UNIVERSITY OF CONNECTICUT

Robust Simulation of Safety-Critical Systems

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Outline

- Introduction & Background
  - What is meant by “robust simulation”?
  - Steady-state vs. dynamical systems
- Preliminaries
  - Problem formulation & foundational results
- New Results
  - Extending steady-state to dynamical
- Conclusions and Future Work

Key Contributor

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PSOR Lab, Dept. of Chemical and Biomolecular Eng.

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Introduction

- A “Robust System” mitigates the effects of uncertainty to ensure performance/safety constraints are satisfied.

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  - Conclude whether or not a system can meet the desired performance/safety constraints in the face of uncertainty using mathematical models

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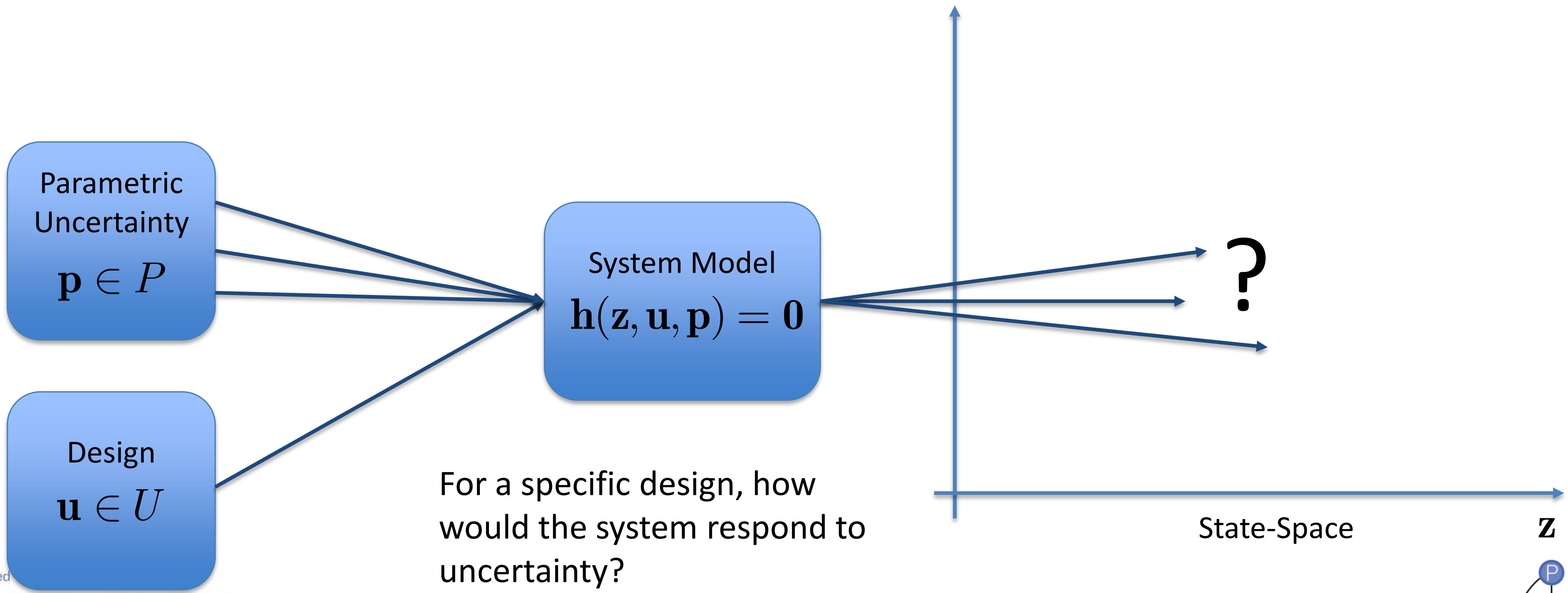
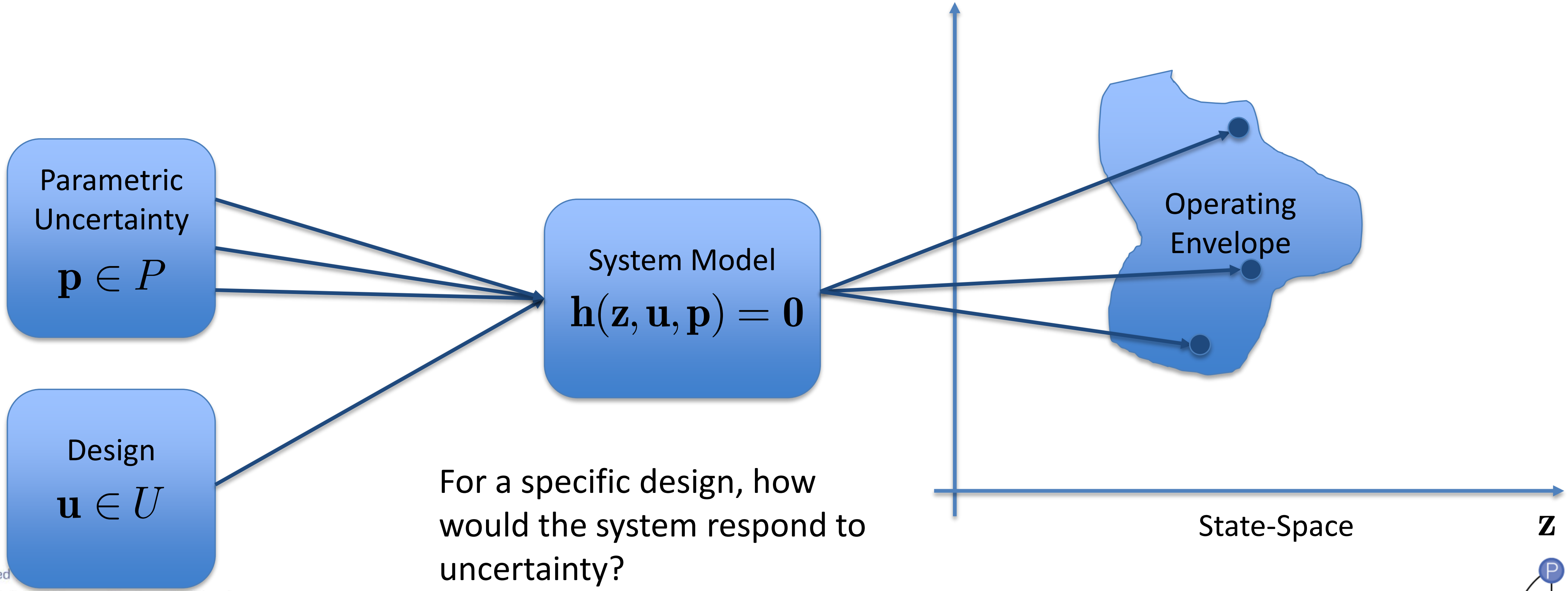
Research Challenge: How can we use model-based optimal design principles to improve reliability and safety of systems at the design stage?

Accounting for Uncertainty



For a specific design, how would the system respond to uncertainty?

