Collocation for Solving Singular ODEs and Higher Index DAEs

Ewa Weinmüller

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Vienna University of Technology

Contents

Models in singular ODEs - shell buckling

Deformation and stress in spherical shell buckling

Gräff, Scheidl, Troger, W. (1985)

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- $s \in (0, \pi)$, $\lambda = \frac{p}{p_{cr}} \in [0, 1]$, f_2, g_2 involve $\int\limits_0^s h(\xi, \beta(\xi)) d\xi$

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- Introduce: $i(s) = \int_0^s h(\xi, \beta(\xi)) d\xi$
- Include: $i'(s) = h(s, \beta(s)),\ i(0) = 0$

Models in singular ODEs - CGL equation

Budd, Koch, W. (2006)

Solve for $u = u(x,t)$, $x \in^3$, $t > 0$:

$$\mathrm{i}\frac{\partial u}{\partial t} + (1 - \mathrm{i}\varepsilon)\Delta u + (1 + \mathrm{i}\delta)|u|^2 u = 0, \quad u(x,0) = u_0(x).$$

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Interested in self-similar solutions

$$u(x,t) = L(\tau)y(\tau),\ \tau = \tau(x,t),\ \lim_{t \to T} L(\tau(x,t)) = \infty$$

where T is the blow-up time and $y = y(\tau)$ satisfies, $\tau > 0$

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

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

Time and space singularities

- Staněk, Pulverer, W. (2008)

  Steady-state of diffusion-reaction of several chemical species

  $$u''(t)g(u(t))u(t) = \lambda u(t), \;\; u(0) = 1, \, u(1) = 1$$

  $g(u(t)) = \sqrt{u(t)}$ becomes zero in $[0, 1]$

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  Genetic composition of population, nucleation theory, nonlinear field theory

  $$u''(t) + \frac{a}{t}u'(t) + \frac{a}{t^2} = f(t, u(t)), \;\; u(1) = 0, \, u'(1) = -1$$

  $f(t, u(t)) = -\frac{1}{\sqrt{t}} - \frac{1}{u(t)^{1/3}}$ becomes unbounded in $t = 0$ and $t = 1$

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- Gschwindl, Rachunková, Staněk, W. (2014)

  Genetic composition of population, nucleation theory, nonlinear field theory

  $$u''(t) + \frac{2}{t}u'(t) = f(t, u(t)), \;\; \lim_{t\to 0} u(t) = \infty,\, u(1) = 0$$

  $f(t, u(t)) = 0.01 + u(t)^{2/3}$ becomes unbounded in $t = 0$

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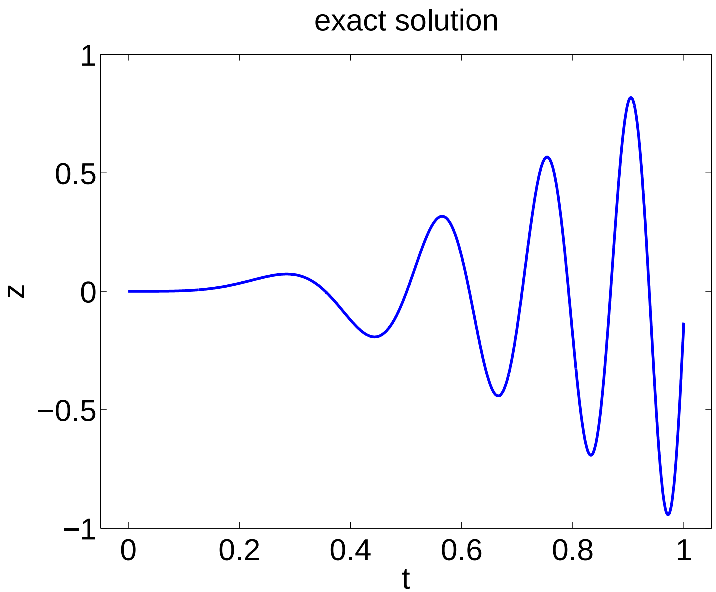
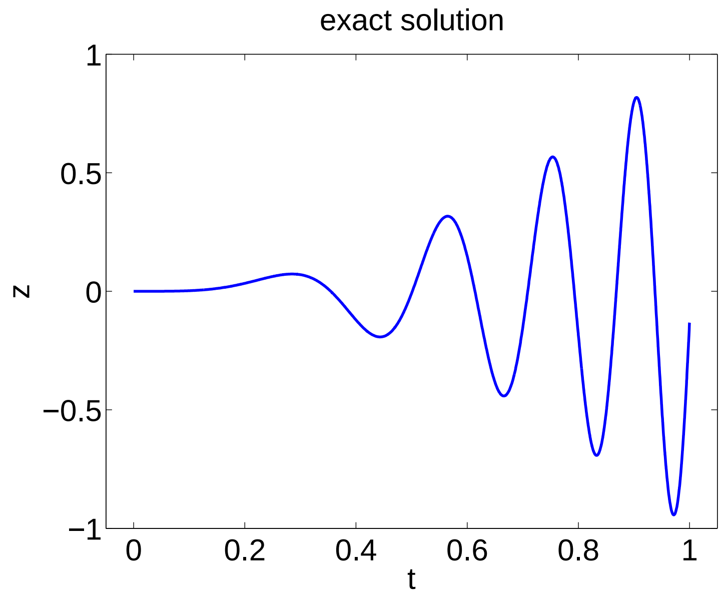
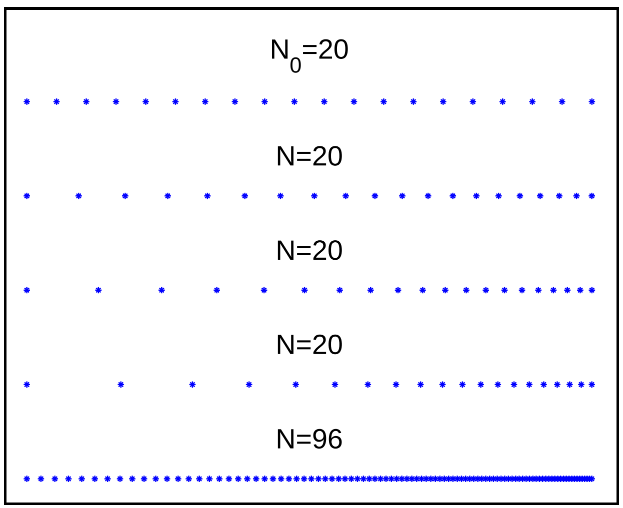
- Adaptive mesh selection:

