Validated Solution of Initial Value Problems for ODEs with Interval Parameters

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Outline

- Motivating Problem: Bioreactor Simulation
- Background
- Overview of Method
- Examples and Results
  - Lotka-Volterra Problem
  - Lorenz Problem
  - Double Pendulum Problem
  - Bioreactor Problem
- Concluding Remarks

Motivating Example – Bioreactor Simulation

- 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

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

Motivating Example – Bioreactor Simulation

- 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			

- Three parameters (μ_m, K_S and K_I) and one initial state (X_0) are uncertain and given by intervals.
- Problem: Determine a validated enclosure of all possible solutions to this ODE system.
- Issue: Standard tools for validated solution of ODEs are designed to deal with interval-valued initial states, not interval-valued parameters.

Problem Definition

- Consider

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta})$$

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0 \in \boldsymbol{X}_0$$

$$\boldsymbol{\theta} \in \boldsymbol{\Theta}$$

  $\boldsymbol{x}$ = state vector (m variables)

  $\boldsymbol{\theta}$ = parameter vector (p parameters)

  $\boldsymbol{X}_0$ = interval enclosure of $\boldsymbol{x}_0$

  $\boldsymbol{\Theta}$ = interval enclosure of $\boldsymbol{\theta}$

- Consider time steps $h_j = t_{j+1} - t_j$, $j = 0, \ldots, N-1$

- Notation: $\boldsymbol{x}(t; t_j, \boldsymbol{x}_j, \boldsymbol{\theta})$ denotes a solution of $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta})$ for the initial condition $\boldsymbol{x} = \boldsymbol{x}_j$ at $t = t_j$ and $\boldsymbol{x}(t; t_j, \boldsymbol{X}_j, \boldsymbol{\Theta})$ is the set of solutions $\boldsymbol{x}(t; t_j, \boldsymbol{X}_j, \boldsymbol{\Theta}) = \{\boldsymbol{x}(t; t_j, \boldsymbol{x}_j, \boldsymbol{\theta}) \mid \boldsymbol{x}_j \in \boldsymbol{X}_j, \boldsymbol{\theta} \in \boldsymbol{\Theta}\}$

- Problem: Determine enclosures $\boldsymbol{X}_j$ of the state variables at each time t_j, $j = 1, \ldots, N$, such that $\boldsymbol{x}(t_j; t_0, \boldsymbol{X}_0, \boldsymbol{\Theta}) \subseteq \boldsymbol{X}_j$

Background – Interval Taylor Series

- In an Taylor series expansion of $\boldsymbol{x}(t)$ with respect to t, the coefficients can be obtained recursively in terms of $\dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta})$ using

$$\begin{aligned}
\boldsymbol{f}^{[0]} &= \boldsymbol{x} \\
\boldsymbol{f}^{[1]} &= \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta}) \\
\boldsymbol{f}^{[i]} &= \frac{1}{i}\left(\frac{\partial \boldsymbol{f}^{[i-1]}}{\partial \boldsymbol{x}}\boldsymbol{f}\right)(\boldsymbol{x}, \boldsymbol{\theta}), \quad i \geq 2.
\end{aligned}$$

- Values of these coefficients can be easily generated using automatic differentiation techniques.

- For an interval Taylor series (ITS), the coefficients $\boldsymbol{F}^{[i]}$ are interval enclosures of $\boldsymbol{f}^{[i]}$.

Background – Taylor Models

- Taylor Model $T_f = (p_f, R_f)$: Bounds a function $f(\boldsymbol{x})$ over $\boldsymbol{X}$ using a q-th order Taylor polynomial p_f and an interval remainder bound R_f, usually from a truncated Taylor series.

$$p_f = \sum_{i=0}^{q} \frac{1}{i!} \left[(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \bigtriangledown\right]^i f(\boldsymbol{x}_0)$$

$$R_f = \frac{1}{(q+1)!} \left[(\boldsymbol{x} - \boldsymbol{x}_0) \cdot \bigtriangledown\right]^{q+1} F\left[\boldsymbol{x}_0 + (\boldsymbol{x} - \boldsymbol{x}_0)\zeta\right]$$

where,

$$\boldsymbol{x}_0 \in \boldsymbol{X}; \quad \zeta \in [0, 1]$$

$$[\boldsymbol{g} \cdot \bigtriangledown]^k = \sum_{\substack{j_1+\cdots+j_m=k \\ 0 \le j_1,\cdots,j_m \le k}} \frac{k!}{j_1!\cdots j_m!} g_1^{j_1} \cdots g_m^{j_m} \frac{\partial^k}{\partial x_1^{j_1} \cdots \partial x_m^{j_m}}$$

- Store and operate on coefficients of p_f only. Floating point errors are accumulated in R_f.

Background – Taylor Model Operations

- Taylor model of $f \pm g$

$$f \pm g \in (p_f, R_f) \pm (p_g, R_g) = (p_f \pm p_g, R_f \pm R_g)$$
$$T_{f\pm g} = (p_{f\pm g}, R_{f\pm g}) = (p_f \pm p_g, R_f \pm R_g)$$

- Taylor model of $f \times g$

$$\begin{aligned} f \times g &\in (p_f, R_f) \times (p_g, R_g) \\ &\subseteq p_f \times p_g + p_f \times R_g + p_g \times R_f + R_f \times R_g \end{aligned}$$

Split $p_f \times p_g$ into q-th order part $p_{f\times g}$ and higher-order terms p_e. Then

$$T_{f\times g} = (p_{f\times g}, R_{f\times g})$$

$$R_{f\times g} = B(p_e) + B(p_f) \times R_g + B(p_g) \times R_f + R_f \times R_g$$

$B(p)$ indicates an interval bound on the function p.

- Reciprocal operation and intrinsic functions can also be defined.

Background – Interval IVPs

- Consider standard ODE system (non-parametric)

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$$

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0 \in \boldsymbol{X}_0$$

- "Standard" approach (step $j+1$): Assuming $\boldsymbol{X}_j$ is known, then
  - Phase 1: Compute a coarse enclosure $\tilde{\boldsymbol{X}}_j$ and prove existance and uniqueness. Use fixed point iteration with Picard operator using high-order interval Taylor series.
  - Phase 2: Refine the coarse enclosure to obtain $\boldsymbol{X}_{j+1}$. Use high-order interval Taylor series with Taylor coefficients bounded using mean value theorem. Reduce wrapping effect using QR-factorization approach.
- Implementations include AWA and VNODE.

