Enclosing All Solutions of TPBVP for ODEs Using Interval Analysis

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Outline

- Background
- Tools
- Methodology
- Examples
- Concluding Remarks

Background

- Given an ODE system: $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}) \qquad t \in [t_0, t_f]$
- Supplemented by boundary conditions: $\boldsymbol{g}(\boldsymbol{x}(t_0), \boldsymbol{x}(t_f), \boldsymbol{\theta}) = \mathbf{0}$
  - Initial Value Problem (IVP)
  - Two-Point Boundary Value Problem (TPBVP)
- A TPBVP may not have a solution or may have a finite number of solutions
- Often also need to determine parameter values for which solutions exist

Background (Cont'd)

- Standard techniques for the numerical solutions of a TPBVP
  - Shooting methods – based on solving related IVPs
  - Finite difference or collocation methods
- Limitation – find a local solution and miss other solutions of interest
- Need a method that can guarantee to enclose all solutions of interest

Tools

- Interval Mathematics
- Taylor Models
- Constraint Propagation
- Validated Solution for Parametric ODEs

Interval Mathematics

- A real interval $X = [a, b] = \{x \in \Re \mid a \leq x \leq b\}$ is a segment in the real number line
- An interval vector $\boldsymbol{X} = (X_1, X_2, \cdots, X_n)^T$ is an n-dimensional rectangle
- Basic interval arithmetic for $X = [a, b]$ and $Y = [c, d]$ is

$$X \text{ op } Y = \{x \text{ op } y \mid x \in X, y \in Y\}$$

- Interval elementary functions (e.g. $\exp(X)$, $\sin(X)$) are also available
- The interval extension $F(\boldsymbol{X})$ encloses all values of $f(\boldsymbol{x})$ for every $\boldsymbol{x} \in \boldsymbol{X}$

$$F(\boldsymbol{X}) \supseteq \{f(\boldsymbol{x}) \mid \boldsymbol{x} \in \boldsymbol{X}\}$$

- Interval extensions computed using interval arithmetic may lead to overestimation of function (”dependence” problem)

Taylor Models

- Taylor Model $T_f = (p_f, R_f)$: Bounds $f(\boldsymbol{x})$ over $\boldsymbol{X}$ using a q-th order Taylor polynomial p_f and an interval remainder bound R_f
- Could obtain T_f using a truncated Taylor series
- Can also compute Taylor models by using Taylor model operations
- Beginning with Taylor models of simple functions, Taylor models of very complicated functions can be computed
- Taylor models often yield sharper bounds for modest to complicated functional dependencies

Taylor Models – Range Bounding

- Exact range bounding of the interval polynomials – NP hard
- Direct evaluation of the interval polynomials – overestimation
- Focus on bounding the dominant part (1st and 2nd order terms)
- Schemes: LDB, QDB, QFB (Makino and Berz, 2004)
- A compromise approach – Exact bounding of 1st order and diagonal elements of 2nd order terms

$$B(p) = \sum_{i=1}^{m} \left[a_i \left(X_i - x_{i0} \right)^2 + b_i (X_i - x_{i0}) \right] + S$$
$$= \sum_{i=1}^{m} \left[a_i \left(X_i - x_{i0} + \frac{b_i}{2a_i} \right)^2 - \frac{b_i^2}{4a_i} \right] + S,$$

where, S is the interval bound of other terms by direct evaluation

Taylor Models – Constraint Propagation

- Consider constraint $c(\boldsymbol{x}) = \mathbf{0}$ over $\boldsymbol{X}$
- Goal – Eliminate parts of $\boldsymbol{X}$ in which constraint cannot be satisfied
- For each $i = 1, 2 \cdots, m$, shrink $\boldsymbol{X}_i$ using

$$
\begin{aligned}
B(T_c) &= B(p_c) + R_c = a_i \left(X_i - x_{i0} + \frac{b_i}{2a_i} \right)^2 - \frac{b_i^2}{4a_i} + S_i = 0 \\
\Longrightarrow \quad & U_i^2 = W_i, \quad \text{with } U_i = X_i - x_{i0} + \frac{b_i}{2a_i} \text{ and } W_i = \left(\frac{b_i^2}{4a_i} - S_i \right) / a_i \\
\Longrightarrow \quad & U_i = \begin{cases} \emptyset & \text{if } \overline{W_i} < 0 \\ \left[-\sqrt{\overline{W_i}}, \sqrt{\overline{W_i}} \right] & \text{if } \underline{W_i} \le 0 \le \overline{W_i} \\ -\sqrt{W_i} \cup \sqrt{W_i} & \text{if } \underline{W_i} > 0 \end{cases} \\
\Longrightarrow \quad & X_i = X_i \cap \left(U_i + x_{i0} - \frac{b_i}{2a_i} \right)
\end{aligned}
$$

