



INVESTMENTS IN EDUCATION DEVELOPMENT

Streamlining the Mathematics Studies at the Faculty of Science of Palacky University in Olomouc

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Numerical Treatment of **Singular** BVPs in ODEs

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Contents

Basic concepts – work by H. Keller ✓

Motivation and introductory remarks ✓

Forward Euler method ✓

Stability ✓

Consistency and convergence ✓

Numerical examples

Collocation method

Existence and uniqueness of the collocation solution

Convergence

Numerical example

Applications

Examples: Convergence of the forward Euler

Example 1: Consider the **linear** problem

$$y''(t) = -\frac{2}{t}y'(t) - \underbrace{n^2 \cos(nt) - \frac{2}{t}n \sin(nt)}_{\text{has a limit for } t \rightarrow 0}, \quad t \in (0, 1],$$

$$y(0) = 2, \quad y'(0) = 0,$$

where $y(t) = 1 + \cos(nt)$, $n = 3$.

Examples: Convergence of the forward Euler

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Example 2: Consider the **nonlinear** problem

$$y''(t) = -\frac{2}{t}y'(t) - y^5(t), \quad t \in (0, 1],$$

$$y(0) = 1, \quad y'(0) = 0,$$

where $y(t) = \frac{1}{\sqrt{1+t^2/3}}$.

Example 1

h	$\ \varepsilon_h\ $	p	c
$1/5$	8.5	0.970	$-4.0 \cdot 10^{+01}$
$1/5 \cdot 2^{-1}$	4.3	0.982	$-4.1 \cdot 10^{+01}$
$1/5 \cdot 2^{-2}$	$2.1 \cdot 10^{-01}$	0.990	$-4.2 \cdot 10^{+01}$
$1/5 \cdot 2^{-3}$	$1.1 \cdot 10^{-01}$	0.995	$-4.3 \cdot 10^{+01}$
$1/5 \cdot 2^{-4}$	$5.5 \cdot 10^{-01}$	0.997	$-4.3 \cdot 10^{+01}$
$1/5 \cdot 2^{-5}$	$2.7 \cdot 10^{-02}$	0.998	$-4.4 \cdot 10^{+01}$
$1/5 \cdot 2^{-6}$	$1.3 \cdot 10^{-02}$	0.999	$-4.4 \cdot 10^{+01}$
$1/5 \cdot 2^{-7}$	$6.9 \cdot 10^{-02}$	0.999	$-4.4 \cdot 10^{+01}$
$1/5 \cdot 2^{-8}$	$3.4 \cdot 10^{-02}$	0.999	$-4.4 \cdot 10^{+01}$
$1/5 \cdot 2^{-9}$	$1.7 \cdot 10^{-03}$	0.999	$-4.4 \cdot 10^{+01}$

Example 2

h	$\ \varepsilon_h\ $	p	c
$1/5$	$2.4 \cdot 10^{-02}$	0.834	$-9.2 \cdot 10^{-01}$
$1/5 \cdot 2^{-1}$	$1.3 \cdot 10^{-02}$	0.921	$-1.1 \cdot 10^{-01}$
$1/5 \cdot 2^{-2}$	$7.1 \cdot 10^{-02}$	0.960	$-1.2 \cdot 10^{-01}$
$1/5 \cdot 2^{-3}$	$3.6 \cdot 10^{-02}$	0.980	$-1.3 \cdot 10^{-01}$
$1/5 \cdot 2^{-4}$	$1.8 \cdot 10^{-03}$	0.990	$-1.4 \cdot 10^{-01}$
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Collocation methods

Consider the following IVP:

