How to approximate singular BVPs in ODEs and DAEs efficiently?

E. Weinmüller

Vienna University of Technology

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Outline

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More general class of problems
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Collocation
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Software development
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Introduction: Problem setting: singular BVPs in ODEs

$$z'(t) = F(t, z(t)), \quad t \in (0, 1]$$
$$b(z(0), z(1)) = 0$$

$F(t, z(t))$ unbounded for $t \to 0$ and not Lipschitz continuous on $[0, 1]$!

Typically, $\lim_{t\to 0} \frac{\partial F(t,z(t))}{\partial z} = \infty$!

Interested in $z \in C[0, 1]$, even $z \in C^p[0, 1]$, $p \geq 1$

Important contributions:

Jamet, Brabston, Keller, Wolfe, Parter, Stein, Shampine, Russell, de Hoog, Weiss, Markowich, Ringhofer, Ascher, Schmeiser, Troger, Abramov, Koniuchova, Lima, März, Winkler, Auzinger, Koch, Cash, Muir, Budd, Stanek, Rachunkova, Amodio, Burkotova, Settanni, Levitina...

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Existence and uniqueness of $z \in C[0,1]$, smoothness, convergence of the polynomial collocation

Linear case:

$$z'(t) = \frac{M(t)}{t} z(t) + f(t), \quad z'(t) = \frac{M(t)}{t^\alpha} z(t) + f(t)$$

Nonlinear case:

$$z'(t) = \frac{M}{t} z(t) + f(t, z(t)), \quad z'(t) = \frac{M}{t^\alpha} z(t) + f(t, z(t))$$

Time singularities

of the first kind $\alpha = 1$, of the second kind $\alpha > 1$

Problems posed on semi-infinite intervals

$z'(t) = f(t, z(t)), \quad t \in [0, \infty)$

Space singularities

$z'(t) = \frac{f(t,z(t))}{g(z(t))}, \quad t \in [a, b], \quad g(z(t_0)) = 0, \; t_0 \in [a, b]$

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‘Regular’ BVPs with singular point: available results

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Models in singular ODEs – CGL equation

Budd, Koch, W. (2006)

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

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

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 $y = y(\tau), \tau > 0$, satisfies

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

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

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More general class of problems with a singularity of the first kind:

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

(Vainikko 2013, 2013, Auzinger, Auer, Burkotová, Rachůnková, Staněk, EW, Wurm 2014, 2017, 2017, 2018, 2021) Analysis for the general linear and nonlinear case

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

Available results: Existence and uniqueness of continuous solutions $z \in C[0, 1]$, smoothness, and convergence of the polynomial collocation

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Crystallization in thin amorphous layers

(Buchner, Schneider 2010) Calculation of the crystallization front propagating through a thin layer of amorphous material on a substrate

The original problem is posed on a semi-infinite interval, we transform

$\tau \in [0, \infty) \to t \in (0, 1]$ by

$$t = 1 - \frac{1}{\sqrt{1+\tau}}$$

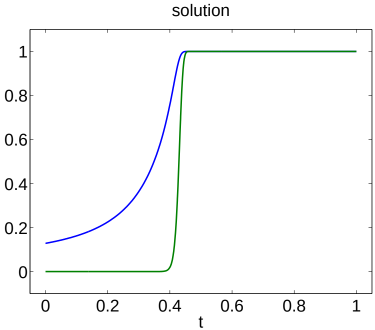
The resulting boundary value problem for the temperature distribution $\Theta(t)$ and the degree of crystallization $\xi(t)$, $t \in [0, 1)$, reads:

$$\Theta'(t) = 2\frac{\Theta(t) - \xi(t)}{(1-t)^3}, \quad \xi'(t) = 2\frac{\lambda^2 G(\Theta(t))g(\xi(t))}{(1-t)^3},$$

$$\Theta(0) = 0{,}1284, \quad \Theta(1) = 1, \quad \xi(0) = 10^{-10}$$

- Essential singularity at $t = 1$
- λ is unknown and related to the speed of the crystallization front
- Third condition: at the beginning tiny crystals may already exist in the material

Crystallization in thin amorphous layers (2)



Graph of the solution components $\Theta(t)$ (blue) and $\xi(t)$ (green) obtained from `bvpsuite1.1` using collocation with $m = 8$ Gaussian points and $Tol_a = Tol_r = 10^{-12}$. Here, $\lambda = 11{,}03605$.