Validated Solution for Parametric ODEs

- Consider the IVP for the parametric ODEs

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}), \quad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \in \boldsymbol{X}_0, \quad \boldsymbol{\theta} \in \boldsymbol{\Theta}$$

- Validated methods:
  - Guarantee there exists a unique solution $\boldsymbol{x}$ in the interval $[t_0, t_f]$, for each $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{x}_0 \in \boldsymbol{X}_0$
  - Compute an interval $\boldsymbol{X}_j$ that encloses all solutions of the ODEs system at t_j for $\boldsymbol{\theta} \in \boldsymbol{\Theta}$ and $\boldsymbol{x}_0 \in \boldsymbol{X}_0$
- Tools are available – AWA, VNODE, COSY VI, VSPODE, etc.

New Method for Parametric ODEs

- Use interval Taylor series to represent dependence on time
- Use Taylor models to represent dependence on uncertain quantities (parameters and initial states)
- Assuming $\boldsymbol{X}_j$ is known, then
  - Phase 1: Compute a coarse enclosure $\widetilde{\boldsymbol{X}}_j$ and prove existence and uniqueness using fixed pointed iteration with Picard operator and high-order interval Taylor series
  - Phase 2: Refine the coarse enclosure to obtain $\boldsymbol{X}_{j+1}$ using Taylor models in terms of the uncertain parameters and initial states
- Implemented in VSPODE (Validating Solver for Parametric ODEs, Lin and Stadtherr, 2006)

Phase 2 of VSPODE

- Represent uncertain initial states and parameters using Taylor model $\boldsymbol{T}_{\boldsymbol{x}_0}$ and $\boldsymbol{T}_{\boldsymbol{\theta}}$, with components

$$T_{x_{i0}} = (m(X_{i0}) + (x_{i0} - m(X_{i0})), [0, 0]), \quad i = 1, \cdots, m$$
$$T_{\theta_i} = (m(\Theta_i) + (\theta_i - m(\Theta_i)), [0, 0]), \quad i = 1, \cdots, p$$

- Bound the interval Taylor series coefficients $\boldsymbol{f}^{[i]}$ by Taylor models $\boldsymbol{T}_{\boldsymbol{f}^{[i]}}$
  - Use mean value theorem
  - Evaluate using Taylor model operations

Phase 2 of VSPODE (Cont'd)

- Reduce "wrapping effect" by using a new type of Taylor model

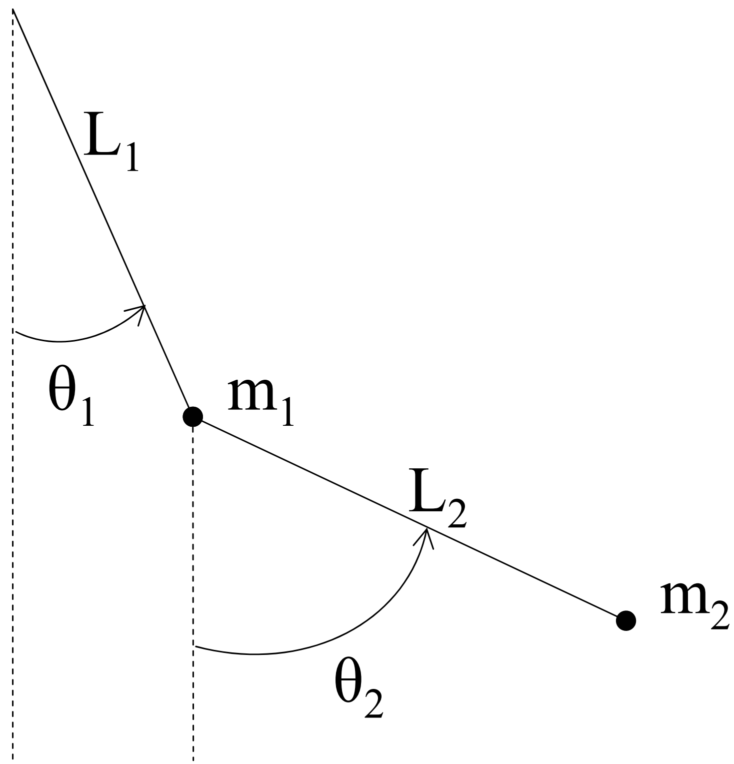
$$\boldsymbol{T}_{\boldsymbol{x}_j} = \widehat{\boldsymbol{T}}_{\boldsymbol{x}_j} + \mathcal{P}_j, \quad \text{where} \quad \mathcal{P}_j = \{\boldsymbol{A}_j \boldsymbol{v}_j \mid \boldsymbol{v}_j \in \boldsymbol{V}_j\}$$

