Safe Learning-based Predictive Control of Low Temperature Plasmas using Deep Neural Networks and Gaussian Processes

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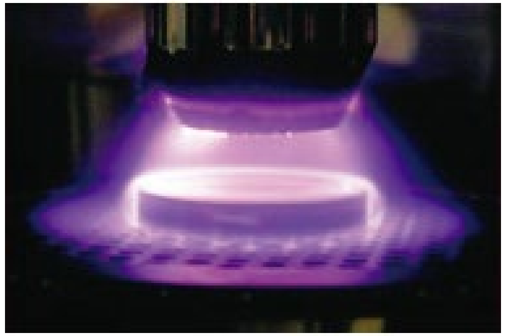
Low Temperature Plasmas (LTPs)

Processing of complex surfaces and interfaces

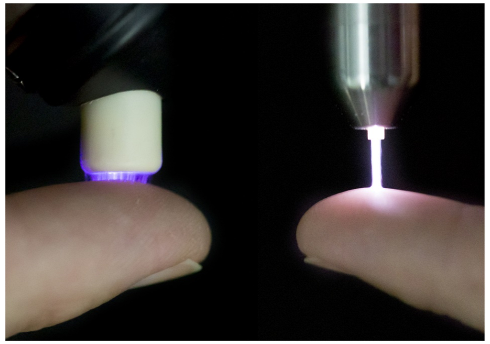
Plasma Etching Process

Surface Coating

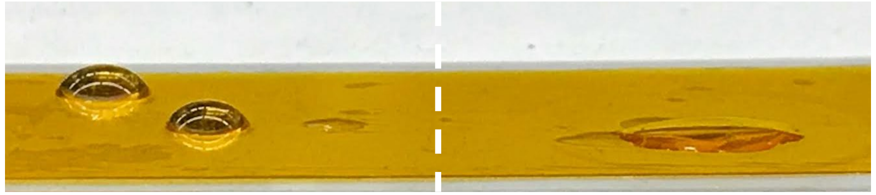
Surface Functionalization



Biomaterials Processing



Water droplets on polyimide film



Not treated Plasma treated

Complex plasma-surface interactions:

- Hard-to-model dynamics across multiple time- and length-scales
- Time-varying surface characteristics
- Lack of real-time diagnostics for surface properties

Grand challenge: Reproducible and precise control of plasma-surface interaction mechanisms

https://www.asbindustries.com/thermal-spray-coatings
http://www.igs.titech.ac.jp/iper/english/iper2/6/detail_44.html
K-D Weltmann and Th von Woedtke, 2016.

Why Advanced Feedback Control for LTPs?

Current practice: Operating protocols for LTP sources devised offline

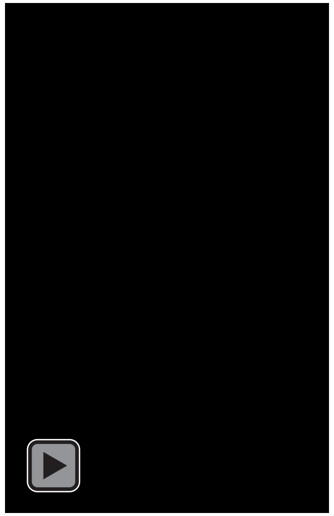
Why go beyond a single operating protocol?

- **Counter disturbances to reproducible plasma operation**
  - Small changes in plasma, surface, or environment can alter fluxes to surface
  - Surface characteristics can vary from point to point and change over time
- **Track plasma-induced surface effects to regulate plasma-surface interactions**
  - Change plasma parameters to optimize delivery of fluxes to surface in real-time

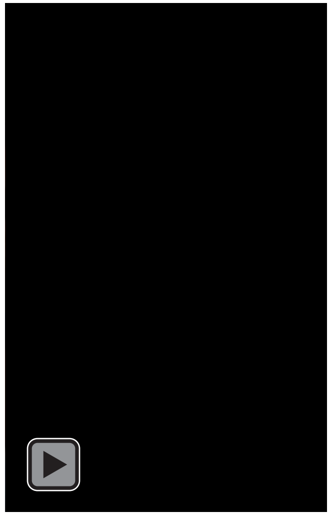
Vision

- Controlled environments for studying plasma effects
- Safe and effective LTP devices for point-of-use applications
- Automated and robotic control for LTP processing of (bio)materials (e.g., using an array of LTP discharges for “large-scale” materials processing)

