Robust Dynamic Optimization via Relaxations of Implicit Integration Schemes

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Robust Dynamic Optimization

**Dynamic SIP Formulation**

\[
\Phi^* = \min_{u} \Phi(u)
\]

Objective

s.t. \( g(x(u, p, t_f), u, p) \leq 0 \)

Performance Constraint(s)

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

Parametric ODEs

\[
x(u, p, t_0) = x_0(u, p)
\]

Initial Condition

\[
t \in I = [t_0, t_f], \forall p \in P
\]

**Assumptions**

- The initial condition \( x_0: P \to D \) is *locally Lipschitz continuous* on \( U \times P \).
- The right hand side \( f \) is \( n \) times continuously differentiable on \( U \times D \times P \).

**Motivation:**

- Determine adequate system performance under worst-case realization of uncertainty.
- Key for safety-critical systems and high-risk defect elimination.
- Prior work rely on heuristic approaches which lose strong guarantees [1,2].

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Relatively general form (via reformulations):

- Applicable to some semi-explicit index-1 DAEs
- Non-autonomous systems

Semi-infinite Programming

- One standard approach to solving SIP’s lies in the discretization the uncertain set [3].

- Restriction-based upper bound incorporated in the SIPres algorithm for nonconvex SIP[4].

- SIPres provides a guaranteed convergence to a global optimal value under Slater-point constraint qualification.

- Adapted to use a hybrid approach which contains an oracle problem that further refines lower and upper bounds at each iteration with a single discretization set per SIP constraint (NOT PICTURED) [5].

Overview of SIPres algorithm [1]

- LBP
  - Converged?
  - Update lower bound
  - LBP Feasible?
  - Update restriction parameter
  - Add to discretization set (or update LLP tolerance)

- LLP 1
  - LBD SIP Feasible?
  - Terminate

- UBP
  - UBD Feasible?
  - LLP 2
  - Update upper bound, restriction parameter, LLP tolerance, and/or discretization set


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In this work.

Overview of SIPres algorithm [4]

- Converged?
  - LBP: Update lower bound
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        - Update restriction parameter
  - Terminate

SIP Subproblems

**LBP**  Lower-Bounding Problem

\[ \Phi^{LBD} = \min_u \Phi(u) \]
\[ \text{s.t. } g(x(u, \bar{p}, t_f), u, \bar{p}) \leq 0 \quad \forall \bar{p} \in P^{disc} \]
\[ u \in U \subset \mathbb{R}^{nu} \]

**UBP**  Upper-Bounding Problem

\[ \Phi^{UBD} = \min_u \Phi(u) \]
\[ \text{s.t. } g(x(u, \bar{p}, t_f), u, \bar{p}) \leq -\epsilon_g \quad \forall \bar{p} \in P^{disc} \]
\[ u \in U \subset \mathbb{R}^{nu} \]

**LLP**  Lower-Level Problem

\[ \Phi^{LLP} = \max_p g(x(\bar{u}, p, t_f), \bar{u}, p) \]
\[ \text{s.t. } p \in P \subset \mathbb{R}^{np} \]

**RES**  Restriction Problem

\[ -\eta^* = \min_{\eta, u} -\eta \]
\[ \text{s.t. } \Phi(u) - \Phi^{RES} \leq 0 \]
\[ g(x(u, \bar{p}, t_f), u, \bar{p}) \leq -\eta \quad \forall \bar{p} \in P^{disc} \]
\[ u \in U \subset \mathbb{R}^{nu} \]

Global Dynamic Optimization

### Reduced-Space Relaxations

**Relax-then-Discretize**

\[
\begin{align*}
\dot{x}^c(t,p) &= f^c(t,p,x^c(t,p),x^{cc}(t,p)), & x^c(t_0,p) &= x_0^c(p) \\
\dot{x}^{cc}(t,p) &= f^{cc}(t,p,x^c(t,p),x^{cc}(t,p)), & x^{cc}(t_0,p) &= x_0^{cc}(p)
\end{align*}
\]

- Development of interval-based differential inequality [10,11]
- Less expansive convex/concave relaxations as well as tighter interval bounds [12,13,14]
- Adaptation of these methods to semi-explicit index-one differential-algebraic systems of equations DAEs [15,16,17]
- Methods of tightening state relaxations by exploiting model redundancy and nonlinear invariants [18,19].