Accounting for Uncertainty



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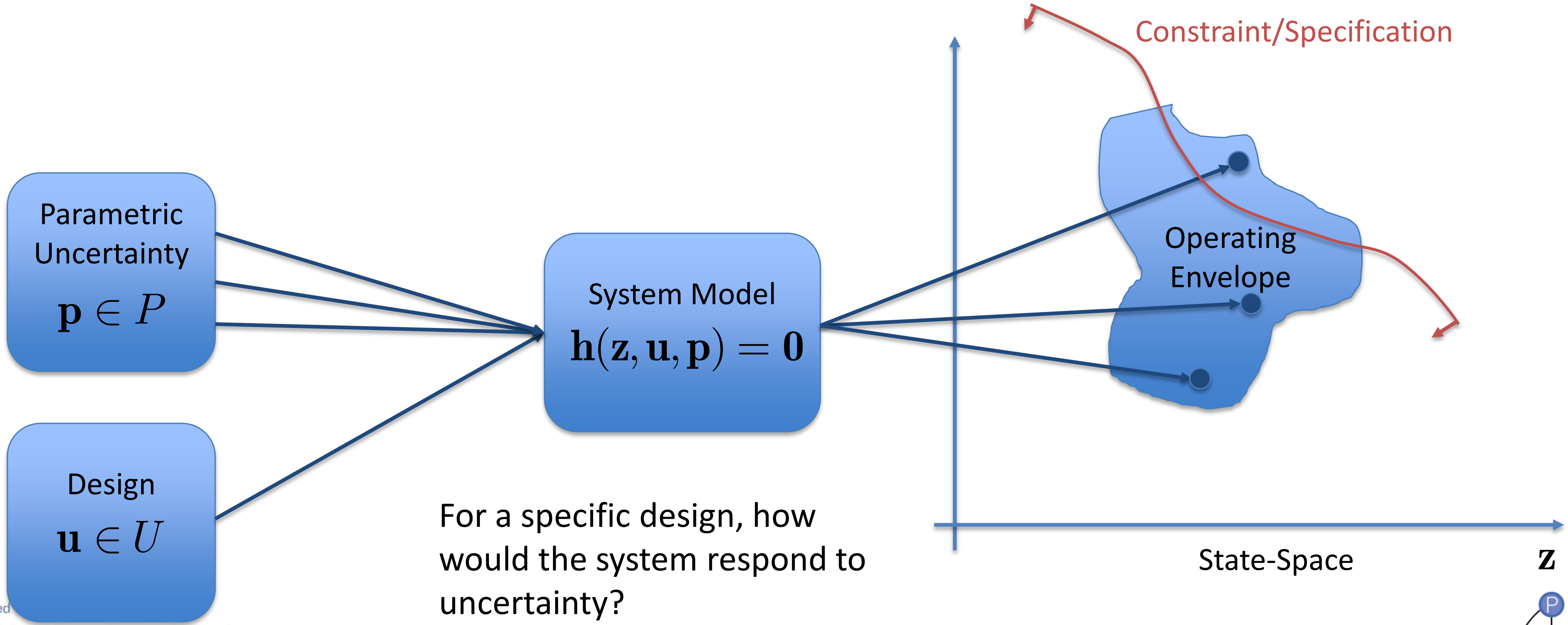

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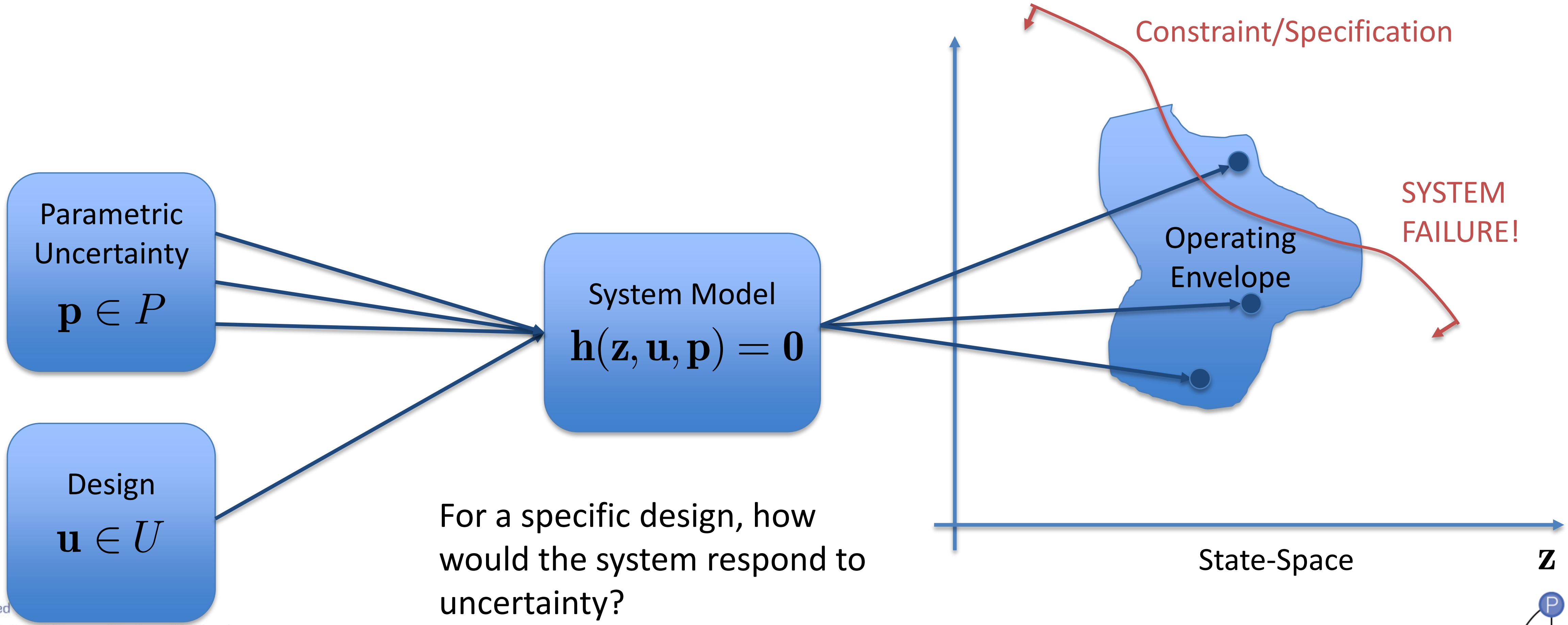

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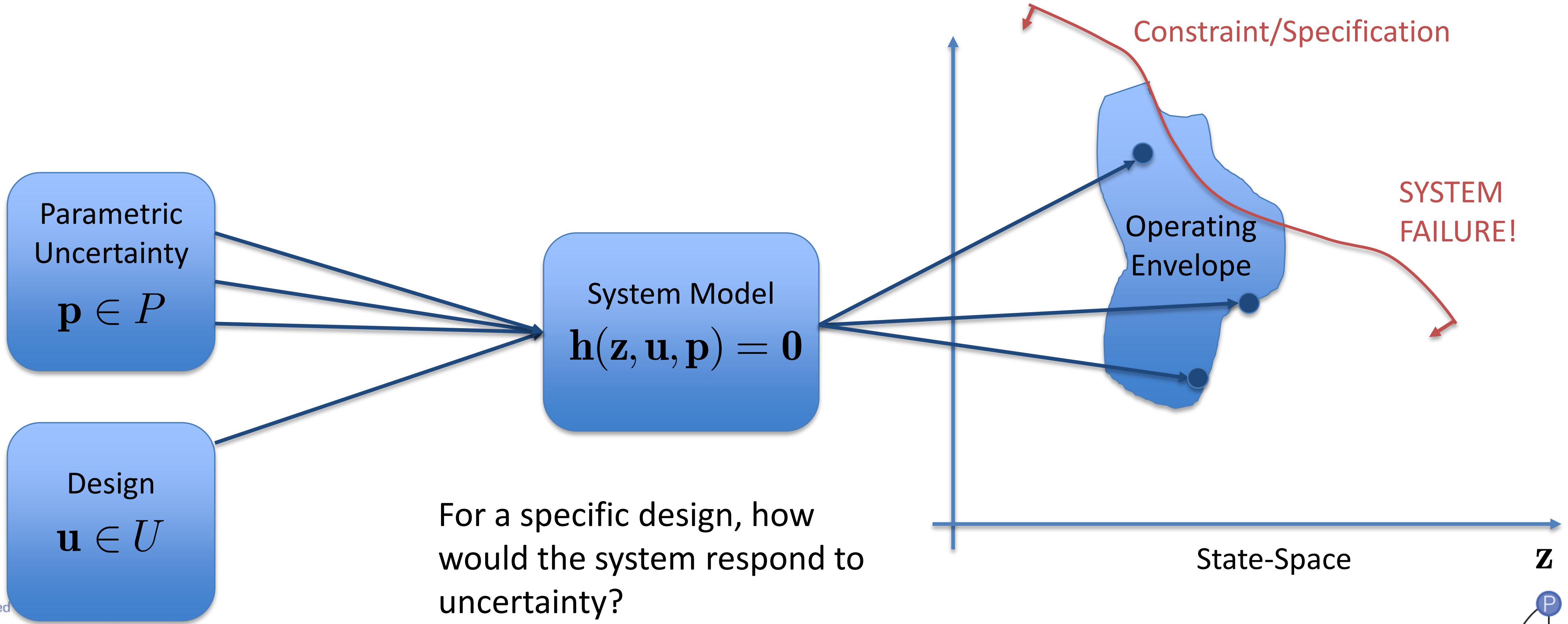