  - The remainder bound is propagated as a parallelepiped (parallelepiped method) or a rotated rectangle (QR-factorization method), instead of intervals

- The result: a Taylor model $\boldsymbol{T}_{\boldsymbol{x}_{j+1}}$ in terms of the initial states $\boldsymbol{x}_0$ and parameters $\boldsymbol{\theta}$

- Compute the enclosure $\boldsymbol{X}_{j+1} = \boldsymbol{B}(\boldsymbol{T}_{\boldsymbol{x}_{j+1}})$ by bounding over $\boldsymbol{X}_0$ and $\boldsymbol{\Theta}$

VSPODE Example 1 – Double Pendulum Problem



$m_1 = m_2 = 1$ kg

$L_1 = L_2 = 1$ m

VSPODE Example 1 – Double Pendulum Problem

- ODE model is

$$\dot{\theta}_1 = \omega_1$$

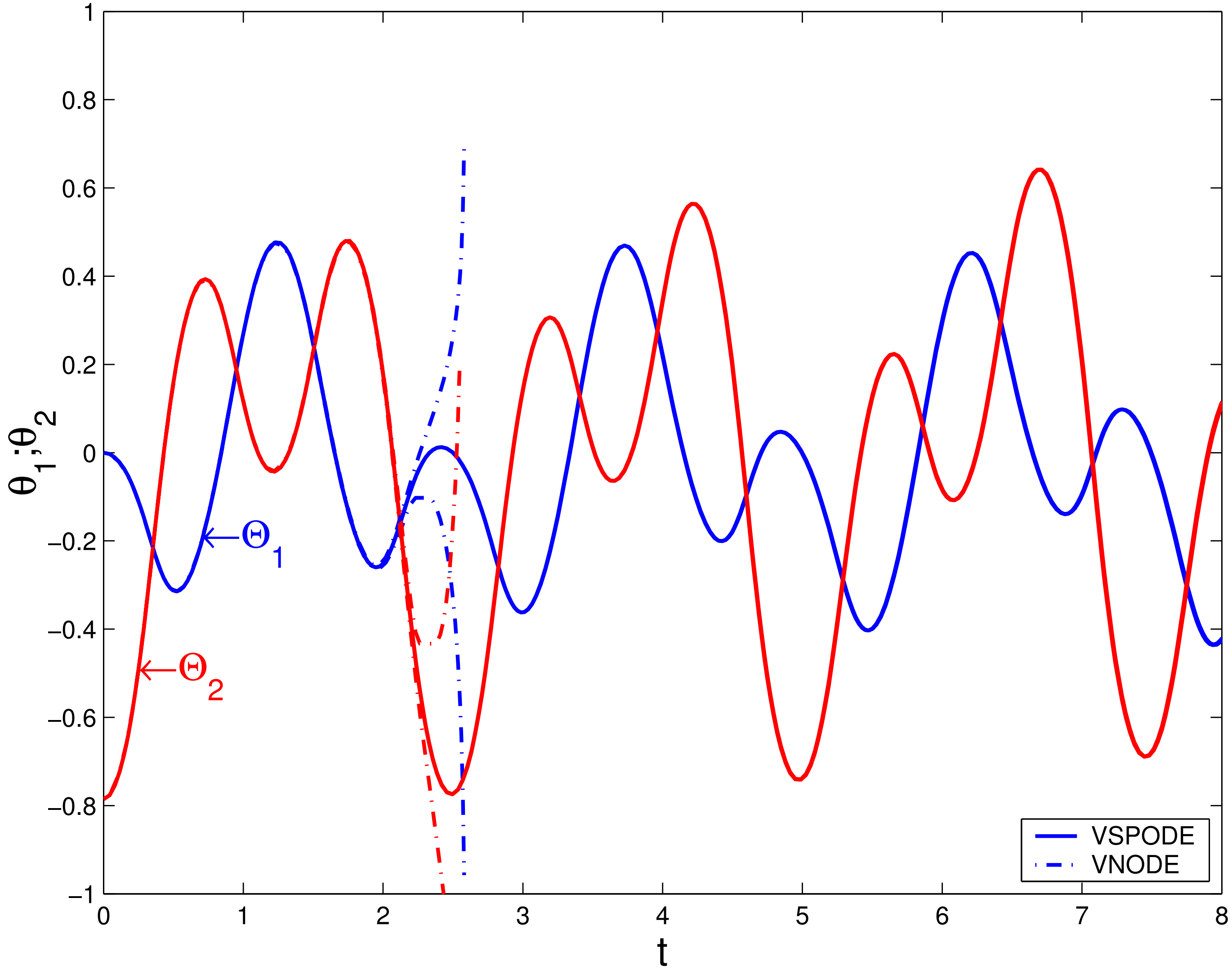
$$\dot{\theta}_2 = \omega_2$$

$$\dot{\omega}_1 = \frac{-g(2m_1 + m_2)\sin\theta_1 - m_2 g\sin(\theta_1 - 2\theta_2) - 2m_2\sin(\theta_1 - \theta_2)\ \ \omega_2^2 L_2 - \omega_1^2 L_1\cos(\theta_1 - \theta_2)}{L_1\left[2m_1 + m_2 - m_2\cos(2\theta_1 - 2\theta_2)\right]}$$

$$\dot{\omega}_2 = \frac{2\sin(\theta_1 - \theta_2)\ \ \omega_1^2 L_1(m_1 + m_2) + g(m_1 + m_2)\cos\theta_1 + \omega_2^2 L_2 m_2\cos(\theta_1 - \theta_2)}{L_2\left[2m_1 + m_2 - m_2\cos(2\theta_1 - 2\theta_2)\right]}$$

- Local acceleration of gravity $g \in [9.79, 9.81]$ m/s^2
- This corresponds roughly to the variation in sea level g between 25° and 49° latitude (i.e. spanning the contiguous United States)
- Initial states: $(\theta_1, \theta_2, \omega_1, \omega_2)_0 = (0, -0.25\pi, 0, 0)$
- Variable step size used in both VSPODE and VNODE

VSPODE Example 1 – Double Pendulum Problem



VSPODE Example 2 – Bioreactor Problem

- In a bioreactor, microbial growth may be described by

$$\dot{X} = (\mu - \alpha D)X$$

$$\dot{S} = D(S^i - S) - k\mu X,$$

where X and S are concentrations of biomass and substrate, respectively.