Substrate Impedance

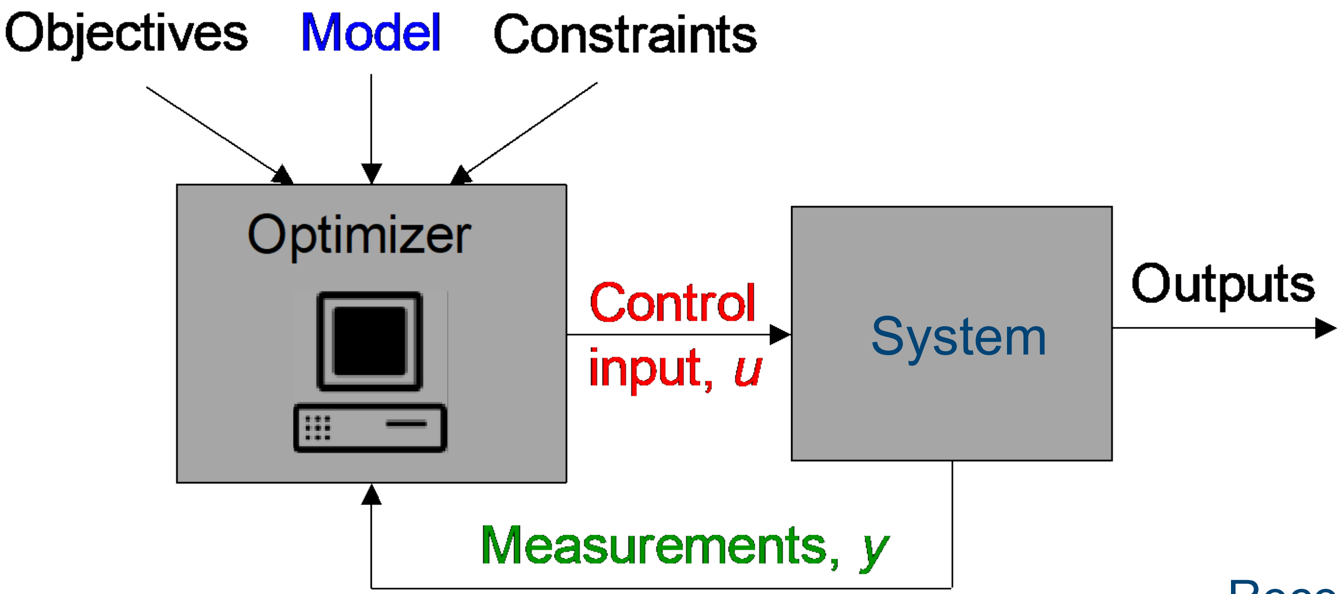


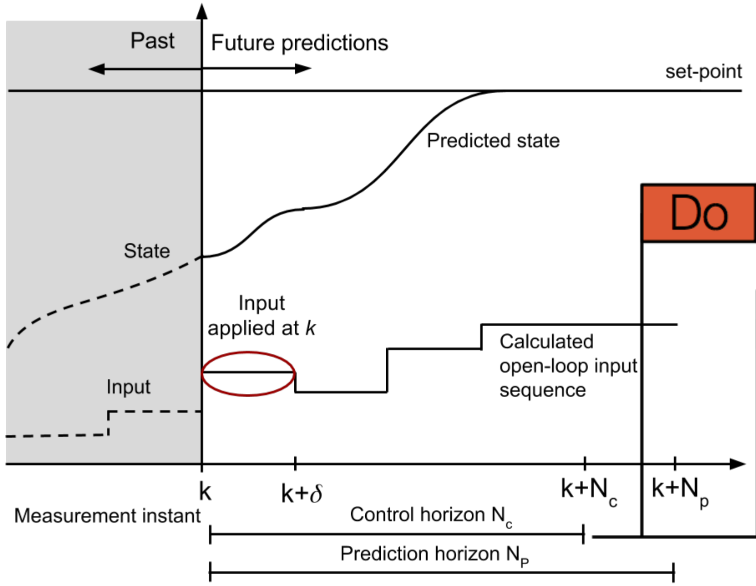
Separation Distance

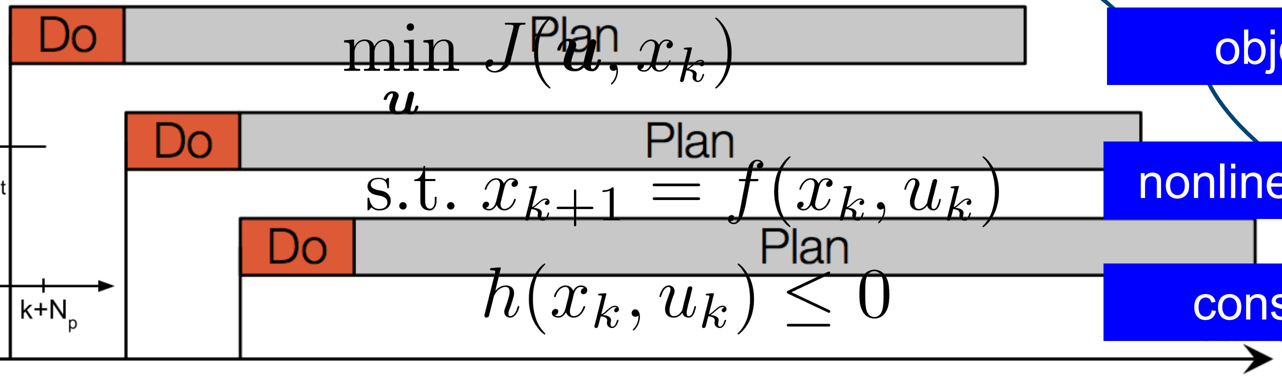


Model Predictive Control (MPC)

An optimization-based feedback control strategy







$$\min_{\boldsymbol{u}} J(\boldsymbol{u}, x_k)$$

$$\text{s.t. } x_{k+1} = f(x_k, u_k)$$

$$h(x_k, u_k) \leq 0$$

objective

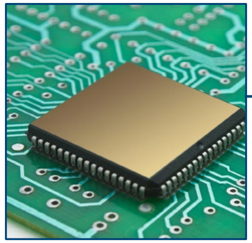
nonlinear model

constraints

Receding-horizon control introduces **feedback**

MPC Applications

Applications over a wide range of length- and time-scales



Embedded systems

Traction control

Chemical processes

Train scheduling

ns
µs
ms
seconds
minutes
hours
days
weeks

Energy systems

Smart buildings

Tissue engineering

Production planning

MPC for Feedback Control of LTP Processing of Complex Surfaces

Key challenges in control of LTP applications

- **Handle hard-to-model and time-varying plasma-induced surface effects:**
  - Predictive models may not be available, thus there is a need for model learning “on the fly”
  - How to explore and exploit the system behavior simultaneously?
- **Handle system uncertainties, imperative in safety-critical and high-performance applications:**
  - Uncertainties arise from disturbances from the environment and model imperfections due to the complex nature of plasma and surface dynamics
  - How to model and incorporate uncertainty into control?
- **Handle fast system dynamics and thus high measurement sampling rates:**
  - There is a need for real-time diagnostics and fast control algorithms
  - How to achieve fast control computations under computational resource limitations?

Leverage stochastic optimal control theory and machine learning to address these challenges towards safe learning-based predictive control for LTPs

Safe Learning-based MPC

Mathematical representation of system dynamics

- **A nominal model is augmented with a function that is learned in real-time to capture unmodeled phenomena using online data:**
  - The nominal model describes our prior knowledge and can be a high-fidelity model or a data-driven model
  - Gaussian process regression is an effective approach for learning the unknown dynamics

$$x_{k+1} = \underbrace{f(x_k, u_k)}_{\text{nominal model}} + B_d\big(\overbrace{g(x_k, u_k)}^{\text{unknown dynamics}} + v_k\big)$$

process noise

unknown dynamics live in the subspace of this matrix

Safe Learning-based MPC

Gaussian processes are non-parametric models and quantify uncertainty of predictions

$$y_j = B_d^{\dagger}(x_{j+1} - f(x_j, u_j)) = g(\overbrace{x_j, u_j}^{z_j}) + v_j$$

Calculate mismatch term over history *M* and store as a new dataset

$$\mathcal{D} = \{\mathbf{y} = [y_1, \ldots, y_M]^\top,\ \mathbf{z} = [z_1, \ldots, z_M]^\top\}$$

Use dataset to train a Gaussian process model that can be used to predict function at any test point

function of full history...

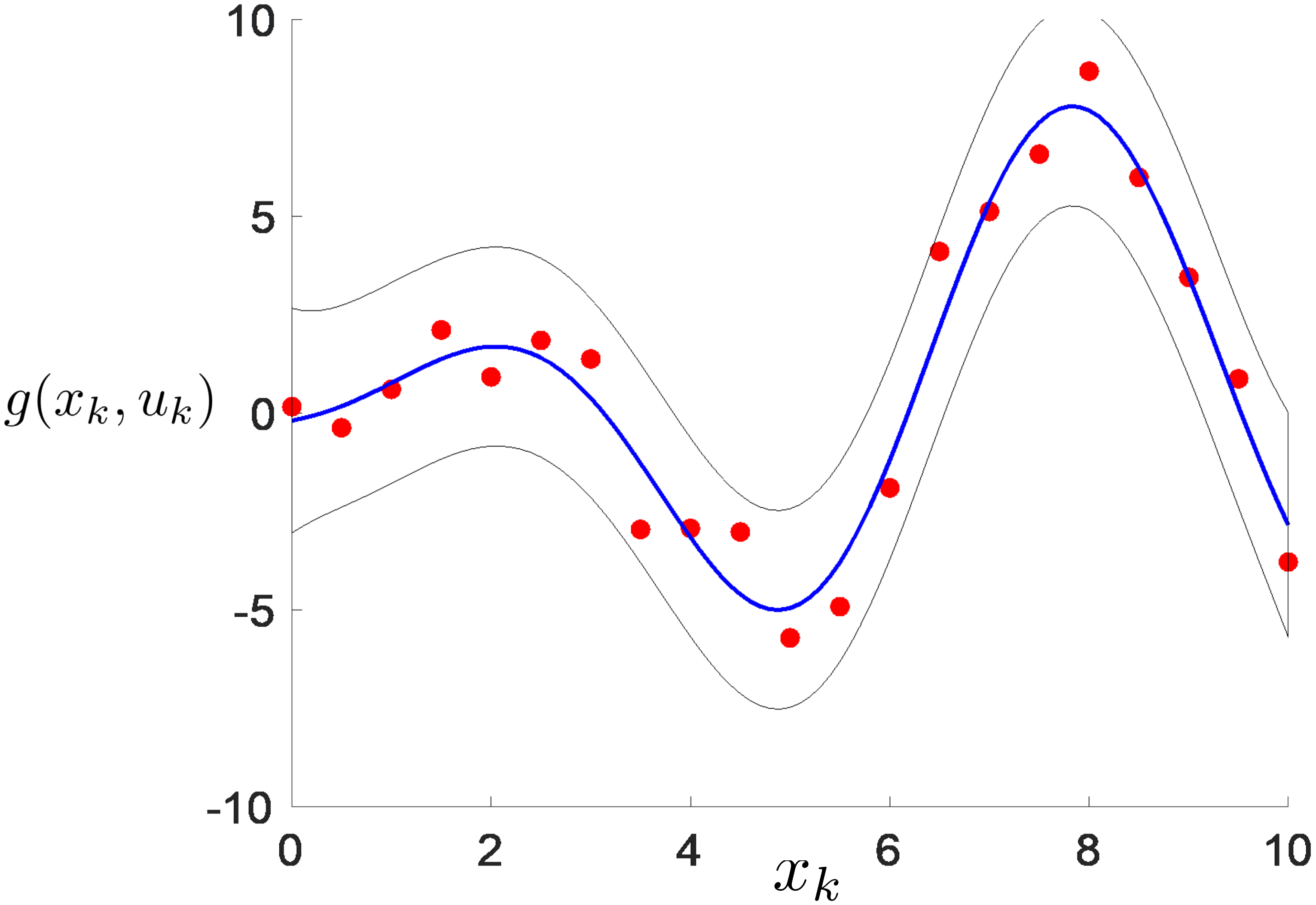
$$\mu^d(z) = m(z) + \mathbf{k}(z)^\top(\mathbf{K} + \sigma^2 I_M)^{-1}\underline{(\mathbf{y} - \mathbf{m})}$$
$$\Sigma^d(z) = k(z, z) - \mathbf{k}(z)^\top(\mathbf{K} + \sigma^2 I_M)^{-1}\mathbf{k}(z)$$

Rasmussen and Williams, 2016.