(Kitzhofer, Koch, Pulverer, Simon, EW 2010)

Now we transform $\tau \in [0, \infty) \to t \in [1, 0)$ by

$$\tau := -\ln t$$

The resulting BVP for the temperature distribution $\Theta(t)$ and the degree of crystallization $\xi(t)$, $t \in [0, 1)$, reads:

$$\Theta'(t) = -\frac{\Theta(t) - \xi(t)}{t}, \quad \xi'(t) = -\frac{\lambda^2 G(\Theta(t)) g(\xi(t))}{t},$$

$$\Theta(1) = 0{,}1284, \quad \Theta(0) = 1, \quad \xi(1) = 10^{-10}$$

- Singularity of the first kind at $t = 0$

Lamour, März, W. (2015)

Consider the DAE

$$x_1'(t) + x_1(t) = 0,$$
$$x_2(t)\, x_2'(t) - x_3(t) = 0,$$
$$x_1(t)^2 + x_2(t)^2 - 1 + \frac{1}{2}\cos(\pi t) = 0,$$

$$x_1(0) - x_1(2) = \alpha, \quad |\alpha| < \frac{1}{2}(1 - \mathrm{e}^{-2}).$$

The solution has to belong to the set

$$\mathcal{M}_0(t) := \{x \in \mathbb{R}^3 : x_1^2 + x_2^2 - 1 + \frac{1}{2}\cos(\pi t) = 0\}.$$

Again, consider

$$x_1'(t) + x_1(t) = 0, \quad x_2(t)\, x_2'(t) - x_3(t) = 0,$$
$$x_1(t)^2 + x_2(t)^2 - 1 + \frac{1}{2}\cos(\pi t) = 0.$$

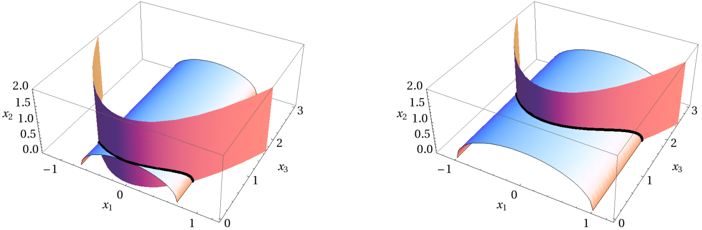
Let $x_*(\cdot)$ be a solution and let us differentiate the last identity. Then,

$$2x_{*1}(t)x_{*1}'(t) + 2x_{*2}(t)x_{*2}'(t) - \pi\frac{1}{2}\sin(\pi t) = 0$$

and finally, $-2x_{*1}(t)^2 + 2x_{*3}(t) - \frac{1}{2}\pi\sin(\pi t) = 0$. Therefore, all solution values $x_*(t)$ must belong to the set

$$\mathcal{H}(t) := \{x \in \mathbb{R}^3 : -2x_1^2 + 2x_3 - \frac{1}{2}\pi\sin(\pi t) = 0\}.$$

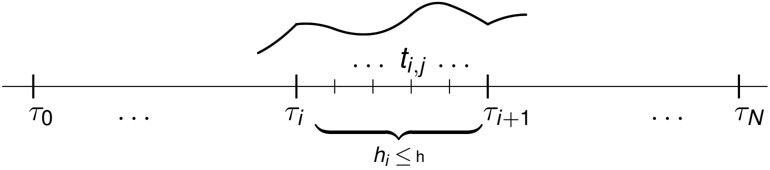
The proper restriction set is
$\mathcal{M}_1(t) := \mathcal{M}_0(t) \cap \mathcal{H}(t) \subset \mathcal{M}_0(t)$.



