UCONN
UNIVERSITY OF CONNECTICUT

Worst-Case Optimization Under Uncertainty With Hybrid Models for Robust Process Systems

Matthew D. Stuber, Robert X. Gottlieb, Dimitri Alston, Matthew E. Wilhelm, and Chenyu Wang

Wednesday, August 16, 2023

MOPTA

Process Systems and Operations Research Laboratory

Outline

1. Worst-case perspective of robust design and operations, optimization under uncertainty
2. Problem formulation
3. Hybrid modeling and optimization of hybrid models
4. Semi-infinite programming with hybrid models
5. Examples
6. Conclusion

Worst-Case Perspective

- Think "safety-critical" systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty

Worst-Case Perspective

- Think "safety-critical" systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty
  - Model validation

Worst-Case Perspective

- Think "safety-critical" systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty
  - Model validation
  - Fault detection and isolation

Worst-Case Perspective

- Think “safety-critical” systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty
  - Model validation
  - Fault detection and isolation
  - Process design under uncertainty

Worst-Case Perspective

- Think “safety-critical” systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty
  - Model validation
  - Fault detection and isolation
  - Process design under uncertainty
  - Process flexibility

Worst-Case Perspective

- Think “safety-critical” systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty

  - Model validation
  - Fault detection and isolation
  - Process design under uncertainty
  - Process flexibility
  - Formal verification

Worst-Case Perspective

- Think “safety-critical” systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty
  - Model validation
  - Fault detection and isolation
  - Process design under uncertainty
  - Process flexibility
  - Formal verification
  - Among others…

Worst-Case Perspective

- Think "safety-critical" systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty **p**

$$\begin{aligned} &\min_{\mathbf{x}\in X\in \mathbb{R}^{n_x}} \ \phi(\mathbf{x}) \\ &\text{s.t.} \ \max_{\mathbf{p}\in P\in \mathbb{R}^{n_p}} \ \max\{g_i(\mathbf{x},\mathbf{p})\} \le 0 \end{aligned}$$

Bilevel program

Worst-Case Perspective

- Think "safety-critical" systems: must ensure feasibility in the face of the worst-case realization(s) of uncertainty **p**

$$\begin{aligned} \min_{\mathbf{x}\in X\in \mathbb{R}^{n_x}} \quad & \phi(\mathbf{x}) \\ \text{s.t.} \quad & \max_{\mathbf{p}\in P\in \mathbb{R}^{n_p}} \max\{g_i(\mathbf{x},\mathbf{p})\} \leq 0 \end{aligned}$$

Bilevel program

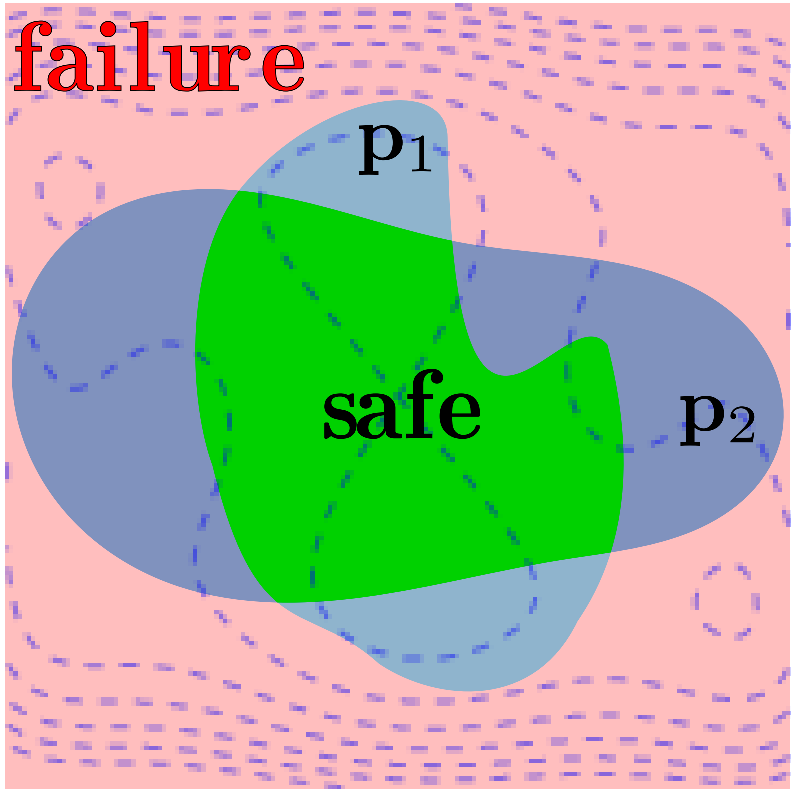
$$\begin{aligned} \min_{\mathbf{x}\in X\in \mathbb{R}^{n_x}} \quad & \phi(\mathbf{x}) \\ \text{s.t.} \quad & \max_{\gamma\in\mathbb{R},\mathbf{p}\in P\in \mathbb{R}^{n_p},\hat{\mathbf{z}}\in\mathbb{R}^{n_z}} \gamma \\ & \quad \text{s.t.} \quad \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\mathbf{p}) = \mathbf{0} \\ & \qquad\quad\ \gamma \leq \max\{g_i(\hat{\mathbf{z}},\mathbf{x},\mathbf{p})\} \end{aligned}$$

Bilevel program with coupling equality constraints

Problem Formulation

- Main challenge: most algorithms do not apply to problems with coupling equality constraints

$$\min_{\mathbf{x}\in X\in\mathbb{R}^{n_x}} \phi(\mathbf{x})$$
$$\text{s.t.} \max_{\gamma\in\mathbb{R},\mathbf{p}\in P\in\mathbb{R}^{n_p},\hat{\mathbf{z}}\in\mathbb{R}^{n_z}} \gamma$$
$$\text{s.t. } \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\mathbf{p}) = \mathbf{0}$$
$$\gamma \le \max\{g_i(\hat{\mathbf{z}},\mathbf{x},\mathbf{p})\}$$

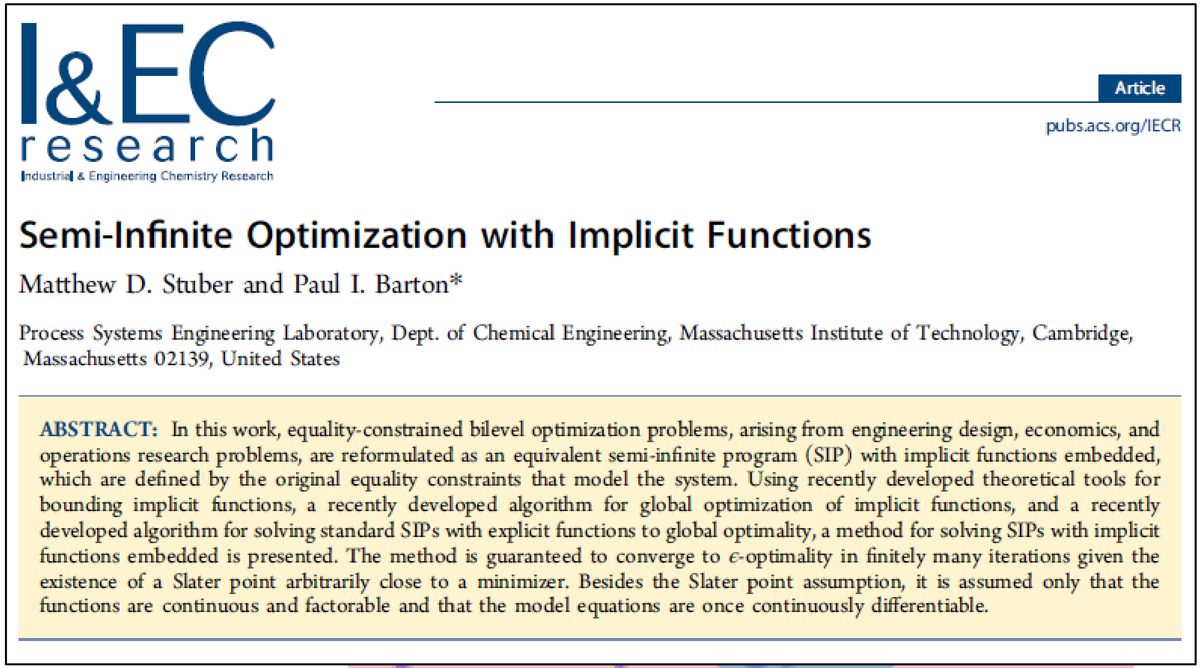


Problem Formulation

- Main challenge: most algorithms do not apply to problems with coupling equality constraints

$$
\begin{aligned}
\min_{\mathbf{x}\in X\in\mathbb{R}^{n_x}} \quad & \phi(\mathbf{x}) \\
\text{s.t.} \quad & \max_{\gamma\in\mathbb{R},\mathbf{p}\in P\in\mathbb{R}^{n_p},\hat{\mathbf{z}}\in\mathbb{R}^{n_z}} \gamma \\
& \quad \text{s.t.} \ \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\mathbf{p}) = \mathbf{0} \\
& \quad \gamma \le \max\{g_i(\hat{\mathbf{z}},\mathbf{x},\mathbf{p})\}
\end{aligned}
$$

$$
\begin{aligned}
&\exists \mathbf{z} : X \times P \to Z \\
&\mathbf{h}(\mathbf{z}(\mathbf{x},\mathbf{p}),\mathbf{x},\mathbf{p}) = \mathbf{0}
\end{aligned}
$$


I&EC research
Industrial & Engineering Chemistry Research

Article

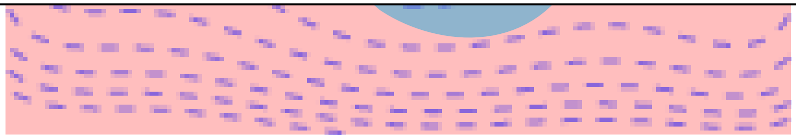
pubs.acs.org/IECR

Semi-Infinite Optimization with Implicit Functions

Matthew D. Stuber and Paul I. Barton*

Process Systems Engineering Laboratory, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States

ABSTRACT: In this work, equality-constrained bilevel optimization problems, arising from engineering design, economics, and operations research problems, are reformulated as an equivalent semi-infinite program (SIP) with implicit functions embedded, which are defined by the original equality constraints that model the system. Using recently developed theoretical tools for bounding implicit functions, a recently developed algorithm for global optimization of implicit functions, and a recently developed algorithm for solving standard SIPs with explicit functions to global optimality, a method for solving SIPs with implicit functions embedded is presented. The method is guaranteed to converge to ϵ-optimality in finitely many iterations given the existence of a Slater point arbitrarily close to a minimizer. Besides the Slater point assumption, it is assumed only that the functions are continuous and factorable and that the model equations are once continuously differentiable.