$$z'(t) - \frac{M}{t}z(t) = f(t), \quad t \in (0, 1], \quad z(0) = 0.$$

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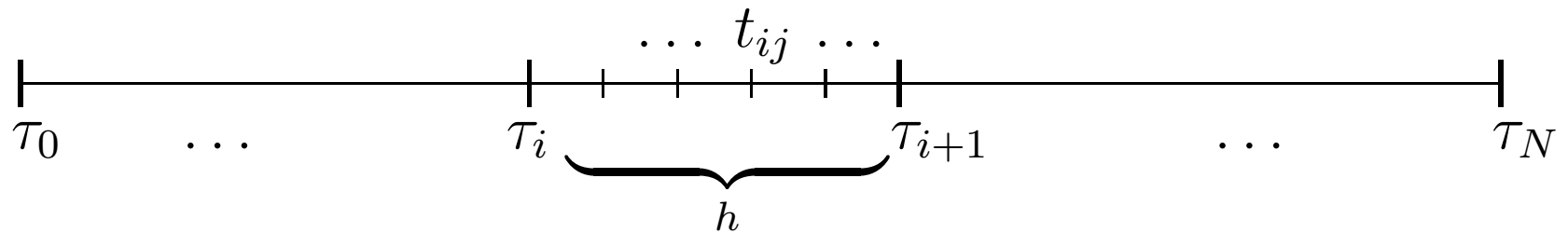
Recall: Let $f \in C[0, 1]$. Then a necessary condition for a solution of the problem to be in $C[0, 1]$ is

$$Mz(0) = 0 \Leftrightarrow z(0) = 0.$$

Moreover $z \in C^1[0, 1]$ and if $f \in C^p[0, 1]$, then $z \in C^{p+1}[0, 1]$.

Collocation scheme

Consider a **mesh** of the interval $[0, 1]$.

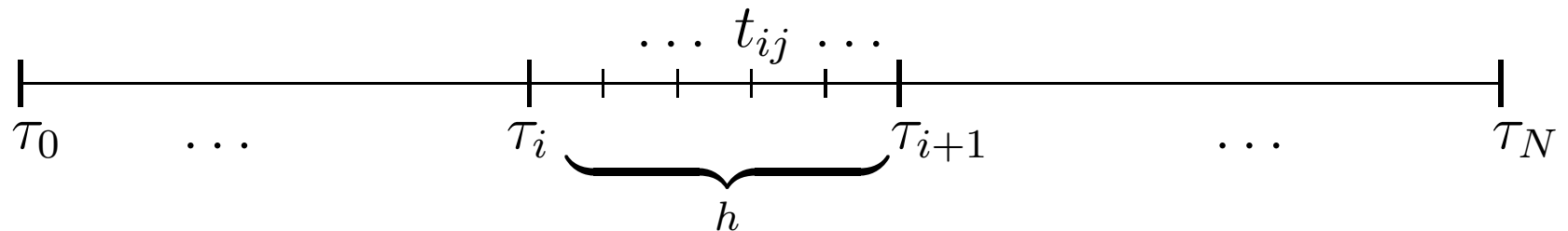


Let

$$\tau_i = ih, \quad i = 0, \dots, N, \quad h := \frac{1}{N}.$$

Collocation scheme

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Introduce the **grid**

$$t_{ij} = \tau_i + \rho_j h, \quad i = 0, \dots, N - 1, \quad j = 1, \dots, m,$$

where $0 < \rho_1 < \rho_2 < \dots < \rho_m < 1$.

Collocation scheme

Let us denote by \mathcal{P}_m the class of **piecewise continuous functions** on $[0, 1]$ which reduce to a **polynomial of degree smaller or equal to m** on each subinterval $[\tau_i, \tau_{i+1}]$,
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 $0 \leq i \leq N - 1$.

Approximate z by a function $p \in \mathcal{P}_m \cap C[0, 1]$ satisfying the **collocation conditions**

$$p'(t_{ij}) - M \frac{p(t_{ij})}{t_{ij}} - f(t_{ij}) = 0, \quad i = 0, \dots, N-1, j = 1, \dots, m,$$

and the IC $p(0) = 0$.

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and the IC $p(0) = 0$.

The aim: **Show the convergence of the scheme.**

Stability

We restrict ourselves to the scalar case and consider the function $u \in \mathcal{P}_m \cap C[0, 1]$ which satisfies

$$u'(t_{ij}) - \lambda \frac{u(t_{ij})}{t_{ij}} = c_{ij}, \quad u(0) = 0,$$
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Note that

$$tu'(t) - \lambda u(t) - t \sum_{j=1}^m l_j \left(\frac{t - \tau_i}{h} \right) c_{ij}$$

is a polynomial of degree $\leq m$, which by the collocation scheme vanishes when $t = t_{ik}$, $k = 1, \dots, m$.

