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*Article*

# Chebfun Solutions to a Class of 1D Singular and Nonlinear Boundary Value Problems.

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**Abstract:** The Chebyshev collocation method (ChC) implemented as Chebfun is used in order to solve a class of second order one-dimensional singular and genuinely nonlinear boundary value problems. Efforts to solve these problems with conventional ChC have generally failed, and the outcomes obtained by finite differences or finite elements are seldom satisfactory. We try to fix this situation using the new Chebfun programming environment. However, for toughest problems we have to loosen the default Chebfun tolerance in Newton's solver as the ChC runs into trouble with ill-conditioning of the spectral differentiation matrices. Although in such cases the convergence is not quadratic the Newton updates decrease monotonically. This fact, along with the decreasing behaviour of Chebyshev coefficients of solutions, suggests that the outcomes are trustworthy, i.e., the collocation method has exponential (geometric) rate of convergence or at least an algebraic rate. We consider first a set of problems that have exact solutions or prime integrals and then another set of benchmark problems that do not possess these properties. Actually, for each test problem carried out we have determined how Chebfun solution converges, its length, the accuracy of the Newton method and especially how well the numerical results overlap with the analytical ones (existence and uniqueness).

**Keywords:** Chebfun; differential equation; non-linearity; singularity; convergence; Bernstein growth; improper integrals; boundary layer

**MSC:** 65L10 65L60 65L70 65D30

## 1. Introduction

The idea of solving as accurate as possible of nonlinear boundary problems by spectral collocation methods is not new to our concerns. Thus we have published the paper [1] and posted the problem [2] on the site of Mathematical Institute of Oxford University. In both situations we have considered nonlinear boundary value problems on the half line.

In this paper we will consider the following class of problems nonlinear and possible singular:

$$\begin{cases} u'' + q(x)f(x,u,u') = 0, \ 0 < x < 1, \\ -au(0) + bu'(0) = 0, \ u(1) = 0, \end{cases} \tag{1}$$

where $a \geq 0, \ b > 0$.

For the main result of existence we will assume the following conditions are satisfied:

$$q \in C[0,1], \ q > 0, \ \int_0^1 q(x) < +\infty \text{ and } f : [0,1] \times (0,\infty) \times R \to R \text{ is continuous.} \tag{2}$$

For the results of the existence and uniqueness of the solutions of these problems, we rely on the paper [3] and the works cited there.

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We must note from the beginning that the mathematical literature abounds with such theoretical results, but their numerical illustration is often lacking. We want to fill this gap as much as possible.

Notice that $f$ may not be a Caratheodory function because of the singular behavior of the $u$ variable, i.e.,$f$ may be singular at $u = 0$. Problems of the above form have been discussed extensively in the literature usually when $f(x, u, z)$ reduces to $f(x, u)$ with $f : (0, 1) \times (0, +\infty) \rightarrow (0, +\infty)$ (see for instance [4]).

The main purpose of our study is to solve numerically such problems as accurately as possible.

In general, attempts are made to attenuate singularity by algebraic manipulations, but these, along with non-linearities, raise serious problems for any numerical algorithm.

Traditionally they have been overcome using variants of the shooting method. *We will never resort to such methods.* As the methods with finite differences, finite elements or volumes, or conventional ChC have shown their limits, we want to show that the use of Chebfun software can solve most of the issues.

The work has the following structure. In Section 2 we elaborate a brief comparison between Chebfun and the conventional ChC method. The central core of the work is the Section 3. Here we report the numerical results of solving eight problems with varying degrees of non-linearity and even singularity. In each case we establish the type of convergence of the Chebyshev collocation method implemented with Chebfun. In Section 4 we draw some conclusions on the usefulness and performance of the Chebfun system. We believe that additional experiments are needed in order to draw even firmer conclusions.