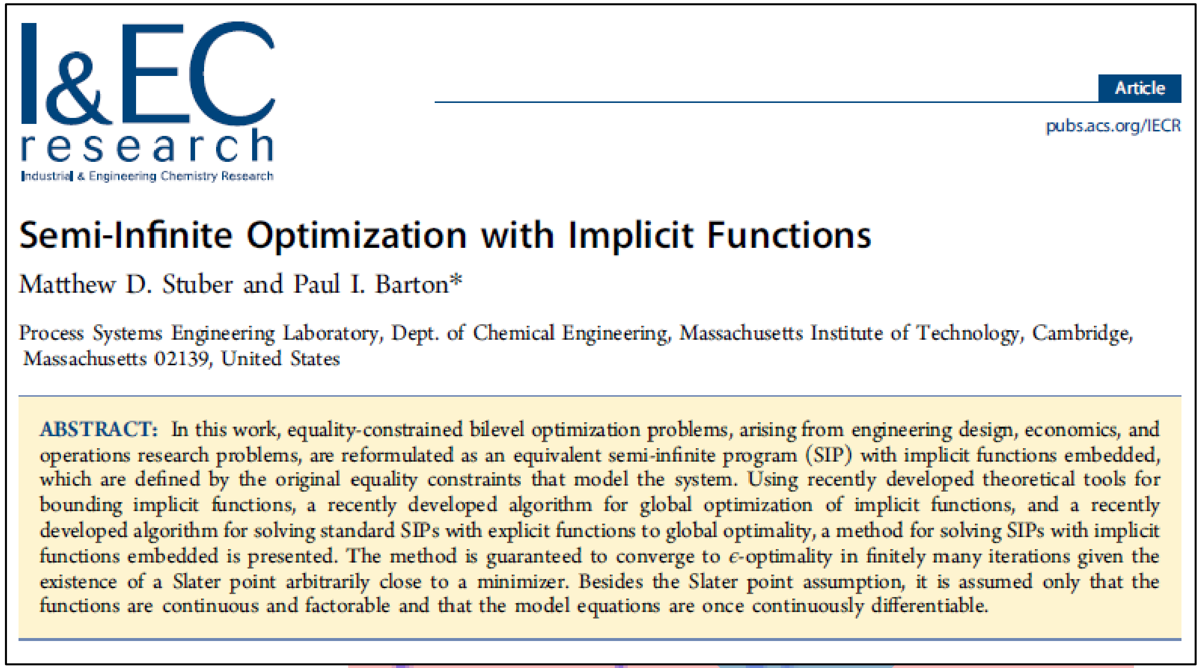


Problem Formulation

- Main challenge: most algorithms do not apply to problems with coupling equality constraints

$$\min_{\mathbf{x} \in X \in \mathbb{IR}^{n_x}} \phi(\mathbf{x})$$
$$\text{s.t.} \;\; \mathbf{g}(\mathbf{z}(\mathbf{x},\mathbf{p}),\mathbf{x},\mathbf{p}) \leq \mathbf{0}, \;\; \forall \mathbf{p} \in P$$

Semi-infinite program with implicit functions embedded


I&EC research
Industrial & Engineering Chemistry Research

Article

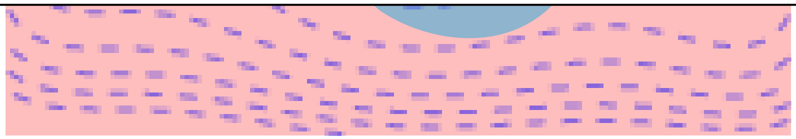
pubs.acs.org/IECR

Semi-Infinite Optimization with Implicit Functions

Matthew D. Stuber and Paul I. Barton*

Process Systems Engineering Laboratory, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States

ABSTRACT: In this work, equality-constrained bilevel optimization problems, arising from engineering design, economics, and operations research problems, are reformulated as an equivalent semi-infinite program (SIP) with implicit functions embedded, which are defined by the original equality constraints that model the system. Using recently developed theoretical tools for bounding implicit functions, a recently developed algorithm for global optimization of implicit functions, and a recently developed algorithm for solving standard SIPs with explicit functions to global optimality, a method for solving SIPs with implicit functions embedded is presented. The method is guaranteed to converge to ϵ-optimality in finitely many iterations given the existence of a Slater point arbitrarily close to a minimizer. Besides the Slater point assumption, it is assumed only that the functions are continuous and factorable and that the model equations are once continuously differentiable.

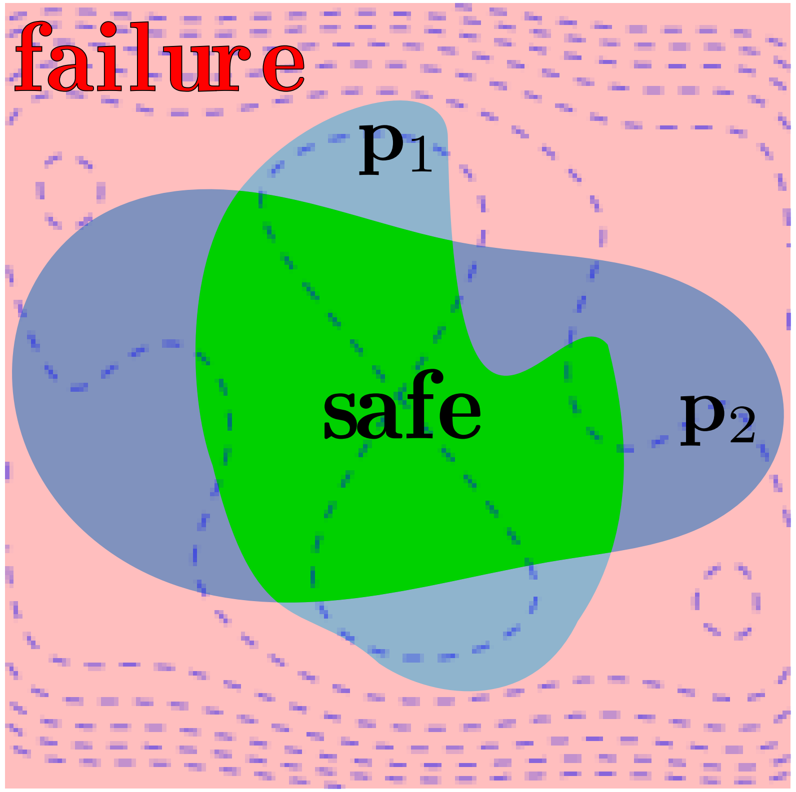


Problem Formulation

- Main challenge: most algorithms do not apply to problems with coupling equality constraints

$$
\begin{aligned}
\min_{\mathbf{x} \in X \in \mathbb{R}^{n_x}} \quad & \phi(\mathbf{x}) \\
\text{s.t.} \quad & \max_{\gamma \in \mathbb{R}, \mathbf{p} \in P \in \mathbb{R}^{n_p}, \hat{\mathbf{z}} \in \mathbb{R}^{n_z}} \quad \gamma \\
& \quad \text{s.t.} \quad \mathbf{h}(\hat{\mathbf{z}}, \mathbf{x}, \mathbf{p}) = \mathbf{0} \\
& \qquad\quad \gamma \leq \max\{g_i(\hat{\mathbf{z}}, \mathbf{x}, \mathbf{p})\}
\end{aligned}
$$

$$
\begin{aligned}
\dot{\mathbf{z}}(\mathbf{u}, \mathbf{p}, t) &= \mathbf{f}(\mathbf{z}(\mathbf{x}, \mathbf{p}, t), \mathbf{x}, \mathbf{p}, t), t \in I \\
\mathbf{z}(\mathbf{x}, \mathbf{p}, 0) &= \mathbf{z}_0(\mathbf{x}, \mathbf{p})
\end{aligned}
$$

