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Guaranteed Relaxations and Bounds on the Solution Sets of Parametric ODEs Via Implicit Linear Multistep Methods

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20 AIChE
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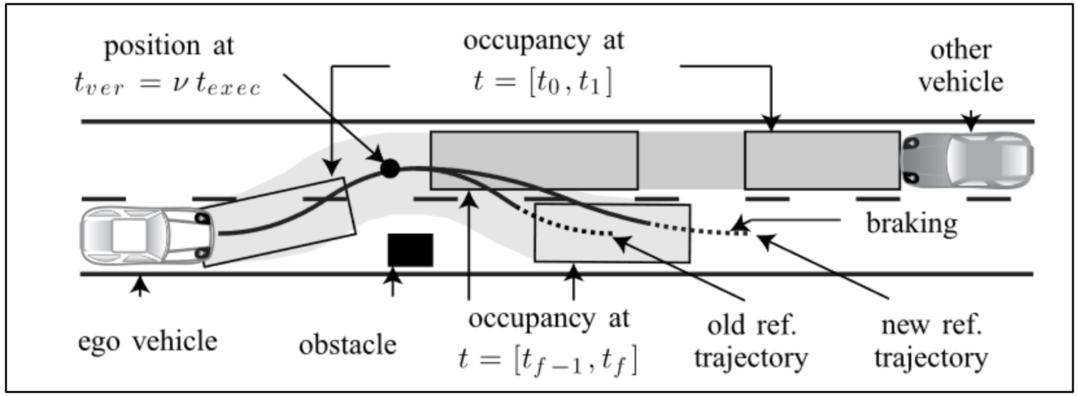
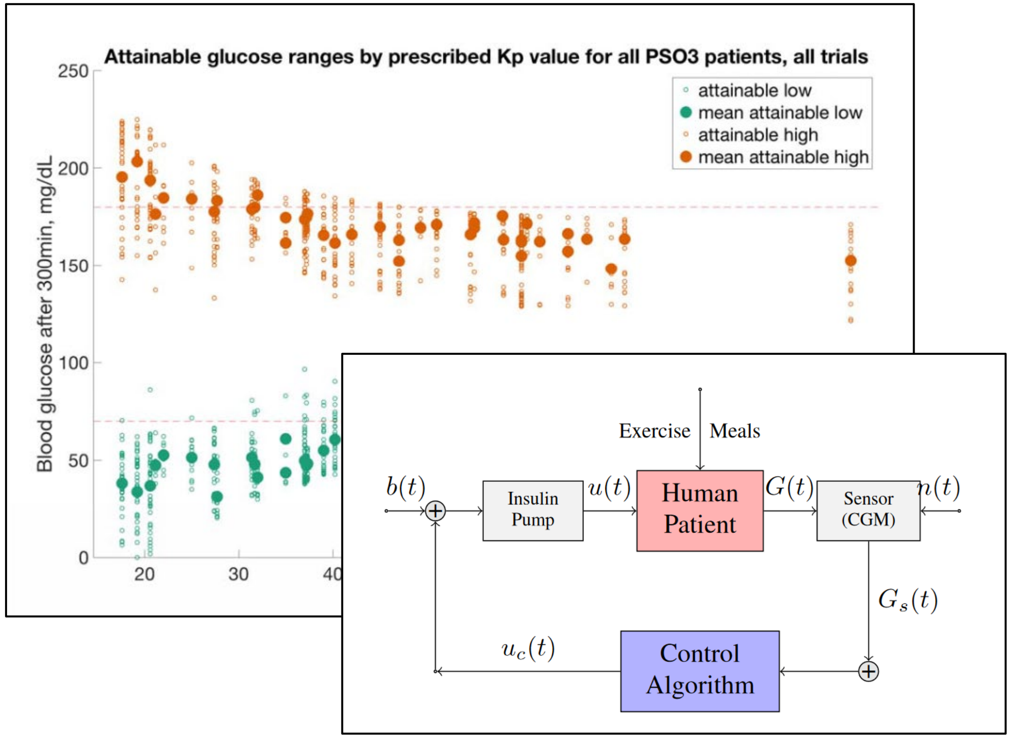
Process Systems and Operations Research Laboratory

Applications: Reachability Analysis

Collison Avoidance – Trajectory Planning[1]



Safety Verification[2]



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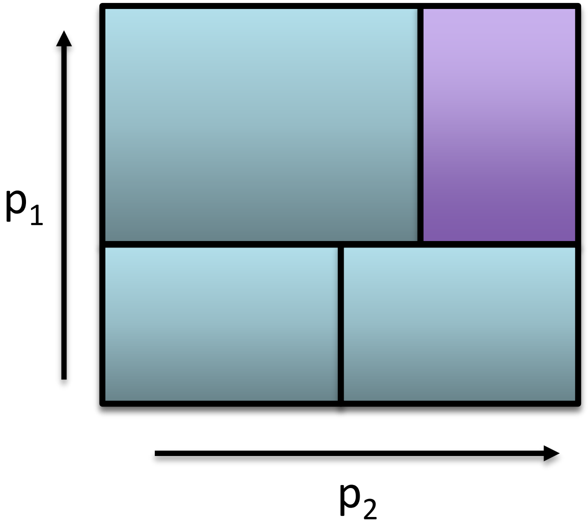
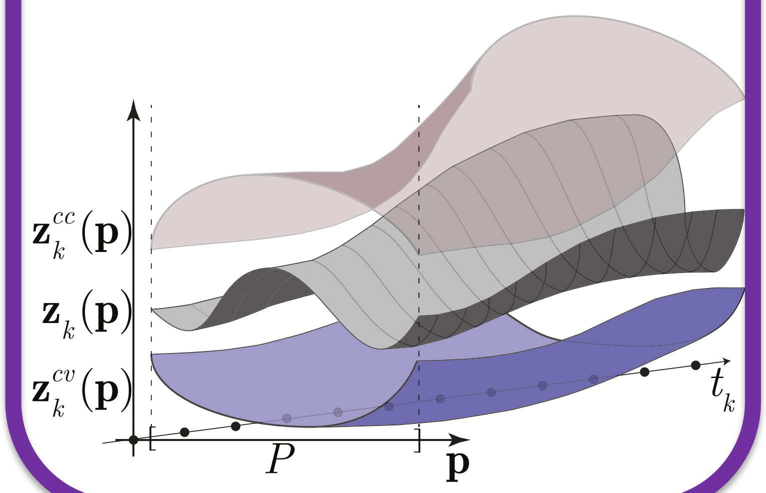
2. Kushner, Taisa, et al. **A data-driven approach to artificial pancreas verification and synthesis.** *2018 ACM/IEEE 9th International Conference on Cyber-Physical Systems (ICCPS)*. IEEE, 2018.

Applications: Global Dynamic Optimization

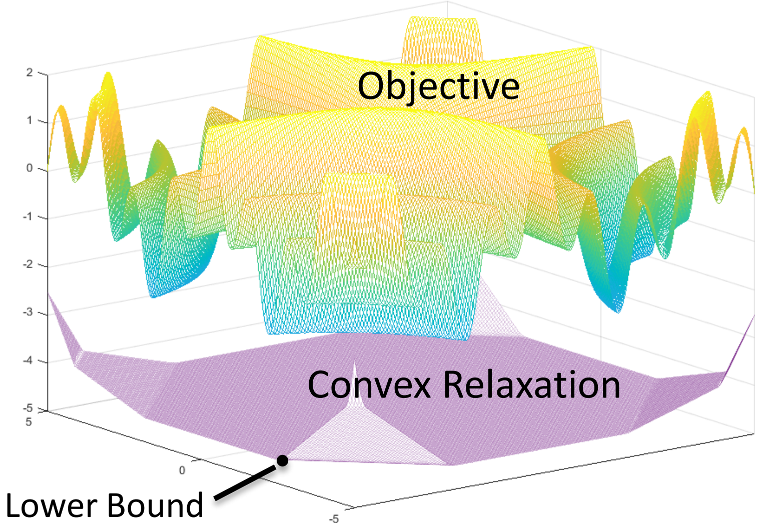
(Selection of Node)



(Relaxation of Intermediate Values)



