Theory, Solution Techniques and Applications of Singular Boundary Value Problems

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Problem Class

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

$$B_a z(0) + B_b z(1) = \beta.$$

Remark: 2nd order problems of the form

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

can be transformed to the first order form by setting

$$z(t) := (y(t), t y'(t)).$$

Applications:

- Chemical reactor theory
- Physics — theory of lasers, computational material science
- Mechanics — buckling of (spherical) shells
- Ecology — run-up of avalanches

Earlier Results

- Order reductions of high-order methods
  - de Hoog, Weiss (1985) — Explicit Runge-Kutta schemes
  - Weinmüller (1986) — standard three-point discretization for 2^{nd} order
  - Frommlet, Weinmüller (2001) — acceleration techniques fail for this scheme
- Local error estimates fail
  - Gräff, Weinmüller (1986) — standard three-point discretization
  - Kofler (1998) — Runge-Kutta methods

Our Current Approaches

- Shooting + **IDeC** based on backward Euler
  - Advantages
    - Classical convergence order
    - Forward integration only
    - Different strategies along interval
  - Disadvantage
    - Restriction of problem class
- Collocation
  - Advantages
    - Stage order holds for **general class**
    - Uniform approximation
  - Disadvantages
    - No superconvergence
    - Computational effort

Fixed points of IDeC are collocation solutions!

Analytical Properties — BVPs

$$z'(t) = \frac{M(t)}{t} z(t) + f(t, z(t)), \tag{1a}$$
$$B_a z(0) + B_b z(1) = \beta, \tag{1b}$$
$$z \in C[0, 1]. \tag{1c}$$

Note:

- (1c) $\Leftrightarrow$ $n - q$ lin. indep. conditions on $z(0)$
- (1b) $\Rightarrow$ (locally) unique solution

Theorem 1: Assume that an isolated solution $z(t)$ of (1) exists and $f \in C^p$, $M \in C^{p+1}$ in a neighborhood of z.

If

- $M(0)$ has no eigenvalues with positive real parts **or**
- all positive real parts of $M(0)$ are $> p + 1$

then

$$z \in C^{p+1}[0, 1].$$

Analytical Properties — IVPs

$$z'(t) = \frac{M(t)}{t} z(t) + f(t, z(t)), \tag{2a}$$
$$B_a z(0) = \beta, \tag{2b}$$
$$z \in C[0,1]. \tag{2c}$$

Note:

- (2c) $\Leftrightarrow z(0) \in \ker M(0) = \mathrm{span}(\tilde{E})$
- ((2b) $\Rightarrow$ unique solution)

  $\Longleftrightarrow B_a \tilde{E}$ nonsingular.

Theorem 2: Assume $f \in C^p$, $M \in C^{p+1}$. Then,

- if $M(0)$ has no eigenvalues with positive real parts $\Rightarrow \exists!\ z \in C^{p+1}[0,1]$,
- **otherwise** (2) does not define a unique continuous solution.

Shooting Methods

IVP equivalent to BVP:

$$
\begin{aligned}
z_s'(t) &= \frac{M(t)}{t} z_s(t) + f(t, z_s(t)), \\
z_s(0) &= \tilde{E}s \in \ker M(0),
\end{aligned}
$$

where s is chosen such that

$$
B_a \tilde{E} s + B_b z_s(1) = \beta.
$$

s is determined using Newton's method $\Rightarrow$ this requires the solution of a set of singular IVPs!

Koch, Weinmüller (2001) —

- Process is **well-defined** and **convergent** if IVPs are well-posed.
- Numerical method of order $O(h^p)$ for IVP $\Rightarrow$ $\mathbf{O(h^p)}$ **solution** for BVP.

Drawback: Restriction of problem class.
Required: High-order integrator for IVPs.

Iterated Defect Correction

$$z'(t) = \frac{M(t)}{t} z(t) + f(t, z(t)),$$
$$z(0) = \beta \in \ker M(0).$$

Numerical solution: $z_h^{[0]} = (z_0^{[0]}, \ldots, z_N^{[0]})$.

Piecewise polynomial interpolant: $p^{[0]}(t)$.

Neighboring problem (NP):

$$y'(t) = \frac{M(t)}{t} y(t) + f(t, y(t)) + d^{[0]}(t),$$
$$y(0) = p^{[0]}(0) = \beta,$$

where

$$d^{[0]}(t) = p^{[0]\prime}(t) - \frac{M(t)}{t} p^{[0]}(t) - f(t, p^{[0]}(t)).$$

Numerical solution: $p_h^{[0]}$.

Yields

- Error estimate $p^{[0]}(t_j) - p_j^{[0]}$
- Improved solution $z_j^{[1]} = z_j^{[0]} + p^{[0]}(t_j) - p_j^{[0]}$.

This process can be iteratively continued!

IDeC — Convergence Results

Theorem 3: If IDeC based on the backward Euler method is used for singular IVPs, then

$$|z_j^{[k]} - z(t_j)| = O(h^{k+1}), \quad k = 0, \ldots, m-1,$$

if piecewise polynomials of degree m are used.