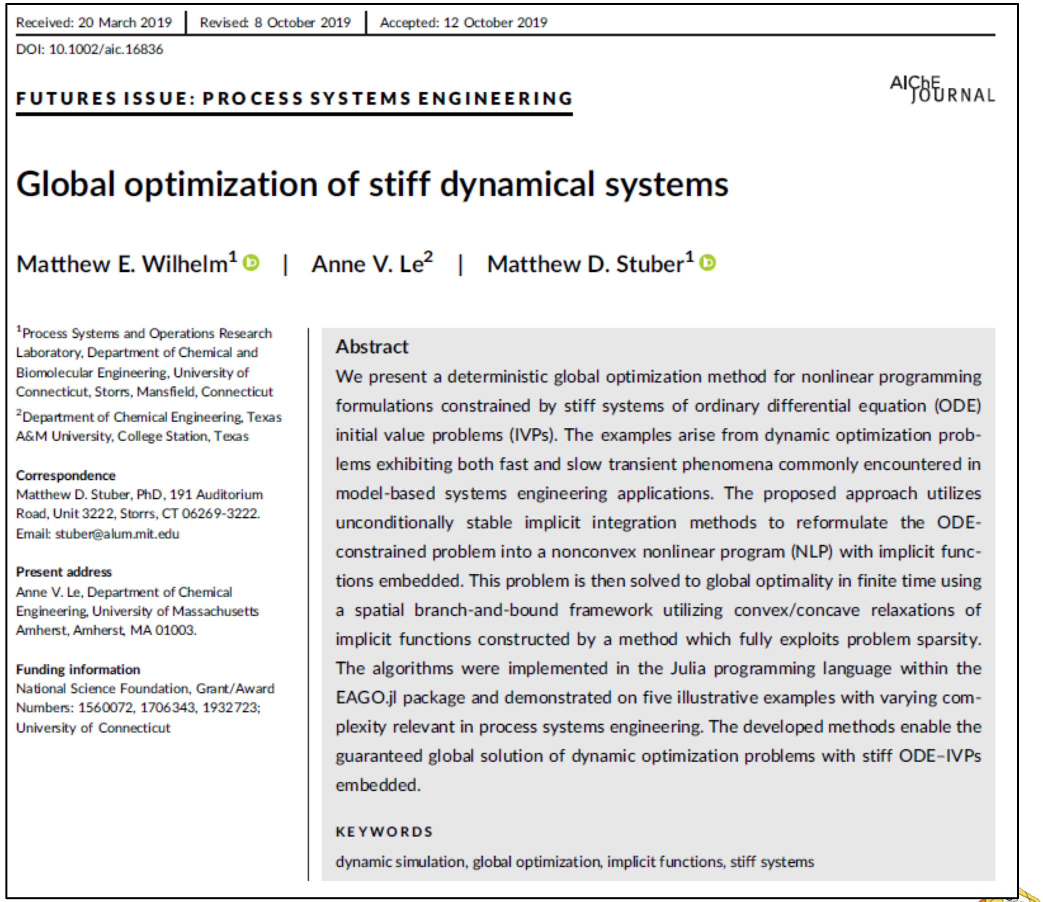


Problem Formulation

- Main challenge: most algorithms do not apply to problems with coupling equality constraints

$$\min_{\mathbf{x}\in X\in \mathbb{R}^{n_x}} \phi(\mathbf{x})$$
$$\text{s.t.} \max_{\gamma\in\mathbb{R},\mathbf{p}\in P\in\mathbb{R}^{n_p},\hat{\mathbf{z}}\in\mathbb{R}^{n_z}} \gamma$$
$$\text{s.t. } \mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\mathbf{p}) = \mathbf{0}$$
$$\gamma \leq \max\{g_i(\hat{\mathbf{z}},\mathbf{x},\mathbf{p})\}$$

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


Received: 20 March 2019 | Revised: 8 October 2019 | Accepted: 12 October 2019
DOI: 10.1002/aic.16836
FUTURES ISSUE: PROCESS SYSTEMS ENGINEERING
AIChE JOURNAL

Global optimization of stiff dynamical systems

Matthew E. Wilhelm[1] | Anne V. Le[2] | Matthew D. Stuber[1]

[1]Process Systems and Operations Research Laboratory, Department of Chemical and Biomolecular Engineering, University of Connecticut, Storrs, Mansfield, Connecticut
[2]Department of Chemical Engineering, Texas A&M University, College Station, Texas

Correspondence
Matthew D. Stuber, PhD, 191 Auditorium Road, Unit 3222, Storrs, CT 06269-3222.
Email: stuber@alum.mit.edu

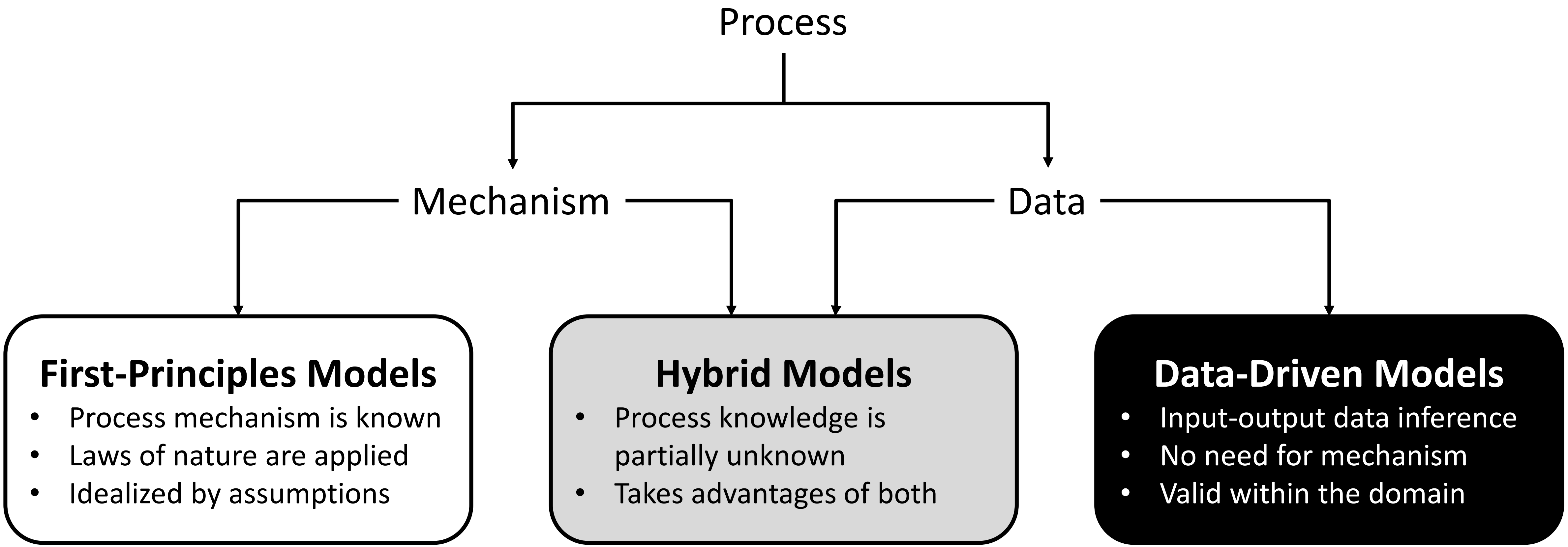
Present address
Anne V. Le, Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA 01003.

Funding information
National Science Foundation, Grant/Award Numbers: 1560072, 1706343, 1932723; University of Connecticut

Abstract
We present a deterministic global optimization method for nonlinear programming formulations constrained by stiff systems of ordinary differential equation (ODE) initial value problems (IVPs). The examples arise from dynamic optimization problems exhibiting both fast and slow transient phenomena commonly encountered in model-based systems engineering applications. The proposed approach utilizes unconditionally stable implicit integration methods to reformulate the ODE-constrained problem into a nonconvex nonlinear program (NLP) with implicit functions embedded. This problem is then solved to global optimality in finite time using a spatial branch-and-bound framework utilizing convex/concave relaxations of implicit functions constructed by a method which fully exploits problem sparsity. The algorithms were implemented in the Julia programming language within the EAGO.jl package and demonstrated on five illustrative examples with varying complexity relevant in process systems engineering. The developed methods enable the guaranteed global solution of dynamic optimization problems with stiff ODE-IVPs embedded.

KEYWORDS
dynamic simulation, global optimization, implicit functions, stiff systems

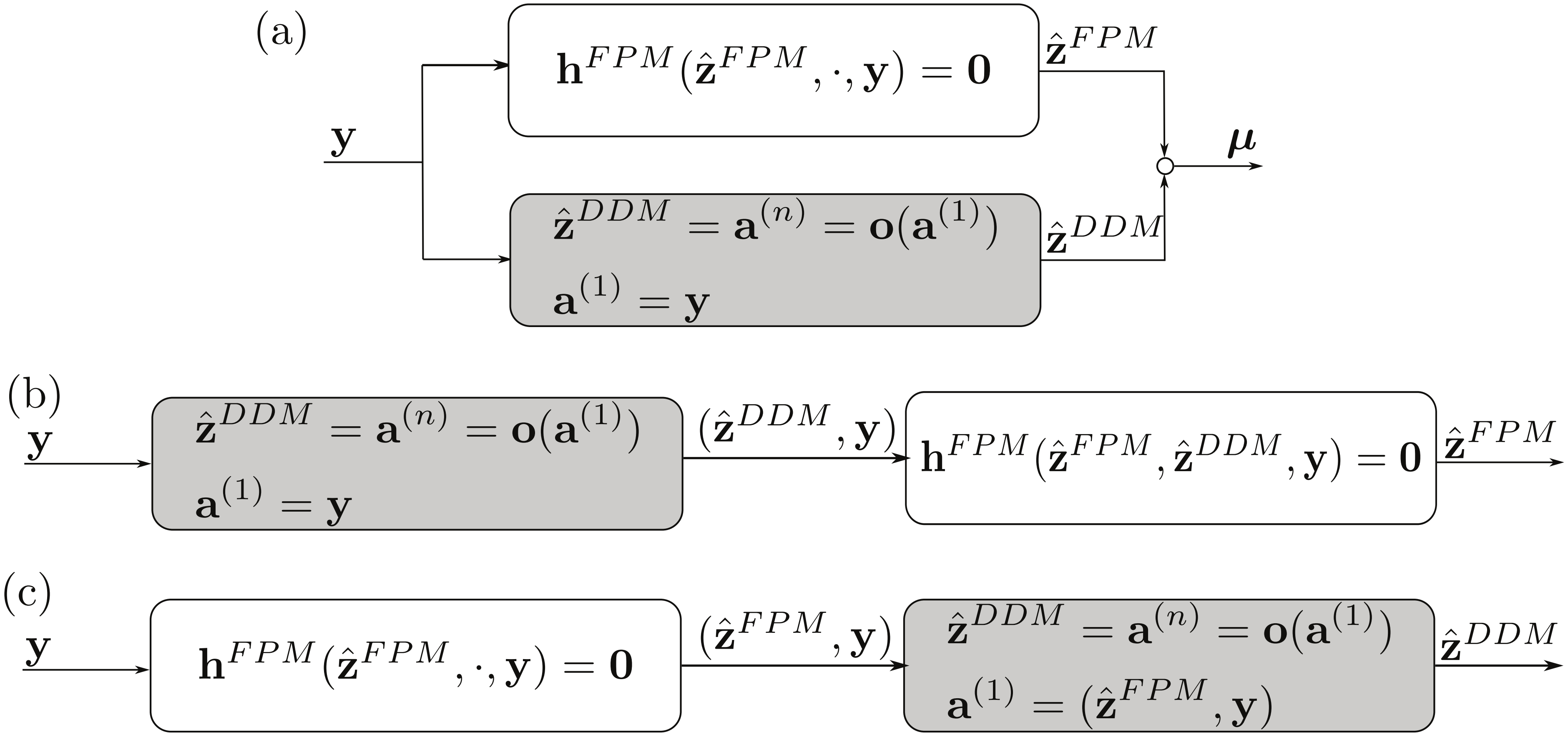
Hybrid Modeling



[1] von Stosch, M.; Oliveira, R.; Peres, J.; de Azevedo, S. F. Hybrid semi-parametric modeling in process systems engineering: Past, present and future. *Computers & Chemical Engineering* 2014,60, 86–101.