**Discretize-then-Relax**

\[
\begin{align*}
x(\tau_{q+1},p) &= x(\tau_q,p) + \sum_{j=1}^{p} \frac{h^j}{j!} f^{(j)}(x(\tau_q,p),p) + \frac{h^{p+1}}{(p+1)!} f^{(p+1)}(X(\tau_q),P)
\end{align*}
\]

- Generalized to two step methods consisting of an existence and uniqueness test and subsequent contraction [21,22].
- Discretize-and-relax approaches with McCormick relaxations [23]
- Taylor-Interval [24], Taylor-McCormick [25] models, and Taylor-Ellipsoid [26] models were introduced which enclosure the remainder term using different set-valued arithmetic.

Prior Work: Stiff Systems and Global Optimization

Wilhelm, ME; Le, AV; and Stuber, MD. "Global Optimization of Stiff Dynamical Systems." AIChe Journal: Futures Issue, 65 (12), 2019

1. INTRODUCTION

Dynamic optimization problems of the form

\[ \min \, J(x) \quad \text{subject to} \quad F(x) = 0, \]

are, in general, and therefore verifying optimality requires deterministic global optimization. The issues in this paper is on solving (1) to guarantee global optimality or demonstration of feasibility. The method developed in this work is of specific importance when the ODE-FV systems is stiff. Methods for solving a system in general/optimal work on the

\[ \xi_k^1 \equiv \hat{z}_{k+1} - \hat{z}_k - \Delta tf(\hat{z}_{k+1}, p) \]

\[ \xi_k^2 \equiv \hat{z}_{k+2} - \frac{4}{3} \hat{z}_{k+1} + \frac{1}{3} \hat{z}_k - \frac{2}{3} \Delta tf(\hat{z}_{k+2}, p) \]

\[ \xi_k^2 \equiv \hat{z}_{k+2} - \hat{z}_{k+1} - \frac{1}{2} \Delta t(f(\hat{z}_{k+2}, p) + f(\hat{z}_{k+1}, p)) \]

Integration Scheme

- Discretize-then-relax algorithm employed.
- Higher-order existence test used\(^{22,29}\).
- Local error per unit step (LEPUS) adaptive step-size control scheme used\(^{30}\).
- **Step 1**: Determines step-size and state relaxations for the entire step (\(t \in [t_j, t_{j+1}]\))\(^{22,30}\).
- **Step 2**: Refines state relaxations at new time (\(t = t_{j+1}\)).

---


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- \textbf{Step 1}: Determines step-size and state relaxations for the \textbf{entire} step ($t \in [t_j, t_{j+1}]$)\textsuperscript{22,30}.
- \textbf{Step 2}: Refines state relaxations at new time ($t = t_{j+1}$).


Adams-Moulton Method\textsuperscript{27,28}

\[ x(p, t_k) = x(p, t_{k-1}) + h \sum_{j=0}^{n} \beta_{jn} f(x(p, t_{k-j}), p) \]
\[ t_{k-n}, ..., t_k \in [t_{k-n}, t_k] \]

Nonlinear System of Equations

\[ h(z(p), p) = x(p, t_k) - x(p, t_{k-1}) - h \sum_{j=0}^{n} \beta_{jn} f(x(p, t_{k-j}), p) = 0 \]
\[ z(p) = [x(p, t_k); x(p, t_{k-1}); ...; x(p, t_{k-n})] \]

- A n-step Adams-Moulton arises from a Lagrange interpolation polynomial appropriating the solution at n+1 points, \( t_{k-n}, ..., t_k \), in the time interval \( [t_{k-n}, t_k] \textsuperscript{27,28} \).
- These methods exhibit preferable regions of stability for stiff systems when compared with many explicit methods\textsuperscript{27,28}.