Method for Parametric ODEs

- Consider again parametric ODE system

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, \boldsymbol{\theta})$$

$$\boldsymbol{x}(t_0) = \boldsymbol{x}_0 \in \boldsymbol{X}_0$$

$$\boldsymbol{\theta} \in \boldsymbol{\Theta}$$

- To apply standard methods, can treat parameters as additional state variables with zero derivative (Lohner, 1988)
- Our method for parametric ODE system: Assuming $\boldsymbol{X}_j$ is known, then
  - Phase 1: Same as “standard” approach. Compute a coarse enclosure $\tilde{\boldsymbol{X}}_j$ and prove existance and uniqueness. Use fixed point iteration with Picard operator using high-order interval Taylor series.
  - Phase 2: Refine the coarse enclosure to obtain $\boldsymbol{X}_{j+1}$. Use Taylor models in terms of the uncertain parameters and initial states.
- Implemented in VSPODE (Validating Solver for Parametric ODEs) (Lin and Stadtherr, 2005).

Method for Phase 2

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

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

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

- Compute Taylor models $\boldsymbol{T}_{\boldsymbol{f}^{[i]}}$ for the interval Taylor series coefficients using Taylor model operations and obtain the polynomial part of $\boldsymbol{T}_{\boldsymbol{x}_{j+1}}$.
- Determine the remainder bound of $\boldsymbol{T}_{\boldsymbol{x}_{j+1}}$ by the mean value theorem and reduce the wrapping effect using a QR factorization approach, where the remainder is represented by $R_{\boldsymbol{x}_{j+1}} = A_{j+1}\boldsymbol{V}_{j+1}$.
- Compute the enclosure $\boldsymbol{X}_{j+1} = B(\boldsymbol{T}_{\boldsymbol{x}_{j+1}})$ by bounding over $\boldsymbol{X}_0$ and $\boldsymbol{\Theta}$.

Examples and Results

- Computations done with Intel Pentium 4 3.2GHz CPU on a Linux workstation.
- For comparsions, VNODE was used, with interval parameters treated as additional state variables
- VSPODE run using

  $\longrightarrow q = 5$ (order of Taylor model)

  $\longrightarrow k = 17$ (order of interval Taylor series)

  $\longrightarrow$ QR
- VNODE run using

  $\longrightarrow k = 17$ order interval Hermite-Obreschkoff

  $\longrightarrow$ QR

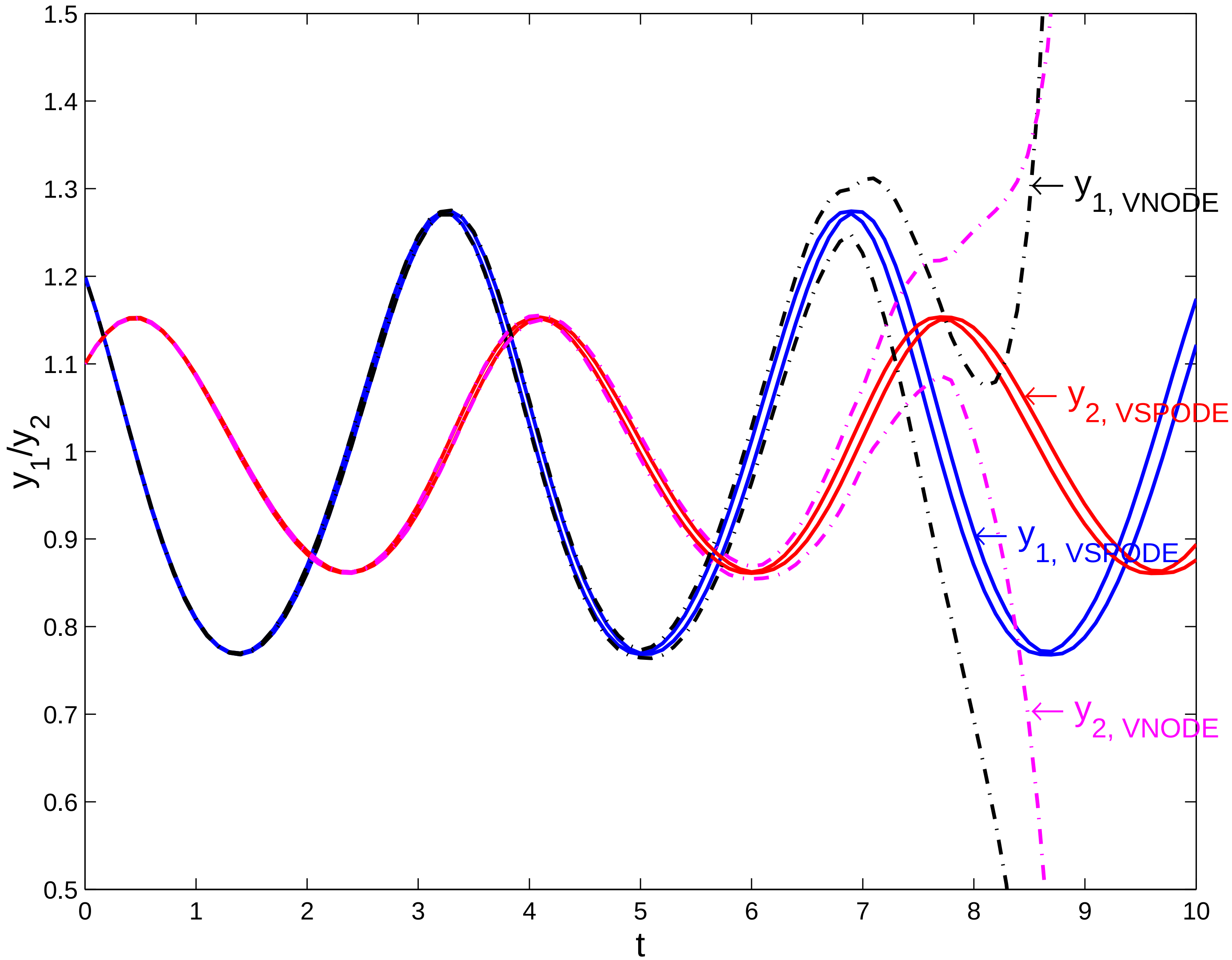
Example 1. Lotka-Volterra Problem

- ODE model is

$$\begin{aligned}\dot{x}_1 &= \theta_1 x_1 (1 - x_2) \\ \dot{x}_2 &= \theta_2 x_2 (x_1 - 1) \\ \boldsymbol{x}_0 &= (1.2, 1.1)^{\mathrm{T}} \\ \theta_1 &\in [2.99, 3.01] \\ \theta_2 &\in [0.99, 1.01]\end{aligned}$$

- Integrate from $t_0 = 0$ to $t_N = 10$.
- Constant step size of $h = 0.1$ used in both VSPODE and VNODE.