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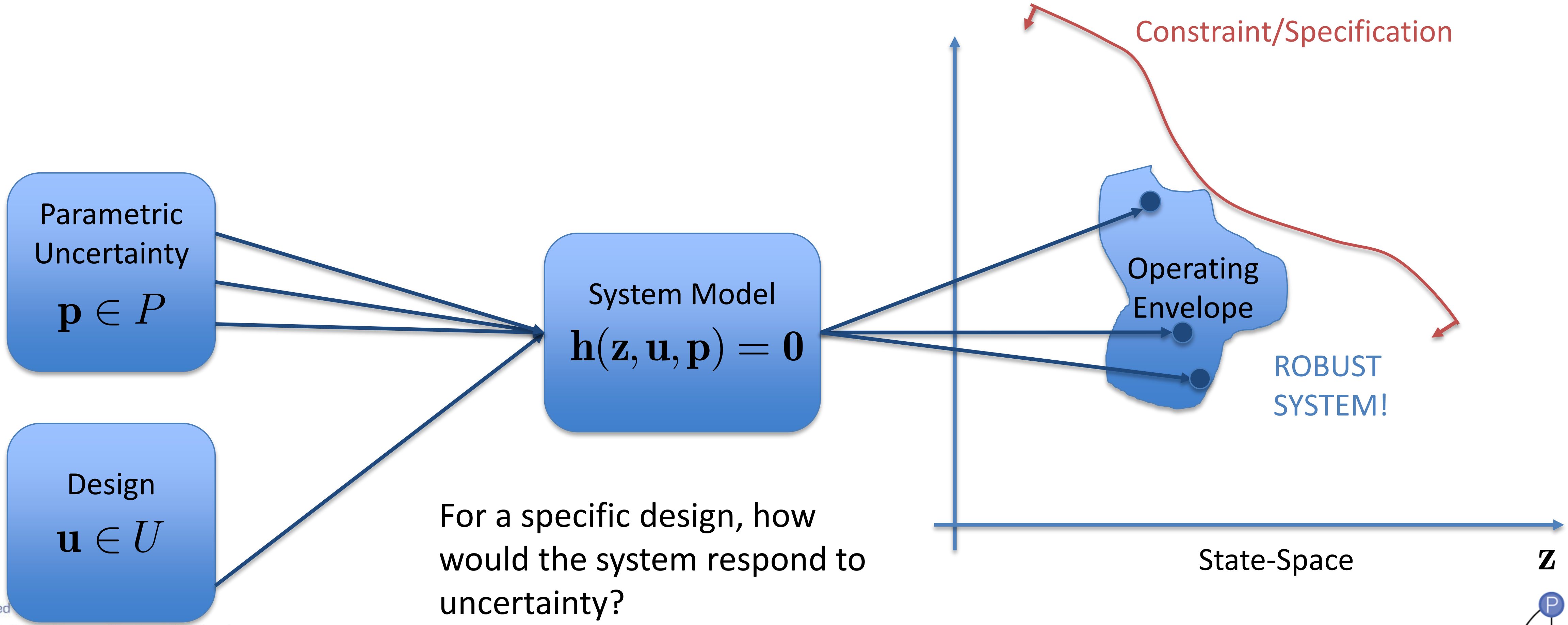


For a specific design, how would the system respond to uncertainty?

Accounting for Uncertainty

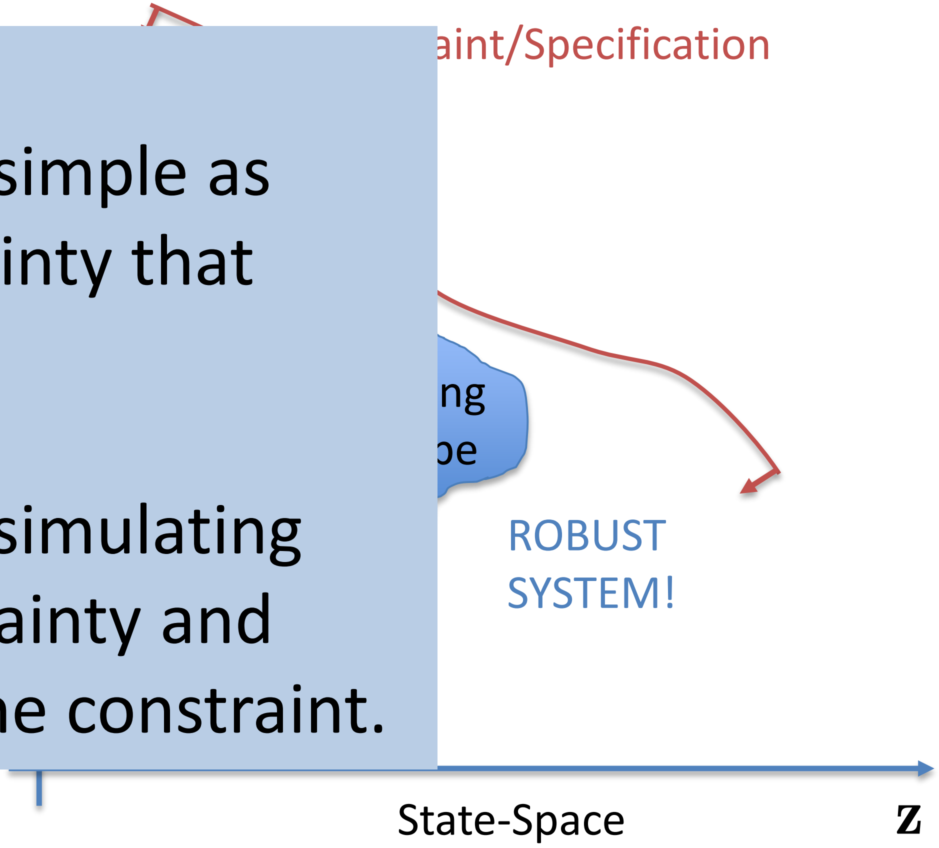
Research Challenge:

Verifying a system is not robust is as simple as finding a single realization of uncertainty that violates the constraint.

Verifying a system is robust requires simulating infinitely-many realizations of uncertainty and ensuring the system never violates the constraint.

Design $\mathbf{u} \in U$

would the system respond to uncertainty?



Introduction

- Steady-state vs. dynamical systems models

System Model

$$\mathbf{h}(\mathbf{z}, \mathbf{u}, \mathbf{p}) = \mathbf{0}$$

nonlinear algebraic system

System Model

$$\dot{\mathbf{x}}(\mathbf{u}, \mathbf{p}, t) = \mathbf{f}(\mathbf{x}(\mathbf{u}, \mathbf{p}, t), \mathbf{u}, \mathbf{p}, t)$$

