Numerical integration of DAE's

seminar

Sandra Allaart-Bruin

sbruin@win.tue.nl

Seminar overview

- February 18 Arie Verhoeven
  “Introduction to DAE’s”

Seminar overview

- February 18 Arie Verhoeven
  “Introduction to DAE’s”
- March 10 Sandra Allaart-Bruin
  “Numerical Integration of DAE’s”

Seminar overview

- February 18 Arie Verhoeven
  “Introduction to DAE’s”
- March 10 Sandra Allaart-Bruin
  “Numerical Integration of DAE’s”
- March 17 Pieter Heres
  “DAE’s in electrical circuits”

Seminar overview

- February 18 Arie Verhoeven
  "Introduction to DAE's"
- March 10 Sandra Allaart-Bruin
  "Numerical Integration of DAE's"
- March 17 Pieter Heres
  "DAE's in electrical circuits"
- March 31 Mikhail Sizov
  "DAE's in Multibody systems"

Seminar overview

- February 18 Arie Verhoeven
  "Introduction to DAE's"
- March 10 Sandra Allaart-Bruin
  "Numerical Integration of DAE's"
- March 17 Pieter Heres
  "DAE's in electrical circuits"
- March 31 Mikhail Sizov
  "DAE's in Multibody systems"
- April 28 Michael Guenther
  "Expert"

Overview

- Test DAE

Overview

- Test DAE
- Trapezoidal rule

Overview

- Test DAE
- Trapezoidal rule
- Backward Differentiation Formulae

Overview

- Test DAE
- Trapezoidal rule
- Backward Differentiation Formulae
- Modified Extended BDF

Overview

- Test DAE
- Trapezoidal rule
- Backward Differentiation Formulae
- Modified Extended BDF
- Codes

Simple test-case

DAE:

$$
\begin{aligned}
x(t) &= \sin(t) \\
x'(t) + y(t) &= 0
\end{aligned}
$$

Simple test-case

DAE:

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

exact solution

$$\begin{aligned} x(t) &= \sin(t) \\ y(t) &= -\cos(t) \end{aligned}$$

Simple test-case

DAE:

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

exact solution

$$\begin{aligned} x(t) &= \sin(t) \\ y(t) &= -\cos(t) \end{aligned}$$

linear constant coefficients: $\mathbf{A}\mathbf{x}'(t) + \mathbf{B}\mathbf{x}(t) = \mathbf{g}(t)$

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} x'(t) \\ y'(t) \end{pmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} \sin(t) \\ 0 \end{pmatrix}$$

Simple test-case

DAE:

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

exact solution

$$\begin{aligned} x(t) &= \sin(t) \\ y(t) &= -\cos(t) \end{aligned}$$

linear constant coefficients: $\mathbf{A}\mathbf{x}'(t) + \mathbf{B}\mathbf{x}(t) = \mathbf{g}(t)$

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{pmatrix} x'(t) \\ y'(t) \end{pmatrix} + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} \sin(t) \\ 0 \end{pmatrix}$$

What is the index?

Differential index

The differential index k of a (non)linear, sufficiently smooth DAE is the smallest k such that

$$\begin{aligned} \mathbf{f}(\mathbf{x}', \mathbf{x}, t) &= \mathbf{0} \\ \frac{d}{dt}\mathbf{f}(\mathbf{x}', \mathbf{x}, t) &= \mathbf{0} \\ &\vdots \\ \frac{d^k}{dt^k}\mathbf{f}(\mathbf{x}', \mathbf{x}, t) &= \mathbf{0} \end{aligned}$$

uniquely determines $\mathbf{x}'$ as a continuous function of $(\mathbf{x}, t)$.

Index

- Differential index $\delta = 2$

Index

- Differential index $\delta = 2$
- Tractability index $\tau = 2$

Index

- Differential index $\delta = 2$
- Tractability index $\tau = 2$
- Perturbation index $\pi = 2$

Index

- Differential index $\delta = 2$
- Tractability index $\tau = 2$
- Perturbation index $\pi = 2$

There always holds that:

$$\delta \leq \tau \leq \delta + 1$$

Consistent Initial Values

$$\mathbf{f}(\mathbf{x}', \mathbf{x}, t) \;=\; \mathbf{0}$$

$\mathbf{x}_0$ is a consistent initial value, if there exists a smooth solution that fullfills $\mathbf{x}(t_0) = \mathbf{x}_0$ and this solution is defined for all t.

Consistent Initial Values

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

$\mathbf{x}_0$ is a consistent initial value, if there exists a smooth solution that fullfills $\mathbf{x}(t_0) = \mathbf{x}_0$ and this solution is defined for all t.

Consistent Initial Values

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

$\mathbf{x}_0$ is a consistent initial value, if there exists a smooth solution that fullfills $\mathbf{x}(t_0) = \mathbf{x}_0$ and this solution is defined for all t.

