Solving strategies for the optimisation of energy systems

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Degrees of freedom of a system

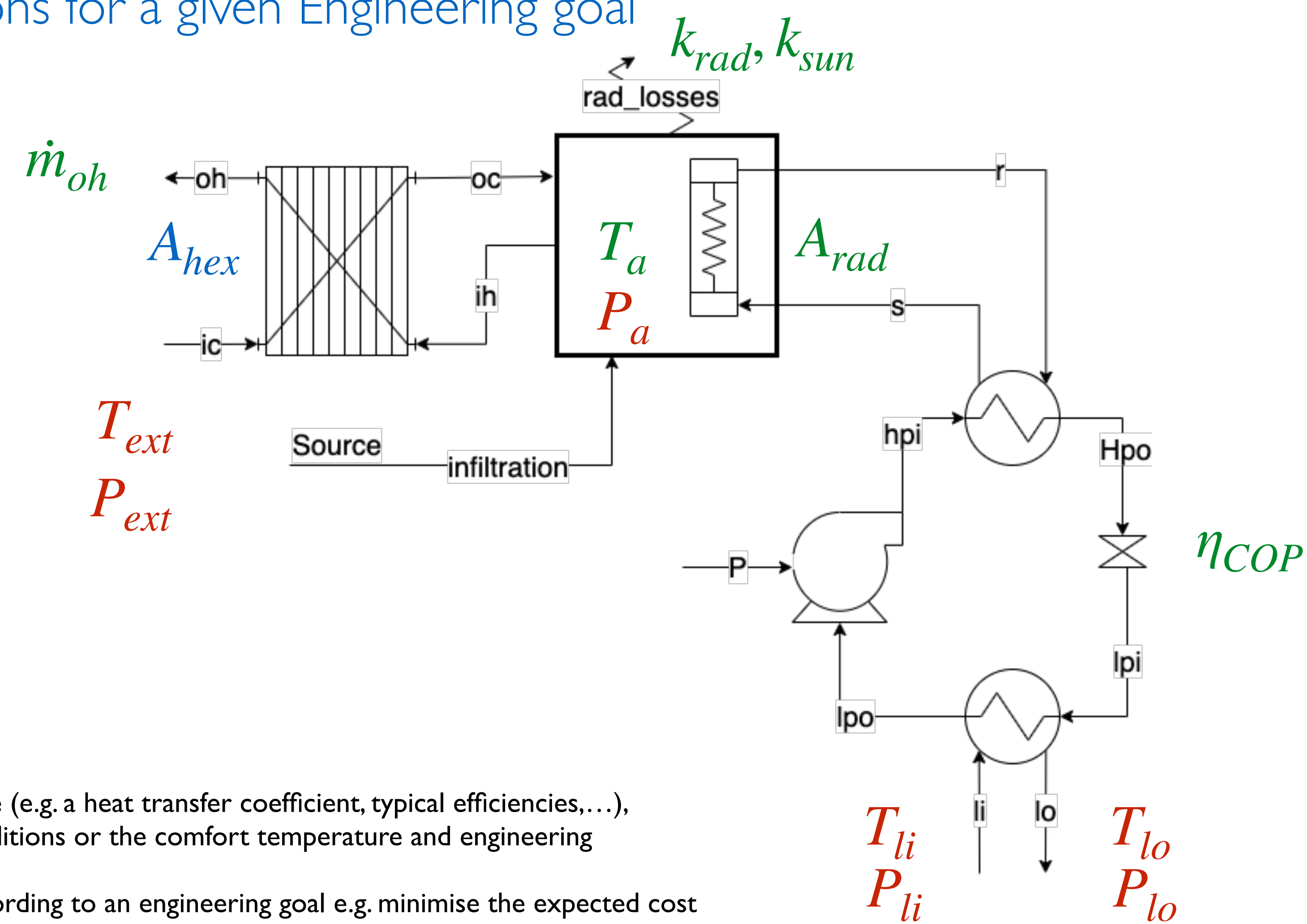
DOF : Degree of freedom of the system

DOF of the system = N_{state variables} - N_{Model equations}

- **State variables** needed to characterise the state
- **Model** define the thermodynamic knowledge
- **DOF** are fixed by specifications: $X - X^* = 0$ or $X = X^*$:
  - Knowledge
    - e.g. parameters of a heat transfer film coefficient correlation
  - Context Specifications
    - e.g. the ambient or the comfort temperature set point
  - Engineering Decisions for a given Engineering goal
    - e.g. minimum expected cost

