Numerical Solution of Singular ODEs

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$$z'(t) = F(t, z(t)) = \frac{1}{t} G(t, z(t)), \;\; t \in (0, 1]$$
$$B_a z(0) + B_b z(1) = \beta$$

$F(t, z(t))$ 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, März, Winkler, Auzinger, Koch, Cash, Muir, Budd, Stanek, Rachunkova, Amodio, Burkotova, Settanni, Levitina...

Typical models for the analysis:
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
$z'(t) = \frac{f(t,z(t))}{g(z(t))}, \quad t \in [a, b], \quad g(z(t_0)) = 0, t_0 \in [a, b]$

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, Auzinger, Auer, Burkotová, Rachůnková, Staněk, EW, Wurm 2014, 2017, 2018, 2021)

Available: Analysis for the general linear and nonlinear case

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

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

Today:
(1) Basic facts about the convergence of collocation, in context of IVPs
(2) MATLAB code `bvpsuite2.0`: pathfollowing module
(3) Collocation vs. Finite Differences

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 exist in the material

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:

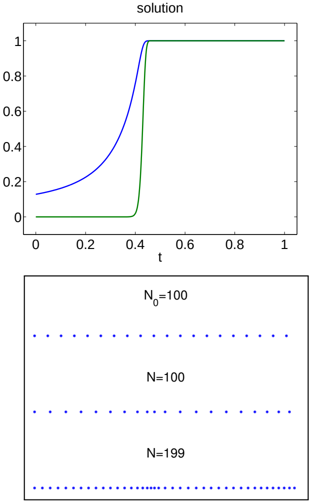
$$\Theta'(t) = -\frac{\Theta(t) - \xi(t)}{t}, \quad \xi'(t) = -\frac{\lambda^2 G(\Theta(t)) g(\xi(t))}{t},$$

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

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

Mesh adaptation

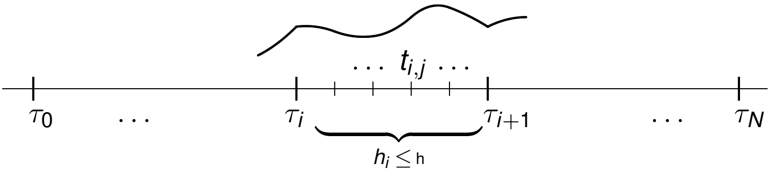
(Kitzhofer, Koch, Pulverer, Simon, EW 2010)



Graph of the solution components $\Theta(t)$ (blue) and $\xi(t)$ (green) obtained from `bvpsuite1.1`.
Method: collocation at 8 Gaussian points with tolerances: $Tol_a = Tol_r = 10^{-12}$.

Collocation method, smooth right hand side f

$$z'(t) - F(t, z(t)) = 0, \quad z'(t) = \frac{1}{t} M z(t) + f(t, z(t)); \; \left(f = \frac{g}{t} \right)$$



- 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
- *Convergence regular case*: $\|p - z\|_\infty = O(\mathrm{h}^m)$ superconvergence at τ_i (de Boor, Swartz 1973)
- *Convergence singular case*: $\|p - z\|_\infty = O(\mathrm{h}^m |\ln \mathrm{h}|^{n_0 - 1})$ no superconvergence (de Hoog, Weiss 1978, Auzinger, Koch, EW 2002, Koch 2005)
- Similar results for $f = g/t$ (Burkotová, Rachunková, EW 2015, 2018, 2021)

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 satisfying the collocation conditions

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

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:

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

Example

$$z'(t) = \frac{M(t)}{t}z(t) + \frac{1}{3}\frac{f(t,z(t))}{t}, \quad M(0)z(0) + \frac{1}{3}f(0,z(0)) = 0$$

$$M(t) = \begin{pmatrix} \lambda_1 + (\exp(t) - 1) & \exp(-t) - 1 \\ \exp(2t) - 1 & \lambda_2 + (\exp(-2t) - 1) \end{pmatrix}$$

$$M(0) = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}, \lambda_1 = -1, \quad \lambda_2 = -2, \quad \beta = 1$$

Function f is specified as follows:

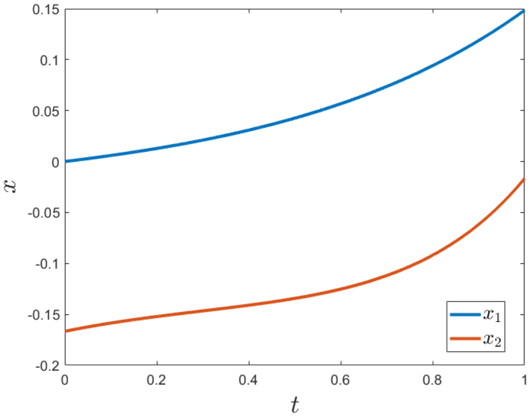
$$f(t,z) = p(t) + H(t)r(t,z), \quad p(t) = \begin{pmatrix} t^2/2 \\ -1 \end{pmatrix}$$

where

$$H(t) = \begin{pmatrix} t & 0 \\ \sin(t) & \cos(t) - 1 \end{pmatrix} \in C[0,1], \quad r(t,z) = \begin{pmatrix} \sin(z_1 + z_2) \\ \cos(z_1 + z_2) \end{pmatrix} \in C[0,1]$$

f satisfies the Lipschitz condition with $L = \frac{2\sqrt{2}}{3} < 1$ and the IVP problem has a unique solution $z \in C^\infty[0,1]$

Numerical experiment (1)



Graph of the solution components

Numerical experiment (2)

$m = 2$		equidistant			Gaussian		
N	h	error	order	const.	error	order	const.
4	2.50e-01	3.0e-3	2.00	4.85e-02	6.3e-5	2.96	3.8e-03
8	1.25e-01	7.5e-4	2.00	4.83e-02	8.1e-6	2.95	3.7e-03
16	6.25e-02	1.9e-4	2.00	4.81e-02	1.1e-6	2.97	3.9e-03
32	3.13e-02	4.7e-5	2.00	4.81e-02	1.4e-7	2.98	4.1e-03

For the Gaussian points the order of global error in the mesh points τ_i is 3.

$m = 3$		equidistant			Gaussian		
N	h	error	order	const.	error	order	const.
4	2.50e-01	8.6e-5	3.94	2.0e-02	2.4e-7	5.53	4.3e-04
8	1.25e-01	5.6e-6	3.99	2.2e-02	4.4e-9	5.37	3.1e-04
16	6.25e-02	3.5e-7	4.00	2.3e-02	1.1e-10	5.16	1.6e-04
32	3.13e-02	2.2e-8	4.00	2.3e-02	3.0e-12	3.69	1.1e-06

For the Gaussian points the order of global error in the mesh points τ_i is 4.

- Main assumption: Analytical problem is

  well-posed with a locally unique smooth solution

- Basic solver: robust with respect to singularity and high order of convergence for smooth problem solutions
  $\Rightarrow$ Collocation (!)

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

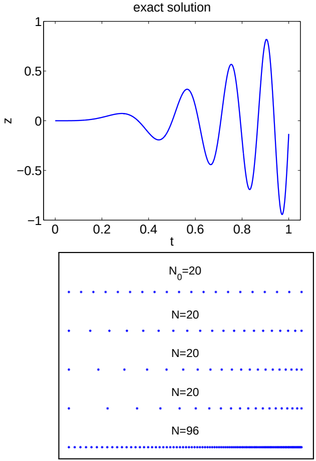
- Error estimate: Robust and asymptotically correct

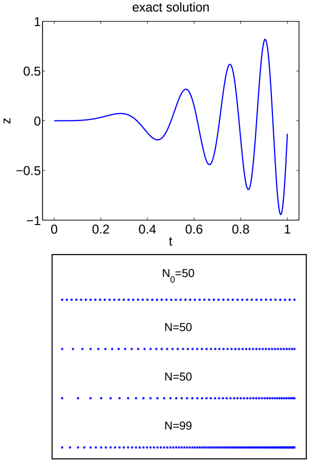
$$\|\text{global error - error estimate}\| = O(h^{m+\gamma}),\ \gamma > 0$$

$\Rightarrow$ Collocation: $h - h/2$ strategy

- Grid adaptation: unaffected (!) by the direction field

Mesh adaptation: robust and unaffected by the non-smooth direction field





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

Pathfollowing problem: pseudo-arclength continuation

(Kitzhofer, Koch, EW 2009, Deuflhard 2004, Auzinger, Burdeos, Fallahpour, Koch, Mendoza, EW 2021)

Find $x \in D \subset \mathbb{R}^\eta$, $\eta \in \mathbb{N}$ such that for $\lambda^* \in \mathbb{R}$,

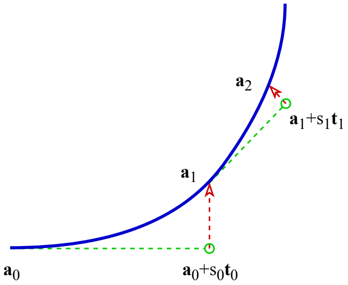
$$F(x, \lambda^*) = 0, \quad F : \mathbb{R}^{\eta+1} \to \mathbb{R}^\eta, \quad \boldsymbol{a} := (x, \lambda^*) \in \mathbb{R}^{\eta+1}$$

Assumptions:

- there exists an isolated path $\boldsymbol{\mathcal{A}}$ of F in $\mathbb{R}^{\eta+1}$,
- given starting solution $\boldsymbol{a}_0$ on the path $\boldsymbol{\mathcal{A}}$

Pseudo-arclength continuation:

- predictor: find $\hat{\boldsymbol{a}}_0 \in \mathbb{R}^{\eta+1}$ close to the path
- corrector: starting at $\hat{\boldsymbol{a}}_0$, we arrive at the corrector $\boldsymbol{a}_1$



Advantage: pathfollowing around turning points is possible

http://www.tuwien.at/mg/asc/weinmueller

History:
sbvp (2003), bvpsuite 1.1 (2009), bvpsuite 2.0 (2018-2021)

- Implicit mixed order (singular) ODEs including unknown parameters
- Eigenvalue Problems
- Index 1 DAEs
- Parameter dependent BVPs in ODEs
- Problems posed on semi-infinite intervals
- Error estimate and mesh adaptation strategy

Shell buckling problem (1)

(Kitzhofer, Koch, EW 2009, MT Fallahpour 2020, private communication with A. Steindl, TU Wien 2020, Auzinger, Burdeos, Fallahpour, Koch, Mendoza, EW 2021)

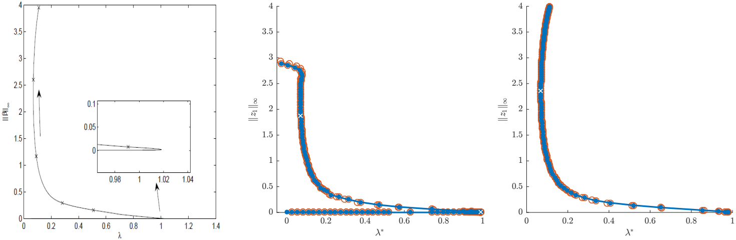
$$z_1''(t) + \cot(t) z_1'(t) + \cot^2(t) f_1(t, z_1(t)) \;= f_2(t, z_1(t), z_2(t), z_3(t), \lambda^*)$$

$$z_2''(t) + \cot(t) z_2'(t) - \cot^2(t) g_1(s, z_1(t)) = g_2(s, z_1(t), z_2(t), z_3(t), \lambda^*)$$

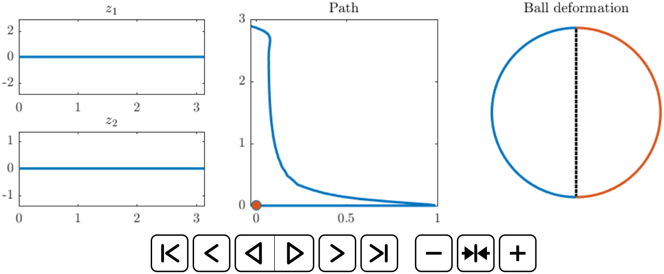
$$z_3(t) = \int_0^t \cos(s - z_1(s)) \sin(s) ds, \quad \lambda* = \frac{p}{p_{cr}} \in [0, 1]$$

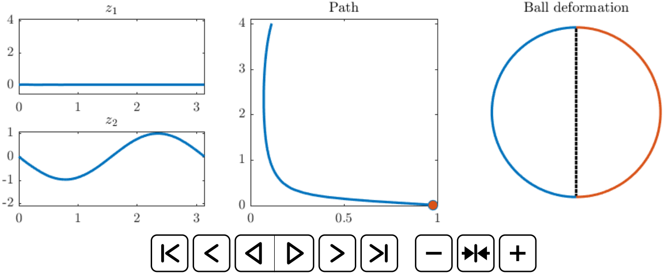
$$z_3'(t) = \cos(t - z_1(t)) \sin(t), \quad t \in (0, \pi),$$

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



Shell buckling problem (2)





- Codes:

  polynomial collocation `bvpsuite2.0` TU Wien

  finite differences `HOFiD_bvp` University of Bari

- We focus on singular BVPs

  $$\boxed{z''(t) = \frac{A_1(t)}{t} z'(t) + \frac{A_0(t)}{t^2} z(t) + f(t)}$$

  Main assumption: Analytical problem is

  well-posed with a locally unique smooth solution

- Convergence:
  Collocation is robust with respect to singularity

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

- Finite differences: no theory for singular problems yet but

  ...

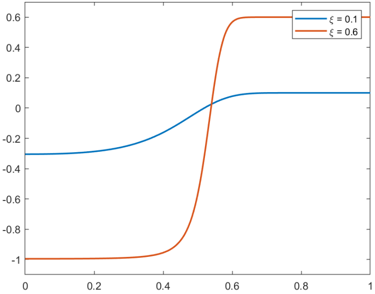
Example 1, problem in hydrodynamics

Formation of microscopic bubbles in a non-homogeneous fluid (vapour inside liquid) (Kitzhofer, Koch, EW 2007)

$$y''(t) + \frac{N-1}{t} y'(t) - 4\lambda^2 (y(t)+1) y(t) (y(t) - \xi) = 0,$$

$$y'(0) = 0, \quad y(\infty) = \xi,$$

where $N = 3$, $\lambda = 1$, and $\xi = 0{,}1, 0{,}6$.