- The growth rate μ may be given by

$$\mu = \frac{\mu_m S}{K_S + S} \quad \text{(Monod Law)}$$

or

$$\mu = \frac{\mu_m S}{K_S + S + K_I S^2} \quad \text{(Haldane Law)}$$

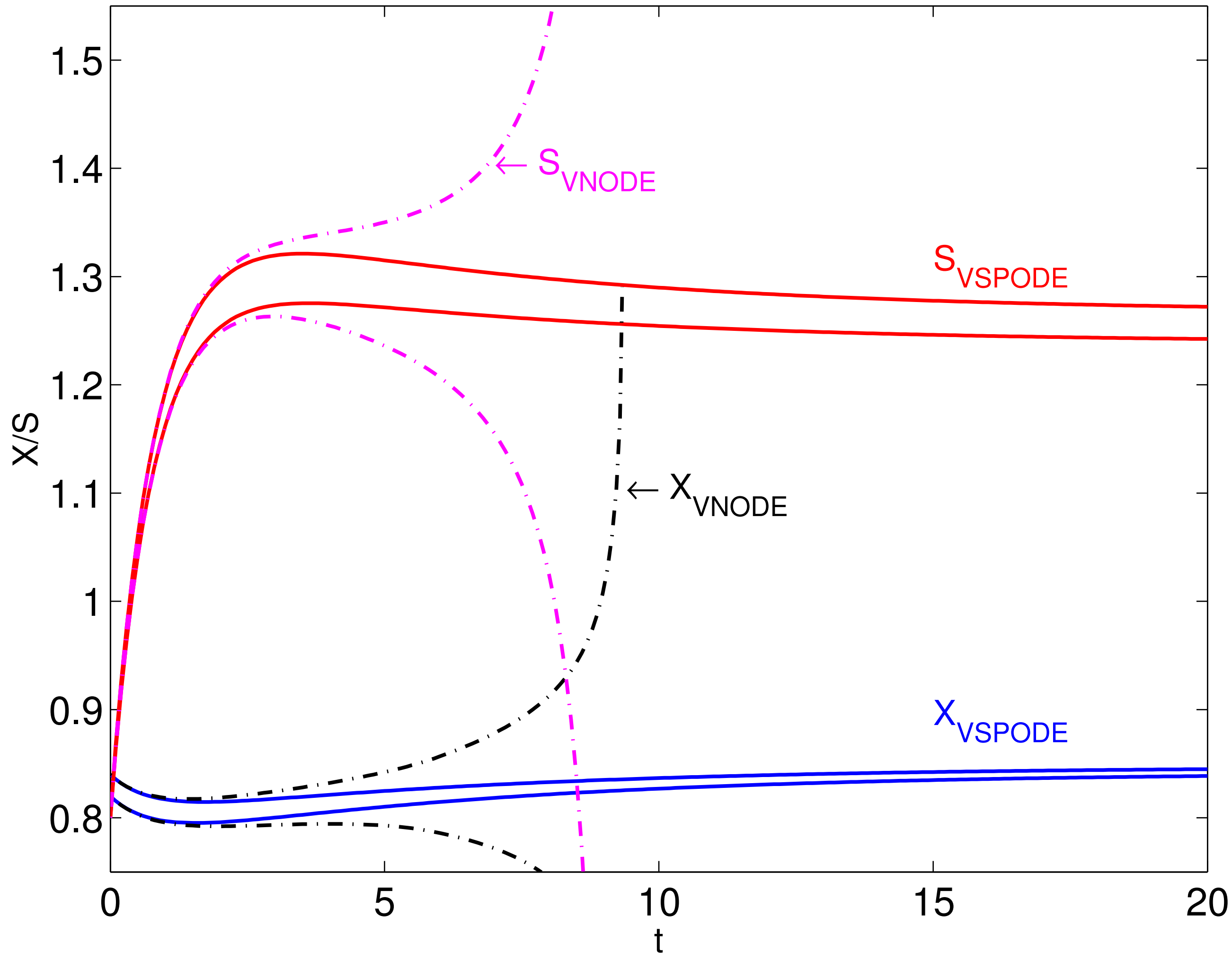
VSPODE Example 2 – Bioreactor Problem

- Problem data

	Value	Units		Value	Units