Truncation Error\textsuperscript{31} (\( \tau \))

\[ \tau(p, \bar{\eta}) = h^{n+1} Y_{n+1} x^{(n+2)}(p, \bar{\eta}) \]
\[ \tau(p, \bar{\eta}) = h^{n+1} Y_{n+1} f^{(n+1)}(x(p, \bar{\eta}), p) \]
\[ \exists \bar{\eta} \in [t_{k-n}, t_k] \]

Adams-Moulton: Pointwise

Adams-Moulton Method\(^{27,28}\)

- Compute relaxation for **truncation error** in standard manner
- Compute relaxation of implicit function using approach of Stuber et al. 2015\(^{32}\) and Wilhelm et al. 2019\(^6\).

\[
h(z(p), p) = x(p, t_k) - x(p, t_{k-1}) - h \sum_{j=0}^{n} \beta_{jn} f(x(p, t_{k-j}), p) = 0
\]

**Nonlinear System of Equations (Defining implicit function)**

\[
h(z(p), p) = x(p, t_k) - x(p, t_{k-1}) - h \sum_{j=0}^{n} \beta_{jn} f(x(p, t_{k-j}), p) + \tau(p, \bar{\eta}) = 0
\]

\[
z(p) = [x(p, t_k); x(p, t_{k-1}); \ldots; x(p, t_{k-n})]
\]

Truncation Error\(^{31}(\tau)\)

\[
h^{n+1} \bar{Y}_{n+1} x^{(n+2)}(p, \bar{\eta})
\]

\[
h^{n+1} \bar{Y}_{n+1} f^{(n+1)}(x(p, \bar{\eta}), p)
\]

6. Wilhelm, ME; Le, AV; and Stuber. MD. Global Optimization of Stiff Dynamical Systems. AIChE Journal: Futures Issue, 65 (12), 2019
Adams-Moulton: Mean Value Form

Mean value form of n-step Adams-Moulton method

\[
x_k = \hat{x}_{k-1} + h \sum_{j=0}^{n} \beta_{jn} f(\hat{x}_{k-j}, \hat{p}) \underbrace{+ R_k(p)}_{D_k(p)} + \sum_{j=0}^{n} h\beta_{jn} \frac{\partial f}{\partial p}(\mu_{k-j}(p), \rho(p))(p - \hat{p})
\]

\[
+ \left( I + h\tilde{\beta}_{1n} \frac{\partial f}{\partial x_{k-1}}(\mu_{k-1}(p), \rho(p)) \right) (x_{k-1} - \hat{x}_{k-1}) + \sum_{j=0}^{n} \sum_{j \neq 1} h\beta_{jn} \frac{\partial f}{\partial x_{k-j}}(\mu_{k-j}(p), \rho(p))(x_{k-j} - \hat{x}_{k-j})
\]

Were we define \( \mu_k \) and \( \rho \) as below

\[
\mu_k(p) = \eta(x_k - \hat{x}_k) + \hat{x}_k
\]
\[
\rho(p) = \eta(p - \hat{p}) + p
\]
\[\eta \in [0,1]\]

**Truncation error** notation and form

\[
R_k(p) = h^{n+2} \tilde{y}_{n+1} f^{(n+1)}(\tilde{x}(p, t_{k-n}; t_k), p)
\]
Adams-Moulton: Interval

Mean value form of n-step Adams-Moulton method

\[ x_k = D_k(p) + J^k_p(p)(p - \hat{p}) + \left( I + J^{k-1}_x(x_{k-1}, P) \right) (x_{k-1} - \hat{x}_{k-1}) + \sum_{j=0}^{n} J^{k-j}_x(x_{k-j}, p)(x_{k-j} - \hat{x}_{k-j}) \]

Interval bounds of n-step Adams-Moulton method

\[ X_k = D_k(P) + J^k_p(P)(P - \hat{p}) + \left( I + J^{k-1}_x(X_{k-1}, P) \right) (X_{k-1} - \hat{x}_{k-1}) + \sum_{j=2}^{n} J^{k-j}_x(X_{k-j}, P)(X_{k-j} - \hat{x}_{k-j}) + J^k_x(X_k, P)(X^0_k - x^0_k) \]

- Uncertain set is propagated as a parallelepiped\(^{22,33}\).
- Namely, that there exist \( A_k \in \mathbb{R}^{n_x \times n_x} \) and \( \delta_k \in \Delta_k \) such that \( x_k(p) - \hat{x}_k = A_k \delta_k \in A_k \Delta_k \).

\[ X_k := \left( D_k(P) + J^k_p(P)(P - \hat{p}) + \left( I + J^{k-1}_x(P) \right) A_{k-1} \Delta_{k-1} + \sum_{j=2}^{n} J^{k-j}_x(X_{k-j}, P) A_{k-j} \Delta_{k-j} + J^k_x(X_k, P)(X^0_k - x^0_k) \right) \cap X^0_k \]