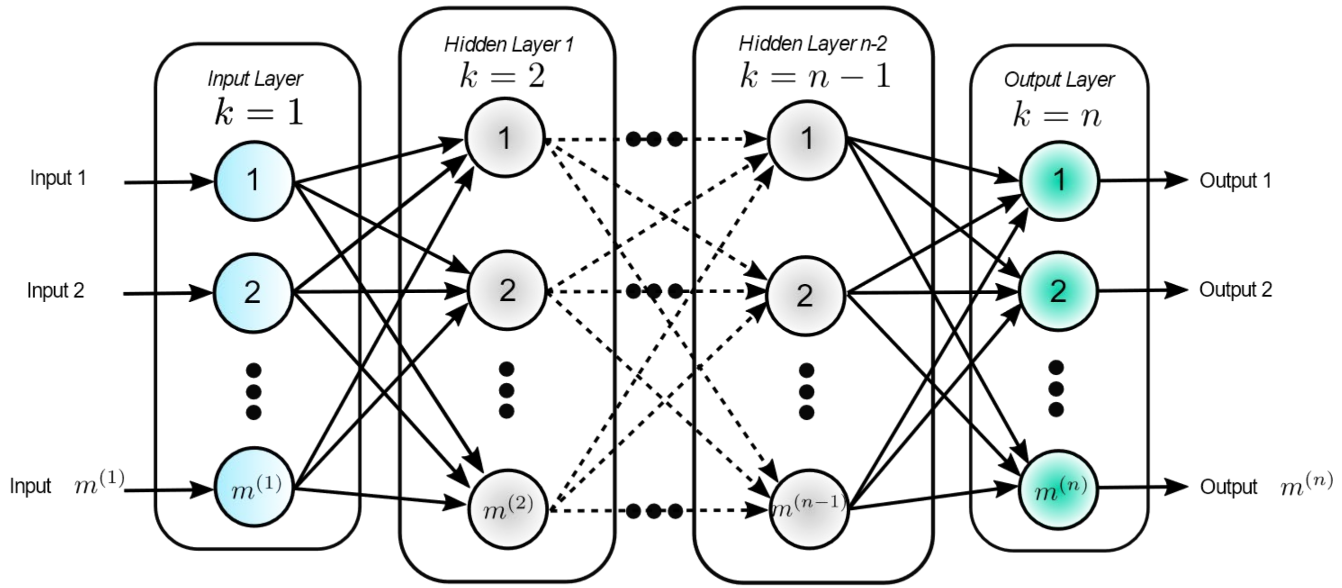
Hybrid Modeling

- Hybrid model architectures



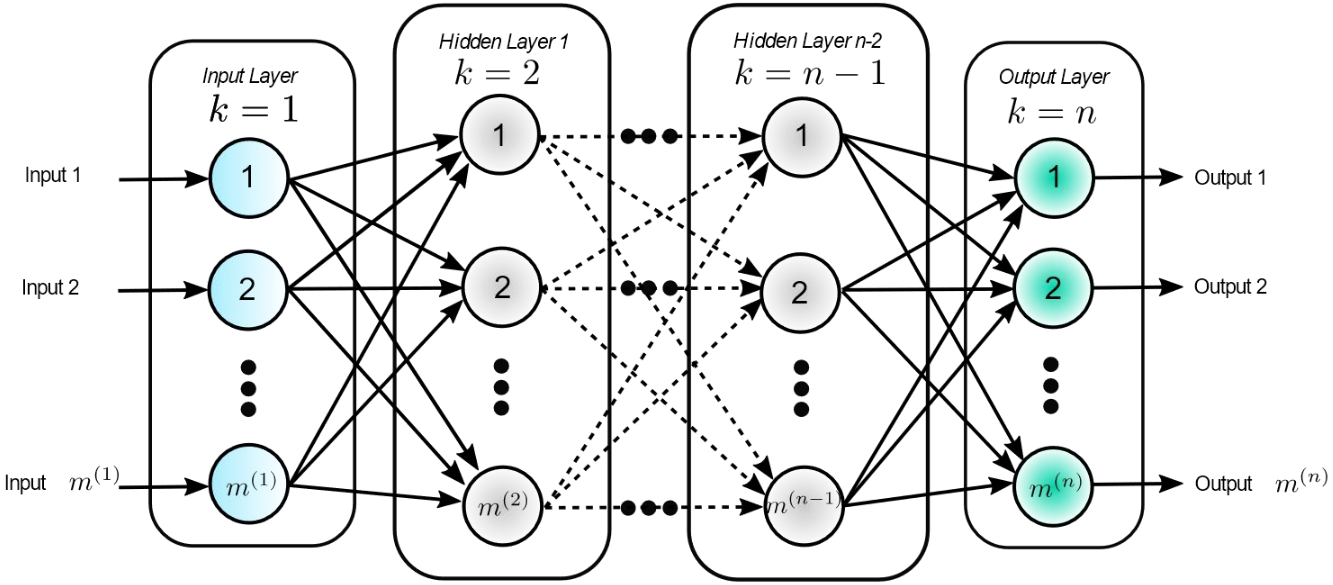
DGO of ANNs

- Hybrid models with artificial neural networks are still nonconvex



DGO of ANNs

- Hybrid models with artificial neural network



Journal of Global Optimization
https://doi.org/10.1007/s10898-022-01228-x

Convex and concave envelopes of artificial neural network activation functions for deterministic global optimization

Matthew E. Wilhelm[1] · Chenyu Wang[1] · Matthew D. Stuber[1]

Received: 30 September 2021 / Accepted: 16 August 2022

Abstract
In this work, we present general methods to construct convex/concave relaxations of the activation functions that are commonly chosen for artificial neural networks (ANNs). The choice of these functions is often informed by both broader modeling considerations balanced with a need for high computational performance. The direct application of factorable programming techniques to compute bounds and convex/concave relaxations of such functions often lead to weak enclosures due to the dependency problem. Moreover, the piecewise formulation that defines several popular activation functions, prevents the computation of convex/concave relaxations as they violate the factorable function requirement. To improve the performance of relaxations of ANNs for deterministic global optimization applications, this study presents the development of a library of envelopes of the thoroughly studied rectifier-type and sigmoid activation functions, in addition to the novel self-gated sigmoid-weighted linear unit (SiLU) and Gaussian error linear unit activation functions. We demonstrate that the envelopes of activation functions directly lead to tighter relaxations of ANNs on their input domain. In turn, these improvements translate to a dramatic reduction in CPU runtime required for solving optimization problems involving ANN models to epsilon-global optimality. We further demonstrate that the factorable programming approach leads to superior computational performance over alternative state-of-the-art approaches.

SIPs with Hybrid Models

- SIP structure is the same, but some decomposition and simplification may be exploited

$$\min_{\mathbf{x}\in X\in \mathbb{R}^{n_x},\hat{\mathbf{z}}\in Z} \phi(\mathbf{x})$$
$$\text{s.t.}\ \max\{g_i(\hat{\mathbf{z}},\mathbf{x},\mathbf{p})\} \leq 0, \forall \mathbf{p}\in P$$
$$\mathbf{h}(\hat{\mathbf{z}},\mathbf{x},\mathbf{p}) = \mathbf{0}, \forall \mathbf{p}\in P$$

Where:

$$\hat{\mathbf{z}} = (\hat{\mathbf{z}}^{\text{FPM}}, \hat{\mathbf{z}}^{\text{DDM}})$$
$$\mathbf{h} = (\mathbf{h}^{\text{FPM}}, \mathbf{h}^{\text{DDM}})$$

SIPs with Hybrid Models

- SIP s… ation may be ex…

$\min_{\mathbf{x}\in X\in\mathbb{IR}^{n_x},\hat{\mathbf{z}}\in\ldots}$

s.t. max…

$\mathbf{h}(\hat{\mathbf{z}},\ldots$

I&EC research
Industrial & Engineering Chemistry Research

pubs.acs.org/IECR

Article

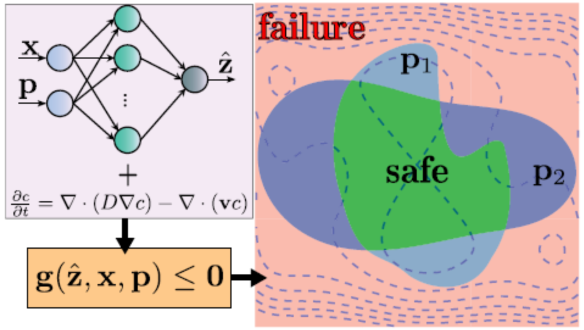
Semi-Infinite Optimization with Hybrid Models