Heat recovery by a double flux heat exchanger

- Specifications
  - Knowledge
  - Context Specifications
  - Engineering Decisions for a given Engineering goal



Degrees of freedom are fixed by knowledge (e.g. a heat transfer coefficient, typical efficiencies,…), context specifications like the ambient conditions or the comfort temperature and engineering decisions (like the heat exchanger area)-
Engineering decisions need to be taken according to an engineering goal e.g. minimise the expected cost

Thermo-economic Model

System model

$$F(X_{state}, \pi) = 0 \quad \text{Model equations}$$
$$S(X_{state}, \pi) = 0 \quad \text{Context specifications}$$
$$with \quad \pi \quad \text{Model parameters}$$
$$X_{state} \quad \text{State variables}$$

DOF : Degree of freedom of the system

DOF of the system = N_{state variables} - N_{Model equations}

N_{Decision variables} = DOF - N_{Context} - N_{Knowledge}

Decision variables :

- Degrees of freedom for which I do not have any rationale to fix its value

- I only know the possible range

$$X_{d,min} \leq X_d \leq X_{d,max}$$

Thermo-economic optimisation

Find the value of the decision variables X_d with a given objective

$$X_{d,min} \leq X_d \leq X_{d,max}$$

"I would like to fix the value of X_d so that it minimise an objective function"

$$\min_{X_{state}} \quad TotalCost(X_{state}, \pi) \quad \rightarrow \text{Objective function}$$

$$\begin{aligned} s.t. \quad & F(X_{state}, \pi) = 0 \Rightarrow \text{equipment model} \\ & S(X_{state}, \pi) = 0 \Rightarrow \text{Specification equations} \\ & G(X_{state}, \pi) \leq 0 \quad \text{Inequality constraints} \\ & X_{state}^{min} \leq X_{state} \leq X_{state}^{max} \quad \text{Bounds} \end{aligned} \quad \rightarrow \text{Constraints}$$

$$where$$

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

X_d is a subset of X_{state}

Typical objective function formula

An objective function defines the relative importance of flows and installed capacity of equipments during the expected lifetime of the system

$$OBJ_o = \sum_{s}^{states} \sum_{f}^{flows} (v_{f,s,o} \, . \, t_{op,s} \, . \, \dot{m}_{f,s}) + \sum_{u}^{units} v_{u,o} \, . \, \frac{1}{\tau_u} \, . \, O_u(S_u)$$

- **with**
  - $\dot{m}_{f,s}$: the flow [kg/s or kW] of resource or product f in the state of operation s
  - $v_{f,s,o}$: the value (relative importance) of $\dot{m}_{f,s}$ for the objective function o
    - $v_{f,s,o}$ can be the expected cost of a flow (e.g. $[CHF/kg$ or $CHF/MJ]$ or the Life Cycle Impact of the flow
  - $t_{op,s}$: a time of operation of the system in the state s of flow $\dot{m}_s$ in [s/year]
  - $v_{u,o}$: the value (relative importance) of the capacity function $O_u(S_u)$ of unit u with the size S_u for the objective function o
  - $\frac{1}{\tau_u}$: annualisation of the installed capacity of unit u over its expected lifetime
    - $O_u(S_u)$ can be the investment cost in $[CHF]$, materials, Life Cycle Inventory e.g. in $[ton_{CO_{2_{eq}}}]$, Land footprint, Life cycle impact associated to construction of unit u