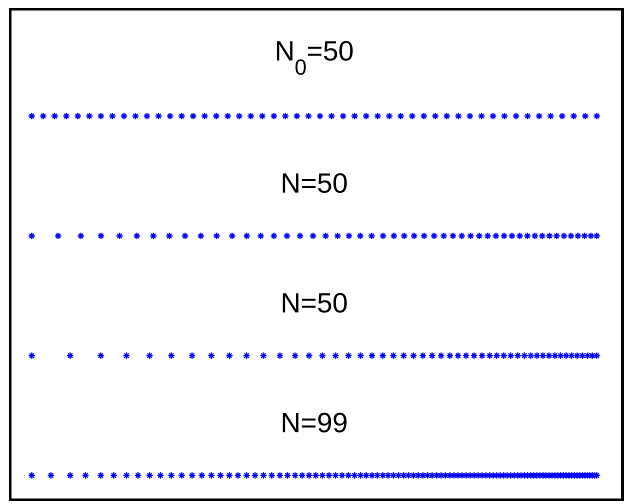
Meshes unaffected by the unsmooth (!) direction field

Computational experiment









Gaussian collocation, order 4, $TOL_a = 10^{-6}$

Collocation

$$z'(t) - F(t, z(t)) = 0, \quad z'(t) = \frac{1}{t} M z(t) + f(t, z(t) \text{ plus BC}$$

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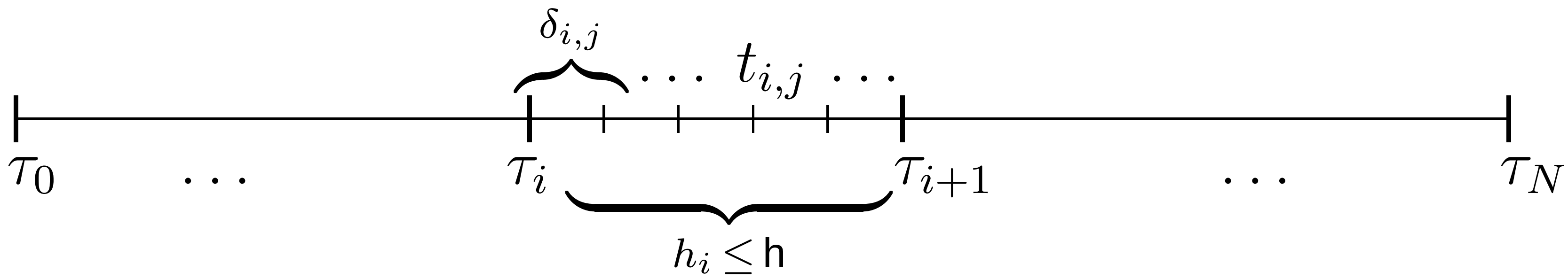

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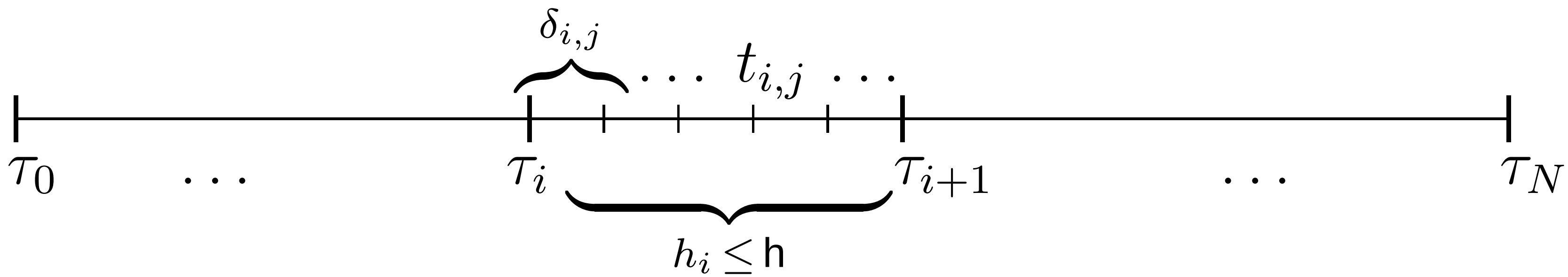

- Piecewise polynomial function $p(t) \in C[0,1]$, maximal degree $\leq m$: $p'(t_{i,j}) - F(t_{i,j}, p(t_{i,j})) = 0$ plus BC

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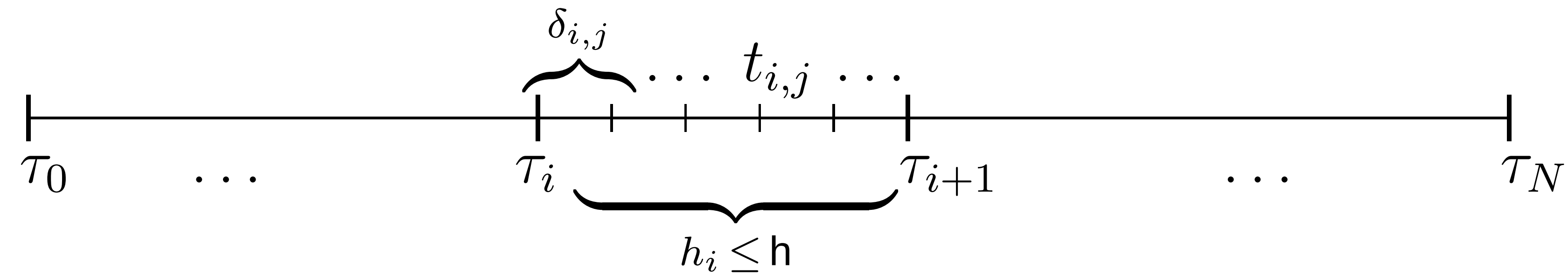

