Laboratoire d'Automatique

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Dynamic Real-Time Optimization via Tracking of the Necessary Conditions of Optimality

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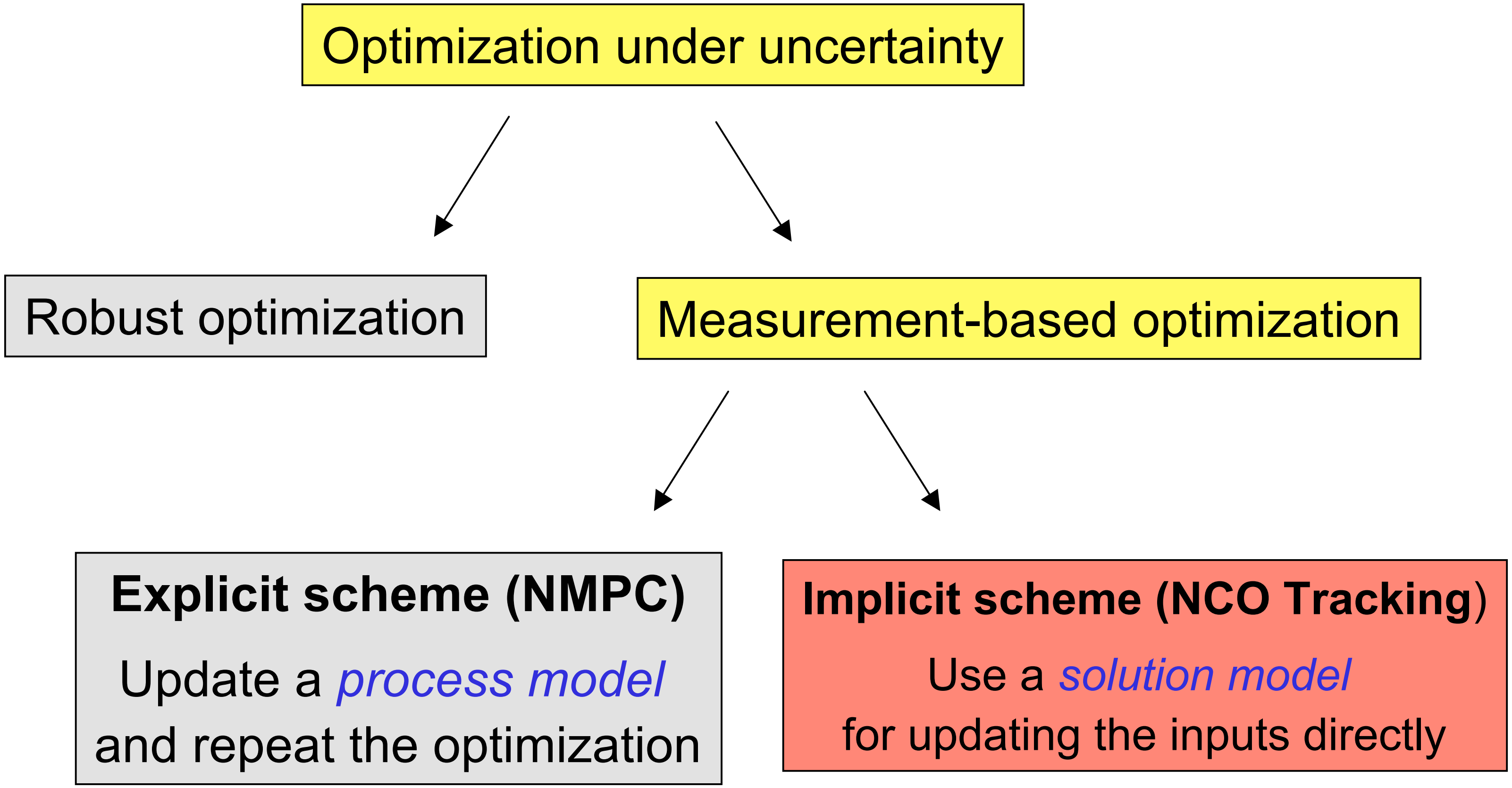
D-RTO under Uncertainty



Outline

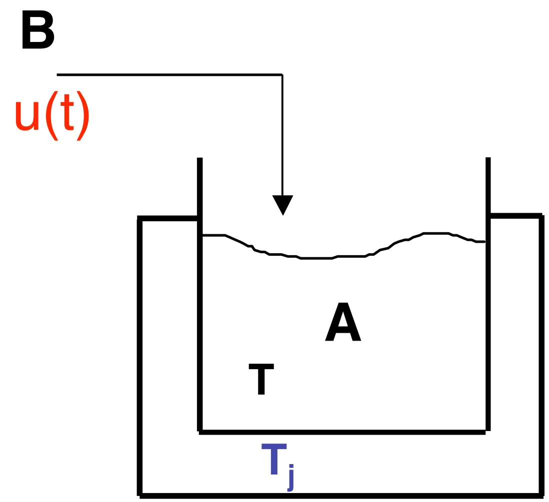
- Optimization and uncertainty
- Tracking the Necessary Conditions of Optimality
  - Turn optimization problem into control problem
  - Decentralized control scheme
  - Simulation results
  - Application projects
- Conclusions