Constraint set $\mathcal{M}_1$ at $t = 0$ and $t = \frac{1}{2}$

Collocation method

Consider a partition of the interval $[0, 1]$,



In $[\tau_i, \tau_{i+1}]$, introduce m inner collocation points t_{ij}

$\mathcal{P}_m$ ... the class of polynomial 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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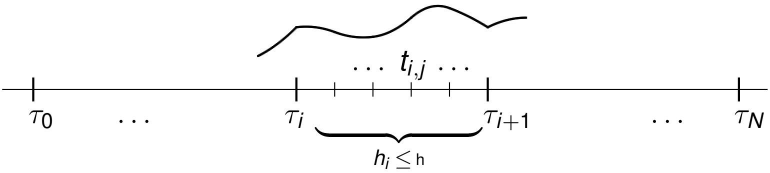

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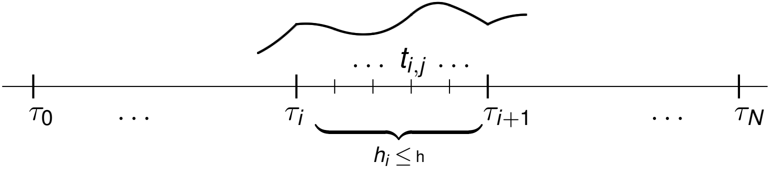

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Consider the IVP

$$z'(t) = \frac{M(t)}{t} z(t) + \frac{f(t, z(t))}{t}, \quad M(0)z(0) + f(0, z(0)) = 0$$

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

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

subject to

$$M(0)p(0) + f(0, p(0)) = 0$$

Theorem: Let $z \in C^{m+1}[0,1]$ be the unique solution of the analytical IVP. For sufficiently small h and $\rho > 0$, the related nonlinear collocation scheme has a unique solution p in the tube $T_\rho(z)$ around z. Moreover, the following estimates hold:

$$\|z - p\|_{[0,1]} = O(h^m),$$
$$\|z' - p'\|_{[0,1]} = O(h^m),$$
$$\left| p'(t) - \frac{M(t)}{t} p(t) - \frac{f(t, p(t))}{t} \right| = O(h^m), \quad t \in [0,1].$$

- First aim:
  Define basic concepts such as *local well-posedness and accurately stated BCs* in context of BVP in DAEs.
- DAEs can be written in a standard, $f(x'(t), x(t), t) = 0$, and advanced form

$$f((Dx)'(t), x(t), t) = 0, \quad x \in \mathbb{R}^m, \quad f \in \mathbb{R}^m.$$

  Matrix function $D = D(t) \in \mathbb{R}^{n\times m}$ indicates which derivatives are involved, $Dx \in \mathbb{R}^n$, $n \le m$.
- Linear version of the DAE

$$A(t)(Dx)'(t) + B(t)x(t) - f(t) = 0,$$
$$A \in \mathbb{R}^{m\times n}, \ D \in \mathbb{R}^{n\times m}, \ B \in \mathbb{R}^{m\times m}.$$

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(Lamour, März, W. 2015)

- Assumptions: $t \in \mathcal{I} = [a, b]$

$$f((Dx)'(t), x(t), t) = 0, \quad g(x(a), x(b)) = 0.$$

- $f(y, x, t)$ is cont. with cont. partial derivatives f_y, f_x.
- The partial Jacobian $f_y(y, x, t)$ is everywhere singular.
- $g \in \mathbb{R}^l$ is cont. differentiable.
- The matrix function D is cont. and $D(t)$ has constant rank r on the given interval $\mathcal{I}$.

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- Classical solution x of the DAE is a functions from

$$\mathcal{C}^1_D(\mathcal{I},\mathbb{R}^m) := \{x \in \mathcal{C}(\mathcal{I},\mathbb{R}^m) : Dx \in \mathcal{C}^1(\mathcal{I},\mathbb{R}^n)\},$$

satisfying the DAE pointwise on $\mathcal{I}$.

This function space setting is the *natural setting* of DAE.