Proof: Koch, Weinmüller (2000).

The update also yields an asymptotically correct estimate of the **global error**.

Reconsidering IDeC

Q: What happens for $k \to \infty$ when h is fixed?

A: Quite frequently, a fixed point of the iteration is reached.

Q: What is the advantage of considering this type of asymptotics?

A: In situations where Theorem 3 is not applicable and the classical order sequence is not observed, the fixed point yields a high-order solution.
Typically, this coincides with a collocation solution.

Fixed Points of IDeC

Theorem 3 is not applicable because BVPs are considered instead of IVPs.

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} z(t) + \begin{pmatrix} 0 \\ 3t\cos(t) - t^2\sin(t) \end{pmatrix},$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ \sin(1) \end{pmatrix},$$

with exact solution

$$z(t) = (t\sin(t), t\sin(t) + t^2\cos(t))^T.$$

h	err_0	p_0	err_1	p_1	err_2	p_2	err_3	p_3
0.0833	2.6e−02		8.9e−03		1.0e−03		1.3e−03	
0.0417	1.2e−02	1.09	2.3e−03	1.95	2.1e−04	2.28	3.4e−04	1.89
0.0208	6.0e−03	1.03	5.8e−04	1.98	5.2e−05	1.97	8.7e−05	1.96
0.0104	3.0e−03	1.01	1.4e−04	1.99	1.4e−05	1.85	2.2e−05	1.98
0.0052	1.5e−03	1.00	3.6e−05	1.99	3.7e−06	1.95	5.5e−06	1.99
0.0026	7.4e−04	1.00	9.1e−06	1.99	9.4e−07	1.98	1.4e−06	1.99

Fixed Points of IDeC (2)

Theorem 3 is not applicable because the box scheme serves as basic method.

$$
\begin{aligned}
z'(t) &= \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(t) \\
&\quad - \begin{pmatrix} 0 \\ 9t\cos(3t) + 3\sin(3t) \end{pmatrix},
\end{aligned}
$$

$$
\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ \cos(3) \end{pmatrix},
$$

with exact solution

$$
z(t) = (\cos(3t), -3t\sin(3t))^T.
$$

h	err_0	p_0	err_1	p_1	err_2	p_2	err_3	p_3
0.0833	3.4e−02		1.7e−03		8.8e−05		4.7e−05	
0.0417	1.0e−02	1.70	4.4e−04	1.93	1.3e−05	2.80	4.6e−07	6.65
0.0208	3.1e−03	1.75	1.1e−04	1.97	3.2e−06	2.00	6.6e−09	6.13
0.0104	8.9e−04	1.79	2.8e−05	1.99	8.0e−07	1.99	1.3e−10	5.63
0.0052	2.5e−04	1.81	7.0e−06	1.99	2.0e−07	1.99	3.8e−11	1.79
0.0026	7.1e−05	1.83	1.7e−06	1.99	5.0e−08	2.00	8.7e−11	

Fixed Points of IDeC (3)

In both cases, however, **fixed point convergence** was observed.

Auzinger, Koch, Weinmüller (2001) — these fixed points coincide with collocation solutions of order 6, respectively.

Thus, a high order solution could be obtained eventually!

Note: In the second case the fixed point was even reached in a finite number of steps. In some situations, such a behavior can in fact be shown analytically!

Direct Approach — Collocation

Collocation equations:

$$q'(t_{i,j}) = \frac{M(t_{i,j})}{t_{i,j}} q(t_{i,j}) + f(t_{i,j}, q(t_{i,j})),$$
$$j = 1, \dots, p,\ i = 0, \dots, N-1,$$
$$B_a q(0) + B_b q(1) = \beta.$$

$q(t)$ ... continuous piecewise polynomial function of maximal degree p.

$t_{i,j}$ ... collocation points distributed equivalently in every subinterval.

de Hoog, Weiss (1978) — (linear) first order systems which are equivalent to a well-posed IVP: The **stage order** $O(h^p)$ is retained, but there is **no superconvergence** in general.

Consequently, we choose **equidistant** collocation at an **even** number of interior points.

Global Error Estimation

- We construct a NP similarly as for IDeC.
- Then we solve for $j = 1, \ldots, p+1$, $i = 0, \ldots, N-1$, the backward Euler schemes

$$\frac{\pi_{i,j} - \pi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = F(t_{i,j}, \pi_{i,j}) + \bar{d}_{i,j},$$
$$B_a \pi_{0,0} + B_b \pi_{N-1,p+1} = \beta,$$

$$\frac{\xi_{i,j} - \xi_{i,j-1}}{t_{i,j} - t_{i,j-1}} = F(t_{i,j}, \xi_{i,j}),$$
$$B_a \xi_{0,0} + B_b \xi_{N-1,p+1} = \beta,$$

where

$$\{t_{i,j} : \; j = 0 \ldots, p+1, \; i = 0, \ldots, N-1\}$$

are the collocation nodes plus the endpoints of each interval.

