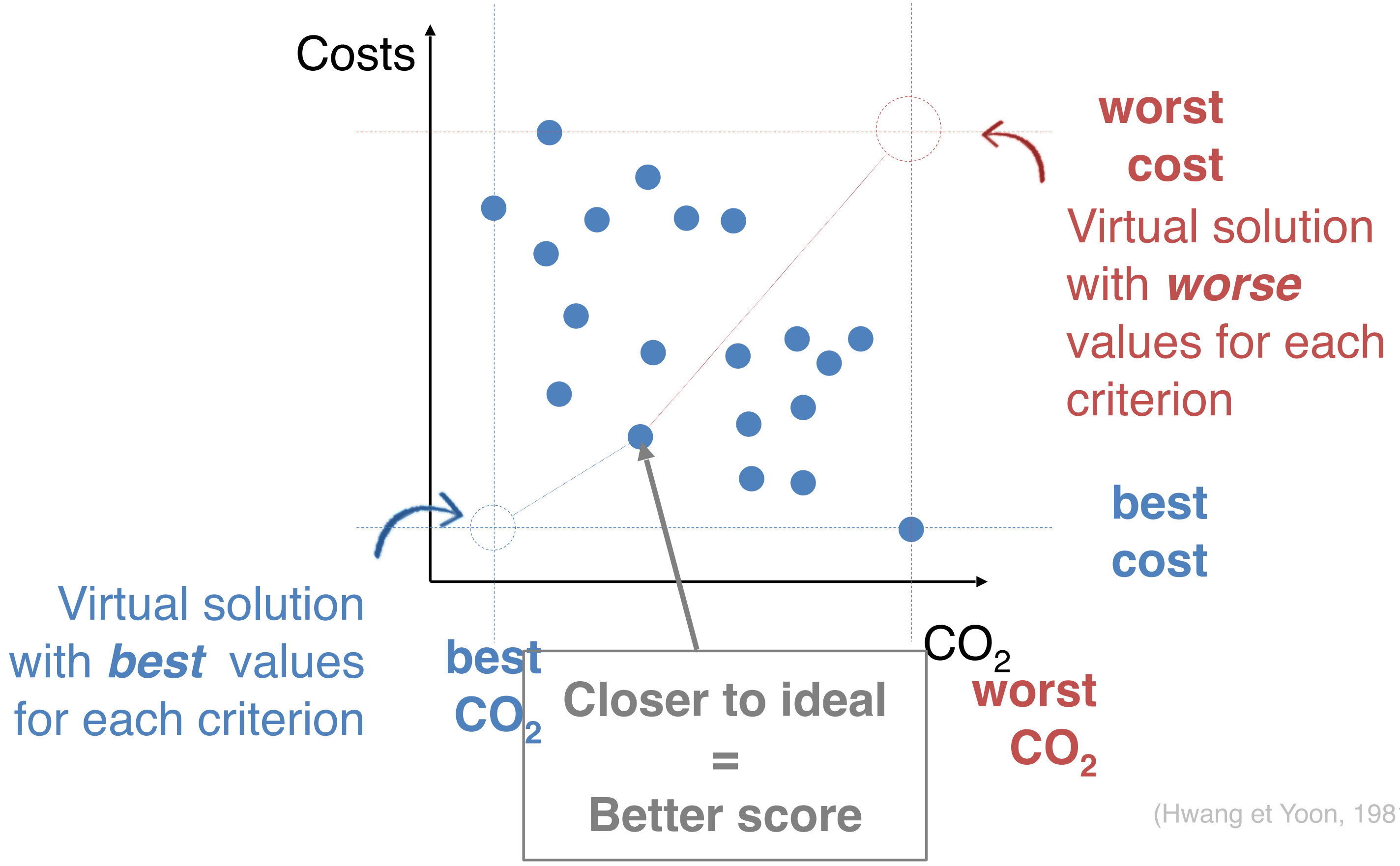
Clustering aims to group objects with similar characteristics into distinct partitions, or clusters.