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\[ x_k = D_k(p) + J_p^k(p)(p - \hat{p}) + \left( I + J_x^{k-1}(x_{k-1}, p) \right)(x_{k-1} - \hat{x}_{k-1}) + \sum_{j=0}^{n} J_x^{k-j}(x_{k-j}, p)(x_{k-j} - \hat{x}_{k-j}) \]

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- Uncertain set is propagated as a parallelepiped\textsuperscript{22,33}.
- Namely, that there exist \( A_k \in \mathbb{R}^{n \times n} \times \mathbb{R} \) and \( \delta_k \in \Delta_k \) such that \( x_k(p) - \hat{x}_k = A_k \delta_k \in A_k \Delta_k \).

\[ X_k := \left( D_k(P) + J_P^k(P)(P - \hat{P}) + \left( I + J_x^{k-1}(P) \right)A_{k-1}\Delta_{k-1} + \sum_{j=2}^{n} J_x^{k-j}(X_{k-j}, P)A_{k-j}\Delta_{k-j} + J_x^k(X_k, P)(X_k^0 - X_k^0) \right) \cap X_k^0 \]


Adams-Moulton: Interval

Initialization for parallelepiped\(^{22,33}\)

\[ A_0 = I \quad \Delta_0 = X_0 - \hat{x}_0 \]

Parallelepiped update at step \( k \)

\[ \Delta_k = A_k^{-1} \left( D_k(P) + J_{P}^k(P)(P - \hat{p}) + (I + J_{X}^{k-1}(P))A_{k-1}\Delta_{k-1} + \sum_{j=2}^{n} J_{X}^{k-j}(X_k, P)A_{k-j}\Delta_{k-j} + J_{X}^{k}(X_k, P)(X_k - \hat{x}_k) \right) \]

Bound truncation error via partition

\[ R_k(P) \equiv h^{n+2} \gamma_{n+1} \bigcup_{j=0}^{n} F^{(n+1)}(\tilde{X}_{k-j}, P) \subseteq h^{n+2} \gamma_{n+1} F^{(n+1)} \bigcup_{j=0}^{n} \tilde{X}_{k-j}, P \]
Adams-Moulton: Interval

Initialization for parallelepiped

\[ A_0 = I \quad \Delta_0 = X_0 - \hat{x}_0 \]

Parallelepiped update at step \( k \)

\[ A_k \text{ update given by taking to be orthogonal matrix } Q \text{ of QR decomposition of } \mid \mid (J_x^k A_{k-1}) \mid \mid^2 \]

\[ \Delta_k = A_k^{-1} \left( D_k(P) + J^k_p(P)(P - \hat{p}) + (I + J^k_x(P)) A_{k-1} \Delta_{k-1} + \sum_{j=2}^{n} J^k_x(X_k, P) A_{k-j} \Delta_{k-j} + J^k_x(X_k, P)(X_k - \hat{x}_k) \right) \]

Bound truncation error via partition

\[ R_k(P) \equiv h^{n+2} \bar{\nu}_{n+1} \bigcup_{j=0}^{n} F^{(n+1)}(\bar{X}_{k-j}, P) \subseteq h^{n+2} \bar{\nu}_{n+1} F^{(n+1)} \left( \bigcup_{j=0}^{n} \bar{X}_{k-j}, P \right) \]


Adams-Moulton: Relaxation

**Interval update** of n-step Adams-Moulton method

\[
X_k := \left( D_k(P) + J_p^k(P)(P - \hat{p}) + \left( I + J_{X}^{k-1}(P) \right) A_{k-1}\Delta_{k-1} + \sum_{j=2}^{n} J_{X}^{k-j}(X_{k-j}, P)A_{k-j}\Delta_{k-j} + J_{X}^{k}(X_0^k, P)(X_0^k - x_k^0) \right) \cap X_k^0
\]