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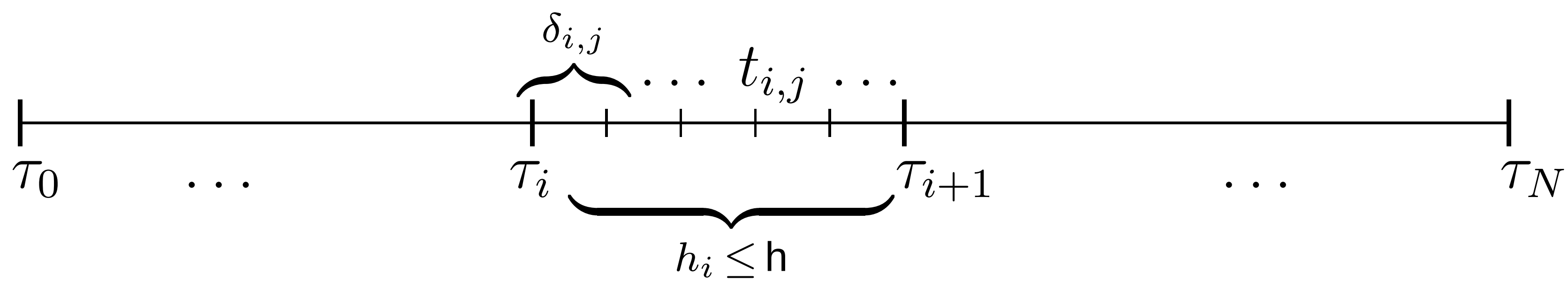

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- *Convergence regular case*: $\|p - z\|_\infty = O(\mathsf{h}^m)$ superconvergence at τ_i de Boor, Swartz (1973)
- *Convergence singular case*: $\|p - z\|_\infty = O(\mathsf{h}^m |\ln \mathsf{h}|^{n_0-1})$ no superconvergence in gen. de Hoog, Weiss (1978), Auzinger, Koch, W. (2002), Koch (2005)

MATLAB code `bvpsuite` – *Scope*

Kitzhofer, Koch, Pulverer, Simon, W. (2009)

http://www.math.tuwien.ac.at/˜ewa/

Implicit nonlinear mixed order system of ODEs

$$F\Big(t, p_1, \dots, p_s, z_1(t), z_1'(t), \dots, z_1^{(l_1)}(t), \dots$$

$$z_n(t), z_n'(t), \dots, z_n^{(l_n)}(t)\Big) = 0$$

$$B\Big(p_1, \dots, p_s, z_1(c_1), \dots, z_1^{(l_1-1)}(c_1), \dots, z_n(c_1), \dots$$

$$z_n(c_q), \dots, z_n^{(l_n-1)}(c_q)\Big) = 0$$

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Unknowns: $z(t) = (z_1(t), z_2(t), \dots, z_n(t))^T$, p_i, $i = 1, \dots, s$

In general, $t \in [a, b]$ or $t \in [a, \infty)$, $a \geq 0$

Main features

- Order of the method, *standard* $m = 2$ *to* $m = 8$, is chosen automatically depending on TOL_a

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- We implemented *Gaussian points (standard)*, Lobatto, and uniform. User's own specification is possible
- Specification of different TOL_a and TOL_r parameters for different solution components is possible
- *Mesh adaptation is the standard choice* but fixed grid is also possible

Applications

Bubbles: Density profile equation in hydrodynamics

Kitzhofer, Koch, Lima, W. (2005)

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

Reformulation for $s \in (0,1]$, $y_1(s) = \rho(s)$, $y_2(s) = \rho(1/s)$:

$$y_1''(s) + \frac{N-1}{s}y_1'(s) = 4(y_1(s)+1)y_1(s)(y_1(s)-\xi)$$

$$y_2''(s) - \frac{N-3}{s}y_2'(s) = 4\frac{1}{s^4}(y_2(s)+1)y_2(s)(y_2(s)-\xi)$$

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Well-posedness $\checkmark$

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Well-posedness ✓

Start animation Bubble!

Generalized Korteweg-de Vries equation

Budd, Koch, Schirnhofer, W. (work in progress)

The generalized Korteweg-de Vries equation, $p \in \mathbb{N}$, $p \geq 2$

$$u_t + u_{xxx} + (u^p)_x = 0, \quad x \in \mathbb{R}, \quad t \geq 0, \qquad u(x,0) = u_0(x)$$

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$$u(x,t) = 1/(T-t)^{2/(3(p-1))} w(\xi), \quad \xi = x/(T-t)^{1/3}$$

where T is the blow-up time and $w = w(\xi)$ satisfies

$$\frac{2}{3(p-1)} w + \frac{\xi}{3} w_\xi + (w_{\xi\xi} + w^p)_\xi = 0, \;\; \xi \in \mathbb{R},$$

$$\frac{2}{3(p-1)} w(\xi) + \frac{\xi}{3} w_\xi(\xi) \xrightarrow{\xi \to \pm\infty} 0, \quad w_{\xi\xi}(\xi) \xrightarrow{\xi \to \infty} 0$$

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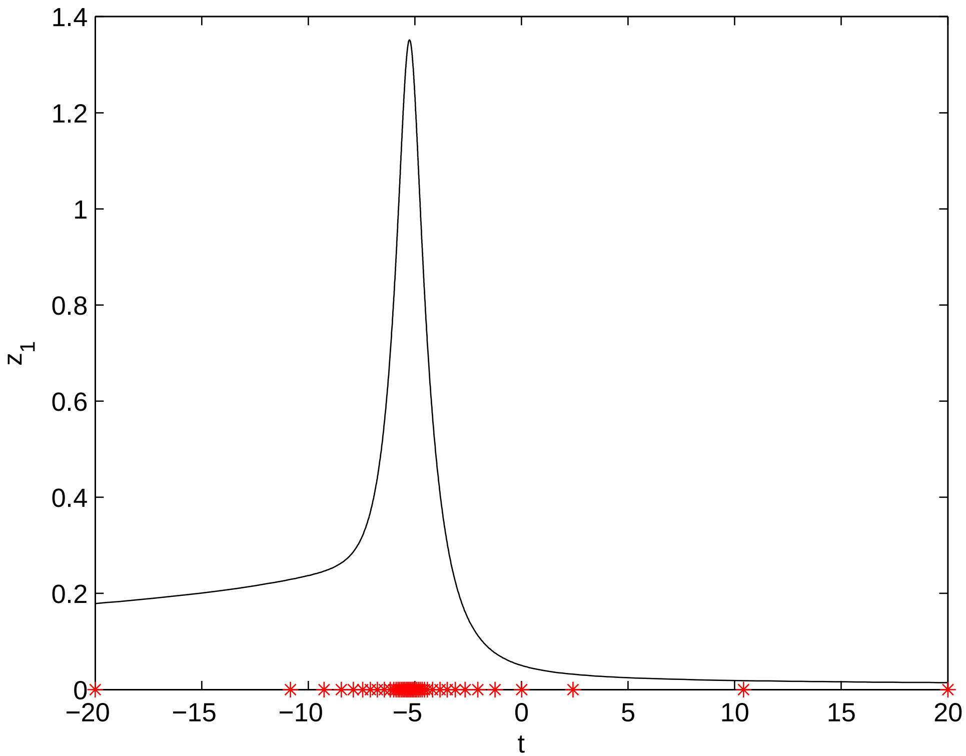
Waves on shallow water surfaces