(Kaufman and Rousseuw, 2009)

K-medoids



Multi-criteria analysis – TOPSIS



(Hwang et Yoon, 1981)

$$n_{ij} = \frac{z_{ij} - \min_i(z_{ij})}{\max_i(z_{ij}) - \min_i(z_{ij})}$$

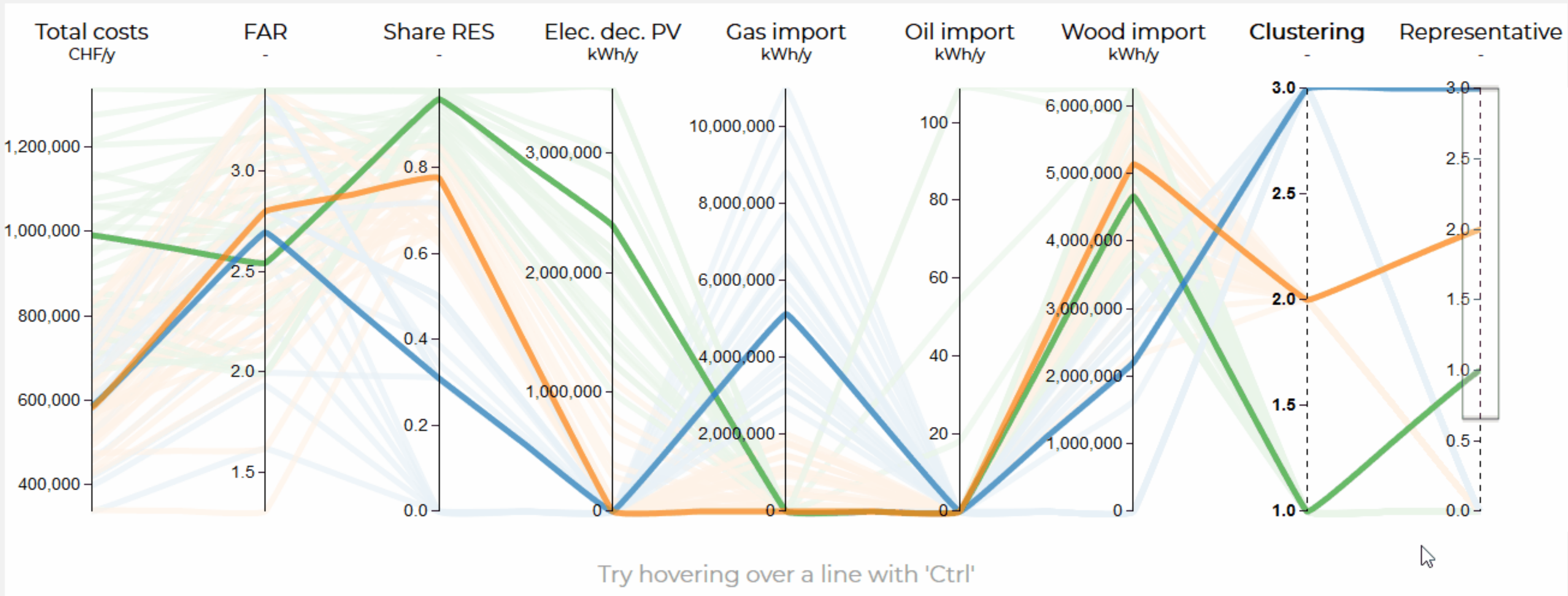
Parallel coordinates to compare solutions

Explore

(TOPSIS)

(Hwang and Yoon, 1981)
(García-Cascales et al, 2012)
(Chakraborty and Yeh, 2009)

Synthesize



Analyze | Generate | Explore | Steer | **Synthesize**

You have currently explored a total of 114 solutions.
Choose some criteria and click on the preferred solutions above to add to the comparer.
Click here to reset. Click here to beautify.

