# Cybersecurity and Quantum Computation in Control of Cyberphysical Systems for Next-Generation Manufacturing

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# PAST EXPERIENCES

- B.S. Chemical Engineering, University of California, Los Angeles
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- M.S. and Ph.D. Chemical Engineering, University of California, Los Angeles
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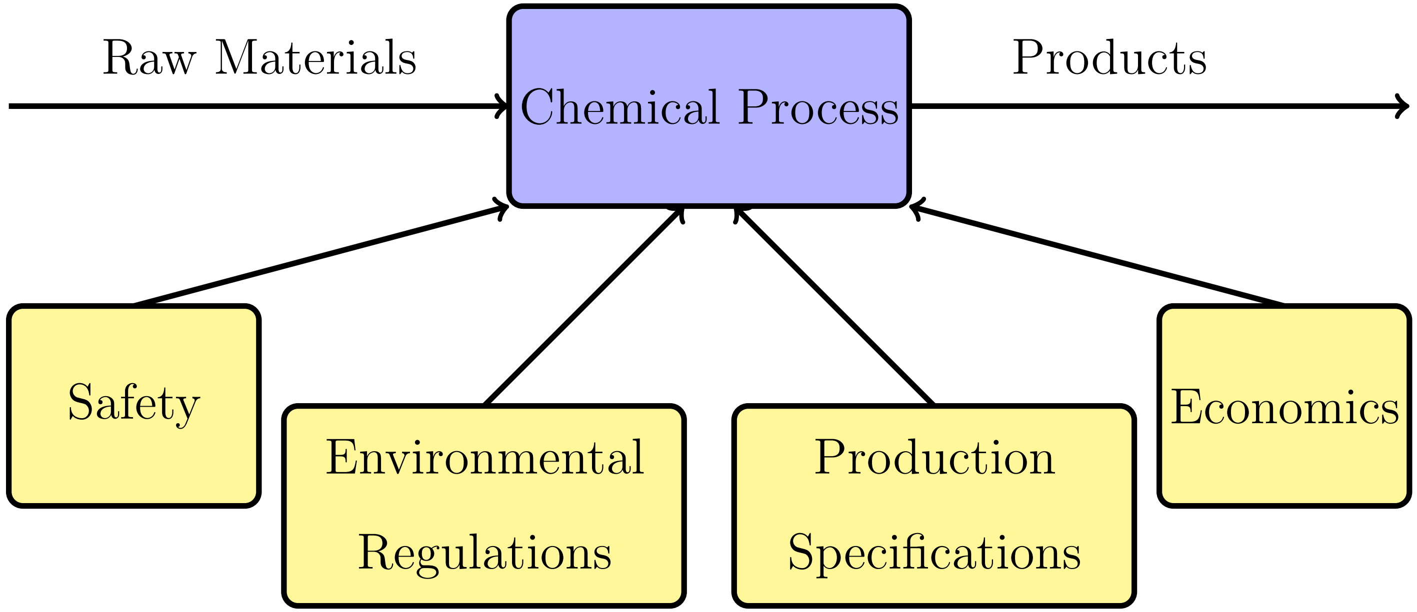
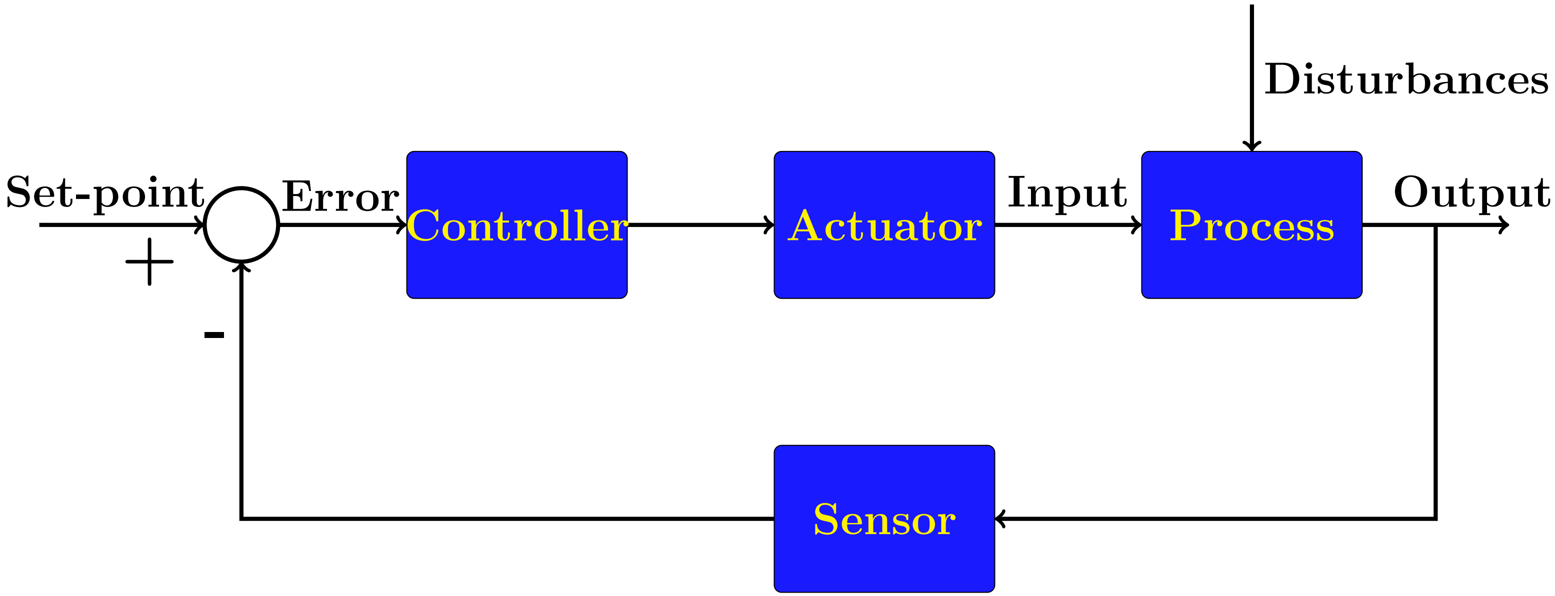
# INTRODUCTION

- Incentives for chemical process control



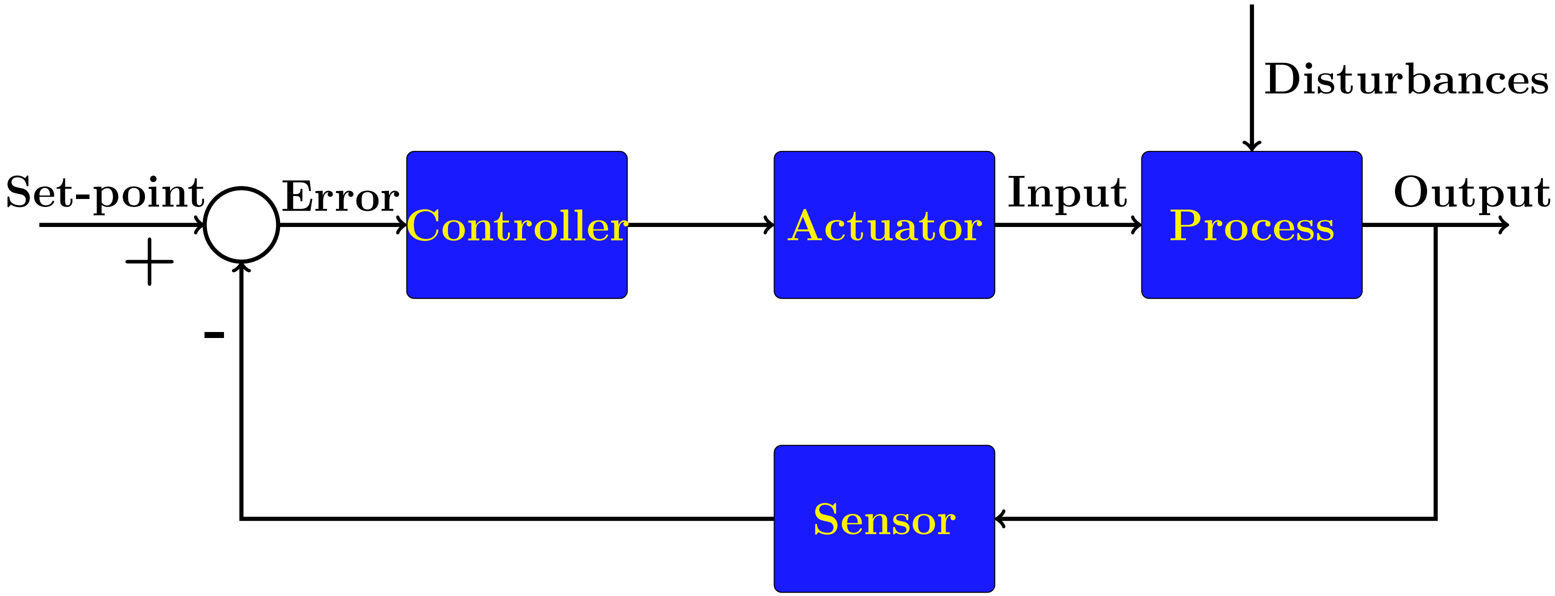

- Need for continuous monitoring and external intervention (process control)
- Objectives of a process control system
  - ◇ Ensuring stability of the process
  - ◇ Suppressing the influence of external disturbances
  - ◇ Optimizing process performance

# FEEDBACK CONTROL LOOP




- How a feedback control loop (closed-loop system) works:
  - ◇ A variable describing the condition of a process (e.g., temperature, pressure, species concentration; known as an output) is measured by a sensor
  - ◇ The error between the measured output value and the desired value of this output (set-point) is calculated and fed to the controller
  - ◇ The controller computes a value of the manipulated input to the process to reduce the error
  - ◇ A control actuator (typically a valve) is used to apply the manipulated input value to the process

# CLASSICAL CONTROL




- Classical control: single-input/single-output (SISO) control design
  - ◇ Proportional-integral-derivative (PID) control (error $e(t)$)
    - ▷ Error reflects difference between measured output and set-point
  - ◇ Input/control action $u(t)$

$$u(t) = \underbrace{K_c e(t)}_{\text{P}} + \underbrace{\frac{1}{\tau_I}\int_0^t e(\tau)d\tau}_{\text{I}} + \underbrace{\tau_D \frac{de(t)}{dt}}_{\text{D}}$$

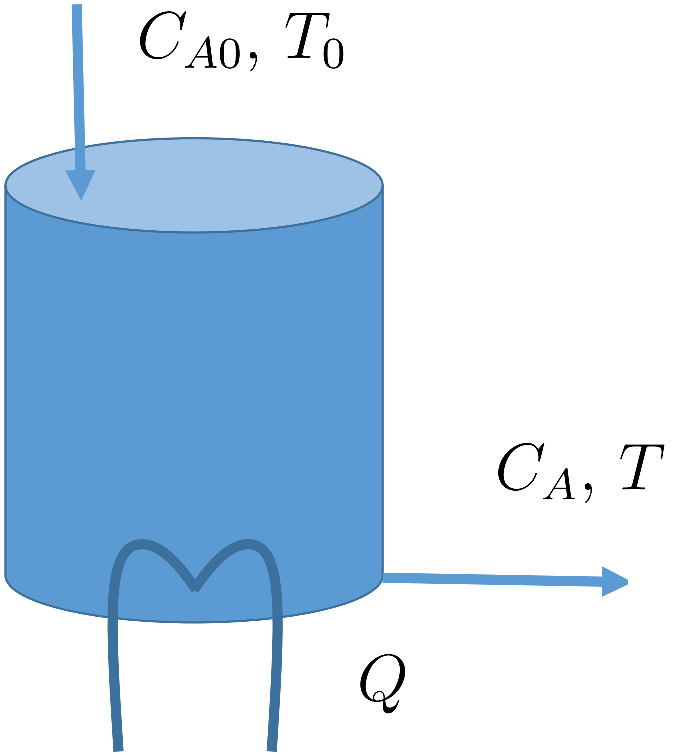
  - ◇ $K_c$, $\tau_I$, $\tau_D$: scalar values that can be picked (tuned)

# ADVANCED MODEL-BASED PROCESS CONTROL

- Advanced process control utilizes a process dynamic model explicitly in the controller design
  - ◇ A mathematical process model is developed:
    - ▷ Constructed from first-principles
    - ▷ Identified from input-output process data
  - ◇ The model describes the process dynamics (variation of the process state variables in time due to disturbances, inputs, and interactions between variables)
  - ◇ Controllers are synthesized based on the process model
- Advantages of model-based control
  - ◇ Possibility of improved closed-loop performance
  - ◇ Model accounts for inherent process characteristics (e.g., nonlinear behavior, multivariable interactions)
  - ◇ Characterization of limitations on achievable closed-loop stability, performance and robustness

# NONLINEAR MODEL-BASED PROCESS CONTROL

- Example: continuous stirred tank reactor (CSTR)




- Model: system of nonlinear ordinary differential equations (ODEs)

$$\frac{dT}{dt} = \frac{F}{V_r}(T_0 - T) + \frac{(-\Delta H)}{\rho C_p} k_0 e^{-E/RT} C_A + \frac{Q}{\rho C_p V_r}$$