nonlinear ODE system

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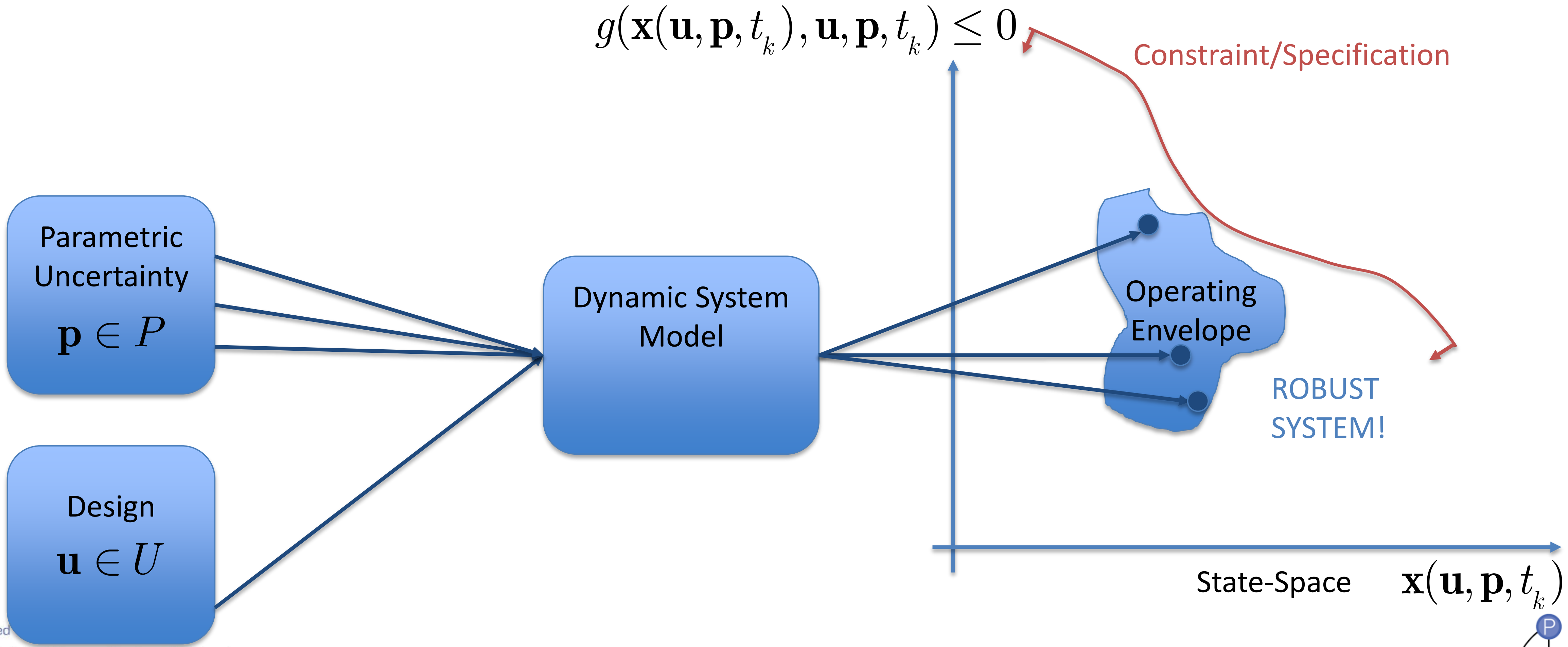
nonlinear ODE system

Now, we must account for the transient response to uncertainty in our design.

Accounting for Uncertainty



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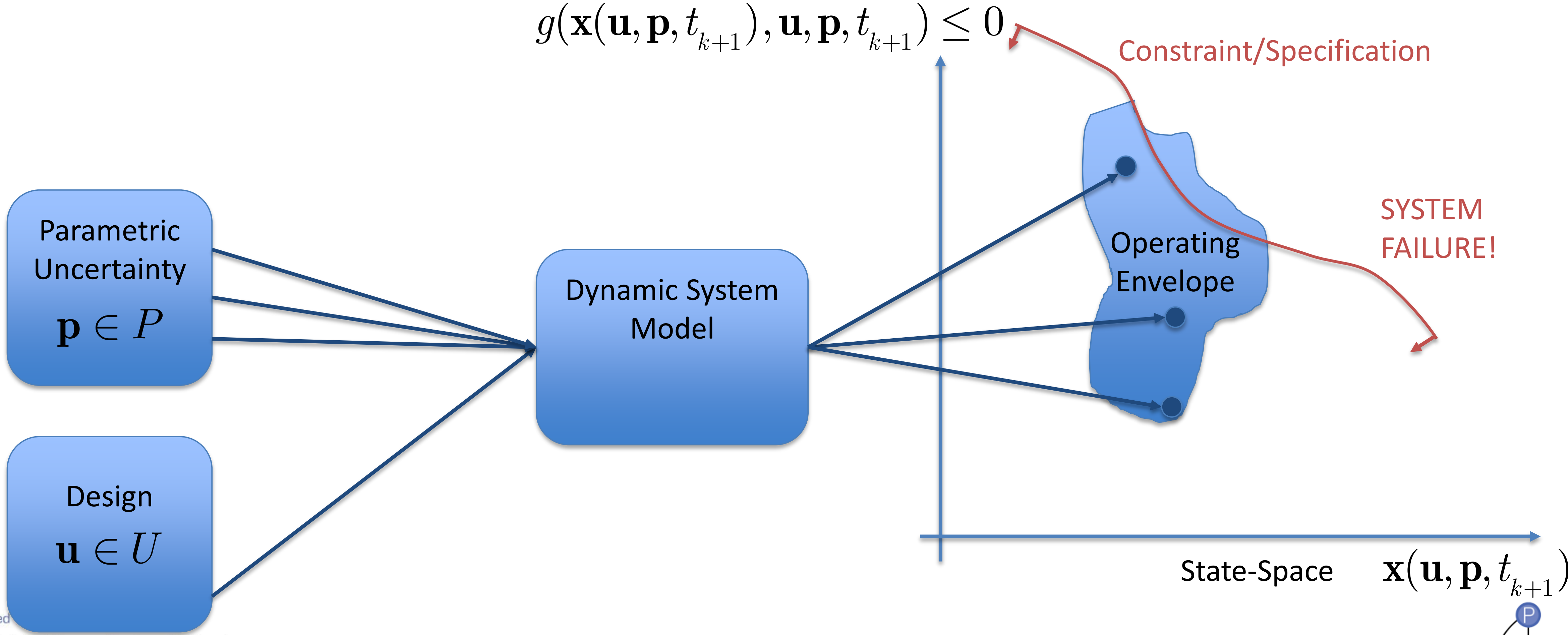

Preliminaries

- From a design perspective, our objective is to verify performance/safety in the face of (the worst-case) uncertainty over the time horizon.

$$\gamma(\mathbf{u}) = \max_{\mathbf{p}\in P, t\in I} g(\mathbf{x}(\mathbf{u},\mathbf{p},t),\mathbf{u},\mathbf{p},t)$$
$$\text{s.t.}\ \dot{\mathbf{x}}(\mathbf{u},\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{u},\mathbf{p},t),\mathbf{u},\mathbf{p},t)$$
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If $\gamma(\mathbf{u}) \leq 0$, we have verified the robustness of our design **u**.

"For a given design, the system does not violate performance/safety at any point in time, even in the face of the worst-case uncertainty"

Preliminaries

Discrete-time reformulation, e.g., implicit Euler:

$$\dot{\mathbf{x}}(\mathbf{u},\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{u},\mathbf{p},t),\mathbf{u},\mathbf{p},t)$$
$$\mathbf{x}(\mathbf{u},\mathbf{p},0) = \mathbf{x}_0(\mathbf{u},\mathbf{p})$$

$\Rightarrow$

$$\mathbf{y}_0 = \mathbf{x}_0(\mathbf{u},\mathbf{p})$$
$$\mathbf{y}_{i+1} = \mathbf{y}_i + h\mathbf{f}(\mathbf{y}_{i+1},\mathbf{u},\mathbf{p},t_{i+1}),\ \ i = 1,\ldots,K$$

Where we have $\mathbf{y}_i(\mathbf{u},\mathbf{p}) \approx \mathbf{x}(\mathbf{u},\mathbf{p},t_i)$

Preliminaries

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$$\gamma(\mathbf{u}) = \max_{\mathbf{p}\in P, t_k\in I, \mathbf{y}} g(\mathbf{y},\mathbf{u},\mathbf{p},t_k)$$
$$\text{s.t.}\ \ \mathbf{y}_0 = \mathbf{x}_0(\mathbf{u},\mathbf{p})$$
$$\underbrace{\begin{array}{l} \mathbf{y}_1 - \mathbf{y}_0 - h\mathbf{f}(\mathbf{y}_1,\mathbf{u},\mathbf{p},t_1) = \mathbf{0} \\ \vdots \qquad \vdots \\ \mathbf{y}_K - \mathbf{y}_{K-1} - h\mathbf{f}(\mathbf{y}_K,\mathbf{u},\mathbf{p},t_K) = \mathbf{0} \end{array}}_{\mathbf{h}(\mathbf{y},\mathbf{u},\mathbf{p}) = \mathbf{0}}$$

