Robustness and Stability Optimization

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based on joint work with
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Joris Gillis (KU Leuven) and Greg Horn

Outline of the Talk

- Motivating Example: Control of Batch Reactors
- Robustification by Linearization
- Lyapunov Differential Equations
- (L-Infinity bounded uncertainty)
- Periodic Orbits for Power Generating Kites
- Open-Loop Stability Optimization

Control of Exothermic Batch Reactors

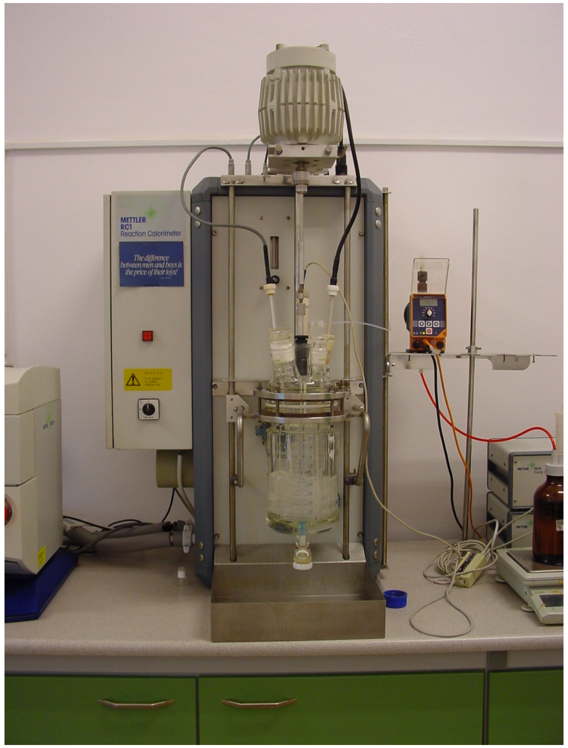
work with ***Peter Kühl*** (now BASF), H.G. Bock (Heidelberg) and ***A. Milewska***, E. Molga (Warsaw)

WARSAW UNIVERSITY OF TECHNOLOGY

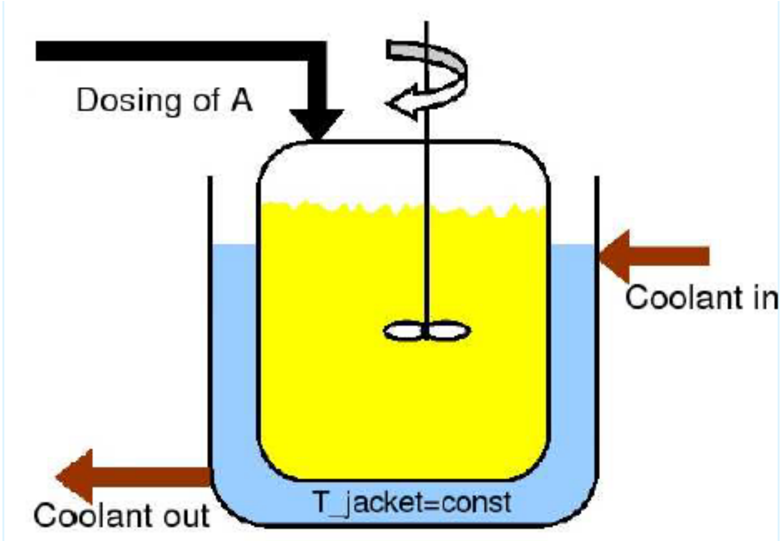
Batch Reactor in Warsaw [Peter Kuehl, Aleksandra Milewska]

Esterification of 2-Butanol (B) by propionic anhydride (A): exothermic reaction, fed-batch reactor with cooling jacket

Aim: complete conversion of B, ***avoid explosion!***



Control: dosing rate of A

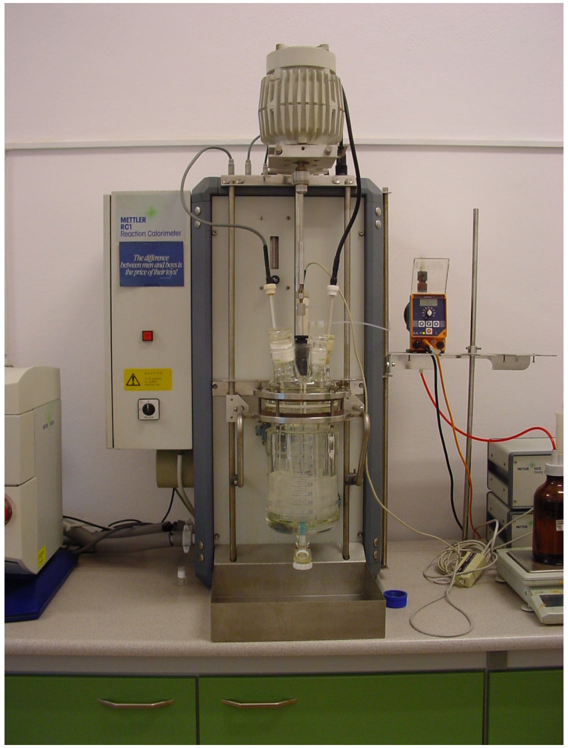


$$A + B \xrightarrow{K} C + D$$

Differential (Algebraic) Equation Model

$$
\begin{aligned}
\dot{n}_A &= u - r\,V \\
\dot{n}_B &= -r\,V \\
\dot{n}_C &= r\,V
\end{aligned}
$$

$$
\begin{aligned}
(C_{p,I} + C_p)\,\dot{T}_R = {} & r\,H\,V - q_{\text{dil}} - U\,\Omega\,(T_R - T_J) \\
& -\alpha(T_R - T_a) - u\,cp_A\,(T_R - T_d),
\end{aligned}
\qquad (1)
$$



$$
\begin{aligned}
\rho_i &= 1000\,M_i \left(P_i\, Q_i^{\left(1-\left(\frac{T_R}{T_{c,i}}\right)^G\right)} \right)^{-1}, \quad i = A, B, C, D \\
cp_i &= a_i + b_i T_R + c_i T_R^2 + d_i T_R^3, \quad i = A, B, C, D \\
C_p &= \sum_{i=A,B,C,D} cp_i n_i \\
C_{p,I} &= C_{p,I1} + \frac{C_{p,I2} - C_{p,I1}}{V_2 - V_1}(V - V_1) \\
V &= 1000 \left(\frac{n_A M_A}{\rho_A} + \frac{n_B M_B}{\rho_B} + \frac{n_C M_C}{\rho_C} + \frac{n_C M_D}{\rho_D} \right) \\
\Omega &= \Omega_{\min} + 4\frac{V - V_{\min}}{1000 d}
\end{aligned}
\qquad (2)
$$

Dynamic Optimization Problem for Batch Reactor

Constrained optimal control problem:

$$
\begin{aligned}
\min_{u} \quad & \int_0^{t_f} n_B(\tau)^2 \, d\tau \\
\text{subject to} \quad & (1),\ (2) \\
& 0 \text{ mol/s} \leq u(t) \leq 0.005 \text{ mol/s} \\
& \int_{t_0=0}^{t_f} u(\tau)\, d\tau = 6.89396 \text{ mol} \\
& T_R(t) \leq 343.15 \text{ K} \\
& S(t) \leq 363.15 \text{ K},
\end{aligned}
$$

$$
S(t) = T_R(t) + \min(n_A, n_B) \frac{H_A}{\rho c_p V}
$$

minimize remaining B

subject to dosing rate and temperature constraints

→

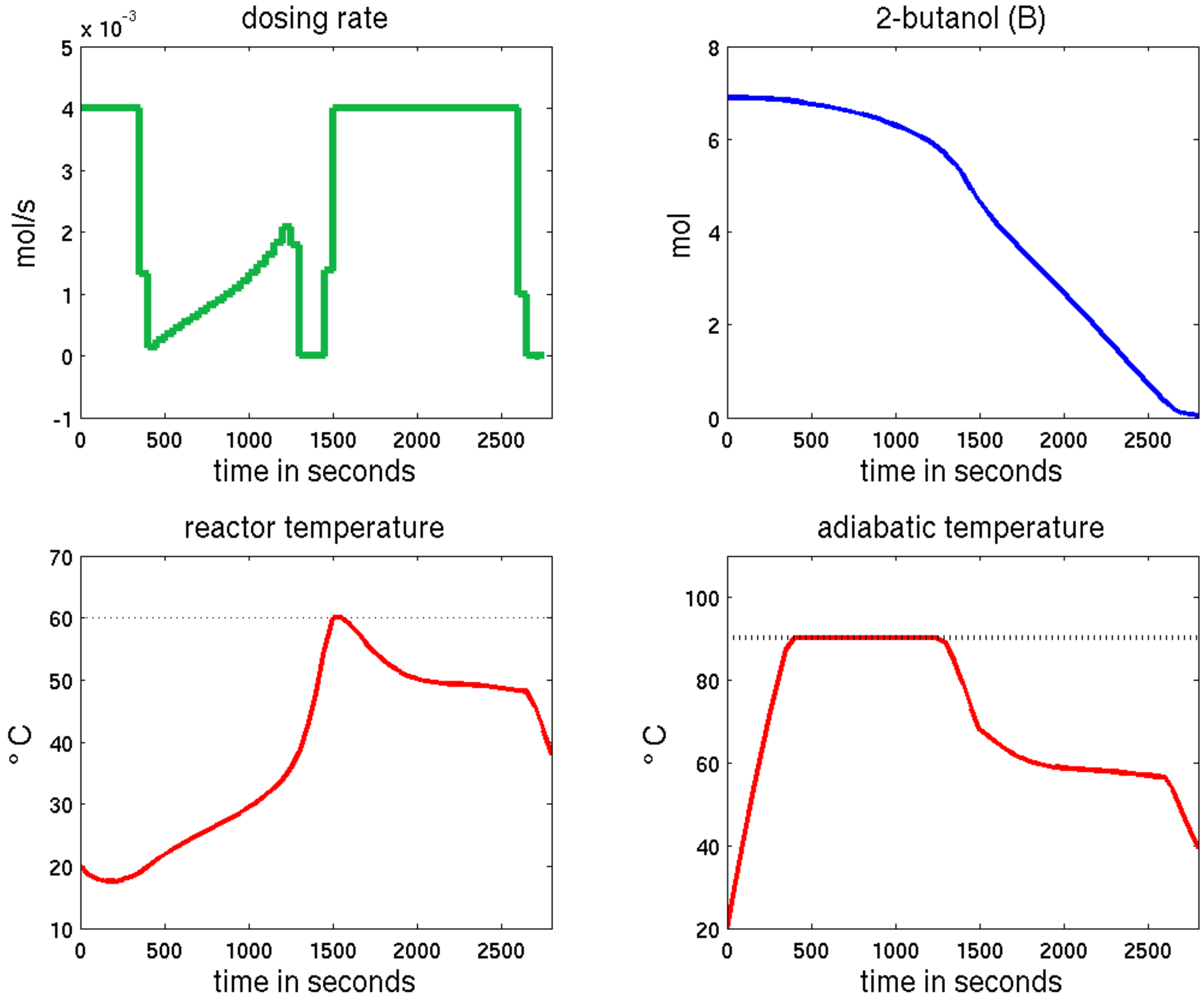
Generic optimal control problem:

$$
\underset{x(\cdot),u(\cdot)}{\text{minimize}} \quad \int_0^T L(x(t),u(t))\,dt \; + \; E\,(x(T))
$$

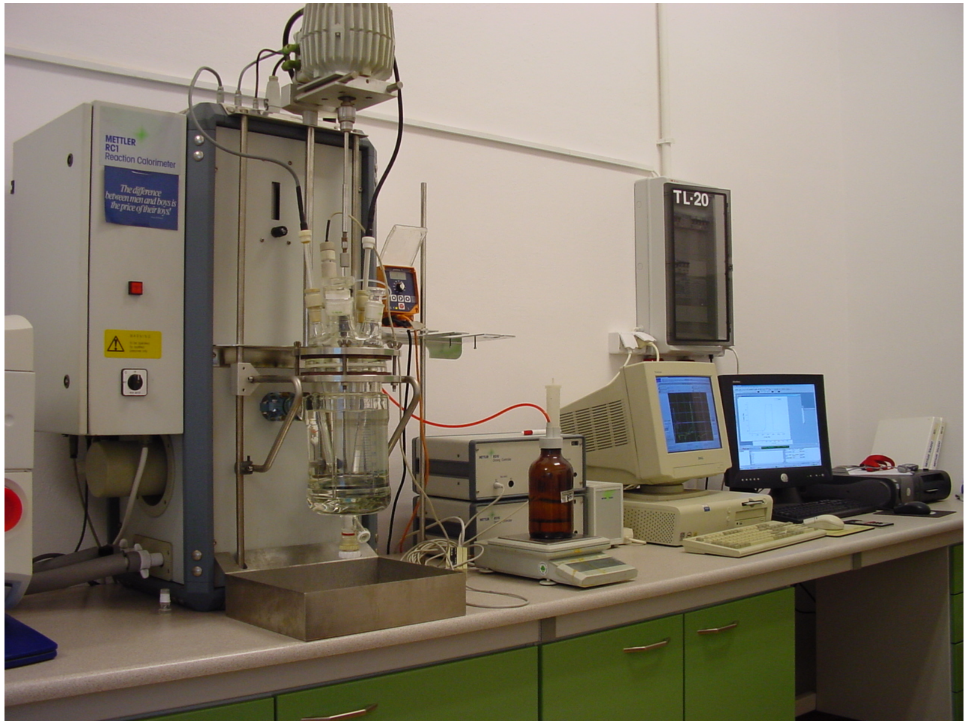
subject to

$$
\begin{aligned}
x(0) - x_0 &= 0, & \\
\dot{x}(t) - f(x(t),u(t)) &= 0, & t \in [0,T], \\
h(x(t),u(t)) &\geq 0, & t \in [0,T], \\
r\,(x(T)) &\geq 0 &
\end{aligned}
$$