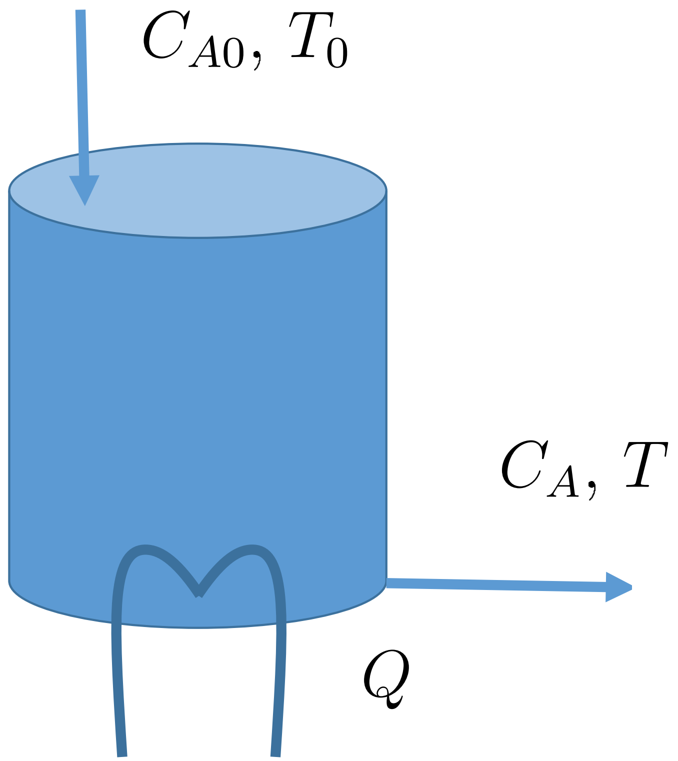
$$\frac{dC_A}{dt} = \frac{F}{V_r}(C_{A0} - C_A) - k_0 e^{-E/RT} C_A$$

$$\Rightarrow x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} T - T_s \\ C_A - C_{As} \end{bmatrix}, \ \dot{x} = \frac{dx}{dt}$$

$$u = Q - Q_s, \ w = C_{A0} - C_{A0s}$$

# NONLINEAR MODEL-BASED PROCESS CONTROL

- Example: continuous stirred tank reactor (CSTR)




- Model: system of nonlinear ordinary differential equations (ODEs)

$$\dot{x} = f(x, u, w)$$

- Techniques for nonlinear controller design for driving the process state to the operating steady-state

  ◇ Lyapunov-based control ◇ Model predictive control

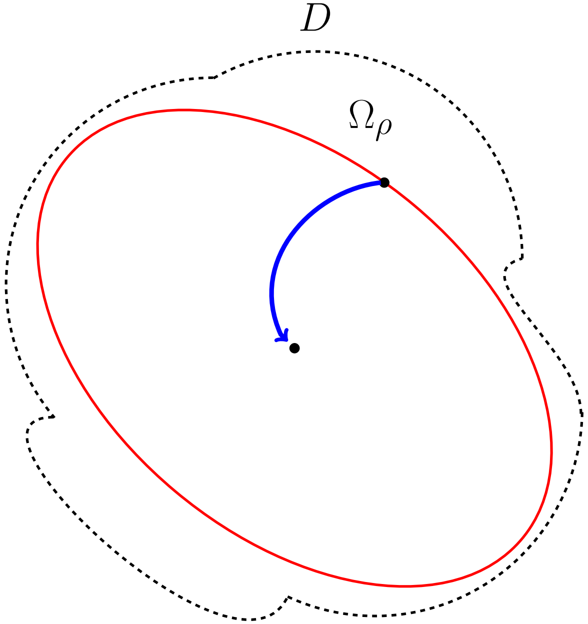
# NONLINEAR PROCESS SYSTEMS

- State-space description

$$\dot{x} = f(x, u, w)$$

  - ◇ $x \in X \subset \mathbb{R}^n$ is the state, $u \in U \subset \mathbb{R}^m$ is the manipulated input, $w \in W \subset \mathbb{R}^l$ is the disturbance, $f$ is a vector function

- Explicit nonlinear feedback control law: $u = h(x)$




  - ◇ Control design technique: Lyapunov-based control
    (Y. Lin and E.D. Sontag, *SCL*, 1991; H. Khalil, *Prentice Hall*, 2002; P. D. Christofides and N. H. El-Farra, *Springer-Verlag*, 2005)
  - ◇ Renders the origin (steady-state) asymptotically stable
  - ◇ There exists a Lyapunov function $V$ which satisfies

$$\dot{V} = \frac{\partial V(x)}{\partial x} f(x, h(x), 0) < 0, \ \forall \, x \in D$$

$V$ : energy of a physical system

  - ◇ Typically, $V(x) = x^T P x$ (quadratic) and $\Omega_\rho \subseteq D$ is a level set of $V$ where state constraints are met (i.e., $\Omega_\rho := \{x \ : \ V(x) \leq \rho\}$)
  - ◇ $u = h(x)$ possesses a degree of robustness to disturbances and uncertainty

- Performance considerations and constraints are not directly/explicitly taken into account

# MODEL PREDICTIVE CONTROL

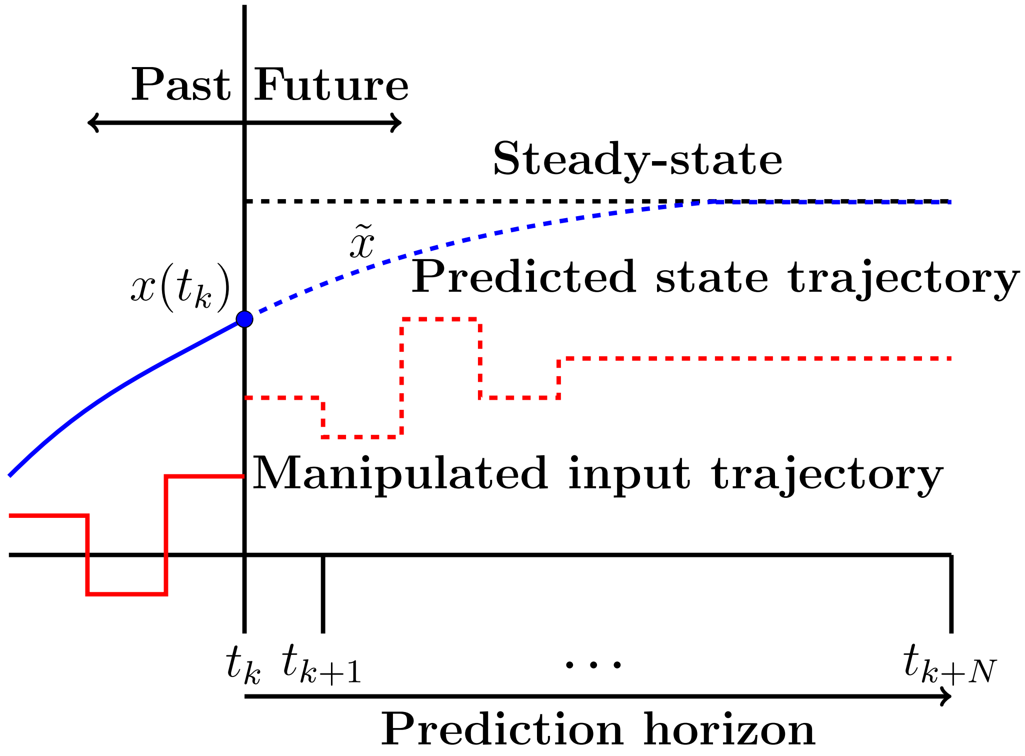
- Model predictive control (MPC)

$$\min_{u \in S(\Delta)} \int_{t_k}^{t_{k+N}} l_T(\tilde{x}(\tau), u(\tau))\, d\tau$$

$$\text{s.t.} \quad \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$

$$\tilde{x}(t_k) = x(t_k)$$

$$u(t) \in U,\ \tilde{x}(t) \in X,\ \forall\ t \in [t_k, t_{k+N})$$




- Quadratic tracking stage cost:

$$l_T(x, u) = x^T Q x + u^T R u$$

  ◇ $Q$, $R$ are positive definite matrices

- Solve the optimization problem every $\Delta$ time units (sampling period)

  ◇ At each sampling time $t_k$

- Solution is a piecewise-constant input trajectory

  ◇ Each piece is held constant for a period $\Delta$

  ◇ Prediction horizon $N$

# MODEL PREDICTIVE CONTROL

- Model predictive control (MPC)

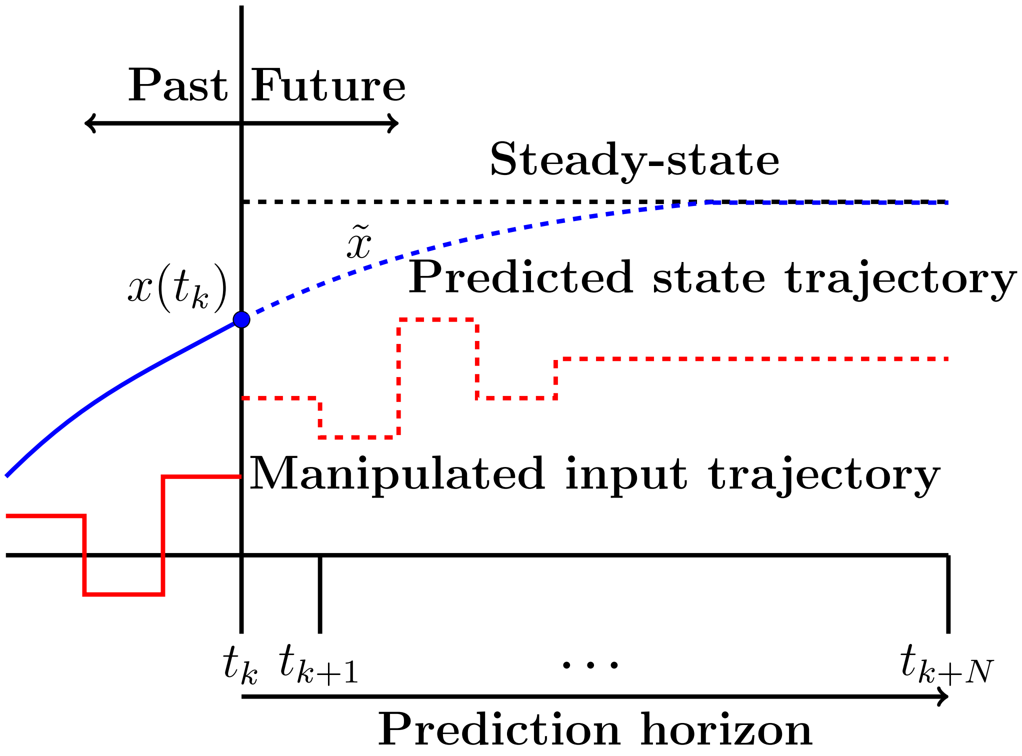
$$\min_{u \in S(\Delta)} \int_{t_k}^{t_{k+N}} \left[ \tilde{x}^T Q \tilde{x} + u^T R u \right] \, d\tau$$

$$\text{s.t.} \quad \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$

$$\tilde{x}(t_k) = x(t_k)$$

$$u(t) \in U, \ \tilde{x}(t) \in X, \ \forall \, t \in [t_k, t_{k+N})$$

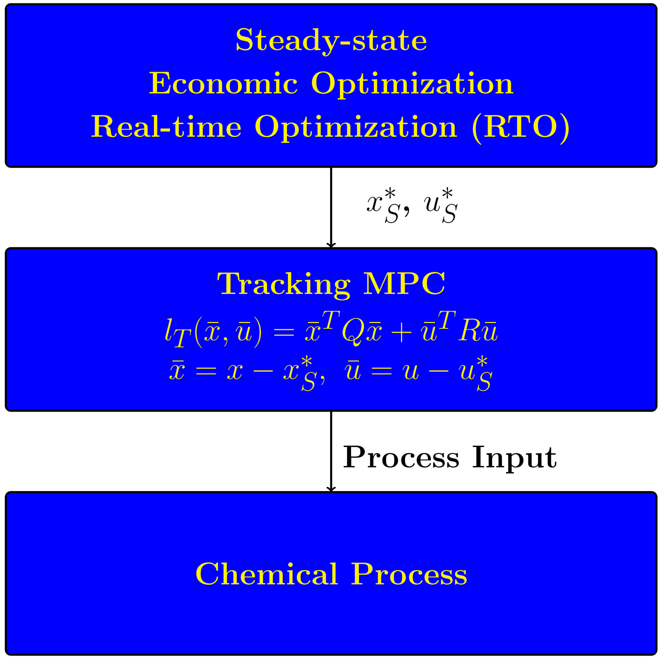
- Receding horizon implementation
  - ◇ Only the first piece of the input trajectory is applied
    - ▷ Allows for feedback at every $\Delta$
    - ▷ Accounts for effects of disturbances and plant/model mismatch on the optimal solution
  - ◇ Longer prediction horizon may improve closed-loop performance




- Closed-loop stability is not guaranteed
- Approaches for closed-loop stability
  - ◇ Infinite/sufficiently long prediction horizon
  - ◇ Terminal cost/constraint
  - ◇ Contractive constraint

# NEXT-GENERATION MANUFACTURING

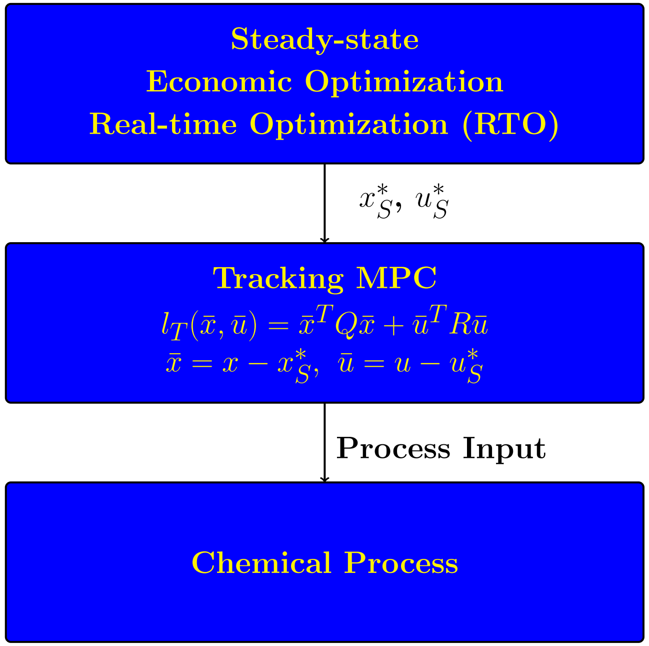
- Next-generation/smart manufacturing objectives (J. Davis, T. Edgar, J. Porter, J. Bernaden and M. Sarli, *Comput. Chem. Eng.*, 2012):
  - Profitability
  - Autonomy
  - Safety and cybersecurity




