Validated Simulation of Differential Algebraic Equations

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Recall of Ordinary differential equations

Given by

$$y' = f(y, t)$$

Initial Value Problems

$$y' = f(y, t), \quad y(0) = y_0$$

Numerical simulation of IVPs till a time t_n

Compute $y_j \approx y(t_j)$ with $t_j \in \{0, t_1, \ldots, t_n\}$

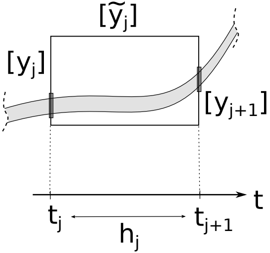
Validated simulation of IVPs

Produces a list of boxes $[y_j]$ and $[\tilde{y}_j]$ such that

- $y(t_j) \in [y_j]$ with $t_j \in \{0, t_1, \ldots, t_n\}$
- $y(t) \in [\tilde{y}_j]$ for all $t \in [t_j, t_{j+1}]$

Method of Lohner

1. Find $[\tilde{y}_j]$ with Picard-Lindelof operator
2. Compute $[y_{j+1}]$ with a validated integration scheme : Taylor (Vnode-LP) or Runge-Kutta (DynIbex)



Differential Algebraic Equations

General form: implicit

$F(t, y, y', \ldots) = 0,\ t_0 \leq t \leq t_{end}$
$y' =$ DAE 1^{st} order, $y'' =$ DAE 2^{nd}, etc.
(all DAEs can be rewritten in DAE of 1^{st} order)

Hessenberg form: Semi-explicit (index: distance to ODE)

$$\boxed{\text{index 1 : } \begin{cases} y' = f(t, x, y) \\ 0 = g(t, x, y) \end{cases}} \qquad \boxed{\text{index 2 : } \begin{cases} y' = f(t, x, y) \\ 0 = g(t, x) \end{cases}}$$

y : state variables, x : algebraic variables

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y : state variables, x : algebraic variables

$\Rightarrow$ Focus on Hessenberg index-1: Simulink, Modelica-like, etc.

Hessenberg index-1

$$\boxed{\text{index 1 : } \begin{cases} y' = f(t,x,y) \\ 0 = g(t,x,y) \end{cases}}$$

Some of dependent variables occur without their derivatives !

Different from ODE + constraint

$$\begin{cases} y' = f(t,y) \\ 0 = g(y,y') \end{cases}, \; t_0 \leq t \leq t_{end}$$

$\Rightarrow$ Direct with contractor approach

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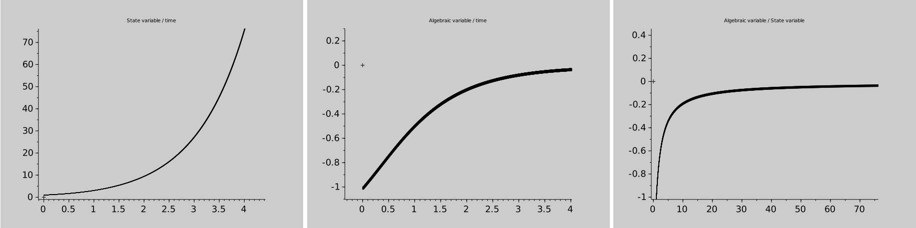
A basic example

System in Hessenberg index-1 form

$$\begin{cases} y' = y + x + 1 \\ (y+1) * x + 2 = 0 \end{cases} \qquad y(0) = 1.0 \text{ and } x(0) = 0.0$$

Simulation $\Rightarrow$ stiffness (in general)



Validated simulation of a DAE

As for ODE: a list of boxes $[y_i]$ and $[\tilde{y}_i]$ such that

- $y(t_i) \in [y_i]$ with $t_i \in \{0, t_1, \ldots, t_n\}$
- $y(t) \in [\tilde{y}_i]$ for all $t \in [t_i, t_{i+1}]$

But in addition: a list of boxes $[x_i]$ and $[\tilde{x}_i]$ such that

- $x(t_i) \in [x_i]$ with $t_i \in \{0, t_1, \ldots, t_n\}$
- $x(t) \in [\tilde{x}_i]$ for all $t \in [t_i, t_{i+1}]$