- The DAE has a properly involved derivative or properly stated leading term:

$$f((Dx)'(t),x(t),t)=0: \ \ker f_y(y,x,t) \oplus \mathrm{im} D(t) = \mathbb{R}^n,$$
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Well-posedness in the sense of Hadamard constitutes the classical basis of a safe numerical treatment. We assume that a solution exist and concentrate on a local variant of well-posedness.

Definition: Let $x_* \in \mathcal{C}^1_D(\mathcal{I}, \mathbb{R}^m)$ be a solution of the original BVP,

$$f((Dx)'(t), x(t), t) = 0, \quad g(x(a), x(b)) = 0.$$

The BVP is said to be *well-posed locally around x_* in its natural setting*, if the BVP

$$f((Dx)'(t), x(t), t) = q(t), \quad g(x(a), x(b)) = \gamma$$

is locally uniquely solvable for arbitrary sufficiently small perturbations $q \in \mathcal{C}(\mathcal{I}, \mathbb{R}^m)$ and $\gamma \in \mathbb{R}^l$, and the solution x satisfies the inequality

$$\|x - x_*\|_{\mathcal{C}^1_D} \leq \kappa(|\gamma| + \|q\|_\infty),$$

with a constant κ.

Otherwise the BVP is said to be *ill-posed in the natural setting*.

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Well-posedness of BVPs in DAEs: Definition

Well-posedness in the sense of Hadamard constitutes the classical basis of a safe numerical treatment. We assume that a solution exist and concentrate on a local variant of well-posedness.

Definition: Let $x_* \in \mathcal{C}_D^1(\mathcal{I}, \mathbb{R}^m)$ be a solution of the original BVP,

$$f((Dx)'(t), x(t), t) = 0, \quad g(x(a), x(b)) = 0.$$

The BVP is said to be *well-posed locally around x_* in its natural setting*, if the BVP

$$f((Dx)'(t), x(t), t) = q(t), \quad g(x(a), x(b)) = \gamma$$

is locally uniquely solvable for arbitrary sufficiently small perturbations $q \in \mathcal{C}(\mathcal{I}, \mathbb{R}^m)$ and $\gamma \in \mathbb{R}^l$, and the solution x satisfies the inequality

$$\|x - x_*\|_{\mathcal{C}_D^1} \leq \kappa(|\gamma| + \|q\|_\infty),$$

with a constant κ.

Otherwise the BVP is said to be *ill-posed in the natural setting*.

Accurately stated BCs: Definition

It is very important to apply exactly the right number of BCs/ICs. This task is more difficult to realize for DAEs than for explicit ODEs.

Definition: Let $x_* \in C^1_D(\mathcal{I}, \mathbb{R}^m)$ be a solution of the original BVP,

$$f((Dx)'(t), x(t), t) = 0, \quad g(x(a), x(b)) = 0.$$

The BVP has *accurately stated boundary conditions* locally around x_* if the BVP with slightly perturbed boundary conditions

$$f((Dx)'(t), x(t), t) = 0, \quad g(x(a), x(b)) = \gamma,$$

is uniquely solvable for arbitrary sufficiently small perturbation $\gamma \in \mathbb{R}^l$, and the solution x satisfies the inequality $\|x - x_*\|_{C^1_D} \leq \kappa|\gamma|$, with a constant κ.

For explicit ODEs, the well-posedness of the BVP is equivalent to the accurately stated BCs, U. Ascher, R. Mattheij, R. Russell (1988). This is not the case for DAEs: well-posedness implies accurately stated boundary conditions but the opposite is not true.

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Example: Well-posedness vs. accurately stated BCs

Consider the following DAEs (index 2):

$$x_1'(t) + x_3(t) = 0, \quad x_2'(t) + x_3(t) = 0, \quad x_2(t) - \sin(t-a) = 0,$$

subject to $x_1(a) + \alpha x_2(a) + \beta x_3(a) = 0, \alpha, \beta \in \mathbb{R}$

The DAE has the following solution:

$$x_{*1}(t) = \beta + \sin(t-a),\ x_{*2}(t) = \sin(t-a),\ x_{*3}(t) = -\cos(t-a).$$

The DAE with the perturbed BC has the following solution:

$$x_1(t) = \beta + \gamma + sin(t-a),\ x_2(t) = \sin(t-a),\ x_3(t) = -\cos(t-a).$$

This means that

$$x(t) - x_*(t) = (\gamma, 0, 0)^T.$$

Therefore, the above BVP has accurately stated BCs.