$p = 6$: Numerical solution $w(\xi)$

We solve the problem using `bvpsuite` by reducing ξ to a finite interval $[-L, L]$ with a sufficiently large L

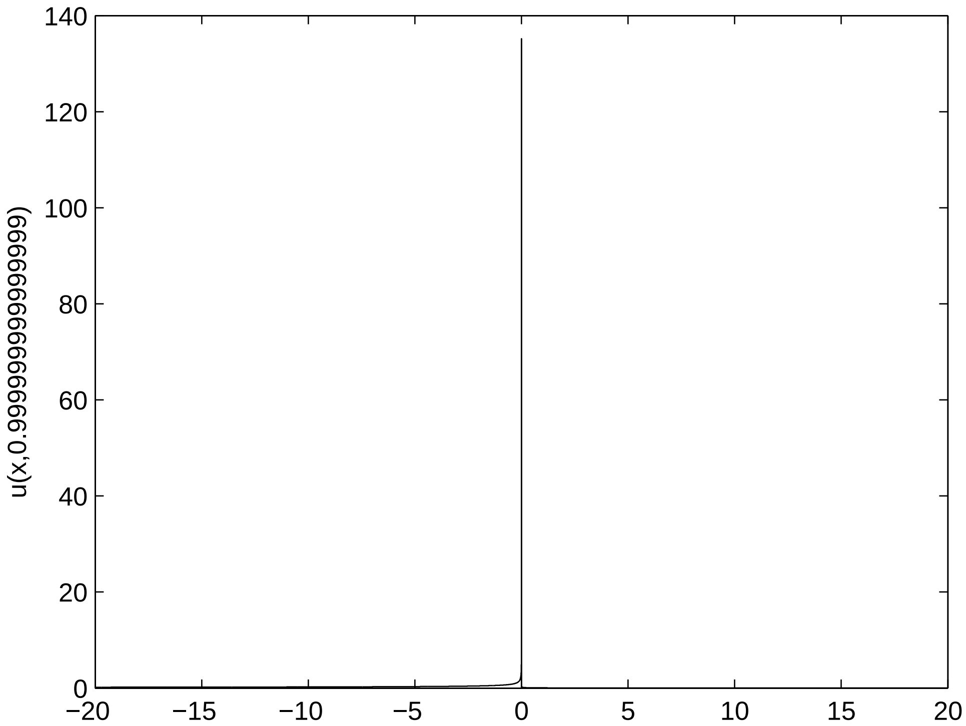


Solution $w(\xi)$ from `bvpsuite` with $TOL_a = TOL_r = 10^{-4}$ and one Gaussian point: adaptive mesh with 40 out of $N = 3332$

For two Gaussian points $N = 558$, for three Gaussian points $N = 264$

$p = 6$: Numerical solution $u(x,t)$, $t = 1 - 10^{-15}$

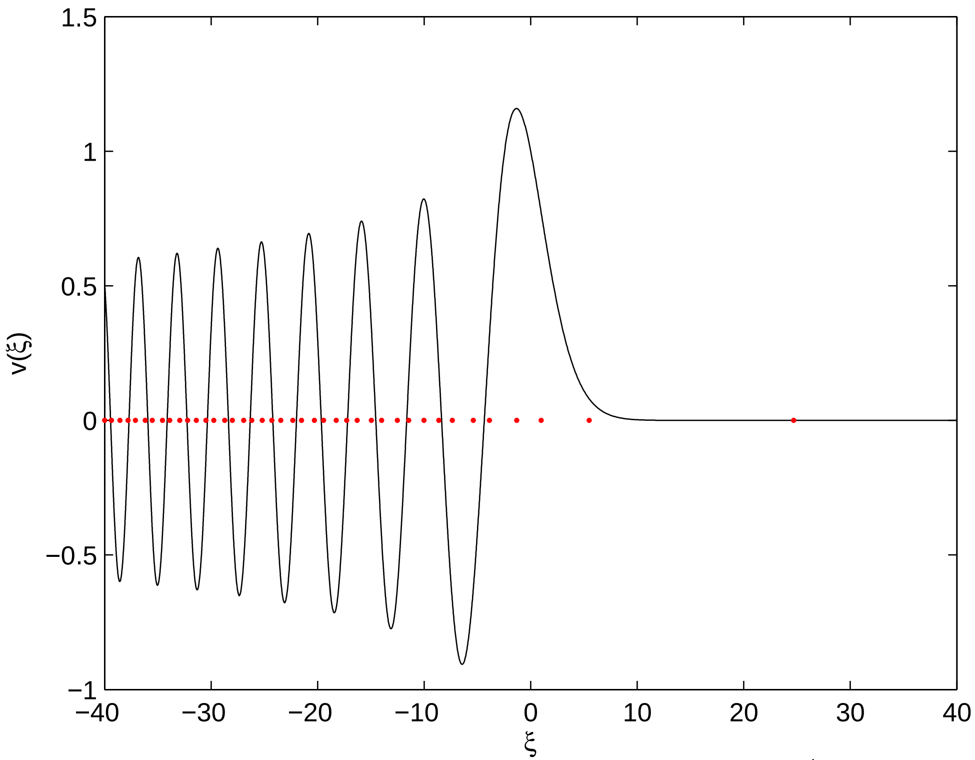
$$u(x,t) = 1/(1-t)^{2/(3(p-1))} w(\xi), \quad \xi = x/(1-t)^{1/3}, \; T = 1$$