Chenyu Wang, Matthew E. Wilhelm, and Matthew D. Stuber*

Cite This: *Ind. Eng. Chem. Res.* 2022, 61, 5239–5254

Read Online

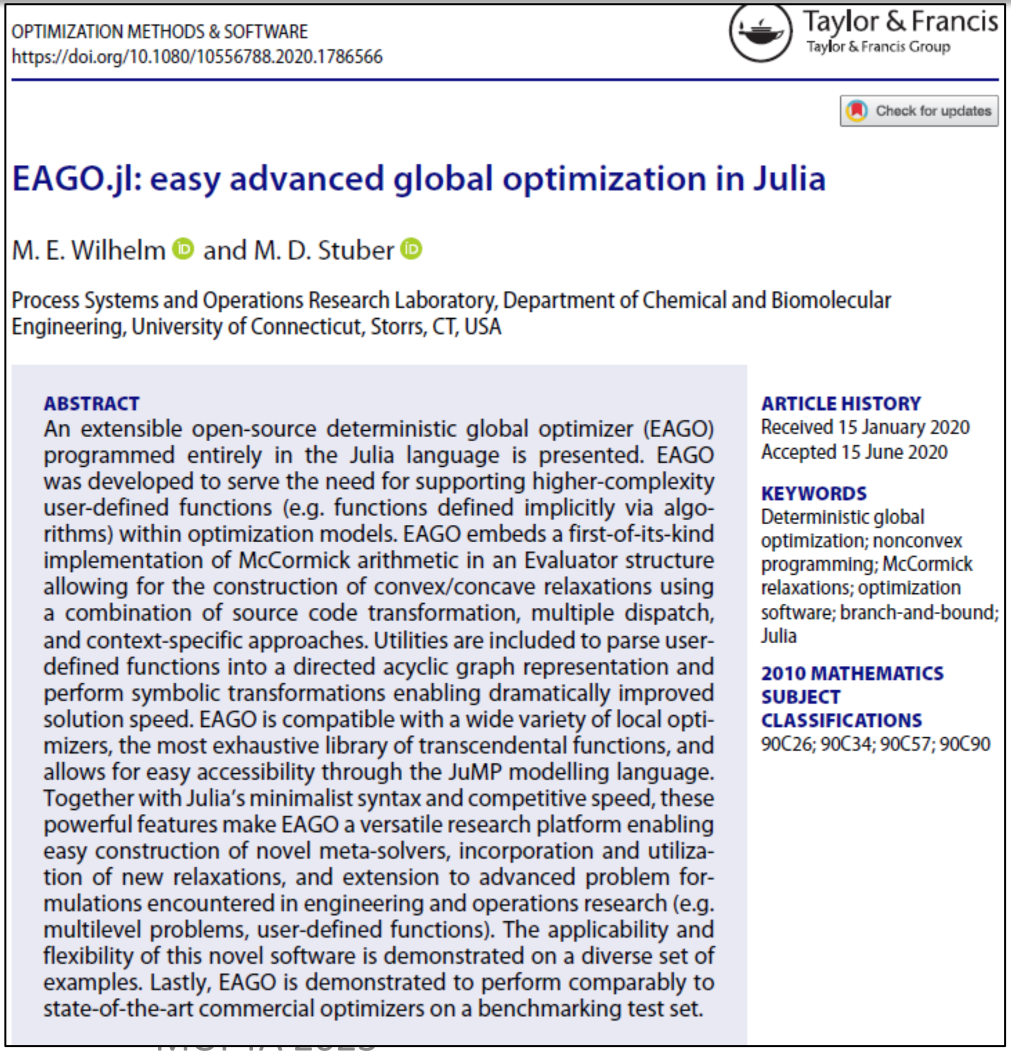
ABSTRACT: The robust design of performance/safety-critical process systems, from a model-based perspective, remains an existing challenge. Hybrid first-principles data-driven models offer the potential to dramatically improve model prediction accuracy, stepping closer to the digital twin concept. Within this context, worst-case engineering design feasibility and reliability problems give rise to a class of semi-infinite program (SIP) formulations with hybrid models as coupling equality constraints. Reduced-space deterministic global optimization methods are exploited to solve this class of SIPs to ϵ-global optimality in finitely many iterations. This approach is demonstrated on two challenging case studies: a nitrification reactor for a wastewater treatment system to address worst-case feasibility verification of dynamical systems and a three-phase separation system plagued by numerical domain violations to demonstrate how they can be overcome using a nonsmooth SIP formulation with hybrid models and a validity constraint incorporated.



SIPs with Hybrid Models

Solution Method

Backbone:
deterministic global optimization solver



OPTIMIZATION METHODS & SOFTWARE
https://doi.org/10.1080/10556788.2020.1786566

Taylor & Francis
Taylor & Francis Group

Check for updates

EAGO.jl: easy advanced global optimization in Julia

M. E. Wilhelm and M. D. Stuber

Process Systems and Operations Research Laboratory, Department of Chemical and Biomolecular Engineering, University of Connecticut, Storrs, CT, USA

ABSTRACT

An extensible open-source deterministic global optimizer (EAGO) programmed entirely in the Julia language is presented. EAGO was developed to serve the need for supporting higher-complexity user-defined functions (e.g. functions defined implicitly via algorithms) within optimization models. EAGO embeds a first-of-its-kind implementation of McCormick arithmetic in an Evaluator structure allowing for the construction of convex/concave relaxations using a combination of source code transformation, multiple dispatch, and context-specific approaches. Utilities are included to parse user-defined functions into a directed acyclic graph representation and perform symbolic transformations enabling dramatically improved solution speed. EAGO is compatible with a wide variety of local optimizers, the most exhaustive library of transcendental functions, and allows for easy accessibility through the JuMP modelling language. Together with Julia's minimalist syntax and competitive speed, these powerful features make EAGO a versatile research platform enabling easy construction of novel meta-solvers, incorporation and utilization of new relaxations, and extension to advanced problem formulations encountered in engineering and operations research (e.g. multilevel problems, user-defined functions). The applicability and flexibility of this novel software is demonstrated on a diverse set of examples. Lastly, EAGO is demonstrated to perform comparably to state-of-the-art commercial optimizers on a benchmarking test set.

ARTICLE HISTORY
Received 15 January 2020
Accepted 15 June 2020

KEYWORDS
Deterministic global optimization; nonconvex programming; McCormick relaxations; optimization software; branch-and-bound; Julia

2010 MATHEMATICS SUBJECT CLASSIFICATIONS
90C26; 90C34; 90C57; 90C90

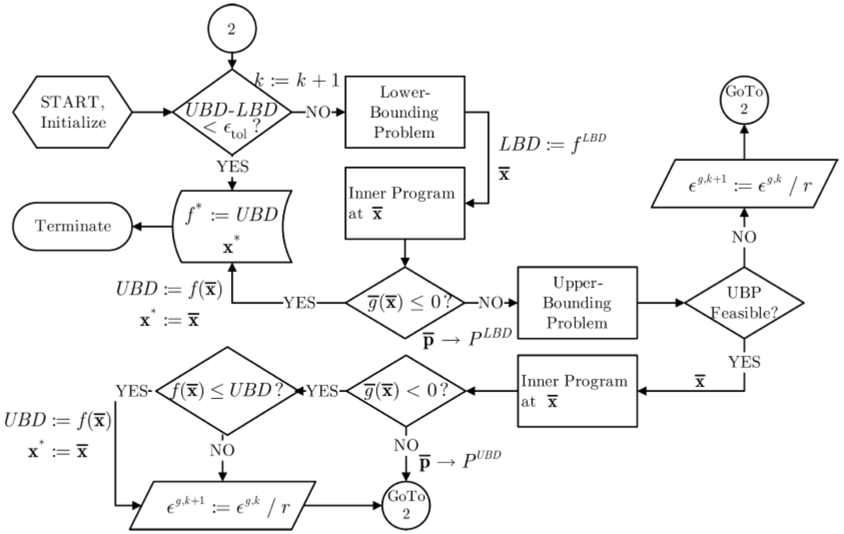
SIPs with Hybrid Models

Solution Method

Backbone:
deterministic global
optimization solver

EAGO

SIP Solver: SIPres
cutting-plane algorithm
(Mitsos, 2011)



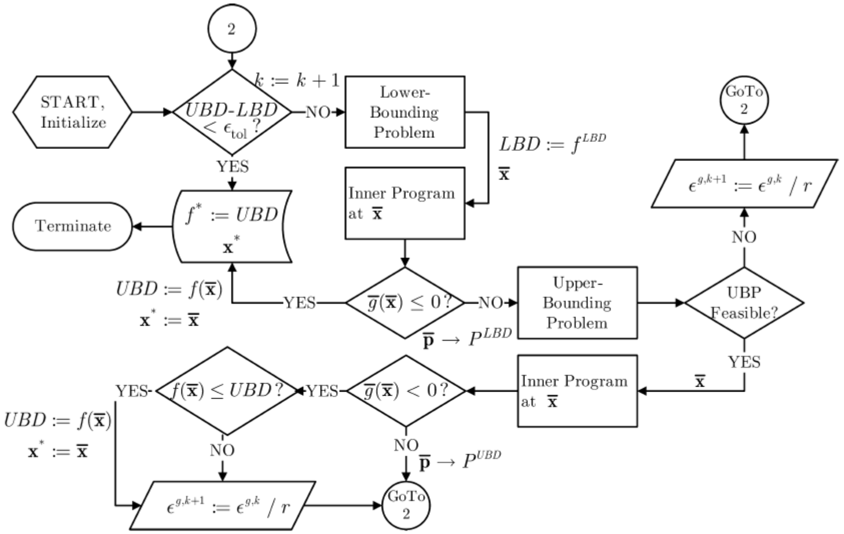
SIPs with Hybrid Models

Solution Method

Backbone: deterministic global optimization solver

EAGO

SIP Solver: SIPres cutting-plane algorithm (Mitsos, 2011)