Illustrative example

Illustrative Example

Semi-batch Chemical Reactor

$$A + B \xrightarrow{k_1} C$$
$$2B \xrightarrow{k_2} D$$



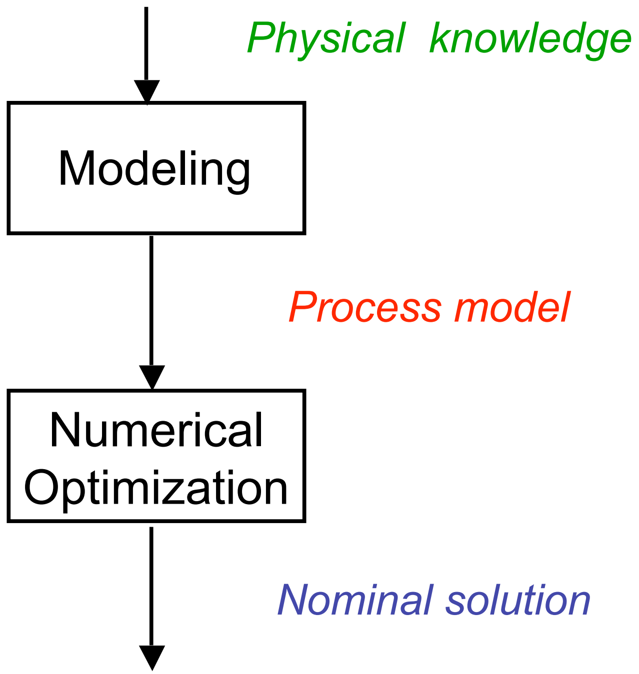
Exothermic reactions -- Isothermal

Terminal objective: Maximize number of moles of C at t_f by adjusting $u(t)$

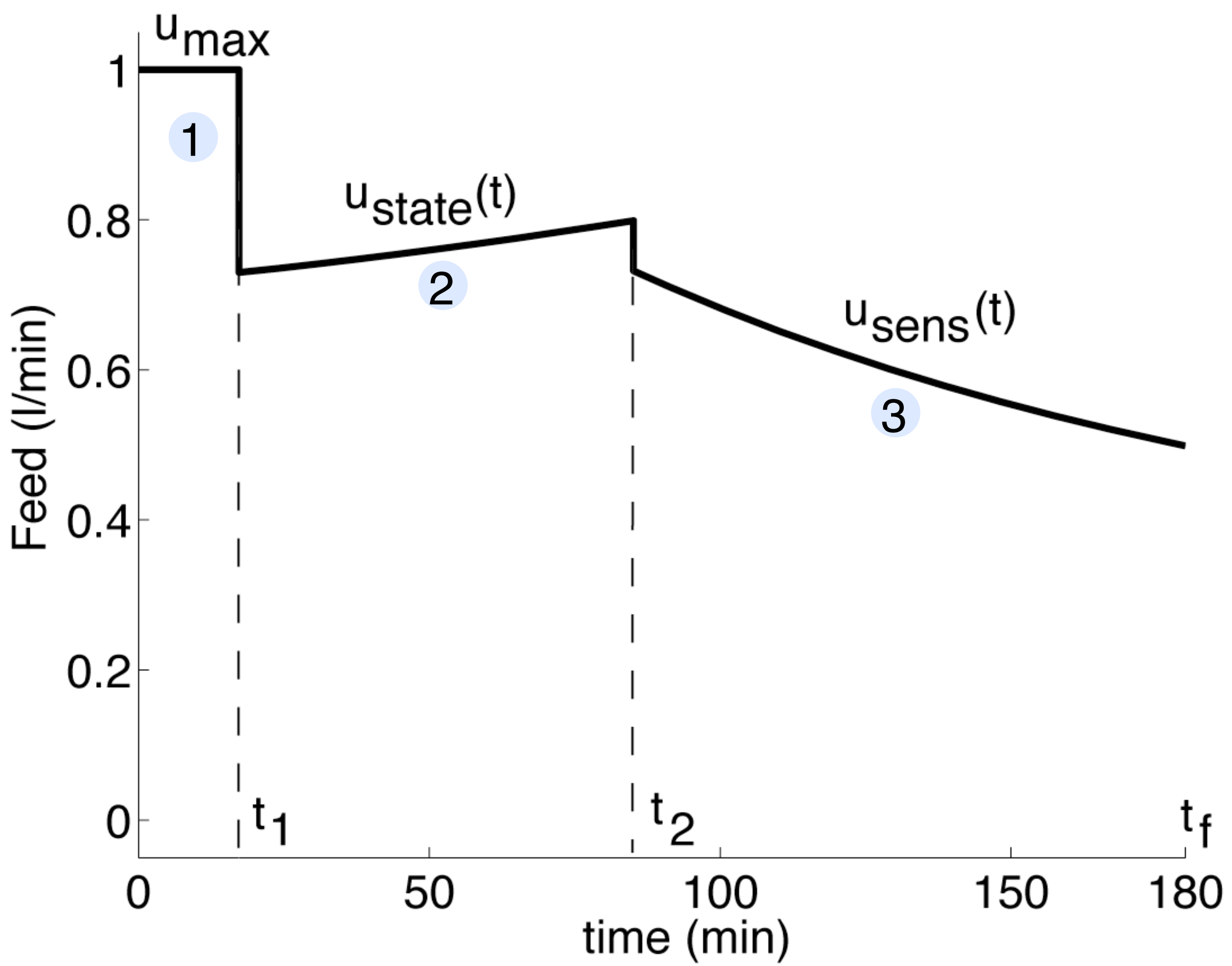
Safety path constraint: Heat removal limitation $T_j \geq T_{j,min}$