## 2. Chebfun vs.conventional ChC method

Feel symbolic but run at the speed of numerics! [5]

This quote contains the essence of the Chebfun system. It is implemented in object-oriented MATLAB and has been introduced in 2004 at Oxford University Mathematical Institute. The algorithms involved amount to spectral collocation methods on Chebyshev grids of automatically determined resolution.

In a latter extension the *chebop* class has been introduced (see [6]). We will extensively use the codes from this class. In [6] the authors observe that "the central principle of the Chebfun system is to evaluate functions in sufficiently many Chebyshev points for a polynomial interpolant to be accurate to machine precision".

The chebop system is implemented by means of four MATLAB classes: *domain*, *chebop*, *oparray*, and *varmat*, the last two classes are not normally relevant at user level. Instead, at the user level one has to specify the domain ($[-1, 1]$ being default), the differential operator along with boundary conditions such that the boundary value problem is well defined, and possible initial guess for Newton's method. Such a Chebfun code contains only a few lines, it is very intuitive and delivers very valuable output parameters relative to the convergence of the method and the evolution of Newton iterations.

Chebfun normally represents solutions $u(x)$ to BVPs by polynomial approximations, typically with an accuracy of about 10 digits, whose degree $N$ (the resolution) may be quite high (actually $0 < N < 4096$). Due to the bad conditioning of Chebyshev differentiation matrices, on a usual computing station the maximum $N$ one can hope for is around 1000. The polynomials can be interpreted as interpolants through a sufficiently large number $N + 1$ of samples at Chebyshev points defined by

$$x_j := \cos(\pi j/N),\ 0 \leq j \leq N\ for\ x \in [-1,\ 1]. \tag{3}$$

From this representation of the solution starts the essential difference from conventional ChC. In the case of the second method, it is impossible to establish this resolution apriori. Thus, although the Chebyshev collocation remains one and the same method, a much performing software leads to considerably better outcomes.

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Moreover, implementing conventional ChC is a much more laborious thing as it appears for instance from our work [1]. First of all, it is a challenging matter of establishing the right resolution. In most cases this is reduced to repeated tests. Imposing less common boundary conditions (mixed or non-local) is another "thorny"issue. Finally, obtaining output parameters similar to those provided by Chebfun requires additional effort, such as a fast Chebyshev transform.

## 3. Numerical Results

### *3.1. A test problem with known solution*

In [7] as well as in [8] the authors are concerned with a problem of type (1). It reads:

$$\begin{cases} u''(x) + \frac{2}{x}u'(x) + [u(x)]^5 = 0,\ 0 < x < 1, \\ u'(0) = 0,\ u(1) = \sqrt{3/4}. \end{cases} \tag{4}$$

The exact solution is known. It reads

$$u(x) = 1/\sqrt{1 + x^2/3}. \tag{5}$$

Among other phenomena, this problem models conductive heat transfer with nonlinear heat generation.

It is important to state that Chebfun works in the physical (values) space, i. e., computes the nodal values of a solution in the nodes $x_j$ defined by (3). At the same time it computes the values of the coefficients of the solution expansion in phase (coefficients) space. The latter reads

$$u_{Chebfun}(x) := \sum_{k=0}^{N-1} u_k T_k(x), \tag{6}$$

where $T_k(x)$ are the usual Chebyshev polynomials and $N$ is the length of solution provided by Chebfun.

The Chebfun solution to this problem is depicted in panel a) of Figure 1. It is clear that it perfectly overlaps with exact solution. The error in the $inf$ norm is of the order $10^{-15}$.

The second panel of this figure shows that the Chebyshev coefficients of the solution decrease almost linearly to the machine precision and the length of solution is $N = 16$. A straight line which bound them from above, the so called *envelope*, is also drawn. This parallelizes the straight line through origin of the equation

$$\log|u_k| = mk,\ 0 \le k \le N-1, \tag{7}$$

where $m \simeq -1$. It means that the (asymptotic) rate of convergence of Chebfun is *exponential* or geometric (see the monograph [9], Chapter 2 for the definition of the rate of convergence).