Example 1. Lotka-Volterra Problem



(Eventual breakdown of VSPODE at $t = 31.8$)

Example 1. Lotka-Volterra Problem

- To allow VNODE to integrate further:
  - Parameters intervals can be subdivided into equal-sized subintervals.
  - Apply VNODE to each parameter subinterval.
  - Final enclosure is the union of enclosures determined from each subinterval.
- VNODE-NN indicates use of NN parameter subintervals.

Example 1. Lotka-Volterra Problem

Method	Final Enclosure ($t = 10$)	Width	CPU time (s)
VSPODE	[1.120873, 1.173607]	0.052734	0.59
	[0.875994, 0.893471]	0.017477	
VNODE–16	[1.110859, 1.182814]	0.071955	1.42
	[0.872528, 0.898407]	0.025879	
VNODE–36	[1.116350, 1.177431]	0.061081	3.14
	[0.874924, 0.895612]	0.020688	
VNODE–64	[1.118151, 1.175692]	0.057541	5.59
	[0.875651, 0.894736]	0.019085	
VNODE–100	[1.118999, 1.174881]	0.055882	8.68
	[0.875975, 0.894337]	0.018362	

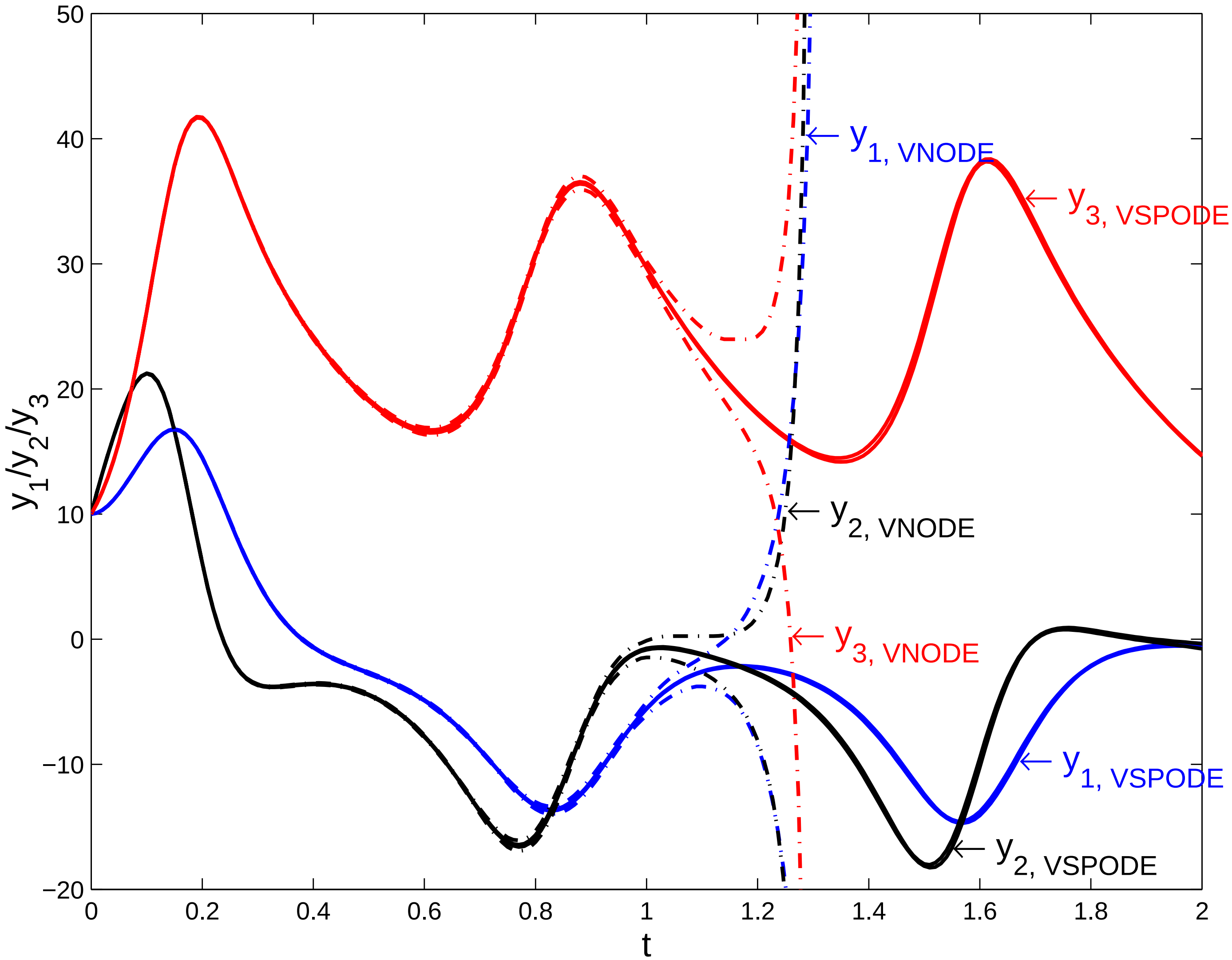
Example 2. Lorenz Problem

- ODE model is

$$\dot{x}_1 = \theta_1(x_2 - x_1)$$
$$\dot{x}_2 = x_1(\theta_2 - x_3) - x_2$$
$$\dot{x}_3 = x_1 x_2 - \theta_3 x_3$$
$$\boldsymbol{x}_0 = (10, 10, 10)^{\mathrm{T}}$$
$$\theta_1 \in 10 + [-0.01, 0.01]$$
$$\theta_2 \in 28 + [-0.01, 0.01]$$
$$\theta_3 \in 8/3 + [-0.01, 0.01]$$

- Integrate from $t_0 = 0$ to $t_N = 2$.
- Constant step size of $h = 0.01$ used in both VSPODE and VNODE.