Algebraic constraint: $x(t) = \sin(t)$

Consistent Initial Values

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

$\mathbf{x}_0$ is a consistent initial value, if there exists a smooth solution that fullfills $\mathbf{x}(t_0) = \mathbf{x}_0$ and this solution is defined for all t.

Algebraic constraint: $x(t) = \sin(t)$

Hidden algebraic constraint: $y(t) = -\cos(t)$

Consistent Initial Values

$$
\begin{aligned}
x(t) &= \sin(t) \\
x'(t) + y(t) &= 0
\end{aligned}
$$

$\mathbf{x}_0$ is a consistent initial value, if there exists a smooth solution that fullfills $\mathbf{x}(t_0) = \mathbf{x}_0$ and this solution is defined for all t.

Algebraic constraint: $x(t) = \sin(t)$

Hidden algebraic constraint: $y(t) = -\cos(t)$

Consistent initial values:

$$
\begin{aligned}
x_0 &= \sin(0) \\
y_0 &= -\cos(0)
\end{aligned}
$$

Trapezoidal rule

Consider the following ODE:

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

The trapezoidal rule applied:

$$\frac{x_{n+1} - x_n}{h} = \frac{1}{2}\left(f(x_{n+1}, t_{n+1}) + f(x_n, t_n)\right)$$

Trapezoidal rule

test DAE

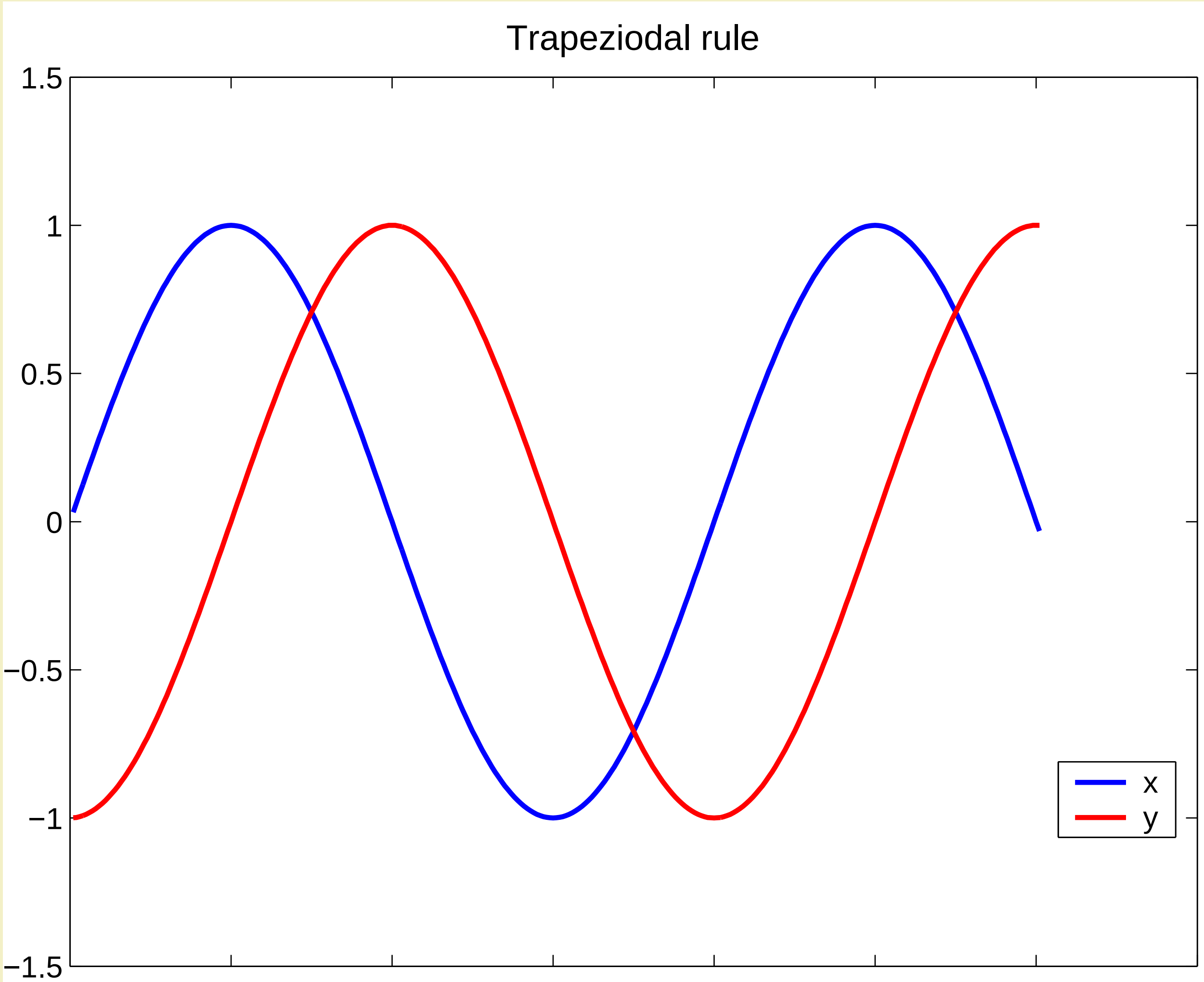
$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