Solution of the original problem calculated using collocation with one Gaussian point

$p = 5$: Numerical solution $w(\xi)$

We solve the problem using `bvpsuite` by reducing ξ to a finite interval $[-L, L]$ with $L = 40$

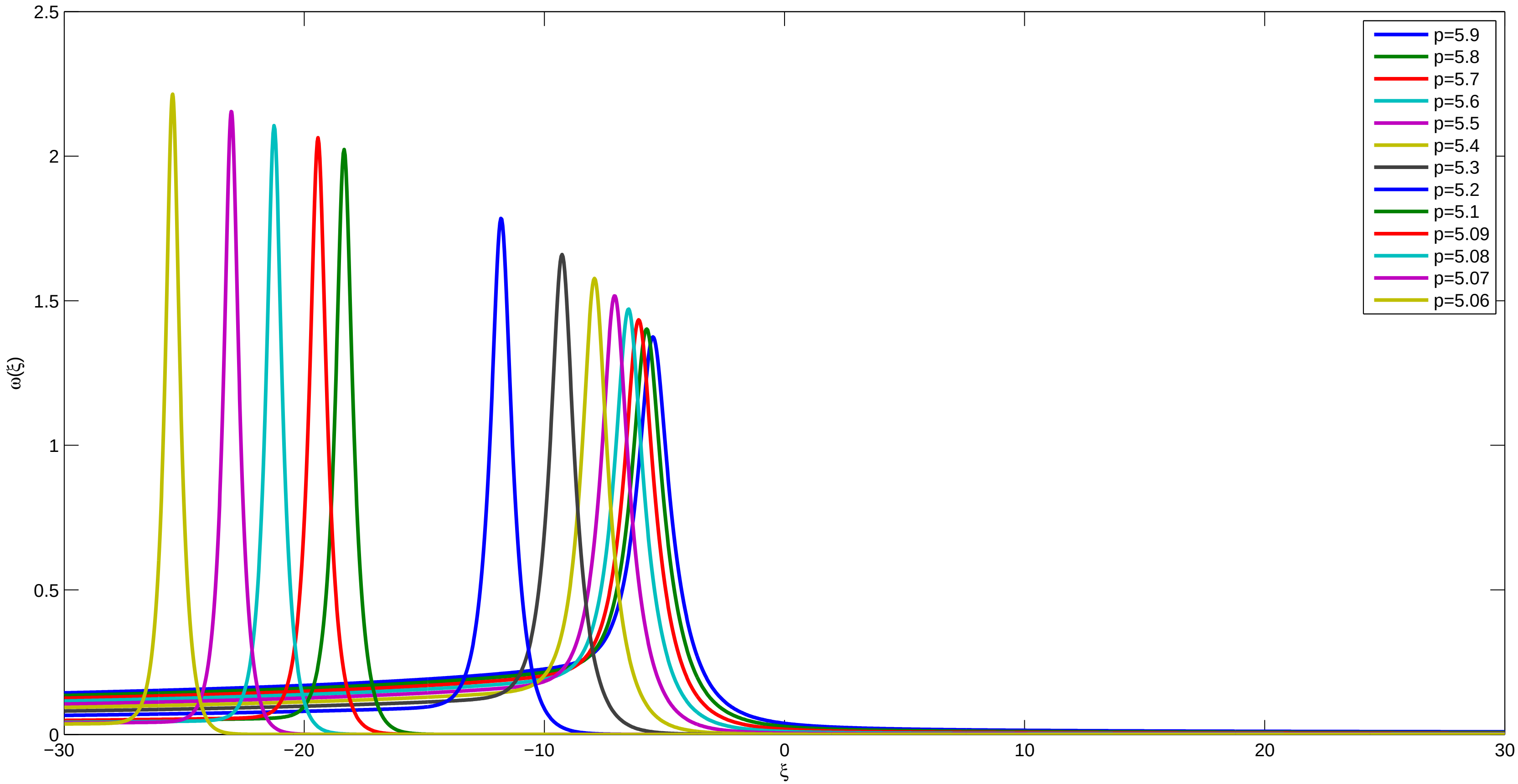


Solution $w(\xi)$ from `bvpsuite` with $TOL_a = TOL_r = 10^{-4}$ and one Gaussian point:

adaptive mesh with 40 out of $N = 4249$ points

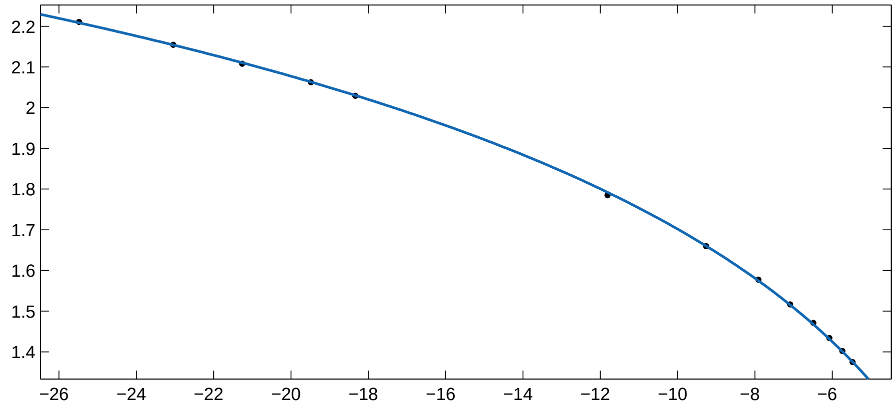
$p = 6 \to 5$: Numerical solution $w(\xi)$