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Consider the original and perturbed DAEs,

$$\begin{aligned} x_1'(t) + x_3(t) &= 0, \\ x_2'(t) + x_3(t) &= 0, \\ x_2(t) - \sin(t-a) &= 0, \\ x_1(a) + \alpha x_2(a) + \beta x_3(a) &= 0, \end{aligned} \qquad \begin{aligned} x_1'(t) + x_3(t) &= q_1(t), \\ x_2'(t) + x_3(t) &= q_2(t), \\ x_2(t) - \sin(t-a) &= q_3(t), \\ x_1(a) + \alpha x_2(a) + \beta x_3(a) &= \gamma. \end{aligned}$$

We can solve the perturbed problem and obtain

$$x(t) - x_*(t) = \begin{bmatrix} \gamma + q_3(t) - q_3(a) + \int_a^t (q_1(s) - q_2(s))ds \\ q_3(t) \\ q_2(t) - q_3'(t) \quad !!! \end{bmatrix}, \quad t \in \mathcal{I}.$$

This means that $x(t) - x_*(t)$ cannot be estimated in terms of $\|q\|_\infty$. Therefore, the above BVP is ill-posed in the natural setting.

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x_2(t) - \sin(t-a) = 0, & x_2(t) - \sin(t-a) = q_3(t), \\
x_1(a) + \alpha x_2(a) + \beta x_3(a) = 0, & x_1(a) + \alpha x_2(a) + \beta x_3(a) = \gamma.
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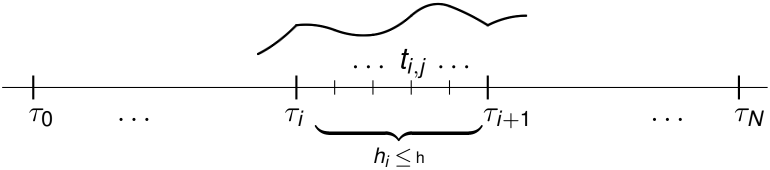
Collocation methods



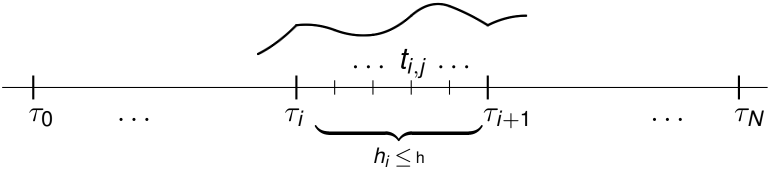
Define a mesh
$\Delta := (\tau_0 = a, \tau_1, \dots, \tau_{N-1}, \tau_N = b)$, and m distinct points $t_{i,j}$ in each subinterval $[\tau_i, \tau_{i+1}]$.

We now discretize the enlarged DAE

$$f(u'(t), x(t), t) = 0, \quad u(t) - D(t)x(t) = 0, \quad g(x(a), x(b)) = 0.$$

Approximations: $u_\Delta, x_\Delta \in \mathcal{P}_{\Delta,m} \cap \mathcal{C}(\mathcal{I}, \mathbb{R}^n)$ approximate u_* and x_*, respectively.

The above collocation scheme results in the classical collocation scheme for the inherent ODE subject to BCs. Therefore, for sufficiently small h, u_Δ and consequently x_Δ exist and are unique.



