Aalto University

# Process dynamics and control

## CHEM-E7190 (was E7140) | 2022

**Francesco Corona** (¬_¬)

Chemical and Metallurgical Engineering
School of Chemical Engineering

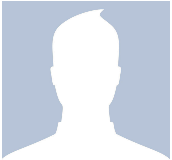
# Overview

We study the mathematical principles and basic computational tools of state-feedback and optimal control theory to manipulate the dynamic behaviour of process systems

- Understanding of feedback control
- Examples from process systems
- (Catchy image from the internet)

The approach is general with application domains in many (bio)-chemical technologies

# Overview (cont.)



**Process control and automation at Aalto University**

**Francesco Corona**

⇝ Professor of process control and automation

- Once and future chemical engineer
- Camouflaged as computer scientist

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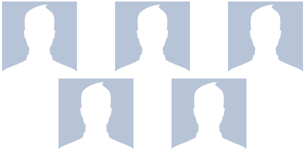
Research and teaching about **computational** and **inferential thinking** of process systems

⇝ **Automatic control and machine learning**

- **Three + one doctoral students**
- **One master's student**

⇝ Production planning and optimisation



Formal methods from automatic control, statistics, and optimisation, plus applications

# Overview (cont.)

- ⇝ Dynamic process modelling and state-space representations
- ⇝ Introduction to state-feedback and optimal control
- ⇝ Introduction to state estimation

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**Outcome 1**

- How to write and analyse a mathematical description of a process system

⇝ The model will be expressed as a set of differential equations

**Outcome 2**

- How to design/synthetise controllers to manipulate the process system

⇝ The design will be based on optimal state-feedback control

**Outcome 3**

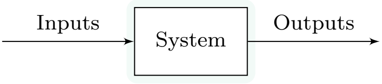
- How to design estimators to reconstruct the process state from data

⇝ The design will be based on optimal state feedback control

# Trajectory

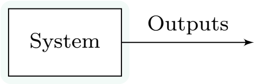
## Input-output (I/O) process modelling of process systems

- I Control variables and disturbances
- O Measurement variables, the data
- ⇝ The system evolves in time
- ⇝ (System/model/process)




## Ordinary differential equations and matrix algebra

- Force-free response (no inputs)
- Numerical integration
- ⇝ Stability



# Trajectory (cont.)

## State-space (SS) process modelling

I/O Inputs $u$, outputs $y$

S State variables $x$

System

$u(t)$ → 

$$\dot{x}(t) = f\left(x(t), u(t), t|\theta_x\right)$$
$$y(t) = g\left(x(t), u(t), t|\theta_y\right)$$

→ $y(t)$

The dynamics of the state vars are represented by some function $f$

- Function $f$ returns $\dot{x}(t)$ at time $t$, given $x(t)$, $u(t)$, and $t$

How the state vars are transformed into measurements, function $g$

- Function $g$ returns $y(t)$ at time $t$, given $x(t)$, $u(t)$, and $t$

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Functions $f$ often derived from a process modelling effort: Mass and energy balances

$$\underbrace{[\text{Stuff in}] - [\text{Stuff out}] + \backslash - [\text{Stuff generated/consumed}]}_{f(x,u,t)} = \underbrace{[\text{Stuff accumulated}]}_{\dot{x}}$$

Functions $g$ often determined by the automation system: Sensors and instruments

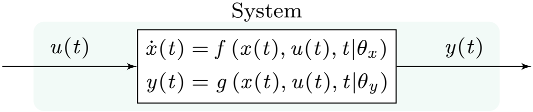
# Trajectory (cont.)