Example 2. Lorenz Problem

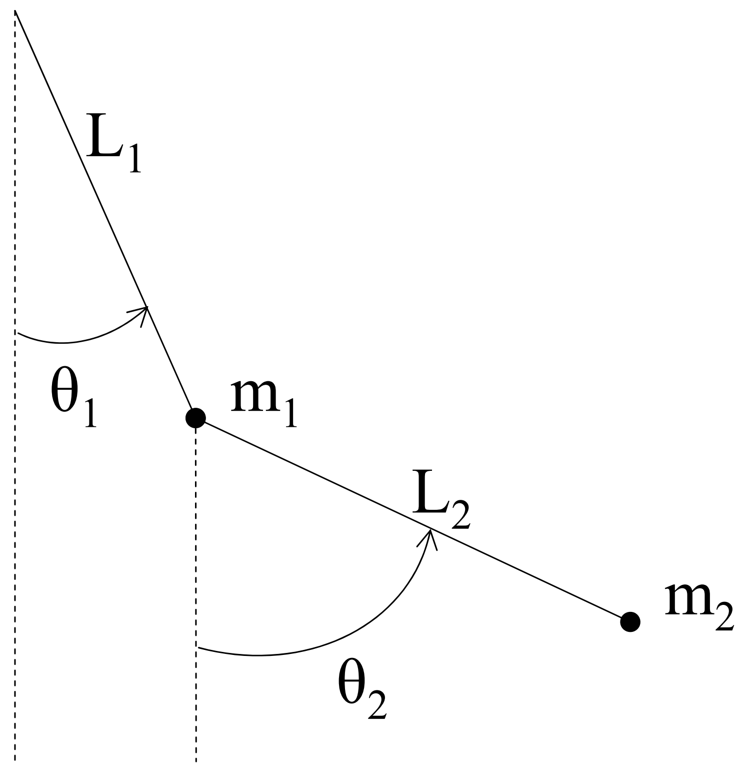


(Eventual breakdown of VSPODE at $t = 2.8$)

Example 2. Lorenz Problem

Method	Final Enclosure ($t = 2$)	Width	CPU time (s)
VSPODE	[-0.582033, -0.342358]	0.2397	2.66
	[-0.769513, -0.369357]	0.4002	
	[14.633803, 14.737535]	0.1037	
VNODE–125	[-8.663336, 7.988072]	16.6514	33.7
	[-10.060512, 8.797511]	18.8580	
	[9.031894, 21.106684]	12.0748	
VNODE–512	[-0.920184, 0.041287]	0.9615	141.5
	[-1.321734, 0.245595]	1.5673	
	[14.352124, 15.010891]	0.6588	
VNODE–1000	[-0.770156, -0.136139]	0.6340	263.1
	[-1.077794, -0.036474]	1.0413	
	[14.502030, 14.869122]	0.3671	

Example 3. Double Pendulum Problem



$$m_1 = m_2 = 1 \text{ kg}$$

$$L_1 = L_2 = 1 \text{ m}$$

Example 3. Double Pendulum Problem

- ODE model is

$$
\begin{aligned}
\dot{\theta}_1 &= \omega_1 \\
\dot{\theta}_2 &= \omega_2 \\
\dot{\omega}_1 &= \frac{-g(2m_1+m_2)\sin\theta_1 - m_2 g\sin(\theta_1-2\theta_2) - 2m_2\sin(\theta_1-\theta_2)\left[\omega_2^2 L_2 - \omega_1^2 L_1\cos(\theta_1-\theta_2)\right]}{L_1\left[2m_1+m_2-m_2\cos(2\theta_1-2\theta_2)\right]} \\
\dot{\omega}_2 &= \frac{2\sin(\theta_1-\theta_2)\left[\omega_1^2 L_1(m_1+m_2) + g(m_1+m_2)\cos\theta_1 + \omega_2^2 L_2 m_2\cos(\theta_1-\theta_2)\right]}{L_2\left[2m_1+m_2-m_2\cos(2\theta_1-2\theta_2)\right]},
\end{aligned}
$$