Safe Learning-based MPC

Gaussian processes are non-parametric models and quantify uncertainty of predictions

$$g(x,u) \sim \mathcal{N}\big(\mu^d(x,u), \Sigma^d(x,u)\big)$$



Safe Learning-based MPC

Control problem that must be solved in real-time

$$\min_{\pi \in \Pi} \quad \mathbb{E}\left\{\sum_{i=0}^{N} J(x_i, u_i)\right\}$$

expected performance (control objective)

system dynamics + uncertainty

$$\text{s.t.} \quad x_{i+1} = f(x_i, u_i) + B_d(\underbrace{g(x_i, u_i)}_{\boxed{\mathcal{N}\left(\mu^d(x,u), \Sigma^d(x,u)\right)}} + v_i)$$

decision variables

$$u_i = \pi(x_i)$$

$$h(x_i, u_i) \leq 0$$

nonlinear state and input constraints

$$x_0 = x$$

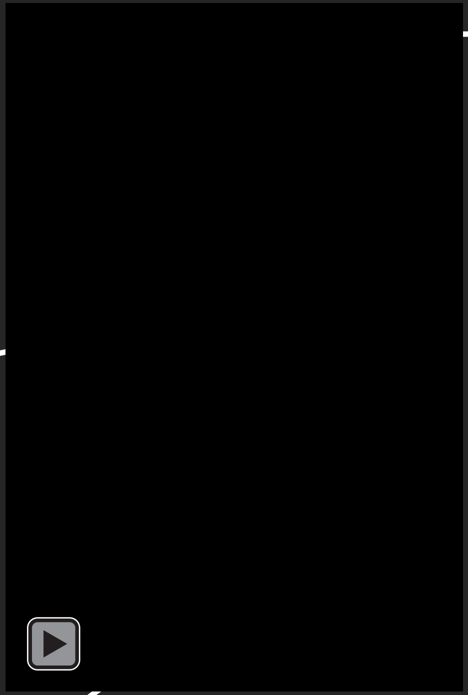
measured state to provide feedback

$$\forall i = 0, \ldots, N-1$$

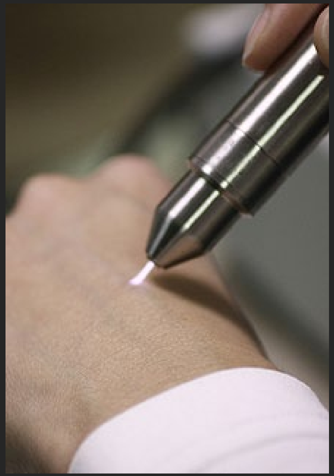
Learning of unmodeled phenomena and uncertainty handling for safe learning are naturally incorporated into online decision-making

Application to a kHz-Excited Atmospheric Pressure Plasma Jet in He

He flow



high-voltage source



safety-critical applications in plasma medicine

1. Identify nominal model

surface temperature & plasma optical intensity

$$x^+ = Ax + Bu$$

He flowrate & applied voltage

2. Train GP model with 100 data points

3. Objective is to deliver thermal effects at the end of treatment time

$$\mathrm{CEM}^+ = \mathrm{CEM} + K^{(43-T_s)}\delta t$$

Delivery of Thermal Effects to Complex Surfaces

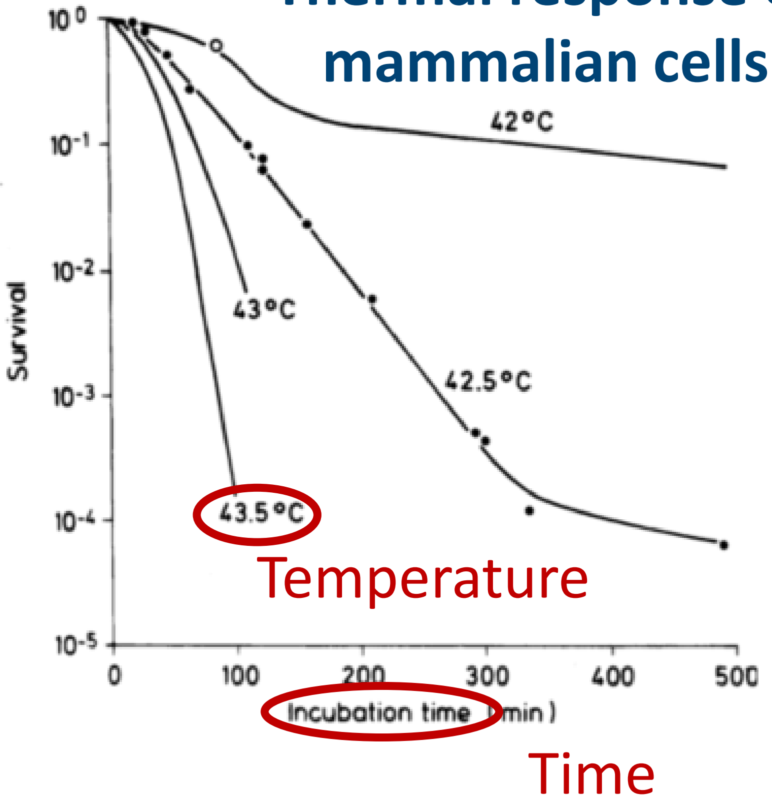
Control the cumulative thermal effects of plasma

Cumulative equivalent minutes (CEM_T)

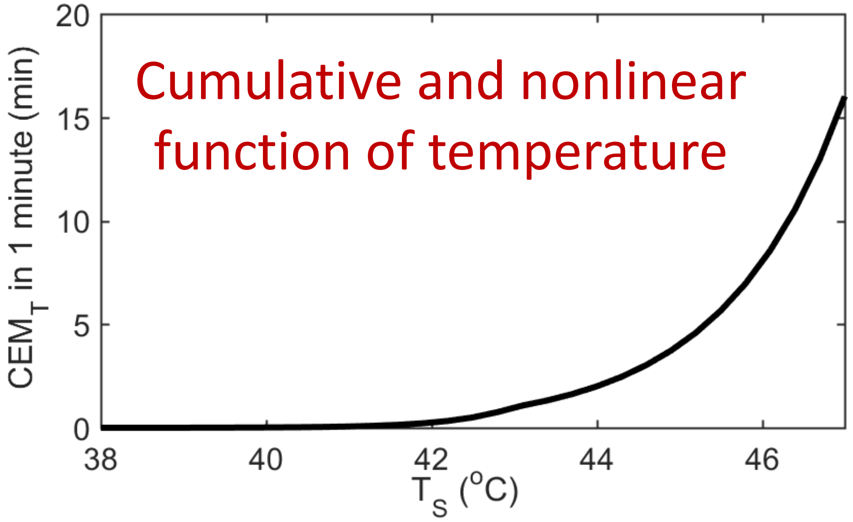
Describes cell death dependence on temperature and exposure time