Example of objective functions : engineering goals

$$TotalCost[CHF/year] = OPEX + CAPEX + Tax$$

$$OPEX = \sum_{p=1}^{n_p} (\sum_{r=1}^{n_r} \dot{m}^+_{r,p} c^+_{r,p} + \dot{E}^+_p c^+_{e,p} - \dot{E}^-_p c^-_{e,p} + \sum_{u=1}^{n_u} f_{u,p} cm_u) d_p$$

$$CAPEX = \sum_{u=1}^{n_u} \frac{1}{\tau(n_{y,u}, i)} (I1_u y_u + I2_u f_u^{max})$$

$$Tax = CO_2^+ \gamma^{CO_2^+}$$

$$CO_2^+ = \sum_{p=1}^{n_p} (\sum_{r=1}^{n_r} \dot{m}^+_{r,p} \epsilon_r^{CO_2} + \dot{E}^+_p \epsilon_{e,p}^{CO_2^+} - \dot{E}^-_p \epsilon_{e,p}^{CO_2^-}) d_p$$

$$Impact = \zeta^{CO_2^+} (CO_2^+ + \sum_{u=1}^{n_u} \frac{1}{n_{y,u}} (\xi_{c_u}^{CO_2} + \xi_{d_u}^{CO_2}) f_u^{max})$$

$$RES = \sum_{p=1}^{n_p} (\sum_{r_{res}=1}^{n_{r_{res}}} \dot{m}^+_{r_{res},p} + \sum_{u=1}^{n_u} f_{u,p} e_{u,p}^{res^+}) d_p$$

$$\dot{E}^+_p + \dot{E}^-_p + \sum_{u=1}^{n_u} f_{u,p} (e_{u,p}^{res^+} - e^-_{u,p}) = 0 \qquad \forall p = 1..n_p$$

Inequality constraints

Constraints limit the search space for the values of X_d

- Operating limits
  - safety, equipment limits,
- Regulation
  - Emission : environment
- Market limits => products quality
- Technology limits and heuristics
  - Materials
- Models limits
  - Correlations
  - Structures and models
- Numerical safety ;Two types
  - **Hard**: numerical validity of the model: i.e. can not be violated otherwise the system state can not be calculated
    - E.g. flow inversion
    - try to place the hard constraints on the variables
  - **Soft**: may be violated during resolution. The state exists but is not expected to be valid as a solution

Different types of problems

- **Optimal operation (Equipment Size is fixed)**
  - Decision : Operation set point
  - Objective : Operating cost (CHF/s)
- **Optimal operation strategy (Equipment Size is fixed)**
  - Decision : Set point strategy + start/stop
  - Objective : Operating cost (CHF/period)
- **Scheduling (Equipment Size is fixed)**
  - Decision : Set points strategy, start/stop, when ?, in which equipment ?
  - Objective : Operating cost (CHF/period)

Different types of problems

- **Optimal sizing (equipment size is decided)**
  - Decision : operating set points, unit sizes, investment
  - Objective : Total cost (CHF, CHF/an)
- **Optimal design (choice and size of equipment is decided)**
  - Decision : operating set points (Operating strategy), unit sizes, investment, configuration
  - Objective : Total cost (CHF, CHF/an)
- **Retrofit (choice and size of some of the equipment is decided, reuse of existing equipment with fixed sizes / configuration)**
  - Decision : operating set points (Operating strategy), unit sizes, configuration, reuse, reconfiguration, investments
  - Objective : total cost

- How do I use a flowsheet model to solve an optimization problem ?

$$F(X_{state}) = 0 \Rightarrow \text{equipment model}$$
$$L(X_{state}) = 0 \Rightarrow \text{linking equations}$$
$$T(X_{state}) = 0 \Rightarrow \text{constitutive equations}$$
$$S(X_{state}) = 0 \Rightarrow \text{Specification equations}$$

Black box method

Optimisation : min $OBJ(X^*_{decision})$

Subject to $G_{inequality}(X^*_{decision}) \geq 0$

$X^*_{decision}$

$OBJ(X^*_{decision})$

$G(X^*_{decision})$ inequality

Status

Model : Solve

$F(X_{dependent}, X_{specification}, X_{decision})=0$

$S(X_{dependent}, X_{specification}, X_{decision})=0 \Rightarrow X(X^*_{decision})$