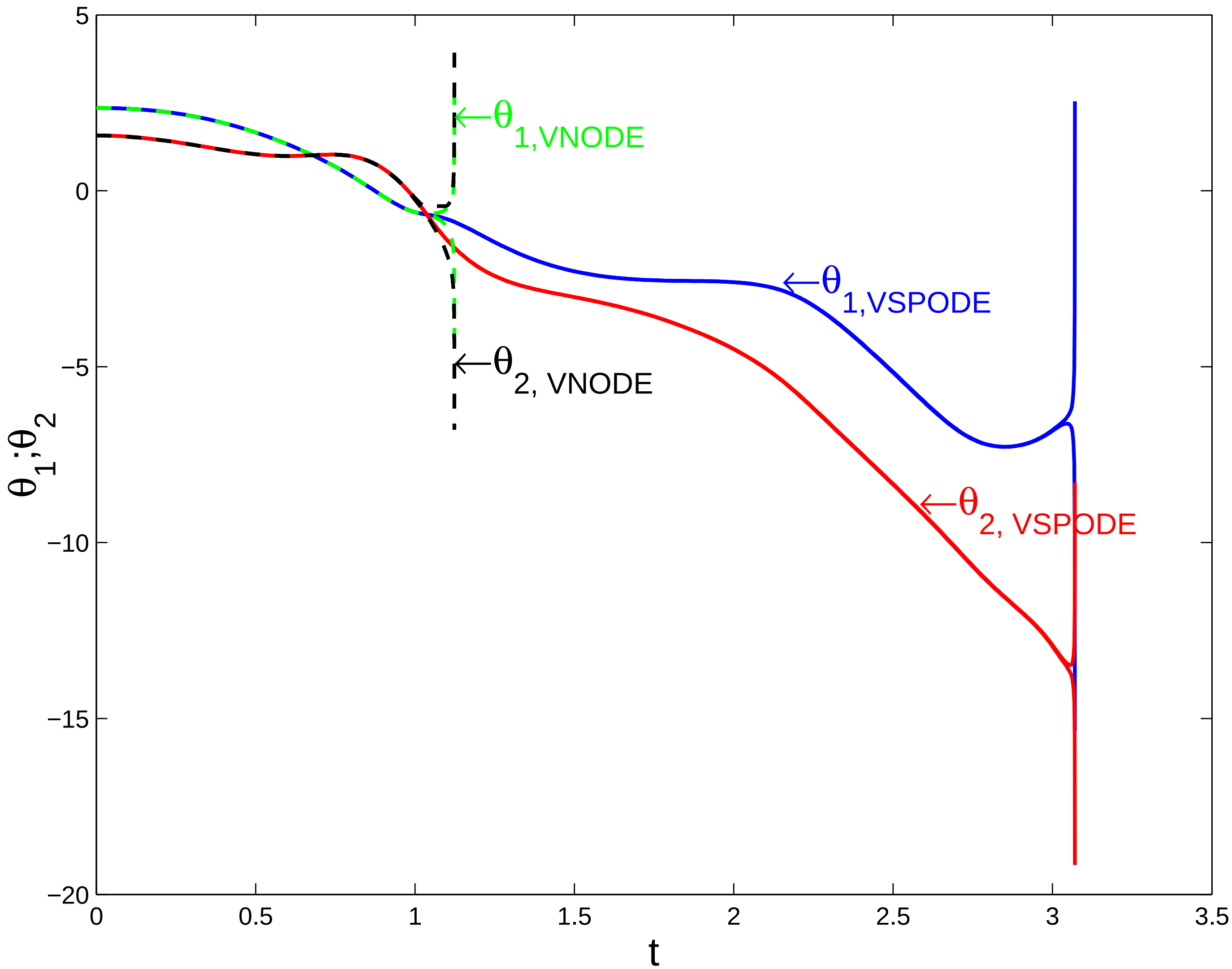
- Local acceleration of gravity $g \in [9.79, 9.81]$ m/s^2.

- This corresponds roughly to the variation in sea level g between 25° and 49° latitude (i.e. spanning the contiguous United States).

- Two cases for initial states:
  - Relatively high energy: $(\theta_1, \theta_2, \omega_1, \omega_2)_0 = (0.75\pi, 0.5\pi, 0, 0)$
  - Relatively low energy: $(\theta_1, \theta_2, \omega_1, \omega_2)_0 = (0, -0.25\pi, 0, 0)$

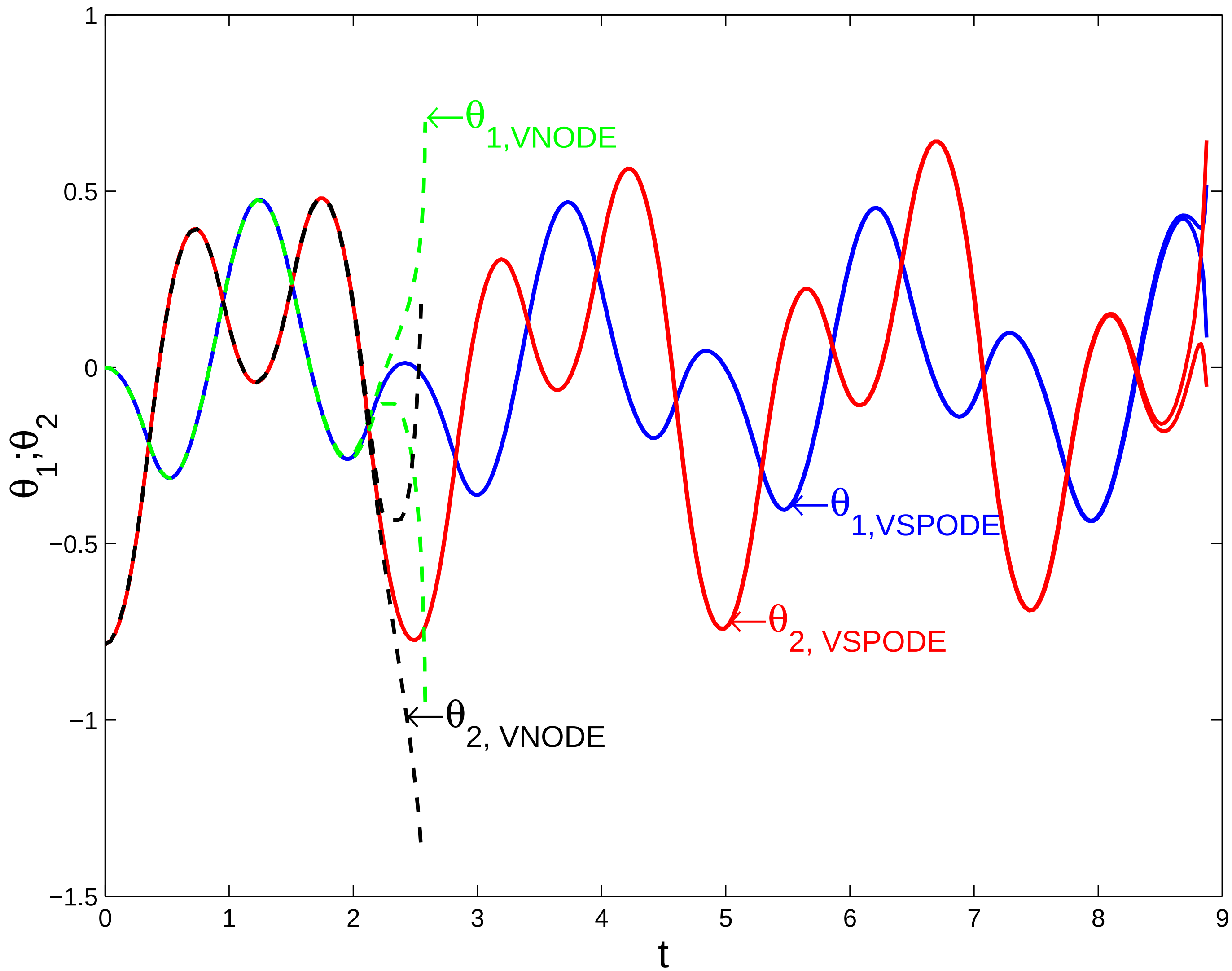
- Variable step size used in both VSPODE and VNODE.