Data-Driven Model: ANN with supported activation functions (NNlib.jl)

flux

PyTorch

SIPs with Hybrid Models

Solution Method

Backbone: deterministic global optimization solver

```
# Objective function
f(x) = (x[1]-3.5)^4 - 5.0*(x[1]-3.5)^3 - 2.0*(x[1]-3.5)^2 + 15.0*(x[1]-3.5)

# SIP constraint
# g(x, y, p) = y + cos(x - p/90) - p
function gSIP(x, p)
    # Call surrogate model to solve for y at the given x and p
    y = scale_output(ANN_model, x[1], p[1])

    # Return g
    return y[1] + cos(x[1] - p[1]/90) - p[1]
end

# Variable bounds for SIP
x_lo_SIP = Float64[0.5]
x_hi_SIP = Float64[8.0]
p_lo_SIP = Float64[80.0]
p_hi_SIP = Float64[120.0]

# Solve SIP
sip_result = sip_solve(SIPRes(), x_lo_SIP, x_hi_SIP, p_lo_SIP, p_hi_SIP,
                       f, Any[gSIP], abs_tolerance = 1E-4)
```

del: ANN
activation
Nlib.jl)

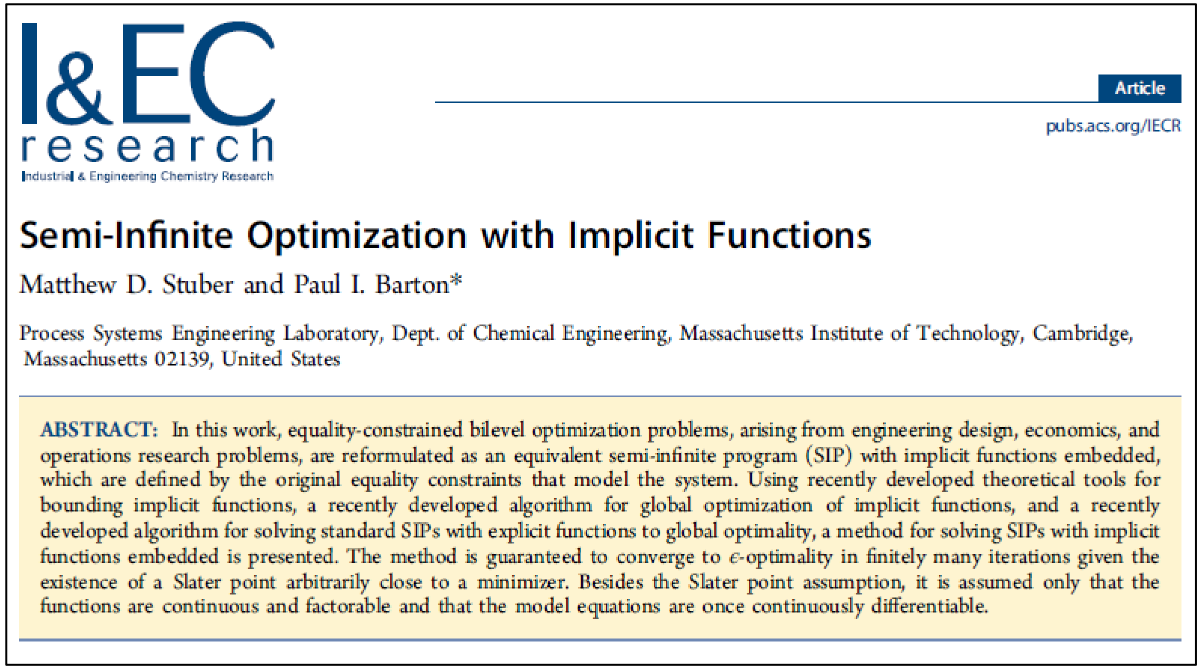
Ex: Simple

- Consider the SIP:

$$\min_{\hat{z}\in Z, x\in X} (x-3.5)^4 - 5(x-3.5)^3 - 2(x-3.5)^2 + 15(x-3.5)$$

$$\text{s.t.} \quad \hat{z} + \cos(x - p/90) - p \leq 0, \forall p \in P$$

$$\hat{z} - (x - x^3/6 + x^5/120)/\sqrt{\hat{z}} = 0, \forall p \in P$$


I&EC research
Industrial & Engineering Chemistry Research
Article
pubs.acs.org/IECR

Semi-Infinite Optimization with Implicit Functions

Matthew D. Stuber and Paul I. Barton*

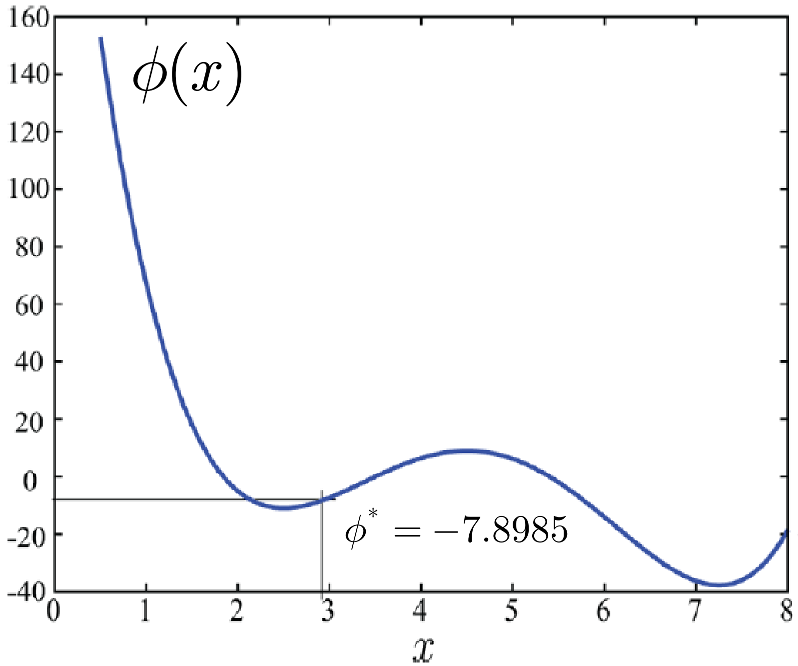
Process Systems Engineering Laboratory, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, United States

ABSTRACT: In this work, equality-constrained bilevel optimization problems, arising from engineering design, economics, and operations research problems, are reformulated as an equivalent semi-infinite program (SIP) with implicit functions embedded, which are defined by the original equality constraints that model the system. Using recently developed theoretical tools for bounding implicit functions, a recently developed algorithm for global optimization of implicit functions, and a recently developed algorithm for solving standard SIPs with explicit functions to global optimality, a method for solving SIPs with implicit functions embedded is presented. The method is guaranteed to converge to ϵ-optimality in finitely many iterations given the existence of a Slater point arbitrarily close to a minimizer. Besides the Slater point assumption, it is assumed only that the functions are continuous and factorable and that the model equations are once continuously differentiable.

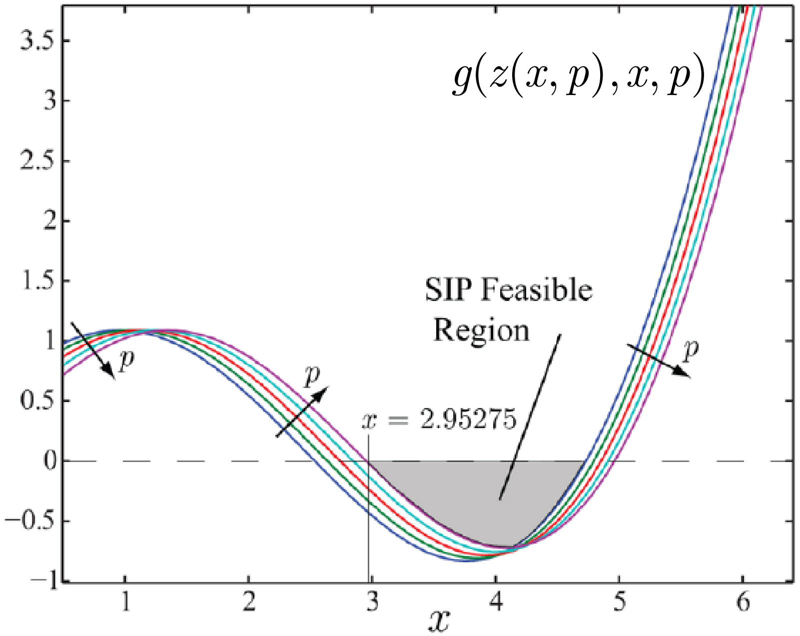
Ex: Simple

- Consider the SIP:

$$\min_{\hat{z}\in Z, x\in X} (x-3.5)^4 - 5(x-3.5)^3 - 2(x-3.5)^2 + 15(x-3.5)$$
$$\text{s.t.}\ \ z(x,p) + \cos(x - p/90) - p \le 0, \forall p \in P$$