Solution of Peter's Batch Reactor Problem

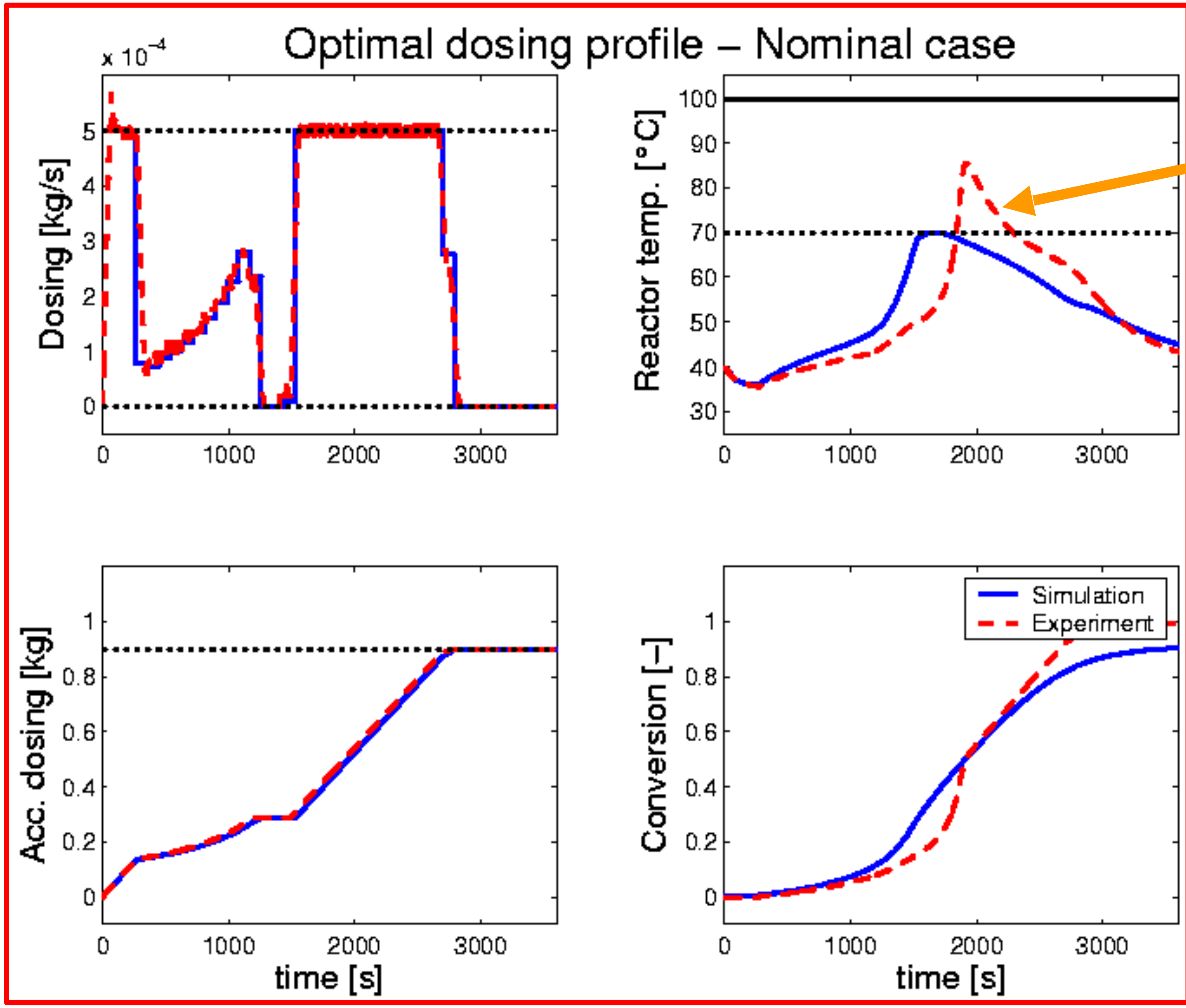


Experimental Results for Batch Reactor



- Mettler-Toledo test reactor R1
- batch time: 1 h
- end volume: ca. 2 l

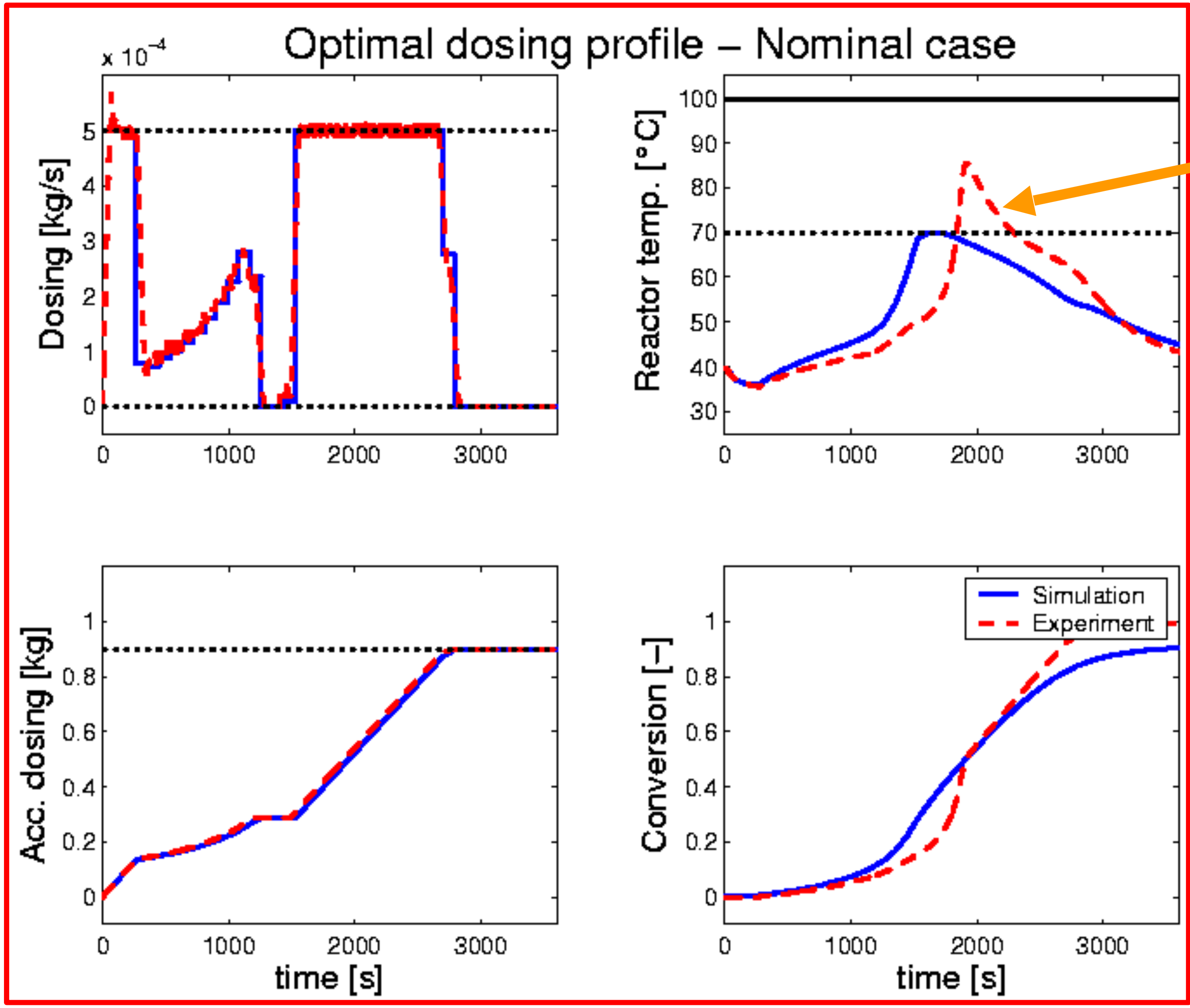
Experimental Results for Batch Reactor (Red)



large model plant mismatch

Safety critical!

Experimental Results for Batch Reactor (Red)



large model plant mismatch

Safety critical!

How can we make Peter 's and Aleksandra's work safer?

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Robust Optimization Framework [Ben-Tal & Nemirovski]

- Uncertain Nonlinear Program (NLP) with controls u, uncertain parameter p, and "states" x (determined by model $g(x,u,p)$)

$$\min_{x\in\mathbb{R}^{n_x}, u\in\mathbb{R}^{n_u}} \quad f_0(x,u) \quad \text{s.t.} \quad \begin{cases} f_i(x,u) \leq 0 & \text{for} \quad i=1,\ldots,n_f, \\ g_j(x,u,p) = 0 & \text{for} \quad j=1,\ldots,n_x. \end{cases}$$

- Idea: let "adverse player" (nature) select p and x, define worst-case constraints and objective:

$$\phi_i(u) \quad := \quad \max_{x\in\mathbb{R}^{n_x}, p\in\mathbb{R}^{n_p}} \quad f_i(x,u) \quad \text{s.t.} \quad \begin{cases} g(x,u,p) = 0, \\ \|p - \bar{p}\| \leq 1. \end{cases}$$

- Formulate "Robust Counterpart" (bi-level problem):

$$\text{(RC)} \qquad \min_{u\in\mathbb{R}^{n_u}} \quad \phi_0(u) \quad \text{s.t.} \quad \phi_i(u) \leq 0 \quad \text{for} \quad i=1,\ldots,n_f.$$

Difficult to tackle numerically for general NLPs!

One Remedy: Linearization of Worst Case

- Approximate worst case by linearization [Nagy et. al '03, D., Bock, Kostina,'06]:

$$\begin{aligned}\tilde{\phi}_i(u) \quad := \quad & \max_{\Delta x \in \mathbb{R}^{n_x}, \Delta p \in \mathbb{R}^{n_p}} \quad f_i(\bar{x}, u) + \frac{\partial f_i}{\partial x}(\bar{x}, u)\Delta x, \\ & \text{s.t.} \qquad \tfrac{\partial g}{\partial x}(\bar{x}, u, \bar{p})\Delta x + \tfrac{\partial g}{\partial p}(\bar{x}, u, \bar{p})\Delta p = 0, \\ & \qquad\qquad\qquad\qquad\qquad\qquad \|\Delta p\| \leq 1.\end{aligned}$$

- Analytical solution (using dual norm):

$$\tilde{\phi}_i(u) = f_i(\bar{x}, u) + \left\| - \left(\frac{\partial g}{\partial p}(\bar{x}, u, \bar{p}) \right)^T \left(\frac{\partial g}{\partial x}(\bar{x}, u, \bar{p}) \right)^{-T} \left(\frac{\partial f_i}{\partial x}(\bar{x}, u) \right)^T \right\|_*$$

One of first papers proposing ODE linearization

Robust Nonlinear Model Predictive Control of Batch Processes

Zoltan K. Nagy
Dept. of Chemical Engineering, "Babes-Bolyai" University of Cluj, 3400, Cluj-Napoca, Romania

Richard D. Braatz
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1776 July 2003 Vol. 49, No. 7 AIChE Journal

Approximated Robust Counterpart

$$\min_{u \in \mathbb{R}^{n_u},\, \bar{x} \in \mathbb{R}^{n_x}} \; f_0(\bar{x}, u) + \left\| \left(\frac{\partial g}{\partial p}\right)^T \left(\frac{\partial g}{\partial x}\right)^{-T} \left(\frac{\partial f_0}{\partial x}\right)^T \right\|_*$$

$$\text{(ARC)} \qquad \text{s.t.} \quad f_i(\bar{x}, u) + \left\| \left(\frac{\partial g}{\partial p}\right)^T \left(\frac{\partial g}{\partial x}\right)^{-T} \left(\frac{\partial f_i}{\partial x}\right)^T \right\|_* \le 0$$

Intelligent safety margins
(influenced by controls)

$$i = 1, \ldots, n_f,$$

$$\text{and} \qquad g(\bar{x}, u, \bar{p}) = 0.$$

- Can be formulated in two sparsity exploiting variants:
  A) Forward derivatives
  B) Adjoint derivatives

  …or in infinite dimensional setting: Lyapunov Differential Equations

A) Forward Derivative Robust Counterpart

$$
\text{(ARC-D)} \quad
\begin{aligned}
\min_{u\in\mathbb{R}^{nu},\, x\in\mathbb{R}^{nx},\, D\in\mathbb{R}^{nx\times np}} \quad & f_0(x,u) + \left\| D^T \left(\frac{\partial f_0}{\partial x}(x,u) \right)^T \right\|_* \\
\text{s.t.} \quad & f_i(x,u) + \left\| D^T \left(\frac{\partial f_i}{\partial x}(x,u) \right)^T \right\|_* \leq 0, \\
& \qquad\qquad\qquad\qquad\qquad\qquad i = 1, \ldots \\
& g(x,u,\bar{p}) = 0, \\
\text{and} \quad & \frac{\partial g}{\partial x}(x,u,\bar{p})\, D + \frac{\partial g}{\partial p}(x,u,\bar{p}) = 0.
\end{aligned}
$$

