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E. Weinmüller

Institute for Analysis and Scientific Computing —  
Vienna University of Technology — TU Wien  
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Institute for Analysis and Scientific Computing  
Vienna University of Technology  
Wiedner Hauptstraße 8–10  
1040 Wien, Austria

**E-Mail:** [admin@asc.tuwien.ac.at](mailto:admin@asc.tuwien.ac.at)  
**WWW:** <http://www.asc.tuwien.ac.at>  
**FAX:** +43-1-58801-10196

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# Collocation – a powerful tool for solving singular ODEs and DAEs

E. B. Weinmüller

*Department for Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstraße 8–10, A-1040 Wien, Austria*

**Abstract.** We discuss how polynomial collocation can be used to solve ordinary differential equations with singularities and differential-algebraic equations of higher index. We introduce the open domain MATLAB code `bvpsuite` and apply it to solve the Korteweg-de Vries equation.

**Keywords:** singular ODEs, time singularity of the first kind, collocation method, DAEs of higher index

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## INTRODUCTION

During recent years, a lot of scientific work concentrated on the analysis and numerical treatment of boundary value problems (BVPs) in ordinary differential equations (ODEs) which can exhibit singularities. Such problems have often the following form:

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

For  $\alpha = 1$  the problem is called singular with a singularity of the first kind, for  $\alpha > 1$  it is essentially singular (singularity of the second kind). We are interested to recover solution  $z$  which is at least continuous,  $z \in C[0, 1]$ . This regularity requirement is equivalent to some additional conditions  $z(0)$  must satisfy. These boundary conditions, augmented by  $b(z(0), z(1)) = 0$  are necessary and sufficient for the solution  $z$  to be isolated and for the problem (1) to be well-posed. We denote this full set of  $n$  boundary conditions by  $B(z(0), z(1)) = 0$ . In particular, problems posed on infinite intervals are frequently transformed to a finite domain taking the form (1) with  $\alpha > 1$ .

The search for efficient numerical methods to solve (1) is strongly motivated by numerous applications from physics, chemistry, mechanics, ecology, or economy. Also, research activities in related fields, like differential algebraic equations (DAEs) [10] or singular Sturm-Liouville eigenvalue problems benefit from techniques developed for problems of the form (1).

## COLLOCATION METHOD AND AVAILABLE SOFTWARE

Motivated by the above applications, a sound theoretical basis for the numerical solution of BVPs with a singularity of the first kind,  $\alpha = 1$ , has been provided. To compute the numerical solution of (1) polynomial collocation was proposed [6]. Consider a mesh  $\Delta = \{\tau_0 < \dots < \tau_i \dots < \tau_N\}$  partitioning the interval  $[0, 1]$  and let  $\tau_i = ih$ ,  $i = 0, \dots, N = 1/h$ . Moreover, let us introduce the grid  $\Gamma = \Delta \cup \{t_{ij}\}$ , where  $t_{ij} = \tau_i + \rho_j h$ ,  $i = 0, \dots, N-1$ ,  $j = 1, \dots, m$ , are the collocation points. Due to the singularity, we place them in the interior of  $[\tau_i, \tau_{i+1}]$  and therefore,  $0 < \rho_1 < \rho_2 < \dots < \rho_m < 1$ . Let us denote by  $\mathcal{P}_m$  the class of piecewise continuous polynomial functions on  $[0, 1]$ . Such function reduces to a polynomial of degree smaller or equal to  $m$  on each subinterval  $[\tau_i, \tau_{i+1}]$ ,  $i = 0, \dots, N-1$ . Then, the solution  $z$  of

$$z'(t) = \frac{M(t)}{t} z(t) + f(t, z(t)), \quad t \in (0, 1], \quad B(z(0), z(1)) = 0, \quad (2)$$

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

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

subject to  $B(p(0), p(1)) = 0$ . The decision to use collocation was motivated by its advantageous convergence properties for (2). For problems with smooth solutions, the convergence order is at least equal to the so-called *stage order* of the method. For the collocation schemes (at equidistant inner points or Gaussian points) this convergence results mean that a collocation scheme with  $m$  inner collocation points constitutes a high order basic solver whose global error is  $O(h^m)$  uniformly in  $t$ . In order to solve the ODE system efficiently, the error estimate and the mesh adaptation strategy have to be provided to correctly reflect the solution behavior. The resulting open domain code MATLAB code `sbvp1.0` for explicit first order singular BVPs has been published in 2002 [2].