Both validate

- $y'(t_i) \in f(t_i, [x_i], [y_i])$
- $\exists x \in [x_i], \exists y \in [y_i] : g(t_i, x, y) = 0$
- $y'(t) \in f(t, [\tilde{x}_i], [\tilde{y}_i]), \forall t \in [t_i, t_{i+1}]$
- $\forall t \in [t_i, t_{i+1}], \exists x \in [\tilde{x}_i], \exists y \in [\tilde{y}_i] : g(t, x, y) = 0$

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Based on Lohner two-step approach

Step 1- A priori enclosure of state and algebraic variables

How find the enclosure $[\tilde{x}]$ on integration step ?

Assume that $\frac{\partial g}{\partial x}$ is locally reversal

we are able to find the unique $x = \psi(y)$ (implicit function theorem), and then:

$$y' = f(\psi(y), y)$$

and finally we could apply Picard-Lindelof to prove **existence and uniqueness**, but...

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$\boxed{\psi \text{ is unknown !}}$

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Step 1- A priori enclosure of state and algebraic variables

Solution

If we are able to find $[\tilde{x}]$ such that
for each $y \in [\tilde{y}], \exists! x \in [\tilde{x}] : g(x, y) = 0$, then $\exists! \psi$ on the neighborhood of $[\tilde{x}]$, and the solution of DAE $\exists!$ in $[\tilde{y}]$ (Picard with $[\tilde{x}]$ as a parameter)

A novel operator Picard-Krawczyk $\mathcal{PK}$:

If $\begin{pmatrix} \mathcal{P}([\tilde{y}], [\tilde{x}]) \\ \mathcal{K}([\tilde{y}], [\tilde{x}]) \end{pmatrix} \subset Int \begin{pmatrix} [\tilde{y}] \\ [\tilde{x}] \end{pmatrix}$ then $\exists!$ solution of DAE

- $\mathcal{P}$ a Picard-Lindelof for $y' \in f([\tilde{x}], y)$
- $\mathcal{K}$ a parametrized preconditioned Krawczyk operator for $g(x, y) = 0, \forall y \in [\tilde{y}]$

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Step 2- Contraction of state and algebraic variables (at $t + h$)

Two contractors in a fixpoint:

- Contraction of $[y_{i+1}]$ (init $[\tilde{y}_i]$)
  - $[\tilde{x}_i]$ as a parameter of function $f(t, x, y)$
    $\Rightarrow$ ODE (stiff + interval parameter)
    $\Rightarrow$ Radau IIA order 3 (fully Implicit Runge-Kutta, A-stable, efficiency for stiff and interval parameters)
- Contraction of $[x_{i+1}]$ (init $[\tilde{x}_i]$)
  - $[y_{i+1}]$ as a parameter of function $g(x, y)$
    $\Rightarrow$ Constraint solving
    $\Rightarrow$ Krawczyk + forward/backward
    (+ any other constraints, from physical context or Pantelides algorithm)

Based on Lohner two-step approach

How to control the stepsize of integration scheme ?

Classical method: Constrained by the Picard success and an evaluation of the truncature error lower than threshold

No specific control w.r.t. the algebraic variable

If x leads to a large evaluation of truncature error: too late !

Solution: force diameter of x grows slower than y

Empirical approach: to improve !

Based on Lohner two-step approach

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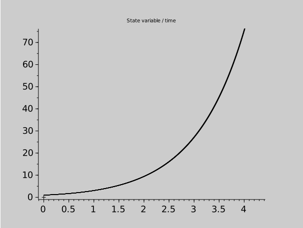
A basic example

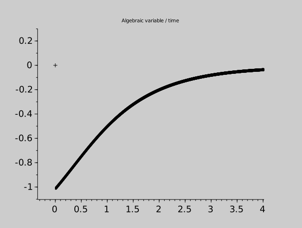
System in Hessenberg index-1 form

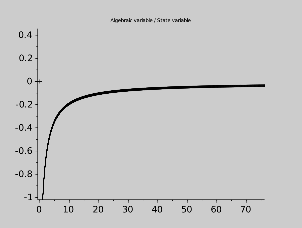
$$\begin{cases} y' = y + x + 1 \\ (y+1) * x + 2 = 0 \end{cases} \qquad y(0) = 1.0 \text{ and } x(0) \in [-2.0, 2.0]$$