- Best if **more constraints** than uncertain parameters

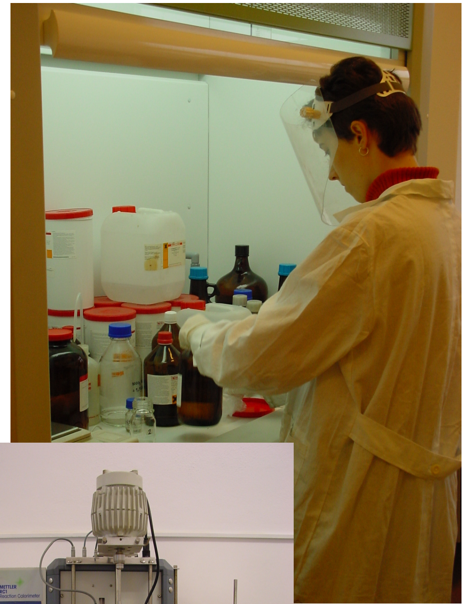
B) Adjoint Derivative Robust Counterpart [D. et al '06]::

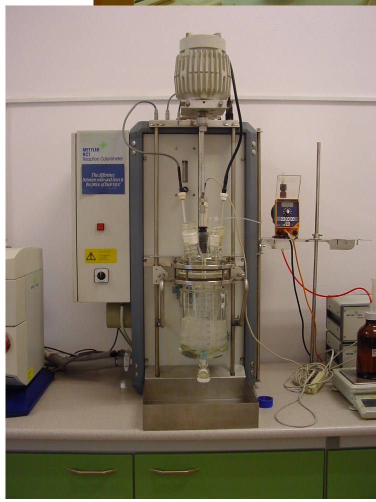
$$
\text{(ARC-A)} \quad
\begin{aligned}
\min_{u\in\mathbb{R}^{n_u},\, x\in\mathbb{R}^{n_x},\, \Lambda\in\mathbb{R}^{n_x\times(1+n_f)}} \quad & f_0(x,u) + \left\| \left(\frac{\partial g}{\partial p}(x,u,p) \right)^T \lambda_0 \right\|_* \\
\text{s.t.} \quad & f_i(x,u) + \left\| \left(\frac{\partial g}{\partial p}(x,u,p) \right)^T \lambda_i \right\|_* \leq 0 \\
& \qquad\qquad\qquad\qquad i = 1, \ldots \\
& \qquad\qquad g(x,u,\bar{p}) = 0, \\
\text{and} \quad & \left(\frac{\partial g}{\partial x}(x,u,\bar{p}) \right)^T \Lambda + \left(\frac{\partial f}{\partial x}(x,u) \right)^T = 0.
\end{aligned}
$$

- Best if **more uncertain parameters** than constraints

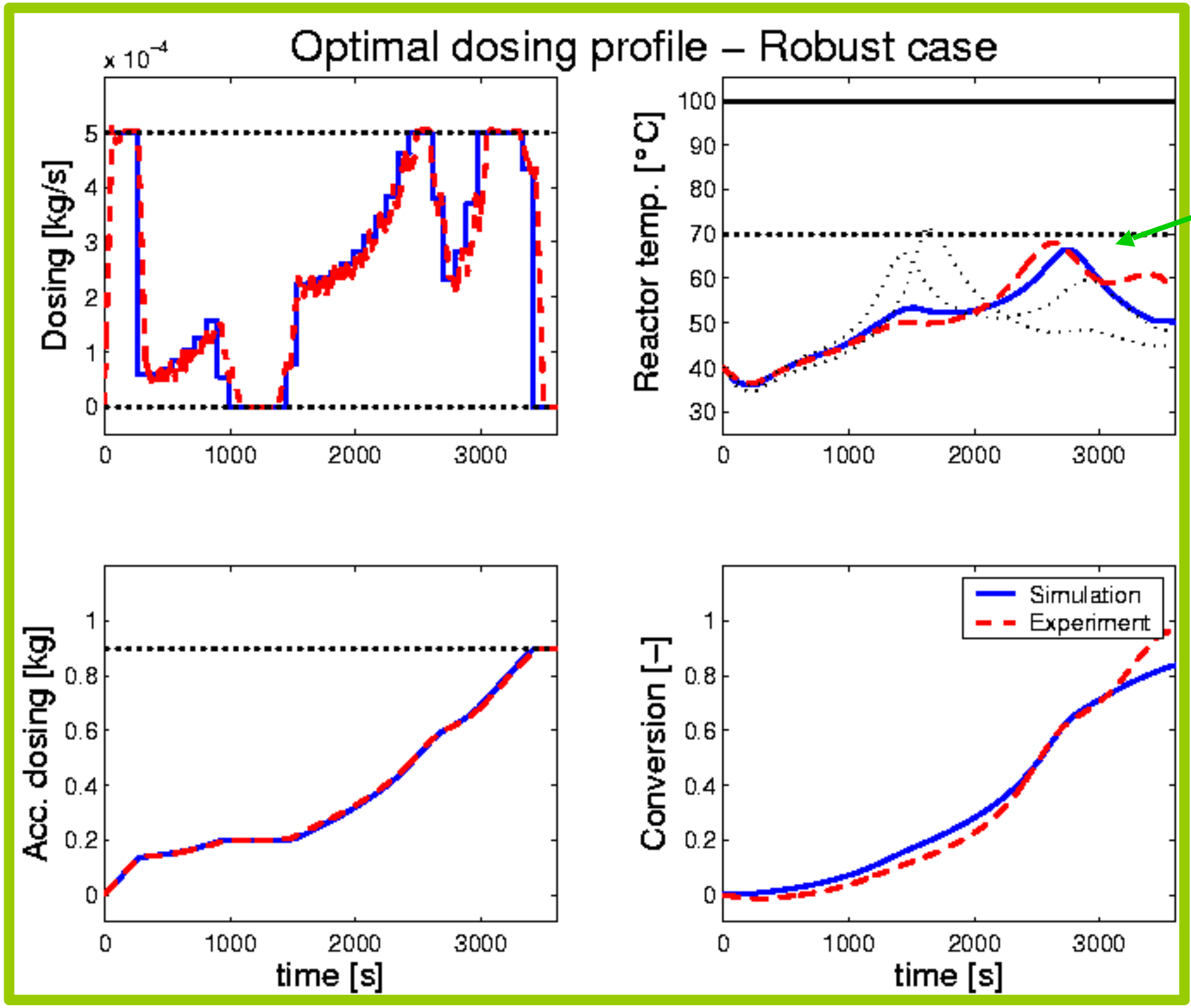
Estimated Parameter Uncertainties for Test Reactor

	Standard deviation
T_{jacket}	0.3 K
$m_{catalyst}$	0.5 g (~10 %)
U_A	10.0 $W/(m^2\,K)$ (~10 %)
u_{offset}	5.0 10^{-5} kg/s (~10 % of upper bound)



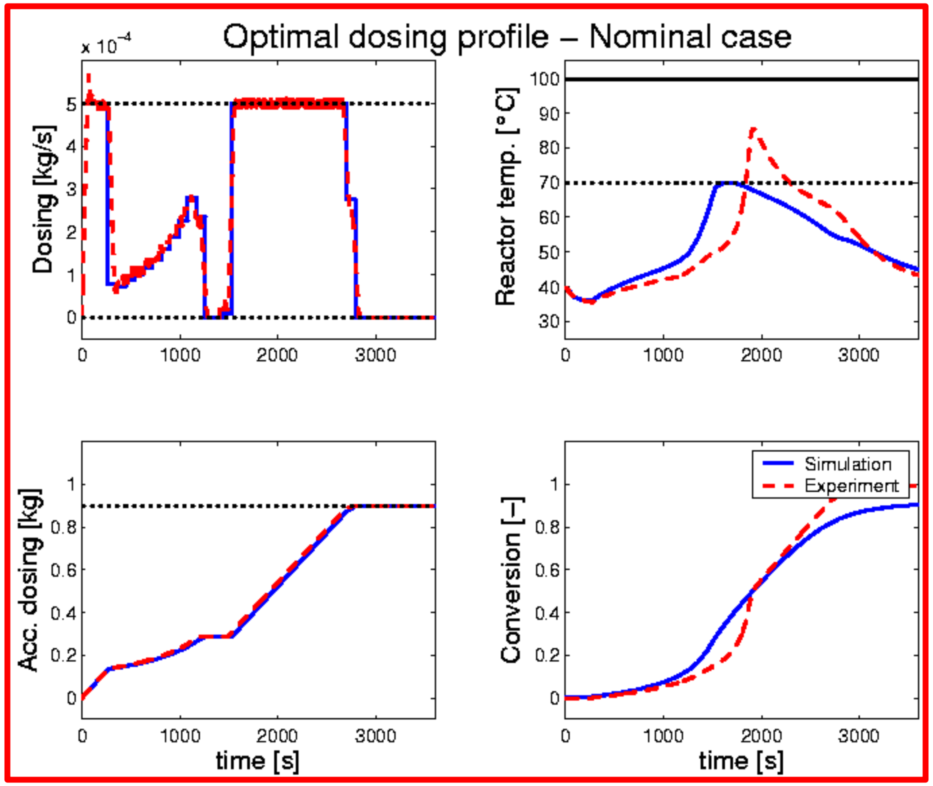


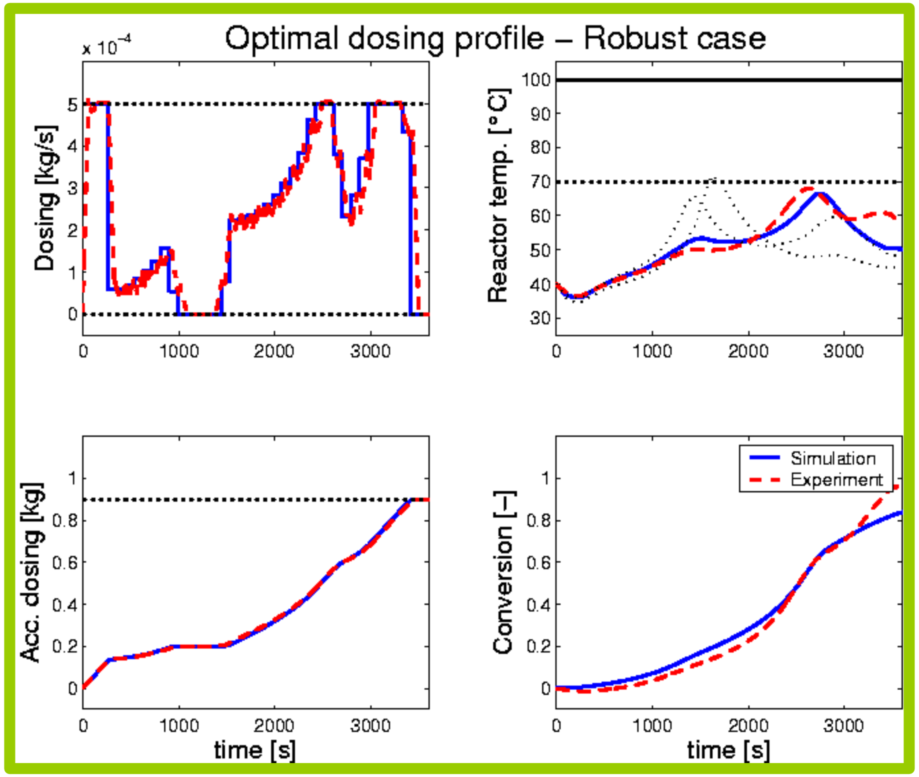
Robust Optimization Result and Experimental Test



Safety margin

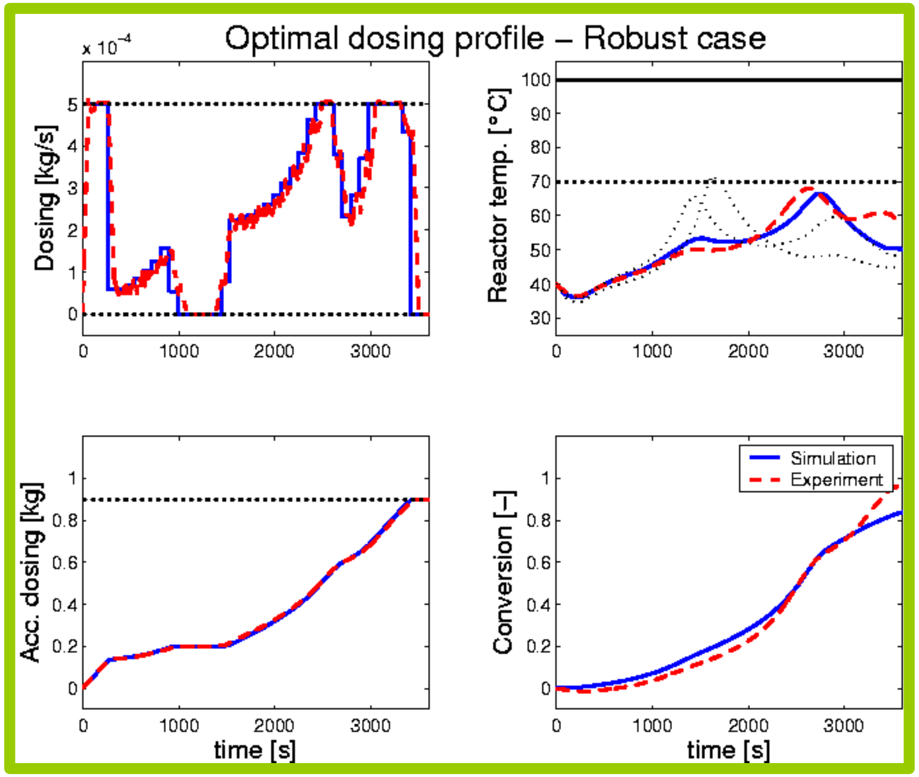
Comparison Nominal and Robust Optimization





Different solution structure. Model plant mismatch and runaway risk considerably reduced. Complete conversion.