- Example: Moving away from a hierarchical approach to optimization and control
  - Upper layer:
    - Determine economically-optimal steady-state (real-time optimization (RTO)) (M. L. Darby, M. Nikolaou, J. Jones and D. Nicholson, *JPC*, 2011)
  - Lower layer:
    - Feedback control drives the state of the process to the optimal steady-state
- Tighter integration of plant operation and process economic optimization

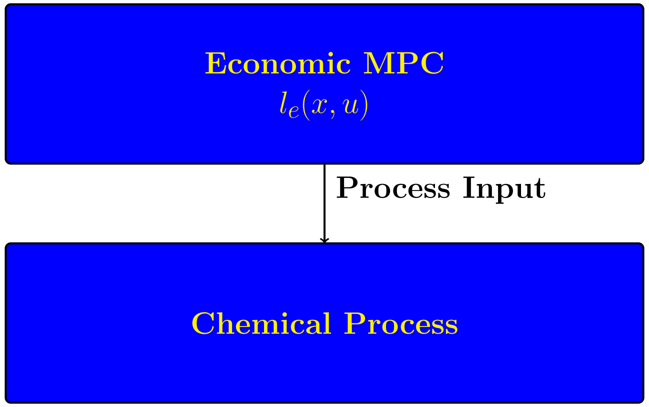
# PROCESS ECONOMICS AND CONTROL

- Traditional Paradigm




**Steady-state operation**

- Integration of economic optimization and process control
- Generalization of MPC
  - ◇ General (economic) stage cost




**Dynamic/time-varying operation**

- Economic MPC (EMPC) potential use cases:
  - ◇ Time-varying objective function or constraints (M. Ellis and P. D. Christofides, *AIChE J.*, 2013; A. Gopalakrishnan and L. T. Biegler, *CACE*, 2013)

(M. Ellis, H. Durand and P. D. Christofides, *JPC*, 2014)

# ECONOMIC MPC FORMULATION

- EMPC formulation:

$$\begin{aligned}
\min_{u(\cdot)\in S(\Delta)} \quad & \int_{t_k}^{t_{k+N}} l_e(\tilde{x}(\tau), u(\tau)) \, d\tau \\
\text{s.t.} \quad & \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0) \\
& \tilde{x}(t_k) = x(t_k) \\
& u(t) \in U, \ \tilde{x}(t) \in X, \\
& \quad \forall \ t \in [t_k, t_{k+N}) \\
& |u(t_j) - u(t_{j-1})| \leq \epsilon_d \\
& j = k, \ldots, k+N-1
\end{aligned}$$

- Components of EMPC:
  - ◇ Economic cost function
  - ◇ Dynamic model
  - ◇ State feedback measurement
  - ◇ Input and state magnitude constraints
  - ◇ Input rate of change constraints

- System equipped with a measure of instantaneous economics $l_e$
- Computes control actions that optimize economics
- Accounts for input and state constraints
  - ◇ Examples: temperature or flow rate bounds
- Prevents rapid variations in inputs which may damage actuators

# LYAPUNOV-BASED ECONOMIC MPC

## Boundedness / Time-varying Operation (Mode 1)

(M. Heidarinejad *et al.*, *AIChE J.*, 2012)

$$\min_{u(\cdot)\in S(\Delta)} \quad \int_{t_k}^{t_{k+N}} l_e(\tilde{x}(\tau), u(\tau))\, d\tau$$

$$\text{s.t.} \quad \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$

$$\tilde{x}(t_k) = x(t_k)$$

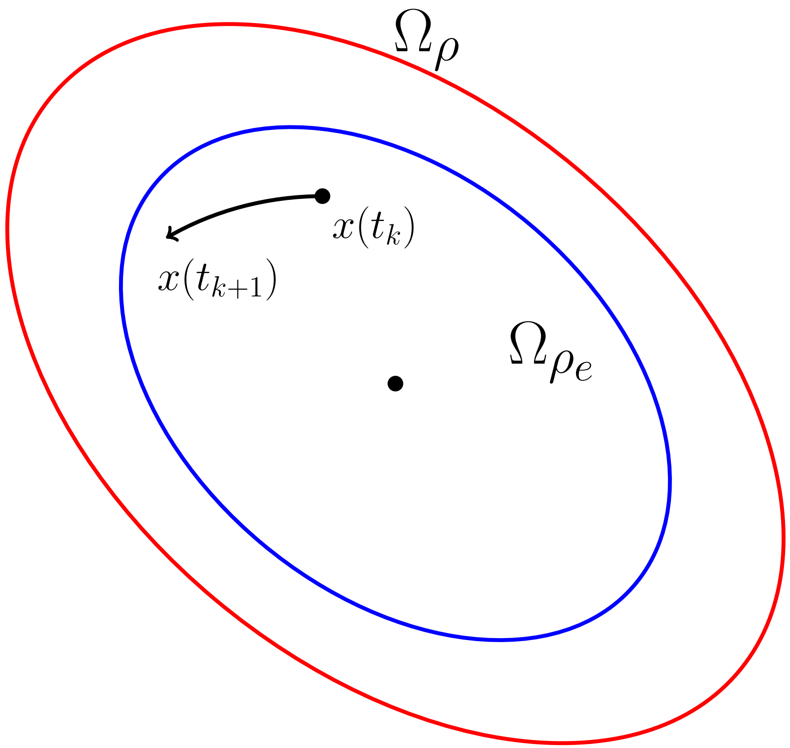
$$u(t) \in U,\ \tilde{x}(t) \in X,\ \forall\, t \in [t_k, t_{k+N})$$

$$|u_i(t_j) - h_i(\tilde{x}(t_j))| \leq \epsilon_r,\ i = 1, \ldots, m,$$

$$j = k, \ldots, k+N-1$$

$$V(\tilde{x}(t)) \leq \rho_e,\ \forall\, t \in [t_k, t_{k+N})$$

$$\text{if } V(x(t_k)) \leq \rho_e \text{ and } t_k < t_s$$




- Provable stability: boundedness of the closed-loop state in $\Omega_\rho$ ($\Omega_{\rho_e} \subset \Omega_\rho$)
- Provable feasibility: $h(x)$ meets all state and input constraints

# LYAPUNOV-BASED ECONOMIC MPC

## Convergence to the Steady-State (Mode 2)

$$\min_{u(\cdot)\in S(\Delta)} \int_{t_k}^{t_{k+N}} l_e(\tilde{x}(\tau), u(\tau))\, d\tau$$

s.t.

$$\dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t), 0)$$

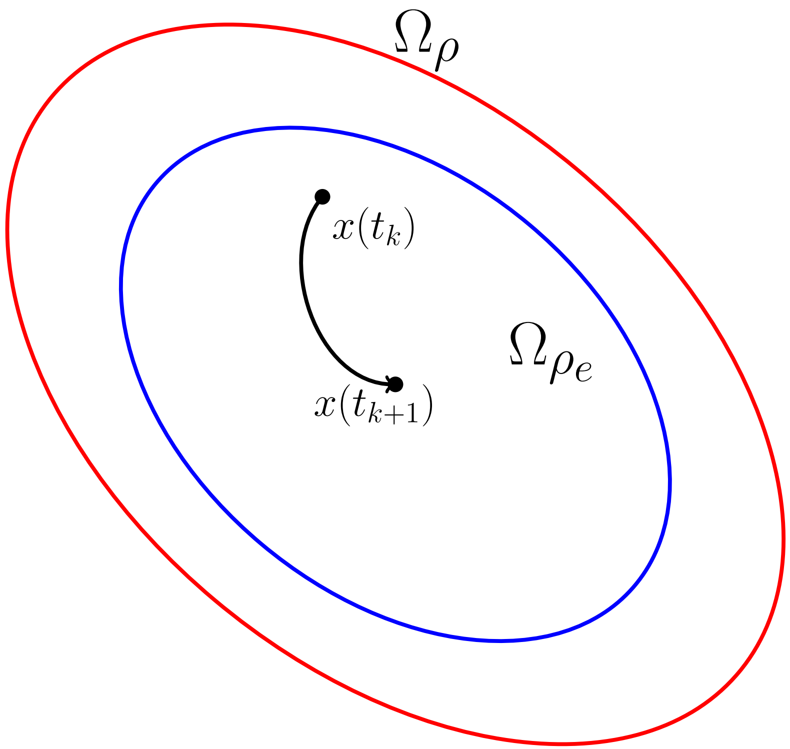
$$\tilde{x}(t_k) = x(t_k)$$

$$u(t) \in U,\ \tilde{x}(t) \in X,\ \forall\, t \in [t_k, t_{k+N})$$

$$|u_i(t_j) - h_i(\tilde{x}(t_j))| \leq \epsilon_r,\ i = 1, \ldots, m,$$
$$j = k, \ldots, k+N-1$$

$$\frac{\partial V(x(t_k))}{\partial x} f(x(t_k), u(t_k), 0) \leq \frac{\partial V(x(t_k))}{\partial x} f(x(t_k), h(x(t_k)), 0)$$

if $V(x(t_k)) > \rho_e$ or $t_k \geq t_s$




- Compute control actions that decrease the Lyapunov function
- Provable stability: convergence to a small neighborhood of the steady-state

# CYBERSECURITY AND PROCESS CONTROL SYSTEMS

- Cyberattacks on control systems seek to impact a physical process and can impact safety, profit, and production rates (A.A. Cárdenas *et al.*, *ASIACCS*, 2011)
- Do cyberattackers care about attacking control and manufacturing systems?
  - ◇ 2010: Stuxnet (trellix.com)
    - ▷ Attack on Iranian nuclear facilities
    - ▷ Worm entered systems via USB sticks and spread
    - ▷ Searched for control system software
    - ▷ Ran centrifuges at conditions that cause breakdown
    - ▷ Falsified information to main controller so that there was no indication of a problem
  - ◇ December 2015: Part of Ukraine power grid (K. Zetter, *Wired*, 2016)
    - ▷ Remote manipulation of circuit breakers
    - ▷ Locking real operators out of their accounts
    - ▷ Malicious firmware prevented operators from un-doing attacks
    - ▷ Turned off backup power for operators
    - ▷ Telephone denial of service to prevent operators from finding out about power outages too quickly

# CYBERSECURITY AND PROCESS CONTROL SYSTEMS

- Cyberattacks on control systems seek to impact a physical process and can impact safety, profit, and production rates (A.A. Cárdenas *et al.*, *ASIACCS*, 2011)
- Do cyberattackers care about attacking control and manufacturing systems?
  - ◇ 2017: Triton (M. Giles, *MIT Technology Review*, 2019)
    - ▷ Malware that can prevent safety instrumented systems from activating when needed
    - ▷ Present on a petrochemical plant in Saudi Arabia
    - ▷ Flaw caused safety systems to act up in a way that revealed it before it could cause an incident
  - ◇ 2021: Florida water treatment plant (J. Bergal, *PEW*, 2021)
    - ▷ Remote user changed sodium hydroxide level to be 100 times higher than it should have been
    - ▷ Operator saw this and changed it back
  - ◇ 2021: Colonial Pipeline (W. Turton and K. Mehrotra, *Bloomberg*, 2021)
    - ▷ Ransom note requesting payment appeared on company computer
    - ▷ Company closed down pipeline due to uncertainty as to whether operational technology was compromised

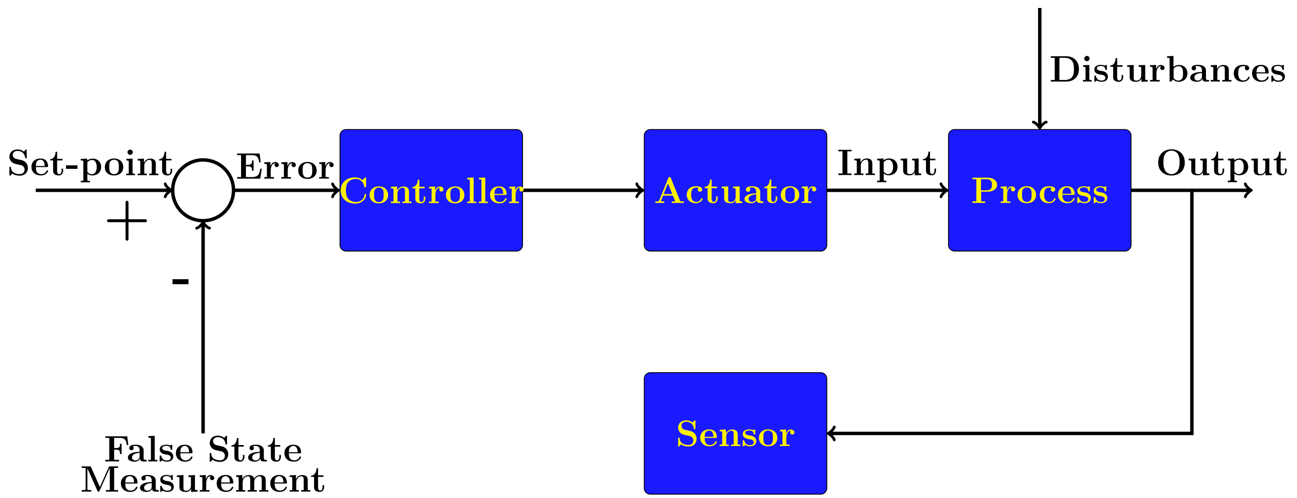
# CYBERATTACK-RESILIENT CHEMICAL PROCESSES