Example 3. Double Pendulum Problem



Relatively high-energy case

Example 3. Double Pendulum Problem



Relatively low-energy case

Example 4. 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

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

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- Problem data

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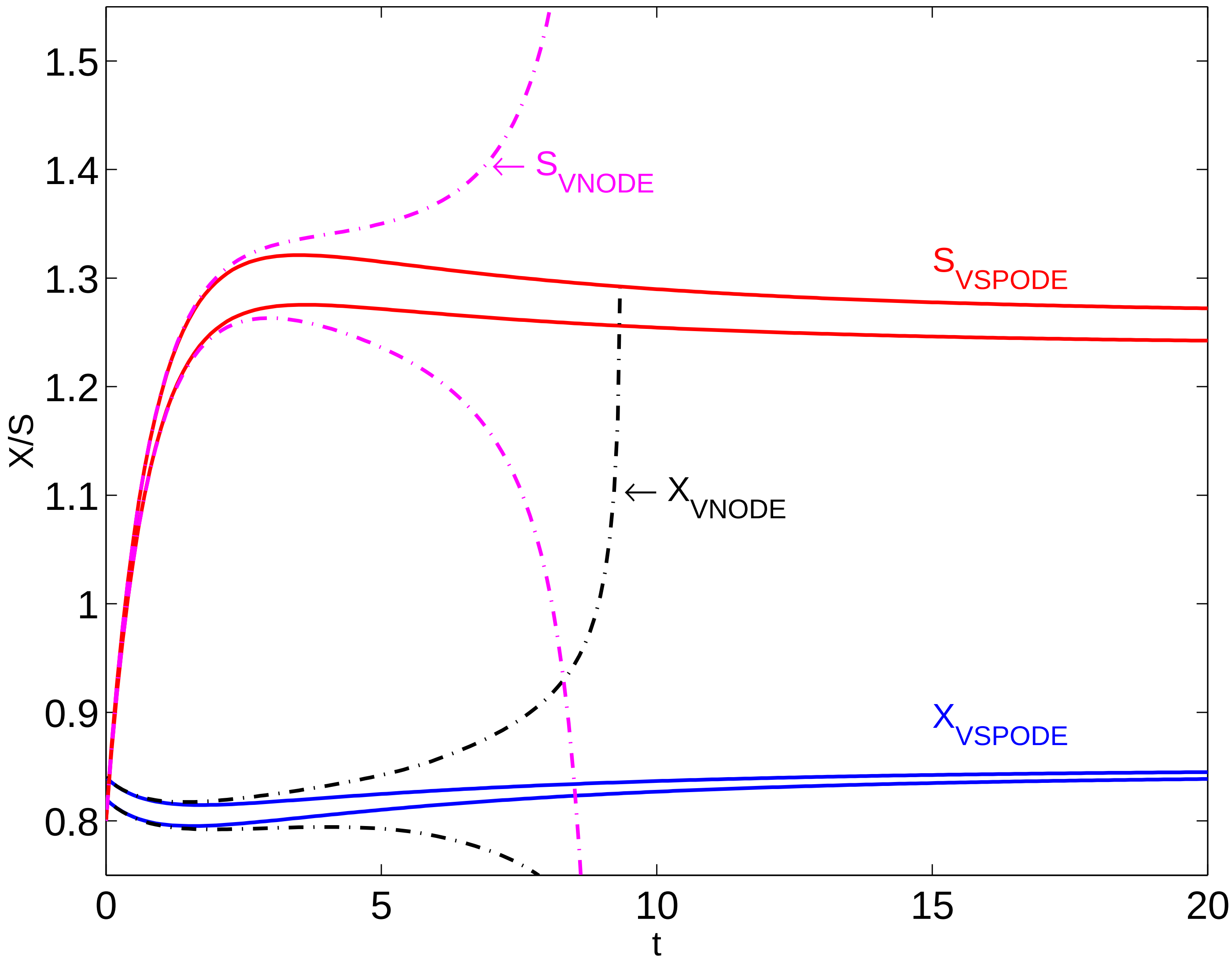
D	0.36	day^{-1}	K_I	[0.49, 0.51]	(g S/l)$^{-1}$
S^i	5.7	g S/l	X_0	[0.82, 0.84]	g X/l
S_0	0.80	g S/l			