ID				

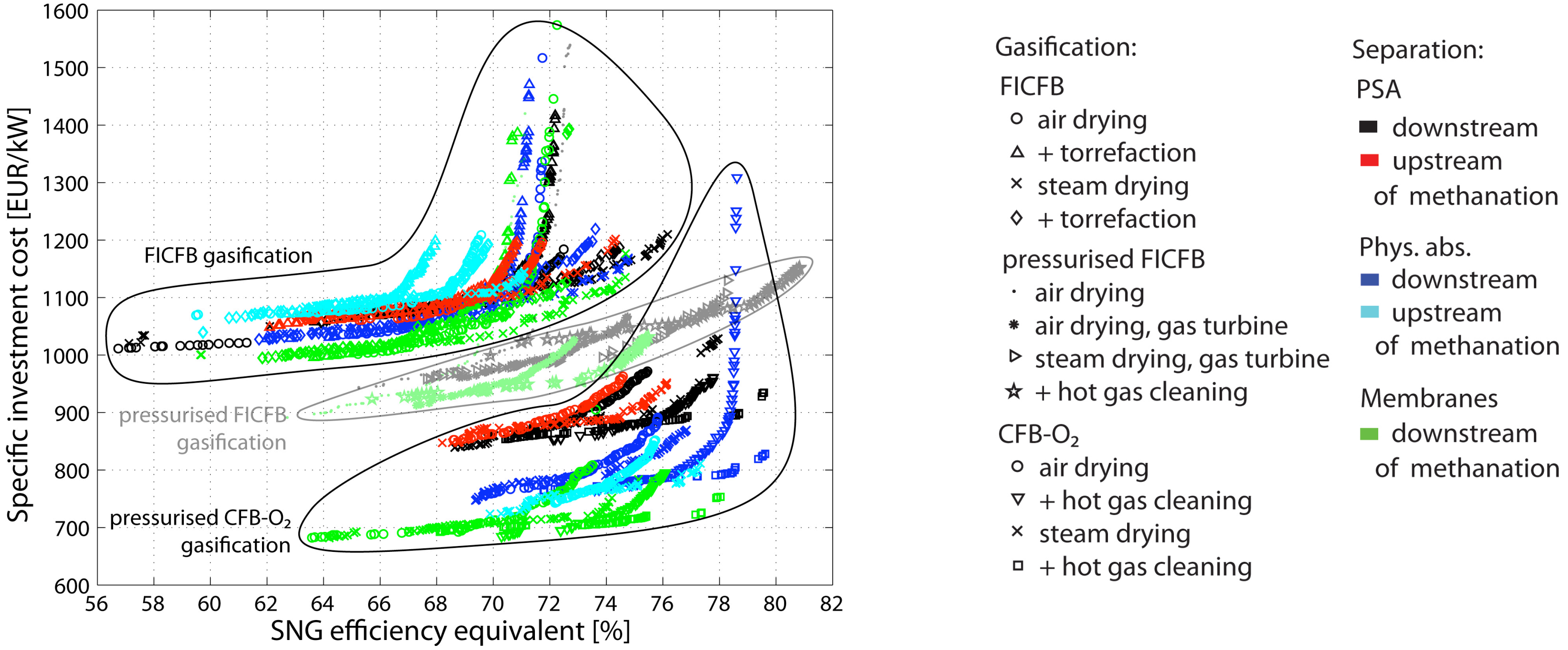
(Gardiner et al, 1997)
(Wolf et al, 2009)
(Piemonti et al, 2017)

8. Analysing the results

François Maréchal – francois.marechal@epfl.ch

- Each point of the Pareto is a process design

Thermo-economic Pareto front (cost vs efficiency):



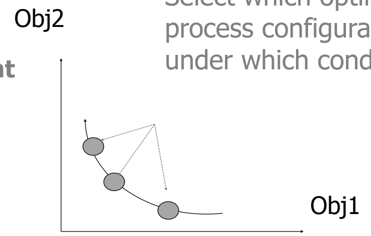
→ *The best solution is the pressurised directly heated gasifier*

Martin Gassner , Ph D Thesis, EPFL, 2010

Decision-making

- Selecting the process in the Pareto set

Pareto optimal front for given economic scenario



Select which optimal process configuration under which conditions ?