Selectivity terminal constraint: Number of moles of D at t_f $n_{Df} \leq n_{Df,max}$

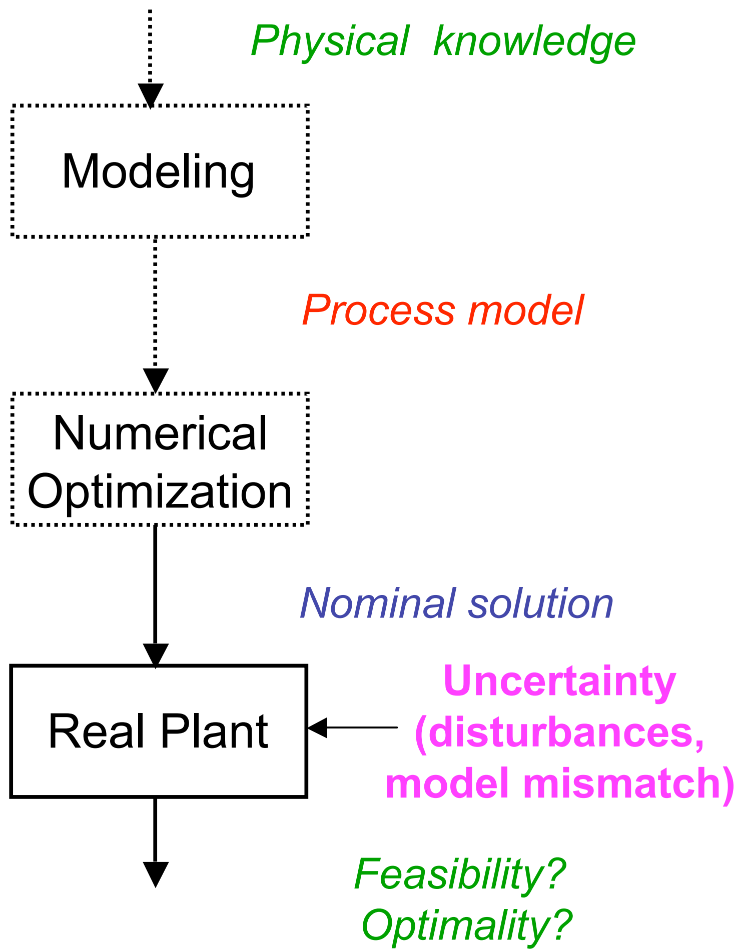
Nominal Optimization



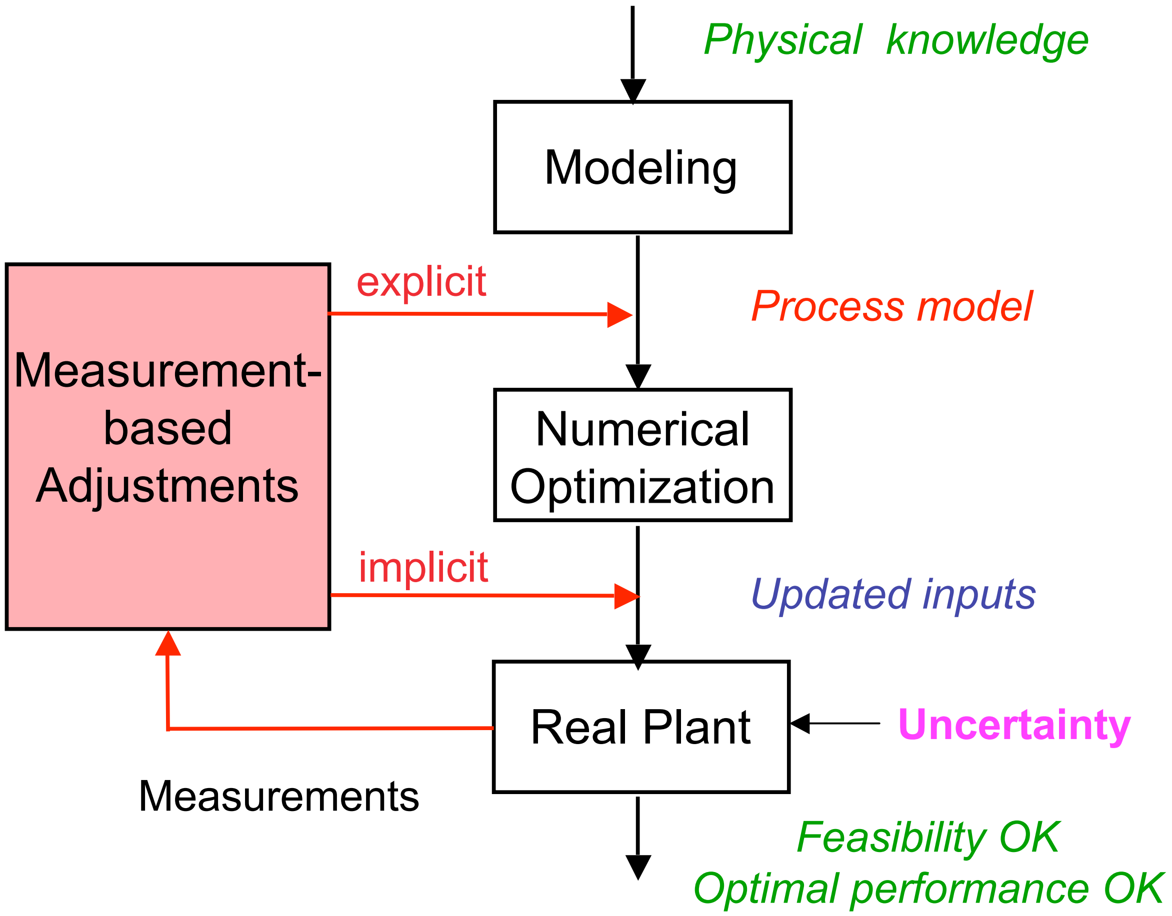
Nominal Optimal Solution



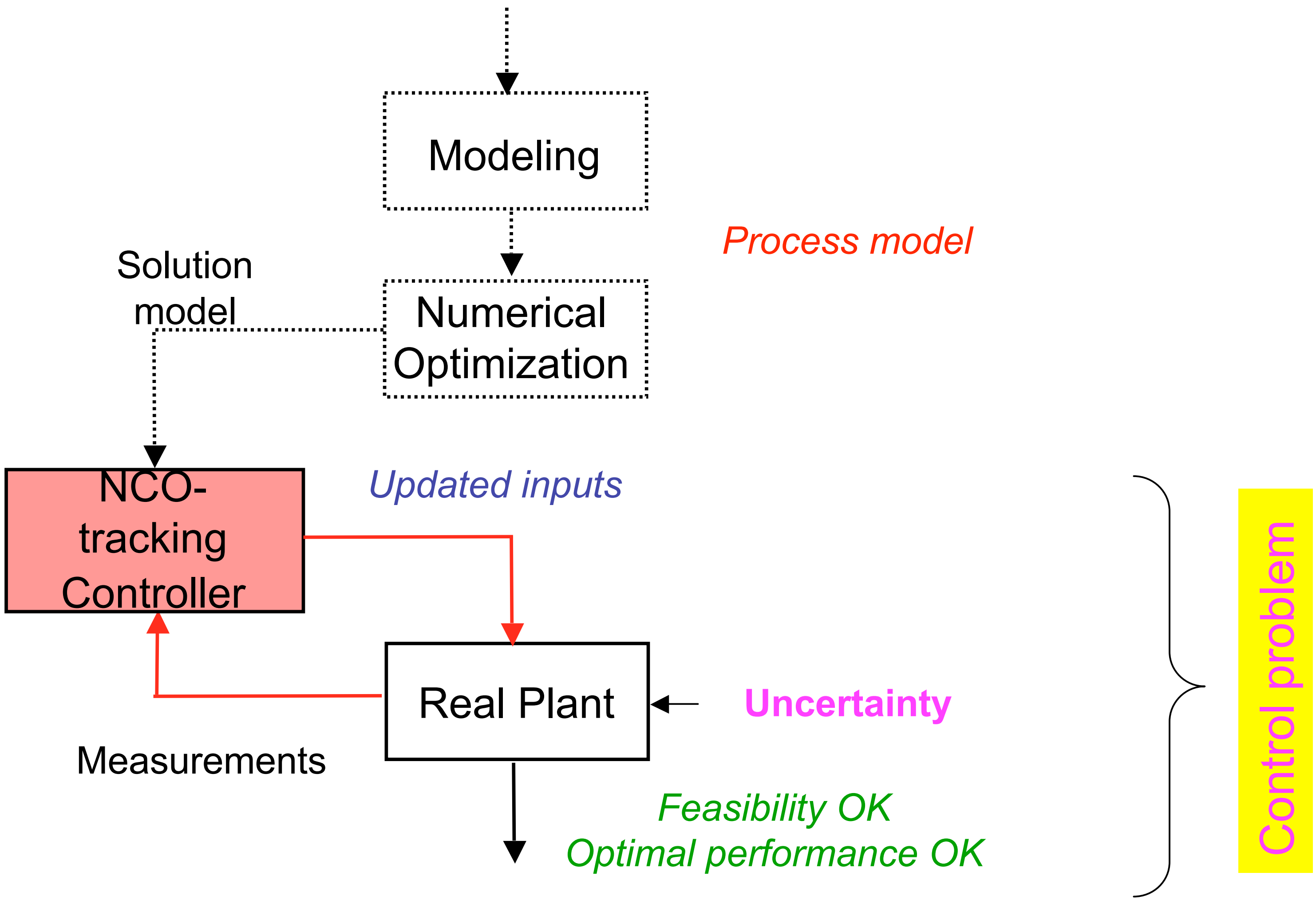
Implementation of the Nominal Solution



Measurement-based Optimization



NCO Tracking: Self-optimizing control structure

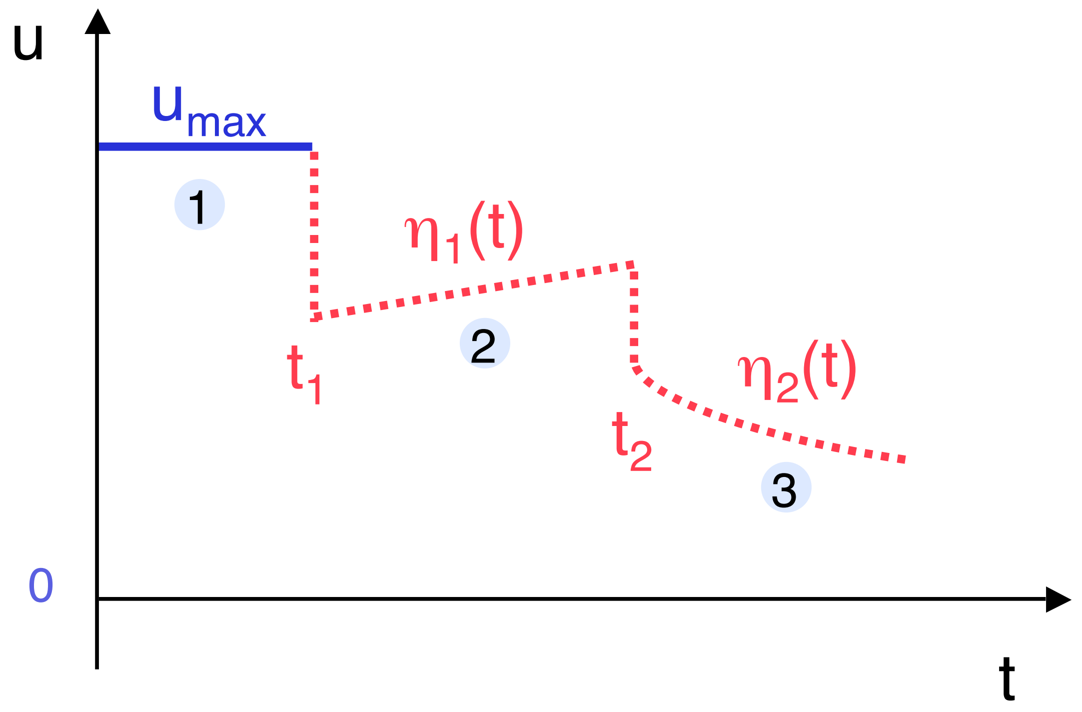


Solution Model

Input representation capable of achieving (near) optimality

- Choice of decision variables
  - Identify arcs and switching times that vary with uncertainty
  - Introduce approximations and parameterization as needed
- Pairing for decentralized control
  - Associate combinations of decision variables with active constraints
  - Associate remaining decision variables with sensitivities

Input Dissection



Model → Fixed part -- u_{max}

Model → Variable parts -- t_1, t_2, $\eta_1(t)$, $\eta_2(t)$ Decision variables

NCO -- Solution Model A

Decision variables: t_1, t_2, $\eta_1(t)$, $\eta_2(t)$

Pairing

	Constraints	Sensitivities
Path Objectives During the run	$T_j = T_{j,min}$	$\partial H / \partial \eta_2 = 0$ H: Hamiltonian
Terminal Objectives End of the run	$n_D(t_f) = n_{Df,max}$	-