We understand dynamic systems as processes that are evolving in time and that can be represented using states that allow to determine the future behaviour of the system

I/O Controls $u$, outputs $y$

S State variables $x$

P Parameters $\theta_{x,y}$

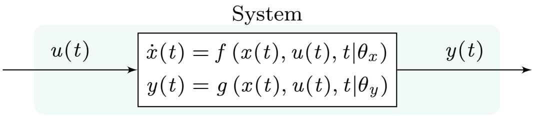



The dynamical system can be controlled by a suitable choice of inputs denoted controls

- The controls should be chosen optimally, in some sense
- They must satisfy certain constraints

This course is about methods and solutions to determine the optimal control inputs

# Trajectory (cont.)



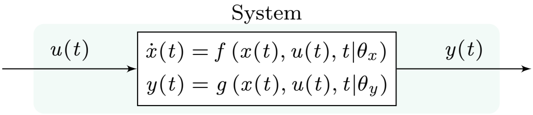

One fundamental element of dynamical systems is represented by state $x(t)$ at time $t$

- The state space $\mathcal{X}$ is the set of all possible values of the state
- It can be continuous, like the usual $\mathcal{R}^{N_x}$ or some manifold
- It can be a discrete countable set such that $|\mathcal{X}| = N_{\mathcal{X}}$
- It can be hybrid, with continuous and discrete states

The other main element of dynamical systems is represented by controls $u(t)$ at time $t$

- The control/action space $\mathcal{U}$ is the set of all possible controls
- It can be continuous, like the usual $\mathcal{R}^{N_u}$ or some manifold
- It can be a discrete countable set such that $|\mathcal{U}| = N_{\mathcal{U}}$
- It can be hybrid, with continuous and discrete actions

# Trajectory (cont.)




The dynamics of the state variables are represented by some nonlinear function $f$

- Function $f$ returns $\dot{x}(t)$ at time $t$, given $x(t)$, $u(t)$, and $t$
- Function $f$ is parameterised, the vector $\theta_x$

How the state variables are transformed into measurements, nonlinear function $g$

- Function $g$ returns $y(t)$ at time $t$, given $x(t)$, $u(t)$, and $t$
- Function $g$ is parameterised, the vector $\theta_y$

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Knowledge of the initial state $x(t_0)$ and of the control trajectory $u(t)$ over some time interval such that $t \in [t_0, T]$ allows to determine the state trajectory $x(t)$ for $t \in [t_0, T]$

- The system model with certain evolution is of the deterministic kind
- Stochastic models describe evolutions that are known statistically

# Trajectory (cont.)

In general, function $f$ and $g$ may change in time ($f$ and $g$ will change with time $t$)

- Typical of process operated under varying conditions
- Important, but we will not discuss those explicitly

We will only consider time-invariant systems,

$\rightsquigarrow$ $\dot{x}(t) = f(x(t), u(t), \not{t}|\theta_x)$

$\rightsquigarrow$ $y(t) = g(x(t), u(t), \not{t}|\theta_y)$

# Trajectory (cont.)

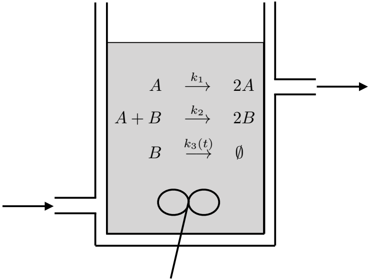
Chemical kinetics are concerned with understanding the evolution of reaction systems

- The system is specified by a set of coupled chemical reactions

The chemical kinetics induce an ordinary differential equation, a dynamical system

# Trajectory (cont.)

## Example




The Lotka-Volterra system is usually used to capture interactions between competing chemical species

$$
\begin{aligned}
A &\xrightarrow{k_1} 2A \\
A + B &\xrightarrow{k_2} 2B \\
B &\xrightarrow{k_3(t)} \emptyset
\end{aligned}
$$

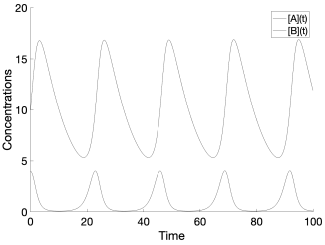
Assuming to be able directly manipulate the rate at which component $B$ is removed,