$z(x,p) : h(z(x,p),x,p) = 0$

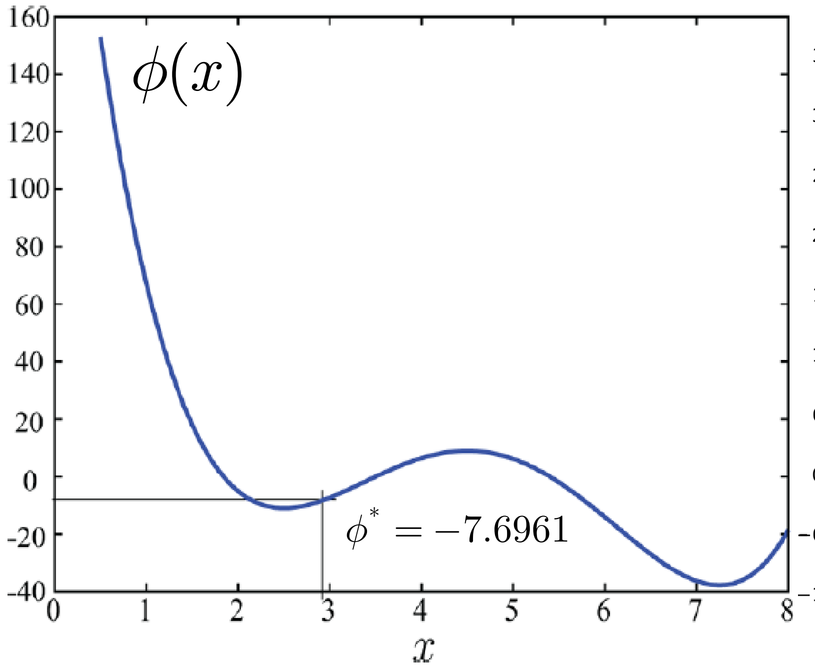


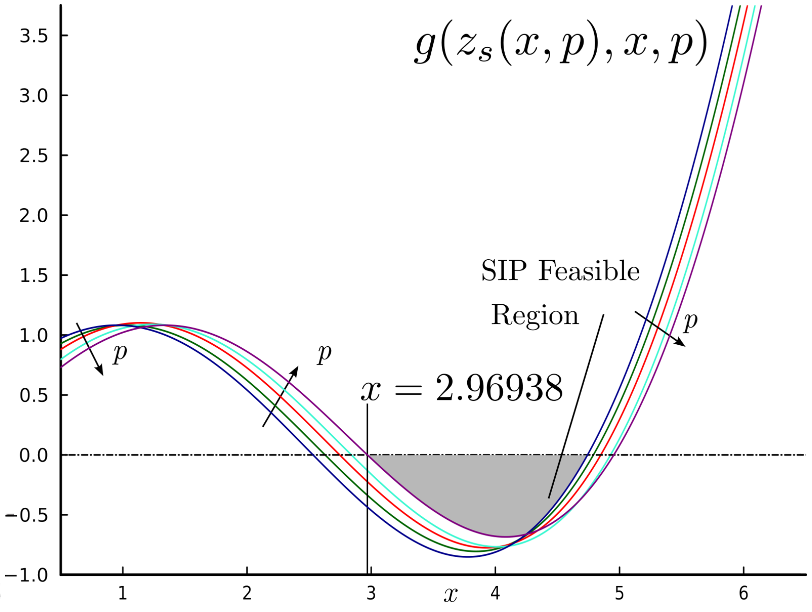
Ex: Simple

- Consider the SIP:

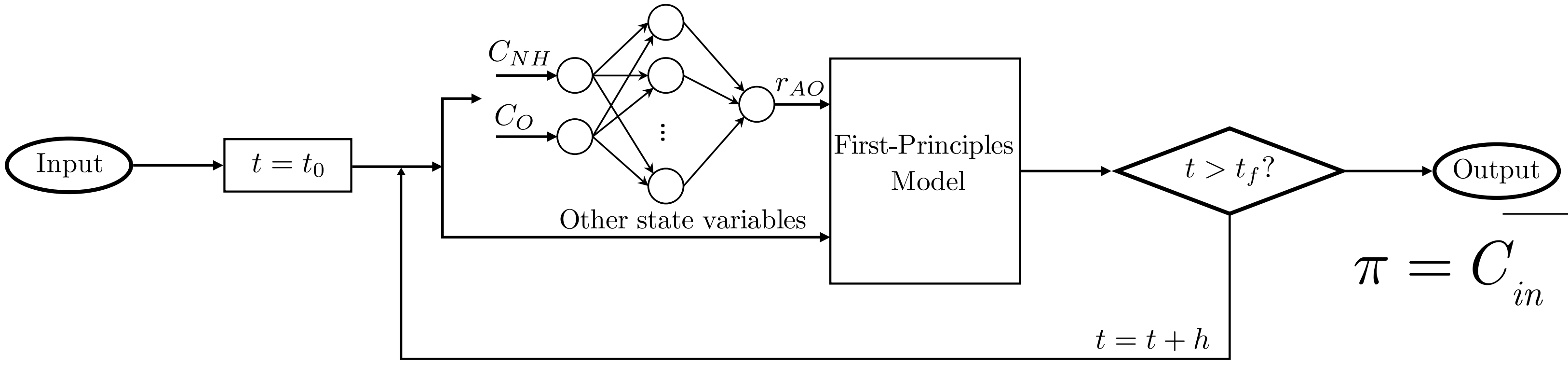
$$\min_{\hat{z}\in Z, x\in X} (x-3.5)^4 - 5(x-3.5)^3 - 2(x-3.5)^2 + 15(x-3.5)$$
$$\text{s.t. } z_s(x,p) + \cos(x - p/90) - p \le 0, \forall p \in P$$

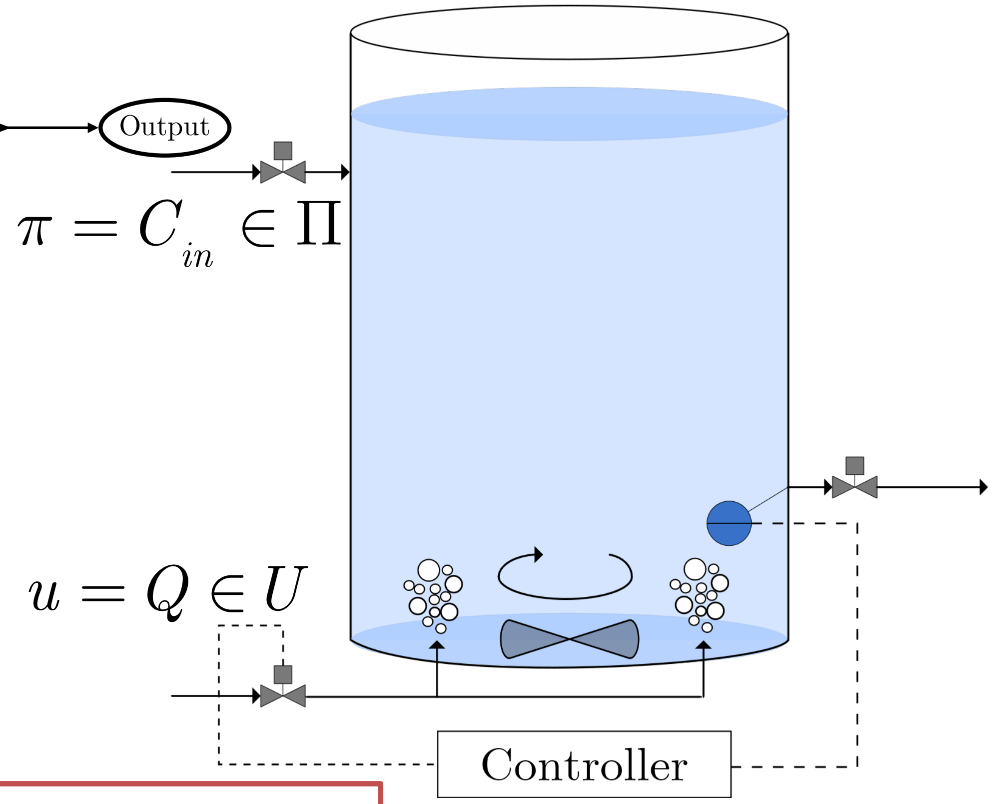
$$z_s(x,p) \approx z(x,p) : h(z(x,p), x, p) = 0$$





Ex: Nitrification CSTR





Model:

$$\frac{dC_{NH}}{dt} = \frac{1}{V}(\dot{m}_{in} C_{in} - \dot{m}_{out} C_{NH}) - r_{AO} X_{AO}$$

$$\frac{dC_{NI}}{dt} = r_{AO} X_{AO} - r_{NO} X_{NO}$$

$$\frac{dC_{NA}}{dt} = r_{NO} X_{NO}$$

$$\frac{dC_{O}}{dt} = -r_{AO} \Psi_{AO} X_{AO} - r_{NO} \Psi_{NO} X_{NO} + k_{la}(C_O^* - C_O)$$

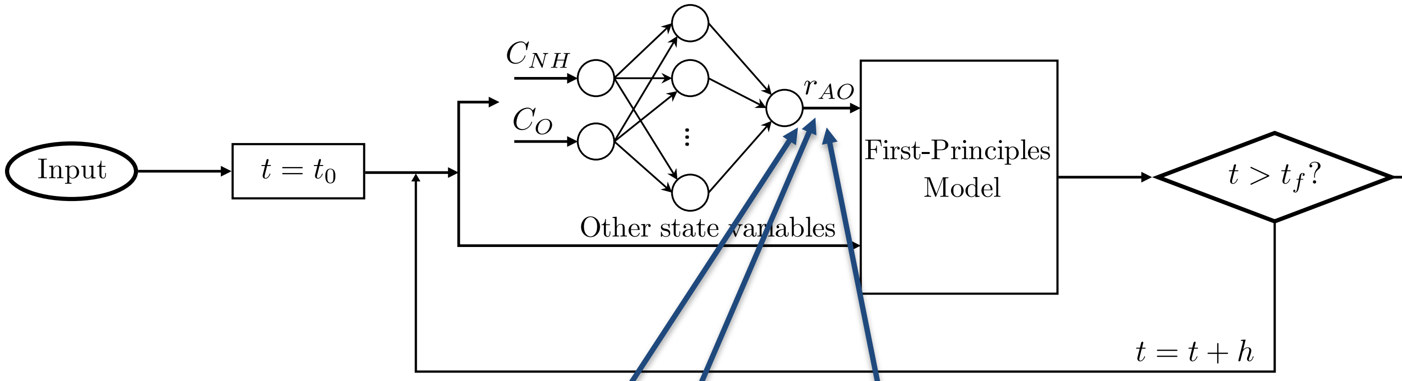
$$k_{la} = \frac{0.2967 Q \cdot \mathrm{SOTE}}{C_O^* \cdot V}$$