$$\mathrm{CEM}_{43} = \int_0^t K^{(43-T_s(\tau))}\, d\tau \quad \textbf{[min]}$$

Thermal response of mammalian cells



Plasma-surface thermal effect

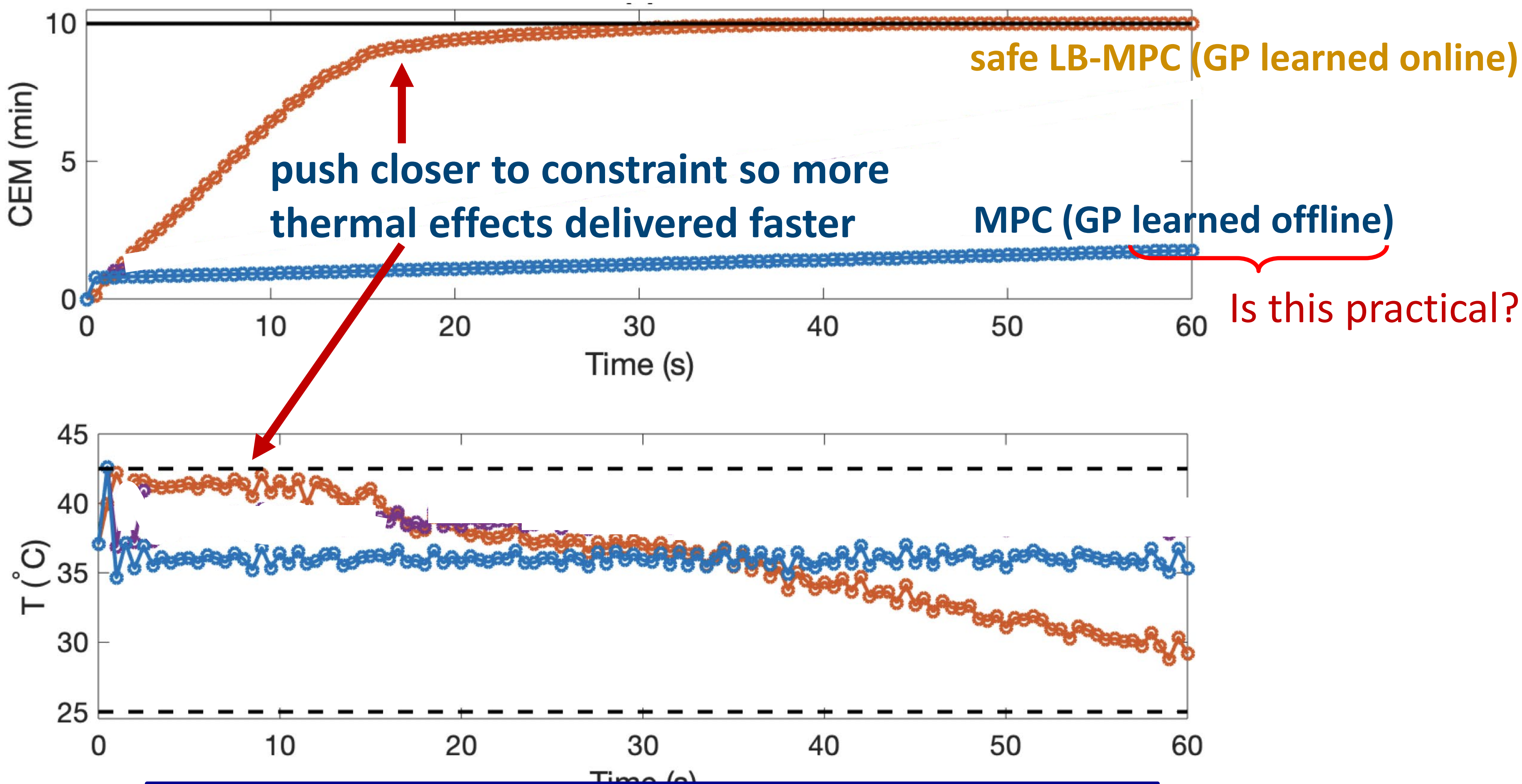


1 min at 43°C = 0.5 min at 44°C
1 min at 43°C = 2 min at 42°C

Sapareto and Dewey, 1984.

Learning-based MPC versus MPC with an Offline Trained Model

Online learning enables significant performance improvement while honoring constraints



Faster LTP treatment without compromising safety

Bonzanini et al., 2021.

Towards Embedded Control Systems for LTPs

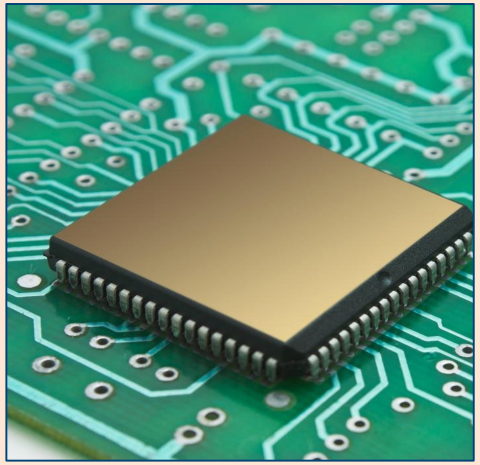
Safe and effective operation of fast sampling LTP devices using inexpensive hardware

Real-time control hinges on fast control computations

- Online solution of the optimization problem can be expensive
- Plasmas have fast dynamics, requiring fast sampling times for feedback control
- Point-of-use and portable LTP devices require control implementations on resource-limited embedded systems

Fast embedded predictive control systems

- Sub-millisecond model predictive control computations
- Control implementations on low-memory and low-power embedded systems
- Inexpensive hardware



Deep Neural Network-based MPC

Towards embedded implementation of deep learning-based controllers

- **Cheap to evaluate**
- **Low memory footprint**

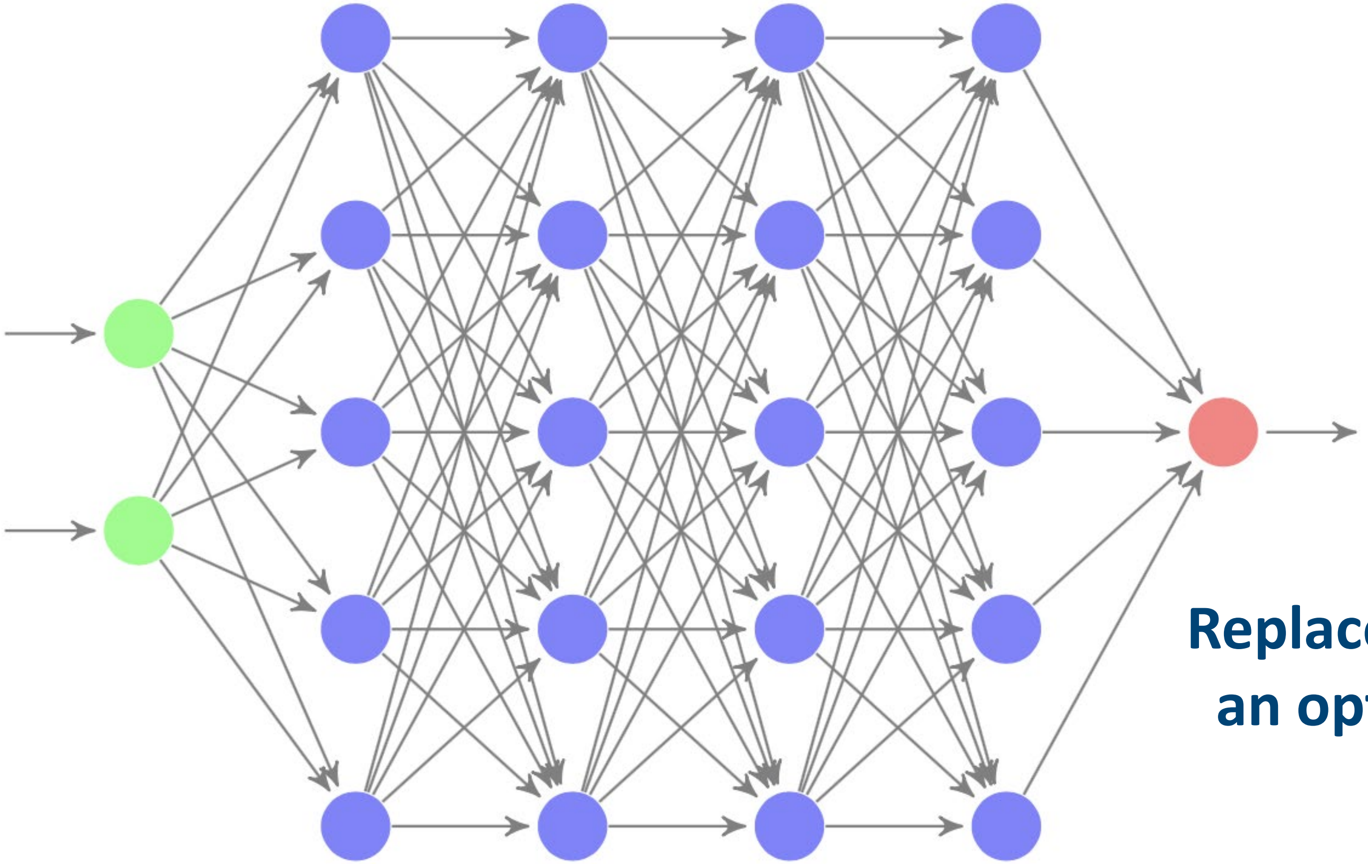
$$\underbrace{\tilde{\kappa}_N(x;p)}_{\text{Explicit control law}} \approx \underbrace{\kappa_N(x)}_{\text{MPC law (implicit function of state)}}$$

(e.g., setpoints)

p

x

(state)

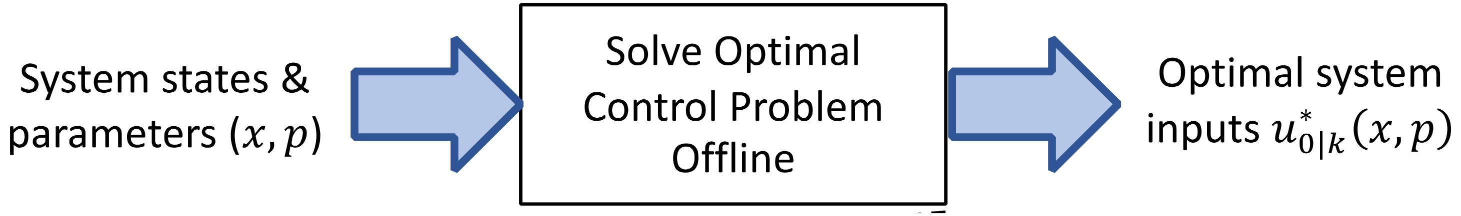


$$\underbrace{\tilde{\kappa}_N(x;p)}_{\text{Replaces online solution of an optimization problem}}$$

Parisini and Zoppoli, 1995
Chen et al., 2018
Karg and Lucia, 2018
Paulson and Mesbah, 2020

Deep Neural Network-based MPC

Towards embedded implementation of deep learning-based controllers



Bonzanini et al., 2020.