The Trapezoidal rule applied:

$$\begin{aligned} x_{n+1} + x_n &= \sin(t_{n+1}) + \sin(t_n) \\ \frac{x_{n+1} - x_n}{h} + \frac{1}{2}(y_{n+1} + y_n) &= 0 \end{aligned}$$

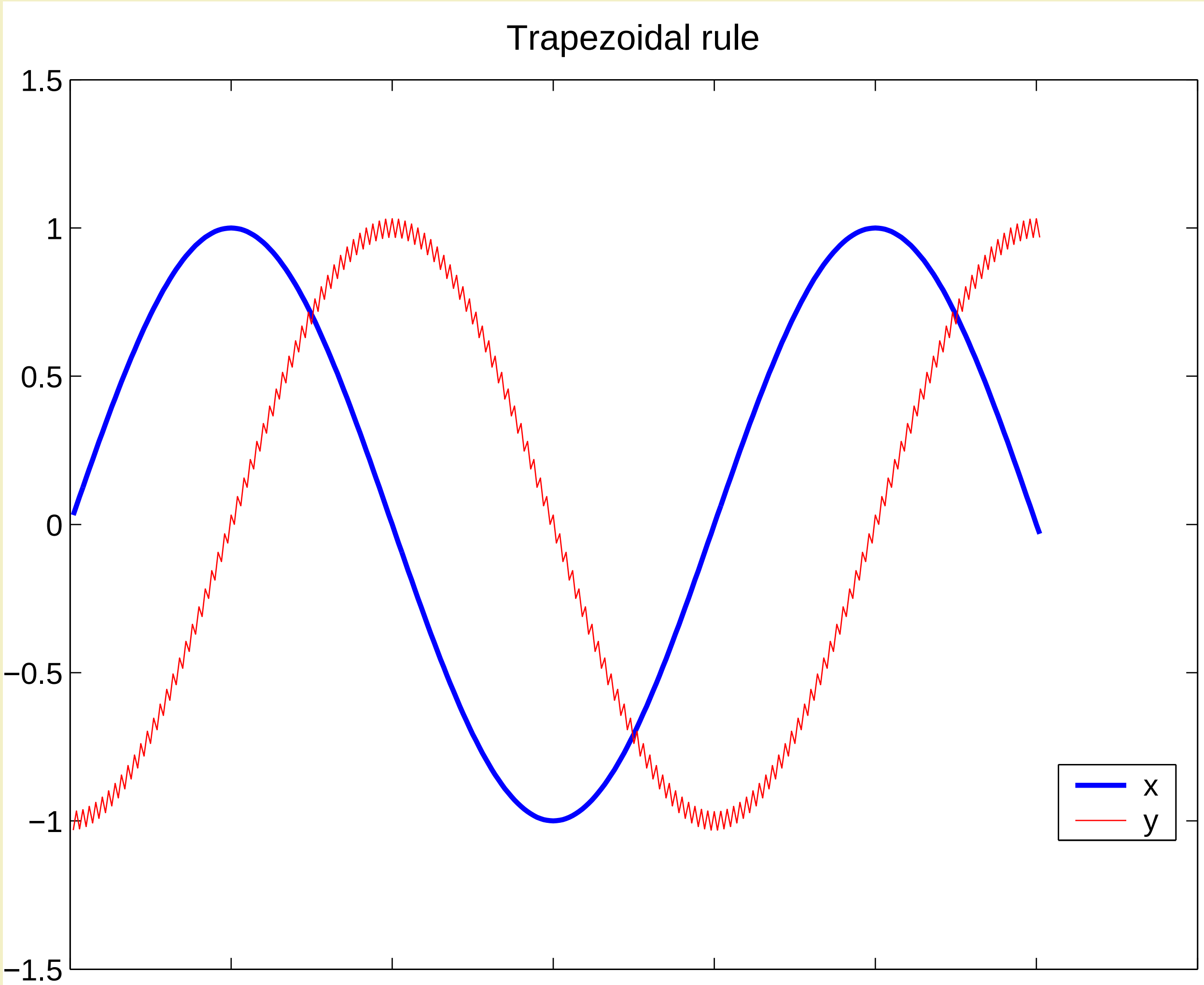
Trapezoidal rule

$$x_0 = \sin(0)$$
$$y_0 = -\cos(0)$$



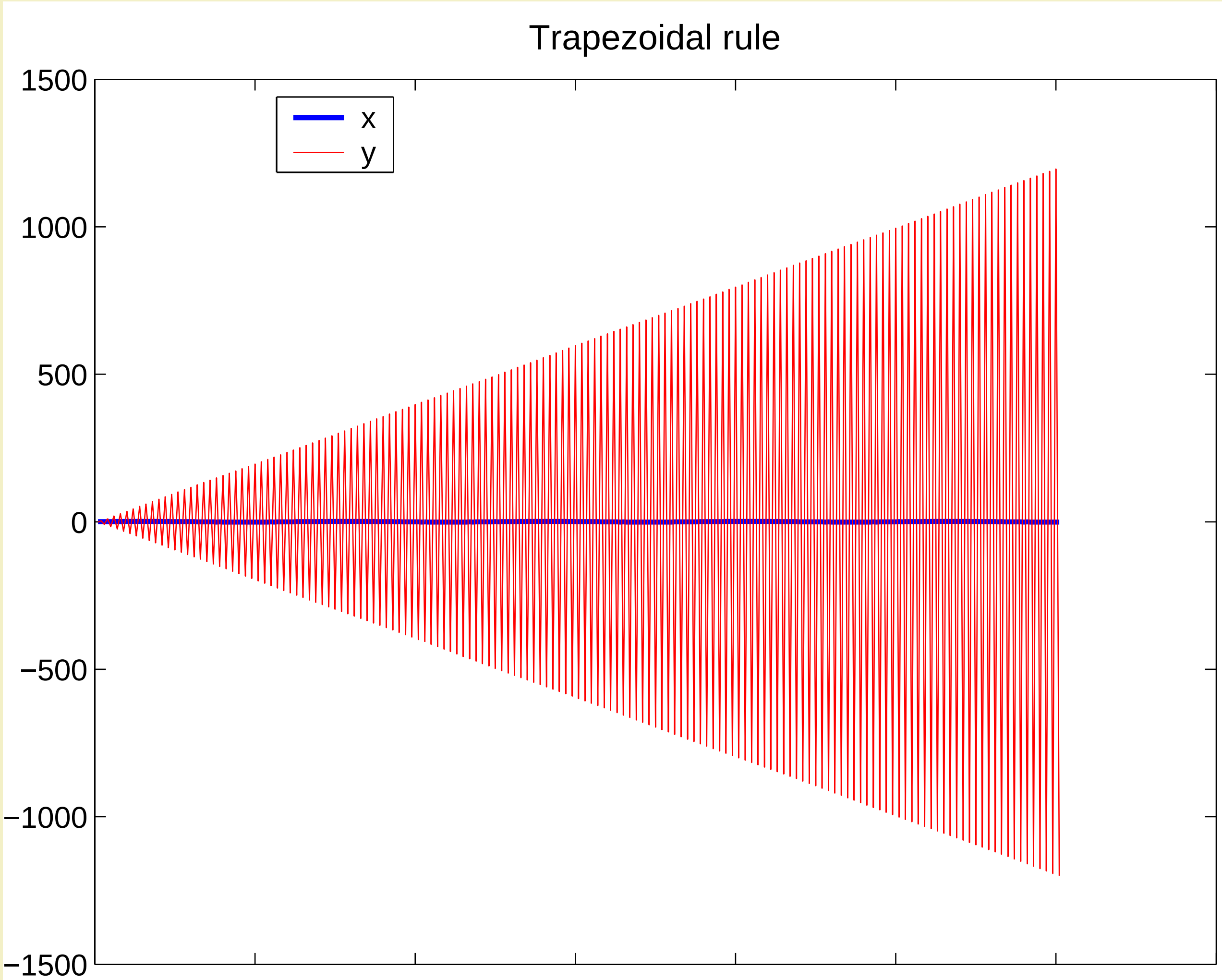
Trapezoidal rule

$$x_0 = \sin(0)$$
$$y_0 = -\cos(0) - h$$



Trapezoidal rule

$$x_0 = h$$
$$y_0 = -\cos(0)$$



Analysis Trapezoidal rule

$$\begin{aligned} x_{n+1} &= \sin(t_{n+1}) + x_n - \sin(t_n) \\ y_{n+1} &= -y_n - \frac{2}{h}(x_{n+1} - x_n) \end{aligned}$$

If $x_0 \neq \sin(0)$ then x_{n+1} is never equal to $\sin(t_{n+1})$.