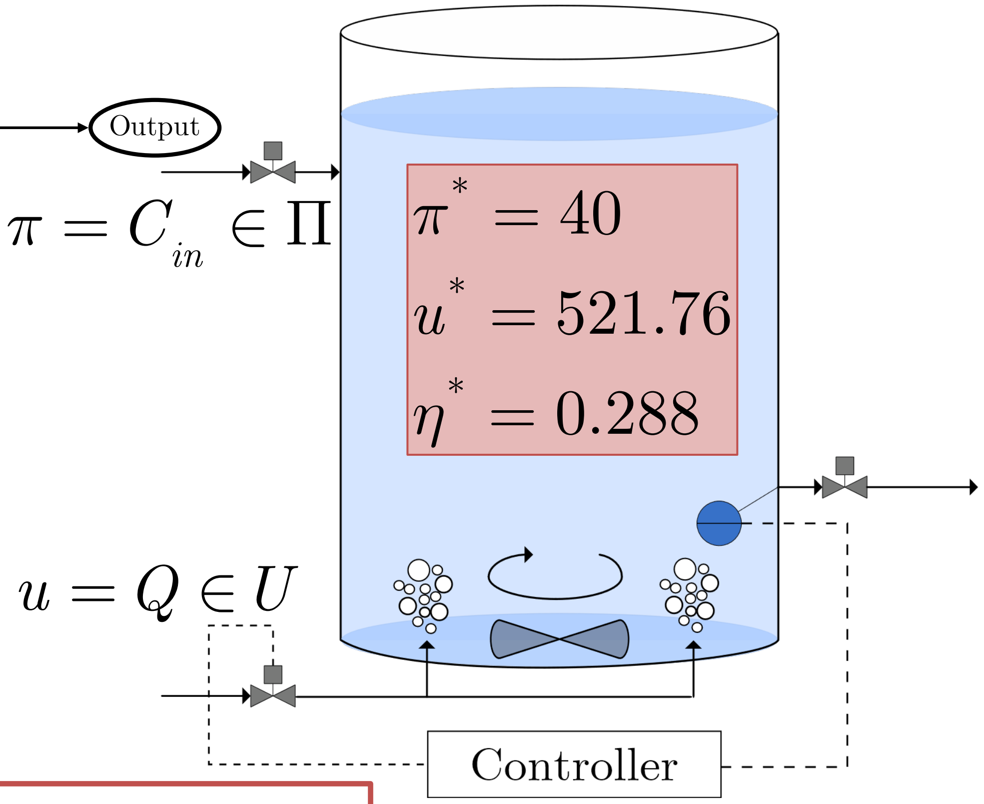
Robust operation:

$$\phi^* = \max_{\pi \in \Pi, \eta \in H} \eta$$

$$\text{s.t.} \quad \eta \le \max\{C_{NH}(t_f, \pi, u) - \mathrm{USL}_{\mathrm{NH}}, C_O(t_f, \pi, u) - \mathrm{USL}_{\mathrm{O}}\}, \forall u \in U$$

Ex: Nitrification CSTR





Model:

$$\frac{dC_{NH}}{dt} = \frac{1}{V}(\dot{m}_{in} C_{in} - \dot{m}_{out} C_{NH}) - r_{AO} X_{AO}$$

$$\frac{dC_{NI}}{dt} = r_{AO} X_{AO} - r_{NO} X_{NO}$$

$$\frac{dC_{NA}}{dt} = r_{NO} X_{NO}$$

$$\frac{dC_O}{dt} = -r_{AO} \Psi_{AO} X_{AO} - r_{NO} \Psi_{NO} X_{NO} + k_{la} (C_O^* - C_O)$$

$$k_{la} = \frac{0.2967 Q \cdot \text{SOTE}}{C_O^* \cdot V}$$

Robust operation:

$$\phi^* = \max_{\pi \in \Pi, \eta \in H} \eta$$

$$\text{s.t.} \quad \eta \leq \max\{C_{NH}(t_f, \pi, u) - \text{USL}_{\text{NH}}, C_O(t_f, \pi, u) - \text{USL}_{\text{O}}\}, \forall u \in U$$

Ex: Remote Separations

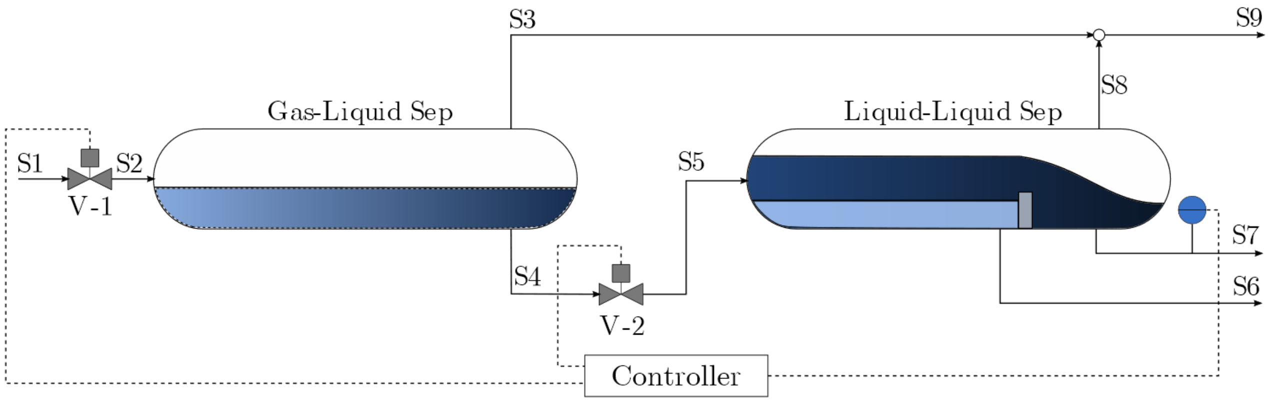
AIChE

Worst-Case Design of Subsea Production Facilities Using Semi-Infinite Programming

Matthew D. Stuber, Achim Wechsung, Arul Sundaramoorthy, and Paul I. Barton
Process Systems Engineering Laboratory, Dept. of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139

DOI 10.1002/aic.14447
Published online April 3, 2014 in Wiley Online Library (wileyonlinelibrary.com)

The problem of designing novel process systems for deployment in extreme and hostile environments is addressed. Specifically, the process system of interest is a subsea production facility for ultra deepwater oil and gas production. The costs associated with operational failures in deepwater environments are prohibitively high and, therefore, warrant the application of worst-case design strategies. That is, prior to the construction and deployment of a process, a certificate of robust feasibility is obtained for the proposed design. The concept of worst-case design is addressed by formulating the design feasibility problem as a semi-infinite optimization problem with implicit functions embedded. A basic model of a subsea production facility is presented for a case study of rigorous performance and safety verification. Relying on recent advances in global optimization of implicit functions and semi-infinite programming, the design feasibility problem is solved, demonstrating that this approach is effective in addressing the problem of worst-case design of novel process systems. *AIChE J*, 60: 2513–2524, 2014
Keywords: robust design, design under uncertainty, verification, global optimization, semi-infinite programming

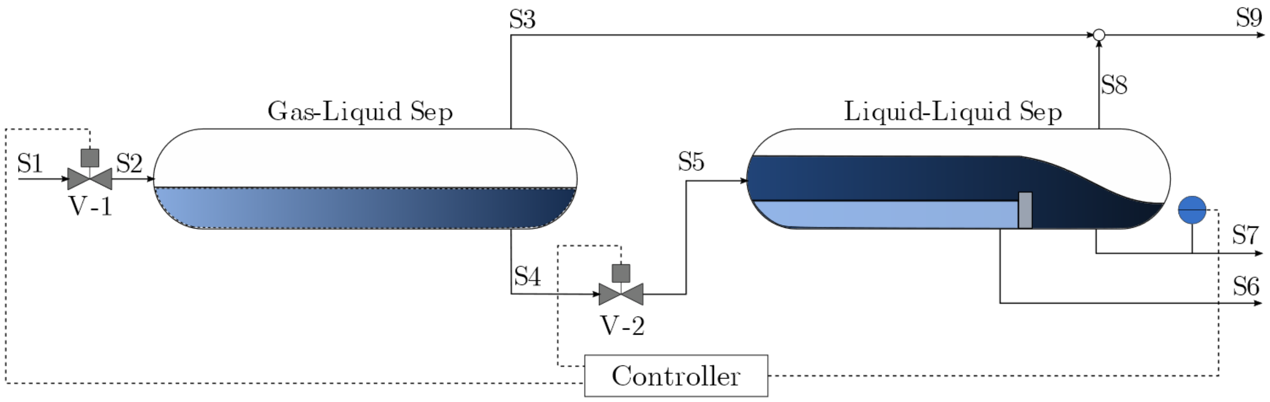


Ex: Remote Separations

$$f(\hat{z}) = \cos^{-1}\left(1 - \frac{\hat{z}}{r}\right), \; r, \hat{z} > 0$$

$$Z_{valid} = [0, 2r]$$

```
julia> acos(-1.1)
ERROR: DomainError with -1.1:
acos(x) not defined for |x| > 1
Stacktrace:
 [1] acos_domain_error(x::Float64)
   @ Base.Math .\special\trig.jl:669
 [2] acos(x::Float64)
   @ Base.Math .\special\trig.jl:699
 [3] top-level scope
   @ REPL[5]:1
```



Conclusions

- Worst-case optimization under uncertainty problems are nonconvex SIPs with coupling equality constraints
- Hybrid modeling approaches can be used to potentially reduce the complexity of the optimization problem
- Toolchain based on EAGO for solving SIPs (with hybrid models)
- Examples illustrate some usage cases for relevant applications in process systems engineering, including:
  - dynamic optimization
  - validity domains

Acknowledgements

Members of the Process Systems and Operations Research Laboratory at the University of Connecticut (https://psor.uconn.edu/)

Process Systems and Operations Research Laboratory

UCONN
UNIVERSITY OF CONNECTICUT

Funding:

National Science Foundation, Award No.: 1932723

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

UCONN
UNIVERSITY OF CONNECTICUT

Thank You!

Process Systems and Operations Research Laboratory