- Examples of attack types: (N. Tuptuk and S. Hailes, *Journal of Manufacturing Systems*, 2018)
  - ◇ Denial of Service: Preventing parts of a network from delivering to others
  - ◇ Eavesdropping: Attackers quietly learn about the system to prepare for more active attacks
  - ◇ False data injection
  - ◇ Time delay attack: Delay occurs in measurements or control actions
  - ◇ Data tampering attack: Data can be altered in storage or transmittal
  - ◇ Replay attack: Correct information from before is sent again
- Cyberattacks on feedback controllers are problematic because they remove associations between state measurements and inputs
  - ◇ Undesired inputs $u \in U$ can be applied at a given state
  - ◇ Defies standard notions of feedback control
- Desirable to understand how elements of a control loop can contribute to detection and handling of attacks
  - ◇ Goal: Understand how and whether control theory-based cyberattack-handling can aid in providing security with flexibility for next-generation manufacturing

# CYBERATTACK-RESILIENT CHEMICAL PROCESSES: A NONLINEAR SYSTEMS DEFINITION

(H. Durand, *Mathematics*, 2018)

- Physical damage from attacks can come from manipulating actuators in a rogue manner (directly or indirectly)
- Focus on sensor and actuator attacks individually to build toward handling both at once
- Cyberattack-resilience for state measurement falsification requires:
  - ◇ There exist no possible input policies given the controllers used and their implementation strategies such that $x(t) \notin X$, for any allowable initial state $x_0 \in \bar{X}$ and $w(t) \in W$, $t \in [0, \infty)$

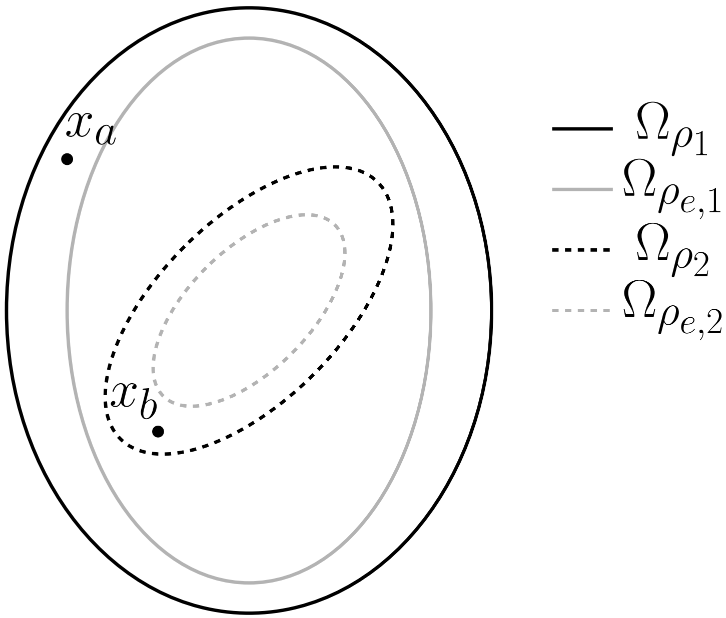


# DISCOVERING PROPERTIES OF CYBERATTACK-RESILIENT PROCESS CONTROL DESIGNS

- The definition of cyberattack-resilient control design is non-constructive
- Developing cyberattack-resilient control strategies will require a better understanding of which designs do and do not work and why
- Explore 2 ideas for cyberattack-resilient controllers:
  - ◇ Controller implementation incorporating randomness
  - ◇ Integrating feedback control/open-loop control
- Conclusions:
  - ◇ Nonlinear systems definition of cyberattack-resilience must be met
    - ▷ Hoping the attacker lacks knowledge about the control design is insufficient
  - ◇ Other techniques (e.g., process design perspectives or techniques which combine control with detection) should be investigated

# CONTROLLER IMPLEMENTATION INCORPORATING RANDOMNESS

- Attacks may be designed by reverse engineering known control laws
  - ◇ Suggests that randomly selecting the controller to be used at a given sampling time may make cyberattack design more difficult
  - ◇ Randomness in control design can only be considered if closed-loop stability is maintained under normal operation
    - ▷ Closed-loop stability and feasibility guarantees can be made with a randomized LEMPC implementation strategy
    - ▷ Cyberattack-resiliency is not guaranteed




- Implementation strategy:
  - ◇ Develop $n_p$ LEMPC's and $h_1(x)$
  - ◇ At each $t_k$, randomly select one of the controllers until one is found for which:
    - ▷ $x(t_k) \in \Omega_{\rho_i}$, $i = 1, \ldots, n_p$, for the $n_p - th$ LEMPC
    - ▷ $x(t_k) \in \Omega_{\rho_1}$ for $h_1(x)$

# CHEMICAL PROCESS EXAMPLE

## Process Description

- Continuous stirred tank reactor (CSTR) with second-order, exothermic, irreversible reaction of the form $A \rightarrow B$:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - k_0 e^{\frac{-E}{RT}} C_A^2$$
$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) + \frac{-\Delta H}{\rho_L C_p} k_0 e^{\frac{-E}{RT}} C_A^2 + \frac{Q}{\rho_L C_p V}$$

- Control objective: regulate the process in an economically optimal time-varying fashion while maintaining closed-loop stability

  ◇ Economic cost:

$$\int_{t_k}^{t_{k+N}} [k_0 e^{-\frac{E}{RT(\tau)}} C_A(\tau)^2] d\tau$$

  ◇ Manipulated input constraints

$$0.5 \leq C_{A0} \leq 7.5 \text{ kmol/m}^3 \qquad -5.0 \times 10^5 \leq Q \leq 5.0 \times 10^5 \text{ kJ / h}$$

  ◇ Deviation variables:

$$x_1 = C_A - C_{As}, \quad x_2 = T - T_s$$

  ◇ Process model in input-affine form $\dot{x} = \tilde{f}(x) + gu$

# CHEMICAL PROCESS EXAMPLE

## Lyapunov-Based Controller Design

- Lyapunov-based controller for the inlet concentration: $h_{1,1}(x) = 0\ \text{kmol/m}^3$
  - ◇ Lyapunov-based controller for the heat rate input:
    - ▷ Sontag's Formula (Y. Lin and E.D. Sontag, *SCL*, 1991)

$$h_{2,1}(x) = \begin{cases} -\dfrac{L_{\tilde{f}}V_1 + \sqrt{L_{\tilde{f}}V_1^2 + L_{g_2}V_1^4}}{L_{g_2}V_1}, & \text{if } L_{g_2}V_1 \neq 0 \\ 0, & \text{if } L_{g_2}V_1 = 0 \end{cases}$$

  - ◇ A quadratic Lyapunov function of the form $V_1(x) = x^T P x$ with:

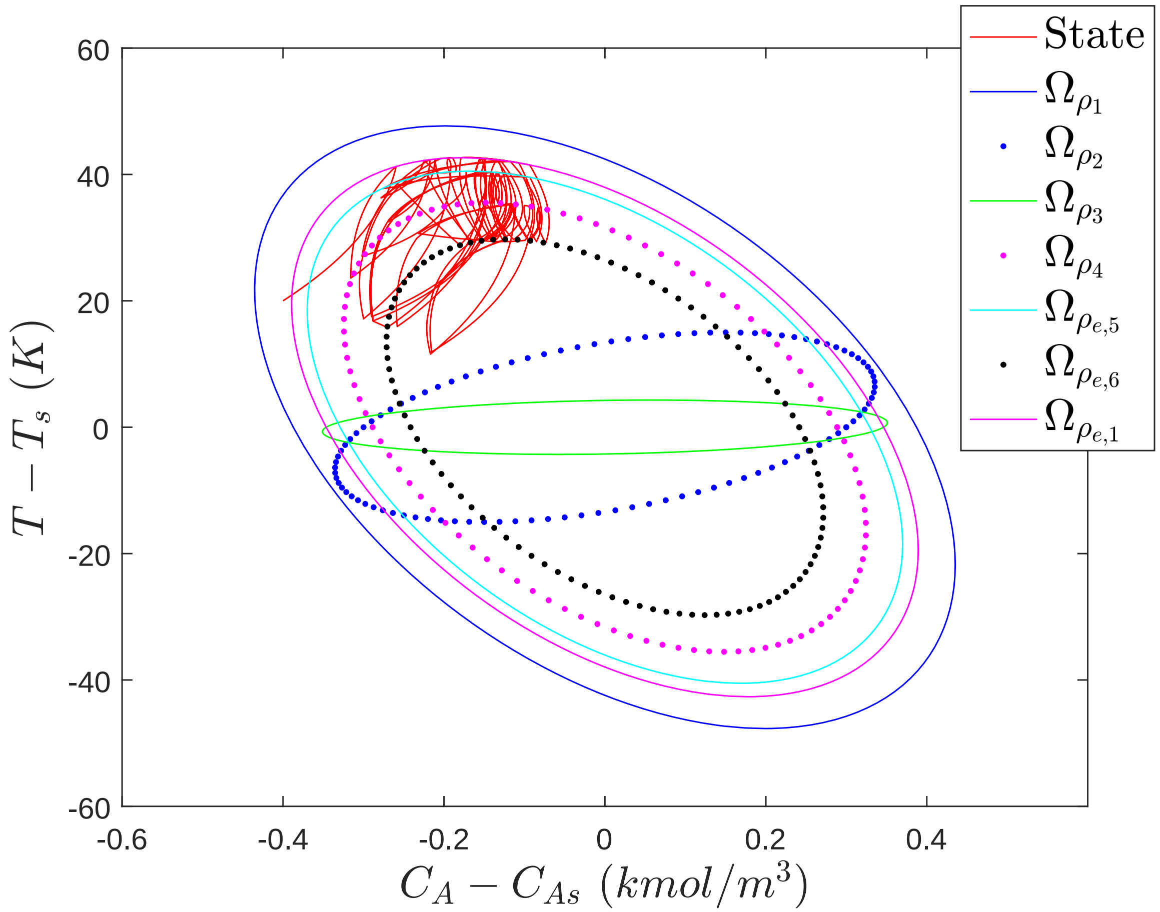
$$P = \begin{bmatrix} 1200 & 5 \\ 5 & 0.1 \end{bmatrix}$$

  - ◇ Stability region $\rho_1 = 180$ (i.e., $\Omega_{\rho_1} = \{x \in R^2 : V_1(x) \leq \rho_1\}$)
- Process state initialized at $x_{init} = [-0.4\ \text{kmol/m}^3\ 20\ \text{K}]^T$
- LEMPC parameters: $N = 10$, $\Delta = 0.01$ h
- Process simulated with an integration step size of $10^{-4}$ h

# CHEMICAL PROCESS EXAMPLE

## Randomized LEMPC Development

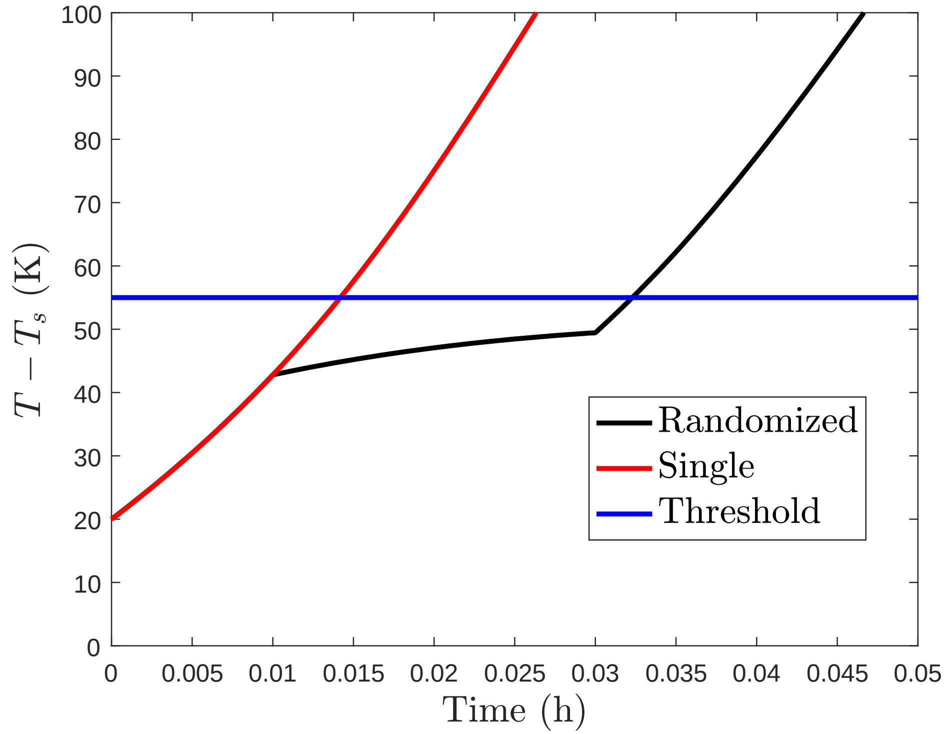
- 6 LEMPC's were designed
  - ◇ $\Omega_{\rho_i} \subseteq \Omega_{\rho_1},\ i = 1, \ldots, 6$
  - ◇ $h_{i,1} = 0$ kmol/m$^3$
  - ◇ $h_{i,2}$ designed via Sontag's control law
  - ◇ Closed-loop state is maintained within $\Omega_{\rho_1}$ throughout 1 h of operation in the absence of a cyberattack



# CHEMICAL PROCESS EXAMPLE

## Randomized LEMPC and LEMPC Under a Cyberattack

- Cyberattack with $x_f = [-0.0521 \text{ kmol/m}^3 \; -8.3934 \text{ K}]^T$ is applied to a single LEMPC and the randomized LEMPC implementation strategy
- Randomized LEMPC results depend on seed to random number generator
- Randomized LEMPC barely delayed the time until $x_2 > 55$ K compared to the single LEMPC (0.0142 h)




| Seed | Time $x_2 > 55$ (h) |
|---|---|
| 5 | 0.0231 |
| 10 | 0.0144 |
| 15 | 0.0142 |
| 20 | 0.0323 |
| 25 | 0.0247 |
| 30 | 0.0142 |
| 35 | 0.0142 |
| 40 | 0.0146 |
| 45 | 0.0247 |
| 50 | 0.0142 |