α	0.5	-	μ_m	[1.19, 1.21]	day^{-1}
k	10.53	g S/ g X	K_S	[7.09, 7.11]	g S/l
D	0.36	day^{-1}	K_I	[0.49, 0.51]	(g S/l)$^{-1}$
S^i	5.7	g S/l	X_0	[0.82, 0.84]	g X/l
S_0	0.80	g S/l			

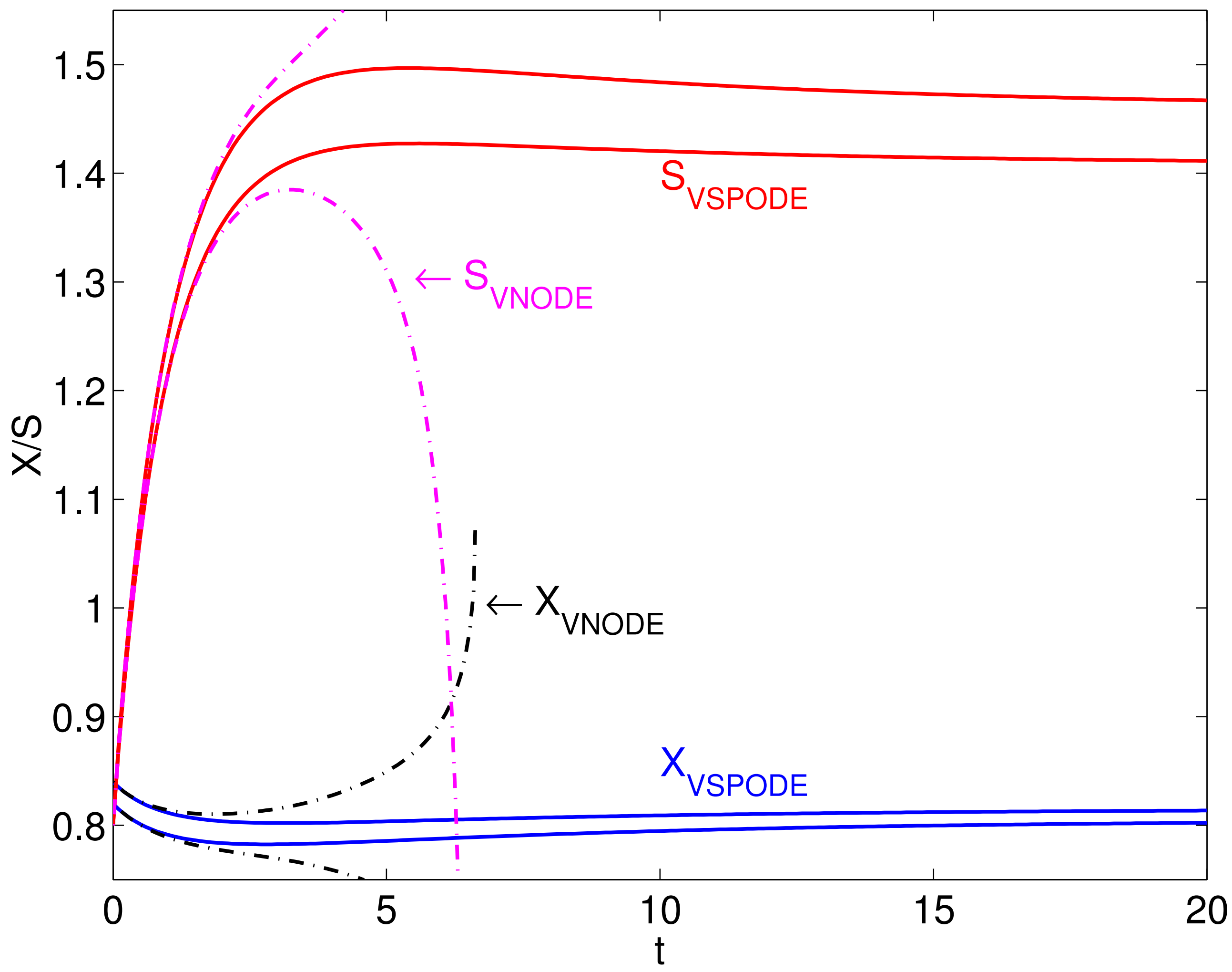
- Integrate from $t_0 = 0$ to $t_N = 20$.
- Constant step size of $h = 0.1$ used in both VSPODE and VNODE.