(Relaxation of Objective and Constraints)



McCormick Operator Arithmetic[3,4,5]

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Parametric ODEs-IVP

Parametric ODE System

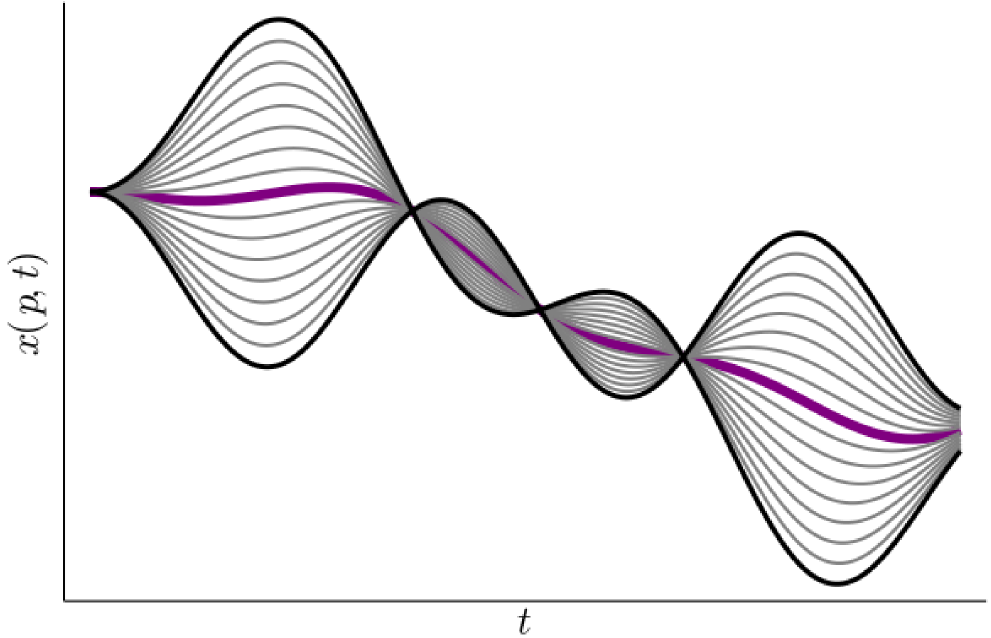
$$\dot{\mathbf{x}}(\mathbf{p},t) = \mathbf{f}(\mathbf{x}(\mathbf{p},t),\mathbf{p}), \quad t \in I = [t_0, t_f],\ \mathbf{p} \in P$$

Initial Condition

$$\mathbf{x}(\mathbf{p},t_0) = \mathbf{x}_0(\mathbf{p}), \ \ \mathbf{p} \in P$$

Assumptions

1. The initial condition $\mathbf{x}_0 : P \to D$ is *locally Lipschitz continuous* on P.
2. The right hand side $\mathbf{f}$ is *n times continuously differentiable* on $D \times \Pi$.



Solution

Any continuous $\mathbf{x} : P \times I \to D$ such that, for every $\mathbf{p} \in P$, $\mathbf{x}(\mathbf{p},\cdot) : \mathrm{T} \to D$ is continuous differentiable and satisfies the parametric ODE-IVP on I.

Prior Work: Nonlinear pODES

Differential Inequalities

$$\boxed{\begin{aligned} \dot{\mathbf{x}}^{cv}(t,\mathbf{p}) &= \mathbf{f}^{cv}(t,\mathbf{p},\mathbf{x}^{cv}(t,\mathbf{p}),\mathbf{x}^{cc}(t,\mathbf{p})), \quad \mathbf{x}^{cv}(t_0,\mathbf{p}) = \mathbf{x}_0^{cv}(\mathbf{p}) \\ \dot{\mathbf{x}}^{cc}(t,\mathbf{p}) &= \mathbf{f}^{cc}(t,\mathbf{p},\mathbf{x}^{cv}(t,\mathbf{p}),\mathbf{x}^{cc}(t,\mathbf{p})), \quad \mathbf{x}^{cc}(t_0,\mathbf{p}) = \mathbf{x}_0^{cc}(\mathbf{p}) \end{aligned}}$$

- Development of interval-based differential inequality [6,7]
- Less expansive convex/concave relaxations as well as tighter interval bounds [8,9,10]
- Adaptation of these methods to semi-explicit index-one differential-algebraic systems of equations DAEs [11,12,13]
- Methods of tightening state relaxations by exploiting model redundancy and nonlinear invariants [14,15].

6. Harrison, Gary W. **Dynamic models with uncertain parameters.** *Proceedings of the first international conference on mathematical modeling. Vol. 1.* University of Missouri Rolla, 1977.
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8. Scott, Joseph K., and Paul I. Barton. **Improved relaxations for the parametric solutions of ODEs using differential inequalities.** *Journal of Global Optimization* 57.1 (2013): 143-176.
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11. Scott, Joseph K., and Paul I. Barton. **Interval bounds on the solutions of semi-explicit index-one DAEs. Part 1: analysis.** *Numerische Mathematik* 125.1 (2013): 1-25.
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14. Shen, Kai, and Joseph K. Scott. **Rapid and accurate reachability analysis for nonlinear dynamic systems by exploiting model redundancy.** *Computers & Chemical Engineering* 106 (2017): 596-608.
15. Shen, Kai, and Joseph K. Scott. **Exploiting nonlinear invariants and path constraints to achieve tighter reachable set enclosures using differential inequalities.** *Mathematics of Control, Signals, and Systems* (2020): 1-27.

Prior Work: Nonlinear pODES

Taylor Series Integration

$$\mathbf{x}(\tau_{q+1},\mathbf{p}) \in \underbrace{\mathbf{x}(\tau_q,\mathbf{p}) + \sum_{j=1}^{p} \frac{h^j}{j!}\mathbf{f}^{(j)}(\mathbf{x}(\tau_q,\mathbf{p}),\mathbf{p})}_{\text{Taylor Series}} + \underbrace{\frac{h^{p+1}}{(p+1)!}\mathbf{f}^{(p+1)}(X(\tau_q),P)}_{\text{Remainder Bound}}$$

- First introduced by Moore [16] based on simple existence test.
- Generalized to two step methods consisting of an existence and uniqueness test and subsequent contraction [17,18].
- Development of shrink wrapping [19] and effective schemes for preconditioning intermediate calculations [20]
- Discretize-and-relax approaches with McCormick relaxations [21]
- Taylor-Interval [22], Taylor-McCormick [23] models, and Taylor-Ellipsoid [24] models were introduced which enclosure the remainder term using different set-valued arithmetics.

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17. Berz, Martin, and Georg Hoffstätter. **Computation and application of Taylor polynomials with interval remainder bounds.** *Reliable Computing* 4.1 (1998): 83-97.
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20. Makino, Kyoko, and Martin Berz. **Suppression of the wrapping effect by Taylor model-based verified integrators: Long-term stabilization by preconditioning.** *International Journal of Differential Equations and Applications* 10.4 (2011).
21. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
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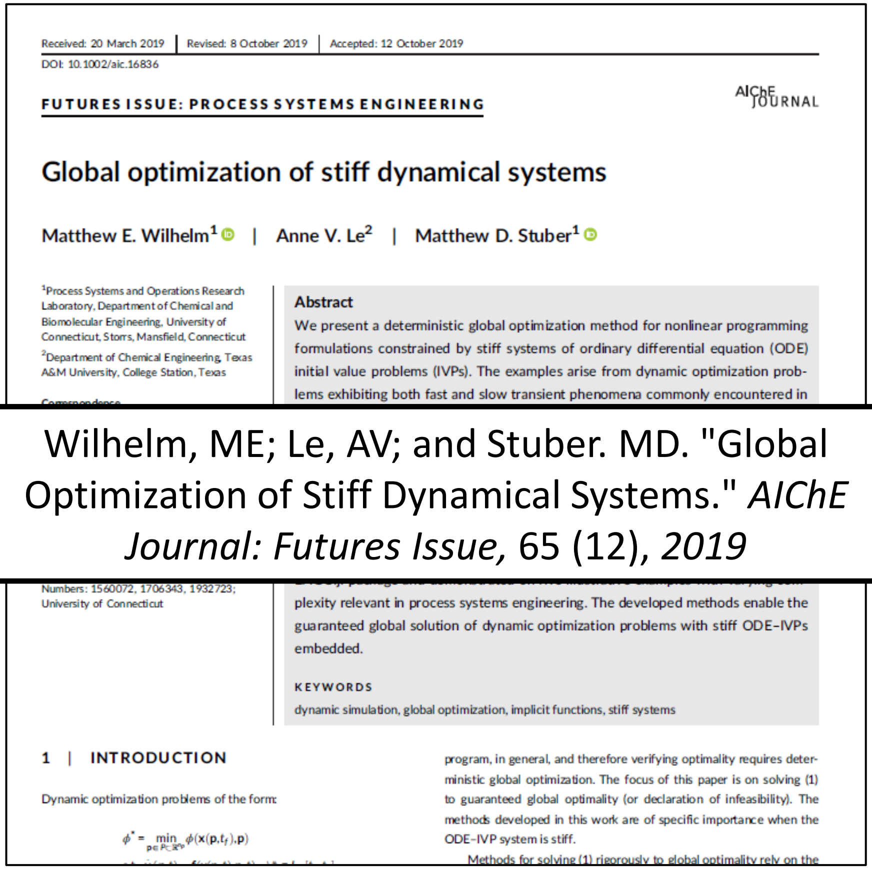
Prior Work: Stiff Systems and Global Optimization