From panel c) of the same figure we understand that the Newton method is of the second order and uses five iterations.

Chebfun provides precise details on the accuracy with which the boundary conditions are enforced. In this case the residue vanishes.

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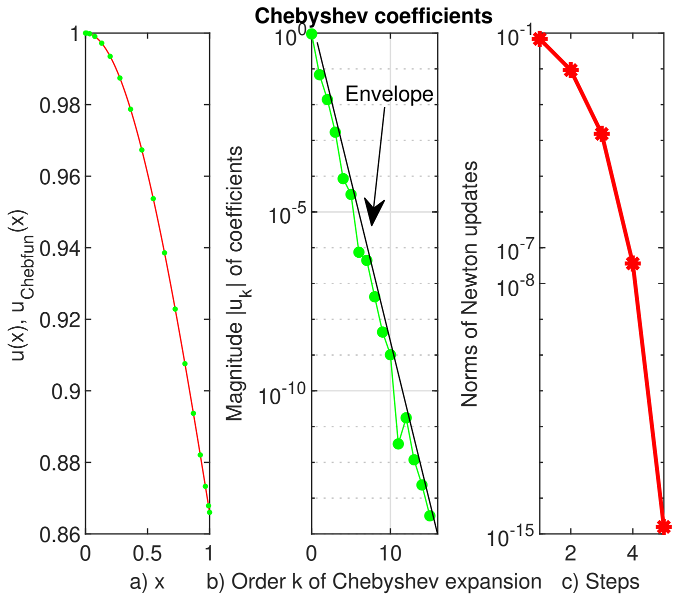


**Figure 1.** (**a**) The exact solutions (5) (green dots) and Chebfun solution (6) to problem (4) are displayed. (**b**) In a log-linear plot the behaviour of $|u_k|$ Chebyshev coefficients of solution to problem (4) (green dots) is reported. The envelope is depicted by a black straight line. (**c**) This panel shows that Newton's method is of second order and uses five iterative steps.

In [7] a classic method with finite differences is used in order to solve this problem and the authors hope to an accuracy of order $10^{-4}$. In a recent paper [8] the authors make use of the Haar wavelet method in order to solve a quasi-linearized version of this problem. Nor do they hope for better accuracy than something of order $10^{-6}$.

Finally we have solved the problem with MATLAB's *bvp4c* routine (see [10] for this routine). In this case we could not find the solution with an error better than $10^{-5}$.

Due to limited space, we will not be able to repeat and report all these comparisons for every problem which follows. However, we will sum up conclusions in the last Section.

### *3.2. A Bernstein type boundary value problem*

In [11] the authors consider a problem of type (1) in which the nonlinear term $f$ satisfies the so called *Bernstein growth condition*. Actually it means that $f$ can grow at most quadratically in its derivative variable.

We will consider the following example from this paper:

$$\left\{ \begin{array}{c} u''(x) - u^3(x) - (u'(x))^2 = \sin(\pi x) + 2\pi^2 \cos(2\pi x),\ 0 < x < 1, \\ u(0) - u'(0) = 2\sqrt{2},\ 2u(1) + 3u'(1) = 4\sqrt{2}. \end{array} \right. \tag{8}$$

The Chebfun solution to this problem is depicted in panel a) of Figure 2. This has exactly the same shape as the one obtained in [11] by shooting along with continuation with respect to the initial data. The Newton's method in solving the Chebfun discretization has second order (see panel b)) and the coefficients of Chebfun solution decrease smoothly and linearly to the level of machine precision. The convergence of the method remains exponential but the slope $m$ approximately equals $-0.3$ in (7), i.e., less optimal than in the previous example.