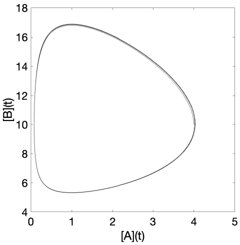
$$
\begin{bmatrix} \dfrac{d[A](t)}{dt} \\ \dfrac{d[B](t)}{dt} \end{bmatrix} = \begin{bmatrix} k_1[A](t) - k_2[A](t)[B](t) \\ k_2[A](t)[B](t) - k_3(t)[B](t) \end{bmatrix}
$$

# Trajectory (cont.)

$$\underbrace{\begin{bmatrix} \dfrac{d[A](t)}{dt} \\ \dfrac{d[B](t)}{dt} \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} k_1[A](t) - k_2[A](t)[B](t) \\ k_2[A](t)[B](t) - k_3(t)[B](t) \end{bmatrix}}_{f(x(t),u(t)|\theta_x)}$$

- State variables $x(t) = (x_1(t), x_2(t)) = ([A](t), [B](t))$
- Control variables $u(t) = u_1(t) = k_3(t)$
- Parameters $\theta_x = (k_1, k_2)$

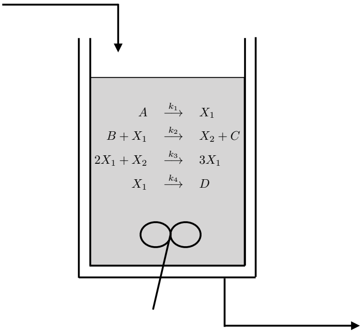



The evolution, for an initial condition $x(0) = x_0$ and sequence of inputs $u(0 \rightsquigarrow T)$ □

# Trajectory (cont.)

## Example




The Brusellator is a theoretical model for certain auto-catalytic reactions

$$
\begin{aligned}
A &\xrightarrow{k_1} X_1 \\
B + X_1 &\xrightarrow{k_2} X_2 + C \\
2X_1 + X_2 &\xrightarrow{k_3} 3X_1 \\
X_1 &\xrightarrow{k_4} D
\end{aligned}
$$

The reaction components $(X_1, X_2)$ are a pair of intermediate state variables

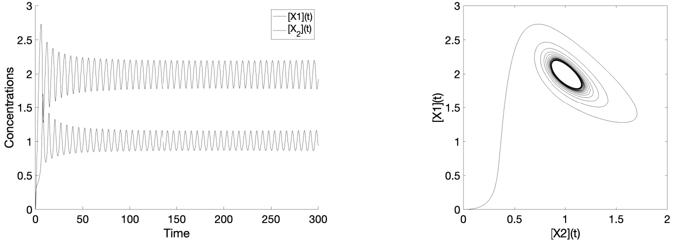
Assuming that the concentration species $A$ and $B$ (and $C$ and $D$) can be manipulated

$$
\begin{bmatrix} \dfrac{d[X_1](t)}{dt} \\ \dfrac{d[X_2](t)}{dt} \end{bmatrix} = \begin{bmatrix} a(t) - b(t)[X_1](t) + [X_1]^2(t)[X_2](t) - [X_1](t) \\ b(t)[X_1](t) - [X_1]^2(t)[X_2](t) \end{bmatrix}
$$

# Trajectory (cont.)

$$\underbrace{\begin{bmatrix} \frac{d[X_1](t)}{dt} \\ \frac{d[X_2](t)}{dt} \end{bmatrix}}_{\dot{x}(t)} = \underbrace{\begin{bmatrix} a(t) - b(t)[X_1](t) + [X_1]^2(t)[X_2](t) - [X_1](t) \\ b(t)[X_1](t) - [X_1]^2(t)[X_2](t) \end{bmatrix}}_{f(x(t),u(t)|\theta_x)}$$