Deep Neural Network-based MPC

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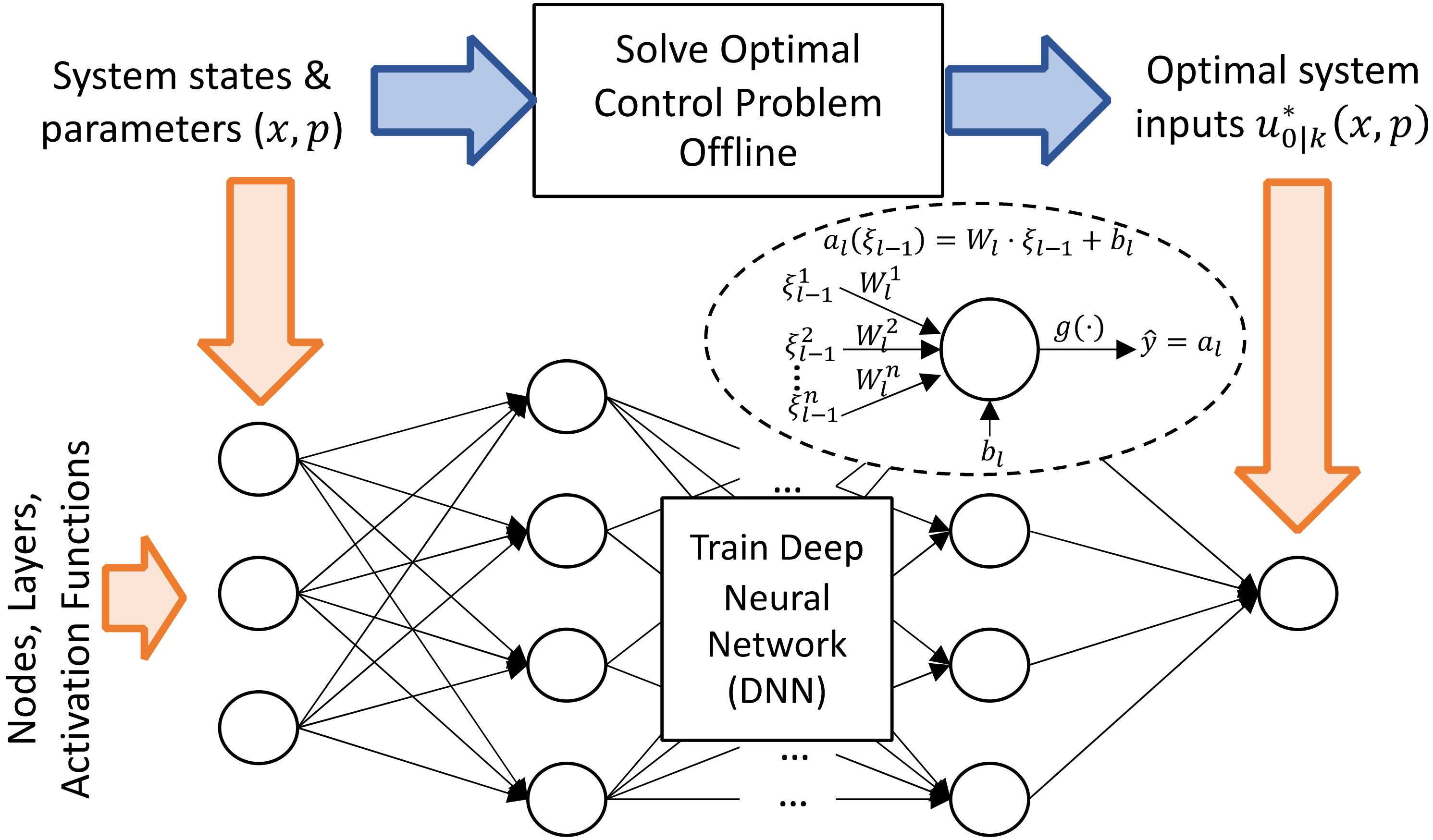

Bonzanini et al., 2020.

Deep Neural Network-based MPC

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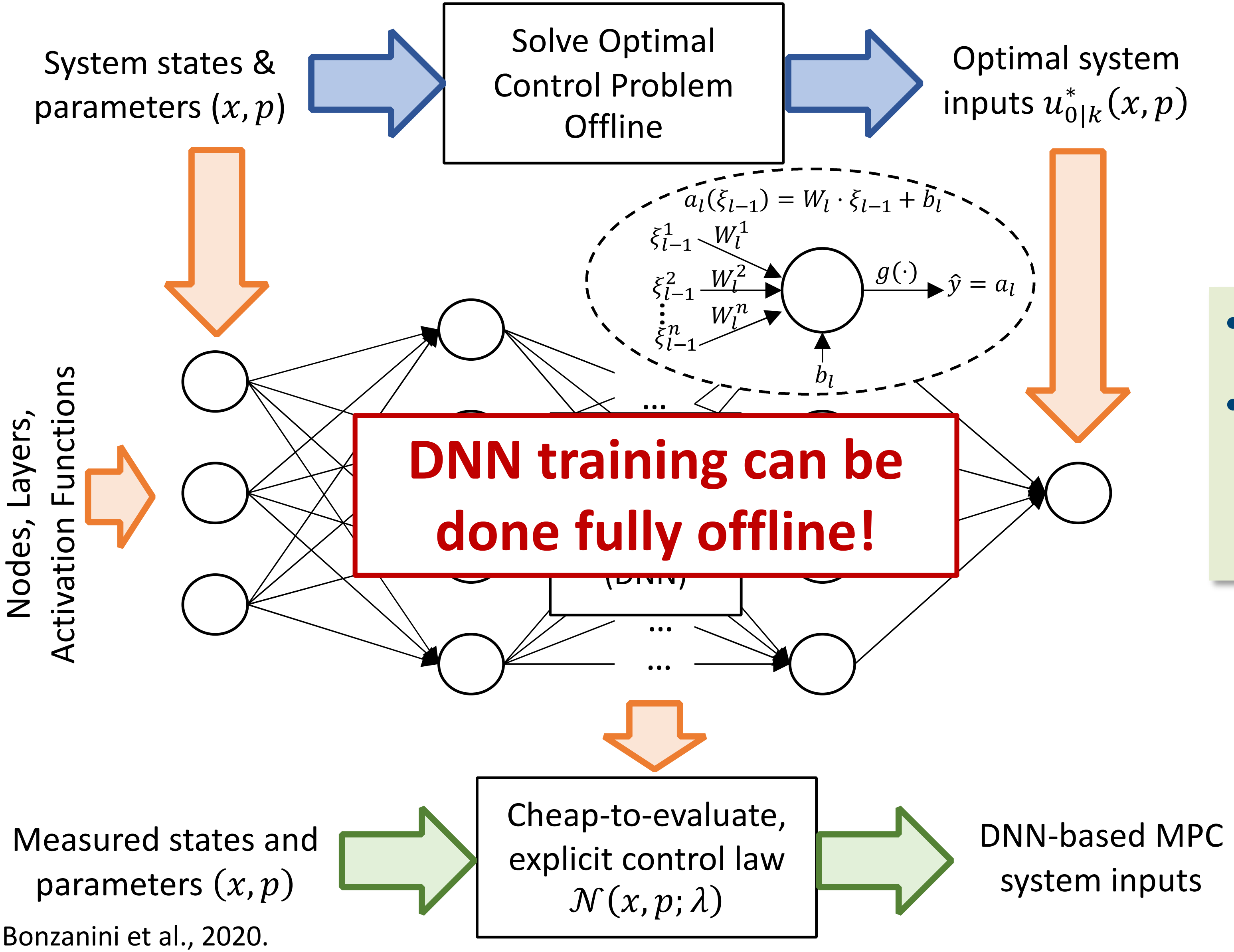