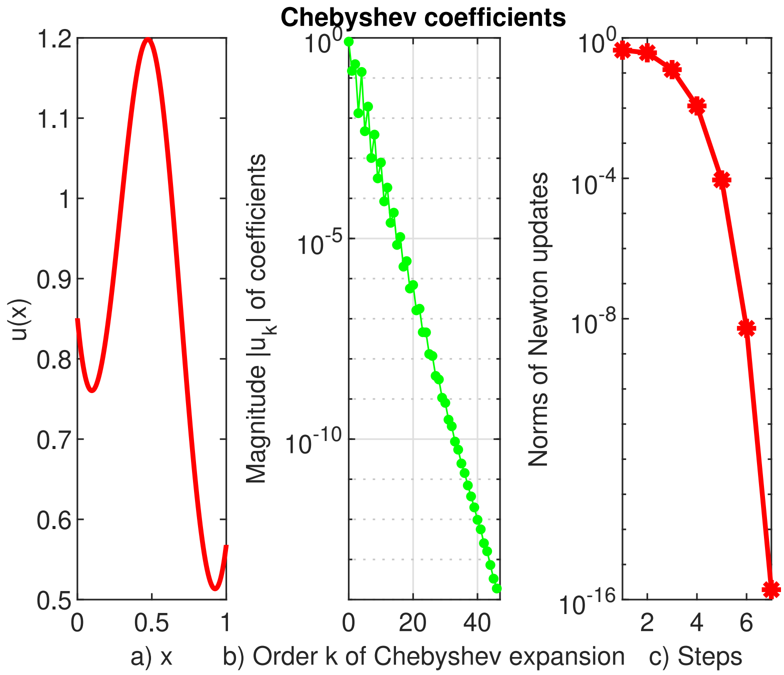


**Figure 2.** (**a**) The Chebfun solution to problem (8) is depicted. (**b**) In this panel we report the behaviour of Chebyshev coefficients of solution to problem (8) when $N = 47$. (**c**) Newton's method appears to be of second order and uses seven iterative steps.

We have intentionally chosen this example from the paper quoted above to show that the enforcement of mixed conditions is extremely simple in Chebfun and especially very precise, i.e., the final error in solving them is of order $10^{-11}$. Such an estimate is practically impossible with conventional ChC or *bvp4c*.

### *3.3. Lane-Emden equation of the second kind*

The equations of Lane-Emden-Fowler type arise in various applications in mechanics, nuclear physics, gas-dynamics, stellar structures, and chemically reacting systems. In [12] the author considers the nonlinear ODE

$$u'' + \frac{k}{x}u' + \delta \exp\left(\frac{u}{1+\varepsilon u}\right) = 0, \tag{9}$$

supplied with boundary conditions

$$u(-1) = u(1) = 0, \text{ for } k = 0, \tag{10}$$

or

$$u'(0) = 0, \; u(1) = 0, \text{ for } k = 1, 2. \tag{11}$$

For $k = 0$ and $\varepsilon > 0$ the problem (9)-(10) admits the following exact first integral

$$\begin{aligned} (u'(x_1))^2 + 2\delta\{\tfrac{e^{1/\varepsilon}}{\varepsilon^2}\mathcal{E}\rangle\left(\tfrac{-1}{\varepsilon(1+\varepsilon u(x_1))}\right) + \left(\tfrac{1}{\varepsilon} + u(x_1)\right)\exp\left(\tfrac{u(x_1)}{1+u(x_1)}\right)\} = \\ (u'(x_2))^2 + 2\delta\{\tfrac{e^{1/\varepsilon}}{\varepsilon^2}\mathcal{E}\rangle\left(\tfrac{-1}{\varepsilon(1+\varepsilon u(x_2))}\right) + \left(\tfrac{1}{\varepsilon} + u(x_2)\right)\exp\left(\tfrac{u(x_2)}{1+u(x2)}\right)\}, \end{aligned} \tag{12}$$

where $-1 \le x_1 \ne x_2 \le 1$ and $\mathcal{E}\rangle(x)$ denotes the exponential integral $\mathcal{E}\rangle(x) := \int_{-\infty}^{x} \frac{e^t}{t} dt$.