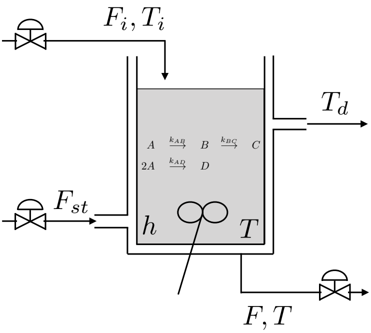
- State variables $x(t) = (x_1(t), x_2(t)) = ([X_1](t), [X_2](t))$
- Control variables $u(t) = (u_1(t), u_2(t)) = (a(t), b(t))$
- Parameters $\theta_x = (k_1, k_2, k_3, k_4)$




The evolution, for an initial condition $x(0) = x_0$ and sequence of inputs $u(0 \rightsquigarrow T)$ □

# Trajectory | System dynamics (cont.)

## Example




$$A \xrightarrow{k_{AB}} B \xrightarrow{k_{BC}} C$$
$$2A \xrightarrow{k_{AD}} D$$

A non-isothermal CSTR (Van de Vusse)

$$\frac{d\rho_A}{dt} = q\left(\rho_{\text{in}}^{(A)} - \rho_A\right) - \left(k_{AB}(T)\rho_A + k_{AD}(T)\rho_A^2\right)$$

$$\frac{d\rho_B}{dt} = -q\rho_B + k_{AB}(T)\rho_A - k_{BC}(T)\rho_B$$

$$\frac{dT}{dt} = q\left(T_{\text{in}} - T\right) + \frac{k_W A_r}{\varrho C_p V_r}(T_d - T) - \frac{1}{\varrho C_p}\left(k_{AB}(T)\rho_A \Delta H_{AB} + k_{BC}\rho_B \Delta H_{BC} + k_{AB}(T)\rho_A^2 \Delta H_{AC}\right)$$

$$\frac{dT_d}{dt} = \frac{1}{m_K C_{pK}} Q + \frac{k_W A_r}{m_K C_{pK}}(T - T_d)$$

□

# Trajectory (cont.)

By definition, the system/model itself is an approximation of the true/real process

$\rightsquigarrow$ We will often need to accept even additional approximations

- Oftentimes, this is a necessary step to be able to proceed
- Otherwise, the mathematics would be too complicated

# Trajectory (cont.)

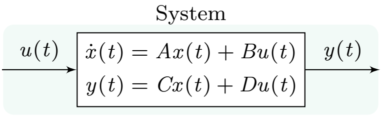
### Approximated process dynamics (linear and time-invariant)

- Function $f$ becomes two matrices

$$f(x(t), u(t)) \approx Ax(t) + Bu(t)$$

- Function $g$ becomes two matrices

$$g(x(t), u(t)) \approx Cx(t) + Du(t)$$

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### Linearisation of nonlinearities around steady-states

⇝ First-order Taylor approximations

⇝ The work-horse of modernity

⇝ Leading tech, since 1700's

# Trajectory (cont.)

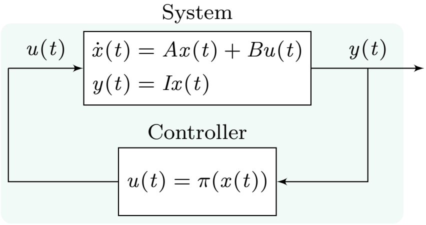
## From (approximated, linear) process dynamics to state-feedback control

We will make some initial assumptions

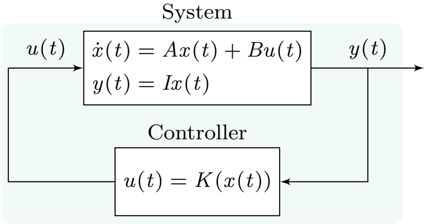
- We can measure the states $x(t)$
- We define control actions $u(t)$