(consistency: $x(0) = -1$)

Simulation till t=4s (30 seconds of computation)







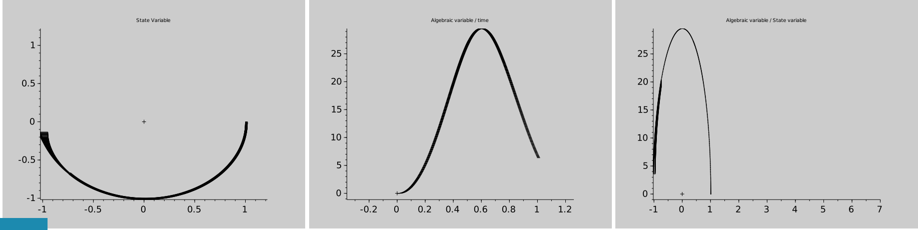
The classical example: Pendulum

$$\begin{cases} p' = u \\ q' = v \\ mu' = -p\lambda \\ mv' = -q\lambda - g \end{cases}$$

$$m(u^2 + v^2) - gq - l^2\lambda = 0$$

$(p, q, u, v)_0 = (1, 0, 0, 0)$ et $\lambda_0 \in [-0.1, 0.1]$ (consistency: $\lambda = 0$)

Simulation till t=1s (2 minutes of computation)



Discussion

Promising first results

- Novel operator Picard-Krawczyk
- Combination of algebraic contractor and integration scheme
- All additive constraints can be considered (from index reduction for example)
- Initial consistency solved by Krawczyk (main issue in DAE community)

But we need

- Higher order Runge-Kutta methods (Radau IIA order 5, Gauss order 6, and more)
- Improvement of global algorithm (stepsize control, contraction (hybrid Krawczyk), first estimation for $[\tilde{x}]$...)

Questions ?

if not several appendices are available...

Radau methods

$$y_{n+1} = y_n + h\sum_{i=1}^{s} b_i k_i, \quad k_i = f\left(t_0 + c_i h, y_0 + h\sum_{j=1}^{s} a_{ij} k_j\right)$$

Butcher tableau Radau IIA order 3

$$\begin{array}{c|cc} 1/3 & 5/12 & \text{-}1/12 \\ 1 & 3/4 & 1/4 \\ \hline & 3/4 & 1/4 \end{array}$$

Butcher tableau Radau IIA order 5

$$\begin{array}{c|ccc} \frac{2}{5} - \frac{\sqrt{6}}{10} & \frac{11}{45} - \frac{7\sqrt{6}}{360} & \frac{37}{225} - \frac{169\sqrt{6}}{1800} & -\frac{2}{225} + \frac{\sqrt{6}}{75} \\ \frac{2}{5} + \frac{\sqrt{6}}{10} & \frac{37}{225} + \frac{169\sqrt{6}}{1800} & \frac{11}{45} + \frac{7\sqrt{6}}{360} & -\frac{2}{225} - \frac{\sqrt{6}}{75} \\ 1 & \frac{4}{9} - \frac{\sqrt{6}}{36} & \frac{4}{9} + \frac{\sqrt{6}}{36} & \frac{1}{9} \\ \hline & \frac{4}{9} - \frac{\sqrt{6}}{36} & \frac{4}{9} + \frac{\sqrt{6}}{36} & \frac{1}{9} \end{array}$$

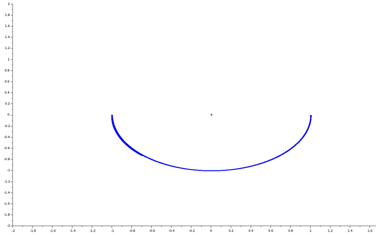
Parametric Krawczyk

Parametric preconditioned Krawczyk operator

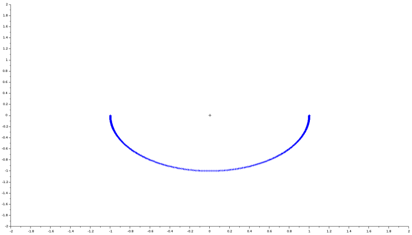
$$\mathcal{K}([\tilde{y}],[\tilde{x}]) = m([\tilde{x}]) - Cg(m([\tilde{x}]), m([\tilde{y}])) - \\ (C\frac{\partial g}{\partial x}([\tilde{x}],[\tilde{y}]) - I)([\tilde{x}] - m([\tilde{x}])) - \\ C\frac{\partial g}{\partial y}(m([\tilde{x}]),[\tilde{y}])([\tilde{y}] - m([\tilde{y}])) \quad (1)$$