(T2.17-T2.18)

Stability

Again

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Hence with a constant ξ_i ,

$$tu'(t) - \lambda u(t) - t \sum_{j=1}^m l_j \left(\frac{t - \tau_i}{h} \right) c_{ij} = \xi_i w \left(\frac{t - \tau_i}{h} \right), \quad t \in [\tau_i, \tau_{i+1}],$$

where $w(s) = (s - \rho_1)(s - \rho_2) \dots (s - \rho_m)$, $s \in (0, 1)$,

and $l_j(s) = w(s) / ((s - \rho_j)w'(\rho_j)) \quad j = 1, \dots, m$.

Stability

For $\lambda < 0$ equation

$$u'(t) - \frac{\lambda}{t} u(t) = \sum_{j=1}^m l_j \left(\frac{t - \tau_i}{h} \right) c_{ij} + \frac{1}{t} \xi_i w \left(\frac{t - \tau_i}{h} \right), \quad t \in [\tau_i, \tau_{i+1}],$$

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$$u(t) = t^\lambda \sum_{j=1}^m \int_0^t s^{-\lambda} l_j \left(\frac{s - \tau_j}{h} \right) ds c_{ij} + t^\lambda \xi_j \int_0^t s^{-\lambda-1} w \left(\frac{s - \tau_j}{h} \right) ds.$$

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On noting that for $i = 0$, $\tau_i = 0$, it follows that

$$\xi_0 = -\lambda \frac{u(0)}{w(0)}.$$

Stability

From the definition of w it follows that

$$w\left(\frac{t - \tau_i}{h}\right) \neq 0, \quad 0 \leq t < \tau_i, \quad i = 1, \dots, N - 1.$$

Stability

From the definition of w it follows that

$$w\left(\frac{t - \tau_i}{h}\right) \neq 0, \quad 0 \leq t < \tau_i, \quad i = 1, \dots, N - 1.$$

Then it is possible to eliminate ξ_i by evaluating

$$u(t) = t^\lambda \sum_{j=1}^m \int_0^t s^{-\lambda} l_j \left(\frac{s - \tau_j}{h}\right) ds c_{ij} + t^\lambda \xi_j \int_0^t s^{-\lambda-1} w\left(\frac{s - \tau_j}{h}\right) ds.$$

at τ_i and this implies

$$u(t) - A(t, \lambda)u(\tau_i) = \sum_{j=1}^m B_j(t, \lambda)c_{ij}, \quad t \in (\tau_i, \tau_{i+1}], \quad i = 0, \dots, N-1.$$

Stability

Theorem: Let all $\lambda(M) < 0$. Then the collocation scheme

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Theorem: Let all $\lambda(M) < 0$. Then the collocation scheme

$$p'(t_{ij}) - M \frac{p(t_{ij})}{t_{ij}} = f(t_{ij}), \quad u(0) = 0, \quad j = 1, \dots, m, \quad i = 0, \dots, N - 1$$

has a unique $p \in \mathcal{P}_m \cap C[0, 1]$ which satisfies

$$|p(\tau_i + \theta h)| \leq \text{const} \{ \tau_{i+1} F_i \}, \quad 0 \leq \theta \leq 1$$

where

$$F_i = \max_{0 \leq l \leq i, 1 \leq j \leq m} |f(t_{lj})|, \quad i = 0, \dots, N - 1.$$

Convergence

Theorem: Let $f \in C^m[0, 1]$ and p and z be solutions of the collocation scheme and the analytical problem, subject to the initial conditions

$$p(0) = 0, \quad z(0) = 0,$$

respectively.

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Then

$$\|p - z\| \leq \text{const } h^m.$$

Proof: Let $e \in \mathcal{P}_m \cap C[0, 1]$ satisfy

$$e'(t_{ij}) = z'(t_{ij}) - p'(t_{ij}), \quad j = 1, \dots, m, \quad i = 0, \dots, N - 1, \\ e(0) = 0.$$

Convergence

Clearly, for $t \in [\tau_i, \tau_{i+1}]$,

$$e'(t) = \sum_{j=1}^m l_j \left(\frac{t - \tau_j}{h} \right) (z'(t_{ij}) - p'(t_{ij})) = \sum_{j=1}^m l_j \left(\frac{t - \tau_j}{h} \right) z'(t_{ij}) - p'(t).$$