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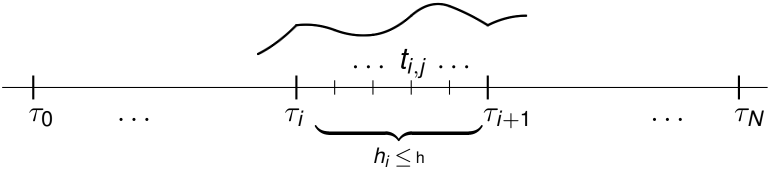

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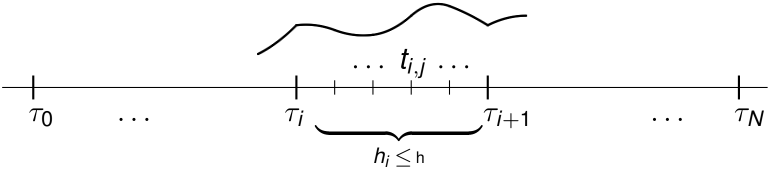

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Convergence result

Let the original BVP

$$f((Dx)'(t), x(t), t) = 0, \ g(x(a), x(b)) = 0, \ \mathrm{im} D(t) = \mathbb{R}^n,$$

be well-posed locally around its solution x_* in the natural setting and let the data of the DAE be sufficiently smooth.

Then, for the above collocation scheme the following statements hold:

- There is a $h_* > 0$, such that, for meshes with $h \leq h_*$, there exists a unique collocation solution u_Δ, x_Δ in the sufficiently close neighborhood of u_*, x_*.
- With a sufficiently good initial guess, the collocation solution can be generated by the Newton method, which converges quadratically.
- Moreover, $\|x_* - x_\Delta\|_\infty = O(h^m), \quad \|u_* - u_\Delta\|_\infty = O(h^m).$
- For Gaussian points, the superconvergence order holds for the smooth component

$$\max_{i=0,\ldots,N} |u_*(\tau_i) - u_\Delta(\tau_i)| = O(h^{2m}).$$

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Numerical results

Nonlinear example

$$x = (x_1, x_2)^T = (x_{11}, x_{12}, x_{21}, x_{22})^T, \quad b(t, x(t)) = Bx(t) + tC(x(t))x(t) + f(t),$$

$$\begin{array}{l} t x_1'(t) + b_1(t, x(t)) = 0, \\ \qquad\quad\; b_2(t, x(t)) = 0, \end{array} \quad B \in \mathbb{R}^{4\times 4},\; C(x) = \begin{pmatrix} \sin x_{12} & 0 & e^{-x_{11}} & 0 \\ 0 & \cos x_{22} & 0 & \sin(x_{11} + x_{21}) \\ x_{12}^3 & 0 & x_{11} & 0 \\ 0 & x_{11}x_{12} & 0 & x_{12}^2 \end{pmatrix},$$

coupled BCs at $t = 0$, $t = 1$, $m = 4$, solution: $x_{11} = t^2 \sin t$, $x_{12} = te^t$, $x_{21} = t\cos t$, $x_{22} = \sin t$.

Uniform Mesh		Error for x_1 at Mesh `tau, eq`			Error for x at Grid `tcol, eq`		
N	**h**	**error**	**order**	**const.**	**error**	**order**	**const.**
10	1.00e−01	2.043e−07			1.127e−06		
20	5.00e−02	1.268e−08	4.0	2.087e−03	7.074e−08	4.0	1.110e−02
40	2.50e−02	7.916e−10	4.0	2.043e−03	4.430e−09	4.0	1.122e−02
80	1.25e−02	4.946e−11	4.0	2.030e−03	2.770e−10	4.0	1.131e−02
160	6.25e−03	3.088e−12	4.0	2.040e−03	1.728e−11	4.0	1.149e−02
320	3.13e−03	1.895e−13	4.0	2.308e−03	1.464e−12	3.6	1.220e−03

Uniform Mesh		Error for x_1 at Mesh `tau, gauss`			Error for x at Grid `tcol, gauss`		
N	**h**	**error**	**order**	**const.**	**error**	**order**	**const.**
10	1.00e−01	7.254e−09			4.215e−07		
20	5.00e−02	2.264e−10	5.0	7.280e−04	2.646e−08	4.0	4.155e−03
40	2.50e−02	7.066e−12	5.0	7.289e−04	1.655e−09	4.0	4.214e−03
80	1.25e−02	2.210e−13	5.0	7.206e−04	1.035e−10	4.0	4.232e−03
160	6.25e−03	7.976e−15	4.8	2.914e−04	6.520e−12	4.0	4.029e−03