In order to see how accurate this integral is satisfied we take first $x_1 := 1$ and $x_{2:} = 0$ and then from the boundary conditions we introduce $u(x_1) = 0$ and $u'(x_2) = 0$ (the symmetry of solution with respect to $x$). The values $u'(x_1)$ and $u(x_2)$ have been computed by Chebfun.

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Thus, in our computation, regardless of the values of parameters $\delta$ and $\varepsilon$, the first integral (12) is satisfied with a precision of order $10^{-13}$.

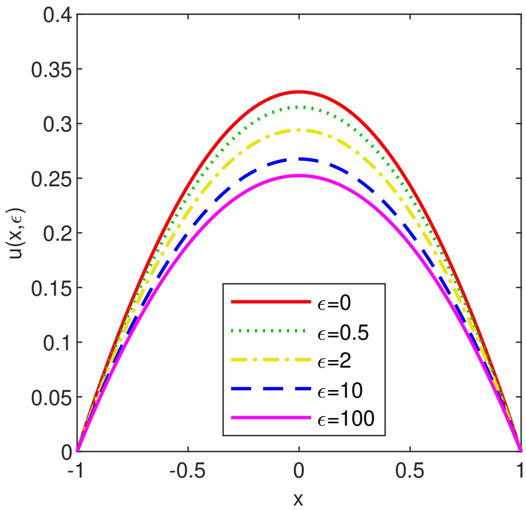


**Figure 3.** Chebfun solutions to problem (9)-(10) when $\delta := 0.5$ for various values of $\epsilon$.

Chebfun has no difficulty solving problems (9)-(10) and (9)-(11). The solutions to the problem (9)-(10) are displayed in Figure 3. The Newton method has effectively the second order and no more than two or three iterations are used in each case.

The convergence of the method is exponential with the slope $m$ approximately equals $-0.3$ in (7). Improper integrals

$$\mathcal{E}\rangle\left(\frac{-1}{\varepsilon(1+\varepsilon u(x_i))}\right),\ i = 1,2,$$

in the first integral (12) are also calculated without any difficulty by Chebfun. It uses $sum$ operator along with option $'splitting',' on'$. In each case the Newton process started from the initial guess $u_0 := 1$.

### *3.4. A singular problem from the theory of the pseudo-plastic fluids*

In [13] the authors consider the existence issue for the problem

$$\begin{cases} u'' + \nu x/u^{1/\nu} = 0,\ 0 < x < 1, \\ -u'(0) = u(1) = 0, \end{cases} \tag{13}$$

where $0 < \nu \leq 1$. The case $\nu := 1$ corresponds to the Newtonian fluid.

This problem is much more difficult than the previous one in the following sense. If in the previous case Chebfun used a tolerance of order $10^{-14}$ for Newton's solver in this case we had to loosen this tolerance to $10^{-6}$ in order to guarantee a convergent procedure.

A set of solutions to problem (13) is displayed in Figure 4.

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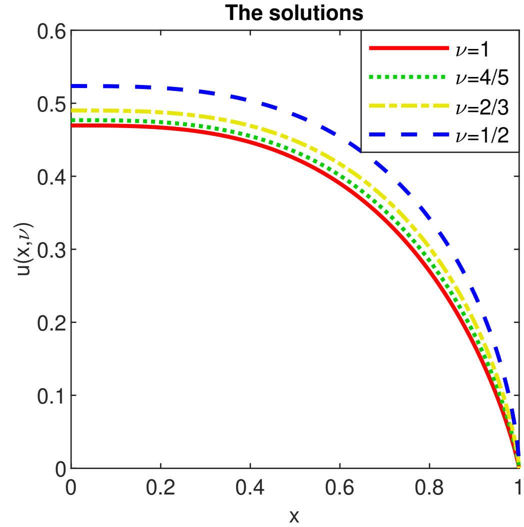


**Figure 4.** Chebfun solutions to problem (13) for various values of $\nu$.

In the left panel of Figure 5 we display the norm of Newton's updates vs. iteration number in the worst case, i.e. $\nu = 1/2$. It is apparent that the order of the Newton's method is much less than 2.