Problems solved on $[-L, L]$ with $L = 30$

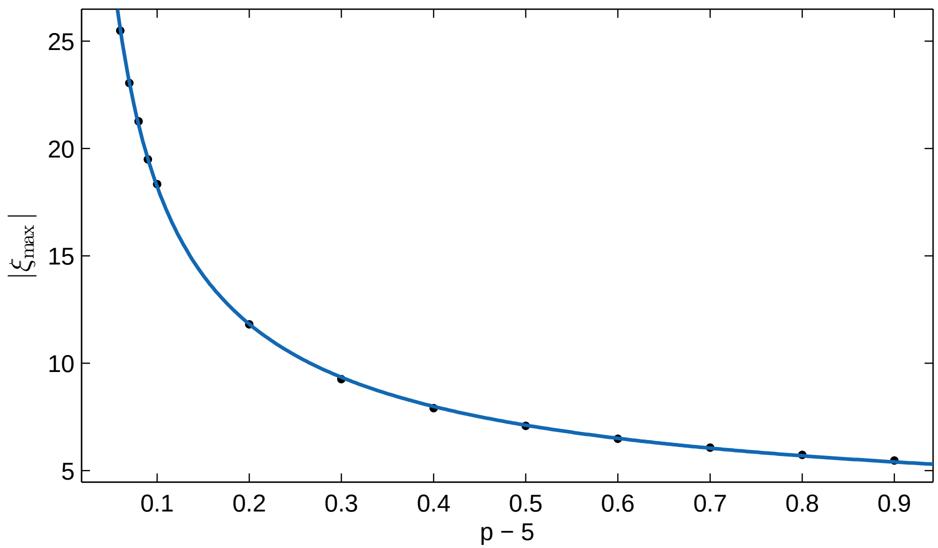


Solution $w(\xi)$ from `bvpsuite` with one Gaussian point

$p = 6 \to 5$: Asymptotics



$\max_\xi w(\xi)$ as a function of ξ fitted to a logarithmic curve



$|\xi_{max}|$ as a function of $p - 5$ fitted to an exponential curve

Remarks on higher index DAEs

Koch, März, Praetorius, W. (2010), Dick, Koch, März, W. (2012)

Hanke, März, Tischendorf, W., Wurm (work in progress)

Consider the index 3 problem

$$
\begin{aligned}
&x_2'(t) + x_1(t) = q_1(t), \\
&\eta t x_2'(t) + x_3'(t) + (\eta + \mathbf{1}) x_2(t) = q_2(t), \quad t \in (0, 1], \\
&\eta t x_2(t) + x_3(t) = q_3(t),
\end{aligned}
$$

with $\eta = 3$ and smooth inhomogeneity, subject to boundary conditions,

$$x_2(0) = 0, \quad x_3(1) = 2\mathrm{e}^{-2}\sin(1) + \mathrm{e}^{-1}\cos(1) - 2x_2(1).$$

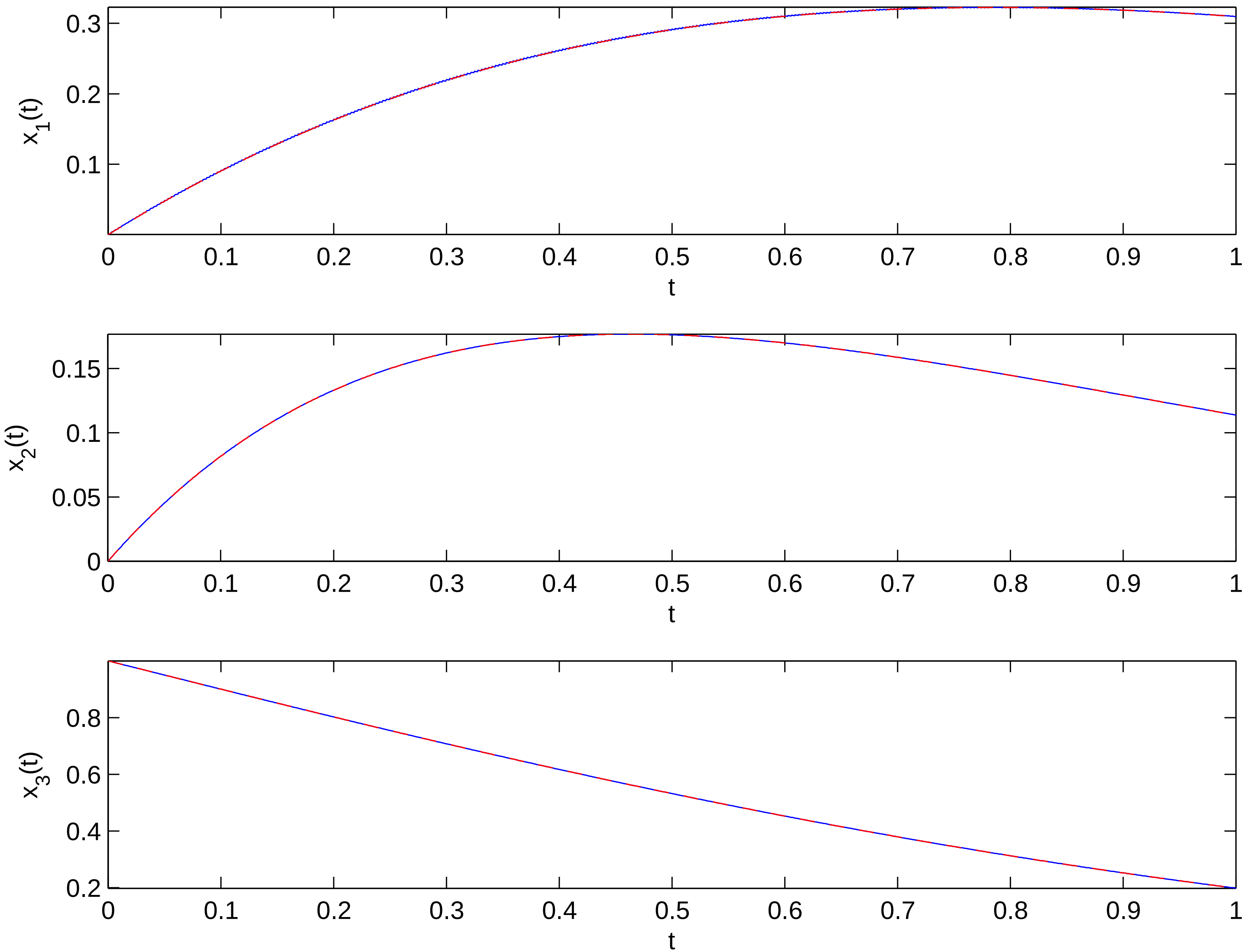
Solution reads:

$$x_1(t) = \mathrm{e}^{-t}\sin(t), \quad x_2(t) = \mathrm{e}^{-2t}\sin(t), \quad x_3(t) = \mathrm{e}^{-t}\cos(t)$$