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Global optimization of stiff dynamical systems

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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

plexity relevant in process systems engineering. The developed methods enable the guaranteed global solution of dynamic optimization problems with stiff ODE–IVPs embedded.

Numbers: 1560072, 1706343, 1932723; University of Connecticut

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

1 | INTRODUCTION

Dynamic optimization problems of the form:

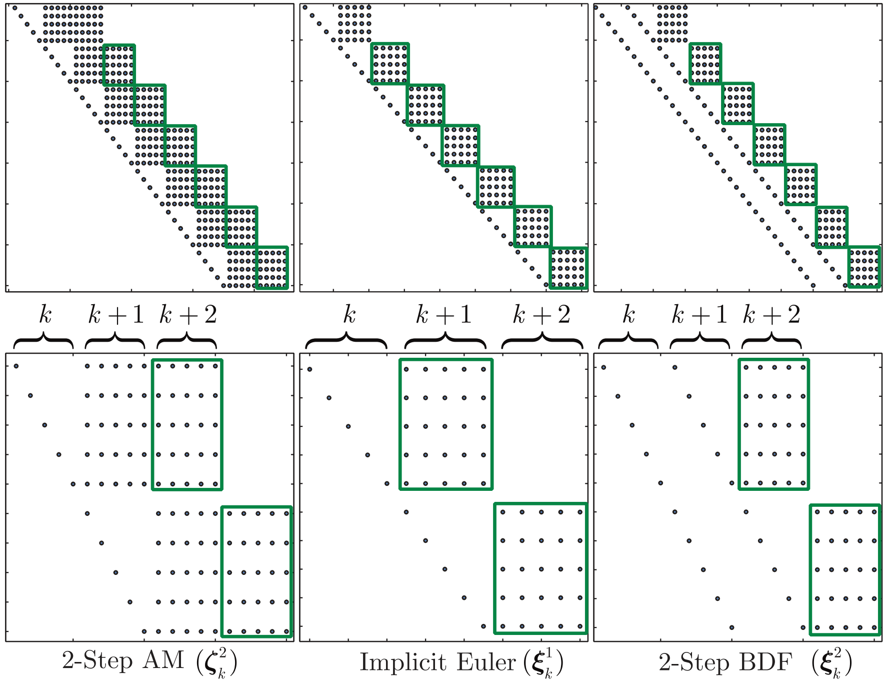
program, in general, and therefore verifying optimality requires deterministic global optimization. The focus of this paper is on solving (1) to guaranteed global optimality (or declaration of infeasibility). The methods developed in this work are of specific importance when the ODE–IVP system is stiff.

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

(Implicit Euler[25,26]) $\boldsymbol{\xi}_k^1 \equiv \hat{\mathbf{z}}_{k+1} - \hat{\mathbf{z}}_k - \Delta t \mathbf{f}(\hat{\mathbf{z}}_{k+1}, \mathbf{p})$

(Two-step Adam-Moulton[25,26]) $\boldsymbol{\xi}_k^2 \equiv \hat{\mathbf{z}}_{k+2} - \frac{4}{3}\hat{\mathbf{z}}_{k+1} + \frac{1}{3}\hat{\mathbf{z}}_k - \frac{2}{3}\Delta t \mathbf{f}(\hat{\mathbf{z}}_{k+2}, \mathbf{p})$

(Two-step BDF[25,26]) $\boldsymbol{\zeta}_k^2 \equiv \hat{\mathbf{z}}_{k+2} - \hat{\mathbf{z}}_{k+1} - \frac{1}{2}\Delta t\big(\mathbf{f}(\hat{\mathbf{z}}_{k+2}, \mathbf{p}) + \mathbf{f}(\hat{\mathbf{z}}_{k+1}, \mathbf{p})\big)$



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26. Hairer E, Wanner G. **Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems**. *Springer, Heidelberg*; 1991.

Integration Scheme

- Discretize-and-relax algorithm employed.
- Higher-order existence test used[21,27].
- Local error per unit step (LEPUS) adaptive step-size control scheme used[28].
- **Step 1:** Determines step-size and state relaxations for the **entire** step ($t \in [t_j, t_{j+1}]$)[21,28].
- **Step 2:** Refines state relaxations at new time ($t = t_{j+1}$).

21. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
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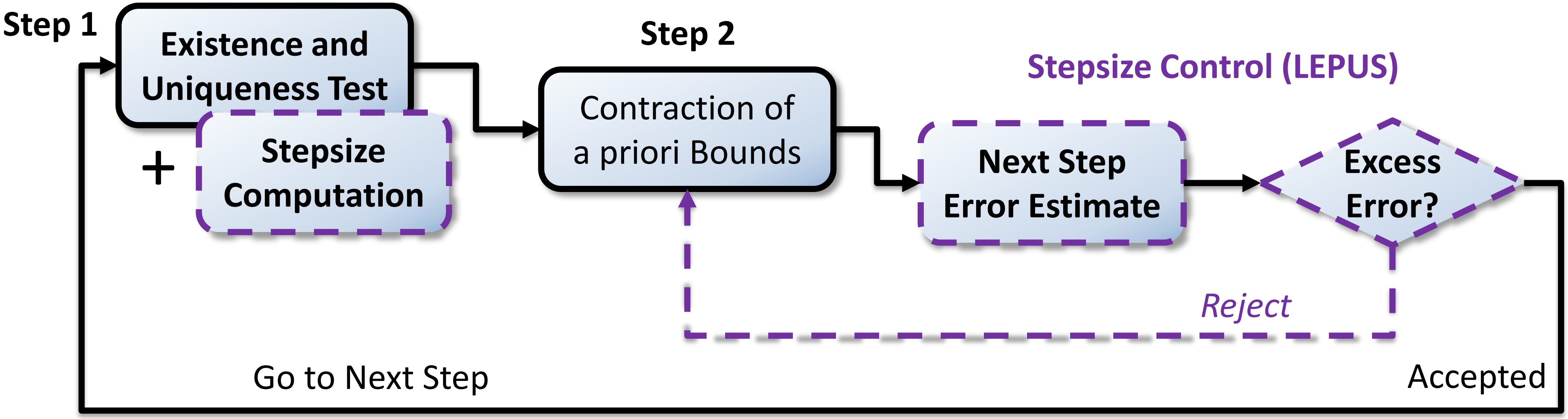