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We know that if $f \in C^m[0, 1]$ then $z \in C^{m+1}[0, 1]$ and so

$$e'(t) = z'(t) - p'(t) + O(h^m),$$

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$$e'(t) = z'(t) - p'(t) + O(h^m),$$

which by integration yields

$$e(t) = z(t) - p(t) + O(h^m t), \quad e(0) = 0.$$

Convergence

On noting that p and z satisfy the collocation scheme and the analytical problem, respectively, it follows that

$$e'(t_{ij}) - M \frac{e(t_{ij})}{t_{ij}} = O(h^m), \quad j = 1, \dots, m, \quad i = 0, \dots, N - 1, \quad e(0) = 0.$$

Convergence

On noting that p and z satisfy the collocation scheme and the analytical problem, respectively, it follows that

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We know, that for

$$p'(t_{ij}) - M \frac{p(t_{ij})}{t_{ij}} = f(t_{ij}), \quad j = 1, \dots, m, \quad i = 0, \dots, N-1, \quad p(0) = 0,$$

$$\|p\| \leq \|F\| = \max_{i,j} |f(t_{ij})| \Rightarrow \|e\| = O(h^m)$$

and

$$\|p - z\| = \|e\| + O(h^m) = O(h^m).$$

Example

Consider the problem

$$z'(t) = -\frac{1}{t}z(t) + 2 \sin t + t \cos t, \quad t \in (0, 1],$$
$$z(0) = 0,$$

with the exact solution $z(t) = t \sin t$.

Example

Numerical experiment with $m = 2$ equidistant points.

Uniform mesh		Error of p at the mesh tau			Error of p at the grid $icol$		
N	h	error	order	err. const.	error	order	err. const.
10	$1.00e - 01$	$3.183e - 04$			$3.183e - 04$		
20	$5.00e - 02$	$7.941e - 05$	2.0	$3.205e - 02$	$7.941e - 05$	2.0	$3.205e - 02$
40	$2.50e - 02$	$1.984e - 05$	2.0	$3.184e - 02$	$1.984e - 05$	2.0	$3.184e - 02$
80	$1.25e - 02$	$4.960e - 06$	2.0	$3.177e - 02$	$4.960e - 06$	2.0	$3.177e - 02$
160	$6.25e - 03$	$1.240e - 06$	2.0	$3.175e - 02$	$1.240e - 06$	2.0	$3.175e - 02$
320	$3.13e - 03$	$3.100e - 07$	2.0	$3.174e - 02$	$3.100e - 07$	2.0	$3.174e - 02$

Example

Numerical experiment with $m = 2$ Gaussian points.

Uniform Mesh		Error of p at the mesh tau			Error of p at the grid $tcoll$		
N	h	error	order	err. const.	error	order	err. const.
10	$1.00e - 01$	$4.617e - 07$			$2.458e - 05$		
20	$5.00e - 02$	$2.891e - 08$	4.0	$4.584e - 03$	$3.073e - 06$	3.0	$2.458e - 02$
40	$2.50e - 02$	$1.808e - 09$	4.0	$4.616e - 03$	$3.840e - 07$	3.0	$2.459e - 02$
80	$1.25e - 02$	$1.130e - 10$	4.0	$4.626e - 03$	$4.800e - 08$	3.0	$2.459e - 02$
160	$6.25e - 03$	$7.064e - 12$	4.0	$4.628e - 03$	$6.000e - 09$	3.0	$2.458e - 02$
320	$3.13e - 03$	$4.415e - 13$	4.0	$4.628e - 03$	$7.500e - 10$	3.0	$2.458e - 02$

Applications

Complex Ginzburg-Landau equation

$$i \frac{\partial u}{\partial t} + (1 - i\varepsilon) \Delta u + (1 + i\delta) |u|^2 u = 0, \quad t \in (0, \infty), \quad x \in \mathbb{R}^3$$

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We are interested in *self-similar blow-up* solutions

Ansatz

$$u(x, t) = L(\tau)y(\tau)$$

$$\tau = \tau(x, t) = \sqrt{\frac{x_1^2 + x_2^2 + x_3^2}{2a(T - t)}}, \quad \lim_{t \rightarrow T} L(\tau(x, t)) = \infty$$

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Nonlinear optics, models of turbulence, superconductivity

Budd, Koch, W. (2006)