Backward Diff. Formula

Consider the following ODE:

$$x'(t) \;=\; f(x(t), t)$$

The Backward Differentiation Formula applied:

$$\sum_{j=1}^{k} \alpha_j x_{n+j} \;=\; h\beta_k f(x_{n+k}, t_{n+k})$$

Remark: 1-step BDF is Euler Implicit ($\alpha_0 = -1$, $\alpha_1 = 1$, $\beta_1 = 1$)

Backward Diff. Formula

test DAE

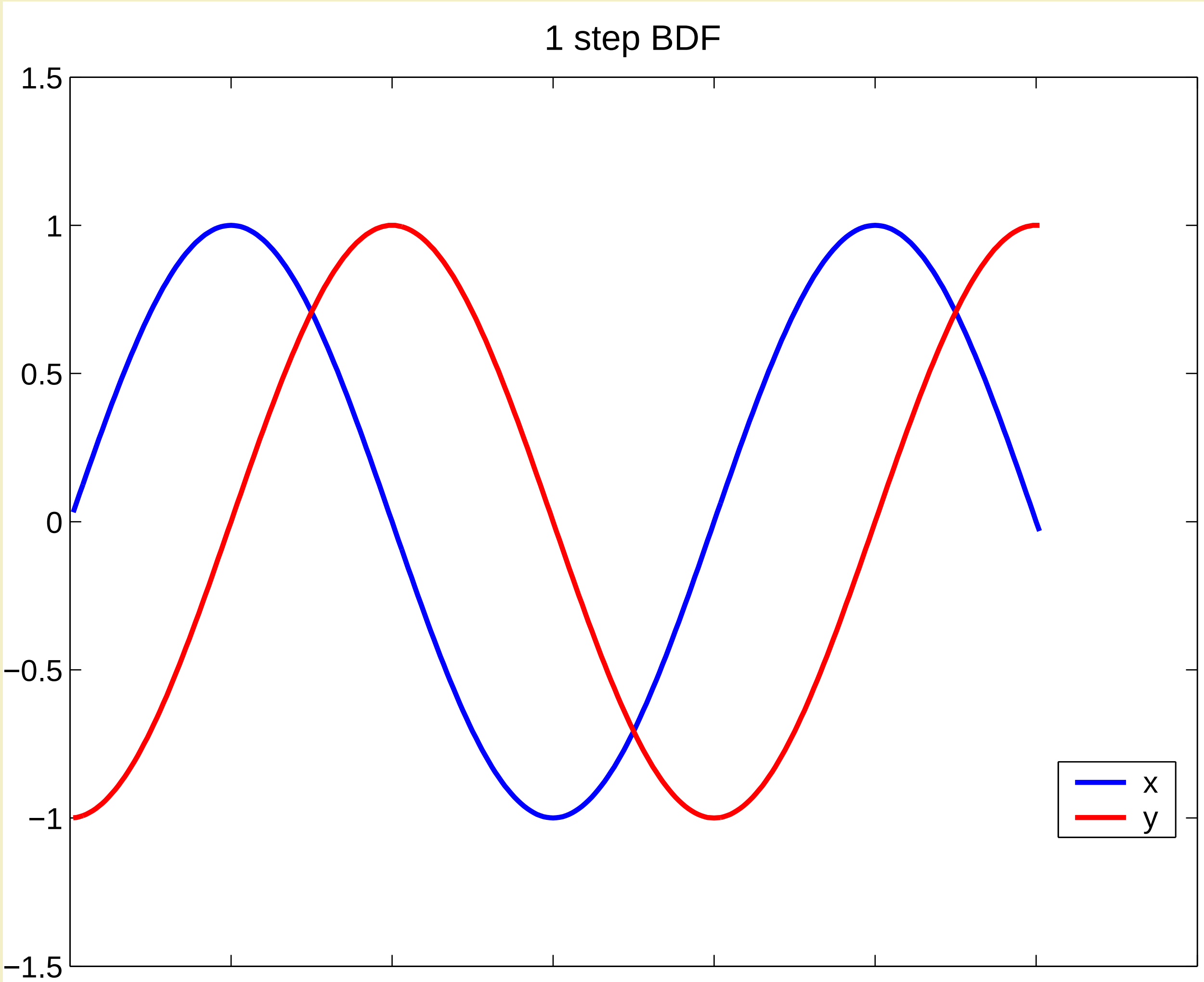
$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

1-step BDF

$$\begin{aligned} x_{n+1} &= \sin(t_{n+1}) \\ \frac{x_{n+1} - x_n}{h} + y_{n+1} &= 0 \end{aligned}$$