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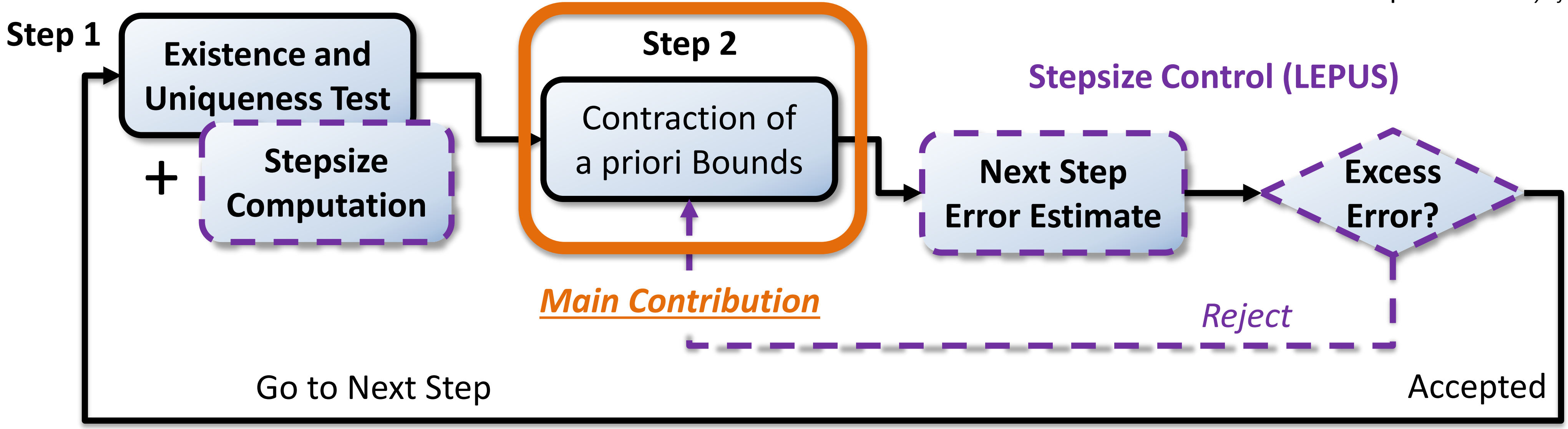

Adams-Moulton: Basic

Adams-Moulton Method[25,26]

$$\mathbf{x}(\mathbf{p}, t_k) = \mathbf{x}(\mathbf{p}, t_{k-1}) + h \sum_{j=0}^{n} \bar{\beta}_{jn}\, \mathbf{f}\big(\mathbf{x}(\mathbf{p}, t_{k-j}), \mathbf{p}\big)$$

$$t_{k-n}, \dots, t_k \in [t_{k-n}, t_k]$$

Truncation Error[29] (τ)

$$\tau(\mathbf{p}, \bar{\eta}) = h^{n+1} \bar{\gamma}_{n+1} \mathbf{x}^{(n+2)}(\mathbf{p}, \bar{\eta})$$

$$\tau(\mathbf{p}, \bar{\eta}) = h^{n+1} \bar{\gamma}_{n+1} \mathbf{f}^{(n+1)}(\mathbf{x}(\mathbf{p}, \bar{\eta}), \mathbf{p})$$

$$\exists \bar{\eta} \in [t_{k-n}, t_k]$$

Nonlinear System of Equations

$$\mathbf{h}(\mathbf{z}(\mathbf{p}), \mathbf{p}) = \mathbf{x}(\mathbf{p}, t_k) - \mathbf{x}(\mathbf{p}, t_{k-1}) - h \sum_{j=0}^{n} \bar{\beta}_{jn}\, \mathbf{f}\big(\mathbf{x}(\mathbf{p}, t_{k-j}), \mathbf{p}\big) = 0$$

- A n-step Adams-Moulton arises form a Lagrange interpolation polynomial appropriating the solution at n+1 points, $t_{k-n}, \dots, t_k$, in the time interval $[t_{k-n}, t_k]$[25,26].
- These methods exhibit preferable regions of stability for stiff systems when compared with many explicit methods[25,26].

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Adams-Moulton: Basic

Adams-Moulton Method[25,26]

$$\mathbf{x}(\mathbf{p}, t_k) = \mathbf{x}(\mathbf{p}, t_{k-1}) + h \sum^{n} \bar{\beta}_{in}\, \mathbf{f}(\mathbf{x}(\mathbf{p}, t_{k-i}), \mathbf{p})$$

$t_{k-n}, \ldots, t_k \in [t_{k-n}$

Truncation Error[29] (τ)

$$\tau(\mathbf{p}, \bar{\eta}) = h^{n+1} \bar{\gamma}_{n+1} \mathbf{x}^{(n+2)}(\mathbf{p}, \bar{\eta})$$

Nonlinear System

$\mathbf{h}(\mathbf{z}(\mathbf{p}), \mathbf{p})$

- **Adam-Moulton:** Order of integration scheme increases with **f** evaluations used (but **f** from prior step may be saved) but nonlinear solve needed
- Existing methods (Lohner's QR[14,30] and Interval Hermite-Obreshkoff[31]) scale with order of Taylor coefficients of **f**
- Approximately *$O(Nk^2)$* complexity to compute the k^{th} Taylor coefficient of **f** where N is the number of operators[28].
    - *$O(N)$* for Adams-Moulton
    - *$O(Nk^2)$* for (k)-order Lohner's QR method
    - *$O(p^2N + q^2N)$* for (p+q+1)-order Hermite Obreshkoff method

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(2017): 777-808.

Adams-Moulton: Basic

Adams-Moulton Method[25,26]

Truncation Error[29] (τ)

$$) = h^{n+1}\bar{\gamma}_{n+1}\mathbf{x}^{(n+2)}(\mathbf{p},\bar{\eta})$$

$$) = h^{n+1}\bar{\gamma}_{n+1}\mathbf{f}^{(n+1)}(\mathbf{x}(\mathbf{p},\bar{\eta}),\mathbf{p})$$

$$[t_{k-n}, t_k]$$

- 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[33].

$$\mathbf{h}(\mathbf{z}(\mathbf{p}),\mathbf{p}) = \mathbf{x}(\mathbf{p},t_k) - \mathbf{x}(\mathbf{p},t_{k-1}) - h\sum_{j=0}^{n}\bar{\beta}_{jn}\,\mathbf{f}\big(\mathbf{x}(\mathbf{p},t_{k-j}),\mathbf{p}\big) = 0$$

32. Stuber, Matthew D., Joseph K. Scott, and Paul I. Barton. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* 30.3 (2015): 424-460.
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Nonlinear System of Equations (Defining implicit function)

$$\mathbf{h}(\mathbf{z}(\mathbf{p}),\mathbf{p}) = \mathbf{x}(\mathbf{p},t_k) - \mathbf{x}(\mathbf{p},t_{k-1}) - h\sum_{j=0}^{n}\bar{\beta}_{jn}\,\mathbf{f}\big(\mathbf{x}(\mathbf{p},t_{k-j}),\mathbf{p}\big) + \boxed{\tau(\mathbf{p},\bar{\eta})} = 0$$

...cal Analysis. *Springer Science* ...ew York; 2012.
...**Solving Ordinary Differential** ...**d Differential-Algebraic** ...*Heidelberg*; 1991.
...Malgorzata A. Jankowska, and ...**n interval predictor-** ...*Numerical Algorithms* 75.3