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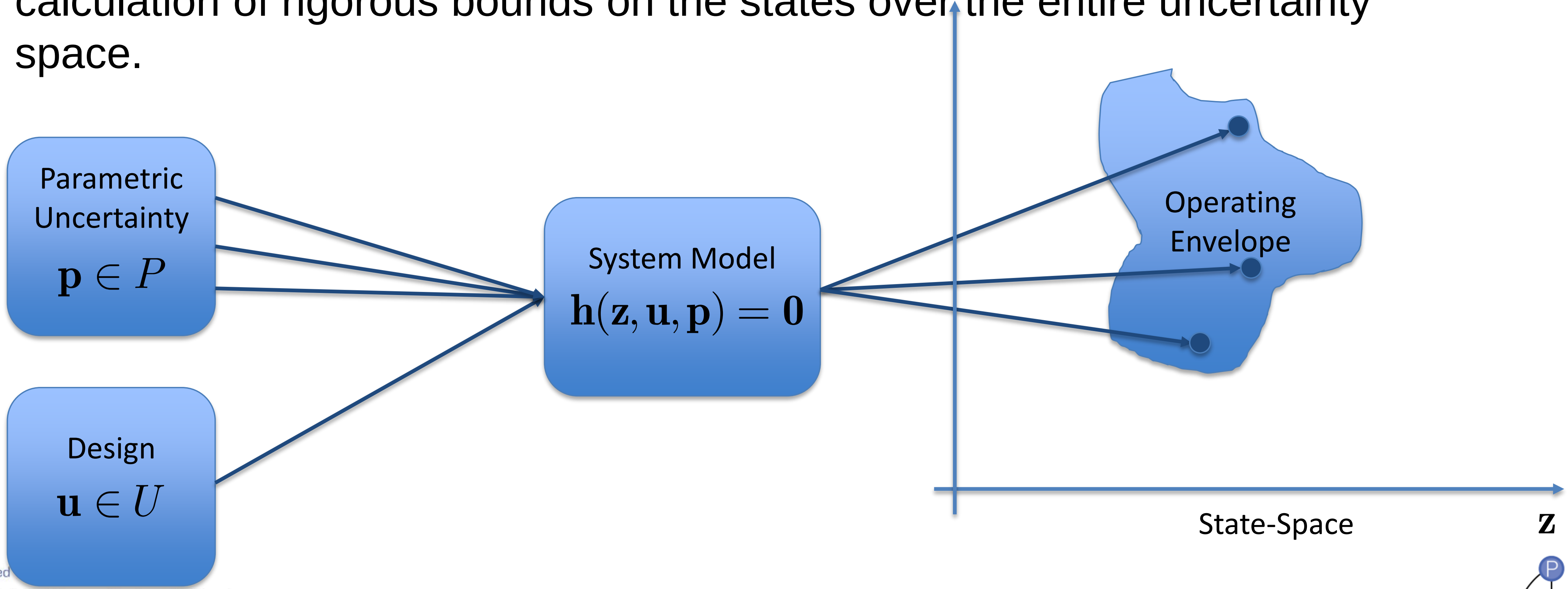
Related to “orthogonal collocation” approach: Biegler (1983)

Robust Steady-State Simulation

- Previous developments: a set-valued mapping theory that enables the calculation of rigorous bounds on the states over the entire uncertainty space.



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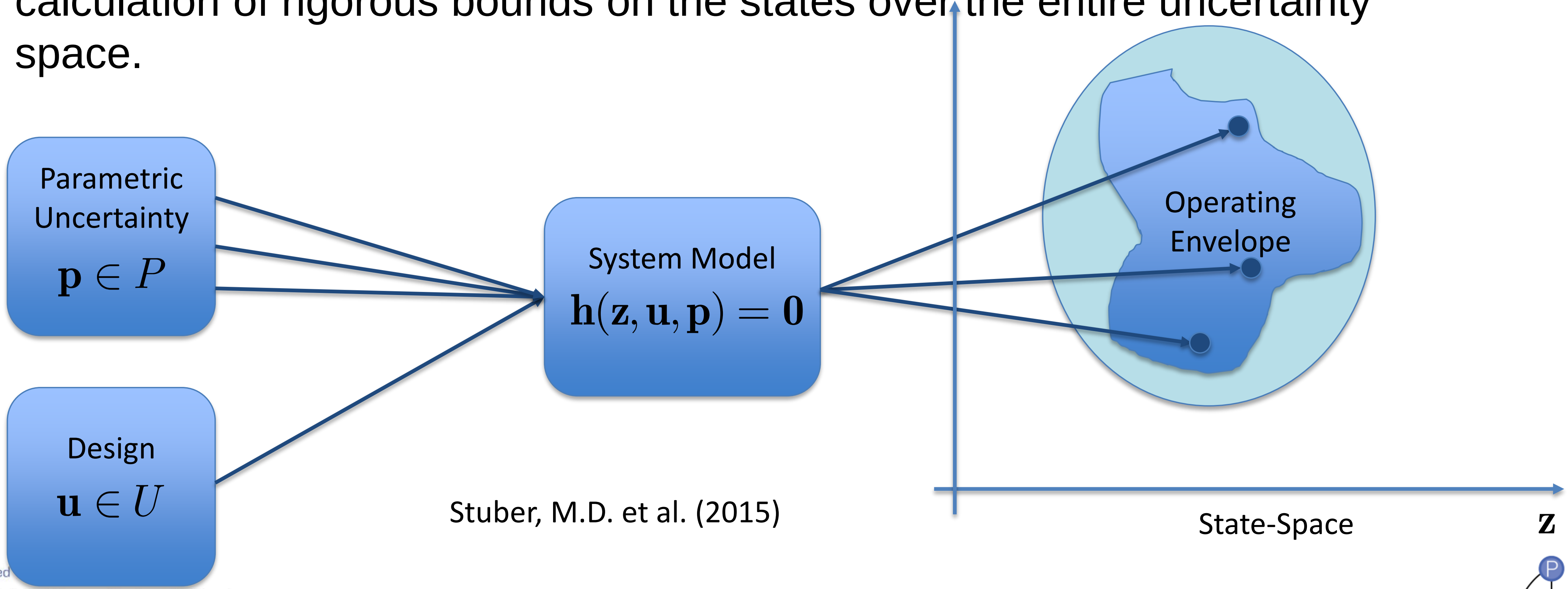


Stuber, M.D. et al. (2015)

Robust Steady-State Simulation

- How does this work mathematically?
  - Implicit function theorem

$$\mathbf{h}(\mathbf{z},\mathbf{u},\mathbf{p}) = \mathbf{0} \Rightarrow \mathbf{z} = \mathbf{x}(\mathbf{u},\mathbf{p}) : \mathbf{h}(\mathbf{x}(\mathbf{u},\mathbf{p}),\mathbf{u},\mathbf{p}) = \mathbf{0}$$

  - (parametric) mean value theorem

$$\mathbf{M}(\mathbf{u},\mathbf{p})(\mathbf{x}(\mathbf{u},\mathbf{p}) - \boldsymbol{\gamma}(\mathbf{u},\mathbf{p})) = -\mathbf{h}(\boldsymbol{\gamma}(\mathbf{u},\mathbf{p}),\mathbf{u},\mathbf{p})$$