Similarity reduction

Find $y : [0, \infty) \rightarrow \mathbb{C}$

$$(1 - i\varepsilon) \left(y''(\tau) + \frac{2}{\tau} y'(\tau) \right) - y(\tau) + ia(\tau y(\tau))' + (1 + i\delta) |y(\tau)|^2 y(\tau) = 0$$

$$y'(0) = 0, \quad \Im y(0) = 0, \quad \lim_{\tau \rightarrow \infty} \tau y'(\tau) = 0$$

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Implicit, parameter dependent ODE with singular points and unknown parameter a posed on a semi-infinite interval

Complex Ginzburg-Landau equation

Pathfollowing for CGL:

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a ... unknown, nonnegative parameter

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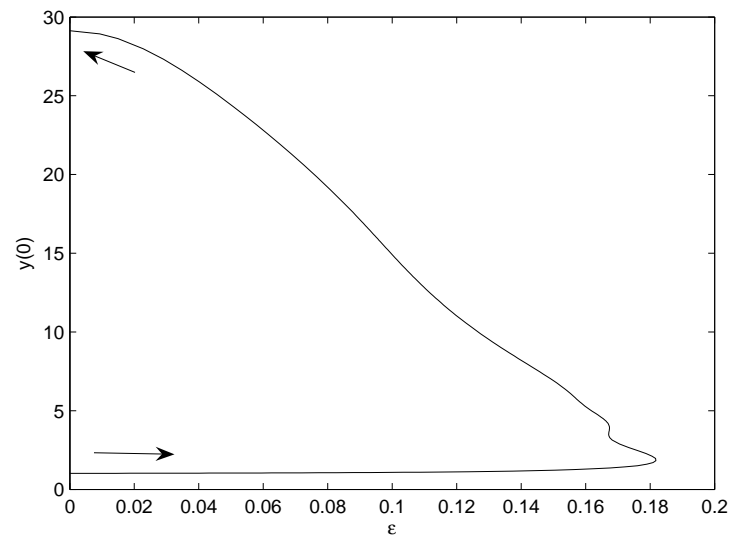
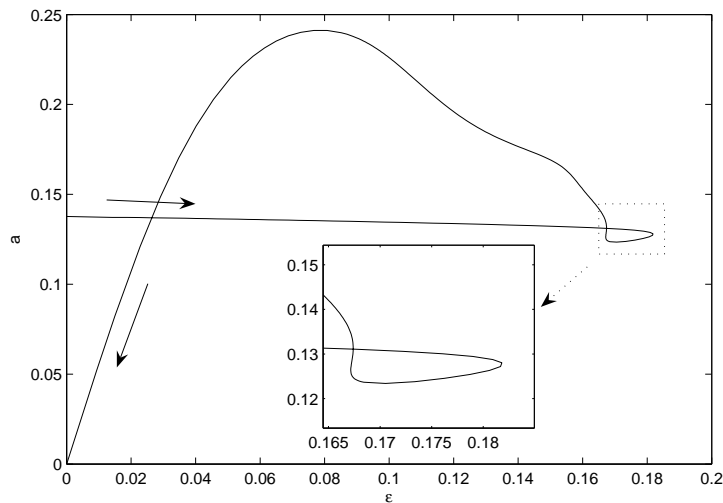
$\varepsilon = \delta = 0$: Nonlinear Schrödinger equation (NLS)

Pathfollowing for CGL

Set $\delta = 0$, vary ε :