Comparison Nominal and Robust Optimization



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Robust Counterpart for Noisy Dynamic Systems

Noisy dynamic systems suffer from “double curse of infinity”:

- infinitely many uncertain parameters (noise w acting on dynamics)
- infinitely many constraints (path constraints)

What to do ?

In linear approximation (and without controls), regard

$$\begin{aligned} \dot{x}(t) &= A(t)x(t) + B(t)w(t) \\ y(t) &= C(t)x(t) \\ x(0) &= B_0 w_0 \end{aligned}$$

with constraints for all i and t: $$y_i(t) \leq 1$$

Assumption:

function space bound $\|\omega\|_W \leq 1$ **on noise** $\omega := (w_0, w(\cdot))$

Easy Case: L2 Bounded Uncertainty [Houska & D. 2007]

- Assume L2 bound $\mathscr{B} := \{\omega \in L_2 \mid \|\omega\|_W \leq 1\}$ on uncertainty,

  based on L2 scalar product

$$
\begin{aligned}
\langle \omega_1 \mid \omega_2 \rangle_W &:= w_{0,1}^T w_{0,2} + \int_0^T w_1(\tau)^T w_2(\tau)\,\mathrm{d}\tau \\
\|\omega_1\|_W &:= \sqrt{\langle \omega_1, \omega_1 \rangle_W}
\end{aligned}
$$

- Note: for L2 Norm, reachable uncertainty sets are also ellipsoids!

- Can easily show that $\max\limits_{\omega \in \mathscr{B}} y_i(t) = \sqrt{C_i(t)P(t)C_i(t)^T}$,

  with P solution of **Lyapunov Differential Equation**

$$
\boxed{
\begin{aligned}
\dot{P}(t) &= A(t)P(t) + P(t)A(t)^T + B(t)B(t)^T \\
P(0) &= B_0 B_0^T
\end{aligned}
}
$$

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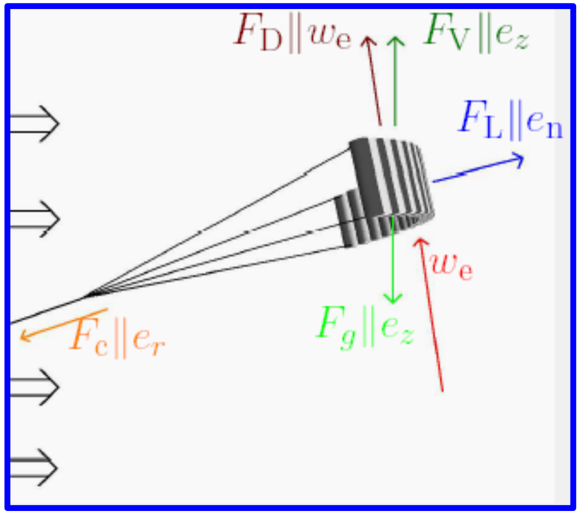
Power Kite Model (with B. Houska)

Includes cable elasticity



forces at kite
(here: 500 m²)

ODE Model with 12 states and 3 controls

- Differential states:
  $x := (r_0\,,\, r\,,\, \phi\,,\, \theta\,,\, \dot{r}_0\,,\, \dot{r}\,,\, \dot{\phi}\,,\, \dot{\theta}\,,\, n\,,\, \Psi\,,\, C_L\,,\, W\,)^T$
- Controls: $u := (\ddot{r}_0\,,\, \dot{\Psi}\,,\, \dot{C}_L)^T$

Control inputs:

- line length
- roll angle (as for toy kites)
- lift coefficient (pitch angle)

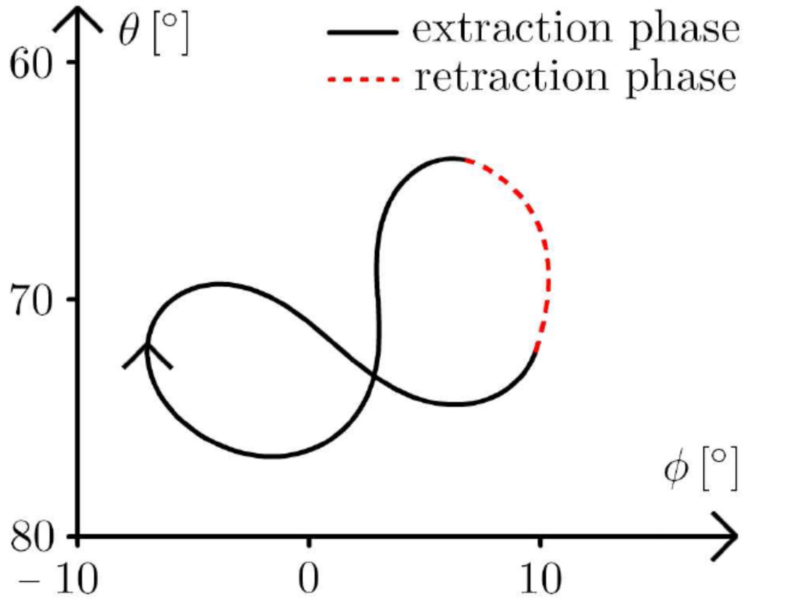
Solution of Periodic Optimization Problem

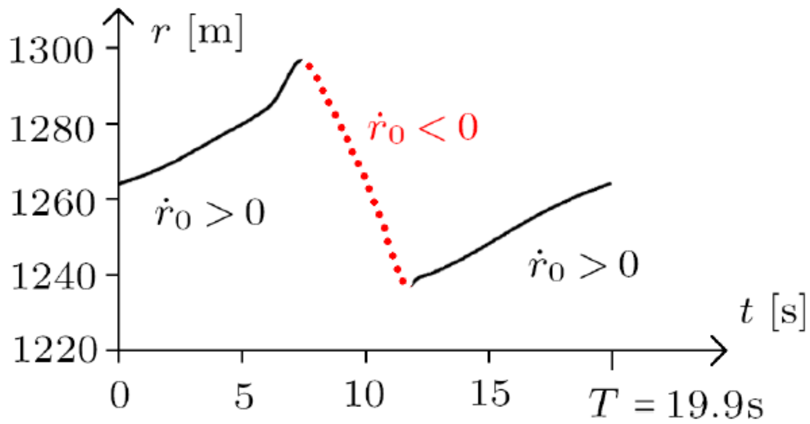
Maximize mean power production:

$$\overline{P} := \frac{1}{T} W(T) := \frac{1}{T} \int_0^T F_c \dot{r}_0 dt$$

by varying line thickness, period duration, controls, subject to periodicity and other constraints:

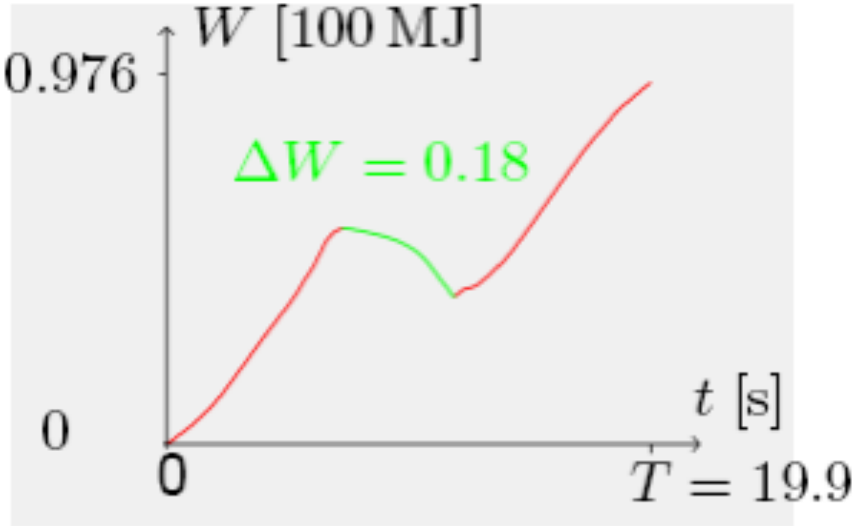
$$\begin{array}{ll} \underset{x(\cdot),u(\cdot),d_c,T}{\text{maximize}} & \overline{P}(x(T),T) \\ \text{subject to:} & \\ \forall t \in [0,T]: & \dot{x}(t) = f(x(t),u(t),d_c) \\ \forall t \in [0,T]: & 0 \succcurlyeq \eta(x(t),u(t),d_c) \\ & 0 = \chi(x(0),x(T)) \end{array}$$

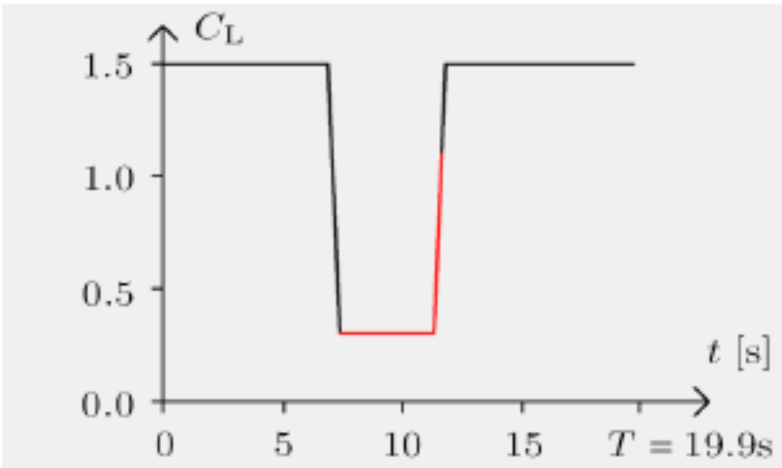




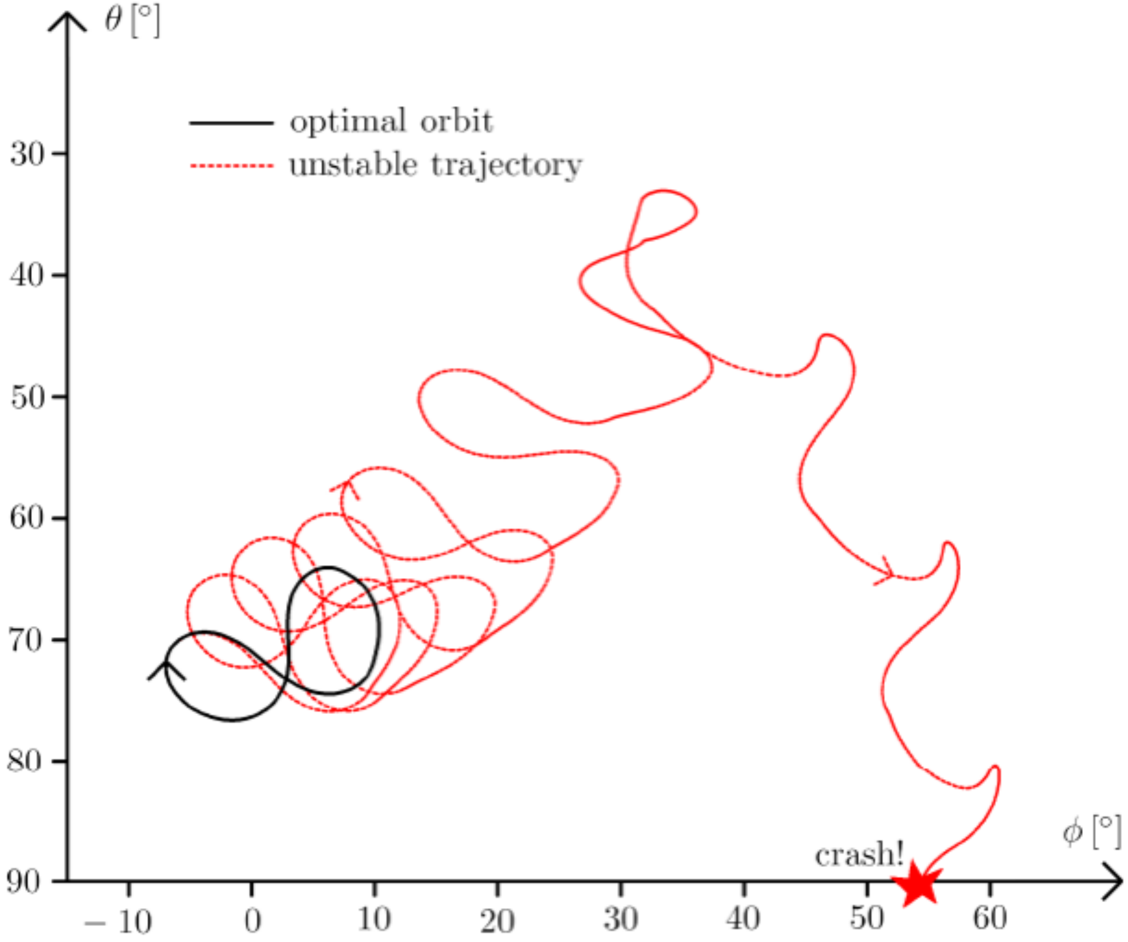
Cable length 1.3km, thickness 7 cm

Periodic Orbit: 5 MW mean power production





Problem: kite orbits unstable. What to do?