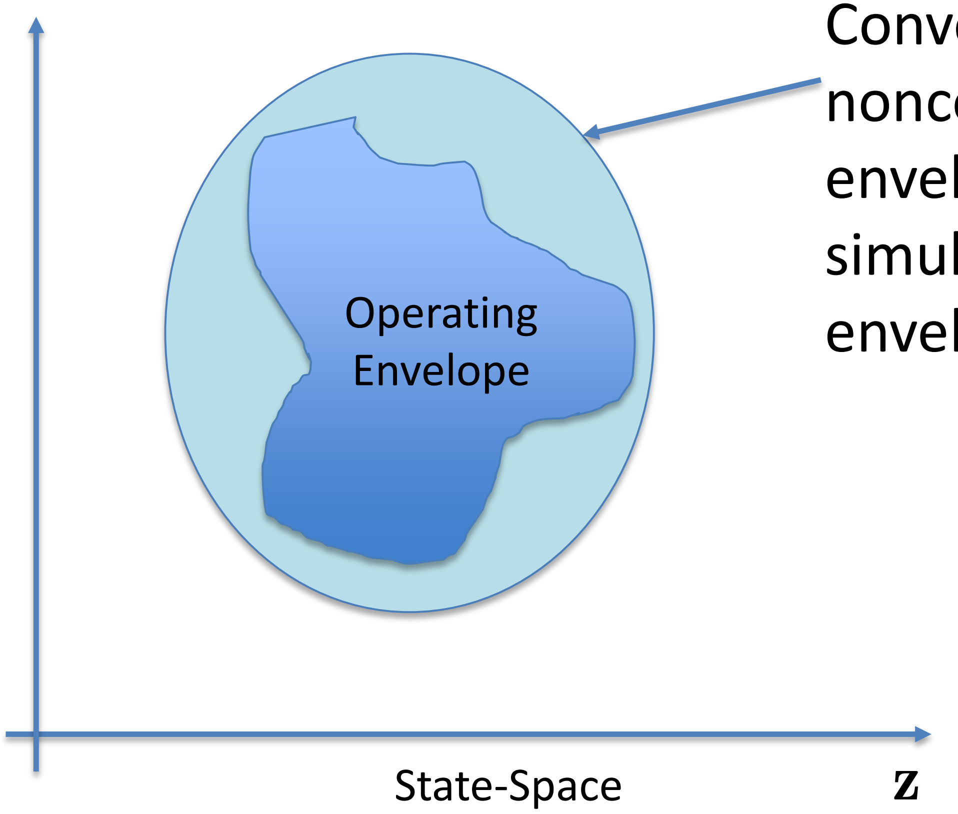
  - Fixed-point iterations

$$\mathbf{x}^{k+1}(\mathbf{u},\mathbf{p}) := \boldsymbol{\Phi}(\mathbf{x}^{k}(\mathbf{u},\mathbf{p}))$$

  - Rigorous (global) set-valued arithmetic
    - Interval arithmetic
    - generalized McCormick convex relaxations

Stuber, M.D. et al. (2015)

Robust Steady-State Simulation



Convex relaxation of nonconvex operating envelope (without actually simulating the operating envelope)

Stuber, M.D. et al. (2015)

Robust Dynamic Simulation

- Our dynamic model is reformulated in the discrete form as a nonlinear algebraic system:

$$\mathbf{h}(\mathbf{y},\mathbf{u},\mathbf{p}) = \begin{pmatrix} \mathbf{y}_0 - \mathbf{x}_0(\mathbf{u},\mathbf{p}) \\ \mathbf{y}_1 - \mathbf{y}_0 - h\mathbf{f}(\mathbf{y}_1,\mathbf{u},\mathbf{p},t_1) \\ \vdots \\ \mathbf{y}_K - \mathbf{y}_{K-1} - h\mathbf{f}(\mathbf{y}_K,\mathbf{u},\mathbf{p},t_K) \end{pmatrix} = \mathbf{0}$$

$$\mathbf{h} : \mathbb{R}^{n_x(K+1)} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \rightarrow \mathbb{R}^{n_x(K+1)}$$

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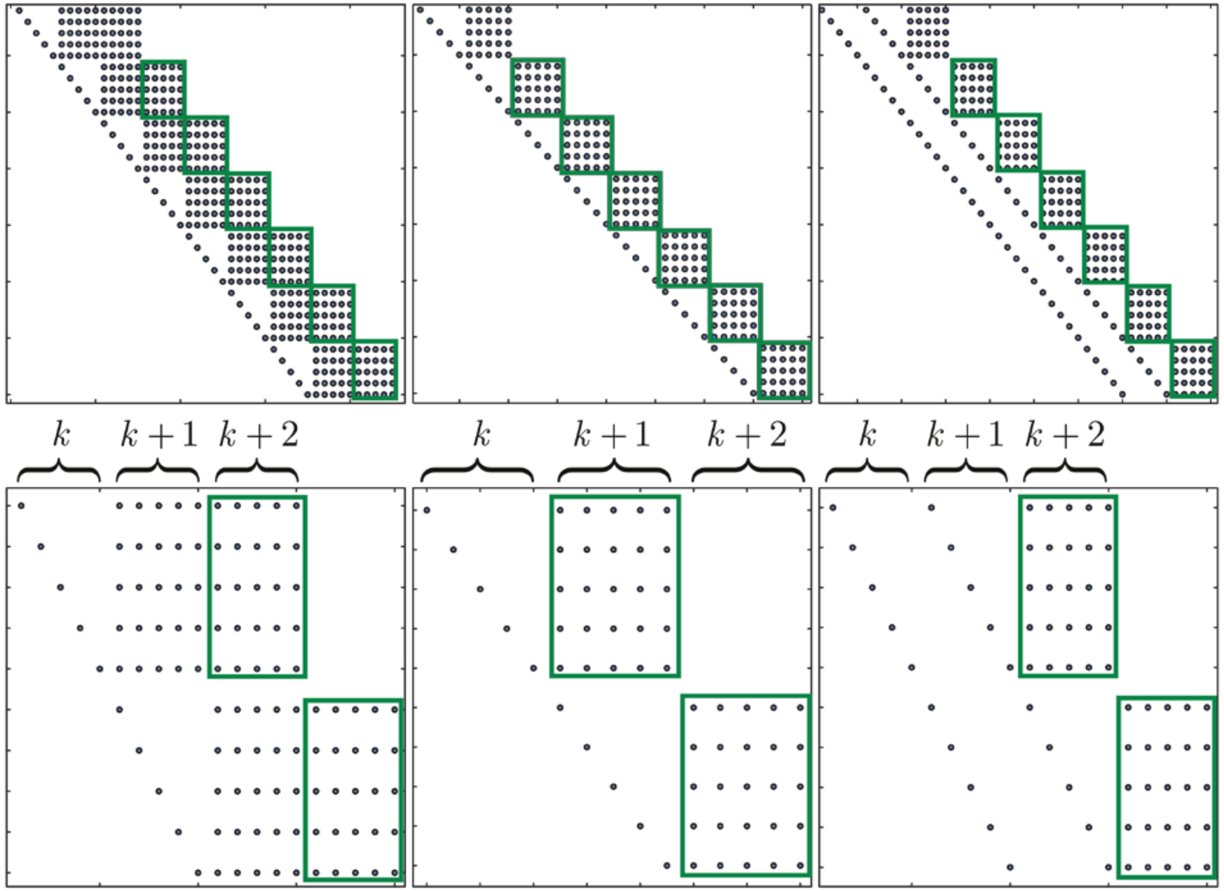
Very large!