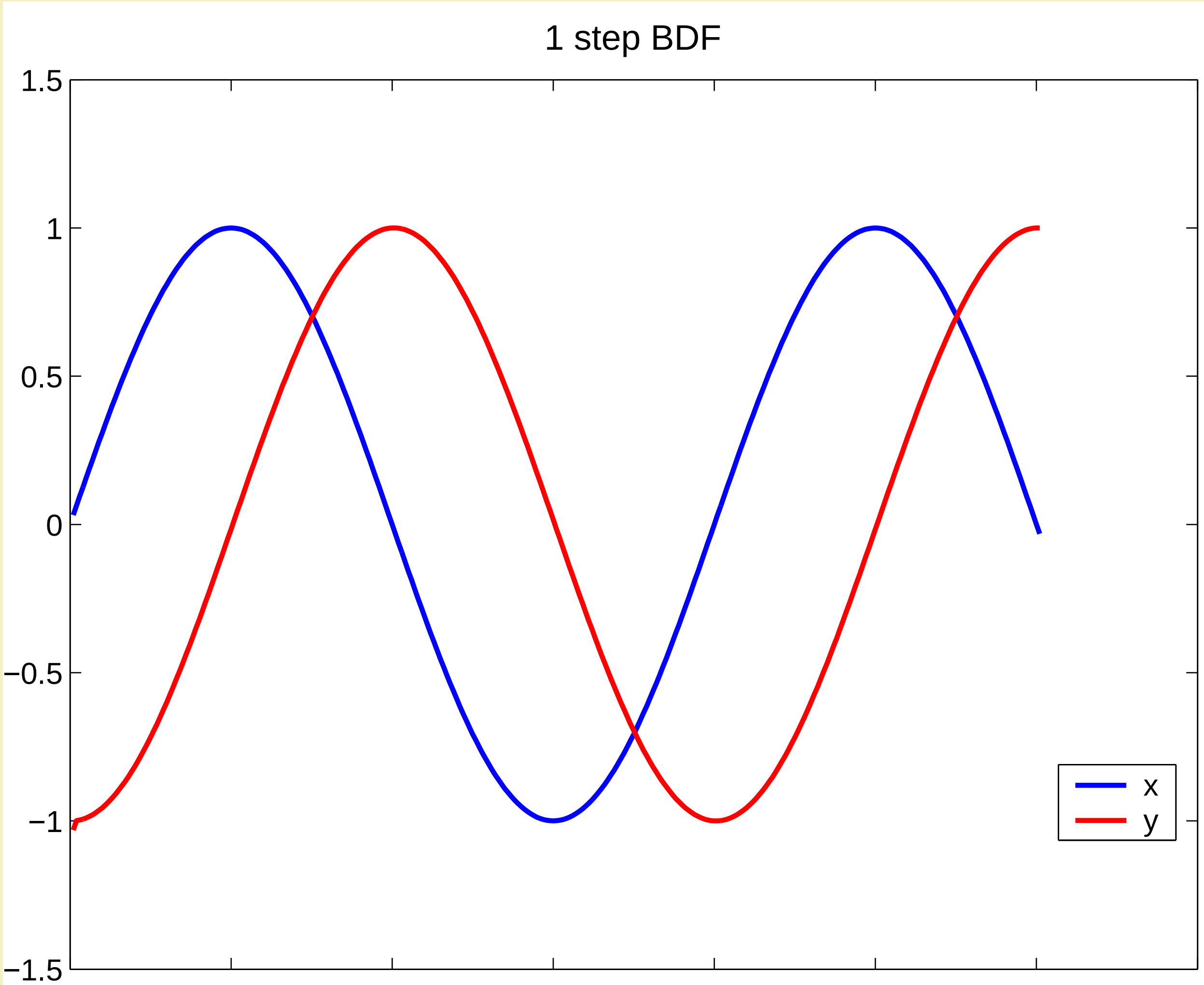
Backward Diff. Formula

$$x_0 = \sin(0)$$
$$y_0 = -\cos(0)$$



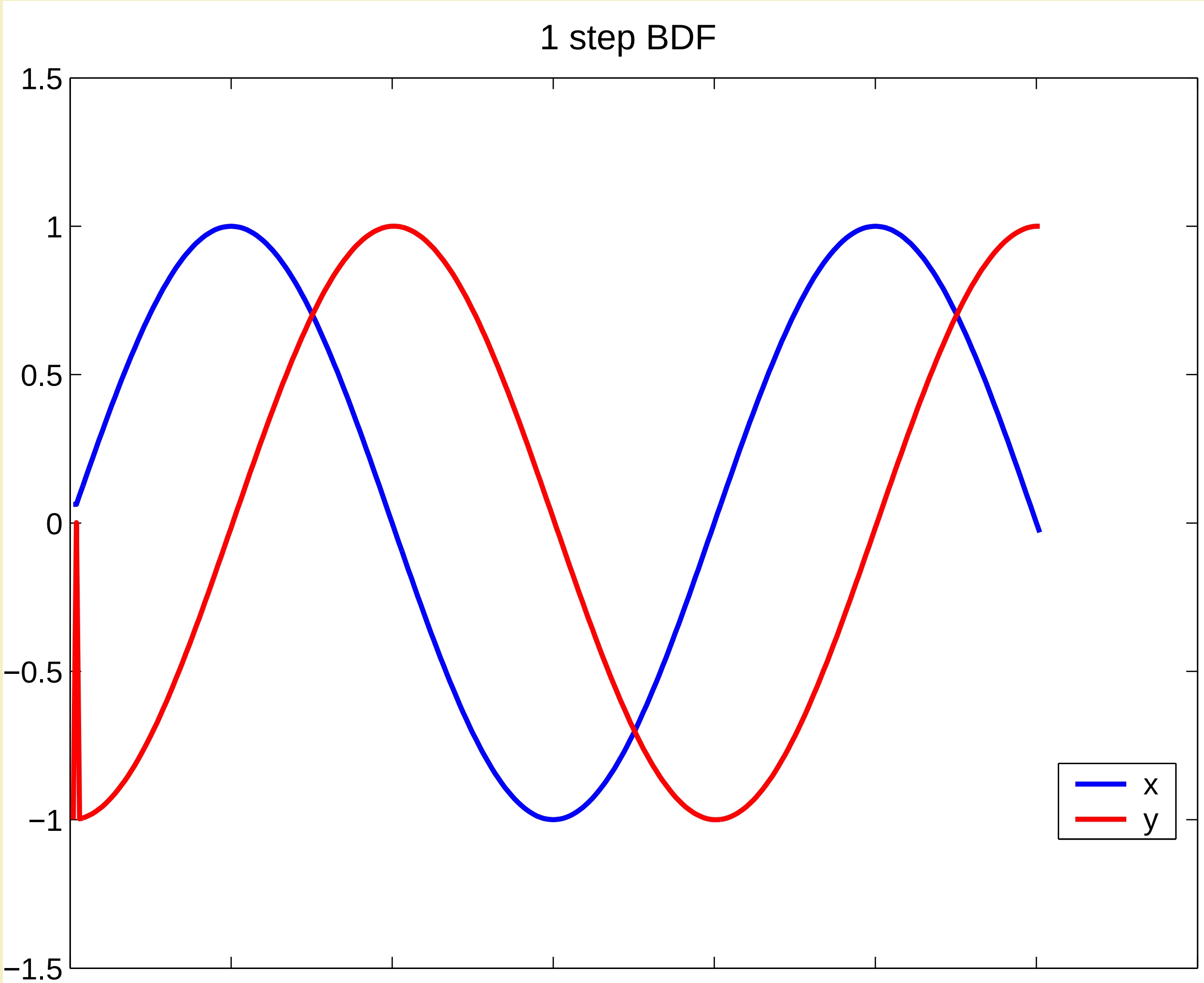
Backward Diff. Formula

$$x_0 = \sin(0)$$
$$y_0 = -\cos(0) - h$$



Backward Diff. Formula

$$x_0 = h$$
$$y_0 = -\cos(0)$$



analysis 1-step BDF

$$
\begin{aligned}
x_{n+1} &= \sin(t_{n+1}) \\
y_{n+1} &= -\frac{x_{n+1} - x_n}{h}
\end{aligned}
$$

analysis 1-step BDF

$$
\begin{aligned}
x_{n+1} &= \sin(t_{n+1}) \\
y_{n+1} &= -\frac{x_{n+1} - x_n}{h}
\end{aligned}
$$

BDF solves the algebraic equation exact!

BDF convergence

A k step BDF with constant stepsize, applied to a const. coeff. DAE with diff. index μ, is convergent with order $p = k$ after $(\mu - 1)k + 1$ steps.

BDF convergence

A k step BDF with constant stepsize, applied to a const. coeff. DAE with diff. index μ, is convergent with order $p = k$ after $(\mu - 1)k + 1$ steps.

What if we use variable stepsizes?

BDF

- BDF method perfect?

BDF

- BDF method perfect?
- A-stable up to order 2 (Dalhquist Barrier).