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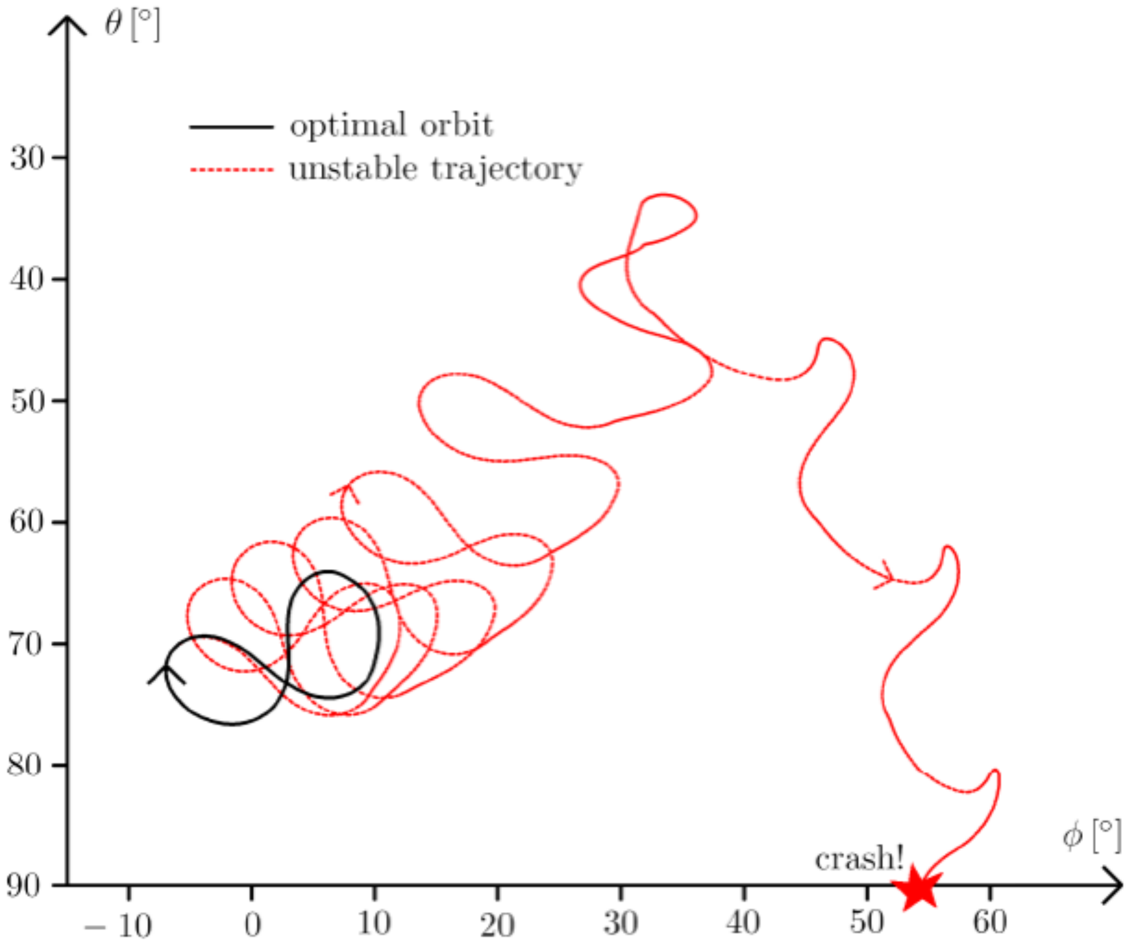
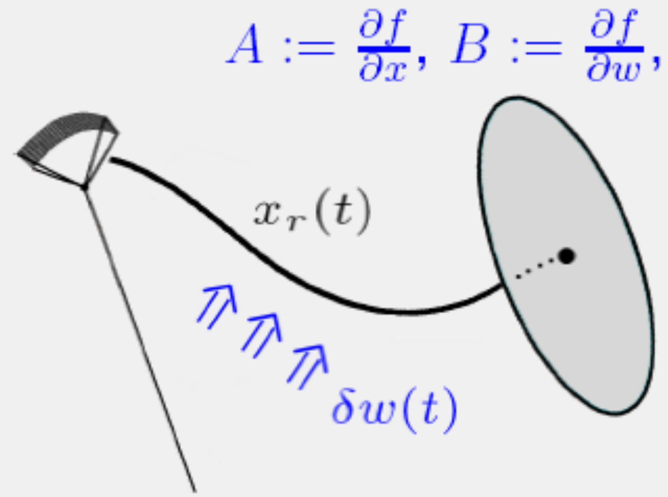


Could we make system stable just by smart choice of **open-loop** controls?

Stability and Robustness Optimization (Houska, D. 2007)

Regard linearized propagation of noise:

$$\dot{\delta x}(t) = A(t)\delta x(t) + B(t)\delta w(t)$$

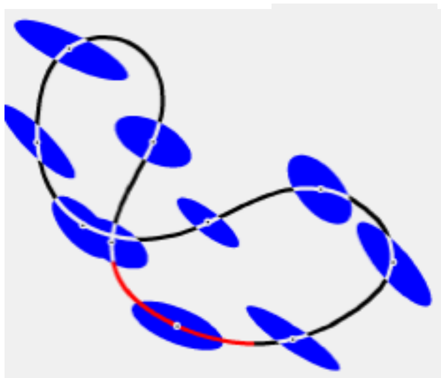


Compute covariance matrix P by Lyapunov Equation:

$$\dot{P}(t) = A(t)P(t) + P(t)A(t)^T + B(t)B(t)^T$$

Infinitely long time: covariance blows up, *or becomes periodic*

$$\boxed{P(0) = P(T)}$$



THEOREM: If periodic Lyapunov solution exists (with $P(0) \succ 0$*), nonlinear system is stable.*

Robust stability optimization problem (Houska & D. 2007)

$$\underset{x_r(\cdot),P(\cdot),u(\cdot),p,T}{\text{minimize}} \quad J[x_r(\cdot), P(\cdot), u(\cdot), p, T]$$

subject to:

$$\dot{x}_r(t) = f(x_r(t), u(t), p, 0)$$
$$x_r(0) = x_r(T)$$

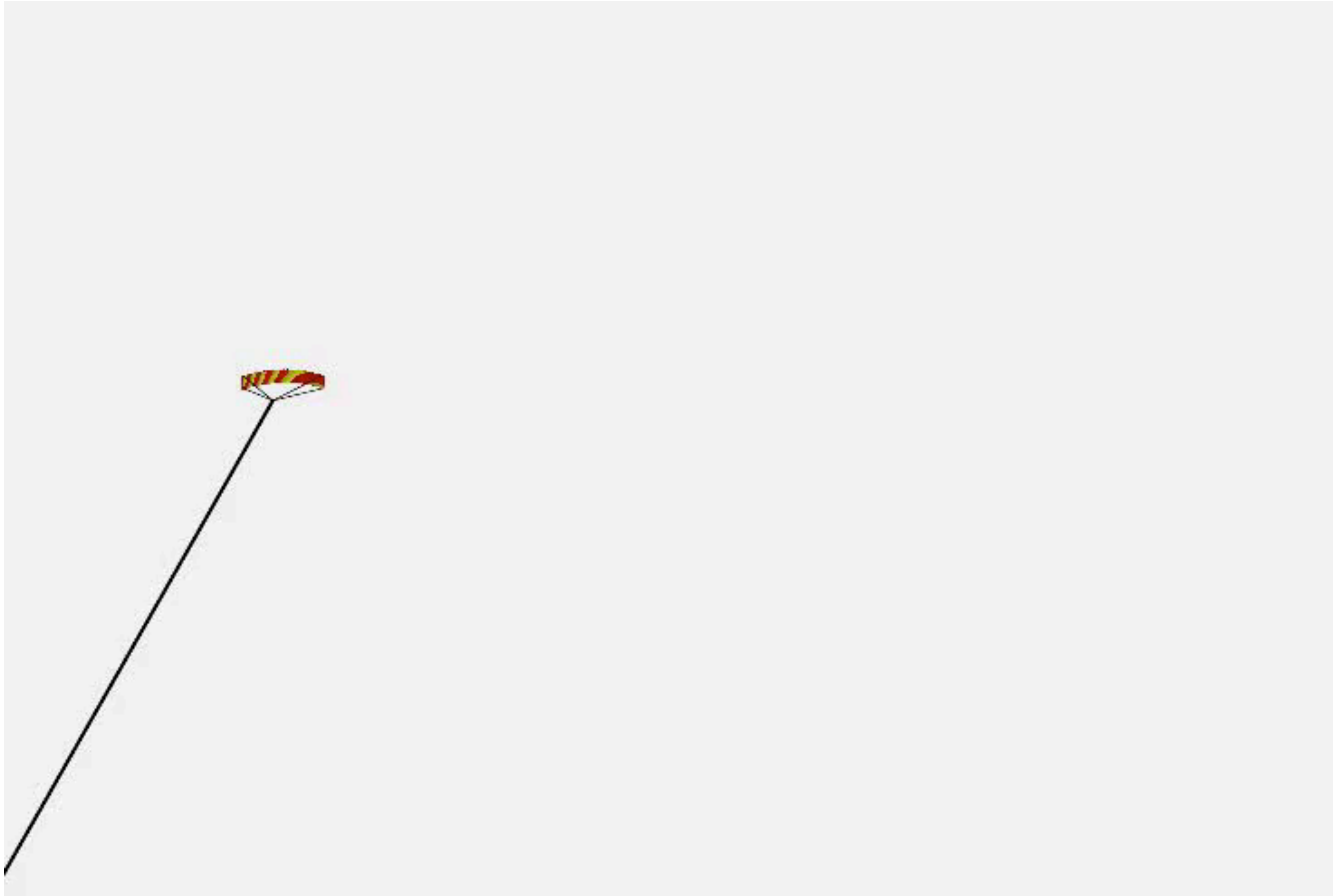
$$\dot{P}(t) = A(t)P(t) + P(t)A(t)^T + B(t)B(t)^T$$
$$P(0) = P(T)$$

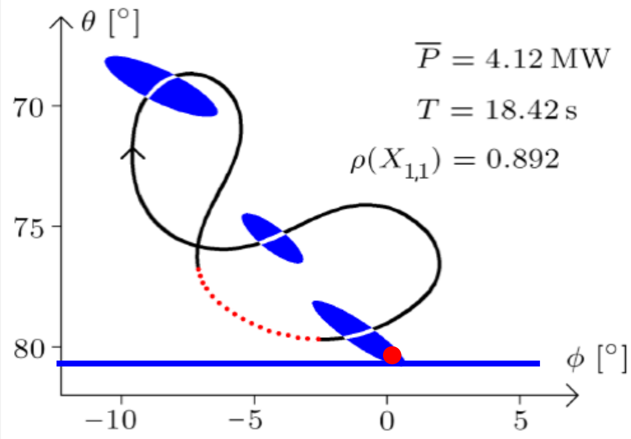
$$0 \geq h_i(x_r(t), u(t), p) \quad + \quad \gamma\sqrt{c_i(t)P(t)c_i(t)^T}$$

for all $t \in [0, T]$, $i \in \{1, ..., n_h\}$, $A := \frac{\partial f}{\partial x}$, $B := \frac{\partial f}{\partial w}$, $c_i := \frac{\partial h_i}{\partial x}$

Allows us to robustly satisfy inequality constraints!

Orbit optimized for stability





Kite does not touch ground

We have **generated** a stable attractor!

Numerical Issues

Main Advantage: formulation avoids non-smoothness, can use advanced optimal control algorithms

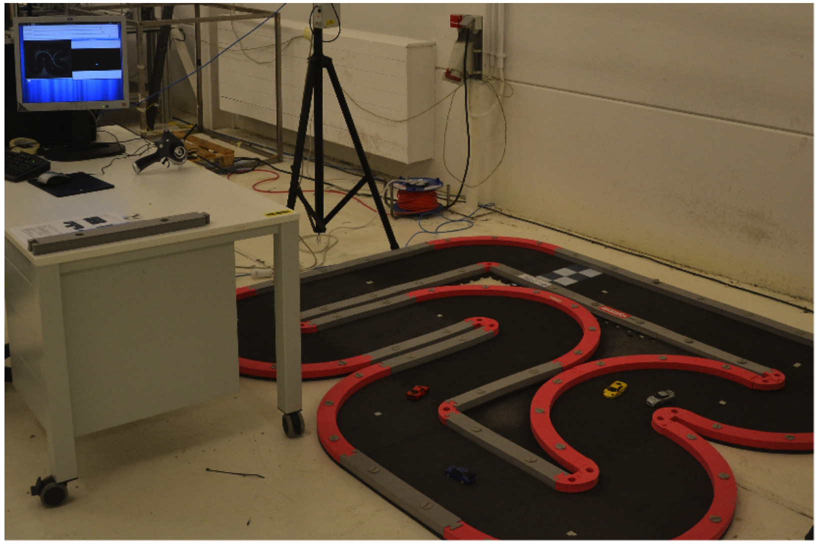
But:

- 1st derivatives in problem: need 2nd derivatives for optimization
- Need homotopy: first use „virtual feedback“, then shrink it

