Second International Conference
Modelling and Development of Intelligent Systems
Sibiu - Romania, September 29 - October 02, 2011

Several methods of approximation for second order nonlinear boundary value problem with boundary conditions at infinity

Daniel N. Pop, Radu T. Trîmbiţaş

Abstract

Consider the problem:

$$\begin{cases} y''(x) + f(x,y) = 0, & 0 < x < \infty, \\ y(0) = \infty, & y(\infty) = 0 \end{cases}$$

where $f(x,y) \in C([0,\infty] \times \mathbb{R}),\ y(x) \in C^1(0,\infty)$. This is not a classical two-points boundary value problem since $y(0) = \infty,\ y(\infty) = 0$. To solve this kind of problems we need to know the values in two inner points $a, b \in (0,\infty)$, $a \neq b$. The aim of this work is to present three approximation procedures:

1. A combined method using collocation method on B-splines of order $(k+2)$ with a $(k+1)$ order *Runge-Kutta* method.
2. A pseudospectral collocation method with *Chebychev* extreme points combined with a *Runge-Kutta* method.
3. MATLAB function `bvp4c` combined with a *Runge-Kutta* method.

Then we give a numerical examples and compare the costs (time U.C) using `MATLAB` functions `tic-toc`.

1 Introduction

Consider the problem (PVP):

$$y''(x) + f(x,y) = 0, \qquad x \in (0,\infty) \tag{1}$$

$$y(a) = \alpha \tag{2}$$

$$y(b) = \beta, \qquad a, b \in (0,\infty),\ a < b. \tag{3}$$

where $f(x,y) \in C((0,\infty) \times \mathbb{R}),\ a, b, \alpha, \beta \in \mathbb{R}$.

We try to solve this problem using three approximation methods:

1. A combined method based on collocation with B-splines of order $(k+2)$ and a *Runge-Kutta* method order $(k+1)$.
2. A pseudospectral collocation method with *Tchebychev* extreme points combined with a *Runge-Kutta* method.
3. MATLAB function `bvp4c` combined with a *Runge-Kutta* method.

The methods are new in this context since the conditions are stated at the interior points of the interval $(0, 1)$. Problems of type (1)+(2)+ (3) occurs in practice. Examples are in semiclassical description of the charge density in atoms of high atomic number (Thomas-Fermi equation) [19, pp.155-156], reaction-diffusion equation [9], frequency domain equation for the vibrating string (Greengard-Rokhlin problem) [11], electromagnetic self interaction theory [4, pp.336-337], the model of the steady concentration of a substrate in an enzyme-catalyzed reaction (Michaelis-Menten kinetics)[19, page 145].

We also consider the problem (BVP):

$$y''(x) + f(x, y) = 0, \qquad x \in [a, b] \tag{4}$$
$$y(a) = \alpha \tag{5}$$
$$y(b) = \beta, \tag{6}$$

Also it is shown that the *Runge-Kutta* method does not degrade the accuracy provided by the collocation method for the (BVP) problem [4, Theorem 5.73 pp219, Theorem 5.140 pp253]. To apply the collocation theory we need to have an isolated solution of (BVP) problem and this occurs if the above linearized problem for $y(x)$ is uniquely solvable.

R.D. Russel and *L.F. Shampine [18]* study the existence and the uniqueness of the isolated solution.

Our methods consists into decomposition of the problem (1)+(2)+(3) into three problems:

1. A (BVP) problem on $[a, b]$ (problem (4)+(5)+(6)).

2. Two (IVPs) on $(0, a]$ and $[b, +\infty)$.

For the existence and uniqueness of an (IVP), see [14, pp: 112-113].

If the problem (BVP) has the unique solution, the requirement $y(x) \in C^1(0, +\infty)$ ensure the existence and the uniqueness of the solution of the problem (PVP). Our choice to use these methods is based on the following reasons:

1. We write the code using the function `spcol` in `Matlab-Spline Toolbox [15]` and the functions `cebdif, cebint, cebdifft` contained in `dmsuite [21].`

2. Theoretical results on the convergence of collocation method are given in ([12], [13]).

3. The accuracy of spectral method is superior to finite elements method (FEM) and finite difference methods (FDM) (the rate of convergence associated with this problems with smooth conditions are $\mathbb{O}(\exp(-CN))$ or $\mathbb{O}(\exp(C\sqrt[2]{N})$ where N is the number of degrees of freedom in the expansions).