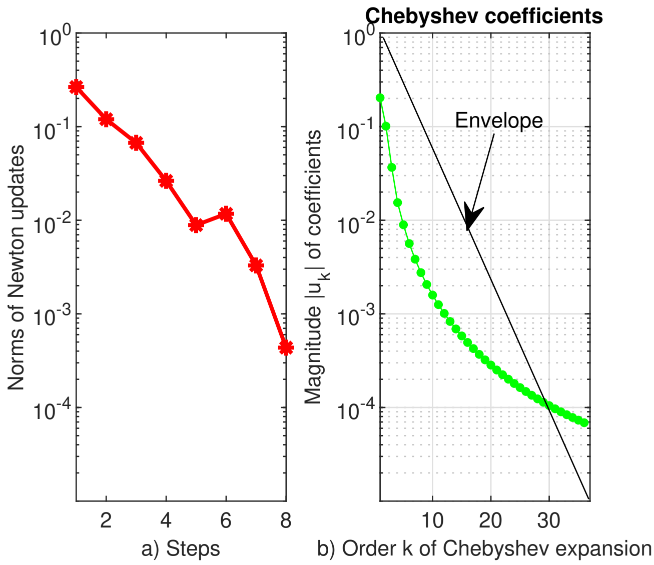


**Figure 5.** (**a**) The convergence of Newton's method in solving problem (13) when $\nu := 1/2$. (**b**) In a log-linear plot we display the decreasing behavior of the Chebyshev coefficients (green dots) of solution to the same problem.

From the right panel of Figure 5 we see that the solution has length 37 and its coefficients decrease smoothly but remain very far from the machine precision level. We also drew the envelope for these coefficients and from the log-linear plot b) of Figure 5 we can only infer that asymptotically, i.e. for large $k$, the coefficients of expansion (6) of solution satisfy

$$|u_k| \sim 1/k^2,$$

which means that the rate of convergence is only *algebraic*.

The point where the envelope intersects the coefficients' curve is (roughly!) the *magnitude of the error*. In fact, the coefficients decrease slightly below the level $10^{-4}$.

The problem of finding an initial guess in order to ensure the convergence of Newton's iterates is not at all simple in this case. Repeated attempts led us to an initial date of form

$$u_0(x) := \left(1 - x^{2n}\right), n = 3, 4, 5.$$

. This initial guess satisfies the boundary conditions of problem (13) and have a curvature close to that of numerical outcomes.

It should be noted that for values of the parameter $\nu$ in the range $(0, 1/2)$ Chebfun completely failed!

In order to solve this problem for arbitrary values of $\nu$ in [14] the authors have introduces an iterative technique which reduces the problem to a sequence of usual eigenvalue problems. We have tested the capabilities of Chebfun in solving various Sturm-Liouville problems in some previous papers thus we are not interested in these iterative techniques (see for instance our contribution [15]).

### *3.5. A nonlinear heat conduction model of the human head*

The analytical study of the problem

$$\begin{cases} -\frac{1}{x^2}\left(x^2 u'\right)' = a \exp(-u),\ 0 < x < 1, \\ u'(0) = 0,\ u'(1) + bu(1) = 0. \end{cases} \tag{14}$$

has been initiated in [16]. Roughly speaking in this model the right hand side is the heat production rate per unit volume, $u(x)$ is the absolute temperature, $x$ is the radial distance from the centre, $a$ is the inverse of the average thermal conductivity inside the head and $b$ is a heat exchange coefficient.

Three solutions $u(x, a, b)$ of this problem are reported in the panel a) of Figure 6.