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

Example 4. Bioreactor Problem – Monod Law

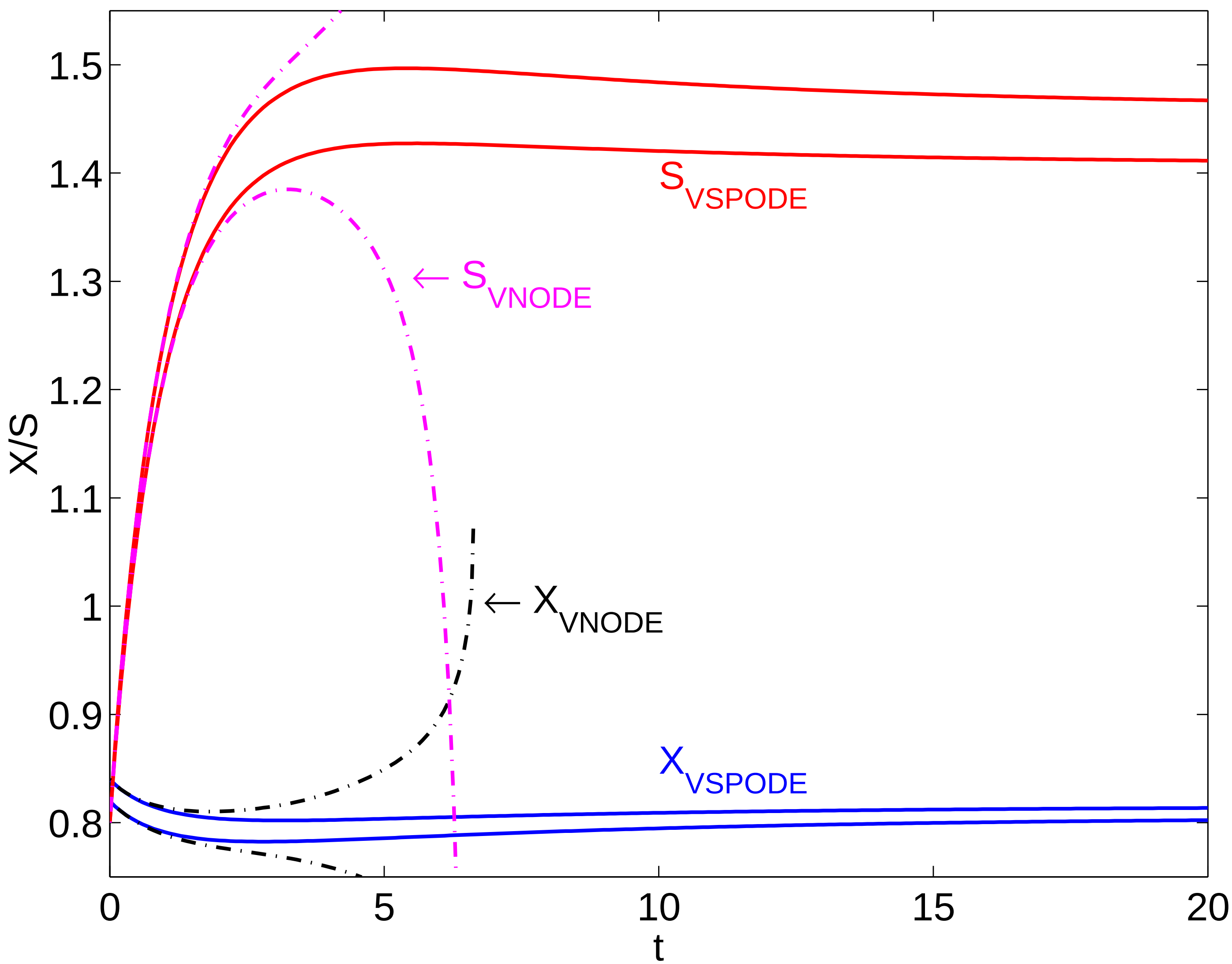


(VSPODE does not break down at longer t)

Example 4. Bioreactor Problem – Monod Law

Method	Final Enclosure ($t = 20$)	Width	CPU time (s)
VSPODE	[0.8386, 0.8450]	0.0064	1.34
	[1.2423, 1.2721]	0.0298	
VNODE–343	[0.8359, 0.8561]	0.0202	68.6
	[1.2309, 1.2814]	0.0505	
VNODE–512	[0.8375, 0.8528]	0.0153	102.8
	[1.2331, 1.2767]	0.0436	
VNODE–1000	[0.8380, 0.8502]	0.0122	263.1
	[1.2359, 1.2732]	0.0373	

Example 4. Bioreactor Problem – Haldane Law



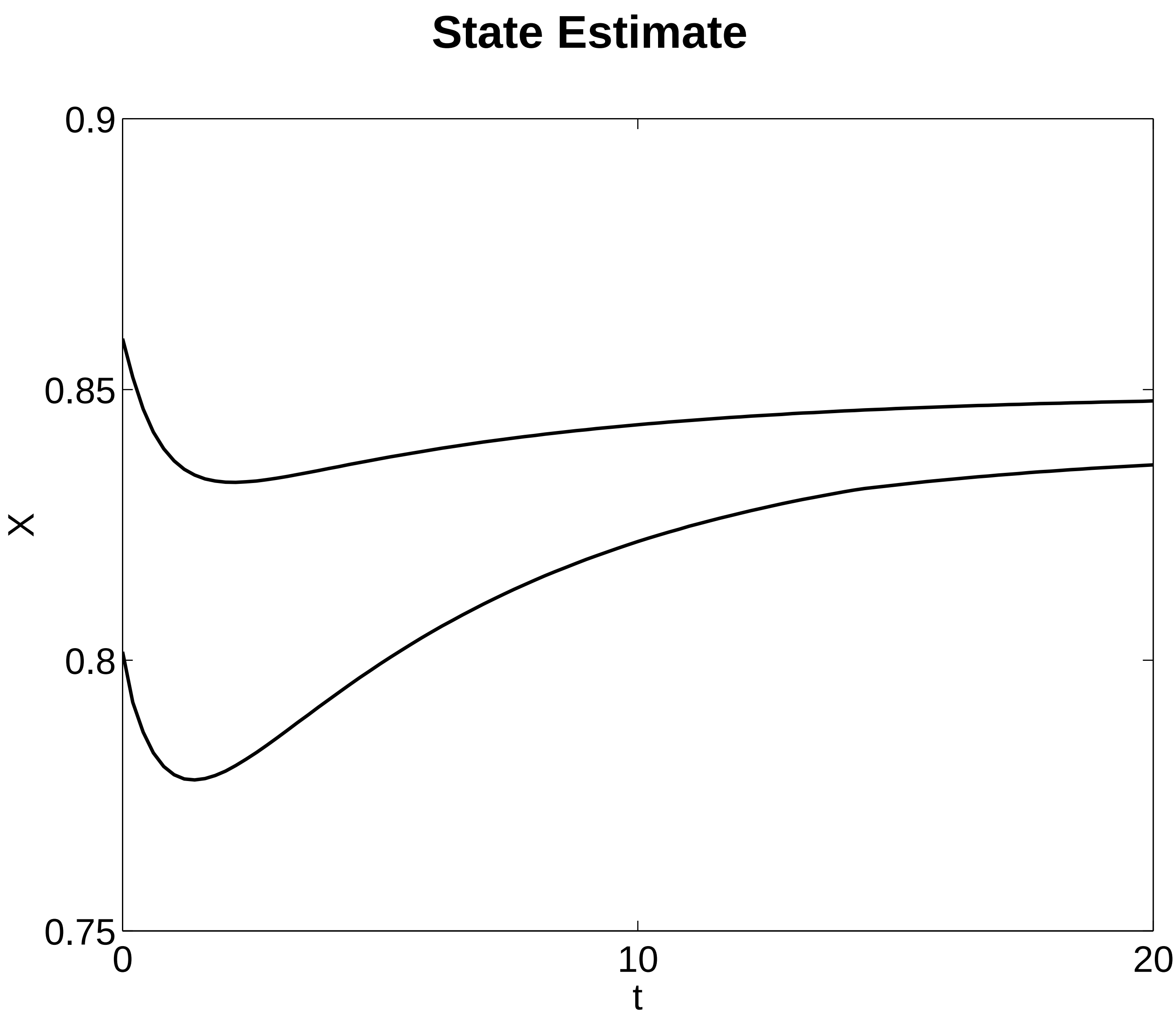
(VSPODE does not break down at longer t)