4. For each *Newton* iteration, the resulting linear algebraic system of equations (after using *Newton* method with quasilinearization) is solved using method given in [8].

2 A combined method using B-splines and Runge-Kutta methods

First we solve the (BVP) problem using the collocation method with B-splines of order $(k + 2)$ presented in [17, Section 2].

Consider the mesh of $[a, b]$:

$$\overline{\Delta} : a = x_0 < x_1 < \cdots < x_N = b, \tag{7}$$

where the multiplicity of a and b is $(k + 2)$ and the multiplicity of inner points is k. So the dimension of spline space is $n = Nk + 2$. Also we construct the collocation points $\xi_j,\ j = 1, 2, ..., n - 2$ like in [17, Section 1] and [2].

We wish to find an approximate solution of the (BVP) problem, having the following form:

$$u_{\overline{\Delta}}(x) = \sum_{i=0}^{n-1} c_i B_{i,k+1}(x), \tag{8}$$

where $B_{i,k+1}(x)$ is the B-spline of order $(k+2)$.

Our approximation method is inspired from [7, Chapter 2,5]. We impose the conditions:

c1 The approximate solution (8) satisfies the differential equation (4) at collocation points:

$$\xi_j,\ j = 1, 2, ...n-2\ .$$

c2 The solution satisfies $u_{\overline{\Delta}}(a) = \alpha,\ u_{\overline{\Delta}}(b) = \beta$.

The above conditions yield a nonlinear system with n equations:

$$\begin{cases} \sum_{i=0}^{n-1} c_i B_{i,k+1}(a) = \alpha, \\ \sum_{i=0}^{n-1} c_i B_i^{''}{}_{,k+1}(\xi_j) + f(\xi_j, \sum_{i=0}^{n-1} c_i B_{i,k+1}(\xi_j)) = 0,\ j = 1, 2, ..., n-2, \\ \sum_{i=0}^{n-1} c_i B_{i,k+1}(b) = \beta, \end{cases}$$

with unknowns $c_i,\ i = 0, \ldots, n-1$. If $F = [F_0, F_{1,}..., F_{N-1}]$ are the functions defined by the equations of the nonlinear system, using the quasilinearization of *Newton* method [4, pp: 52-55], we find the next approximation by means of

$$c^{(k+1)} = c^{(k)} - w^{(k)},$$

where $c^{(k)}$ is the vector of unknowns obtained at the $k-$th step and $w^{(k)}$ is the solution of the linear system

$$F^{'}(c^{(k)})w = F(c^{(k)}).$$

To solve the (BVP) problem we use the method presented in [20] and the initial approximation $u^{(0)} \in C^1[0,1]$ is required. The successful stopping criterion [3] is:

$$\left\| u^{(k+1)} - u^{(k)} \right\| \leq abstol + \left\| u^{(k+1)} \right\| reltol,$$

where *abstol* and *reltol* is the absolute and the relative error tolerance, respectively and the norm is the usual uniform convergence norm. The reliability of the error-estimation procedure being used for stopping criterion was verified in [8]. For the solution of two IVPs on $(0, a]$ and $[b, +\infty)$ we use a *Runge-Kutta* method of appropriate order, this need good approximation of $y'(a)$ and $y'(b)$, which could be obtained with noadditional effort during the collocation method.

The stability and convergence of *Runge-Kutta* method are guaranteed in [10, Theorem 5.3.1 page 285, Theorem 5.3.2 page 288]. A $(k+1)$ order explicit *Runge-Kutta* method is consistent and stable, so is convergent. The convergence and accuracy of our combined method to whole interval $(0, +\infty)$ was proved in [17, Section 3, Theorem 3.1] and the total costs of this method was studied in [17, Section 4].