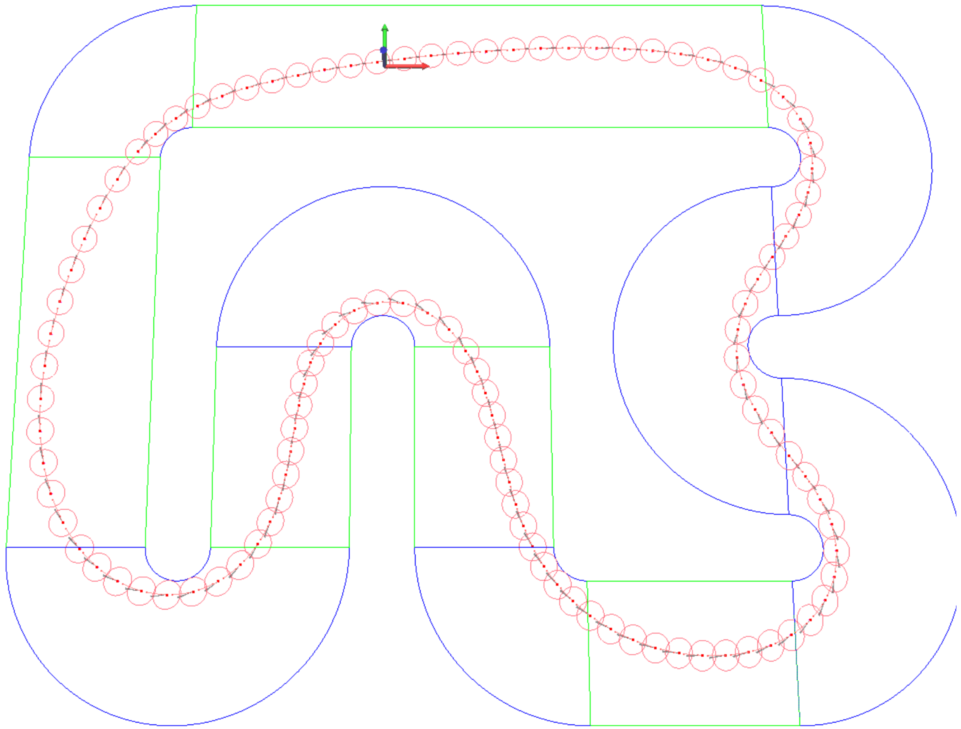
$$\dot{P}(t) = (A(t) - \sigma I)\, P(t) + P(t)\, (A(t) - \sigma I)^T + B(t) B(t)^T$$

- Can solve periodic Lyapunov equation (a large, but linear system) with periodic Schur decomposition (Varga 1997), implemented as CasADi function, CPU savings up to factor 100 possible (PhD thesis Joris Gillis 2015)

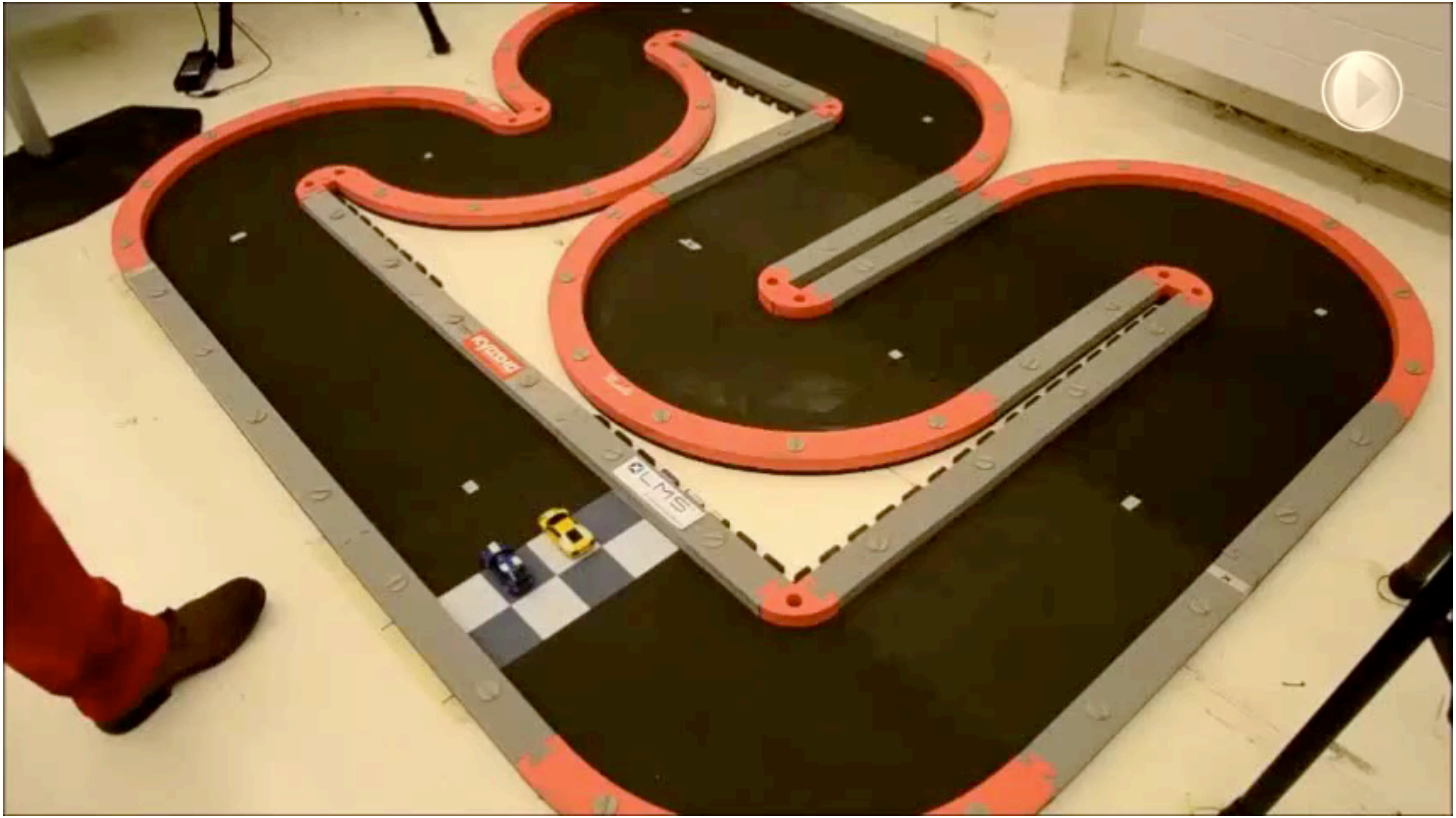
Robust Control of Control Race Cars (Greg Horn, Joris Gillis, Robin Verschueren)



- 6 states, i.e. $n_x = 6$
- 100 time steps, i.e. $N = 100$
- 6 disturbances, i.e. $n_w = 600$
- 2 controls and 4 feedback gains, i.e. $n_u = 204$
- solved in 40 seconds using CasADi and IPOPT

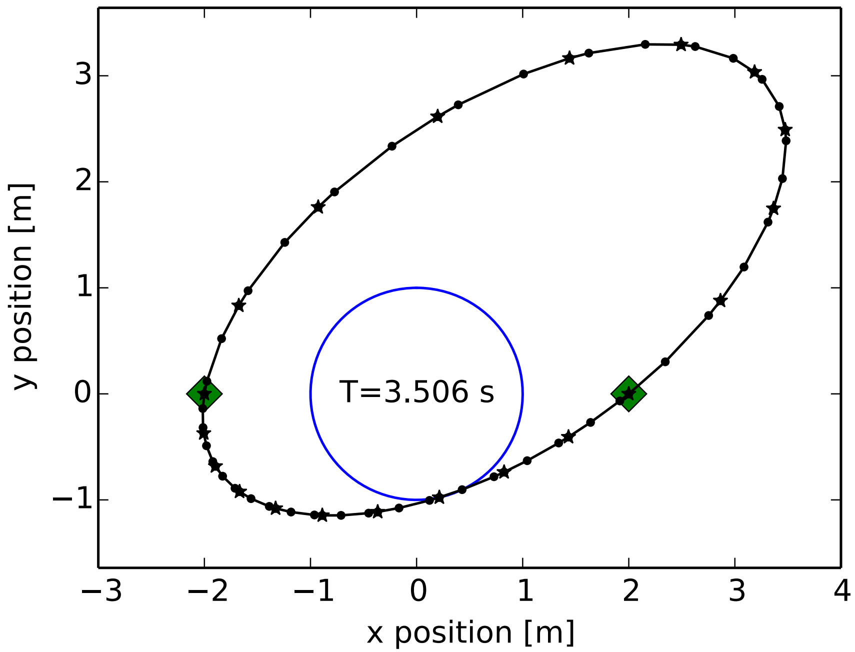


Robust Control of Control Race Cars (Greg Horn, Joris Gillis, Robin Verschueren)

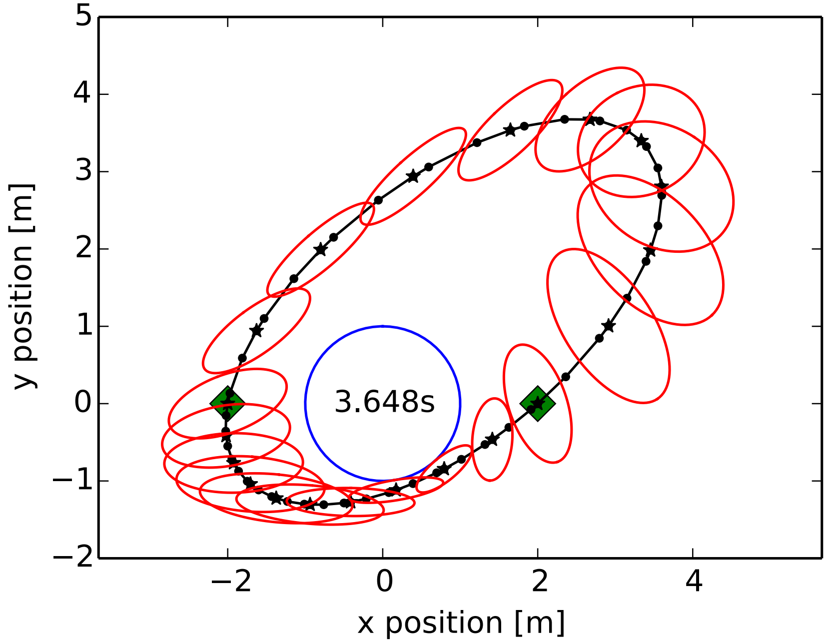


Quadcopter flight around obstacle (Joris Gillis)

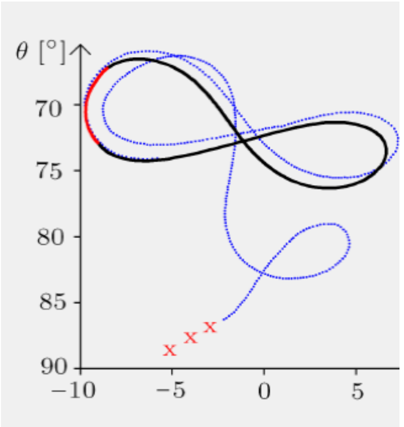
Nominal Solution

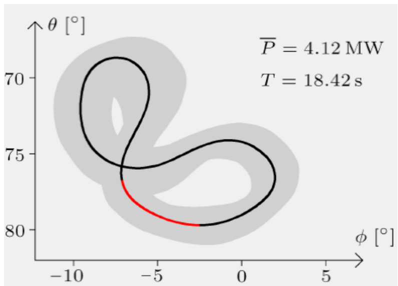


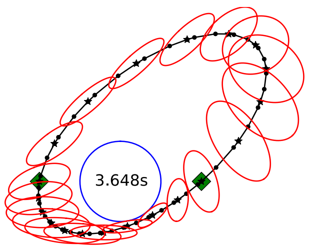
Robustified Solution



Summary: from Nominal to Robust Optimal Control





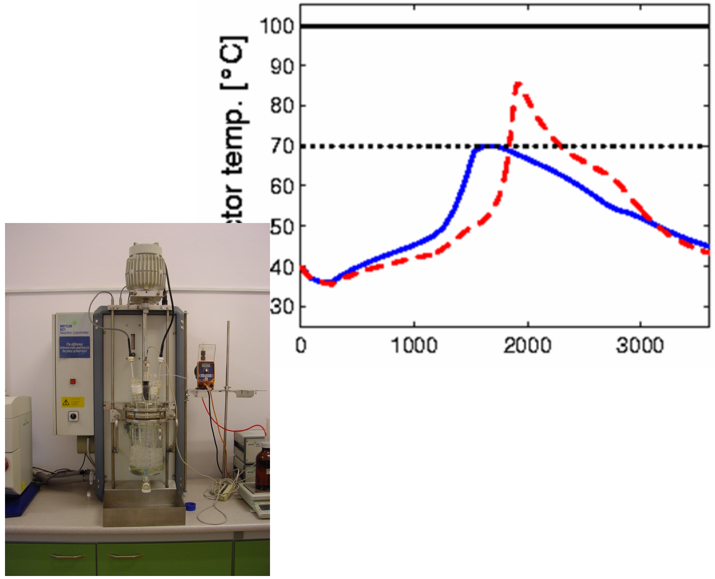


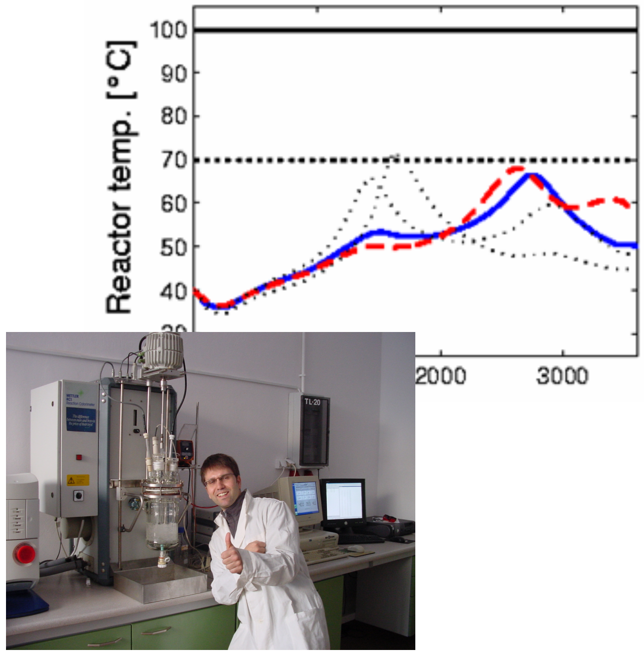
Nominal Optimal Control
(prone to model-plant-mismatch)

↓

Robust Open-Loop Optimal Control

- finite dimensional:
  - forward (many outputs)
  - adjoint (many inputs)
- infinite dimensional:
  Lyapunov Differential Equations, even allow periodic stability optimisation
- can optimise feedback parameters





Outline of the Talk

- Motivating Example: Control of Batch Reactors
- Robustification by Linearization
- Lyapunov Differential Equations
- **(L-Infinity bounded uncertainty — omitted)**
- Periodic Orbits for Power Generating Kites
- Open-Loop Stability Optimization

Thank you !