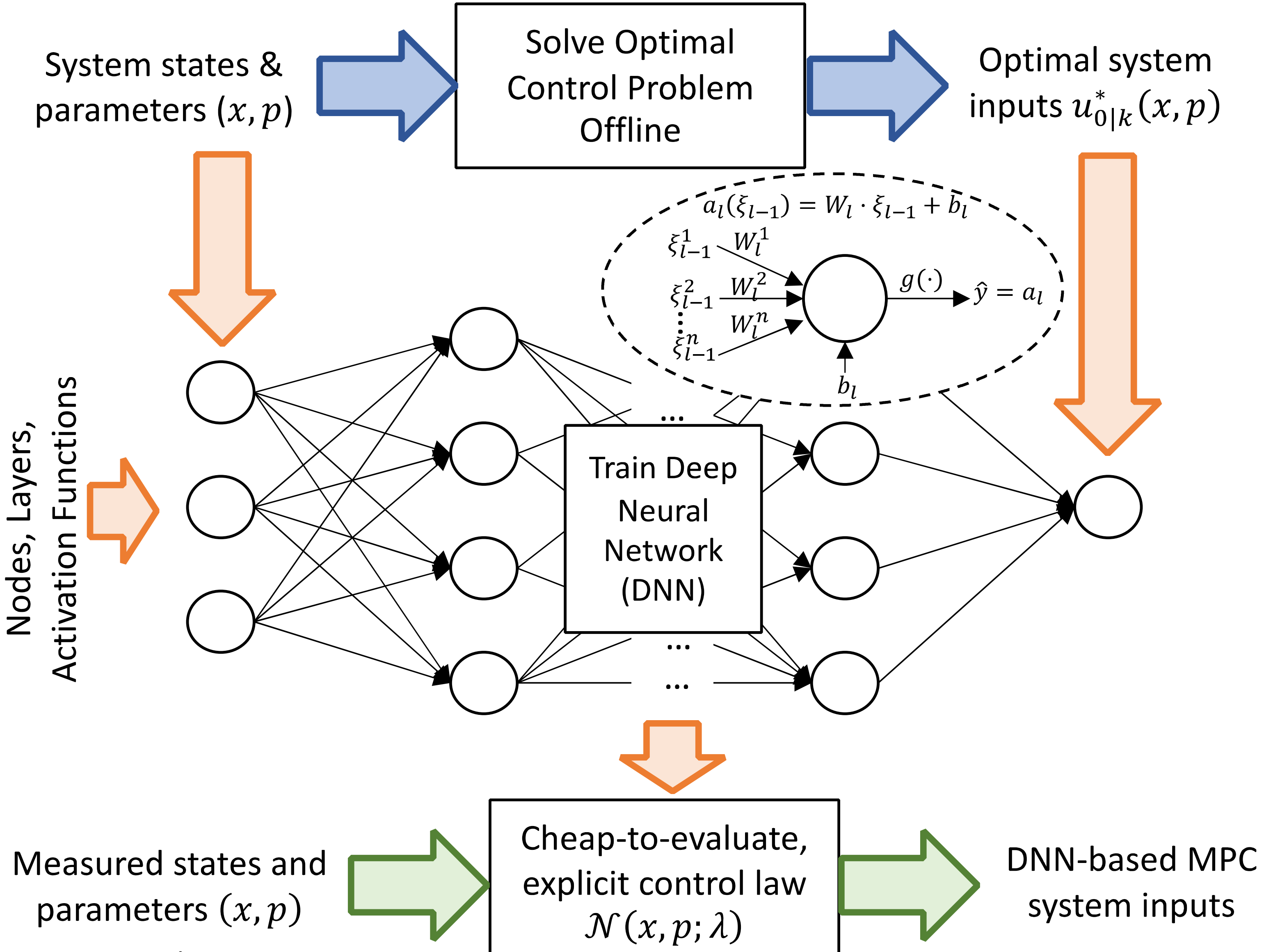
- **Fast control computations**
- **Control inputs may no longer be robustly feasible (no guarantees on state constraint satisfaction)**

Unsafe control!

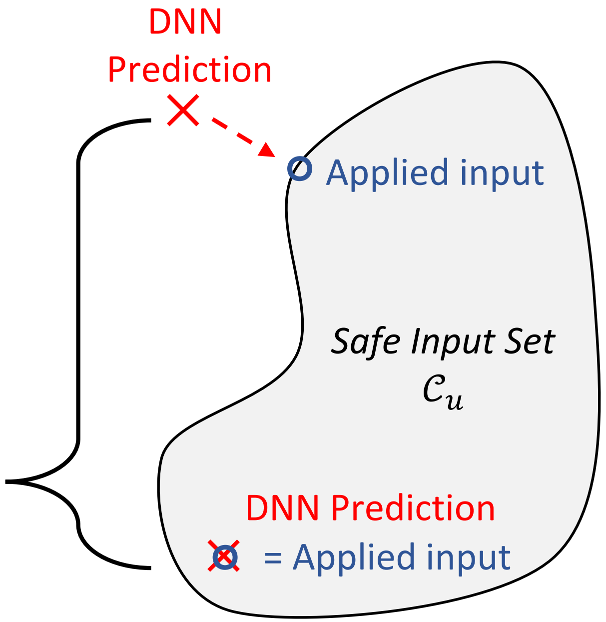
Bonzanini et al., 2020.

Deep Neural Network-based MPC

Towards embedded implementation of deep learning-based controllers



Projection of DNN-based control inputs onto a safe input set



Bonzanini et al., 2020.

Deep Neural Network-based MPC

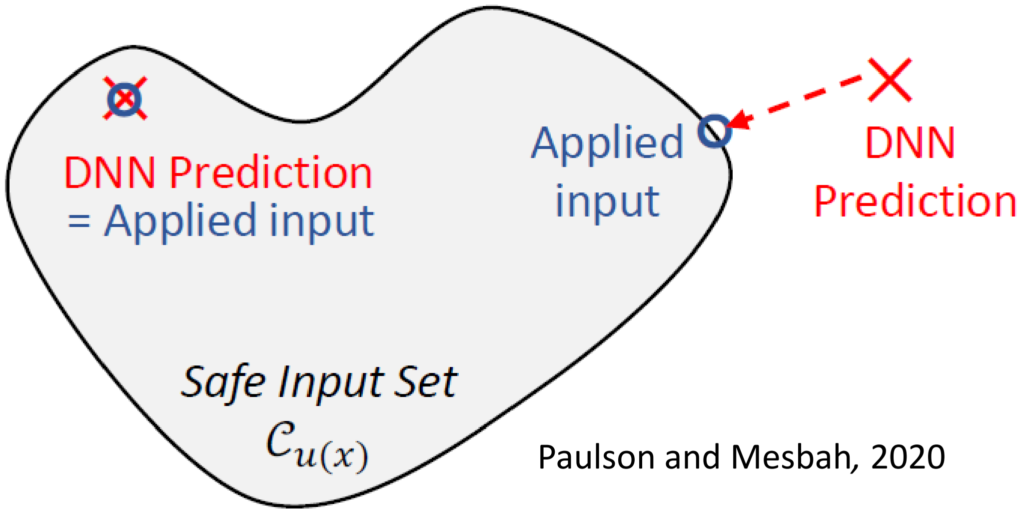
Towards embedded implementation of deep learning-based controllers

Safe input set

$$\overbrace{\mathcal{C}_u(x)} = \{u \in \mathcal{U} : f(x,u,w) \in \underbrace{\mathcal{C}}, \;\; \forall w \in \mathcal{W}\}$$

Robust control invariant (RCI) set

RCI sets for linear and hybrid systems can be calculated via already-established methods



Paulson and Mesbah, 2020

there exists feasible input

for all possible disturbances

$$\forall x \in \mathcal{C} \Rightarrow \exists u \in \mathcal{U} : f(x,u,w) \in \mathcal{C}, \;\; \forall w \in \mathcal{W}$$