⇝ The (static) controller, $\pi$

⇝ Controllability




## State-feedback optimal control (again linear dynamics, plus quadratic costs)




We introduce performance measures

- Control accuracy

$$\left\| x(t) - x_{\text{target}} \right\|_Q^2$$

- Control effort

$$\left\| u(t) - u_{\text{reference}} \right\|_R^2$$

# Trajectory (cont.)

## Optimal state-feedback, estimation, and control (again, linear and quadratic)

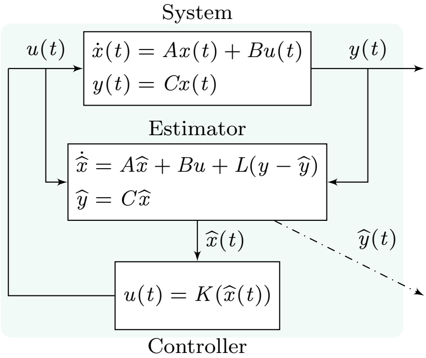
We will relax some initial assumptions

- Cannot measure the states $x(t)$
- Must estimate them, from data

⇝ The estimator, $\varphi$

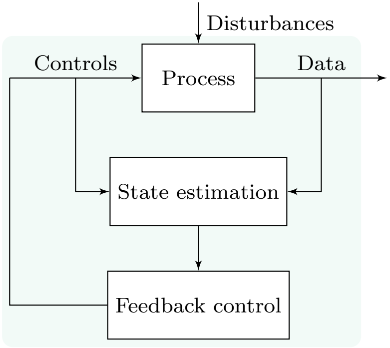
⇝ Observability

We then define control actions, $u(t)$



# Trajectory (cont.)

## Optimal state-feedback, estimation, and control (the general framework)




A general structure, each block can be treated using different technologies

- First-principles (physics)
- Empirical (data-derived)

It scales (it can be solved) reasonably well with the process size (complexity)

**Process control** is a field about methods for sensing, learning, reasoning, and actuating

# Trajectory (cont.)

**Sensing**, ‘observing, getting measurements’
**Learning**, ‘making statistical inferences’
**Reasoning**, ‘making optimal decisions’
**Actuating**, ‘implementing decisions’

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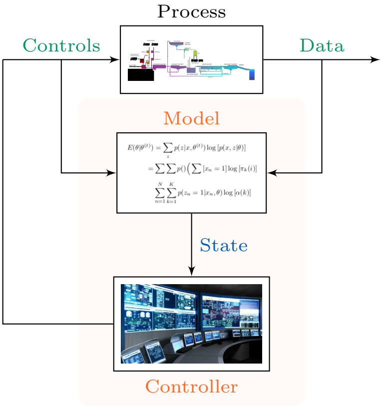
**Process control** is applied **automatic control**, **optimisation**, and **statistics** to **(bio-)chem eng**




Key factor is that the approach needs be automatic, interpretable, general and efficient

- Full-scale industrial and environmental systems (that is, constraints)

# Why should I care? An example: Control4Reuse

Present wastewater treatment technologies are designed to produce a disposable WW

- Discharged wastewater is expected to be poor in solids and nutrients
- Low carbon (C), nitrogen (N) and phosphorus (P) concentration

Increasing water scarcity requires us to reuse treated WW, a non conventional resource

- At present there exists no standardised solution for urban WWTPs that explicitly aim at delivering a treated wastewater that fulfils the requirements for reuse
- ⇝ In agriculture, high N and P contents and absence of micro-pollutants, pathogens and antibiotic resistant bacteria (ARB), and antibiotic resistance genes (ARG)