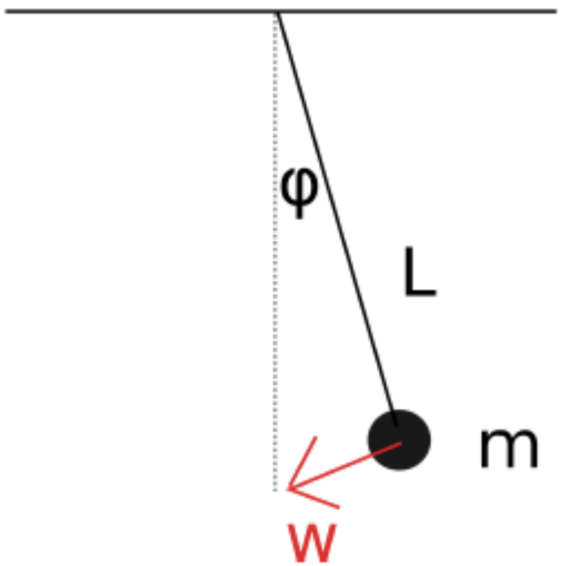
Difficult Case: L-Infinity Bounded Uncertainty

- Assumption:

$$\dot{x}(t) = A(t)x(t) + B(t)w(t) \quad \text{with} \quad x(0) = 0$$

Uncertainty satisfies $\|w(t)\|_\infty \leq 1$ for all $t \in [0, T]$

- Example:



Linearized Pendulum:

$$\begin{aligned} \dot{\varphi}(t) &= \omega(t) \\ \dot{\omega}(t) &= -\frac{g}{L}\varphi(t) + \frac{w(t)}{mL^2} \end{aligned}$$

The torque w is unknown.

Worst Case Reachable States

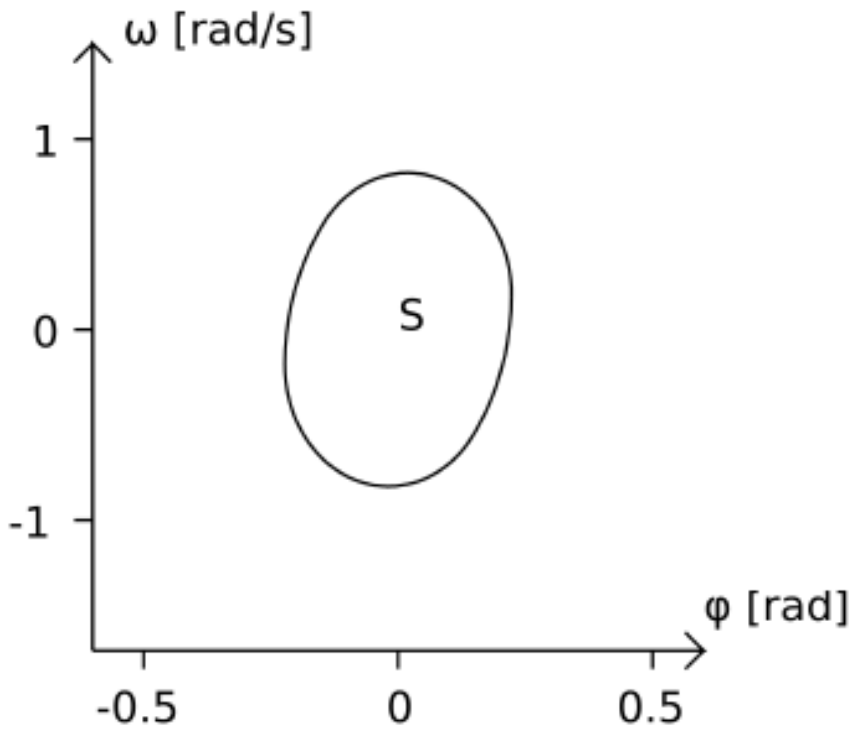
The Uncertainty Tube:

- Pick a time $t \in [0, T]$.
- Define $S(t)$

$$S(t) := \left\{ x(t) \in \mathbb{R}^{n_x} \;\middle|\; \begin{array}{l} \forall \tau \in [0,T] : \\ \dot{x}(\tau) = A(\tau)x(\tau) + B(\tau)w(\tau) \\ x(0) \;=\; 0 \\ \|w(\tau)\|_\infty \leq 1 \end{array} \right\}$$

- $S(t) \;=\;$ set of reachable states at time t.
- $S(t)$ is convex.

Uncertainty Tube for Pendulum



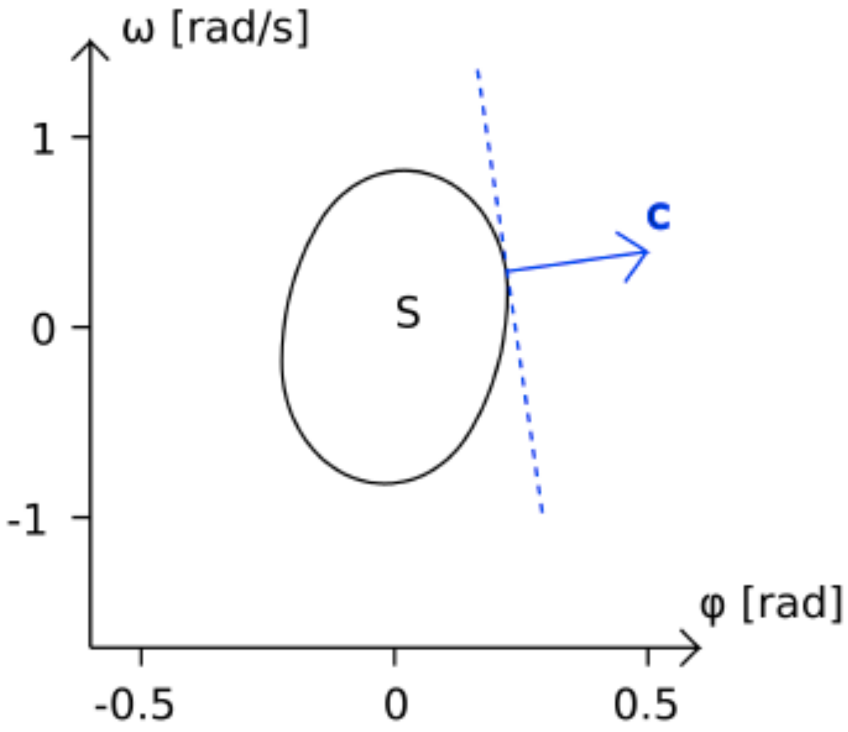
Example:

- The set $S(t)$ for the linearized pendulum.

t [s]	L [m]	g [m/s^2]	m [kg]
1.2	1	9.81	1

Question: How can we compute the set $S(t)$?

Uncertainty Tube for Pendulum



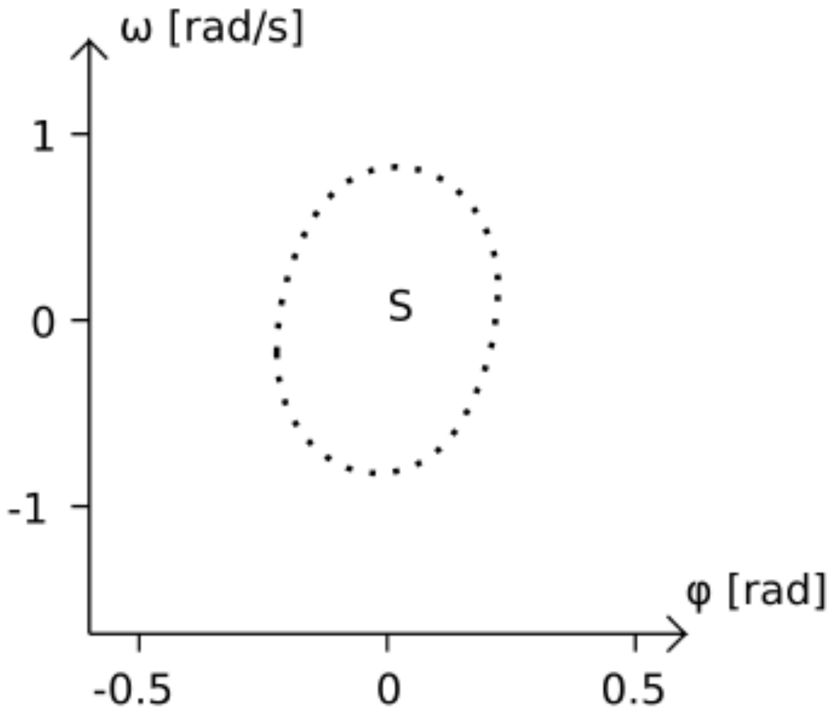
Solution: Solve the LP

$$\max_{x(\cdot),w(\cdot)} \quad c^T x(t)$$
$$\text{s.t.} \begin{cases} \dot{x}(\tau) = Ax(\tau) + Bw(\tau) \\ x(0) \; = \; 0 \\ \|w(\tau)\|_\infty \leq 1 \quad \tau \in [0,t]. \end{cases}$$

for all directions c.

Question: How can we compute the set $S(t)$?

Uncertainty Tube for Pendulum



CPU-time:

- Solve 100 LP's.
- Need approximately 1s for computing $S(t)$.

Problem: Computing $S(t)$ exactly takes very long if $n_x \gg 2$.

Dual of Infinite Dimensional LP

- Consider the Linear Program for a given c:

$$\begin{aligned} V(t) \quad &:= \quad \max_{x(\cdot),w(\cdot)} \quad c^T x(t) \\ &\qquad \text{s.t. } \dot{x}(\tau) = A(\tau)x(\tau) + B(\tau)w(\tau) \\ &\qquad\qquad x(0) = 0 \qquad \|w(\tau)\|_\infty^2 \leq 1 \end{aligned}$$

- Reformulation step 1:

$$\begin{aligned} V(t) \quad &= \quad \max_{w(\cdot)} \int_0^t c^T H_t(\tau) w(\tau) \mathrm{d}\tau \ \text{ s.t. } \|w_i(\tau)\|^2 \leq 1 \\ &= \quad \inf_{\lambda(\cdot)>0} \max_{w(\cdot)} \int_0^t \left[c^T H_t(\tau) w(\tau) - \sum_i \lambda_i(\tau) \left(w_i(\tau)^2 - 1 \right) \right] \mathrm{d}\tau \end{aligned}$$

Maximize dual function and transform further…

- Reformulation step 2:

$$V(t) \; = \; \inf_{\Lambda(\cdot)\succ 0} \int_0^t \frac{c^T H_t(\tau)\Lambda(\tau)^{-1} H_t(\tau)^T c}{4} \, \mathrm{d}\tau + \int_0^t \mathrm{Tr}\left[\, \Lambda(\tau) \,\right] \mathrm{d}\tau \; .$$

with

$$\Lambda(\tau) \; := \; \mathrm{diag}(\lambda(\tau)) \in \mathbb{D}^{n_w}_{++} \; .$$

- Main idea: use a variable transformation of the form

$$\forall \tau \in [0,t] : \quad R(\tau) \quad := \quad \frac{1}{\kappa} \Lambda(\tau) \exp\left(\int_\tau^t \frac{\mathrm{Tr}\left[\, \Lambda(\tau') \,\right]}{\kappa - \int_{\tau'}^t \mathrm{Tr}\left[\, \Lambda(s) \,\right] \mathrm{d}s} \, \mathrm{d}\tau' \right)$$

with $\kappa > \int_0^t \mathrm{Tr}\left[\, \Lambda(s) \,\right] \mathrm{d}s$ being a sufficiently large constant.

…and introduce Lyapunov Equations again!

THEOREM [Houska & D. 2010]:

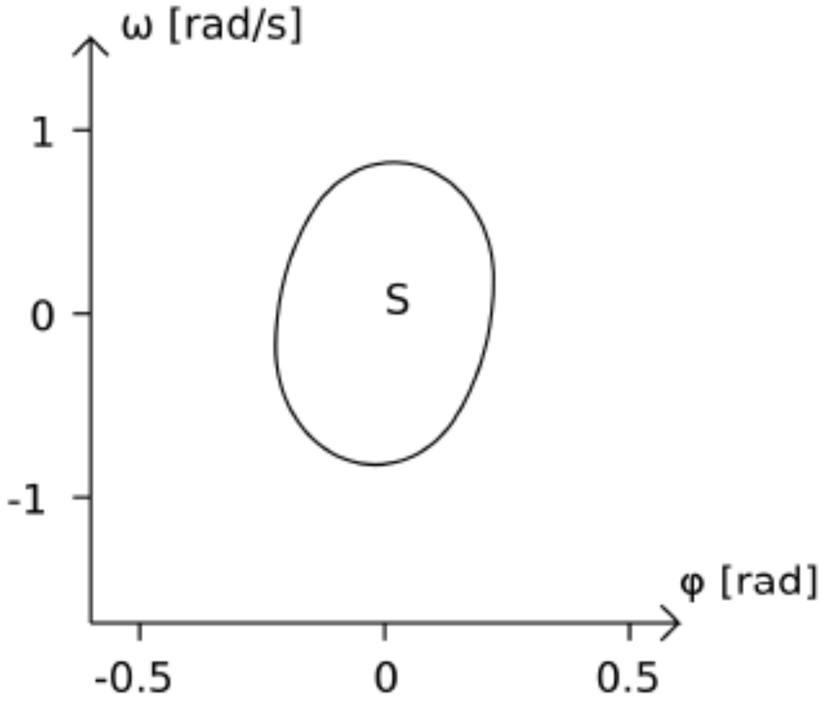
The function V can equivalently be expressed as

$$V(t) \;=\; \inf_{P(\cdot),\theta(\cdot),R(\cdot)\in\mathbb{D}^{nw}_{++}} \sqrt{1-\theta(\tau)}\sqrt{c^T P(t) c}$$

$$\text{s.t.} \quad \begin{cases} \dot{P}(\tau) & = & A(\tau)P(\tau) + P(\tau)A(\tau)^T + \operatorname{Tr}\left[\, R(\tau) \,\right]\, P(\tau) \\ & & +B(\tau)R^{-1}(\tau)B(\tau)^T \\ P(0) & = & 0 \\ \dot{\theta}(\tau) & = & -\operatorname{Tr}\left[\, R(\tau) \,\right]\, \theta(\tau) \\ \theta(0) & = & 1\,. \end{cases}$$

Note: worst case minimization problem, useful for robust counterpart!