Adams-Moulton: Mean Value Form

Mean value form of n-step Adams-Moulton method

$$\mathbf{x}_{\mathrm{k}} = \underbrace{\hat{\mathbf{x}}_{\mathrm{k}-1} + \mathrm{h}\sum_{\mathrm{j}=0}^{\mathrm{n}} \bar{\beta}_{jn}\, \mathbf{f}\left(\hat{\mathbf{x}}_{\mathrm{k}-\mathrm{j}}, \hat{\mathbf{p}}\right) + \overset{\text{truncation error}}{\boxed{\mathbf{R}_{\boldsymbol{k}}(\mathbf{p})}}}_{\mathbf{D}_{\boldsymbol{k}}(\mathbf{p})} + \underbrace{\sum_{j=0}^{n} \mathrm{h}\bar{\beta}_{jn} \frac{\partial \mathbf{f}}{\partial \mathbf{p}}\left(\boldsymbol{\mu}_{\mathrm{k}-\mathrm{j}}\,(\mathbf{p}), \boldsymbol{\rho}(\mathbf{p})\right)}_{\mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{p})} (\mathbf{p} - \hat{\mathbf{p}}) +$$

$$\underbrace{\left(\mathbf{I} + \mathrm{h}\bar{\beta}_{1n} \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{\mathrm{k}-1}}\left(\boldsymbol{\mu}_{\mathrm{k}-1}\,(\mathbf{p}), \boldsymbol{\rho}(\mathbf{p})\right)\right)}_{\mathbf{I}+\mathbf{J}_{\mathrm{x}}^{\mathrm{k}-1}(\mathbf{p})} (\mathbf{x}_{\mathrm{k}-1} - \hat{\mathbf{x}}_{\mathrm{k}-1}) + \sum_{\substack{j=0 \\ j\neq 1}}^{n} \underbrace{\mathrm{h}\,\bar{\beta}_{jn} \frac{\partial \mathbf{f}}{\partial \mathbf{x}_{\mathrm{k}-\mathrm{j}}}\left(\boldsymbol{\mu}_{\mathrm{k}-\mathrm{j}}\,(\mathbf{p}), \boldsymbol{\rho}(\mathbf{p})\right)}_{\mathbf{J}_{\mathrm{x}}^{\mathrm{k}-\mathrm{j}}(\mathbf{p})} (\mathbf{x}_{\mathrm{k}-\mathrm{j}} - \hat{\mathbf{x}}_{\mathrm{k}-\mathrm{j}})$$

Were we define $\boldsymbol{\mu}_{\mathrm{k}}$ and $\boldsymbol{\rho}$ as below

$$\boldsymbol{\mu}_{\mathrm{k}}\,(\mathbf{p}) = \eta(\mathbf{x}_{\mathrm{k}} - \hat{\mathbf{x}}_{\mathrm{k}}) + \hat{\mathbf{x}}_{\mathrm{k}}$$

$$\boldsymbol{\rho}(\mathbf{p}) = \eta(\mathbf{p} - \hat{\mathbf{p}}) + \mathbf{p}$$

$$\eta \in [0,1]$$

Truncation error notation and form

$$\mathbf{R}_{\boldsymbol{k}}(\mathbf{p}) = \mathrm{h}^{\mathrm{n}+2}\,\bar{\gamma}_{\mathrm{n}+1}\mathbf{f}^{(\mathrm{n}+1)}(\tilde{\mathbf{x}}(\mathbf{p}, t_{k-n}; t_k), \mathbf{p})$$

Adams-Moulton: Interval

Mean value form of n-step Adams-Moulton method

$$\mathbf{x}_{\mathrm{k}} = \mathbf{D}_{k}(\mathbf{p}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{p})(\mathbf{p} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-1}(\mathbf{x}_{\mathrm{k}-1}, \mathbf{p})\right)(\mathbf{x}_{\mathrm{k}-1} - \hat{\mathbf{x}}_{\mathrm{k}-1}) + \sum_{\substack{j=0 \\ j\neq 1}}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-\mathrm{j}}(\mathbf{x}_{\mathrm{k}-\mathrm{j}}, \mathbf{p})(\mathbf{x}_{\mathrm{k}-\mathrm{j}} - \hat{\mathbf{x}}_{\mathrm{k}-\mathrm{j}})$$

Interval bounds of n-step Adams-Moulton method

$$\mathbf{X}_{\mathrm{k}} = \mathbf{D}_{k}(\mathbf{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-1}(\mathbf{X}_{\mathrm{k}-1}, \mathbf{P})\right)(\mathbf{X}_{\mathrm{k}-1} - \hat{\mathbf{x}}_{\mathrm{k}-1}) + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-\mathrm{j}}(\mathbf{X}_{\mathrm{k}-\mathrm{j}}, \mathbf{P})(\mathbf{X}_{\mathrm{k}-\mathrm{j}} - \hat{\mathbf{x}}_{\mathrm{k}-\mathrm{j}}) + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}(\mathbf{X}_{\mathrm{k}}, \mathbf{P})(\mathbf{X}_{k}^{0} - \mathbf{x}_{k}^{0})$$

- ☐ Uncertain set is propagated as a parallelepiped[14,30].
- ☐ Namely, that there exist $\mathbf{A}_{\mathrm{k}} \in \mathbb{R}^{n_x \times n_x}$ and $\boldsymbol{\delta}_{\mathrm{k}} \in \Delta_{\mathrm{k}}$ such that $\mathrm{x}_{\mathrm{k}}(\mathbf{p}) - \hat{\mathrm{x}}_{\mathrm{k}} = \mathbf{A}_{\mathrm{k}}\boldsymbol{\delta}_{\mathrm{k}} \in \mathbf{A}_{\mathrm{k}}\Delta_{\mathrm{k}}$.

$$\mathbf{X}_{\mathrm{k}} = \left(\mathbf{D}_{k}(\mathbf{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-1}(\mathbf{P})\right)\mathbf{A}_{\mathrm{k}-1}\Delta_{\mathrm{k}-1} + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k}-\mathrm{j}}(\mathbf{X}_{\mathrm{k}-j}, \mathbf{P})\mathbf{A}_{\mathrm{k}-\mathrm{j}}\Delta_{\mathrm{k}-\mathrm{j}} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}(\mathbf{X}_{k}^{0}, \mathbf{P})(\mathbf{X}_{k}^{0} - \hat{\mathbf{x}}_{k}^{0})\right) \cap \mathbf{X}_{k}^{0}$$

14. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
30. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.

Adams-Moulton: Interval

Mean value form of n-step Adams-Moulton method

$$\mathbf{x}_{\mathrm{k}} = \mathbf{D}_k(\mathbf{p}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{p})(\mathbf{p} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathbf{x}_{\mathrm{k-1}}, \mathbf{p})\right)(\mathbf{x}_{\mathrm{k-1}} - \hat{\mathbf{x}}_{\mathrm{k-1}}) + \sum_{\substack{j=0 \\ j\neq 1}}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathbf{x}_{\mathrm{k-j}}, \mathbf{p})(\mathbf{x}_{\mathrm{k-j}} - \hat{\mathbf{x}}_{\mathrm{k-j}})$$

Interval bounds of n-step Adams-Moulton method

$$\mathbf{X}_{\mathrm{k}} = \mathbf{D}_k(\mathbf{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathbf{X}_{\mathrm{k-1}}, \mathbf{P})\right)(\mathbf{X}_{\mathrm{k-1}} - \hat{\mathbf{x}}_{\mathrm{k-1}}) + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathbf{X}_{\mathrm{k-j}}, \mathbf{P})(\mathbf{X}_{\mathrm{k-j}} - \hat{\mathbf{x}}_{\mathrm{k-j}}) + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}(\mathbf{X}_{\mathrm{k}}, \mathbf{P})(\mathbf{X}_k^0 - \mathbf{x}_k^0)$$

- Uncertain set is propagated as a parallelepiped[14,30].
- Namely, that there exist $\mathbf{A}_{\mathrm{k}} \in \mathbb{R}^{\mathrm{n_x} \times \mathrm{n_x}}$ and $\boldsymbol{\delta}_{\mathrm{k}} \in \Delta_{\mathrm{k}}$ such that $\mathrm{x}_{\mathrm{k}}(\mathbf{p}) - \hat{\mathrm{x}}_{\mathrm{k}} = \mathbf{A}_{\mathrm{k}}\boldsymbol{\delta}_{\mathrm{k}} \in \mathbf{A}_{\mathrm{k}}\Delta_{\mathrm{k}}$.

$$\mathbf{X}_{\mathrm{k}} = \left(\mathbf{D}_{\boldsymbol{k}}(\mathbf{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathbf{P})\right)\mathbf{A}_{\mathrm{k-1}}\Delta_{\mathrm{k-1}} + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathbf{X}_{\mathrm{k}-j}, \mathbf{P})\mathbf{A}_{\mathrm{k-j}}\Delta_{\mathrm{k-j}} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}(\mathbf{X}_{\boldsymbol{k}}^{\mathbf{0}}, \mathbf{P})(\mathbf{X}_{\boldsymbol{k}}^{\mathbf{0}} - \hat{\mathbf{x}}_{\boldsymbol{k}}^{\mathbf{0}})\right) \cap \mathbf{X}_{\boldsymbol{k}}^{\mathbf{0}}$$

14. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
30. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.