Solution Model A

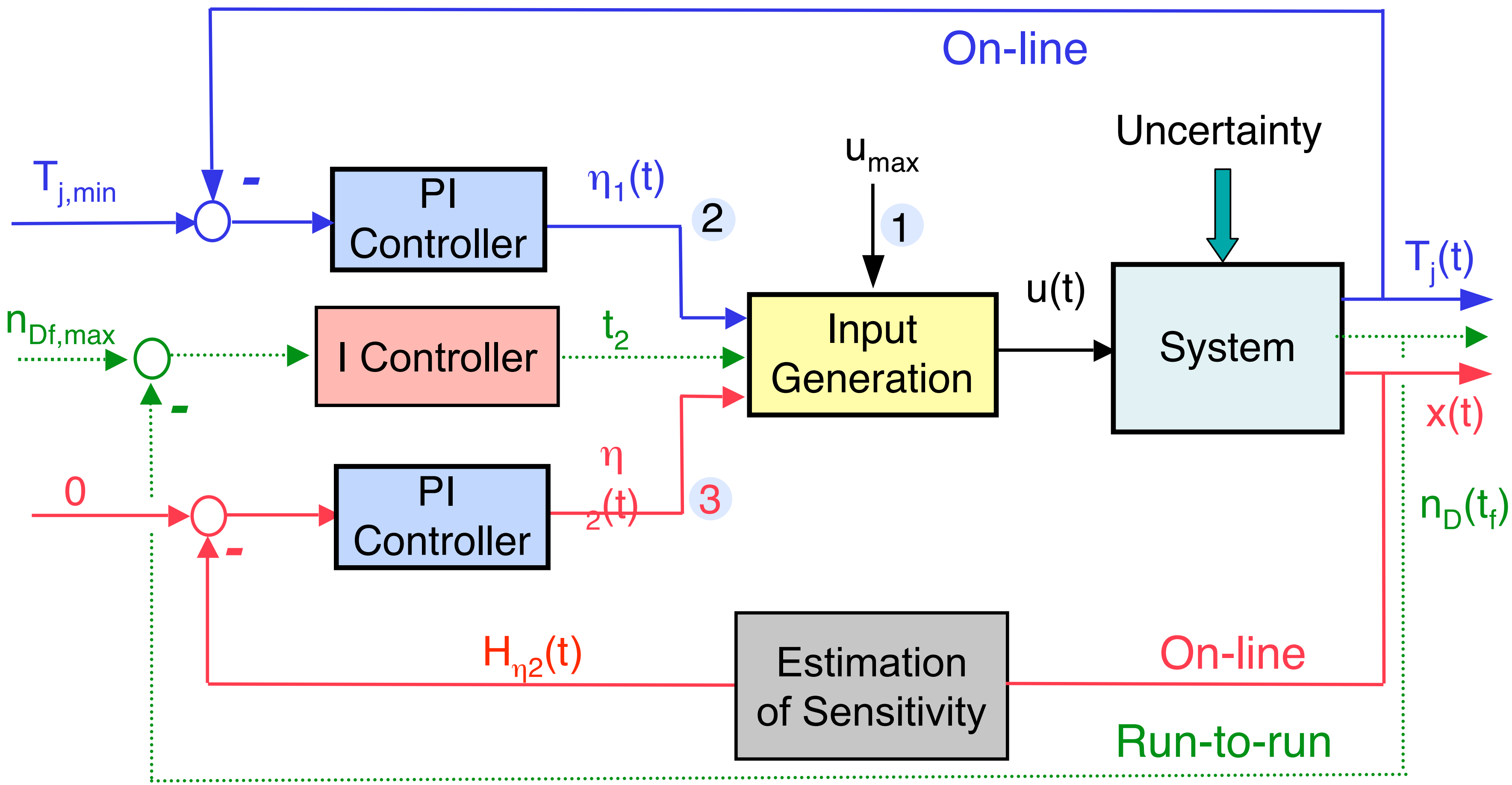
- Invariant part -- u_{max}
- Path constraint -- $T_j = T_{j,min}$ -- $t_1, \eta_1(t)$
- Terminal constraint -- $n_D(t_f) = n_{Df,max}$ -- t_2
- Sensitivity -- $\partial H / \partial \eta_2 = 0$ -- $\eta_2(t)$

$$u = \begin{cases} u_{max} & 0 \le t \le t_1 \\ K_\eta (T_{j,min} - T_j) & t_1 < t \le t_2 \\ G_\eta (\partial H / \partial \eta_2) & t_2 < t \le t_f \end{cases}$$

$$t_1 = t \quad with \quad T_j(t) = T_{j,min} \quad and \quad T_j(t\_) > T_{j,min}$$

$$t_2 = R_\pi (n_{Df,max} - n_D(t_f))$$

NCO-tracking Scheme for Solution Model A



NCO -- Solution Model C

Decision variables: t_1, t_2, $\eta_1(t)$, $\eta_2(t)$

Different pairing

	Constraints	Sensitivities
Path Objectives During the run	$T_j = T_{j,min}$	-
Terminal Objectives End of the run	$n_D(t_f) = n_{Df,max}$	$\partial n_C(t_f)/\partial t_2 = 0$