Pathfollowing for CGL

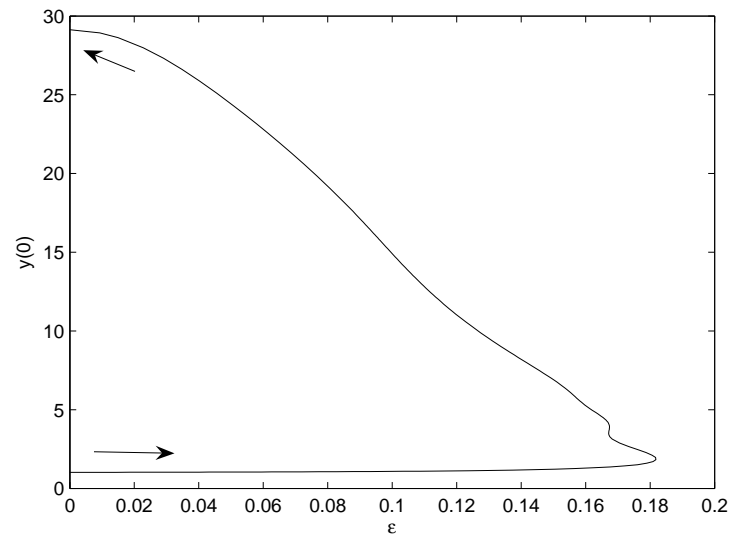
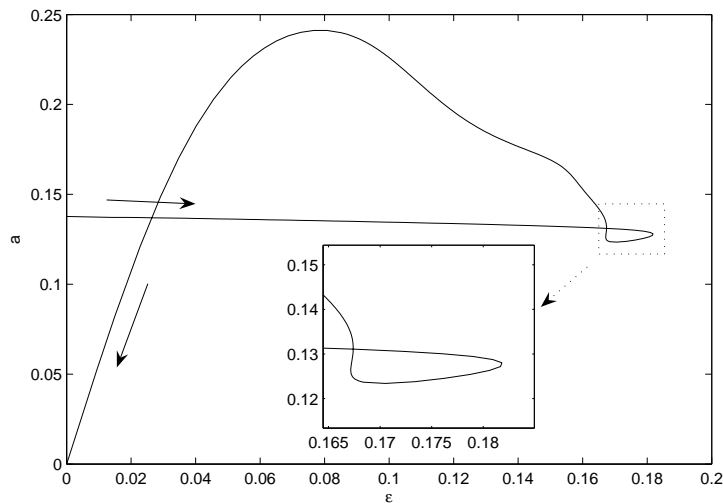
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Values of a (left) and $y(0)$ (right) along a branch bifurcating from the NLS

Pathfollowing for CGL

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Values of a (left) and $y(0)$ (right) along a branch bifurcating from the NLS

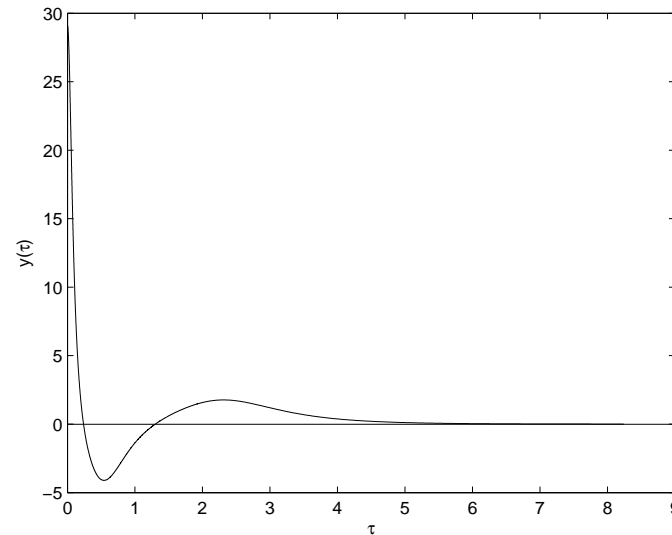
Γ has three turning points, but no bifurcation points

Pathfollowing for CGL

Path Γ terminates at a real-valued, multi-bump solution of the NLS

Pathfollowing for CGL

Path Γ terminates at a real-valued, multi-bump solution of the NLS



Real solution of the NLS computed by pathfollowing

Density profile equation in hydrodynamics

Bubbles: Density profile equation in hydrodynamics

Kitzhofer, Koch, Lima, W. (2005)

$$\rho''(r) + \frac{N-1}{r} \rho'(r) = 4(\rho(r) + 1)\rho(r)(\rho(r) - \xi), \quad r \in (0, \infty)$$

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Density profile equation in hydrodynamics

Bubbles: Density profile equation in hydrodynamics

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Start animation Bubble!