Adams-Moulton: Interval

Initialization for parallelepiped[14,30]

$$\mathbf{A}_0 = \mathbf{I} \qquad \Delta_0 = \mathbf{X}_0 - \hat{\mathbf{x}}_0$$

Parallelepiped update at step k

14. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
30. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.

$\mathbf{A}_\mathrm{k}$ update given by taking to be orthogonal matrix Q of QR decomposition of $\mathrm{mid}(\mathbf{J}_\mathrm{x}^\mathrm{k}\mathbf{A}_{\mathrm{k}-1})$[14,30]

$$\Delta_\mathrm{k} = \mathbf{A}_\mathrm{k}^{-1}\left(\mathbf{D}_k(\mathbf{P}) + \mathbf{J}_\mathrm{p}^\mathrm{k}(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_\mathrm{x}^{\mathrm{k}-1}(\mathbf{P})\right)\mathbf{A}_{\mathrm{k}-1}\Delta_{\mathrm{k}-1} + \sum_{j=2}^{n} \mathbf{J}_\mathrm{x}^{\mathrm{k}-\mathrm{j}}(\mathbf{X}_\mathrm{k}, \mathbf{P})\mathbf{A}_{\mathrm{k}-\mathrm{j}}\Delta_{\mathrm{k}-\mathrm{j}} + \mathbf{J}_\mathrm{x}^\mathrm{k}(\mathbf{X}_\mathrm{k}, \mathbf{P})(\mathbf{X}_\mathrm{k} - \hat{\mathbf{x}}_\mathrm{k})\right)$$

Bound truncation error via partition

$$\mathbf{R}_k(\mathbf{p}) = \mathrm{h}^{\mathrm{n}+2}\,\overline{\gamma}_{\mathrm{n}+1}\mathbf{f}^{(\mathrm{n}+1)}\left(\bigcup_{j=0}^{n}\mathbf{X}_{\mathrm{k}-\mathrm{j}}, \mathbf{P}\right) = \mathrm{h}^{\mathrm{n}+2}\,\overline{\gamma}_{\mathrm{n}+1}\left(\bigcup_{j=0}^{n}\mathbf{f}^{(\mathrm{n}+1)}(\mathbf{X}_{\mathrm{k}-\mathrm{j}}, \mathbf{P})\right)$$

Adams-Moulton: Interval

Initialization for parallelepiped[14,30]

$$\mathbf{A}_0 = \mathbf{I} \qquad \Delta_0 = \mathbf{X}_0 - \hat{\mathbf{x}}_0$$

parallelepiped update at step k

14. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.
30. Lohner, Rudolf J. **Computation of guaranteed enclosures for the solutions of ordinary initial and boundary value problems.** *Institute of mathematics and its applications conference series.* Vol. 39. Oxford University Press, 1992.

$\mathbf{A}_k$ update given by taking to be orthogonal matrix Q of QR decomposition of $\mathrm{mid}(\mathbf{J}_x^k \mathbf{A}_{k-1})$[14,30]

$$\Delta_k = \mathbf{A}_k^{-1}\left(\mathbf{D}_k(\mathbf{P}) + \mathbf{J}_p^k(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_x^{k-1}(\mathbf{P})\right)\mathbf{A}_{k-1}\Delta_{k-1} + \sum_{j=2}^{n} \mathbf{J}_x^{k-j}(\mathbf{X}_k, \mathbf{P})\mathbf{A}_{k-j}\Delta_{k-j} + \mathbf{J}_x^k(\mathbf{X}_k, \mathbf{P})(\mathbf{X}_k - \hat{\mathbf{x}}_k)\right)$$

Bound truncation error via partition

$$\mathbf{R}_k(\mathbf{p}) = h^{n+2}\,\bar{\gamma}_{n+1}\mathbf{f}^{(n+1)}\left(\bigcup_{j=0}^{n} \mathbf{X}_{k-j}, \mathbf{P}\right) = h^{n+2}\,\bar{\gamma}_{n+1}\left(\bigcup_{j=0}^{n} \mathbf{f}^{(n+1)}(\mathbf{X}_{k-j}, \mathbf{P})\right)$$

Adams-Moulton: Relaxation

Interval update of n-step Adams-Moulton method

$$\mathbf{X}_{\mathrm{k}} = \left(\mathbf{D}_{\boldsymbol{k}}(\mathbf{P}) + \mathbf{J}_{\mathrm{p}}^{\mathrm{k}}(\mathbf{P})(\mathbf{P} - \hat{\mathbf{p}}) + \left(\mathbf{I} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k-1}}(\mathbf{P})\right)\mathbf{A}_{\mathrm{k-1}}\Delta_{\mathrm{k-1}} + \sum_{j=2}^{n} \mathbf{J}_{\mathrm{x}}^{\mathrm{k-j}}(\mathbf{X}_{\mathrm{k}-j}, \mathbf{P})\mathbf{A}_{\mathrm{k-j}}\Delta_{\mathrm{k-j}} + \mathbf{J}_{\mathrm{x}}^{\mathrm{k}}\left(\mathbf{X}_{\boldsymbol{k}}^{\mathbf{0}}, \mathbf{P}\right)\left(\mathbf{X}_{\boldsymbol{k}}^{\mathbf{0}} - \mathbf{x}_{\boldsymbol{k}}^{\mathbf{0}}\right) \right) \cap \mathbf{X}_{\boldsymbol{k}}^{\mathbf{0}}$$

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

Analogous computation of convex/concave relaxations. Let ($[\mathbf{g}^{\mathbf{cv}}, \mathbf{g}^{\mathbf{cc}}](\mathbf{p})$ denote the convex and concave relaxations of $\mathbf{g}$ at $\mathbf{p}$:

$$\begin{aligned}[\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{x}_{\mathbf{k}}^{\boldsymbol{cc}}](\mathbf{p}) = {} & [\mathbf{D}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{D}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}) + [\mathbf{J}_{\mathbf{p}}^{\mathbf{k,cv}}, \mathbf{J}_{\mathbf{p}}^{\mathbf{k,cc}}](\mathbf{p})(\mathbf{p} - \hat{\mathbf{p}}) + \left(\mathbf{I} + [\mathbf{J}_{\mathbf{x}}^{\mathbf{k-1,cv}}, \mathbf{J}_{\mathbf{x}}^{\mathbf{k-1,cc}}](\mathbf{p})\right) \otimes \mathbf{A}_{\mathrm{k-1}}[\Delta_{\mathrm{k-1}}^{\mathrm{cv}}, \Delta_{\mathrm{k-1}}^{\mathrm{cc}}](\mathbf{p}) \\ & + \sum_{j=2}^{n} [\mathbf{J}_{\mathbf{x}}^{\mathbf{k-j,cv}}, \mathbf{J}_{\mathbf{x}}^{\mathbf{k-j,cc}}](\mathbf{p})\mathbf{A}_{\mathrm{k-j}}[\Delta_{\mathrm{k-1}}^{\mathrm{cv}}, \Delta_{\mathrm{k-1}}^{\mathrm{cc}}](\mathbf{p}) + [\mathbf{J}_{\mathrm{x}}^{\mathrm{k,cv}}, \mathbf{J}_{\mathrm{x}}^{\mathrm{k,cc}}](\mathbf{p})\left([\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cv}}, \mathbf{x}_{\mathbf{k}}^{\mathbf{0,cc}}](\mathbf{p}) - \hat{\mathbf{x}}_{\boldsymbol{k}}^{\mathbf{0}}\right)\end{aligned}$$

$$[\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{x}_{\mathbf{k}}^{\boldsymbol{cc}}](\mathbf{p}) = \mathrm{intersect}\left([\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}}, \mathbf{x}_{\mathbf{k}}^{\boldsymbol{cc}}](\mathbf{p}), \mathbf{X}_{\mathbf{k}}^{\mathbf{0}}\right)$$

Adams-Moulton: Relaxation

Generalization of Intersection:

Compute intersect$\left([\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}),[\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cc}}](\mathbf{p})\right)$ and update $[\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p})$ as follows:

Step 1: $[\boldsymbol{\phi}_{\mathbf{l}}^{\mathbf{cv}},\boldsymbol{\phi}_{\mathbf{l}}^{\mathbf{cc}}](\mathbf{p}) \longleftarrow \min([\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}),[\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cc}}](\mathbf{p}))$

Step 2: $[\boldsymbol{\phi}_{\mathbf{u}}^{\mathbf{cv}},\boldsymbol{\phi}_{\mathbf{u}}^{\mathbf{cc}}](\mathbf{p}) \longleftarrow \max([\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}),[\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{0,cc}}](\mathbf{p}))$

Step 3: $[\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}) \longleftarrow [\boldsymbol{\phi}_{\mathbf{l}}^{\mathbf{cv}},\boldsymbol{\phi}_{\mathbf{u}}^{\mathbf{cc}}](\mathbf{p})$

Bound truncation error via partition

$$[\mathbf{R}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{R}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}) = \mathrm{h}^{\mathrm{n}+2}\,\bar{\gamma}_{\mathrm{n}+1}\mathrm{intersect}\left(\mathrm{intersect}\left(\mathbf{f}^{(\mathrm{n}+1)}([\mathbf{x}_{\mathbf{k}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k}}^{\mathbf{cc}}](\mathbf{p}),\mathbf{p}),\ldots\right),\mathbf{f}^{(\mathrm{n}+1)}([\mathbf{x}_{\mathbf{k-n}}^{\mathbf{cv}},\mathbf{x}_{\mathbf{k-n}}^{\mathbf{cc}}](\mathbf{p}),\mathbf{p})\right)$$

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].

14. Sahlodin, Ali M., and Benoit Chachuat. **Discretize-then-relax approach for convex/concave relaxations of the solutions of parametric ODEs.** *Applied Numerical Mathematics* 61.7 (2011): 803-820.

Implementation

- Algorithm implemented in our DynamicBounds.jl package available at https://github.com/PSORLab/DynamicBounds.jl[34]

- Branch and bound algorithm as an extension to the EAGO global optimizer available at https://github.com/PSORLab/EAGODynamicOptimizer.jl[35]

- **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.

https://github.com/PSORLab/EAGO.jl

34. Wilhelm, M. E., **DynamicBounds.jl**, (2020), GitHub repository, https://github.com/PSORLab/DynamicBounds.jl
35. Wilhelm, M. E., **EAGODynamicOptimizer.jl**, (2020), GitHub repository, https://github.com/PSORLab/EAGODynamicOptimizer.jl
36. Wilhelm, M. E., **McCormick.jl**, (2020), GitHub repository, https://github.com/PSORLab/McCormick.jl
37. Wilhelm, M. E., and M. D. Stuber. **EAGO. jl: easy advanced global optimization in Julia.** *Optimization Methods and Software* (2020): 1-26.
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Illustration of Trajectories

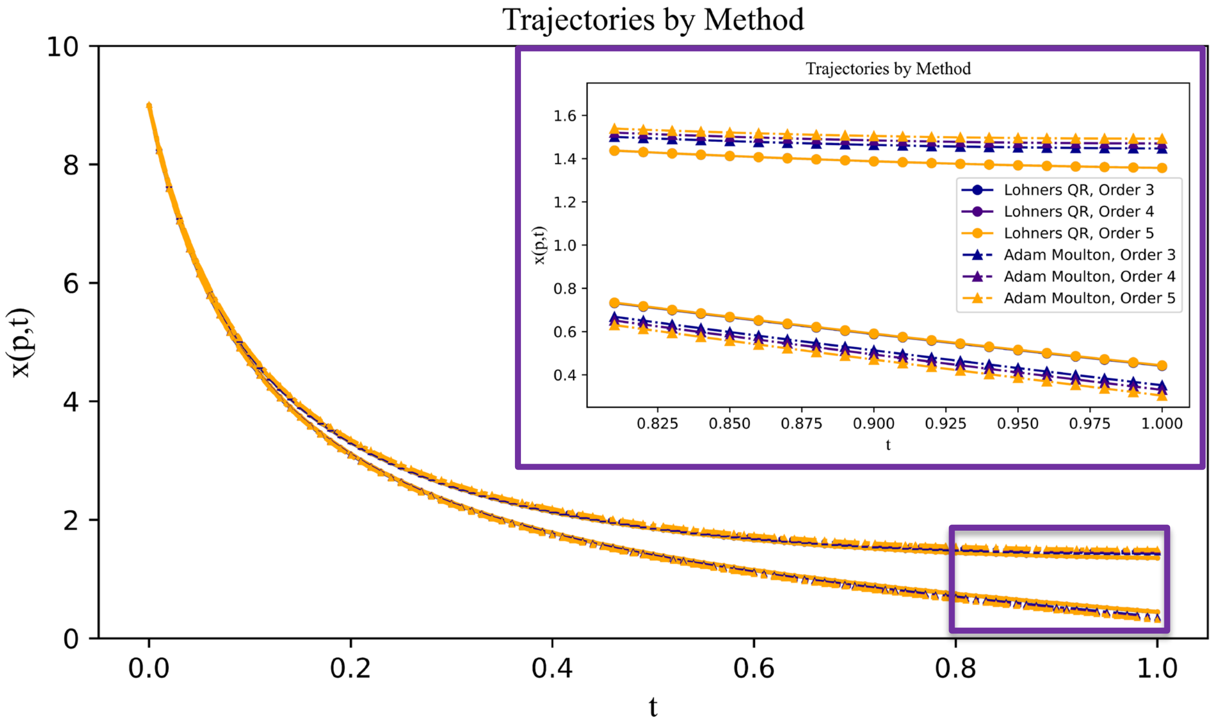
Basic 1D pODE-IVP:

$$\frac{dx}{dt}(p,t) = -x^2 + p \qquad t \in [0,1],\ \ p \in P = [-1,1]$$

$$x_o(p) = 9 \qquad x \in X = [0.1,9]$$

Comparison of interval bounds obtained between the PILMs method and Lohner's QR

Method	Order	CPU Time (ms)	Width @ t = 1
Lohner's QR	3	1.370	0.91560
Lohner's QR	4	2.450	0.91375
Lohner's QR	5	3.891	0.91376
PILMS, Adams-Moulton	3	0.420	1.095998
PILMS, Adams-Moulton	4	0.552	1.13989
PILMS, Adams-Moulton	5	0.717	1.18881



Kinetic Problem - Formulation

(Objective Function)

$$f^* = \min_{\boldsymbol{p}\in P} \sum_{i=1}^{n} \left(\mathrm{I}^i - \mathrm{I}^i_{\mathrm{data}}\right)^2$$

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

(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[33]

(pODE IVP)

$$\dot{\mathrm{x}}_{\mathrm{A}} = \mathrm{k}_1 \mathrm{x}_{\mathrm{Z}} \mathrm{x}_{\mathrm{Y}} - \mathrm{c}_{\mathrm{O2}}(\mathrm{k}_{2\mathrm{f}} + \mathrm{k}_{3\mathrm{f}})\mathrm{x}_{\mathrm{A}} + (\mathrm{k}_{2\mathrm{f}}/\mathrm{K}_2)\mathrm{x}_{\mathrm{D}} + (\mathrm{k}_{3\mathrm{f}}/\mathrm{K}_3)\mathrm{x}_{\mathrm{B}} - \mathrm{k}_5 \mathrm{x}_{\mathrm{A}}^2,$$

$$\dot{\mathrm{x}}_{\mathrm{B}} = \mathrm{k}_{3\mathrm{f}} \mathrm{c}_{\mathrm{O2}} \mathrm{x}_{\mathrm{A}} - (\mathrm{k}_{3\mathrm{f}}/\mathrm{K}_3 + \mathrm{k}_4)\mathrm{x}_{\mathrm{B}}, \qquad \dot{\mathrm{x}}_{\mathrm{D}} = \mathrm{k}_{2\mathrm{f}} \mathrm{c}_{\mathrm{O2}} \mathrm{x}_{\mathrm{A}} - (\mathrm{k}_{2\mathrm{f}}/\mathrm{K}_2)\mathrm{x}_{\mathrm{D}},$$

$$\dot{\mathrm{x}}_{\mathrm{Y}} = -\mathrm{k}_{1\mathrm{s}} \mathrm{x}_{\mathrm{Y}} \mathrm{x}_{\mathrm{Z}}, \qquad \dot{\mathrm{x}}_{\mathrm{Z}} = -\mathrm{k}_1 \mathrm{x}_{\mathrm{Y}} \mathrm{x}_{\mathrm{Z}},$$