Related Problem – State and Parameter Estimation

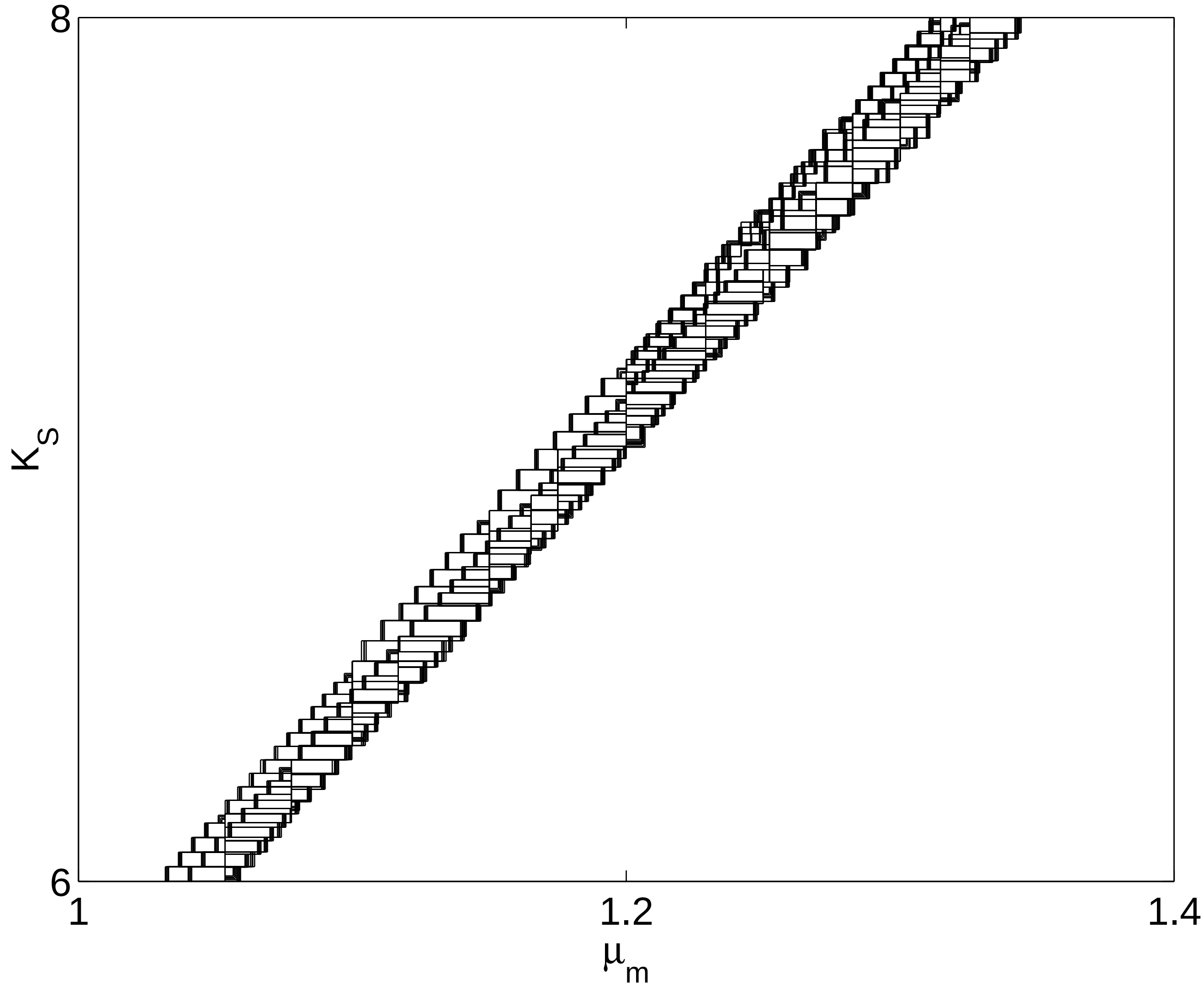
- Consider again the bioreactor problem.
- Bounded-error (1%) measurements of S at $t_j, j = 1, \ldots, N$ are available.
- Estimate the other state variable X and the parameters μ_m, K_S and K_I.
- New problem data

	Value	Units		Value	Units
α	0.5	-	μ_m	[1.0, 1.4]	day^{-1}
k	10.53	g S/ g X	K_S	[6, 8]	g S/l
D	0.36	day^{-1}	K_I	[0.0025, 0.01]	(g S/l)$^{-1}$
S^i	5.7	g S/l	X_0	[0.4, 1.2]	g X/l
S_0	0.8 $\times$ [0.99, 1.01]	g S/l			

- Use VSPODE with constraint propagation procedure on Taylor models (Lin and Stadtherr, 2006).


State Estimate
0.9
0.85
0.8
0.75
X
0
10
20
t

Parameter Estimate



Concluding Remarks

- The validated solution of parametric ODEs is a subproblem in many applications of interest.
- An approach was demonstrated for the direct handling of uncertainty in model parameters in the validated solution of ODEs.
- A standard two-phase approach was used
  - The dependence on t was handled using an interval Taylor series approach, as in standard methods (e.g. VNODE).
  - The dependence on parameters (and initial states) was handled using Taylor models in Phase 2 of the approach.
- Significant performance improvements were observed in comparison with VNODE.

- Funding
  - Indiana 21st Century Research & Technology Fund
  - U. S. Department of Energy