Pendulum with Dymola

Our method:



Dymola:

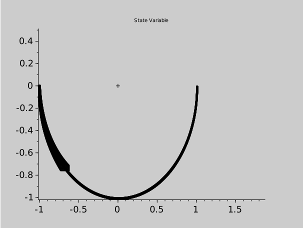


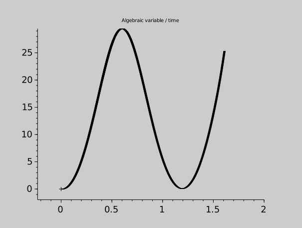
Pantelides on pendulum

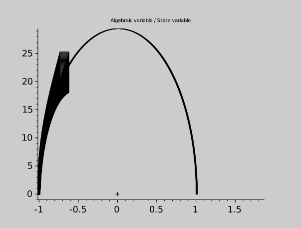
$$\begin{cases} p^2 + q^2 - l^2 = 0 \\ p * u + q * v = 0 \\ m * (u^2 + v^2) - g * q^2 - l^2 * p = 0 \end{cases}$$

Pendulum to 1.6s, $tol = 10^{-18}$

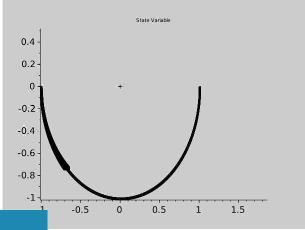
28 minutes...

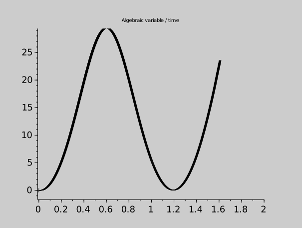


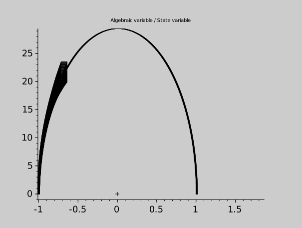




With csp: 27 minutes...







Frobenius theorem

Let X and Y be Banach spaces, and $A \subset X$, $B \subset Y$ a pair of open sets. Let
$F : A \times B \to L(X, Y)$
be a continuously differentiable function of the Cartesian product (which inherits a differentiable structure from its inclusion into $X \times Y$) into the space L(X,Y) of continuous linear transformations of X into Y. A differentiable mapping $u : A \to B$ is a solution of the differential equation
$y' = F(x, y)$ (1)
if $u'(x) = F(x, u(x))$ for all $x \in A$. The equation (1) is completely integrable if for each $(x_0, y_0) \in A \times B$, there is a neighborhood U of x0 such that (1) has a unique solution u(x) defined on U such that u(x0)=y0. The conditions of the Frobenius theorem depend on whether the underlying field is R or C. If it is R, then assume F is continuously differentiable. If it is C, then assume F is twice continuously differentiable. Then (1) is completely integrable at each point of $A \times B$ if and only if
$D_1F(x, y) \cdot (s_1, s_2) + D_2F(x, y) \cdot (F(x, y) \cdot s_1, s_2) = D_1F(x, y) \cdot (s_2, s_1) + D_2F(x, y) \cdot (F(x, y) \cdot s_2, s_1)$ for all $s1, s2 \in X$. Here D1 (resp. D2) denotes the partial derivative with respect to the first (resp. second) variable; the dot product denotes the action of the linear operator $F(x, y) \in L(X, Y)$, as well as the actions of the operators $D1F(x, y) \in L(X, L(X, Y))$ and $D2F(x, y) \in L(Y, L(X, Y))$.

Dieudonné, J (1969). Foundations of modern analysis. Academic Press. Chapter 10.9.