Bioreactor Problem – Monod Law



(VSPODE does not break down at longer t)

Bioreactor Problem – Haldane Law



(VSPODE does not break down at longer t)

Methodology for Solutions of TPBVP

- A type of shooting method based on branch and reduce framework
- Find variables z (unknown initial state and parameters)
- The initial interval vector of $Z^{(0)}$ is divided into a sequence of subintervals.
- Certain subintervals are dynamically refined while others are excluded from consideration based on solution criteria (Boundary Conditions)

Methodology for Solutions of TPBVP (Cont'd)

- Iteration: for a particular subinterval $\boldsymbol{Z}^{(k)}$
  - Obtain the Taylor model of $\boldsymbol{X}_f$ using VSPODE
  - Perform the CPP on boundary conditions ($\boldsymbol{g} = 0$) to reduce $\boldsymbol{Z}^{(k)}$
    * If $\boldsymbol{Z}^{(k)} = \emptyset$, go to next subinterval in the test list $\mathcal{L}$
    * If $\text{Width}(Z) \leq \epsilon_x$ or $|B(\boldsymbol{g})| \leq \epsilon_g$, store $\boldsymbol{Z}^{(k)}$ in the result list $\mathcal{R}$ and go to next subinterval in the test list $\mathcal{L}$
    * If $\boldsymbol{Z}^{(k)}$ is sufficiently reduced, repeat
    * Otherwise, bisect $\boldsymbol{Z}^{(k)}$ and store the resulting two subintervals in the test list $\mathcal{L}$
- Termination
  - The test list $\mathcal{L}$ is empty
  - All solutions of interest are stored in the result list $\mathcal{R}$

Methodology for Solutions of TPBVP (Cont'd)

- One of drawback of shooting methods is that the solution of IVP with some variables may not exist in $[t_0, t_f]$, i.e. state becomes unbounded before reaching t_f
- VSPODE would FAIL in such a case
- May be associated with the abnormal value of state
- Introduce bounds on the state, i.e. natural bounds.
- Check state bounds on each integration step of VSPODE, and discard those subintervals that will result in violation of the state bounds.