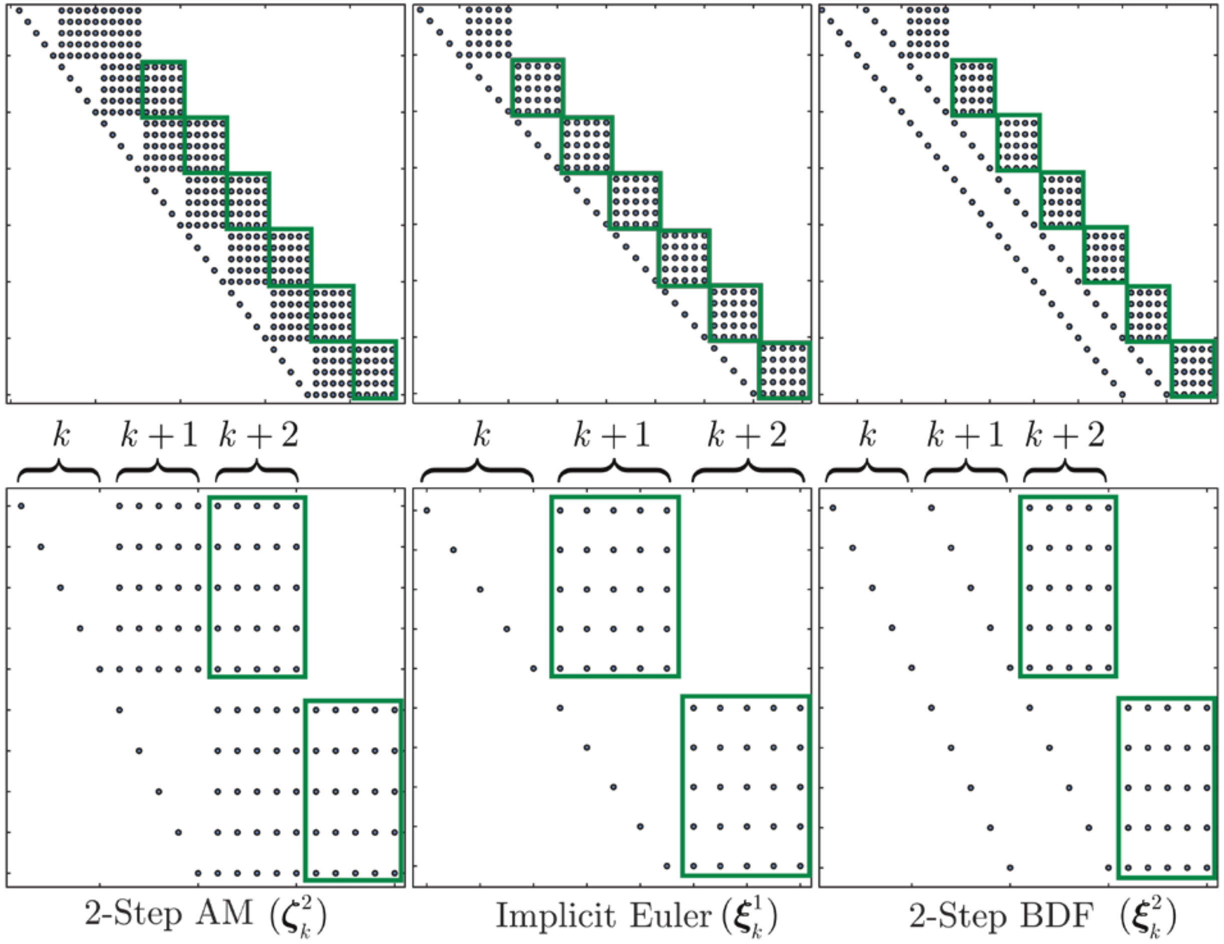
$$\mathbf{h} : \mathbb{R}^{n_x(K+1)} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x(K+1)}$$

Robust Dynamic Simulation



2-Step AM (ζ_k^2)   Implicit Euler (ξ_k^1)   2-Step BDF (ξ_k^2)

Robust Dynamic Simulation

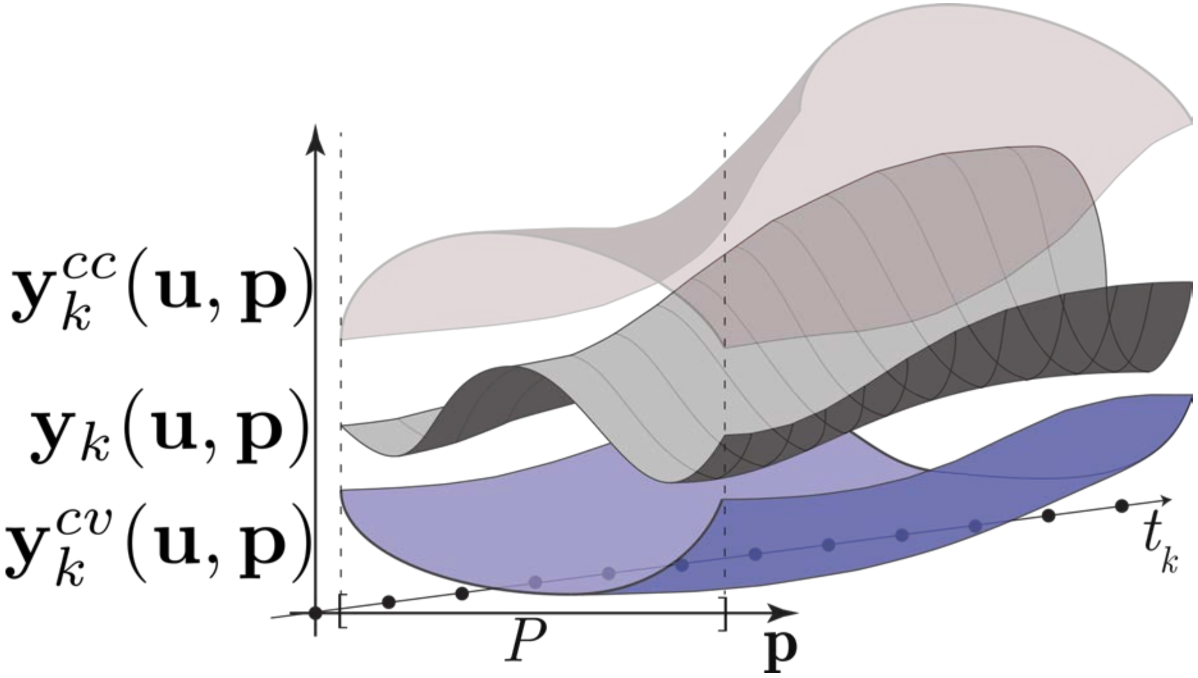


Here, we have 5 states. For a system with K=1000, we would need to account for a 5000-dimension system simultaneously.

Each block of unknowns only depends on the previous timesteps (known). Thus, we only need to account for a single 5-dimensional system sequentially.

Robust Dynamic Simulation

Apply the theory introduced previously for robust steady-state simulation to our system $\mathbf{h}(\mathbf{y}, \mathbf{u}, \mathbf{p}) = \mathbf{0}$ to calculate rigorous bounds on the state variables over the range of uncertainty variables **p** and design variables **u**, block-by-block.



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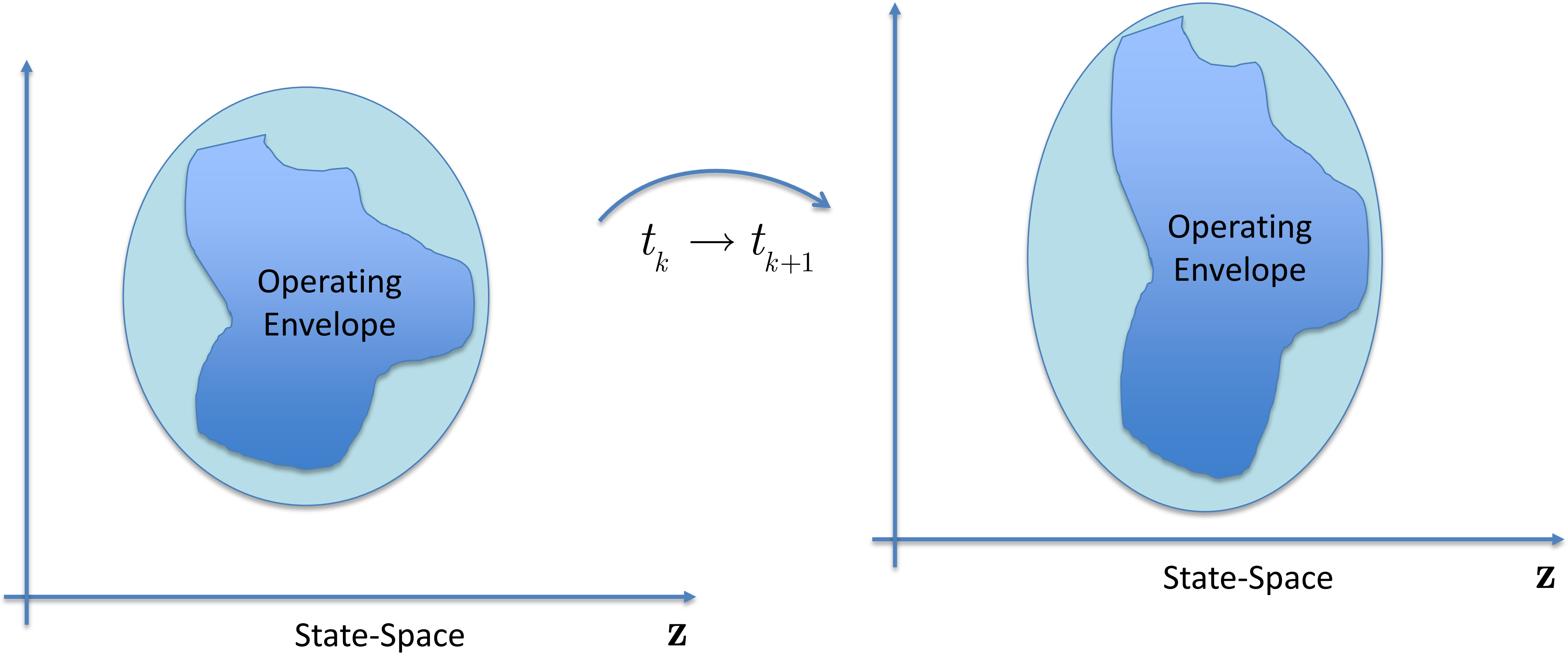