# INTEGRATING FEEDBACK CONTROL/OPEN-LOOP CONTROL

- Randomized LEMPC implementation strategy could not guarantee that no problematic inputs could be applied over time (even for steady-state tracking)
- Cyberattack resilience against state measurement falsification could be achieved for systems with an open-loop stable steady-state
  - ◇ Applying the steady-state input $u_s$ bypasses the issues with cyberattacks on feedback and drives the closed-loop state to the origin
  - ◇ Loses benefits of feedback control
- Cyberattack-resilience definition must be met
- Three concepts for utilizing LEMPC to attempt to detect attacks were explored (H. Durand and M. Wegener, *Mathematics*, 2020; H. Oyama and H. Durand, *AIChE J.*, 2020)
  - ◇ LEMPC with random control law modifications to probe for cyberattacks
  - ◇ State feedback LEMPC with an attack detection strategy based on state predictions at each sampling time
  - ◇ Output feedback LEMPC (M. Ellis, J. Zhang, J. Liu and P. D. Christofides, *SCL*, 2014; L. Lao, M. Ellis, H. Durand and P. D. Christofides, *AIChE J.*, 2015) with an attack detection strategy based on redundant state estimators

# OBSERVABILITY ASSUMPTION

- $M$ sets of measurements are continuously available:

$$y_i(t) = k_i(x(t)) + v_i(t)$$

  - ◇ $k_i$ is vector-valued function, and $v_i$ represents the measurement noise associated with the measurements $y_i$
  - ◇ $v_i \in V_i \subset \mathbb{R}_i^q$ $(|v_i| \leq \theta_{v,i})$, $i = 1, \dots, M$

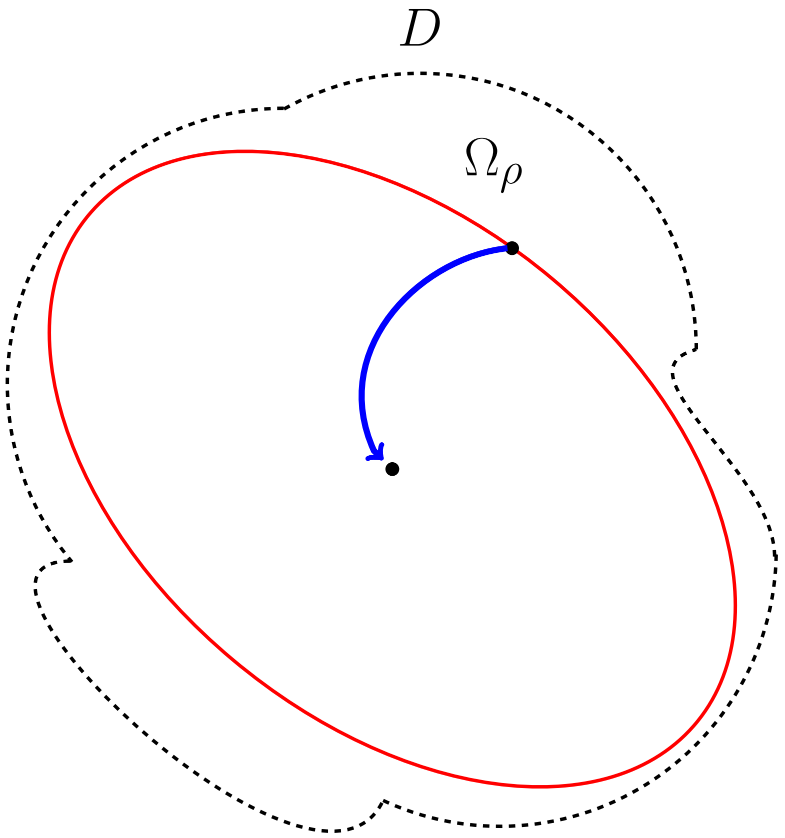
- A deterministic observer exists for each of the $M$ sets of measurements:

$$\dot{z}_i = F_i(\epsilon_i, z_i, y_i)$$

  - ◇ Observer estimate $z_i$; $\epsilon_i > 0$

- Assumptions:
  - ◇ For an initial state estimate with sufficiently low error between $z_i$ and $x$, $h(z_i)$ maintains the closed-loop state in $\Omega_\rho$
  - ◇ There exists a time $t_{bi}$ such that:

$$|z_i(t) - x(t)| \leq \epsilon_{mi}$$



# CYBERATTACK-RESILIENT OUTPUT FEEDBACK LEMPC

- Cyberattacks on state measurements could impact the state estimate used by the LEMPC
- If the estimate is sufficiently incorrect, the closed-loop state may exit $\Omega_\rho$
- Estimator properties suggest an attack detection methodology
  - $|z_i(t) - x(t)| \leq \max\{e_{mi}\}$, $i = 1, \ldots, M$
  - Implies $|z_i(t) - z_j(t)| \leq \epsilon_{\max}$, $i, j = 1, \ldots, M$, when no attack occurs
  - Condition can be used with redundant estimators to attempt to flag falsified sensor measurements

$$
\begin{aligned}
\min_{u(t) \in S(\Delta)} \quad & \int_{t_k}^{t_{k+N}} l_e(\tilde{x}(\tau), u(\tau))\, d\tau \\
\text{s.t.} \quad & \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t)) \\
& \tilde{x}(t_k) = z_1(t_k) \\
& \tilde{x}(t) \in X, \; \forall\, t \in [t_k, t_{k+N}) \\
& u(t) \in U, \;\; \forall\, t \in [t_k, t_{k+N}) \\
& V(\tilde{x}(t)) \leq \rho_{e,1}, \;\; \forall\, t \in [t_k, t_{k+N}), \\
& \qquad \text{if } \tilde{x}(t_k) \in \Omega_{\rho_{e,1}} \\
& \frac{\partial V(\tilde{x}(t_k))}{\partial x} (f(\tilde{x}(t_k), u(t_k))) \\
& \leq \frac{\partial V(\tilde{x}(t_k))}{\partial x} (f(\tilde{x}(t_k), h(x(t_k)))) \\
& \quad \text{if } \tilde{x}(t_k) \in \Omega_\rho / \Omega_{\rho_{e,1}}
\end{aligned}
$$

# CYBERATTACK-RESILIENT OUTPUT FEEDBACK LEMPC

- Consider that at least one state estimate is not impacted by an attacker
- If $|z_i(t) - z_j(t)| > \epsilon_{\max}$, $i, j = 1, \ldots, M$, flag an attack
- If $|z_i(t) - z_j(t)| \leq \epsilon_{\max}$, $i, j = 1, \ldots, M$, but an attack occurred:
  - ◇ Closed-loop state will be maintained in $\Omega_\rho$ over the subsequent sampling period under sufficient conditions
    - ▷ Examples: sufficiently small $\rho_{e,1}$, $\theta$, and $\Delta$

$$
\begin{aligned}
\min_{u(t) \in S(\Delta)} \quad & \int_{t_k}^{t_{k+N}} l_e(\tilde{x}(\tau), u(\tau))\, d\tau \\
\text{s.t.} \quad & \dot{\tilde{x}}(t) = f(\tilde{x}(t), u(t)) \\
& \tilde{x}(t_k) = z_1(t_k) \\
& \tilde{x}(t) \in X, \forall\, t \in [t_k, t_{k+N}) \\
& u(t) \in U, \ \forall\, t \in [t_k, t_{k+N}) \\
& V(\tilde{x}(t)) \leq \rho_{e,1}, \ \ \forall\, t \in [t_k, t_{k+N}), \\
& \qquad \text{if } \tilde{x}(t_k) \ \in \ \Omega_{\rho_{e,1}} \\
& \frac{\partial V(\tilde{x}(t_k))}{\partial x}(f(\tilde{x}(t_k), u(t_k))) \\
& \leq \frac{\partial V(\tilde{x}(t_k))}{\partial x} \ (f(\tilde{x}(t_k), h(x(t_k)))) \\
& \ \text{if } \ \tilde{x}(t_k) \in \Omega_\rho / \Omega_{\rho_{e,1}}
\end{aligned}
$$

# MOTIVATION FOR HANDLING SIMULTANEOUS ACTUATOR AND SENSOR ATTACKS

- Continuous stirred tank reactor (CSTR) with second-order $A \rightarrow B$ reaction:

$$\frac{dC_A}{dt} = \frac{F}{V}(C_{A0} - C_A) - k_0 e^{\frac{-E}{RT}} C_A^2$$
$$\frac{dT}{dt} = \frac{F}{V}(T_0 - T) + \frac{-\Delta H}{\rho_L C_p} k_0 e^{\frac{-E}{RT}} C_A^2 + \frac{Q}{\rho_L C_p V}$$

- Control objective: Optimize process economics while maintaining the closed-loop state in $\Omega_{\rho_1}$

  - ◇ Economic cost:

$$\int_{t_k}^{t_{k+N}} [k_0 e^{-\frac{E}{RT(\tau)}} C_A(\tau)^2] d\tau$$

  - ◇ Manipulated input constraint

$$0.5 \leq C_{A0} \leq 7.5 \text{ kmol/m}^3$$

  - ◇ Deviation variables:

$$x_1 = C_A - C_{As}, \quad x_2 = T - T_s$$

  - ◇ Process model in input-affine form $\dot{x} = \tilde{f}(x) + gu$

# MOTIVATION FOR HANDLING SIMULTANEOUS ACTUATOR AND SENSOR ATTACKS

- Lyapunov-based controller: $h(x) = -1.6x_1 - 0.01x_2$ (M. Heidarinejad, J. Liu, and P. D. Christofides, *SCL*, 2012)
  - ◇ A quadratic Lyapunov function of the form $V_1(x) = x^T P x$ with:

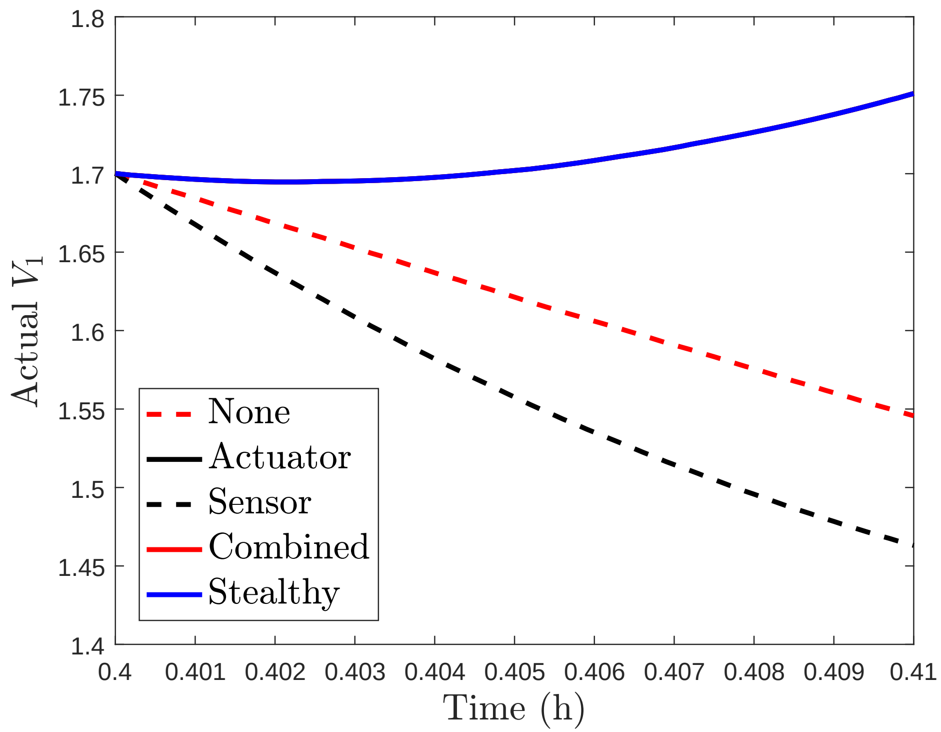
$$P = \begin{bmatrix} 110.11 & 0 \\ 0 & 0.12 \end{bmatrix}$$

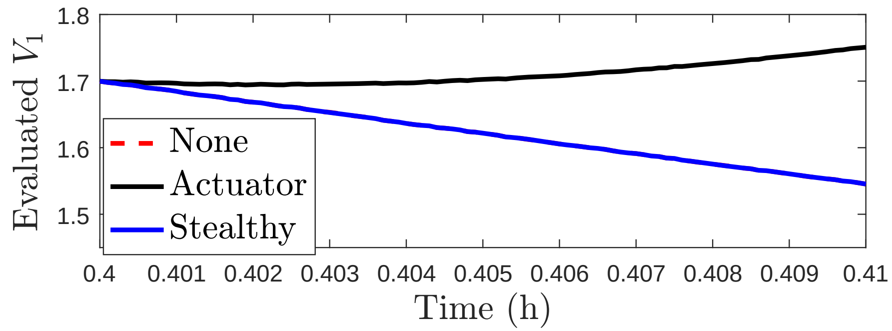
  - ◇ Stability region $\rho_1 = 440$ (i.e., $\Omega_{\rho_1} = \{x \in R^2 : V(x) \leq \rho_1\}$)
  - ◇ $\Omega_{\rho_{e_1}} \subset \Omega_\rho$, $\rho_{e_1} = 330$
- LEMPC parameters: $N = 10$, $\Delta = 0.01$ h
- Process simulated with an integration step size of $10^{-3}$ h
- The LEMPC receives full state feedback with the full system state $x = [x_1 \; x_2]^T$
- Attack detection policy (initialized at 0.4 h when attack begins): Check if Lyapunov function evaluated at the state measurement decreases over $\Delta$

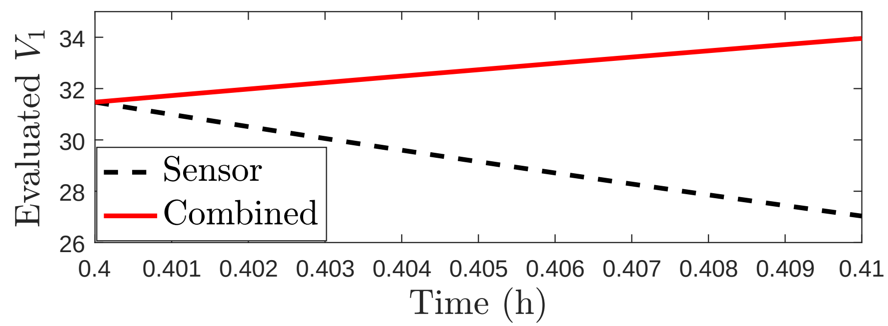
# VARIOUS ATTACK POLICIES

(H. Oyama, D. Messina, K. K. Rangan, and H. Durand, *Frontiers in Chemical Engineering*, 2022)