3 A combined method using a pseudospectral collocation with Tchebychev extreme points and Runge-Kutta methods

Consider the grid:

$$\Delta : 0 = x_{-q} < ... < x_{-1} < a = x_0 < x_1 < ... < x_N = b < x_{N+1} < ... < x_{N+p}. \tag{9}$$

Our second method is a combined a pseudospectral method for the (BVP) problem and a *Runge-Kutta* method for the two IVPs on $(0, a]$ and $[b, +\infty)$. The approximate solution of (BVP) problem follow the ideas presented in [5]. Let $y(x)$ of this problem and considering the *Lagrange* basis (l_k) we have:

$$y(x) = \sum_{k=0}^{N} l_k(x) y(x_k) + (R_N y)(x),\ x \in [a, b]$$

where :

$$(R_N y)(x) = \frac{y^{(N+1)}(\xi)}{(N+1)!}(x-x_0)...(x-x_N)$$

is the remainder of *Lagrange* interpolation. Since $y(x)$ fulfills the differential equation (4) we obtain:

$$\sum_{k=0}^{N} l_k''(x)y(x_k) + (R_N y)''(x) = -f(x_i, y(x_i)),\ i = 1, 2, ..., N-1.$$

Setting $y(x_k) = y_k$ and ignoring the rest, one obtains the nonlinear system:

$$\sum_{k=0}^{N} l_k''(x)y(x_k) = -f(x_i, y(x_i)),\ i = 1, 2, ..., N-1, \tag{10}$$

with unknowns $y_k,\ k = 1, ..., N-1$, here $y_0 = y(a) = \alpha$ and $y_N = y(b) = \beta$. The approximate solution (that is the collocation polynomial for (BVP) problem), is the *Lagrange* interpolation polynomial at nodes $\{x_k\},\ k = 0, 1, 2, ...N$:

$$y_N(x) = \sum_{k=0}^{N} l_k(x)y(x_k). \tag{11}$$

The nonlinear system (10) can be rewritten as:

$$AY_N = F(Y_N) + b_N$$

where:

$$A = [a_{ik}],\ a_{ik} = l_k''(x_i),\ k, i = 1, 2, ..., N-1,$$

$$F(Y_N) = \begin{bmatrix} -f(x_1, y_1) \\ -f(x_2, y_2) \\ \vdots \\ -f(x_{N-1}, y_{N-1}) \end{bmatrix}, b_N = \begin{bmatrix} -\alpha l_0''(x_1) - \beta l_N''(x_1) \\ -\alpha l_0''(x_2) - \beta l_N''(x_2) \\ \vdots \\ -\alpha l_0''(x_{N-1}) - \beta l_N''(x_{N-1}) \end{bmatrix}.$$

If the nodes $\{x_k\},\ k = 0, 1, ...N$ are symmetric with respect of $(a+b)/2$, A is centro-symmetric [6, for proof], so nonsingular. So we choose the nodes given by:

$$x_i = \frac{(b-a)\cos\frac{\pi i}{N} + b + a}{2},\ i = 1, 2, ..., N, \tag{12}$$

i.e. the Chebyshev-*Lobatto* nodes. We introduce :

$$G(Y) = A^{-1}F(Y) + A^{-1}b_N. \tag{13}$$

To solve numerically (PVP) problem on Δ given by (9) we apply pseudo-spectral collocation method at points $[a, b]$ and a *Runge-Kutta* method to other points. To apply the *Runge-Kutta* method for the solution of two (IVP) on $(0, a]$ and $[b, +\infty)$ we need the derivatives $y'(a)$ and $y'(b)$, this can be computed by deriving the formula (11). In work [5], the authors prove the existence of unique solution of the system (10) which can be calculated by successive approximation method:

$$Y^{(N+1)} = G(Y^{(N)}),\ n \in N^*,$$

with $Y^{(0)}$ fixed and G given by (13), also they estimate the error:

$$\|Y - Y_N\| \leq \frac{\|A^{-1}\| \|R\|}{1 - \|A^{-1}\| L}$$

where

$$Y = [y(x_1), y(x_2), ..., y(x_{N-1})]^T \ ,$$

$y(x)$ is the exact solution of (BVP) problem,

$$Y_N = [y_1, y_2, ..., y_{N-1}]^T \ ,$$

y_i are the values of approximated solution at x_i computed by (12),

$$R = [-(R_N y)''(x_1), -(R_N y)''(x_2), ..., -(R_N y)''(x_{N-1})]^T,$$

and L is the *Lipschitz* constant. Combining these results with the stability and convergence of *Runge-Kutta* methods in [16, Theorem 2.3] the authors prove the convergence of this method and occurs:

$$|y_N(a) - y'(a)| = \mathbb{O}(h^k),$$
$$|y_N(b) - y'(b)| = \mathbb{O}(h^k),$$

and for each points x_i in Δ giving by (9):

$$|y_N(x_i) - y_i| = \mathbb{O}(h^k), \ i = -q, ..., N + p.$$

If the *Runge-Kutta* method is stable and has the order k, then the final solution has the same accuracy.

4 MATLAB solver `bvp4c` and Runge-Kutta methods

MATLAB solver `bvp4c` is a strong solver based on collocation. It allows a flexible description of the ODEs, various kind of boundary conditions, parameters and options (jacobian, tolerances, vectorization and so on). It requires a guess solution. As a side effect it provides an approximation of the derivative of the solution. This allows us to combine `bvp4c` with an IVP solver.

5 Numerical examples

For the both methods we implemented the ideas in `MATLAB 2010a [15],` for the first method our code use `Matlab Spline Toolbox,`the function `spcol` allows us to compute easily the collocation matrix and for (IVP) problems the solver `ode23tb` works fine (when the problem is stiff)`.`To avoid the error propagation, we choose for (BVP) problem B-splines of order 4 (degree 3) or order 5 (degree 4), in this we implemented the function `polycalnlinRK`.

The second method was implemented in `MATLAB` using the functions `cebdif,cebint` and `cebdiff` contained in `dmsuite` and described in [21], we write the function `solvepolylocalceb` who solve the nonlinear system and call the *Runge-Kutta* solver `ode23tb`. The derivatives at a and b were computed by calling `cebdifft`. The third method following the idea given by [19].

In order to compare the costs (run-times) experimentally we use `Matlab` functions `tic` and `toc.`

- **The first example is the case where we know the exact solution**

  Consider the (BVP) problem:

$$\begin{cases} y''(x) + 2\pi^2 \exp(-y(x)) = 0, \ 0 < x < \infty, \\ y(1/10) = 2\ln\sin\pi/10, \\ y(9/10) = 2\ln\sin 9\pi/10 = 2\ln\sin\pi/10. \end{cases} \tag{14}$$

  The exact solution of this problem is:

$$y(x) = 2\ln(\sin(\pi x)),$$

and we see that the exact solution is a periodic function of the period $T = 1$. Using step control algorithm [1] we determined that problem (14) has singularities in $x = 0$ and in $x = 1$. We have set the tolerance to $\varepsilon = 10^{-10}$, we took $N = 1025$ and maximum number of iterations $NMAX = 50$. The start solution are obtained using the *Lagrange* interpolation polynomial with nodes: $1/4, 5/24, 1/6$. The results we have obtained after 10 iterations, run times are:

$Tolerance$	$1st\ Method$	$2nd\ Method$	$3rd\ Method$
10^{-10}	0.777144	7.204652	1.350691

The graph of approximate solution are presented in Figure 1, and the errors in semi-logarithmic scale for the first method in Figure 2(a), for the second in Figure 2(b) and for the third in Figure 2(c), respectively.