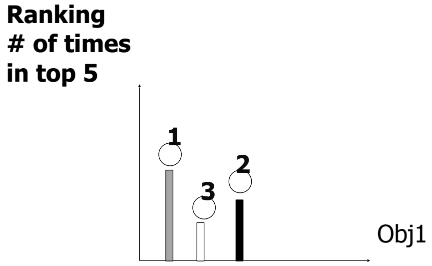
Economic parameters

Distribution functions → Randomly generate a set of uncertain parameters → Calculate the value of the objective function for all the Pareto optimal configurations

For each evaluation : give 1 point if in the top 10

repeat 3000 times

Solutions ranking based on probability
→ Decision-making support



Decision-making

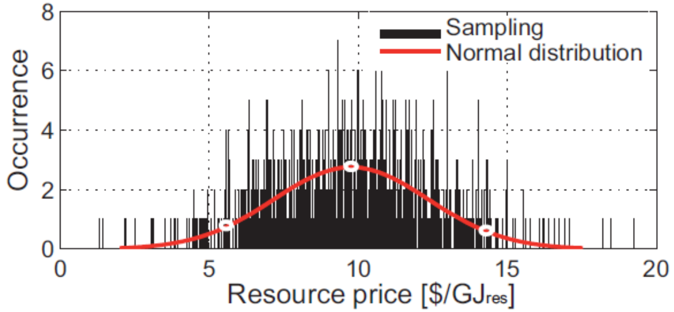
- Uncertainty of the economical conditions
  - Economic assumptions probability distribution functions
    - Normal, uniform, beta distribution

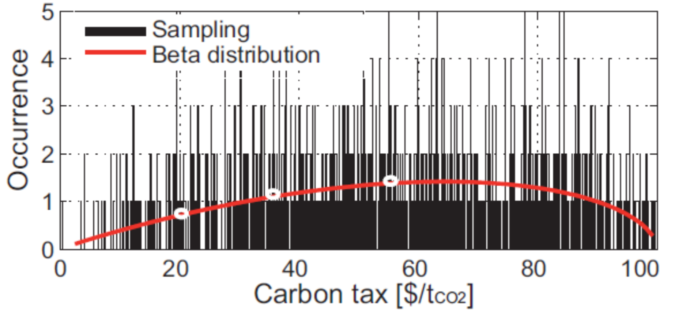
Scenario [IEA, EU, ZEP,...]	Base	Low	High
Resource price [$/GJ$_{res}$]	9.7	14.2	5.5
Carbon tax [$/t$_{CO2}$]	35	20	55
Yearly operation [h/y]	7500	4500	8200
Expected lifetime [y]	25	15	30
Interest rate [%]	6	4	8
Investment cost [%]	-30%	-	+30%

$$f(x;\mu,\sigma^2) = \frac{1}{\sigma\sqrt{2\Pi}}e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