$X_{decision} - X^*_{decision} = 0$

then calculate $OBJ(X(X^*_{decision}))$

$G(X(X^*_{decision}))$

Black Box strategy

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

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

$$where$$

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

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

NxN problem

$$F(X_{state}, \pi) = 0 \Rightarrow \text{model equations}$$

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

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

$$where$$

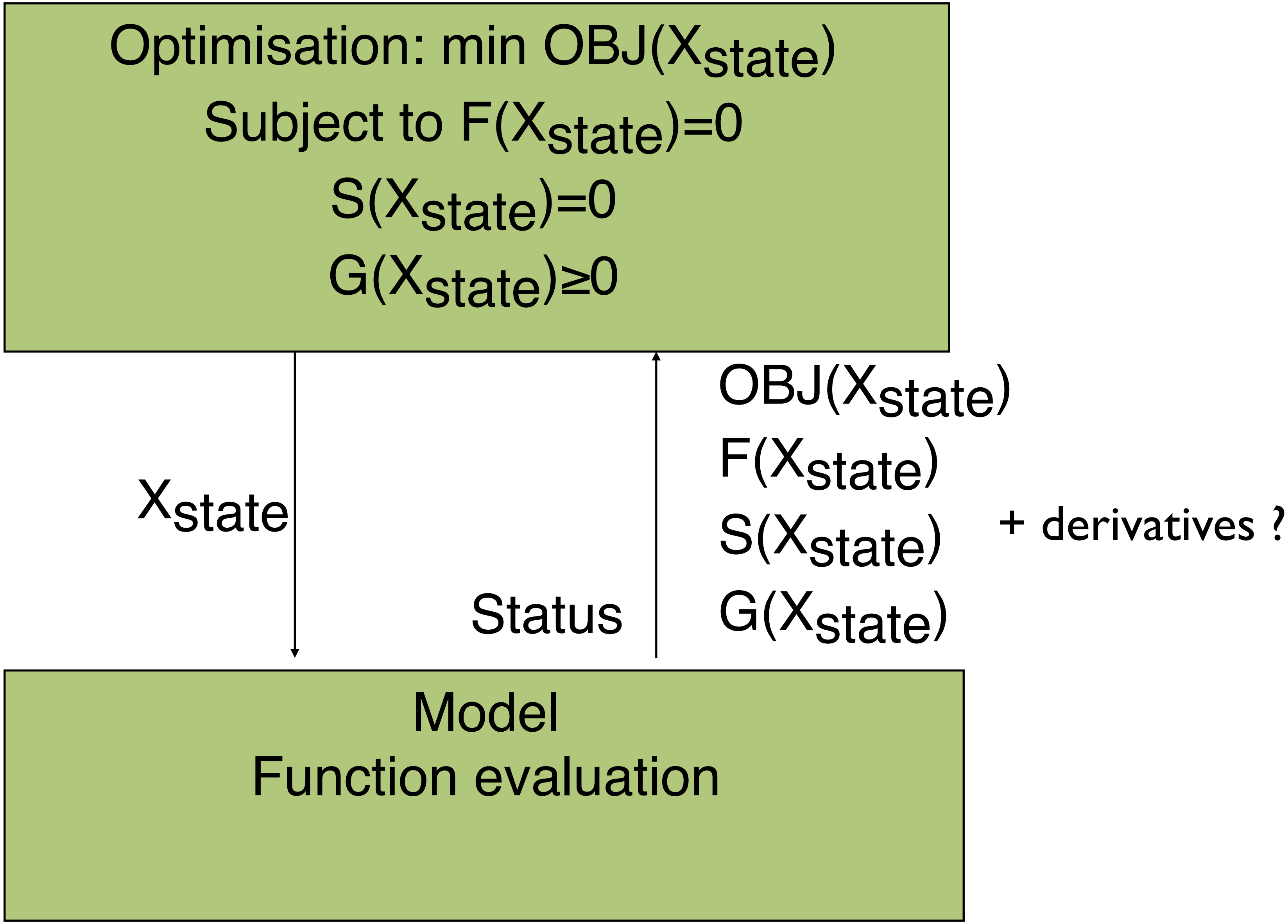
$$X_{state} = \{x_{StateVariables}, x_{UnitParameters}, y_{decision} \epsilon \{0,1\}\}$$