Due to the robustness of collocation, this method was used in one of the best established standard FORTRAN codes for (regular) BVPs, COLNEW [1], as well as in `bvp4c`, the standard MATLAB module for (regular) ODEs with an option for singular problems [11] and BVP SOLVER [12]. The scope of `bvpsuite` is much wider than that of `sbvp`, COLNEW, `bvp4c`, and the BVP SOLVER and includes, among others, fully implicit form of the ODE system with multi-point boundary conditions, arbitrary mixed order of the differential equations including zero, module for dealing with infinite intervals, module for eigenvalue problems, free parameters, and a path-following strategy for parameter-dependent problems with turning points [7].

## NONSTANDARD SINGULAR BVPS

In this section, we discuss a more general class of singular ODEs. The first aim is to investigate the analytical properties of linear BVPs of the form,

$$y'(t) = \frac{M}{t}y(t) + \frac{f(t)}{t}, \quad t \in (0, 1], \quad B_0y(0) + B_1y(1) = \beta. \quad (3)$$

The BVPs of type (3) arise in the modelling of the avalanche run up [8] and occur when the system of regular ODEs  $u'(x) = Mu(x) + g(x)$ , posed on the semi-infinite interval  $x \in [0, \infty)$ , is transformed by  $x = -\ln t$  to a finite domain  $t \in (0, 1]$ .

Again, we are interested to find out under which circumstances the above problem has a solution  $y \in C[0, 1]$ . It turns out that constant matrices  $B_0$  and  $B_1$  are subject to certain restrictions for a problem to be well-posed. The analytical properties of (3) and the convergence of the collocation in context of the initial value problems (IVP),  $B_0y(0) = \beta$ , have been discussed in [13]. For smooth solutions of such IVPs, the polynomial collocation described above converges with at least the stage order uniformly in  $t$ . Similar result can be shown for the terminal value problem (TVP),  $B_1y(1) = \beta$ . Let all eigenvalues of  $M$  be positive and let  $y \in C^{m+1}[0, 1]$  be a solution of the well-posed TVP. Moreover, let  $p \in \mathcal{P}_m \cap C[0, 1]$  be a solution of the associated collocation scheme. Then  $|p(t) - y(t)| \leq \text{const} \cdot h^m$ ,  $t \in [0, 1]$ . The proof follows by using techniques developed for IVPs [13, 14].

We illustrate this result with an example of the form  $y'(t) = \frac{M}{t}y(t) + \frac{f(t)}{t}$ ,  $B_1y(1) = \beta$ , where the data is chosen in such a way that the eigenvalues of  $M$  are  $\lambda_1 = 0.5$ ,  $\lambda_2 = 1$ , and  $\lambda_3 = 0$ . Since the smoothness of  $y$  is determined by the smallest positive eigenvalue of  $M$ ,  $y \in C[0, 1]$  behaves as  $y(t) \sim \sqrt{t}$ . We solved this model problem using `bvpsuite` on coherently refined meshes to empirically estimate the order of the scheme with  $m = 2$  collocation points and observed the expected order reduction down to  $O(h^{0.5})$ . The clear remedy for this lack of smoothness is a transformation of the independent variable,  $t = x^\mu$ ,  $\mu > 1$ . Solving the problem on an equidistant mesh in  $x$  can be interpreted as solving the original problem on an appropriately adapted mesh in  $t$  [4]. Since the solution of the transformed problem is sufficiently smooth, we now observe high convergence orders predicted by the theory.

## HIGHER INDEX DAEs

Higher index DAEs constitute a really challenging class of problems due to the involved differentiation which is a critical operation to carry out numerically. A possible technique to master the problem is to pre-handle the DAE system in such a way that the transformed problem is of index one and less difficult to solve. Since this approach is technically involved, it is worth to try to avoid it and provide a method which can be applied directly to the original DAE system of high index. At present, there are only some experimental results available, but they are quite encouraging and therefore, we shall briefly discuss them here [5]. To this aim, we restrict our attention to a models of index 3,

$$x_2'(t) + x_1(t) = q_1(t), \quad \eta t x_2'(t) + x_3'(t) + (\eta + 1)x_2(t) = q_2(t), \quad \eta t x_2(t) + x_3(t) = q_3(t), \quad \eta \in \mathbb{R},$$

**TABLE 1.**  $\eta = 3$ : Convergence orders for the collocation method with two Gaussian collocation points

$m = 2$		error for $x_1$ at $\Gamma$			error for $x_1$ at $\Delta$		
$N$	$h$	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 $x_2$ at $\Gamma$			error for $x_2$ at $\Delta$		
$N$	$h$	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 $x_3$ at $\Gamma$			error for $x_3$ at $\Delta$		
$N$	$h$	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