BDF

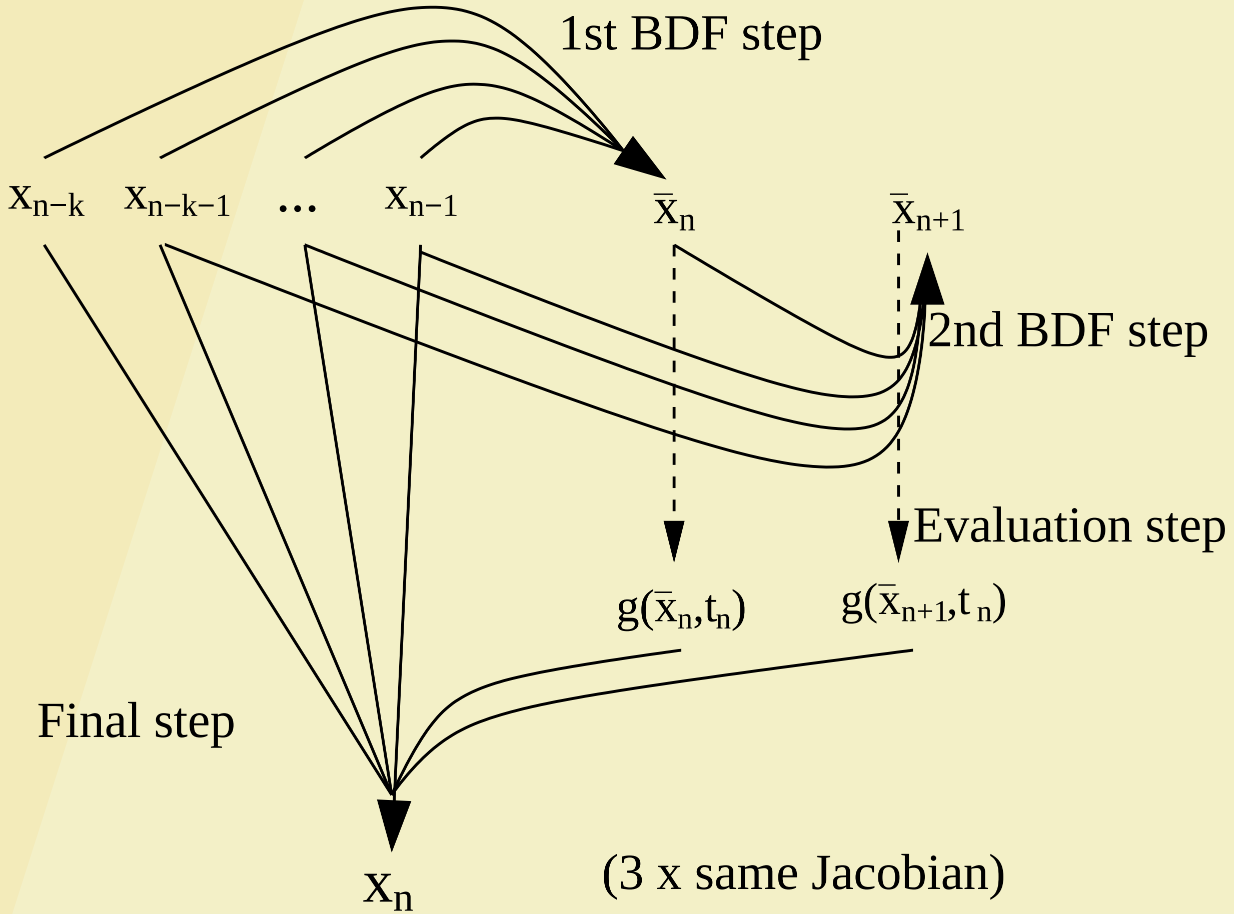
- BDF method perfect?
- A-stable up to order 2 (Dalhquist Barrier).
- A(α) stable up to order 6.

BDF

- BDF method perfect?
- A-stable up to order 2 (Dalhquist Barrier).
- A(α) stable up to order 6.
- other methods?

Modified Extended BDF

$$A\mathbf{x}'(t) + \mathbf{g}(\mathbf{x}(t), t) \;=\; 0$$



Order reduction

k-step method	Convergence order		consistent solutions
	index-1 DAE	index-2 DAE	
BDF	k	k	+
MEBDF	k+1	k	+

Available codes

code	method	authors	DAE_{index}	IDE
RADAU	IRK	Hairer, Wanner	≤ 3	-
GELDA	BDF,RK	Mehrmann		+
MEBDFI	MEBDF	Abdulla, Cash	≤ 3	+
DASSL	BDF	Petzold	≤ 1	+
PSIDE	IRK	De Swart a.o.	≤ 3	+
GAMD	BVM	Iavernaro, Mazzia	≤ 3	+

Available codes

http://www-iam.mathematik.hu-berlin.de/~lamour/

code for index reduction and computing consistent initial values.

Available codes

http://www-iam.mathematik.hu-berlin.de/~lamour/

code for index reduction and computing consistent initial values.

index 2:

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

Available codes

http://www-iam.mathematik.hu-berlin.de/~lamour/

code for index reduction and computing consistent initial values.

index 2:

$$\begin{aligned} x(t) &= \sin(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

index 1:

$$\begin{aligned} x(t)' &= \cos(t) \\ x'(t) + y(t) &= 0 \end{aligned}$$

Summary

- Trapezoidal rule is not suited for DAE's.

Summary

- Trapezoidal rule is not suited for DAE's.
- BDF with fixed stepsize is suited for DAE's.

Summary

- Trapezoidal rule is not suited for DAE's.
- BDF with fixed stepsize is suited for DAE's.
- Index of DAE is important for convergence results.

Summary

- Trapezoidal rule is not suited for DAE's.
- BDF with fixed stepsize is suited for DAE's.
- Index of DAE is important for convergence results.
- There are a lot of different codes available for DAE's with index ≤ 3.

References

- Ordinary Differential Equations in Theory and Practice, Mattheij and Molenaar
- Solving Ordinary Differential Equations II, Hairer and Wanner
- Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations, Brenan, Campbell and Petzold
- http://pitagora.dm.uniba.it/~testset

Questions?