Tight Outer Approximating Ellipsoids



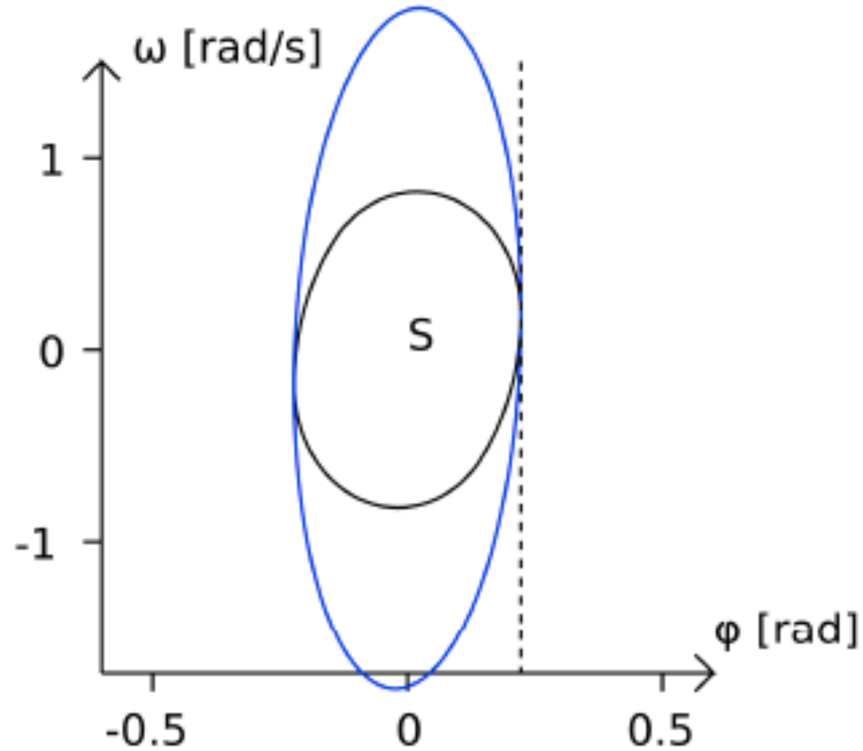
- Solve the above problem for any direction c and set

$$Q(t) := (1 - \theta(t))\, P(t) \, .$$

Then we have

$$S(t) \subseteq \left\{ Q(t)^{\frac{1}{2}} v \;\middle|\; v^T v \leq 1 \right\}$$

Tight Outer Approximating Ellipsoids



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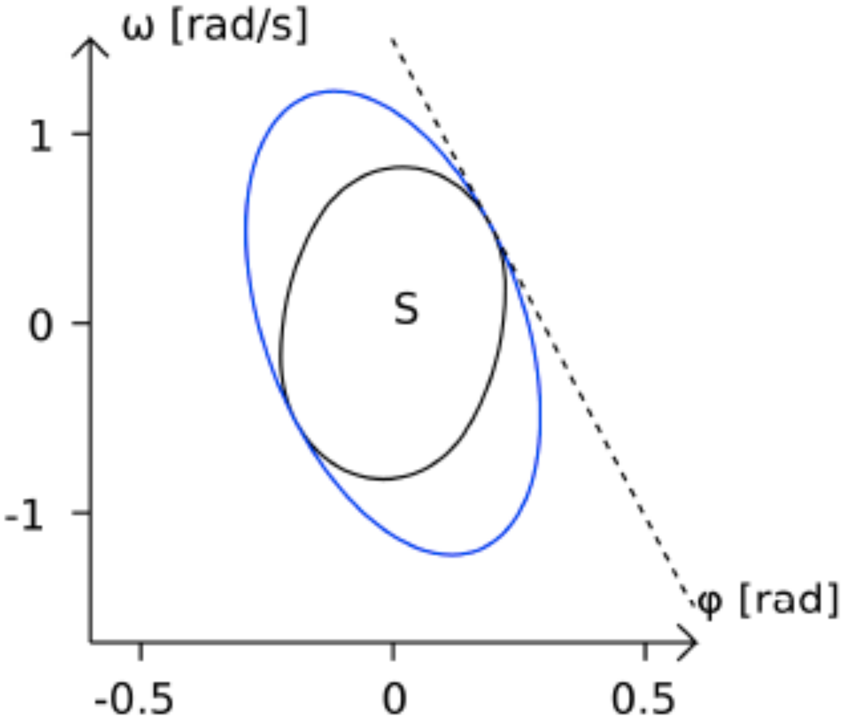

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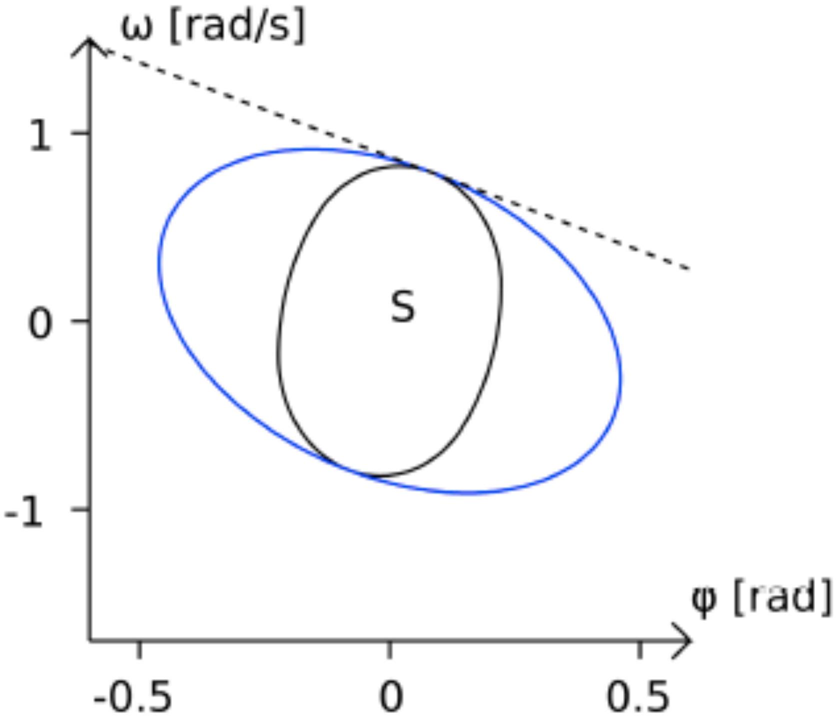

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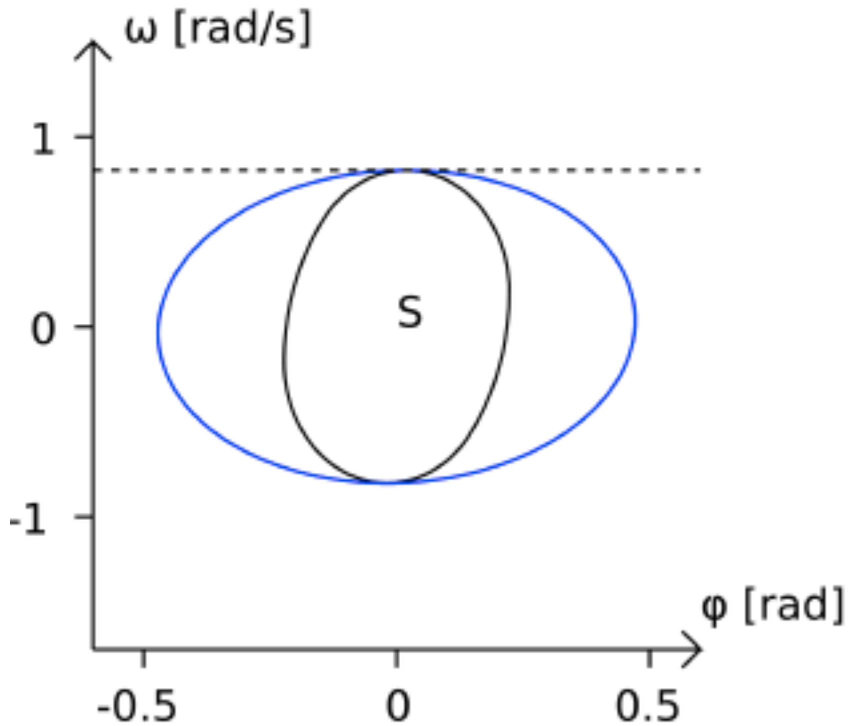

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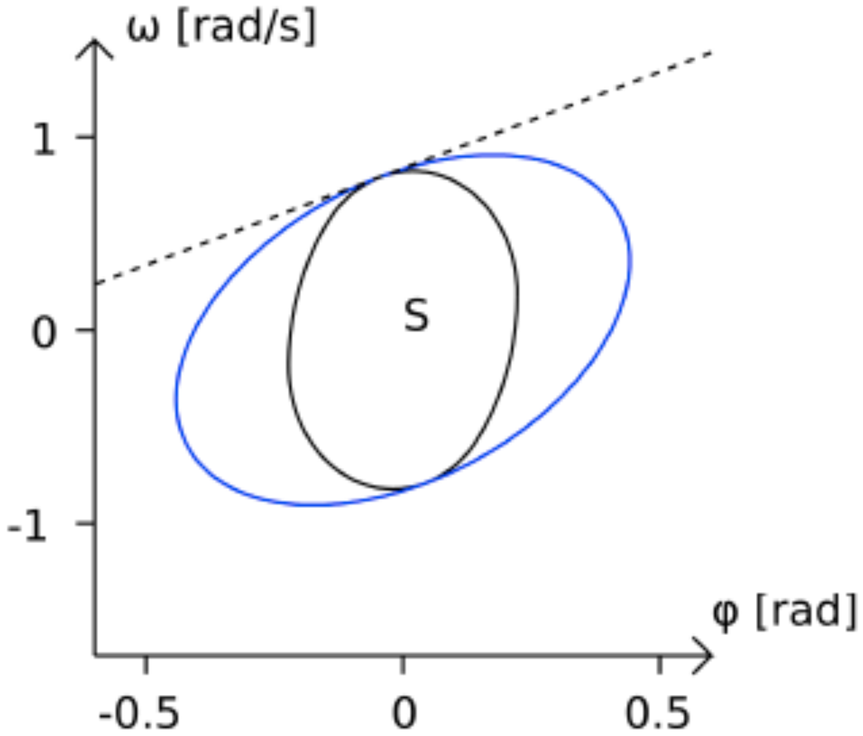
Tight Outer Approximating Ellipsoids



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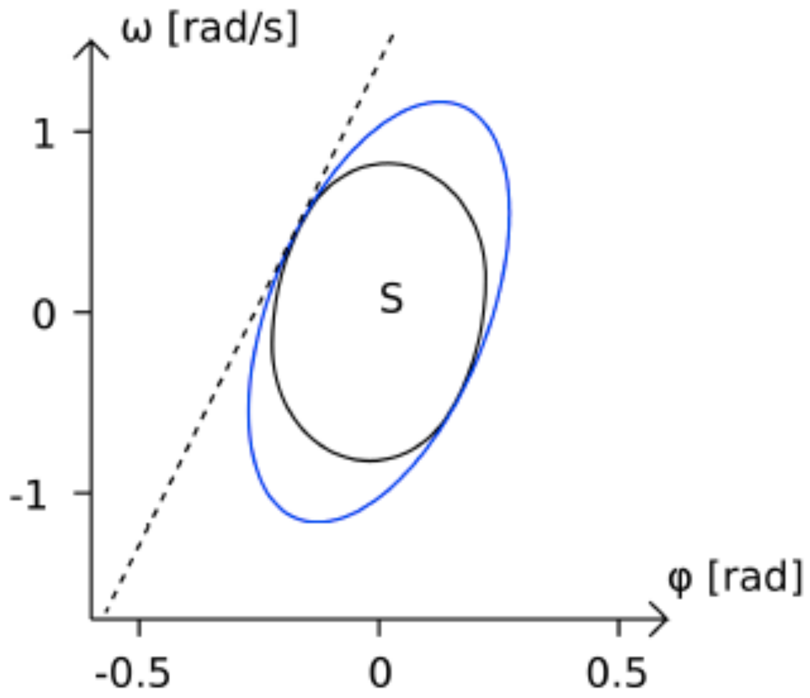

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Summary: The above theorem yields ellipsoidal outer-approximations of the set of reachable states, which are exact in a given direction c.