- Actuator attack ($u = 0.5$ kmol/m$^3$): Discoverable
- False sensor measurement ($x_1 + 0.5$ kmol/m$^3$): Not discoverable (no safety issue)
- Combined actuator and sensor attack: Discoverable
- Stealthy actuator and sensor attack (sensor measurements follow trajectory they should have taken): Not discoverable
  - ◇ State moves closer to safe operating region boundary



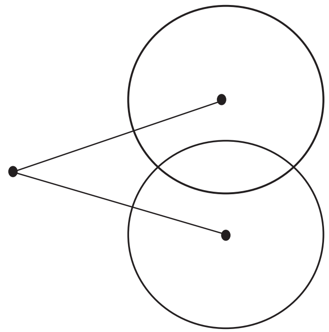
# PREVENTING SAFETY ISSUES DURING SIMULTANEOUS ATTACKS

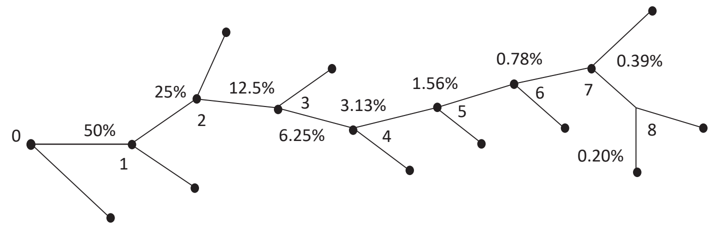
- Multiple detector types can be used to aid in cornering an attacker
  - Examples:
    - Redundant estimators and forcing the decrease of the Lyapunov function across a sampling period
    - Redundant estimators and state predictions with a redundant control law
  - Resilient under sufficient conditions
    - Closed-loop state cannot leave a safe operating region in the presence of individual or simultaneous attacks before attack detection
    - Potentially challenging to obtain reasonable control law parameters satisfying resilience theory
- Fundamental notion of cyberattack discoverability:
  - Whether it is possible to distinguish between a state trajectory coming from attacked sensors and/or actuators and the actual
  - Integrated control and detection policies attempt to use the controller to force differences to show themselves

# EXAMPLE OF DISCOVERABILITY-INSPIRED CYBERATTACK DETECTION

(H. Oyama et al., *Digital Chemical Engineering*, 2023)

- Need a strategy for detecting attacks on sensors that might flag them even with all sensors being compromised
- Set up expectations for measurements that would be "hard" to fake
  - ◇ At every sampling time, two control actions are available
  - ◇ Should result in non-overlapping potential sets of measured states
  - ◇ One of the two is randomly selected
- Random selection many times in a row
  - ◇ May make it challenging to predict how to not get "caught"

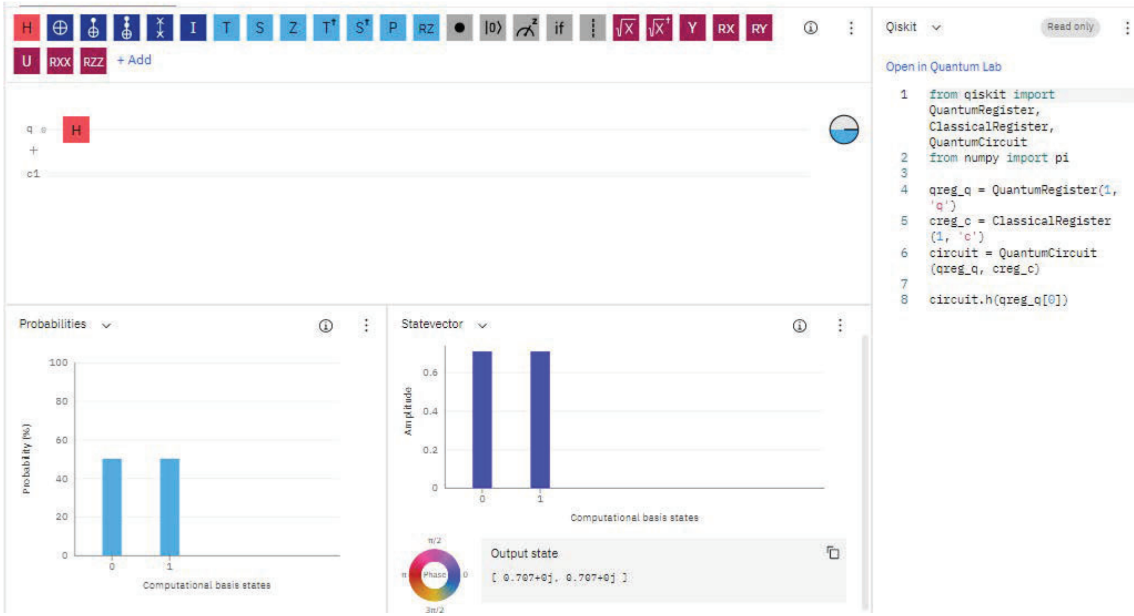




# IMPLEMENTING CONTROL ON QUANTUM COMPUTERS

## Quantum Computing

- Quantum computing is a technology of recent interest in chemical engineering (D.E Bernal et al., AIChE J., 2022)
- Quantum computers exist today of different types




- Quantum annealing
  - ◇ Hardware designed to solve certain optimization problems
- Gate-based computers
  - ◇ Considered a path toward "universal" computation

# QUANTUM MECHANICS FOR QUANTUM COMPUTING VS. CHEMISTRY

- Reminders from chemistry:
  - "Time-independent Schrödinger equation" (eigenvalue-eigenvector relationship)
  $$\hat{H}(x,t)\psi(x,t) = E\psi(x,t)$$
  - Time-dependent Schrödinger equation
  $$\hat{H}(x,t)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$
- $\hat{H}(x,t)$: Hamiltonian (total energy operator)
- Energy $E$
- $\hbar$: Reduced Planck constant
- $\psi(x,t)$: Wavefunction of the quantum system
  - Contains information about position of a quantum system
  - Example: $\psi(x,t)$ is the wavefunction of an electron
    - $\psi(x_0,t_0)^*\psi(x_0,t_0)dx$ conveys the probability that the quantum particle will be found in a spatial interval with width $dx$ around $x_0$ at time $t_0$ (T. Engel, *Prentice Hall*, 2010)

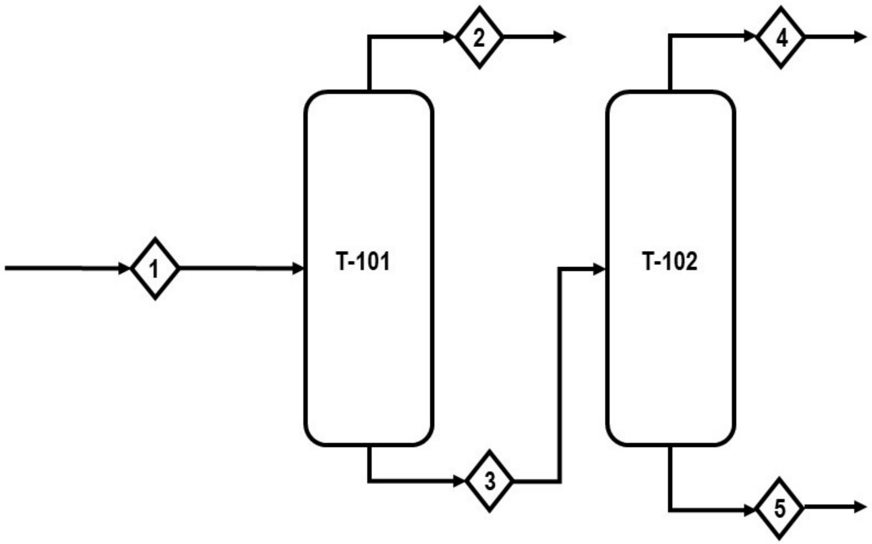
# QUANTUM MECHANICS FOR QUANTUM COMPUTING VS. CHEMISTRY

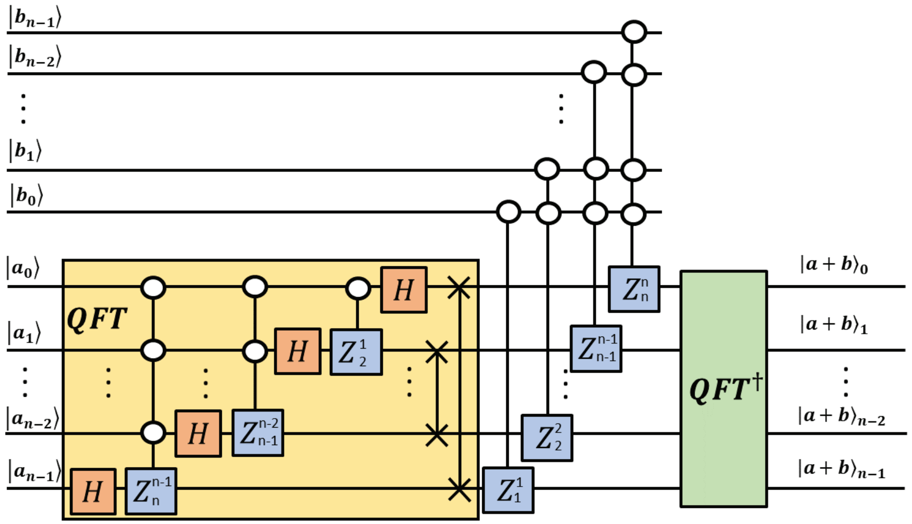
- Wavefunctions are derived from a more fundamental notion of "quantum states"
  - ◇ "Time-independent Schrödinger equation" (eigenvalue-eigenvector relationship)
$$\bar{H}(t)\left|\Psi(t)\right\rangle = E\left|\Psi(t)\right\rangle$$
  - ◇ Time-dependent Schrödinger equation
$$\bar{H}(t)\left|\Psi(t)\right\rangle = i\hbar\frac{\partial\left|\Psi(t)\right\rangle}{\partial t}$$
- $\left|\Psi(t)\right\rangle$ is the "quantum state"
  - ◇ "Dirac notation"
- Wavefunctions are derived from the quantum state in a way that makes them particularly good for representing information about position
- Position is continuous
- Gate-based quantum computers generally stay with the binary concept of classical computing
  - ◇ We only want to have 2 possible quantum states for the system
  - ◇ Position will not work for this

# QUANTUM MECHANICS FOR QUANTUM COMPUTING VS. CHEMISTRY

- Wavefunctions are derived from a more fundamental notion of "quantum states"
  - ◇ "Time-independent Schrödinger equation" (eigenvalue-eigenvector relationship)
  $$\bar{H}(t)\,|\Psi(t)\rangle = E\,|\Psi(t)\rangle$$
  - ◇ Time-dependent Schrödinger equation
  $$\bar{H}(t)\,|\Psi(t)\rangle = i\hbar\frac{\partial\,|\Psi(t)\rangle}{\partial t}$$
- $|\Psi(t)\rangle$ is the "quantum state"
  - ◇ "Dirac notation"
- Wavefunctions are derived from the quantum state in a way that makes them particularly good for representing information about position
- Position is continuous
- Gate-based quantum computers generally stay with the binary concept of classical computing
  - ◇ Wavefunctions are not used in quantum computing
  - ◇ Two possible quantum states: $|0\rangle$ and $|1\rangle$ (regardless of actual implementation)

# CONCEPTUALIZING QUANTUM CIRCUITS

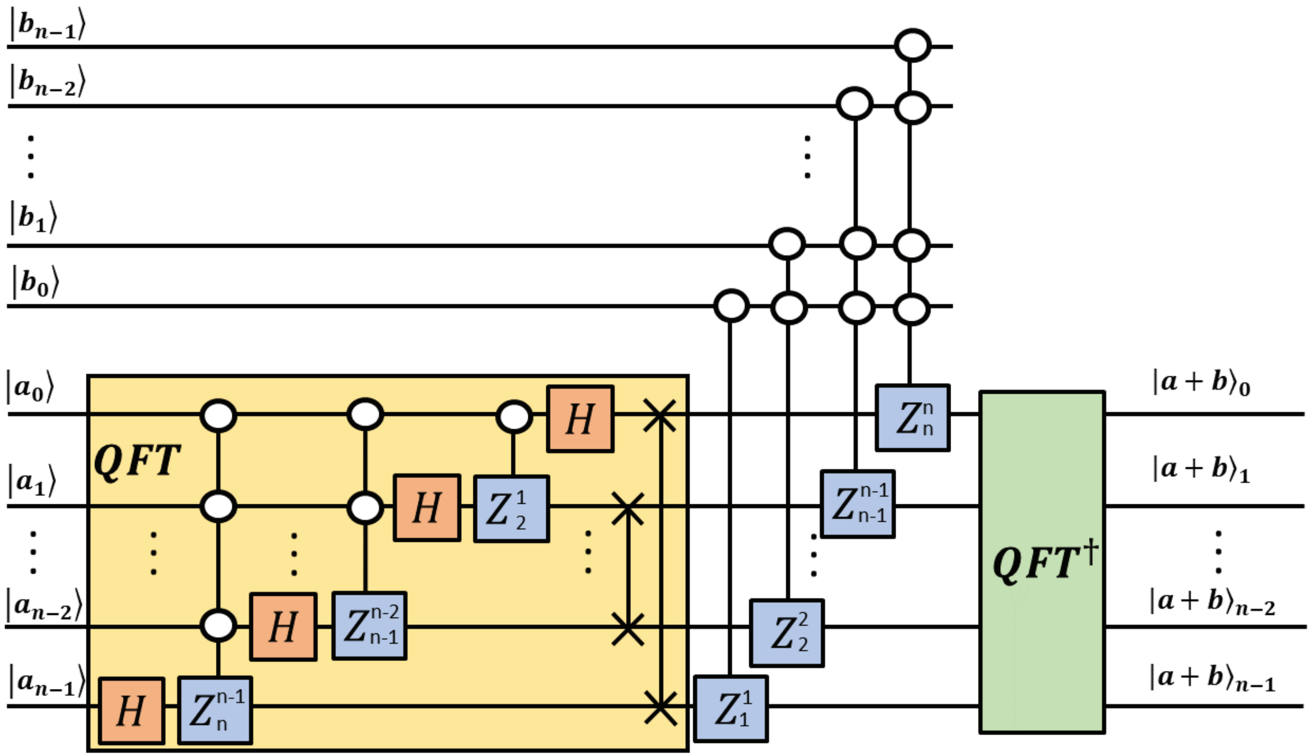



- Each unit of a chemical plant changes the state of a process stream
  - ◇ Symbols and labeling for process units create meaning for chemical engineers regarding the expected state changes
- Each block ("gate") in a quantum circuit changes the state of a quantum system
  - ◇ Symbols and labeling for the gates create meaning regarding the expected state changes
  - ◇ Example: *H* gate puts a qubit in an equal superposition of two states