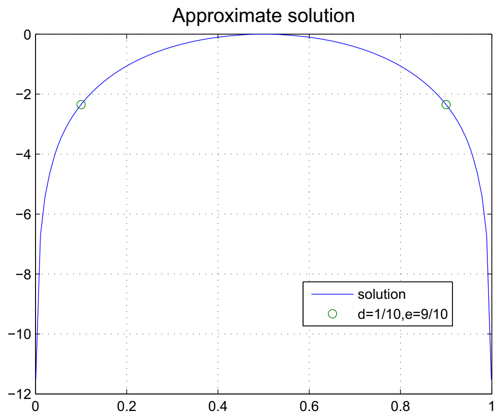
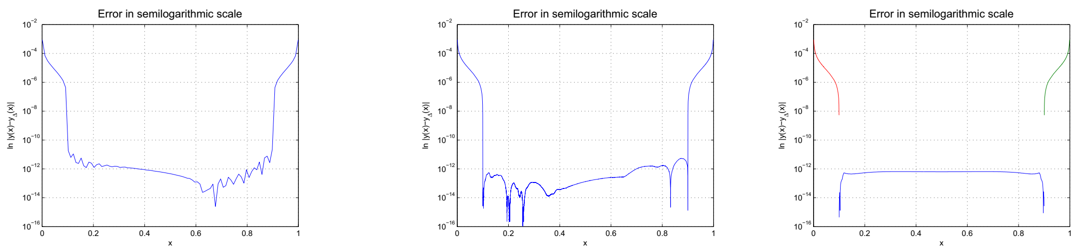


Figure 1: Approx-solution



(a) B-splines+Runge-Kutta (b) C.C+Runge-Kutta (c) `bvp4c`+Runge-Kutta

Figure 2: Errors

- **The second example is the case of unknown exact solution**

$$y''(x) = x^{-1/2} y^{3/2}, \tag{15}$$

with boundary conditions:

$$y(0) = +\infty, \quad y(\infty) = 0. \tag{16}$$

This (BVP) arises in a semiclassical description of the charge density in atoms of high atomic number. There are difficulties at both end points. These difficulties are discussed at length in *Davis* (1962) and in *Bender and Orszag* (1999). *Davis* discusses series solutions for:

$$y(x) \text{ as } x \to 0.$$

It is clear that there are fractional powers in the series. That is because, with $y(0) = 1$, ODE requires:

$$y''(x) \sim x^{-1/2} \text{ as } x \to 0,$$

and hence there be a term $\frac{4}{3}x^{3/2}$ in series for $y(x)$. Of course, there must also be lower-order terms so as to satisfy the boundary condition at $x = 0$. Bender and Orszag discuss the asymptotic behavior of $y(x)$, $x \to 0$. Verify that trying a solution of the form

$$y(x) \sim ax^{\alpha},$$

yields for the start solution:

$$y_0(x) = 144x^{-3}.$$

We use for inner points $a = 0.015$, and $b = 59$. The results we have obtained after 12 iterations, run times are:

Tolerance	*1st Method*	*2nd Method*	*3rd Method*
10^{-10}	0.493448	1.204652	0.838735

The graph of approximate nonlinear solution of *Fermi-Thomas* problem is presented in Figure 3.

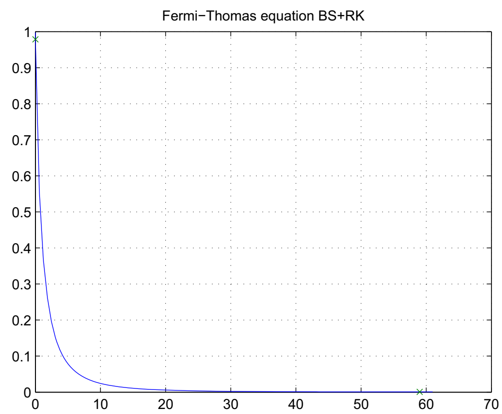


Figure 3: The charge density in atoms of high atomic number

6 Conclusions

The running time for B-spline collocation is the shortest, because its collocation matrix is banded. Tchebychev collocation has the longest time, since its collocation matrix is full. The `bvp4c` solver has an intermediary position, since it has a different type collocation. Nevertheless, further tests are necessary.

References

[1] O.Agratini, I.Chiorean, G.Coman, R.Trîmbiţaş, *Analiză numerică şi Teoria Aproximării* , Presa Universitară Clujeană, Cluj-Napoca, 2002.