**Convex/concave relaxation update** of n-step Adams-Moulton method

Let \( \{g^{cv}, g^{cc}\}(p) \) denote the tuple of convex and concave relaxations of \( g \) on \( P \) evaluated at \( p \in P \):

\[
\begin{align*}
\{x_k^{cv}, x_k^{cc}\}(p) := & \{D_k^{cv}, D_k^{cc}\}(p) + \{J_p^{k, cv}, J_p^{k, cc}\}(p)(p - \hat{p}) + \left( I + \{J_{X}^{k-1, cv}, J_{X}^{k-1, cc}\}(p) \right) \otimes A_{k-1}\{\Delta_{k-1}^{cv}, \Delta_{k-1}^{cc}\}(p) \\
& + \sum_{j=2}^{n} \{J_{X}^{k-j, cv}, J_{X}^{k-j, cc}\}(p)A_{k-j}\{\Delta_{k-j}^{cv}, \Delta_{k-j}^{cc}\}(p) \{J_{X}^{k, cv}, J_{X}^{k, cc}\}(p)(\{x_k^{0, cv}, x_k^{0, cc}\}(p) - \hat{x}_k^0) \\
\{x_k^{cv}, x_k^{cc}\}(p) := & \text{intersect(} \{x_k^{cv}, x_k^{cc}\}(p), X_k^0 \)
\end{align*}
\]
Adams-Moulton: Relaxation

Generalization of Union:

Compute union \( \left( \{ x_k^{cv}, x_k^{cc} \}(p), \{ x_k^{0,cv}, x_k^{0,cc} \}(p) \right) \) and update \( \{ x_k^{cv}, x_k^{cc} \}(p) \) as follows:

Step 1: \( \{ \varphi_1^{cv}, \varphi_1^{cc} \}(p) \leftarrow \min(\{ x_k^{cv}, x_k^{cc} \}(p), \{ x_k^{0,cv}, x_k^{0,cc} \}(p)) \)

Step 2: \( \{ \varphi_u^{cv}, \varphi_u^{cc} \}(p) \leftarrow \max(\{ x_k^{cv}, x_k^{cc} \}(p), \{ x_k^{0,cv}, x_k^{0,cc} \}(p)) \)

Step 3: \( \{ x_k^{cv}, x_k^{cc} \}(p) \leftarrow \{ \varphi_1^{cv}, \varphi_u^{cc} \}(p) \)

Bound truncation error via partition

\( \{ R_k^{cv}, R_k^{cc} \}(p) = h^{n+2} \bigcup_{n+1} \text{union} \left( \text{union}(f^{(n+1)}(\{ x_k^{cv}, x_k^{cc} \}(p), p), \ldots), f^{(n+1)}(\{ x_{k-n}^{cv}, x_{k-n}^{cc} \}(p), p) \right) \)

Subgradient-based tightening of state bounds:

Update interval bounds at \( k \) by using interval extension of affine relaxations compute at \( p_{ref} \) if an improvement \(^{14}\).
Implementation

Customizable Global and Robust Optimization Routines

EAGO

Implicit Linear Multistep Relaxations

EAGODynamicOptimizer.jl

Implementation

Customizable Global and Robust Optimization Routines

EAGO

Abstract Layer for Dynamic Problems

DynamicBounds.jl

- DynamicBounds.jl – Wrapper for dependent modules
- DynamicBoundsBase.jl – Abstraction Layer
- DynamicBoundspODEsDiscrete.jl
  – Discrete time approaches
- DynamicBoundspODEsIneq.jl
  -- Continuous time approaches

- Implicit Linear Multistep Relaxations

36. Wilhelm, M. E., McCormick.jl, (2020), GitHub repository, [https://github.com/PSORLab/McCormick.jl](https://github.com/PSORLab/McCormick.jl)
Customizable Global and Robust Optimization Routines

- **IntervalArithmetic.jl** for validated interval calculations.
- Relaxations from McCormick.jl\(^{36}\) submodule of **EAGO.jl**\(^{37}\).
- All simulations run on single thread of Intel Xeon E3-1270 v5 3.60/4.00GHz processor with 16GM ECC RAM, Ubuntu 18.04LTS using Julia v1.5.1\(^{38}\). Intel MKL 2019 (Update 2) for BLAS/LAPACK.

### Abstract Layer for Dynamic Problems

- **DynamicBounds.jl**
- **DynamicBoundsBase.jl** – Abstraction Layer
- **DynamicBoundspODEsDiscrete.jl** – Discrete time approaches
- **DynamicBoundspODEsIneq.jl** – Continuous time approaches

**Implicit Linear Multistep Relaxations**

- **DynamicBounds.jl**
  - IntervalArithmetic.jl for validated interval calculations.
  - Relaxations from McCormick.jl\(^{36}\) submodule of **EAGO.jl**\(^{37}\).