The estimate for the global error is given by

$$\varepsilon_{i,j} := \pi_{i,j} - \xi_{i,j}.$$

Global Error Estimation (2)

However, in contrast to the IDeC, the defect is chosen in locally integrated form:

$$\begin{aligned}\bar{d}_{i,j} \;:=\; & \frac{q(t_{i,j}) - q(t_{i,j-1})}{t_{i,j} - t_{i,j-1}} - \\ & - \sum_{k=1}^{p+1} \alpha_{j,k} F(t_{i,k}, q(t_{i,k})).\end{aligned}$$

Here, the $\alpha_{j,k}$ define a quadrature rule,

$$\frac{1}{t_{i,j}-t_{i,j-1}} \int_{t_{i,j-1}}^{t_{i,j}} \varphi(\tau)\, d\tau = \sum_{k=1}^{p+1} \alpha_{j,k} \varphi(t_{i,k}) + O(h_i^{p+1}).$$

Theorem 4: For regular problems, this estimate is asymptotically correct,

$$\begin{aligned}|(q(t_{i,j}) - z(t_{i,j})) - (\pi_{i,j} - \xi_{i,j})| = O(h_i^{p+1}), \\ j = 0, \dots, p+1,\; i = 0, \dots, N-1.\end{aligned}$$

Proof: Auzinger, Koch, Weinmüller (2001).

Conclusions & Future Work

A Fortran 90 shooting code is currently being developed:

- (equidistant) IDeC near the singular point.
- Embedded Runge-Kutta pairs with local step-size control away from singularity.

The IDeC subroutine will also be employed for the solution of a singular IVP occurring in the modeling of the run-up amd run-out of avalanches due to
McClung, Mears (1995).

Conclusions & Future Work (2)

We have recently developed a Matlab BVP solver based on collocation, see Auzinger, Kneisl, Koch, Weinmüller (2001).

Our global error estimation procedure is used for adaptive mesh selection which is robust with respect to the singularity.

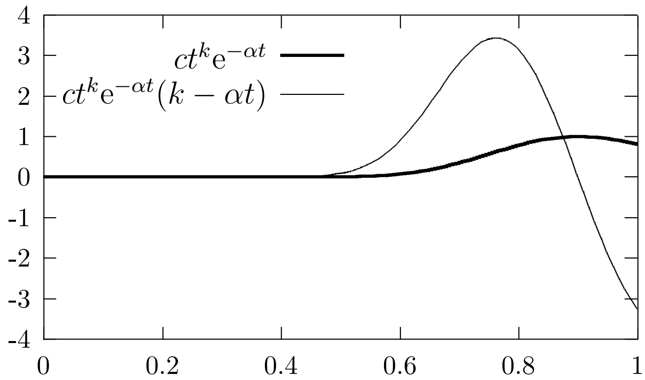
Example

$$z'(t) = \frac{1}{t}\begin{pmatrix} 0 & 1 \\ 1+\alpha^2 t^2 & 0 \end{pmatrix} z(t) +$$

$$+ \begin{pmatrix} 0 \\ c t^{k-1} \mathrm{e}^{-\alpha t}(k^2 - 1 - \alpha t(1+2k)) \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} z(0) + \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} z(1) = \begin{pmatrix} 0 \\ c\mathrm{e}^{-\alpha} \end{pmatrix},$$

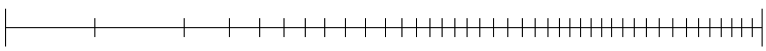
where $\alpha = 40,\ k = 36$ and $c = \left(\frac{\alpha}{k}\right)^k \mathrm{e}^k$.



Mixed tolerance with rTOL=aTOL=10^{-6}.

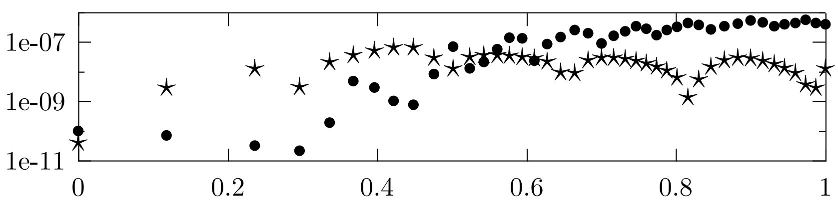
Polynomial degree $p = 4$.

Final mesh:



Evaluation on final mesh: $\star$ exact global error,

$\bullet$ error estimate.



Conclusions & Future Work (3)

At the moment we try to use our knowledge of singular IVPs to speed up calculations for the solution of the

radial Schrödinger equation

in the context of

computational material science

— Walter Kohn's

Density Functional Theory,

see for example Eschrig (1996).

Aim: Performance comparison of

- IDeC,
- Collocation,
- Transformation to a regular problem on a large interval (employed in a standard FORTRAN 77 code).