Black Box approach

+ Can be used in any kind of optimisation method
  Heuristic, direct et indirect (derivatives)
+ Solving method to be defined => problem analysis
+ Selection of $X^*_{decision}$ by the user
+ Robustness
+ Non convergence analysis
+ Gives a list of system states
- Flexibility
- Computation time
- Inequality might be a problem when not on decision variables
- Derivative calculation (especially when done in iterative loops)

$$\frac{\partial f}{\partial x_i} = \frac{f(X + \Delta x_i) - f(X)}{\Delta x_i}$$

Simultaneous method



Simultaneous strategy

$$
\begin{aligned}
\min_{X_{state}} \quad & TotalCost(X_{state}, \pi) \\
s.t. \quad & F(X_{state}, \pi) = 0 \Rightarrow \text{equipment model} \\
& S(X_{state}, \pi) = 0 \Rightarrow \text{Specification equations} \\
& G(X_{state}, \pi) \leq 0 \quad \text{Inequality constraints} \\
& X_{state}^{min} \leq X_{state} \leq X_{state}^{max} \quad \text{Bounds} \\
where \quad & \\
& X_{state} = \{x_{statevariables}, x_{UnitParameters}, y_{decision} \epsilon \{0, 1\}\}
\end{aligned}
$$

Requires : Non Linear Constrained Optimisation solving method

X_d is not defined (hidden in X_{state})

Simultaneous approach

+ Optimisation under constraints

=> indirect method with 2nd derivatives if possible

+ Flexibility : different pbm with the same model (changing specification set and not the model)

+ Efficient and robust for on-line optimisation systems

Bounds definition !

+ Computing time

+ Automatic DOF analysis and sensitivity analysis

+ Hard and soft inequality constraints

- Initialisation !
- Derivatives calculation (during function evaluation, symbolic ?)
- No system state when no convergence
- Scaling !
- No explanations when the problem does not converge !
- Push button system?

Two levels approach

Optimisation:

$$\min OBJ(X^*_{decision}, X^*_{specification})$$

$$\text{Subject to } H(X^*_{decision}, X^*_{specification})=0$$

$$G(X^*_{decision}, X^*_{specification})\geq 0$$

Requires a constrained optimisation solver

↓ $X^*_{decision}$, $X^*_{specification}$

↑ Status

$OBJ(X^*_{decision}, X^*_{specification})$

$H(X^*_{decision}, X^*_{specification})$

$G(X^*_{decision}, X^*_{specification})$

+ derivatives ?

Modèle

$$X_{dependent} = \Phi(X^*_{decision}, X^*_{specification})$$

Two level strategy

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

$$s.t. \quad H(X^*_{decision}, X^*_{Specs}, X(X^*_{decision}, X^*_{Specs}), \pi) = 0 \quad \text{some equality constraints}$$

$$G(X^*_{decision}, X^*_{Specs}, X(X^*_{decision}, X^*_{Specs}), \pi) \leq 0 \quad \text{inequality constraints}$$

$where$

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

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

(N+Ns)x(N+Ns) problem

$$F(X_{state}, \pi) = 0 \Rightarrow \text{system model}$$

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

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

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

$where$

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

Two levels strategy

+ Best of both world
+Robustness of unit models (single calculation mode)
+Code Maintenance
+Derivative chaining is possible
    Analytical calculation is possible
+ Soft inequality constraints
+ Sensitivity analysis
- Conditional simulation
- Computing time (solving the lower level iteratively)
- Hard bounds (except when they are at the decision variable level).
- Noise in derivatives evaluation
    Internal iterative calculations