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Kinetic Problem - Formulation

(Objective Function)

$$\Phi^* = \min_{p \in P} \sum_{i=1}^{n} (I^i - I_{\text{data}}^i)^2$$

s. t.  
$$I^i = x_A^i + \frac{2}{21} x_B^i + \frac{2}{21} x_D^i$$

(Description of Problem)

➢ Fit the rate constants ($k_{2f}$, $k_{3f}$, $k_4$) of oxygen addition to cyclohexadienyl radicals to data.\(^{39}\)
➢ First addressed by global by Singer et al.\(^{40}\)
➢ Explicit Euler form solved by Mitsos\(^{3}\)
➢ Implicit Euler form addressed in Stuber\(^{32}\)
➢ Two-step PILMS forms addressed in Wilhelm\(^{6}\)

(pODE IVP)

\[
\begin{align*}
\dot{x}_A &= k_1 x_Z x_Y - c_{O2} (k_{2f} + k_{3f}) x_A + (k_{2f}/K_2) x_D + (k_{3f}/K_3) x_B - k_5 x_A^2, \\
\dot{x}_B &= k_{3f} c_{O2} x_A - (k_{3f}/K_3 + k_4) x_B, \\
\dot{x}_Y &= -k_1 s x_Y x_Z, \\
\dot{x}_Z &= -k_1 x_Y x_Z,
\end{align*}
\]

(Decision Variables)  
$$u = (k_{2f}, k_{3f}, k_4)$$

(State Variables)  
$$x = (x_A, x_B, x_D, x_Y, x_Z)$$

(Parameters)  
$$k_1, k_{1s}, k_5, K_2, K_3, c_{O2}, \Delta t, n$$

(Initial Condition)  
$$x(t = 0) = (0, 0, 0, 0.4, 140)$$

Kinetic Problem - Formulation

(Objective Function) \[
\Phi^* = \min_{\mathbf{p} \in \mathcal{P}} \sum_{i=1}^{n} (I_i - \hat{I}_{\text{data}})^2
\]

(Description of Problem)

- Fit the rate constants (k₂₅, k₃₆, k₄) of oxygen addition to cyclohexadienyl radicals to data. \(^\text{39}\)
- Affine relaxations used to compute lower bound (CPLEX 12.8).
- Upper-bound computed by integrating ODE at midpoint of active node then evaluating objective & constraints.
- Duality-based bound tightening was performed in all cases.
- Absolute and relative convergence tolerances for the B&B algorithm of \(10^{-2}\) and \(10^{-5}\), respectively.

3. Mitsos et al. \(^\text{M1}\)
6. Wilhelm, ME; Le, AV; and Stuber, MD. \(^\text{W1}\)
32. Stuber, M.D. et al. \(^\text{S1}\)
39. J. W. Taylor, et al. \(^\text{T1}\)
40. A. B. Singer et al., \(^\text{S2}\)

\[s. t. \quad I_i = x_A + 2x_B + x_D, \quad \text{for } i = 1, \ldots, n\]

\[\mathbf{p} = (k_2 f, k_3 f, k_4)\]

\[\mathbf{x}_0 = (x_A, x_B, x_D, x_Y, x_Z)\]

\[\mathbf{x}_\Delta t = (x_3, c_{\text{O}_2}, \Delta t, n)\]

\[\mathbf{x}_0 = (0, 0, 0.4, 140)\]
A comparison of our new approach is made to existing methods. The 200 step numerical Adams-Moulton (AM, 2nd order) approach of Wilhelm 2019 is compared to the exact bounds of the solution set with the novel method. Differential inequality used approaches using the CVODE Adams integrator (SUNDIALS) are included for comparison.