for all states in RCI

such that successor states in RCI

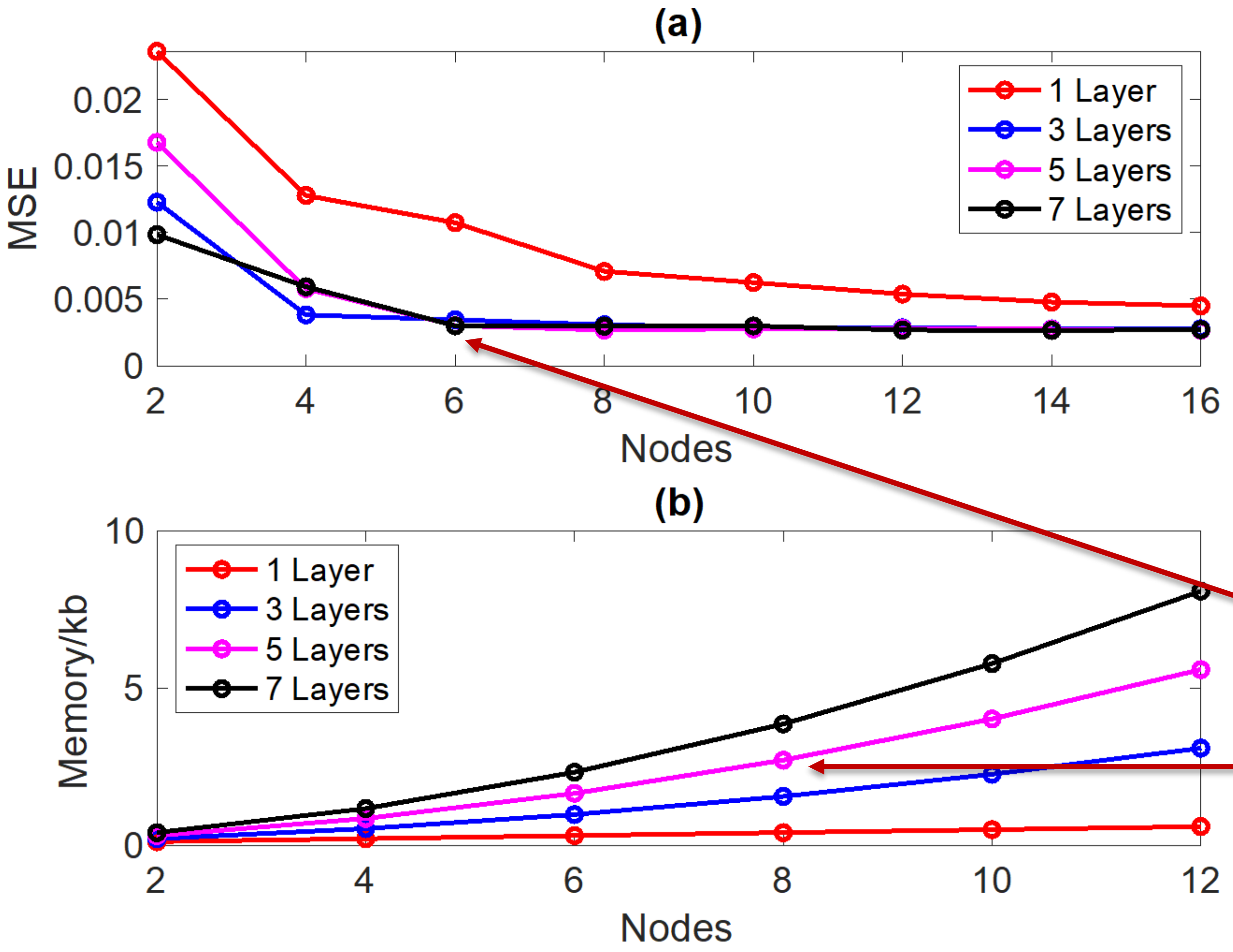
$$\kappa_N^{\text{proj}}(x) = \underset{u \in \mathcal{C}_u(x)}{\operatorname{argmin}} \; \|u - \tilde{\kappa}_N(x)\|_2^2$$

Safe operation guaranteed

This can be solved as a mp-QP for faster online evaluation!

Training of Deep Neural Network-based MPC

Trade-off between low error and low memory requirement



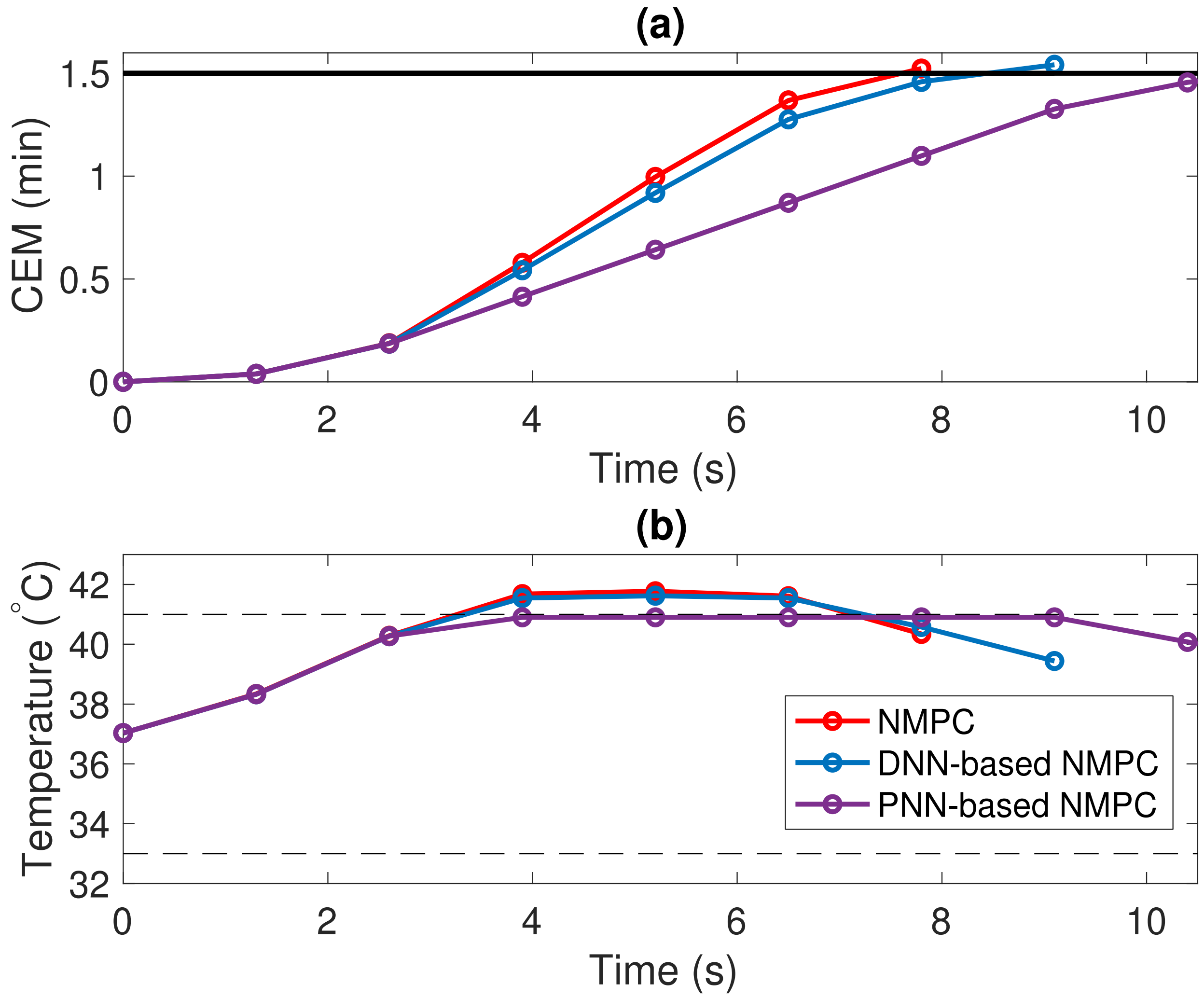
- Trained the DNN **offline** using multiple combinations of hyperparameters
- MSE decreases as number of layers and number of nodes per layer increase
- At the same time more nodes and layers correspond to a larger memory footprint
- Trade-off between accuracy and memory requirement

$$N_{\text{layers}} = 5$$
$$N_{\text{nodes}} = 6$$

Bonzanini et al., 2020.

Closed-loop Simulations

DNN-based MPC provides accurate approximation



NMPC and DNN-based NMPC

- Practically indistinguishable performance
- DNN provides an accurate approximation
- Constraint violation → **may compromise safety**!