# QFT-BASED ADDITION

(Ruiz-Perez, L., Garcia-Escartin, J.C., *Quantum Information Processing*, 2017)

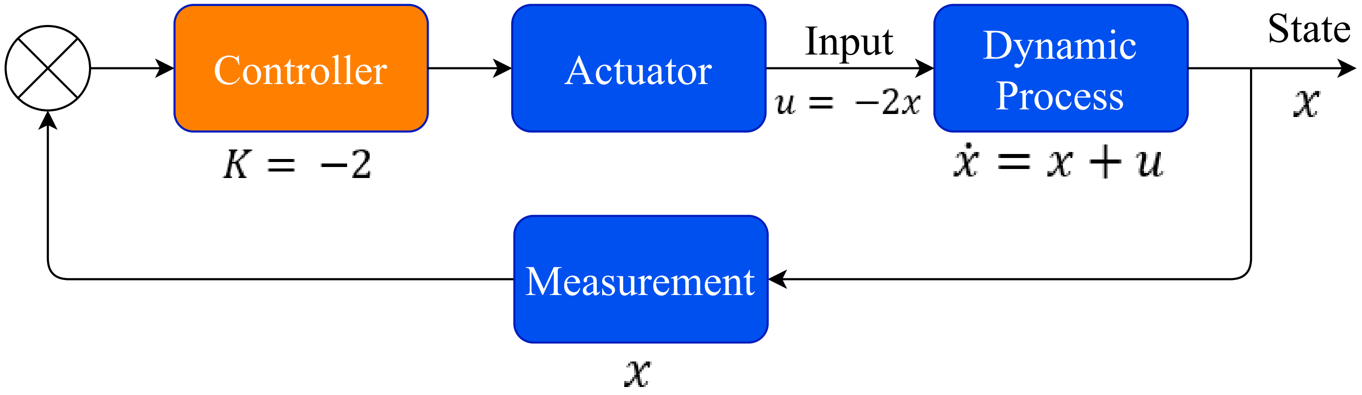



- QFT-based addition: Add two integers $a$ and $b$ (S. Anagolum, Github)
- Binary representations of both numbers are translated to qubit states
- Quantum gates are applied (including those in the inverse QFT, QFT$^\dagger$) to obtain final qubit states representative of the bits of the sum

# QUANTUM COMPUTING-IMPLEMENTED CONTROL EXAMPLE

## Motivation

(K. K. Rangan *et al.*, *DYCOPS*, 2022; K. Nieman, K. K. Rangan, and H. Durand, *IECR*, 2022)

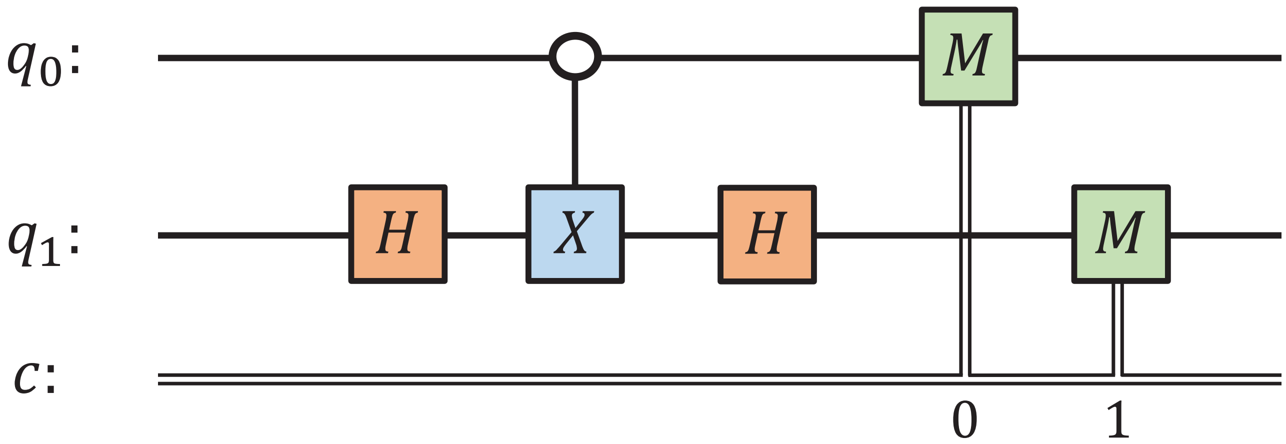



- Today's quantum computers are noisy
  - ◇ Can cause results of a series of gates to be non-deterministic in practice even if it should be deterministic in theory
- If control was implemented on today's quantum computers, noise could make applied inputs non-deterministic for deterministic process behavior
  - ◇ Raises question of when control could be implemented on quantum computers
- Initial study of these effects: a linear dynamic process, $\dot{x} = x + u$, classically stabilized using the control law $u = -2x$

# QUANTUM COMPUTING-IMPLEMENTED CONTROL EXAMPLE

## Noise Model

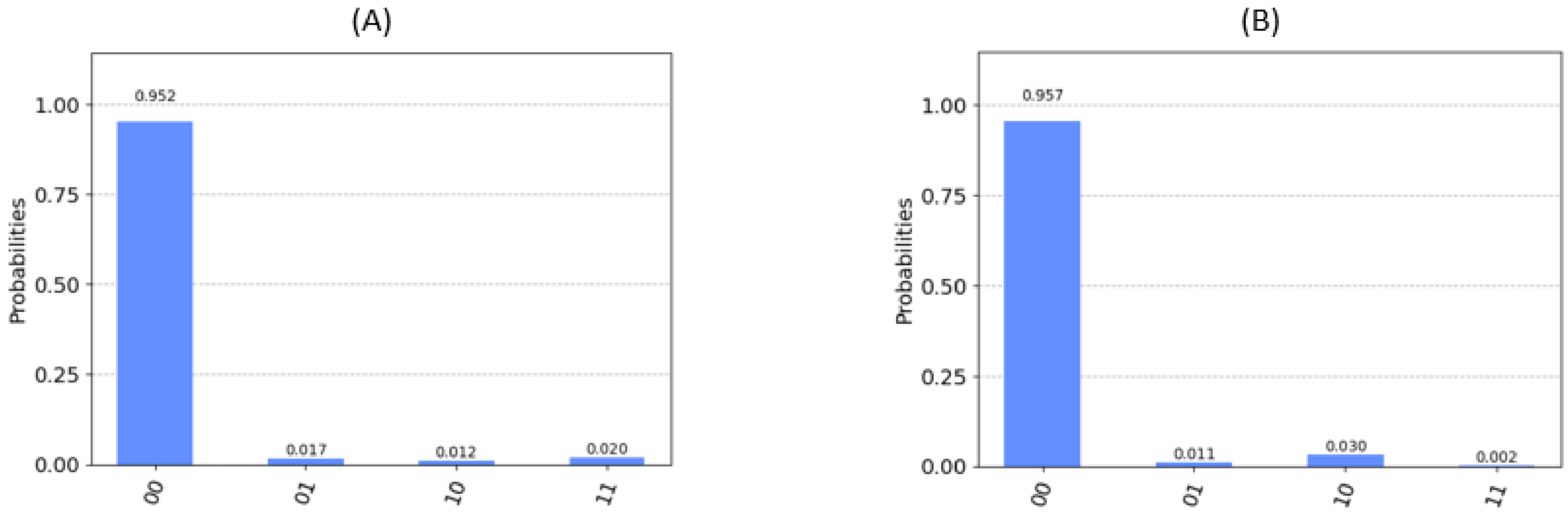
(Garcia-Escartin, J.C., Chamorro-Posada, P., *arXiv*, 2011)




- $u = -2x$ is evaluated using a quantum simulator (qasm_simulator) accessed via Qiskit
  - ◇ Use QFT-based addition to compute $u = -2x$ from $x + x$
- Quantum simulator does not inherently have noise
  - ◇ Required to select a noise model
  - ◇ Evaluated using a controlled $Z$ gate implementation (2 $H$ gates and CNOT gate) as a special case of a controlled phase rotation $Z_k$

# QUANTUM COMPUTING-IMPLEMENTED CONTROL EXAMPLE

## Noise Models

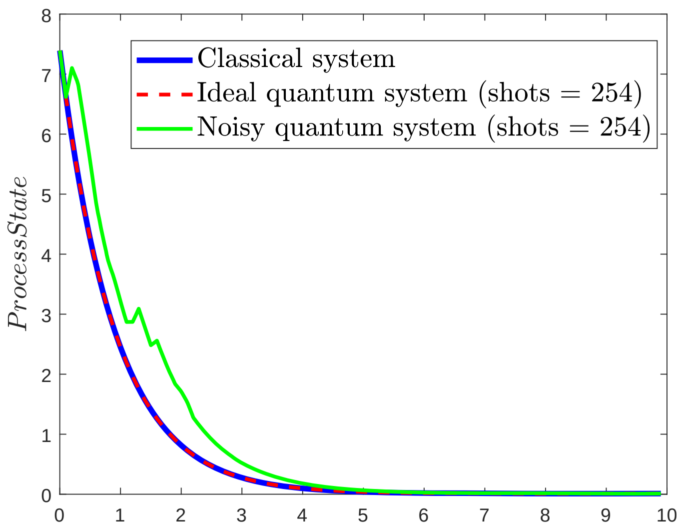


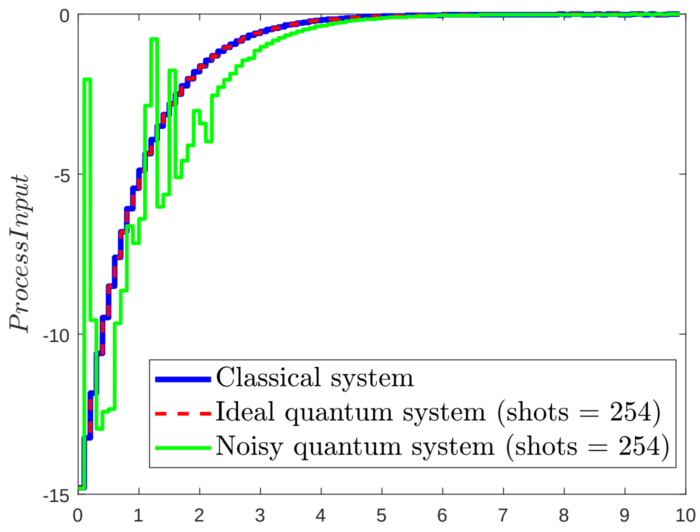

- A depolarizing error parameter for qasm_simulator was selected using command for modeling the noise from the 5-qubit quantum device, ibmq_manila, on the qasm_simulator
  - ◇ The controlled $Z$ gate was simulated with both the qasm_simulator using this noise model from the device backend and with the depolarizing error parameter set to a fixed value on qasm_simulator
- A depolarizing error parameter of 0.05 was determined to sufficiently approximate the results from the simulations based on ibmq_manila

# QUANTUM COMPUTING-IMPLEMENTED CONTROL

## Results

- Comparison between the state trajectories (left) and input trajectories (right) when run with 254 shots for $x(0) = 7.4$
  - ◇ Classical computer (“Classical system”),
  - ◇ Quantum simulator with 254 shots and no noise (“Ideal quantum system”)
  - ◇ Quantum simulator with 254 shots and noise (“Noisy quantum system”)
- Some deviation is observed between the noisy system and the other two, related to the size (in binary) of the state measurement and number of shots