Reaction-diffusion systems

Staněk, Pulverer, W. (2008)

$$u''(t) = \lambda g(u(t)) = \frac{\lambda}{\sqrt{u(t)}}, \quad t \in [0, 1]$$

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Problem: Characterize the relation between the values of λ and number and type of solutions, *positive, pseudo dead core, and dead core!*

Dead core solutions

Original formulation

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Dead core solutions

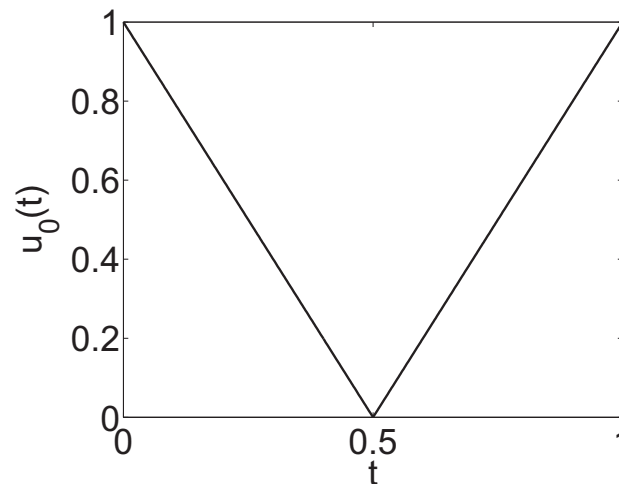
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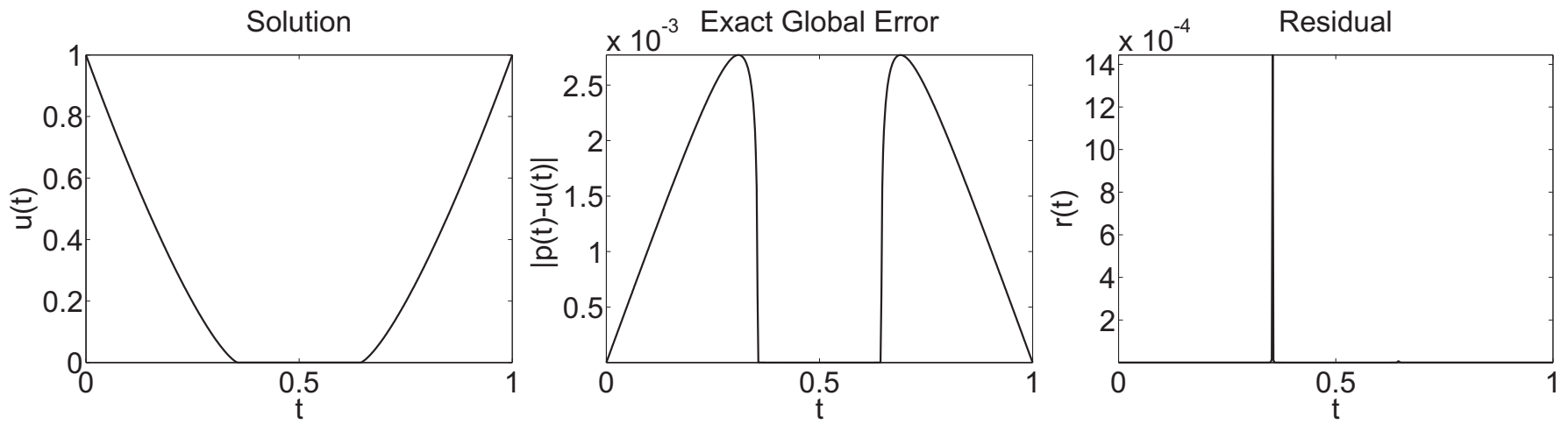
New formulation