PNN-based NMPC

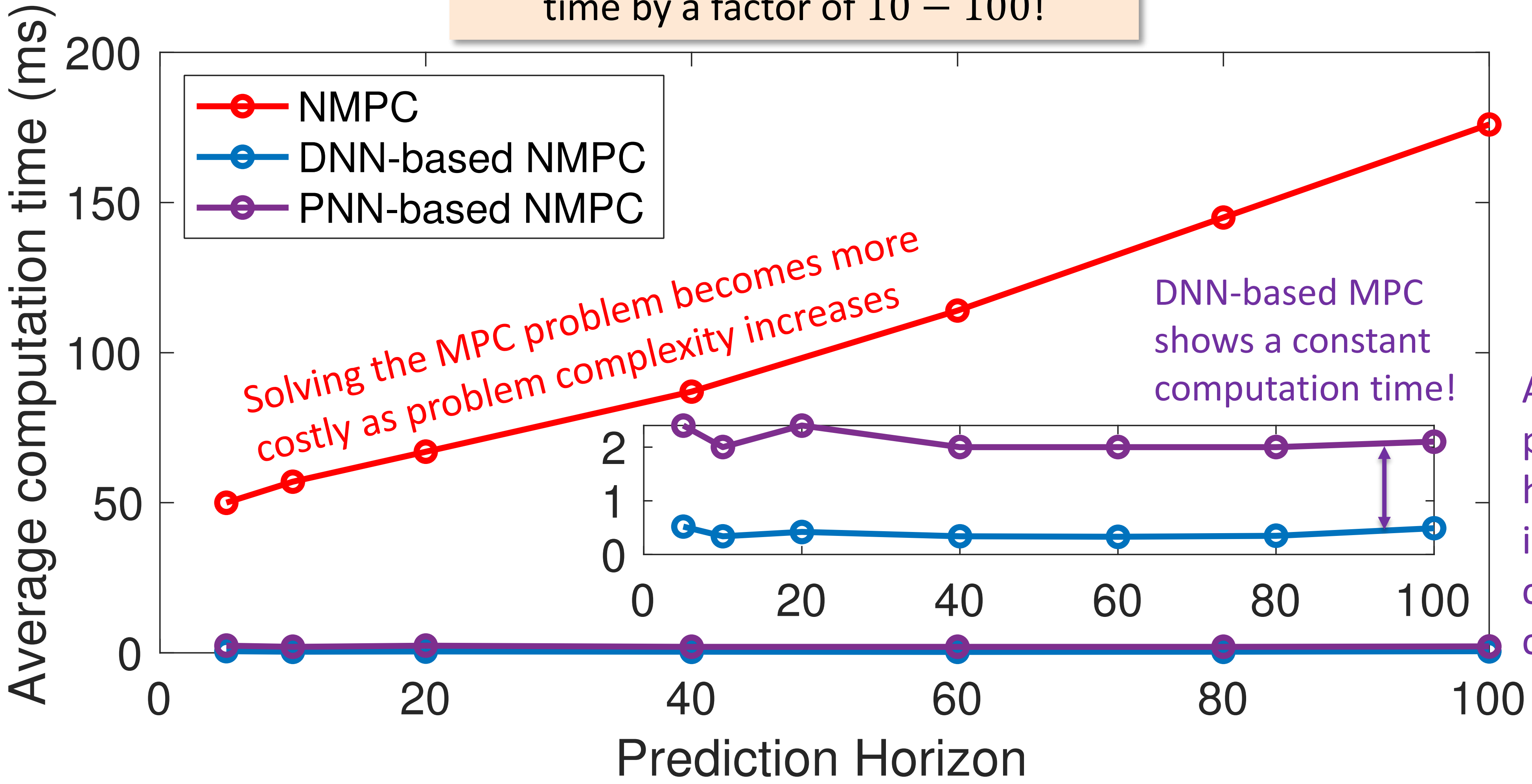
- Worse performance (longer treatment time)
- No constraint violation
- Trade-off between robustness and performance

Bonzanini et al., 2020.

Computation Times

Average computation time reduced by up to a factor of 100

Reduction of average computation time by a factor of $10 - 100$!

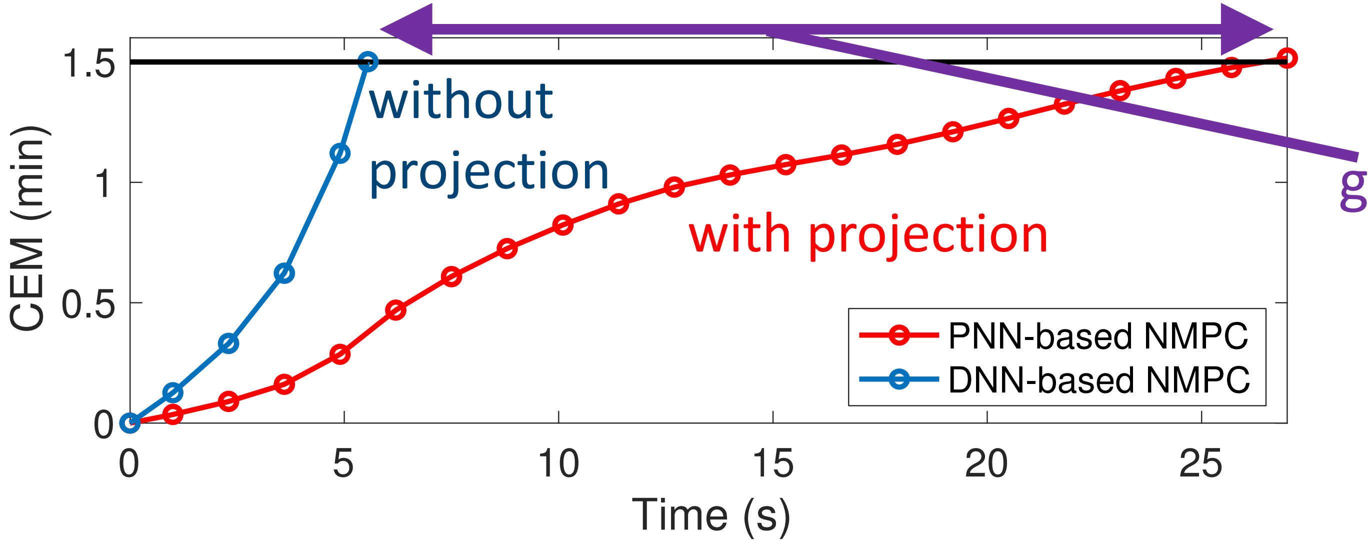


Adding the projection step has a small impact on computational cost

Bonzanini et al., 2020.

Real-time Control Experiments

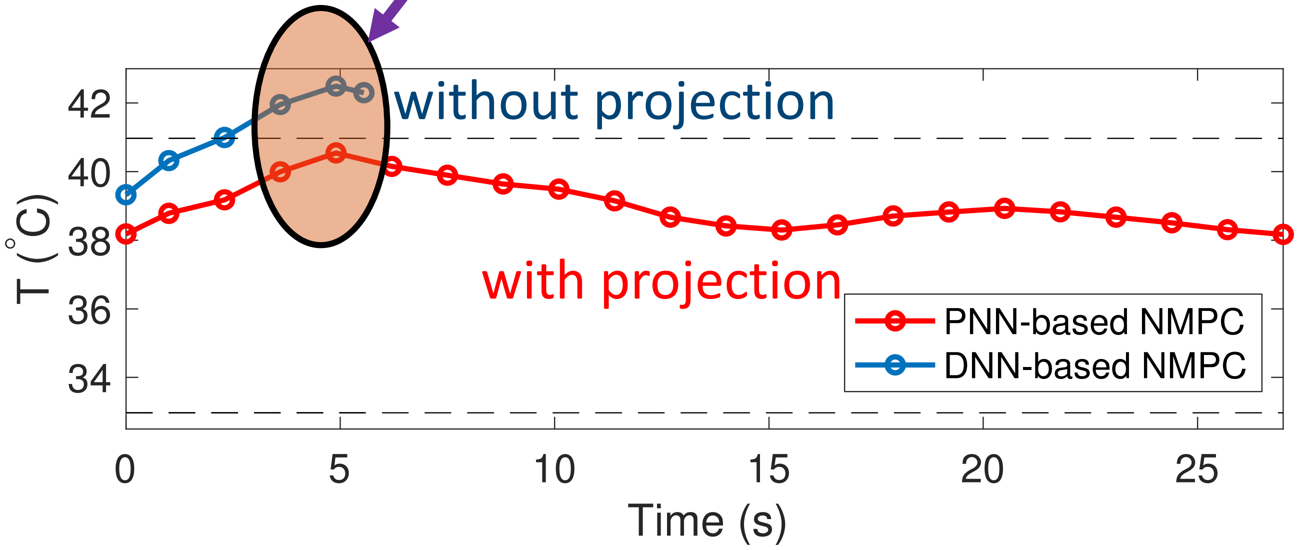
Safety achieved at the expense of performance



Performance loss due to guaranteed constraint satisfaction under uncertainty

Constraint violation avoided by projecting onto a safe set

- Computation time: 2 ms
- Memory footprint: 1 kb



Bonzanini et al., 2020.

Takeaways

- **Predictive control is essential for effective LTP treatment of complex surfaces:**
  - Controlled environments for studying plasma effects
  - Safe and effective LTP devices for point-of-use applications
  - Automated and robotic control for LTP processing of (bio)materials
- **Learning-based methods can create unique opportunities for:**
  - Leveraging high-fidelity LTP models along with data-driven approaches to learn and control hard-to-model plasma and surface phenomena
  - Handling uncertainties in real-time decision making towards ensuring safe and repeatable LTP treatments