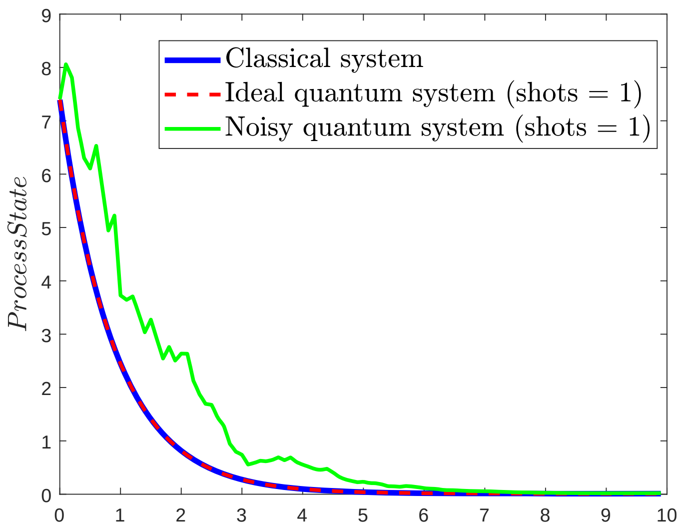


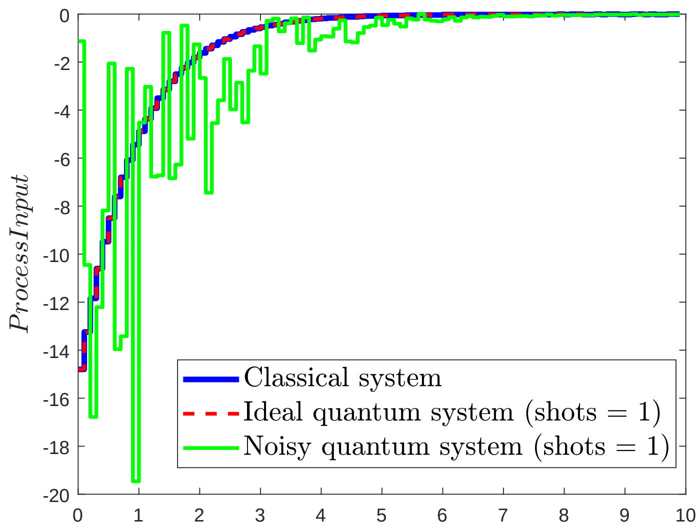



# QUANTUM COMPUTING-IMPLEMENTED CONTROL

## Results

- Comparison between the state trajectories (left) and input trajectories (right) when run with 1 shot for $x(0) = 7.4$
  - ◇ Classical computer ("Classical system"),
  - ◇ Quantum simulator with 1 shot and no noise ("Ideal quantum system")
  - ◇ Quantum simulator with 1 shot and noise ("Noisy quantum system")
- A significant deviation is observed between the noisy system and the other two, related to the size (in binary) of the state measurement and number of shots

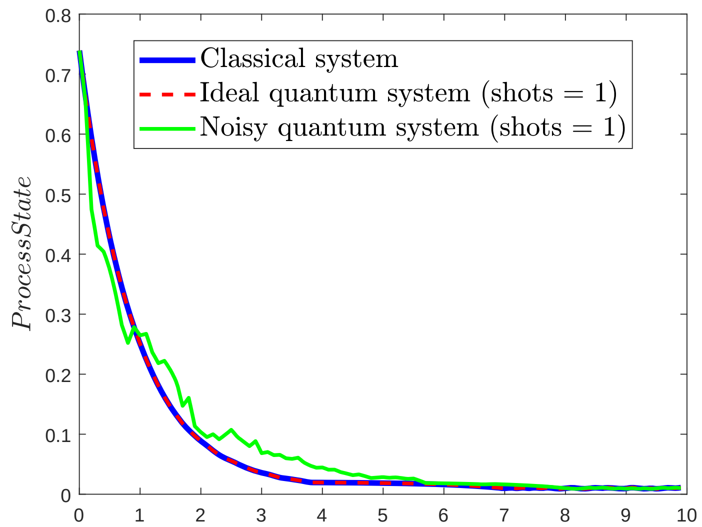


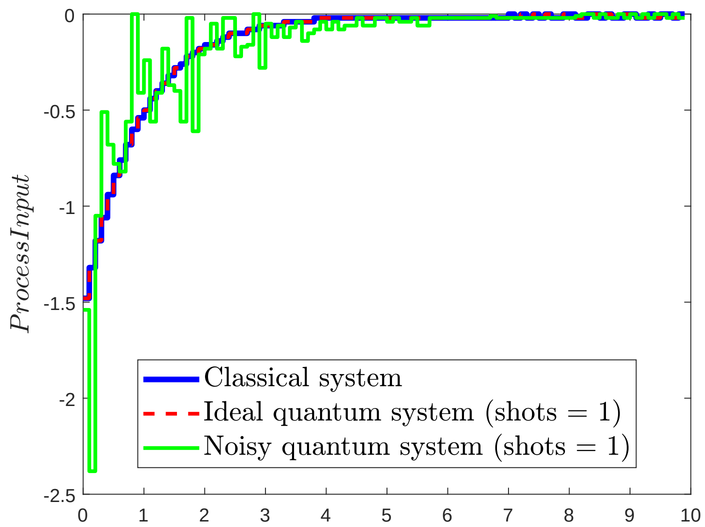



# QUANTUM COMPUTING-IMPLEMENTED CONTROL

## Results

- Comparison between the state trajectories (left) and input trajectories (right) when run with 1 shot for $x(0) = 0.74$
  - ◇ Classical computer ("Classical system"),
  - ◇ Quantum simulator with 1 shot and no noise ("Ideal quantum system")
  - ◇ Quantum simulator with 1 shot and noise ("Noisy quantum system")
- A significant deviation is observed between the noisy system and the other two as a result of the small number of shots

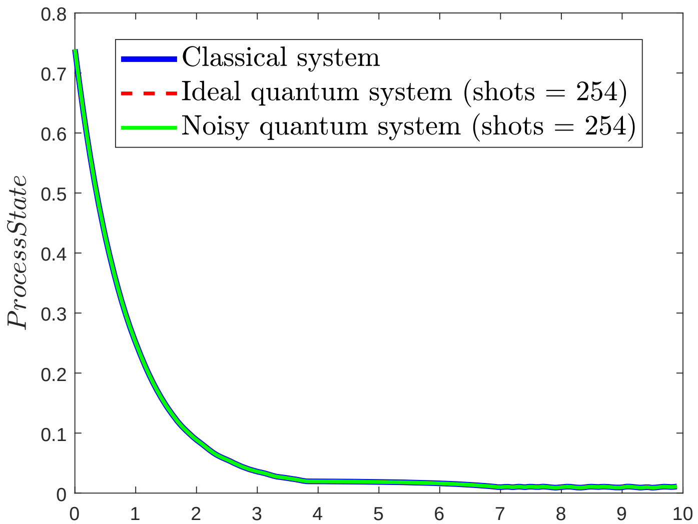


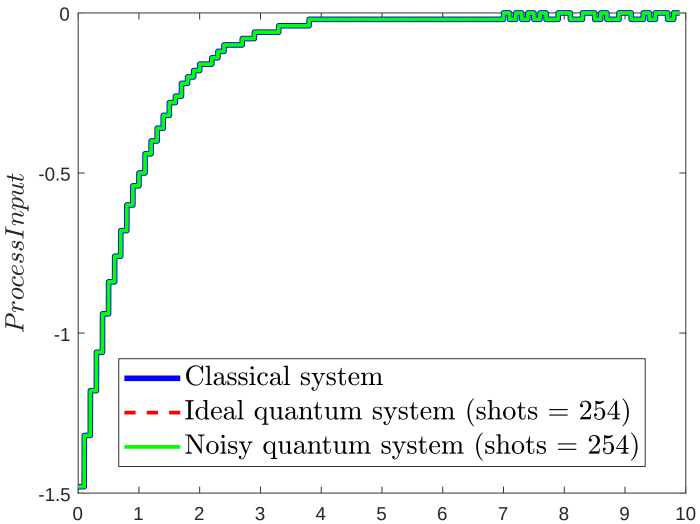



# QUANTUM COMPUTING-IMPLEMENTED CONTROL

## Results

- Comparison between the state trajectories (left) and input trajectories (right) when run with 254 shots for $x(0) = 0.74$
  - ◇ Quantum simulator with 254 shots and noise ("Noisy quantum system")
- No deviation is observed between the noisy system and the other two as a result of the number of shots
- Should we put controllers on quantum computers?
  - ◇ Trying algorithms and evaluating theory to show benefits/limitations



# ADVANCED CONTROL AND QUANTUM COMPUTATION

- Rigorous theory for LEMPC makes it attractive for considering the implications of non-deterministic inputs on stability guarantees
  - ◇ Initial investigations of closed-loop stability of quantum computing-implemented inputs should focus on simple quantum computing algorithms

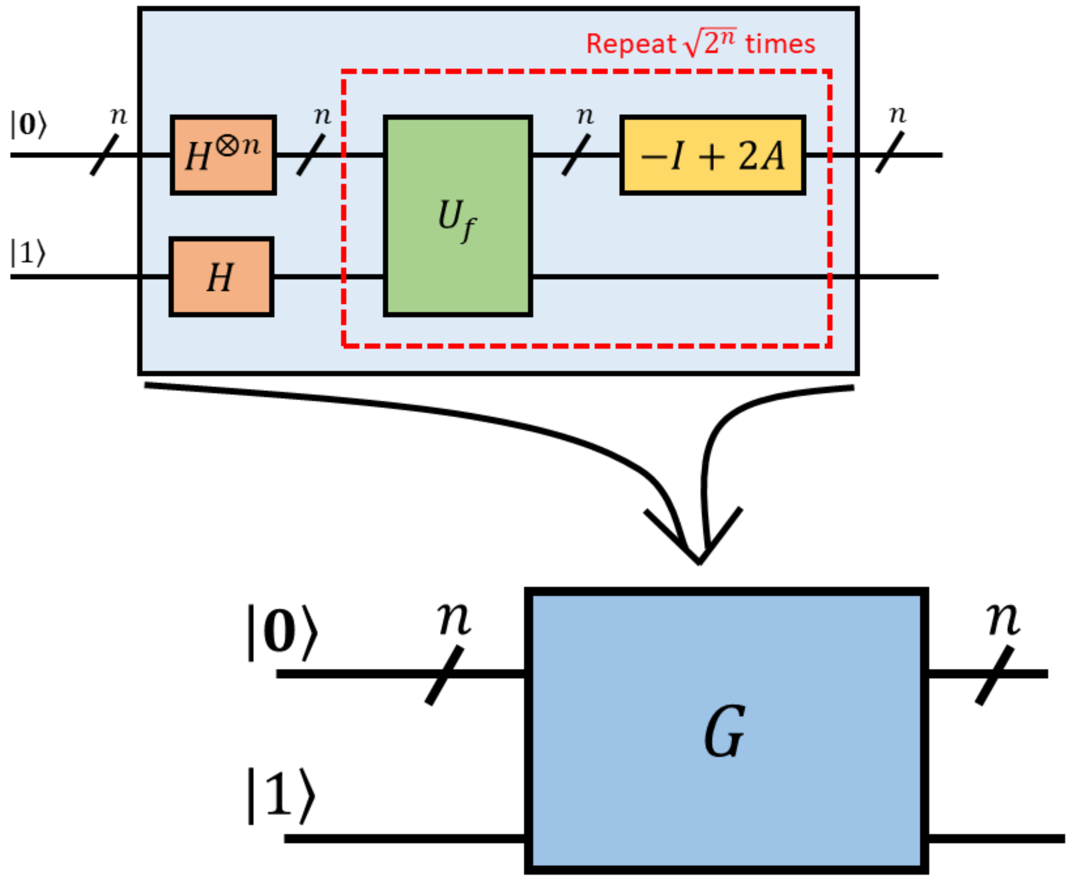
Table 1: LEMPC solution lookup table

| State Measurement | Control Action |
|---|---|
| 0000 | 1111 |
| 0001 | 1110 |
| 0010 | 1010 |
| ⋮ | ⋮ |

- Consider LEMPC solutions in a look-up table
  - ◇ For relating to quantum computing, must express state measurements and inputs in binary
  - ◇ Requires quantization of state measurements for LEMPC
  - ◇ Also quantize control actions output by LEMPC

# SEARCHING AN LEMPC LOOKUP TABLE VIA MODIFIED GROVER'S SEARCH

- Grover's search algorithm is a quantum computing algorithm for searching an unsorted list (Yanofsky and Mannucci, *Cambridge University Press*, 2008)
- A modified version of Grover's algorithm could be used to search the LEMPC lookup table
  - ◇ Not efficient for solving this problem
  - ◇ Show how non-deterministic inputs can be generated by a quantum computing algorithm tied to LEMPC




- Modified Grover's algorithm implementation strategy:
  - ◇ Use a series of controlled Grover blocks to represent the state/input pairings
  - ◇ Measurements return the "correct" input with probability $\lambda$

# IMPLICATIONS FOR CLOSED-LOOP STABILITY

- Probability of obtaining the expected control action from Grover's algorithm: $\lambda$
- Consider $x(t)$ and $\bar{x}(t) \in \Omega_{\rho_e}$
  - ◇ Control action computed by the LEMPC on a classical computer would maintain $x(t_k)$ and $\bar{x}(t_k)$ in $\Omega_\rho$ for $t \in [t_k, t_{k+1})$
  - ◇ The modified Grover algorithm would return the same control action as the classical computer with probability $\lambda$
  - ◇ Conclusion:
    - ▷ $\mathbf{P}(x(t), \bar{x}(t) \in \Omega_\rho \forall\ t \in [t_k, t_{k+1})) \geq \lambda$
- Consider $x(t)$ and $\bar{x}(t) \in \Omega_\rho / \Omega_{\rho_e}$
  - ◇ Control action computed by the LEMPC on a classical computer would maintain $x(t_k)$ and $\bar{x}(t_k)$ in $\Omega_\rho$ for $t \in [t_k, t_{k+1})$
  - ◇ The modified Grover algorithm would return the same control action as the classical computer with probability $\lambda$
  - ◇ Conclusion:
    - ▷ $\mathbf{P}(x(t), \bar{x}(t) \in \Omega_\rho \forall\ t \in [t_k, t_{k+1})) \geq \lambda$

# CONCLUSIONS

- Next-generation manufacturing values flexibility and profitability
  - ◇ Facilitated by automation advances such as economic model predictive control
  - ◇ Flexible and profitable systems may not be secure
    - ▷ Attacks on control systems may undermine process safety
- Integrated detection and control policies geared toward nonlinear systems have potential to enable attacks of various types to be detected before causing safety issues
  - ◇ Requires sufficient control-theoretic conditions
  - ◇ May require at least some sensors to be secure
    - ▷ Handling attacks after detection likely requires some actuators to be secure
- Fundamental notions of cyberattack-resilience and discoverability for nonlinear systems provide insights into potential future directions for securing controllers
- Quantum computing provides another interesting potential direction for the future of next-generation manufacturing
  - ◇ Control theory and practice require further exploration to determine if benefit exists for quantum computing-implemented control

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