[2] U.Ascher, S.Pruess and R.D. Russel, On spline basis selection for solving differential equations, *SIAM J. Numer. Anal. 20 nr:1*, 1983.

[3] U.Ascher, Solving boundary value problems with spline collocation code, Journal of computational physics, 34 , Nr:3, pp: 401-415, 1980.

[4] U. Ascher, R.M. Mattheij, and R.D. Russel, *Numerical Solution of Boundary Value Problems for Ordinary Differential Equations*, SIAM, 1997.

[5] F.A.Costabile, A.Napoli, A coolocation method for global approximation of general second order BVPs, *Computing Letters* 3, pp: 23-24, 2007.

[6] F.A.Costabile, F.Dell-Accio, On the nonsingularity of a special class of centrosymmetric matrices arising in spectral method in BVPs, *Applied Mathematics and Computation*, 206, pp: 991-993, 2008.

[7] C.de Boor, *A practical guide to splines*, Springer-Verlag, Berlin, Heidelberg, New-York, 1978.

[8] C.de Boor, R.Weiss, *Solveblock: A package for solving almost block diagonal linear systems, with applications on the numerical solution of odinary differential equations* , MCR#TSR 1625, Madison,Wisconsin, 1976.

[9] M.A. Diminescu, V. Nistorean, *Gospodărirea durabilă a resurselor de apă, Conf. Internaţ. Energie-Mediu,* CIEM , Bucureşti, 2005.

[10] W.Gautschi, *Numerical Analysis, An Introduction*, Birkhauser Verlag, Basel, 1997.

[11] L.Greengard, V.Rohlin *On the Numerical Solution of Two-Point Boundary Value Problems, Comm.Pure Appl.Math.XLIV* , pp:419-452,1991.

[12] W.Heinrichs, Strong convergence estimates for pseudospectral methods, *Applications of Mathematics*, 37(6), pp:24-37, 1992.

[13] E.Houstis, A collocation method for systems of nonlinear ordinary differential equations, *J. Math. Anal. Appl.*, 62, pp:24-37, 1978.

[14] P. Henrici, *Discrete Variable Methods in Ordinary Differential Equations*, John Willey and Sons, New York, 1962.

[15] Mathlab 2010a, *Set of manuals,* , MathWorks, Inc., Natick, MA, 2010.

[16] Ion Păvăloiu, Daniel N.Pop, Radu T.Trîmbiţaş, Solution of polylocal problem with a pseudospectral method, *Annals of "Tiberiu Popoviciu" Seminar of functional equations, approximation and convexity*, vol 8, pp: 53-65, Cluj-Napoca, 2010.

[17] Daniel N.Pop, Radu T.Trîmbiţaş, An approximation methods for second order nonlinear value polylocal problems using B-splines and Runge-Kutta metods, N.A.A.T. 2010, *Studia Universitas "Babes-Bolyai", Series Mathematica*, Vol.LVI, Number 2, pp:515-527, June 2011.

[18] R.D.Russel, L.F.Shampine, A Collocation Method for Boundary Value Problems, *Numer. Math.*, 19, Springer-Verlag, pp: 1-28, 1972.

[19] L. F. Shampine, I. Gladwell, S. Thompson, Solving ODEs with MATLAB, Cambridge University Press, 2003.

[20] R.Stover, Collocation methods for solving linear-algebraic boundary value problem, *Numer.Math.* 88, pp:771-795, 2001.

[21] J.A.C Weideman, S.C Reddy, A MATLAB Differentiation Matrix Suite, *ACM Trans. on Math. Software*, 26, pp: 465-519, 2000.

Daniel N.Pop
Romanian-German University Sibiu
Faculty of economic engineering
in electric, energy, electronic
Calea Dumbravii street nr: 28-32
Romania
E-mail: *popdaniel31@yahoo.com*

Radu T. Trîmbiţaş
"Babeş-Bolyai" University Cluj-Napoca
Faculty of Mathematics and Computer
Science
Mihail Kogalniceanu street nr. 1
Romania
E-mail: *tradu@math.ubbcluj.ro*