Table of errors for $m = 2$

m=2		error for x_1 on Γ			error for x_1 on Δ		
N	h	error	order	const.	error	order	const.
320	3.13e-003	1.11e-003	1.0	3.57e-001	6.11e-004	1.1	4.07e-001
640	1.56e-003	5.53e-004	1.0	3.56e-001	2.87e-004	1.1	3.29e-001
1280	7.81e-004	2.76e-004	1.0	3.55e-001	1.38e-004	1.1	2.66e-001
m=2		error for x_2 on Γ			error for x_2 on Δ		
N	h	error	order	const.	error	order	const.
320	3.13e-003	5.76e-007	2.0	5.89e-002	3.93e-007	2.0	4.70e-002
640	1.56e-003	1.44e-007	2.0	5.89e-002	9.73e-008	2.0	4.36e-002
1280	7.81e-004	3.60e-008	2.0	5.89e-002	2.42e-008	2.0	4.17e-002
m=2		error for x_3 on Γ			error for x_3 on Δ		
N	h	error	order	const.	error	order	const.
320	3.13e-003	5.15e-007	2.0	5.27e-002	1.18e-008	2.9	1.90e-001
640	1.56e-003	1.29e-007	2.0	5.27e-002	1.63e-009	2.9	1.64e-001
1280	7.81e-004	3.22e-008	2.0	5.27e-002	2.24e-010	2.9	1.80e-001

Comparing the numerical with the exact solution for $m = 2$, $N = 320$



Index 3 problem – continued

Petzold (1982), März (1992)

Consider the case $\eta = -\mathbf{1/2}$

$$x_2'(t) + x_1(t) = q_1(t),$$
$$-\mathbf{1/2}\, t x_2'(t) + x_3'(t) + \mathbf{1/2}\, x_2(t) = q_2(t),$$
$$-\mathbf{1/2}\, t x_2(t) + x_3(t) = q_3(t),$$

with smooth inhomogeneity, subject to initial conditions,

$$x_2(0) = 0, \quad x_3(0) = 1$$

Solution reads:

$$x_1(t) = \mathrm{e}^{-t}\sin(t), \quad x_2(t) = \mathrm{e}^{-2t}\sin(t), \quad x_3(t) = \mathrm{e}^{-t}\cos(t)$$

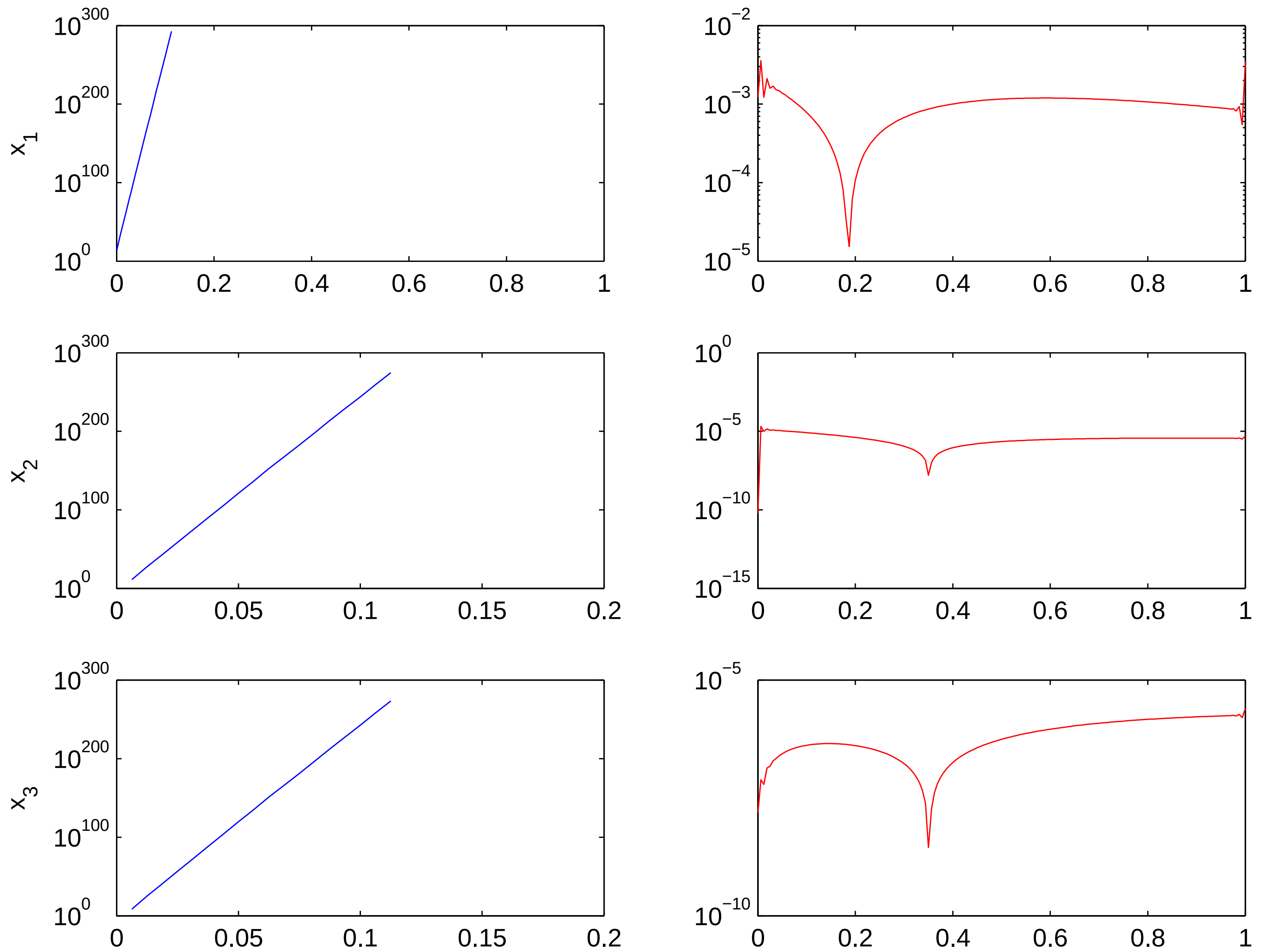
Table of errors for $m = 2$

uniform mesh		error for x_1 (classic coll.)		error for x_1 (overdet coll.)	
N	h	error	order	error	order
160	6.25e-03	Inf	-Inf	3.58e-03	0.97
320	3.13e-03	3.65e+171	Inf	1.81e-03	0.98
640	1.56e-03	2.09e+307	-450.98	9.11e-04	0.99

