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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Introduction

• A “Robust System” mitigates the effects of uncertainty to ensure performance/safety constraints are satisfied.
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• “Robust Simulation” refers to the ability to rigorously account for the impacts of uncertainty via a model-based (i.e., simulation) approach
  – Conclude whether or not a system can meet the desired performance/safety constraints in the face of uncertainty using mathematical models
Introduction

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- “Robust Simulation” refers to the ability to rigorously account for the impacts of uncertainty via a model-based (i.e., simulation) approach
  - Conclude whether or not a system can meet the desired performance/safety constraints in the face of uncertainty using mathematical models

**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?

System Model

$$h(z, u, p) = 0$$

Parametric Uncertainty
$$p \in P$$

Design
$$u \in U$$

State-Space

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

\[ \mathbf{h}(\mathbf{z}, \mathbf{u}, \mathbf{p}) = 0 \]
Accounting for Uncertainty

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Parametric Uncertainty
\[ p \in P \]

Design
\[ u \in U \]

Constraint/Specification

State-Space

Operating Envelope
Accounting for Uncertainty

System Model

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

Constraint/Specification

SYSTEM FAILURE!
Accounting for Uncertainty

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

Parametric Uncertainty \( p \in P \)

Design \( u \in U \)

System Model

\[ h(z, u, p) = 0 \]
Accounting for Uncertainty

Parameter Uncertainty

\( \mathbf{p} \in P \)

Design

\( \mathbf{u} \in U \)

System Model

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

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

Constraint/Specification

ROBUST SYSTEM!

State-Space
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.
Introduction

• Steady-state vs. dynamical systems models

System Model

\[ h(z, u, p) = 0 \]

nonlinear algebraic system

System Model

\[ \dot{x}(u, p, t) = f(x(u, p, t), u, p, t) \]

nonlinear ODE system
Introduction

- Steady-state vs. dynamical systems models

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

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\[ g(x(u, p, t_k), u, p, t_k) \leq 0 \]

Parametric Uncertainty
\( p \in P \)

Design
\( u \in U \)

Dynamic System Model

Operating Envelope

State-Space
\( x(u, p, t_k) \)

Constraint/Specification

ROBUST SYSTEM!
Accounting for Uncertainty

Parametric Uncertainty \( \mathbf{p} \in P \)

Design \( \mathbf{u} \in U \)

Dynamic System Model

\[
g(x(u, p, t_{k+1}), u, p, t_{k+1}) \leq 0
\]

Constraint/Specification

SYSTEM FAILURE!
Preliminaries

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

\[
\gamma(u) = \max_{p \in P, t \in I} g(x(u, p, t), u, p, t)
\]

s.t. \[
\dot{x}(u, p, t) = f(x(u, p, t), u, p, t)
\]

\[
x(u, p, 0) = x_0(u, p)
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Preliminaries

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\]

If \(\gamma(u) \leq 0\), 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:

\[
\begin{align*}
\dot{x}(u, p, t) &= f(x(u, p, t), u, p, t) \\
x(u, p, 0) &= x_0(u, p)
\end{align*}
\]

Where we have \( y_i(u, p) \approx x(u, p, t_i) \)

\[
\begin{align*}
y_0 &= x_0(u, p) \\
y_{i+1} &= y_i + hf(y_{i+1}, u, p, t_{i+1}), \quad i = 1, \ldots, K
\end{align*}
\]
Preliminaries

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x(u, p, 0) = x_0(u, p)
\]

\[
\gamma(u) = \max_{p \in P, t_k \in I, y} g(y, u, p, t_k) \\
\text{s.t. } y_0 = x_0(u, p) \\
y_1 - y_0 - hf(y_1, u, p, t_1) = 0 \\
\vdots \\
y_K - y_{K-1} - hf(y_K, u, p, t_K) = 0 \\
h(y, u, p) = 0
\]
Preliminaries

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

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h(y, u, p) = 0
\]

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.

\[ h(z, u, p) = 0 \]

- Parametric Uncertainty: \( p \in P \)
- Design: \( u \in U \)
- Operating Envelope
- State-Space

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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.

Stuber, M.D. et al. (2015)
Robust Steady-State Simulation

- How does this work mathematically?
  - Implicit function theorem
    \[ h(z, u, p) = 0 \Rightarrow z = x(u, p) : h(x(u, p), u, p) = 0 \]
  - (parametric) mean value theorem
    \[ M(u, p)(x(u, p) - \gamma(u, p)) = -h(\gamma(u, p), u, p) \]
  - Fixed-point iterations
    \[ x^{k+1}(u, p) := \Phi(x^k(u, p)) \]
  - 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:

\[
\begin{align*}
    h(y, u, p) &= \begin{pmatrix}
        y_0 - x_0(u, p) \\
        y_1 - y_0 - hf(y_1, u, p, t_1) \\
        \vdots \\
        y_K - y_{K-1} - hf(y_K, u, p, t_K)
    \end{pmatrix} = 0 \\
    h : \mathbb{R}^{n_x(K+1)} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} &\rightarrow \mathbb{R}^{n_x(K+1)}
\end{align*}
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\mathbf{y}_0 - \mathbf{x}_0(\mathbf{u}, \mathbf{p}) \\
\mathbf{y}_1 - \mathbf{y}_0 - h\mathbf{f}(\mathbf{y}_1, \mathbf{u}, \mathbf{p}, t_1) \\
\vdots \\
\mathbf{y}_K - \mathbf{y}_{K-1} - h\mathbf{f}(\mathbf{y}_K, \mathbf{u}, \mathbf{p}, t_K)
\end{bmatrix} = 0 \\
h : \mathbb{R}^{n_x(K+1)} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x(K+1)}
\end{align*}
\]

Very large!
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 $h(y, u, p) = 0$ to calculate rigorous bounds on the state variables over the range of uncertainty variables $p$ and design variables $u$, block-by-block.
Robust Dynamic Simulation

Operating Envelope

State-Space

$t_k \rightarrow t_{k+1}$

Operating Envelope

State-Space
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”

\[
\gamma(u) = \max_{p \in P, t \in I} g(x(u, p, t), u, p, t) \\
\text{s.t. } \dot{x}(u, p, t) = f(x(u, p, t), u, p, t) \\
x(u, p, 0) = x_0(u, p)
\]

\[
\min_{u \in U, \eta \in \mathbb{R}} \eta \\
\text{s.t. } \eta \geq \max_{p \in P, t \in I} g(x(u, p, t), u, p, t) \\
\text{s.t. } \dot{x}(u, p, t) = f(x(u, p, t), u, p, t) \\
x(u, p, 0) = x_0(u, p)
\]
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\textsuperscript{nd}-order) methods
  - Much greater accuracy than implicit Euler
  - Unconditionally stable
Thank you!

Any Questions?

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