Solutions for $\xi = 0{,}1$ and $\xi = 0{,}6$.

Example 1

order	TOL	mesh	abs. error
$\xi = 0{,}1$			
6	1e-8	51	2.8471e-14
8	1e-8	51	1.4489e-15
10	1e-8	51	2.2298e-13
$\xi = 0{,}6$			
6	1e-8	51	7.6069e-10
8	1e-8	51	2.7590e-12
10	1e-8	51	6.1910e-12

$\xi = 0{,}1$ and $\xi = 0{,}6$: Results obtained from `bvpsuite2.0`.

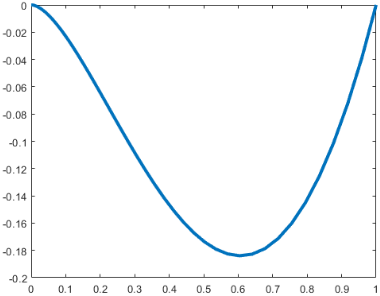
Kitzhofer, Koch, W. (2004)

order	TOL	mesh	abs. error	rel. error
6	1e-8	247	4.6386e-09	3.5608e-09
8	1e-8	86	8.2062e-09	6.2899e-09
10	1e-8	48	1.2494e-08	9.5763e-09

$\xi = 0{,}1$: Results obtained from `HOFiD_bvp`.

Example 2

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



Exact solution $y(t) = t^2 \ln t$

Example 2

order	TOL	mesh	error est.	abs. error	rel. error
6	1e-8	51	6.1013e-10	3.3430e-14	6.1490e-15
8	1e-8	51	6.6641e-10	1.7964e-13	3.3029e-14
10	1e-8	51	9.2947e-10	1.1065e-11	2.0351e-12
6	1e-8	21	3.4399e-09	2.8829e-13	5.2993e-14
8	1e-8	21	7.3561e-09	1.8116e-13	3.3168e-14
10	1e-8	21	7.3319e-09	1.0511e-11	1.9334e-12

Results from `bvpsuite2.0`

order	TOL	mesh	error est.	abs. error	rel. error
6	1e-8	918	9.3704e-09	7.6807e-08	7.6806e-08
8	1e-8	474	9.8446e-09	1.0902e-07	1.0902e-07
10	1e-8	571	9.9055e-09	1.3958e-07	1.3958e-07

Results from `HOFiD_bvp`

Why those fine meshes?

Why those fine meshes?

- Order reduction for the finite difference scheme, down to 2!
- Grid adaptation techniques are based on different principles

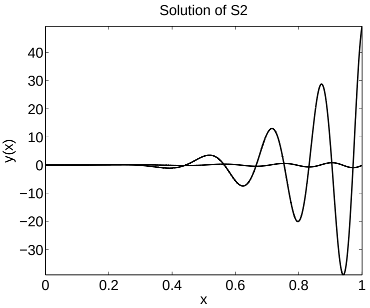
Grid adaptation in `bvpsuite2.0`

Example S2: Söderlind, Polsterer, W. (2001)

$$y'(x) = \frac{1}{x}\begin{pmatrix} 0 & 1 \\ 2 & 6 \end{pmatrix} y(x) - \begin{pmatrix} 0 \\ 4k^4x^5\sin(k^2x^2) + 10x\sin(k^2x^2) \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} y(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} y(1) = \begin{pmatrix} 0 \\ \sin(k^2) \end{pmatrix}$$

$k = 5$



Grid adaptation in `bvpsuite2.0`

TOL	equidistant	nga	bvpsuite
1e-6	3 844	1 583	14 018
1e-7	8 281	3 354	44 329
1e-8	17 842	7 079	76 012

Problem BVP S2, $m = 2$. Number of grid points necessary to satisfy the tolerance on an equidistant grid and the non-equidistant grids provided by `nga`, `bvpsuite`, and `sbvp`

TOL	equidistant	nga	bvpsuite
1e-6	209	93	188
1e-7	331	145	335
1e-8	526	226	398

Problem BVP S2, $m = 4$

TOL	equidistant	nga	bvpsuite
1e-6	57	42	43
1e-7	78	59	62
1e-8	106	80	92

Problem BVP S2, $m = 6$

Conclusion

- Software for singular problems based on collocation is standard
- Separation of finding the grid density function and the number of grid points to satisfy the tolerance results (in general) in coarser grids

Thank you for listening!