(Decision Variables) $\mathbf{p} = (\mathrm{k}_{2\mathrm{f}}, \mathrm{k}_{3\mathrm{f}}, \mathrm{k}_4)$

(State Variables) $\mathbf{x} = (\mathrm{x}_{\mathrm{A}}, \mathrm{x}_{\mathrm{B}}, \mathrm{x}_{\mathrm{D}}, \mathrm{x}_{\mathrm{Y}}, \mathrm{x}_{\mathrm{Z}})$

(Parameters) $\mathrm{k}_1, \mathrm{k}_{1\mathrm{s}}, \mathrm{k}_5, \mathrm{K}_2, \mathrm{K}_3, \mathrm{c}_{\mathrm{O2}}, \Delta\mathrm{t}, \mathrm{n}$

(Initial Condition) $\dot{\mathbf{x}}(\mathrm{t} = 0) = (0, 0, 0, 0.4, 140)$

39. J. W. Taylor, et al. **Direct measurement of the fast, reversible addition of oxygen to cyclohexadienyl radicals in nonpolar solvents**, *Phys. Chem. A*, 108 (2004), pp. 7193–7203.
40. A. B. Singer et al., **Global dynamic optimization for parameter estimation in chemical kinetics** A. B. Singer et al., *J. Phys. Chem. A*, 110 (2006), pp. 971–976
3. Mitsos et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601
32. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460
33. Wilhelm, ME; Le, AV; and Stuber. MD. "**Global Optimization of Stiff Dynamical Systems.**" *AIChE Journal: Futures Issue,* 65 (12), *2019*

Kinetic Problem - Formulation

(Objective Function)

$$f^* = \min_{\boldsymbol{p}\in P} \sum^{n} \left(\mathrm{I}^i - \mathrm{I}^i_{\ldots}\right)^2$$

$s.t. \quad \mathrm{I}^i = \ldots$

(pODE IVP)

$\dot{\mathrm{x}}_{\mathrm{A}} = \mathrm{k}_1 \ldots$

$\dot{\mathrm{x}}_{\mathrm{B}} = \mathrm{k}_{3f} \ldots$

$\dot{\mathrm{x}}_{\mathrm{Y}} = -\mathrm{k} \ldots$

(Description of Problem)

- Fit the rate constants (k_{2f}, k_{3f}, k_4) of oxygen addition to cyclohexadienyl radicals to data. [39]

$\ldots, \mathrm{k}_4)$

$\ldots, \mathrm{x}_{\mathrm{Y}}, \mathrm{x}_{\mathrm{Z}})$

$\ldots \mathrm{K}_3, \mathrm{c}_{\mathrm{O2}}, \Delta\mathrm{t}, \mathrm{n}$

$\ldots, 0, 0, 0.4, 140)$

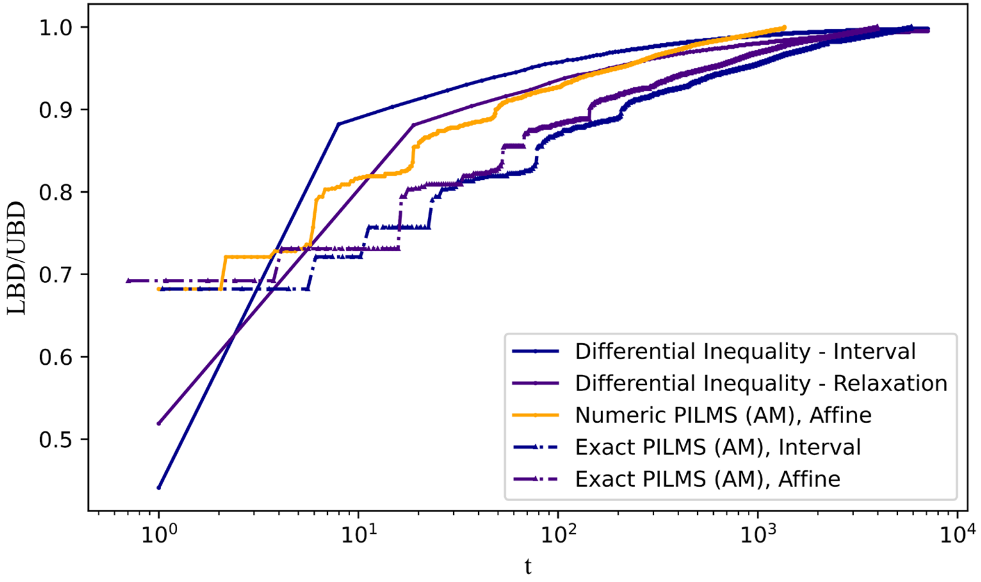
- Affine relaxations used to compute lower bound (CPLEX 12.8).
- Upper-bound computed by integrating ODE at midpoint of active node then evaluating objective & constraints.
- Duality-based bound tightening was performed in all cases.
- Absolute and relative convergence tolerances for the B&B algorithm of 10^{-2} and 10^{-5}, respectively.

39. J. W. Taylor, … , 108 (2004), pp. 7193–7203.
40. A. B. Singer et al., … , pp. 971–976
3. Mitsos et al. **McCormick-based relaxations of algorithms.** *SIAM Journal on Optimization*, SIAM (2009) 20, 73-601
32. Stuber, M.D. et al. **Convex and concave relaxations of implicit functions.** *Optimization Methods and Software* (2015), 30, 424-460
33. Wilhelm, ME; Le, AV; and Stuber. MD. "**Global Optimization of Stiff Dynamical Systems.**" *AIChE Journal: Futures Issue,* 65 (12), *2019*

Kinetic Problem - Results

- A comparison of our new approach is made to existing methods.
- The 200 step numerical Adams-Moulton (AM, 2^{nd} 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)[41] are included for comparison.

Method	Lower Bound	Final Relative Gap	Time (s)	Iterations
Exact PILMS, Adams-Moulton	Interval	None	5983	>800,000
Exact PILMS, Adams-Moulton	Affine	None	3976	>350,000
Numerical, Adams-Moulton, 200 step	Affine	None	1356	6068
Differential Inequality	Interval[6,7,9]	1.9E-3	>7200	>1,300,000
Differential Inequality	Affine[8]	4.5E-3	>7200	>475,000



41. Serban, Radu, and Alan C. Hindmarsh. **CVODES: the sensitivity-enabled ODE solver in SUNDIALS.** *International Design Engineering Technical Conferences and Computers and Information in Engineering Conference*. Vol. 47438. 2005.
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6. Harrison, Gary W. **Dynamic models with uncertain parameters.** *Proceedings of the first international conference on mathematical modeling.* Vol. 1. University of Missouri Rolla, 1977.
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9. Scott, Joseph K., and Paul I. Barton. **Bounds on the reachable sets of nonlinear control systems.** *Automatica* 49.1 (2013): 93-100.
8. Scott, Joseph K., and Paul I. Barton. **Improved relaxations for the parametric solutions of ODEs using differential inequalities.** *Journal of Global Optimization* 57.1 (2013): 143-176.

Next Steps

Extend approaches to partitioned pODEs.

- ❑ ***General form of partitioned pODEs:***

$$\frac{dx}{dt} = f_1(x,p) + f_2(x,p)$$

- ❑ ***Implicit-explicit (IMEX) pODEs***:

f_1 is a stiff, f_2 is a nonstiff

- ❑ ***Linear-nonlinear (LNL) pODEs:***

f_1 is linear, f_2 is nonlinear/nonstiff

Apply lower order to PILMS method to solve parametric parabolic PDEs.

- *Analogous approach to Crank-Nicolson methods.*
- *Implicit-explicit methods (IMEX)*

Further integration into dynamic global/robust optimization algorithms.

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