Petzold (1982), März (1992)

Consider

$$
\begin{aligned}
&x_2'(t) + x_1(t) = q_1(t),\\
&-1/2tx_2'(t) + x_3'(t) + 1/2x_2(t) = q_2(t),\\
&-1/2tx_2(t) + x_3(t) = q_3(t),
\end{aligned}
$$

with a smooth $q(t)$. This system has no inherent ODE (no BCs necessary) and the solution reads:

$$
x_1(t) = q_1(t) - q_2'(t) + q_3''(t), \quad x_2(t) = q_2(t) - q_3'(t),
$$

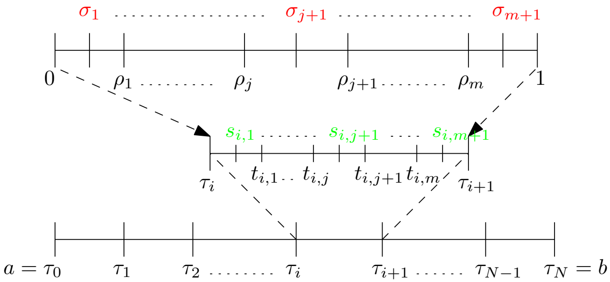
$$
x_3(t) = q_3(t) + \frac{1}{2}tx_2(t),
$$

or equivalently,

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

$$
x_3(t) = \mathrm{e}^{-t}\cos(t).
$$

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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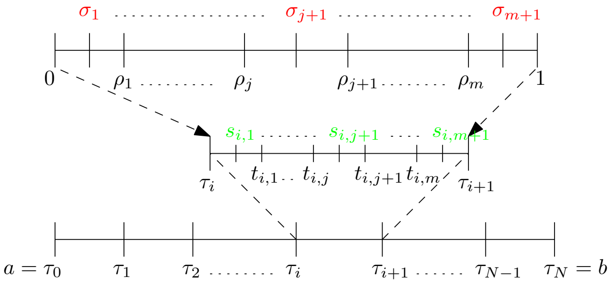

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Table of errors for $m = 2$

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

History:

sbvp (2003), bvpsuite 1.1 (2009), bvpsuite 2.0 (2018-2020)

http://www.asc.tuwien.ac.at/~ewa/

Implicit mixed order (singular) ODEs including unknown parameters

- BVPs in ODEs on finite and semi-infinite intervals
- EVPs in ODEs on finite and semi-infinite intervals
- Index-1 DAEs on finite and semi-infinite intervals
- Pathfollowing for BVPs and EVPs in ODEs on finite and semi-infinite intervals for parameter dependent BVPs in ODEs

Error estimate and mesh adaptation strategy

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sbvp (2003), bvpsuite 1.1 (2009), bvpsuite 2.0 (2018-2020)

http://www.asc.tuwien.ac.at/~ewa/

Implicit mixed order (singular) ODEs including unknown parameters

- BVPs in ODEs on finite and semi-infinite intervals
- EVPs in ODEs on finite and semi-infinite intervals
- Index-1 DAEs on finite and semi-infinite intervals
- Pathfollowing for BVPs and EVPs in ODEs on finite and semi-infinite intervals for parameter dependent BVPs in ODEs

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well-posed with a locally unique smooth solution

- Numerical method: Robust with respect to singularity

  $$\|\text{global error}\| = O(h^m), \;\; m \text{ reasonably large}$$

  Our choice is *polynomial collocation*

- Error estimation: Robust and asymptotically correct

  $$\|\text{global error - error estimate}\| = O(h^{m+\gamma}), \;\; \gamma > 0$$

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- Adaptive mesh selection:
  Meshes unaffected by the nonsmooth (!) direction field