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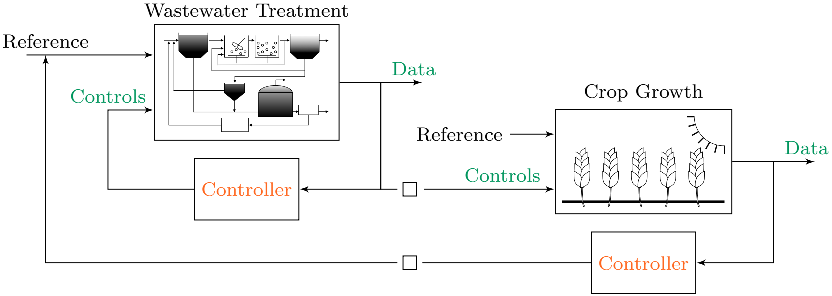
Most of water withdrawal goes to agriculture

**Can we operate a large-scale WWTP to produce reuse water of different grades, on demand?**

Wastewater not as a waste but as a resource

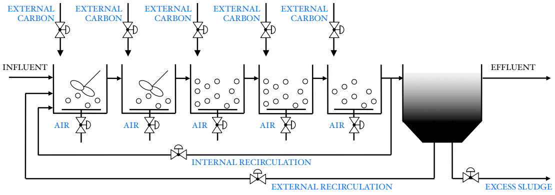
Water JPI

# Control4Reuse (cont.)

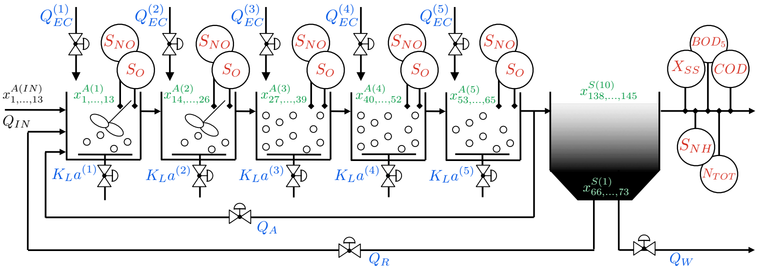



## Benchmark Simulation Model no. 1 (BSM1)

- 5 bio-reactors (ASMs)
- 1 settler (TAKACS')



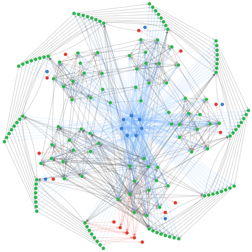
# Control4Reuse (cont.)




Analysis of the dynamics and control flexibility of activated sludge plants

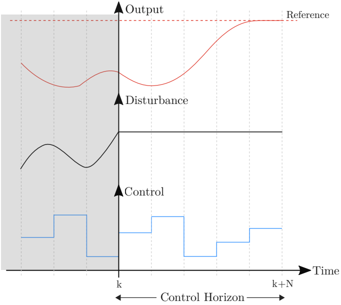
- ⇝ **Full-state controllability**
- ⇝ **Full-state observability**
- ⇝ **Online optimal control**

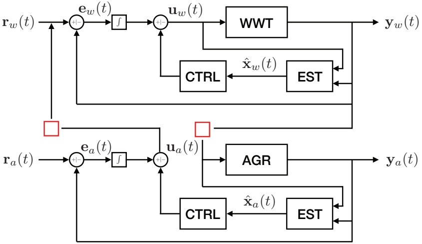
Neto et al. in ECC + IFAC (2020), ADCHEM (2021), DYCOPS + JPC (2022)



# Control4Reuse (cont.)

- ASPs are controllable but unobservable, in a structural sense
- ASPs are uncontrollable and unobservable in a classical sense




- A cascade of optimal controllers

There will be a guest seminar on how to control wastewater treatment plants for reuse

# Overview

CHEM-E7190 is a set of **lectures (approx. 24h)** and **exercises (approx. 24h)**

⇝ The objective is to provide a modern view on process control

**To pass CHEM-E7190 you must pass the exam (65% of the total points)**

**The remaining points (35%) can be collected from the exercises**

*We encourage you to collaborate in figuring out answers and help others solve the problems, yet we ask you to submit your work individually and to explicitly acknowledge those with whom you collaborated. We are assuming that you take the responsibility to make sure you personally understand the solution to work arising from collaboration*