<table>
<thead>
<tr>
<th>Method</th>
<th>Lower Bound</th>
<th>Final Relative Gap</th>
<th>Time (s)</th>
<th>Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact PILMS, Adams-Moulton</td>
<td>Interval</td>
<td>None</td>
<td>5983</td>
<td>&gt;800,000</td>
</tr>
<tr>
<td>Exact PILMS, Adams-Moulton</td>
<td>Affine</td>
<td>None</td>
<td>3976</td>
<td>&gt;350,000</td>
</tr>
<tr>
<td>Numerical, Adams-Moulton, 200 step</td>
<td>Affine</td>
<td>None</td>
<td>1356</td>
<td>6068</td>
</tr>
<tr>
<td>Differential Inequality</td>
<td>Interval6,7,9</td>
<td>1.9E-3</td>
<td>&gt;7200</td>
<td>&gt;1,300,000</td>
</tr>
</tbody>
</table>

32. Wilhelm, ME; Le, AV; and Stuber. MD. “Global Optimization of Stiff Dynamical Systems.” AIChE Journal: Futures Issue, 65 (12), 2019
**Robust Design - SIP**

**CSTR with Aeration**

Inlet with Uncertain Nitrogen Concentration (p) → Effluent required to be less than SP

**Goal**

Minimize aeration cost while ensuring constraint satisfaction at final time ($t = 500$ s) if step-change feed disturbance occurs

$$\Phi^* = \min_{u \in U} u$$

s.t. $x_1(t_f, u, p) − SP \leq 0, \forall p \in P$

**Initial Condition**

Steady-state operation with $x_1 = 30$ (mg/L)

**Mass balance**

$$\frac{dx_1}{dt} = \tau^{-1}(p − x_1) − r_{AO}X_{AO}$$

$$\frac{dx_2}{dt} = r_{AO}X_{AO} − r_{NO}(x_2, x_4)X_{NO}$$

$$\frac{dx_3}{dt} = r_{NO}(x_2, x_4)X_{NO}$$

$$\frac{dx_4}{dt} = −r_{AO}\Psi_{AO}X_{AO} − r_{NO}(x_2, x_4)\Psi_{NO}X_{NO} + ku(C_o^* − x_4)$$

**Rate Law**

$$r_{NO} = r_{NO,max} \frac{x_2}{K_{SNO} + x_2 + x_2^2 / K_{INO}} \frac{x_4}{K_{DONO} + x_4}$$

**Variable Range**

$$P = [31, 40], \quad U = [440, 2000], \quad t = [0, 500]$$

---

Comparison of Methods

- Optimal aeration rate found to be $u = 704 \, L/s$ via algorithms compared.
- Exact PILMs methods faster than numerical approximation.
- Exact PILMs comparable to differential inequality method.

<table>
<thead>
<tr>
<th>Method</th>
<th>Lower Bound</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exact PILMS, Adams-Moulton</td>
<td>Interval</td>
<td>55</td>
</tr>
<tr>
<td>Exact PILMS, Adams-Moulton</td>
<td>Affine</td>
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</tr>
<tr>
<td>Numerical, Adams-Moulton, 200 step</td>
<td>Interval</td>
<td>323</td>
</tr>
<tr>
<td>Numerical, Adams-Moulton, 200 step</td>
<td>Affine</td>
<td>118</td>
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<tr>
<td>Differential Inequality</td>
<td>Interval</td>
<td>38</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residence time ($t$)</td>
<td>4136</td>
<td></td>
</tr>
<tr>
<td>Concentration of AOB ($X_{AO}$)</td>
<td>505</td>
<td></td>
</tr>
<tr>
<td>Concentration of NOB ($X_{NO}$)</td>
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</tr>
<tr>
<td>Maximum Nitrite Consumption Rate ($r_{NO,max}$)</td>
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</tr>
<tr>
<td>Stoichiometric ratio O$_2$:NH$<em>4$ ($\Psi</em>{AO}$)</td>
<td>2.5</td>
<td></td>
</tr>
<tr>
<td>Stoichiometric ratio O$_2$:NO$<em>2$ ($\Psi</em>{NO}$)</td>
<td>0.32</td>
<td></td>
</tr>
<tr>
<td>Inhibition constant of NO$<em>2$ for NOB ($K</em>{INO}$)</td>
<td>13000</td>
<td></td>
</tr>
<tr>
<td>Monod constant of O$<em>2$ for NOB ($K</em>{ONO}$)</td>
<td>1.5</td>
<td></td>
</tr>
</tbody>
</table>

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6. Wilhelm, ME; Le, AV; and Stuber. MD. “Global Optimization of Stiff Dynamical Systems.” AIChE Journal: Futures Issue, 65 (12), 2019
Acknowledgements

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