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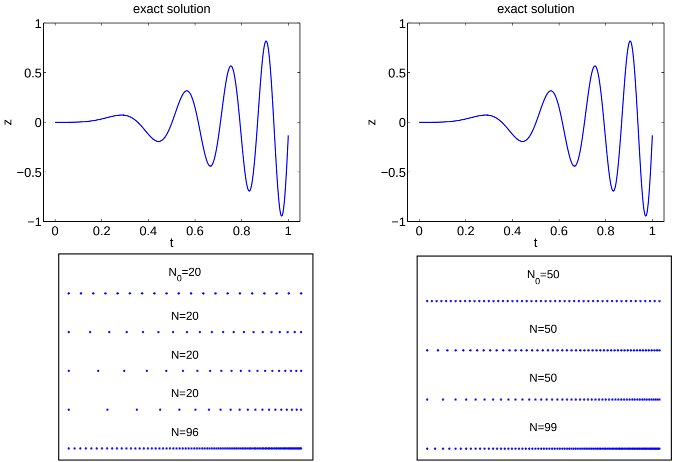
Computational experiment – grid adaptation



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

An application: Shell buckling problem 1

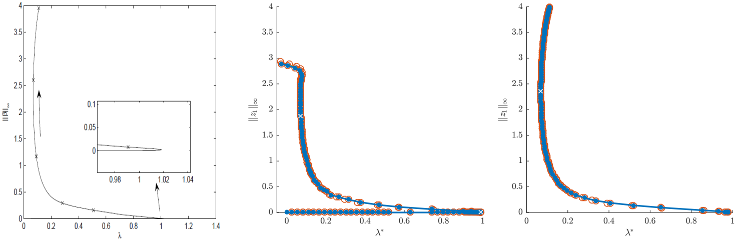
Kitzhofer, Koch, EW 2009, MT Fallahpour 2020, private kommunikation with A. Steindl, TU Wien 2020, Auzinger, Burdeos, Fallahpour, Koch, Mendoza, EW submitted

$$
\begin{aligned}
z_1''(t) + \cot(t) z_1'(t) + \cot^2(t) f_1(t, z_1(t)) &= f_2(t, z_1(t), z_2(t), z_3(t), \lambda^*) \\
z_2''(t) + \cot(t) z_2'(t) - \cot^2(t) g_1(s, z_1(t)) &= g_2(s, z_1(t), z_2(t), z_3(t), \lambda^*)
\end{aligned}
$$

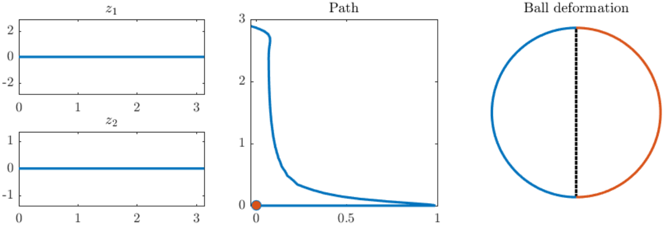
$$
z_3(t) = \int_0^t \cos(s - z_1(s)) \sin(s) ds, \quad \lambda * = \frac{p}{p_{cr}} \in [0, 1]
$$

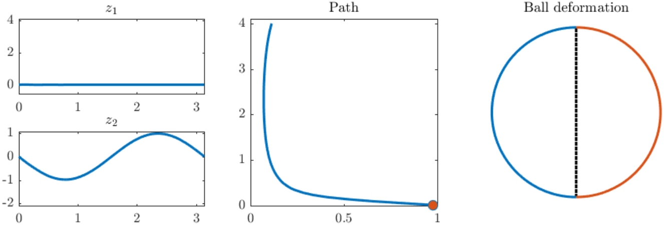
$$
z_3'(t) = \cos(t - z_1(t)) \sin(t), \quad t \in (0, \pi),
$$

$$
z_1(0) = z_1(\pi) = 0, \quad z_2(0) = z_2(\pi) = 0, \quad z_3(0) = 0.
$$



Shell buckling problem 2





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- Existence, uniqueness and smoothness results of solutions $z \in C[0,1]$ of

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  subject to correctly posed BCs are available. For IVPs with all eigenvalues of $M(0)$ being negative, the correctly posed ICs are

$$M(0)z(0) + f(0, z(0)) = 0$$

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