Solution Model C

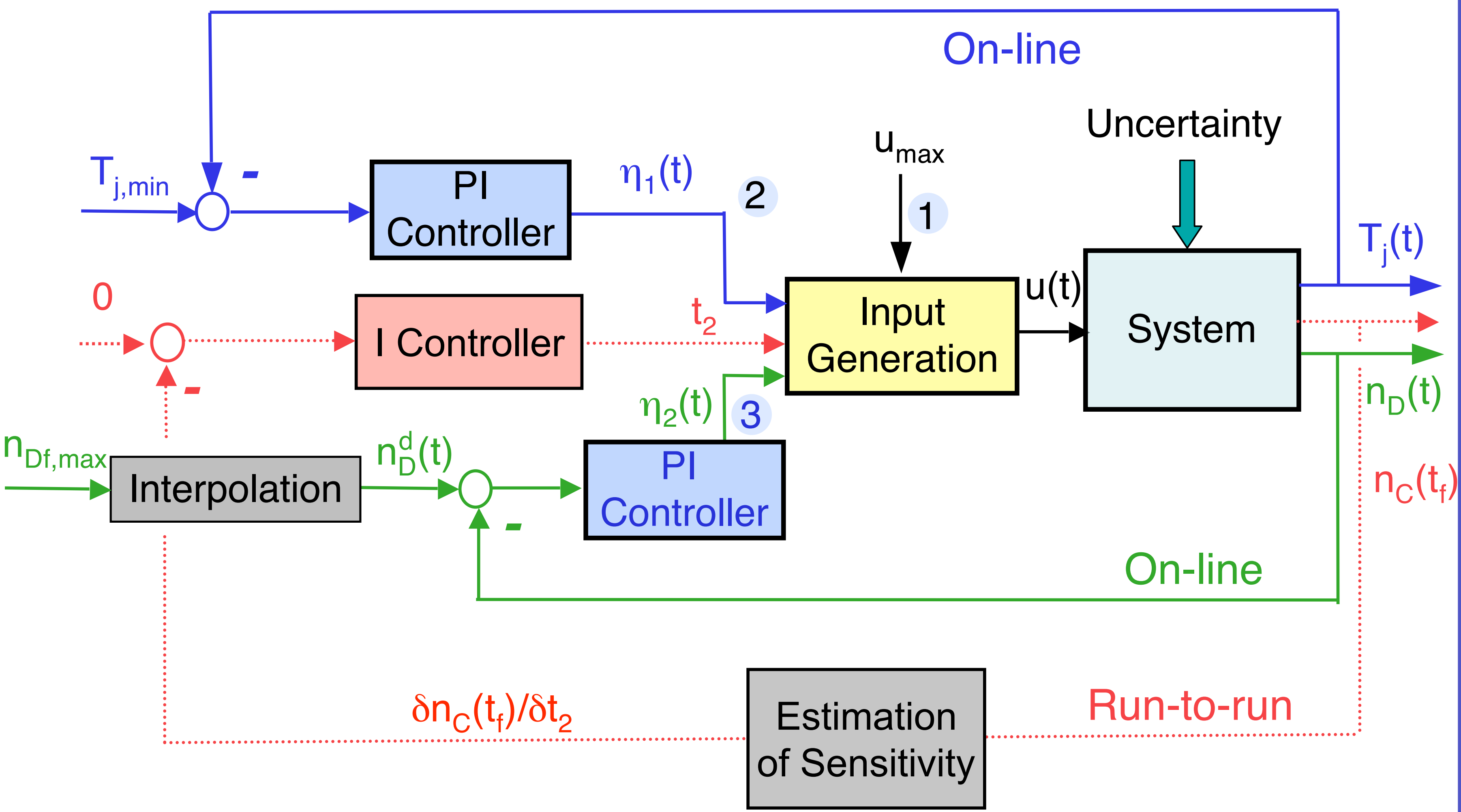
- Invariant part -- u_{max}
- Path constraints -- $T_j = T_{j,min}$ -- t_1, $\eta_1(t)$
- Terminal constraints -- $n_D(t_f) = n_{Df,max}$ -- $\eta_2(t)$
- Sensitivity -- $\partial n_C(t_f)/\partial t_2 = 0$ -- t_2

$$u = \begin{cases} u_{\max} & 0 \le t \le t_1 \\ K_\eta (T_{j,\min} - T_j) & t_1 < t \le t_2 \\ T_\eta (n_{Df,\max} - n_{Df}^{pred}(t)) & t_2 < t \le t_f \end{cases}$$