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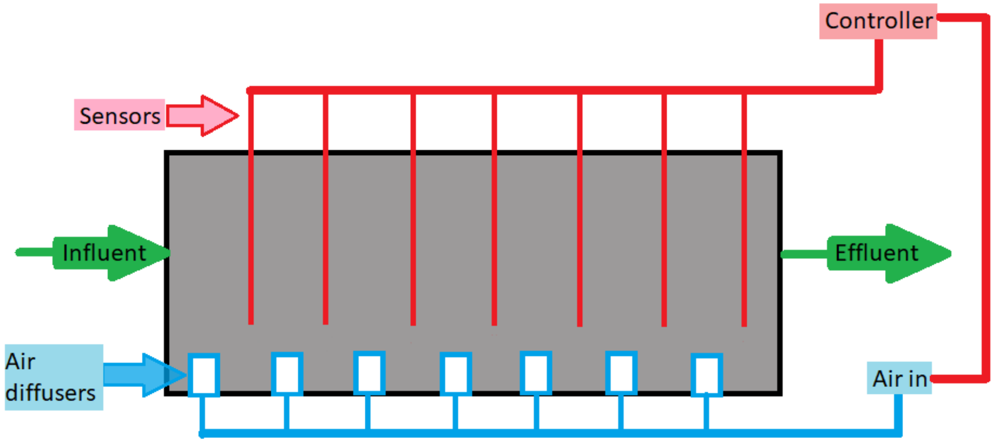
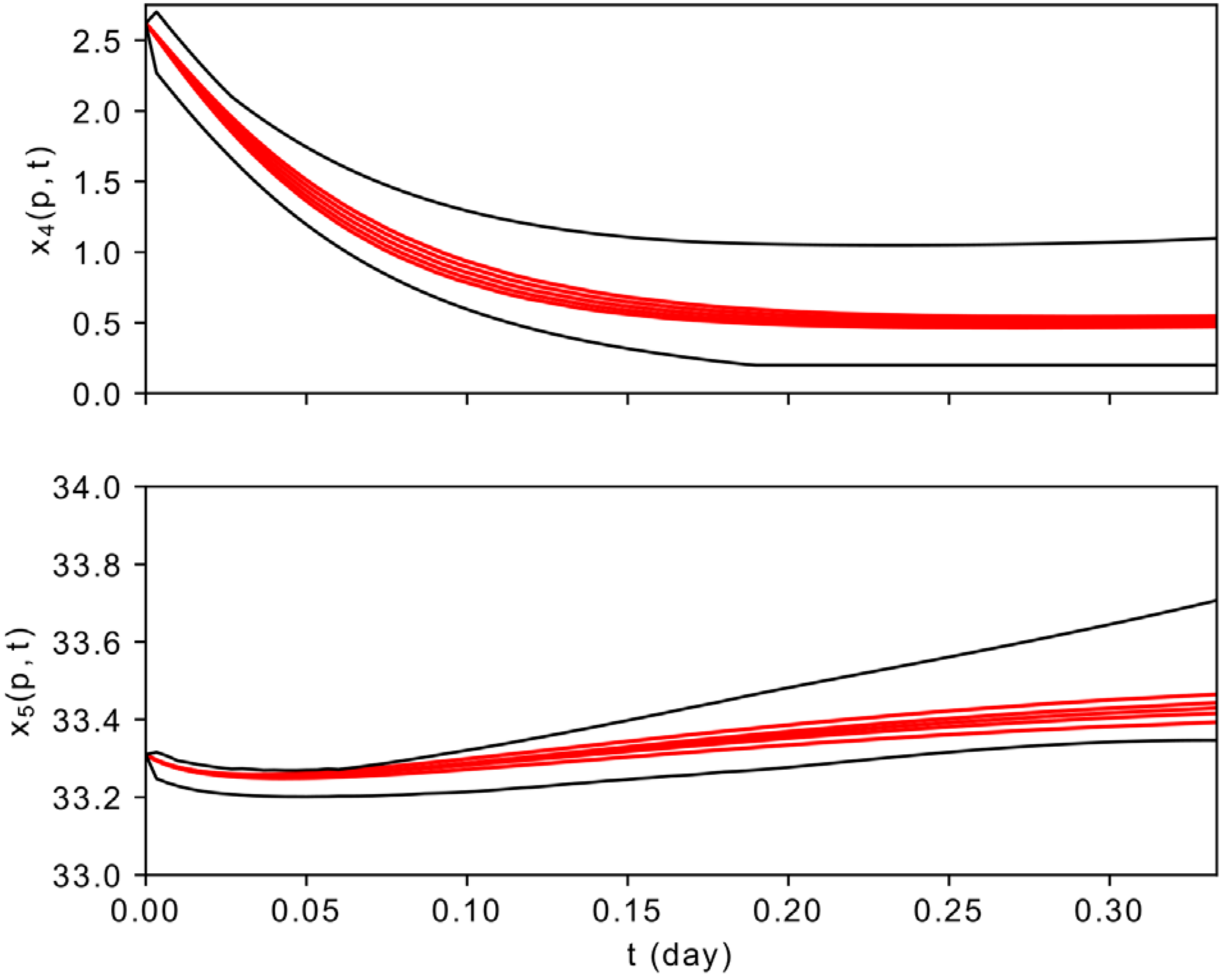


Control of a 9-species biological reaction for wastewater treatment.



Future Work

- Extend the worst-case uncertainty verification to the robust design problem to “minimize the maximum impact of uncertainty”

$$
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\end{aligned}
$$

$$
\begin{aligned}
\min_{\mathbf{u}\in U, \eta\in\mathbb{R}} \; & \eta \\
\text{s.t.} \;\; & \eta \geq \max_{\mathbf{p}\in P, t\in I} g(\mathbf{x}(\mathbf{u},\mathbf{p},t),\mathbf{u},\mathbf{p},t) \\
& \qquad \text{s.t.} \;\; \dot{\mathbf{x}}(\mathbf{u},\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{u},\mathbf{p},t),\mathbf{u},\mathbf{p},t) \\
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\end{aligned}
$$

Conclusion

- We have developed a method for rigorously bounding the operating envelope of a dynamical system
- We enable a simulation-based approach with deterministic global optimization for worst-case safety verification
- We have developed the theory for higher-order implicit integration methods (parametric implicit linear multistep methods).
- Focused on two-step (2^{nd}-order) methods
  - Much greater accuracy than implicit Euler
  - Unconditionally stable

Thank you!

Any Questions?

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