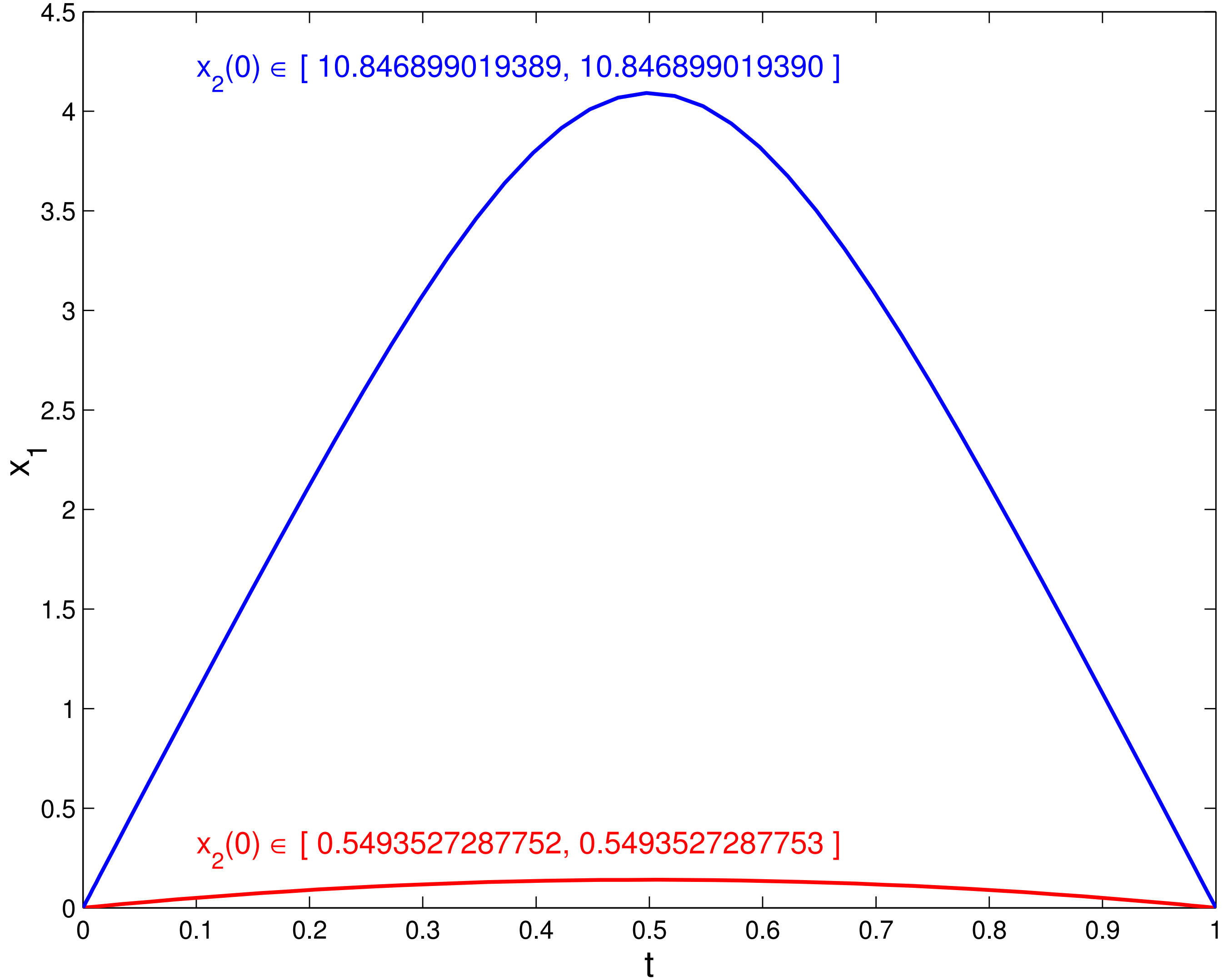
Example 1 – Bratu's Equation

- Arises in a model of spontaneous combustion: $x'' + \lambda \exp(x) = 0$

$$\begin{aligned} x_1' &= x_2 \\ x_2' &= -\exp(x_1) \\ t &\in [0, 1] \\ x_1(0) &= 0 \\ x_1(1) &= 0 \\ x_2(0) &\in [0, 20] \end{aligned}$$

- Two solutions in less than 2 seconds CPU time

Example 1 – Bratu's Equation (Cont'd)