$$f(x) = \frac{1}{a-b}$$

$$f(x;a,b) = cst \cdot x^{a-1} \cdot (1-x)^{b-1}$$





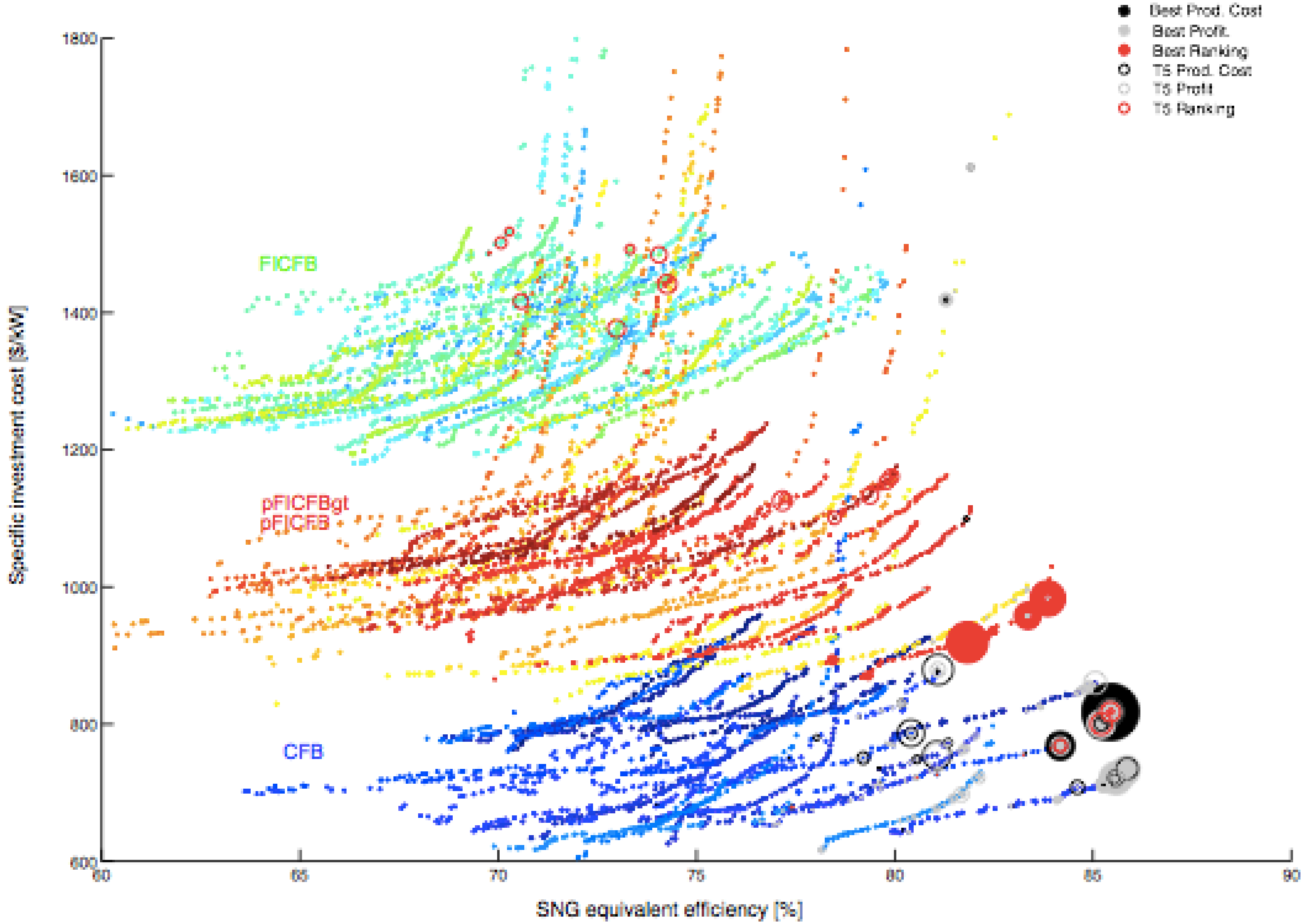
data for the biomass case

Table 6: Definition of the economic scenarios and parameters of the distribution functions for the economic assumptions.

	Distribution functions parameters			
	Distribution	Param. A	Param. B	Param. C
Biomass price [$/MWh$_{BM}$]	Normal	μ=28.6	σ=3.5	-
$\dot{E}$ price [$/MWh$_e$]	Normal	μ=145	σ=15	-
$\dot{E}$ price (green) [$/MWh$_e$]	Normal	μ=165	σ=20	-
Distributed heat price [$/MWh]	Beta	a=5.3	b=1.37	c=92
SNG price (automotive fuel) [$/MWh$_{SNG}$]	Normal	μ=110	σ=20	-
Biodiesel price [$/MWh$_{FAME}$]	Normal	μ=105	σ=20	-
Yearly operation [-]	Normal	μ=0.9	σ=0.1	-
Interest rate [%]	Normal	μ=0.06	σ=0.01	-
Investment cost [%]	Uniform	a=-0.3	b=0.3	-

What is the best process design ?

Pareto optimal configurations => new process model for the energy system design



(1)

ision Support for Ranking Pareto Optimal Process Designs under Uncertain Market Conditions. *Computers & Chemical Engineering* **2015**, *83*, 165–175. https://doi.org/10.1016/j.compchemeng.2015.06.009.