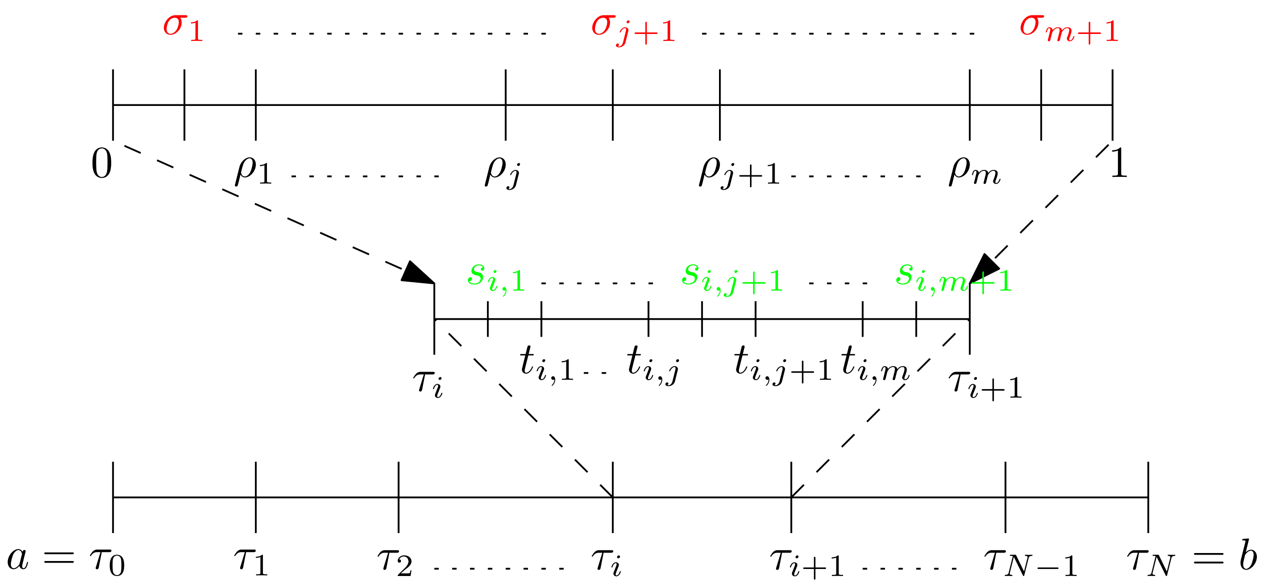
uniform mesh		error for x_2 (classic coll.)		error for x_2 (overdet coll.)	
N	h	error	order	error	order
160	6.25e-03	5.11e+274	-716.36	2.04e-05	1.97
320	3.13e-03	6.05e+153	401.71	5.14e-06	1.99
640	1.56e-03	5.76e+289	-451.71	1.29e-06	1.99

uniform mesh		error for x_3 (classic coll.)		error for x_3 (overdet coll.)	
N	h	error	order	error	order
160	6.25e-03	2.80e+273	-717.97	2.51e-06	2.00
320	3.13e-03	9.03e+151	403.59	6.28e-07	2.00
640	1.56e-03	8.35e+287	-451.67	1.57e-07	2.00

Comparing the classic collocation with the overdetermined variant for $m = 2$, $N = 160$

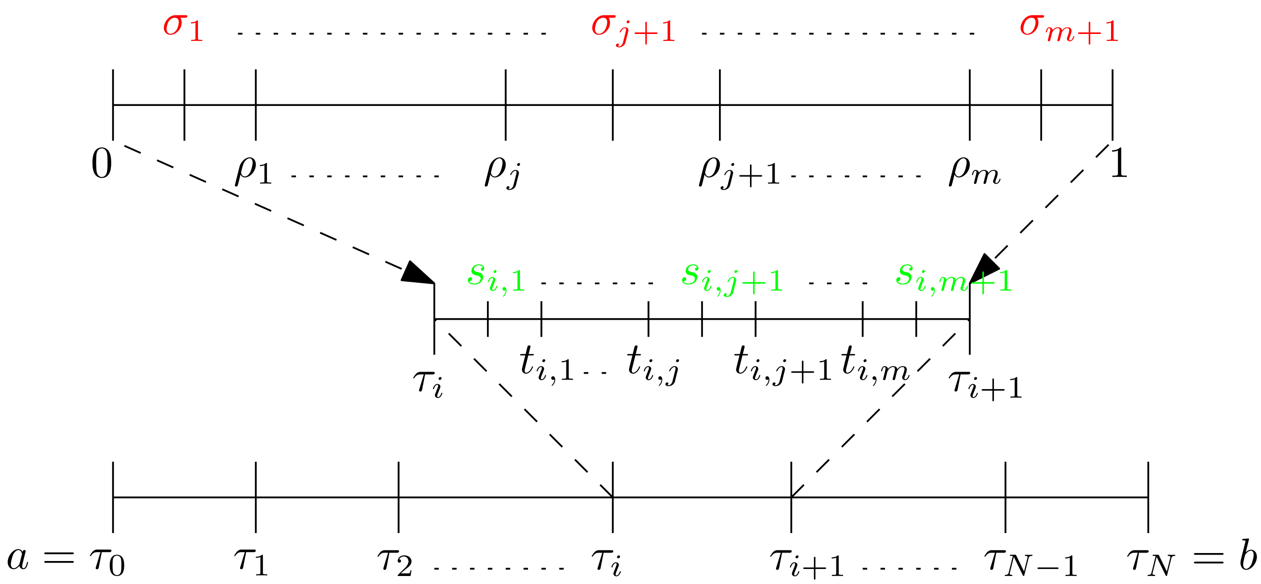


Overdetermined variant of collocation



Without increasing the degree of the collocation polynomial, additional conditions are required to hold

Overdetermined variant of collocation



Without increasing the degree of the collocation polynomial, additional conditions are required to hold

The overdetermined system is then solved in the least squares sense

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Future activities

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Future activities

- Convergence theory: Space singularities and singularities on both interval ends

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Future activities

- Convergence theory: Space singularities and singularities on both interval ends
- Convergence analysis: Higher index DAEs