$$u''(t) \sqrt{u(t)u(t)} = \lambda u(t), \quad u(0) = 1, \quad u(1) = 1$$

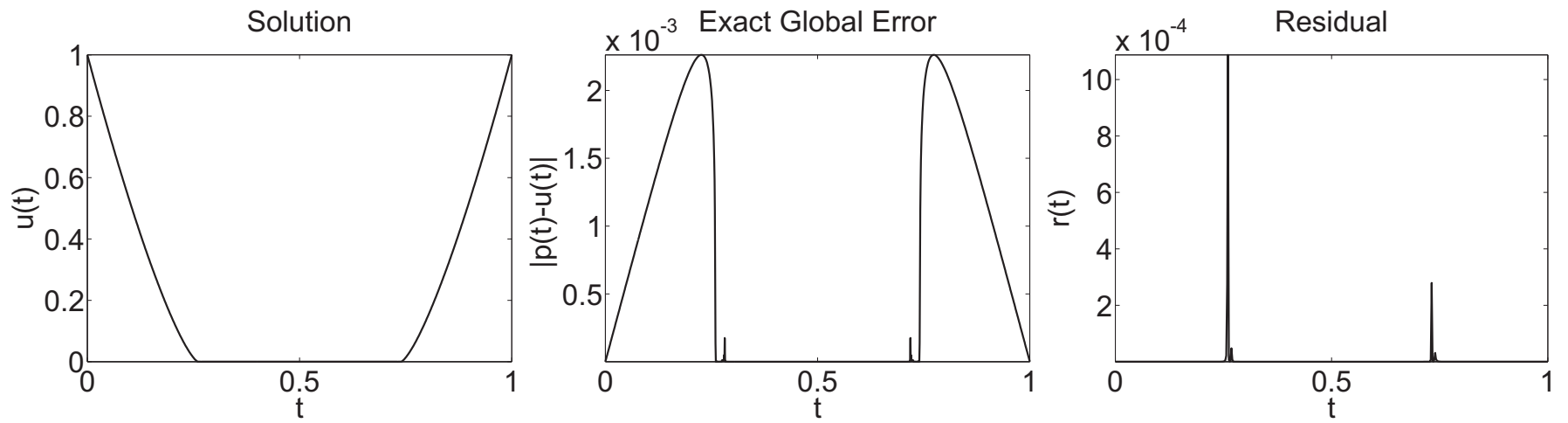
Initial profile



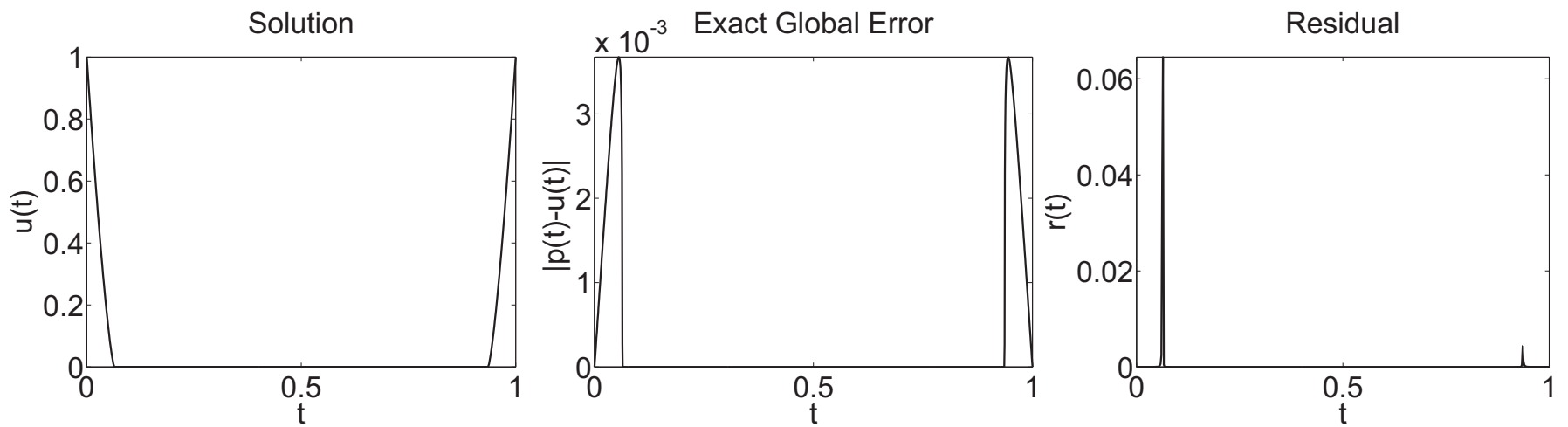
Dead core solution, $\lambda = \frac{32}{9}$



Dead core solution, $\lambda = \frac{60}{9}$



Dead core solution, $\lambda = \frac{1000}{9}$



Summary

We discussed convergence of two numerical schemes applied to

$$z'(t) = \frac{M}{t}z(t) + f(t), \quad t \in (0, 1], \quad z(0) = 0, \quad \lambda(M) < 0.$$

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- ▶ Open question: Convergence of collocation for the singularity of second kind.