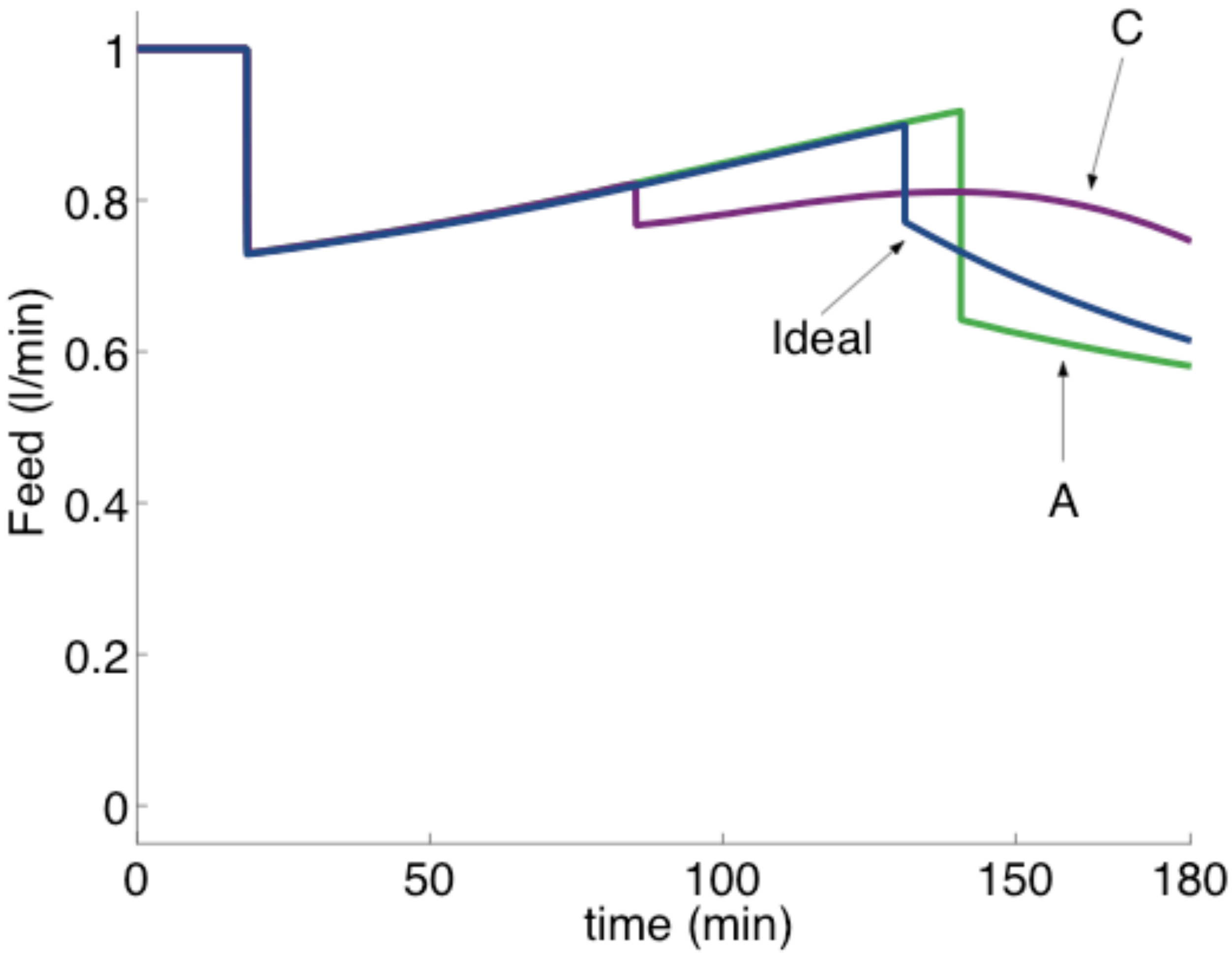
$$t_1 = t \quad with \quad T_j(t) = T_{j,\min} \quad and \quad T_j(t\_) > T_{j,\min}$$

$$t_2 = G_\pi (\partial n_C(t_f)/\partial t_2)$$

NCO-tracking Scheme for Solution Model C



NCO-tracking -- Input Profiles



NCO-tracking Results

Model and run index	Minimum jacket temperature 10 °C	Maximal final amount of D 100 mol	Final amount of C Cost (mol)
A 1	10.0	79.6	376.4
A 5	10.0	96.2	389.8
A 10	10.0	99.6	392.2
C 1	10.0	100	391.8
C 5	10.0	100	391.8
C 10	10.0	100	391.8

Ideal cost: 392.3

Open-loop nominal cost: 374.6

NCO Tracking in Practice

- Features of NCO tracking
  - No need of a process model for implementation
  - Need appropriate process measurements
  - Approximations can (must) be introduced in solution model
- Practical observations
  - Complexity depends on the number of inputs (not system order)
  - For many terminal-time dynamic optimization problems, the solution is often determined by the constraints of the problem
- Practical extensions
  - Measurement noise → backoff
  - Unknown active constraints → superstructure

Projects Implementing NCO Tracking

- On-line optimization
  - Semi-batch reactor with safety constraint (***Novartis Basel***; *Bayer-RWTH*)
  - Discontinuous wastewater treatment plant (*Firmenich Geneva*)
  - Fed-batch fermenter (**Bioengineering Lab EPFL**)
  - Batch distillation column (**Engineering School Fribourg**)
  - Grade transitions in polymerization (*Bayer-RWTH*; *CEPRI Thessaloniki*)
- Run-to-run optimization
  - Emulsion copolymerization reactor (***Aqua+Tech Geneva***)
  - Electro-discharge machining (***Charmilles Geneva***)
  - Batch reactive distillation column (INPT Toulouse)
  - Fed-batch fermenter (*Novozymes Denmark*)

Bold: experimental *Italics*: industrial

Conclusions

- Real-time optimization under uncertainty
  - Turn optimization problem into control problem
  - Considerable prior information goes into solution model
  - How robust is this information wrt. uncertainty ?

    → solution model must remain valid over uncertainty
  - Considerable potential for industrial applications
- Further work
  - Rigorous mathematical framework
  - Application to large-scale processes

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