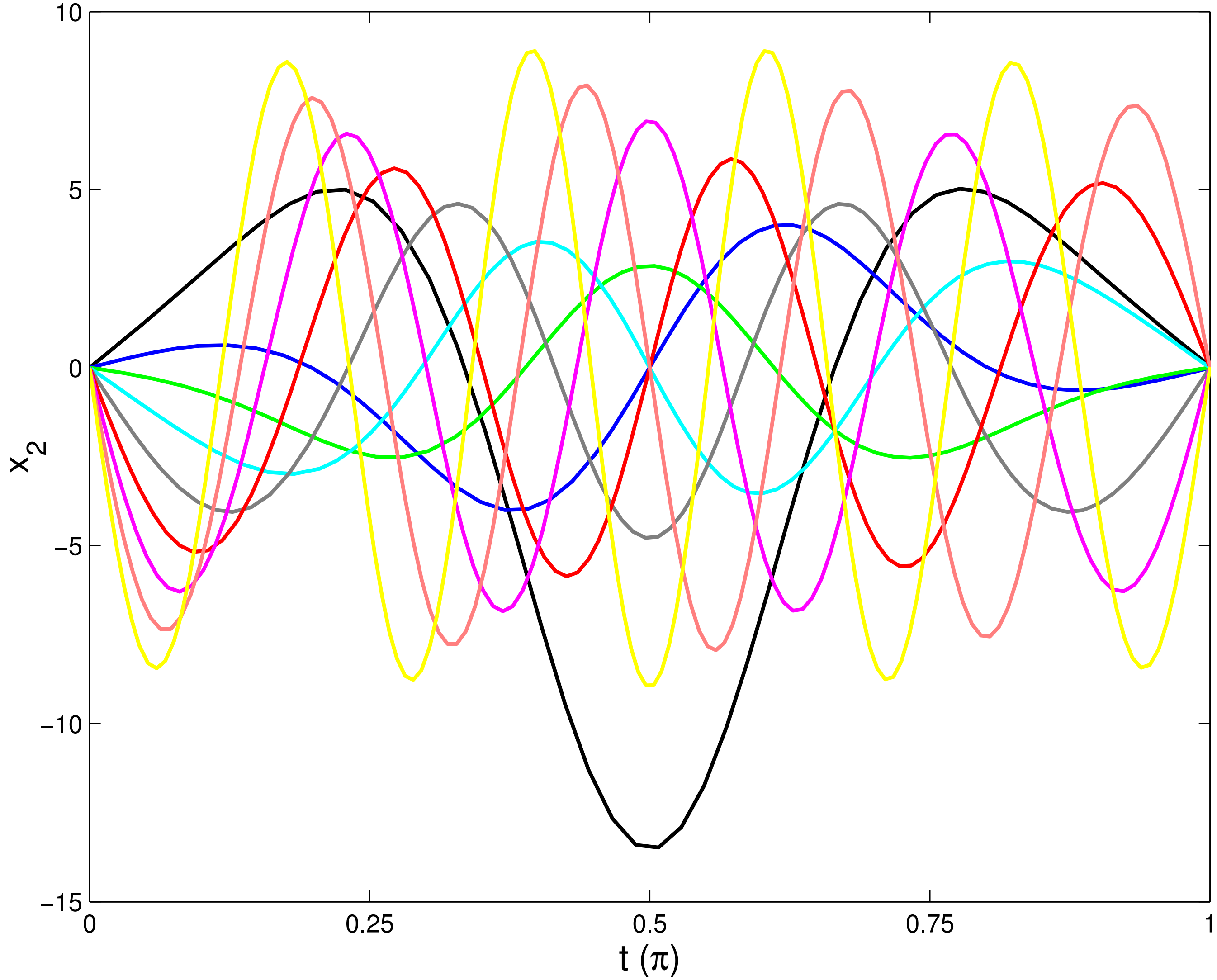
Example 2 – Mathieu's equation

- Arises arises in separation of variables of the Helmholtz differential equation in elliptic cylindrical coordinates: $x'' + (\lambda - 2r\cos 2t)x = 0$

$$
\begin{aligned}
x_1' &= x_2 \\
x_2' &= -(\lambda - 10\cos(2x_3))x_1 \\
x_3' &= 1 \\
t &\in [0, \pi] \\
\boldsymbol{x}(0) &= (1, 0, 0)^T \\
x_2(\pi) &= 0 \\
\lambda &\in [0, 100]
\end{aligned}
$$

- 9 solutions are found in 6.56 seconds of CPU time

Example 2 – Mathieu's equation (Cont'd)



Example 3 – Steady State Brusselator with Diffusion

- Arises in an autocatalytic, oscillating chemical reaction

$$
\begin{aligned}
x_1' &= x_2 \\
x_2' &= L^2/D_1\left[(B+1)x_1 - A - x_1^2 x_3\right] \\
x_3' &= x_4 \\
x_4' &= L^2/D_2\left(x_1^2 x_3 - B x_1\right) \\
t &\in [0,1] \\
x_1(0) &= x_1(1) = A \\
x_3(0) &= x_3(1) = B/A \\
x_2 &\in [-25,25], \quad x_4 \in [-25,25] \\
x_1 &\geq 0, \quad x_3 \geq 0
\end{aligned}
$$

- Constants: $D_1 = 0.0016$, $D_2 = 0.008$, $A = 2$, and $B = 4.6$

Example 3 – Steady State Brusselator with Diffusion

- Depending on the value of L, there exists a differing number of solutions

L	Solutions	CPU (s)
0.1	2	2303
0.15	2	10545
0.2	6	9696
0.22	6	12683
0.25	6	30185
0.3	5	130603

Concluding Remarks

- We propose a type of shooting method based on branch and reduce framework to enclose all solutions of interest of TPBVP
  - A new validated solver for parametric ODEs is used to produce guaranteed bounds on the solutions of IVPs for ODEs with interval-valued parameters and initial states
  - A constraint propagation strategy on the Taylor models is used to efficiently eliminate incompatible domain of variables
- Future work
  - Computing Bifurcations
  - Optimal control problems

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