**TABLE 2.**  $\eta = -0.5$ : The standard collocation shows divergent behaviour (left). Convergence orders for the  $L_2$  variant of the collocation (right)

uniform mesh		error for $x_1$ (standard)		error for $x_1$ (overdetermined)	
$N$	$h$	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 $x_2$ (standard)		error for $x_2$ (overdetermined)	
$N$	$h$	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 $x_3$ (standard)		error for $x_3$ (overdetermined)	
$N$	$h$	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

subject to boundary conditions,  $x_2(0) = 0$ ,  $x_3(1) = 2e^{-2} \sin(1) + e^{-1} \cos(1) - 2x_2(1)$ . The smooth inhomogeneity  $q$  is chosen in such a way that the solution of the model reads:  $x_1(t) = e^{-t} \sin(t)$ ,  $x_2(t) = e^{-2t} \sin(t)$ ,  $x_3(t) = e^{-t} \cos(t)$ . We solve the problem for  $\eta = 3$  and  $\eta = -0.5$  using `bvpsuite` and coherently refine meshes to estimate the convergence order for  $m = 2$  equidistant and Gaussian collocation points, cf. Table 1. As we can see collocation can successfully solve the problem showing very satisfactory convergence behaviour. The situation changes for  $\eta = -0.5$ . As already observed in [9], the BDF methods cannot cope with the problem and this is also the case for standard collocation, see Table 2. We can still solve the problem successfully using another realization of the collocation method. Without increasing the degree of the collocation polynomial  $m + 1$  additional collocation conditions at points  $s_{ik}$  placed in  $[\tau_i, \tau_{i+1}]$ ,  $\tau_i < s_{i1} < t_{i1} < \dots < s_{ij} < t_{ij} < \dots < t_{im} < s_{i,m+1} < \tau_{i+1}$ , are required to hold. The resulting overdetermined system of equations is solved in the least squares sense.

## AN APPLICATION: GENERALIZED KORTEWEG-DE VRIES EQUATION

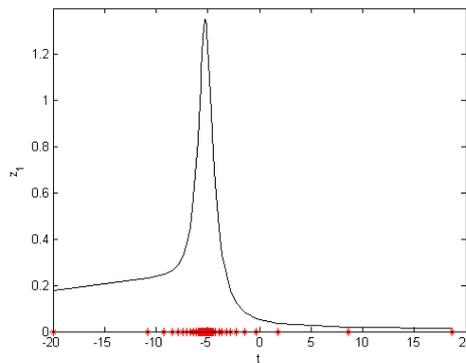
The generalized Korteweg-de Vries (GKdV) equation has the form

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

where  $p \in \mathbb{N}$ ,  $p \geq 1$ . The aim is to calculate the so-called self-similar solutions,  $u(x, t) = 1/(T - t)^{2/(3(p-1))} w(\xi)$ , where  $T$  is the blow-up time and the function  $w = w(\xi)$ ,  $\xi = x/(T - t)^{1/3}$ , the similarity profile, satisfies the following nonlinear BVP:

$$\frac{2}{3(p-1)} w + \frac{\xi}{3} w_\xi + (w_{\xi\xi} + w^p)_\xi = 0, \quad \xi \in \mathbb{R}, \quad \frac{2}{3(p-1)} w(\xi) + \frac{\xi}{3} w_\xi(\xi) \xrightarrow{\xi \rightarrow \pm\infty} 0, \quad w_{\xi\xi}(\xi) \xrightarrow{\xi \rightarrow \infty} 0.$$

Then  $u(x, t)$  is a solution of the GKdV equation blowing-up as  $t \rightarrow T$  [3]. We solve the problem using our MATLAB code `bvpsuite` by reducing  $\xi$  to a finite interval  $[-L, L]$  with a sufficiently large  $L$ . The solution  $w(\xi)$  can be found in Figure 1.



**FIGURE 1.** Korteweg-de Vries equation: Solution  $w(\xi)$  obtained from `bvpsuite` with  $TOL_a = TOL_r = 10^{-4}$  and the adaptive mesh with 40 out of 3332 subintervals necessary for the collocation with one Gaussian collocation point to satisfy the tolerances. For two Gaussian points the number of subintervals in the final mesh reduces to 558, for three Gaussian points to 264

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