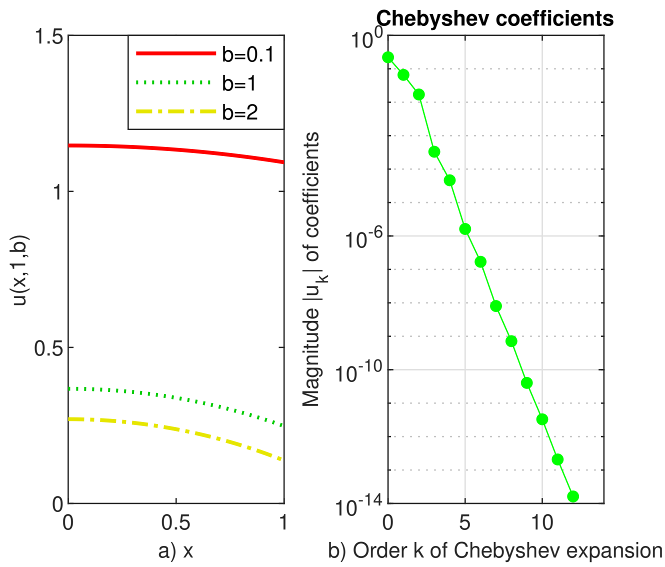


**Figure 6.** (**a**) Three solutions $u(x, 1, b)$ to the problem (14). (**b**)) This panel shows that when $b := 2$ the Chebyshev coefficients of solution decrease almost linearly, close to the machine precision level, with a slope a little bit larger than $-1$.

The behavior of Chebyshev coefficients in the panel b) of Figure 6 shows that the rate of convergence is definitely exponential.

Although the problem has received some attention over time, we have not found numerical results with which to compare ours. In any case, in its solution Newton's method keeps the second order and does not use more than six iterative steps.

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### 3.6. Membrane buckling

In [17] the authors consider, among other problems, the following nonlinear and singular problem:

$$\begin{cases} \left(x^3 u'\right)' + x^3/u^2 = 0,\ 0 < x < 1, \\ u'(0) = 0,\ u'(1) + (1-\nu)u(1) = 0, \end{cases} \tag{15}$$

which describes a flat, circular elastic membrane which is deformed by an axisymmetric pressure applied to its surface. The edge of the membrane is restrained from deforming normal to its mid-plane. Either a compressive radial thrust or a contractile radial displacement is applied to the edge. The dependent variable $u(x)$ stands for the radial stress and $x$ is the dimensionless radius. The parameter $\nu$ stands for Poisson ration of the membrane material.

Two solutions to the problem (15) are displayed in Figure 7.

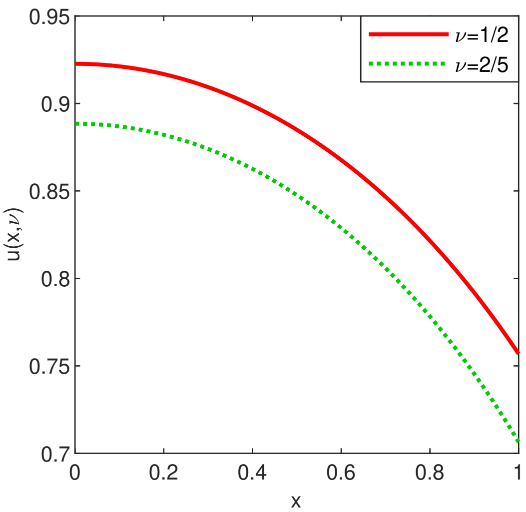


**Figure 7.** Two solutions $u(x,\nu)$ to the problem (15).

The calculation of the two solutions differs fundamentally. In the first case ($\nu = 1/2$) Chebfun produces the solution in five iterations and the Newton's method has the second order. In the other case, Chebfun produces the solution in 86 iterations and the order of Newton's method is far from order two. This aspect is visible in the left panel of Figure 8.

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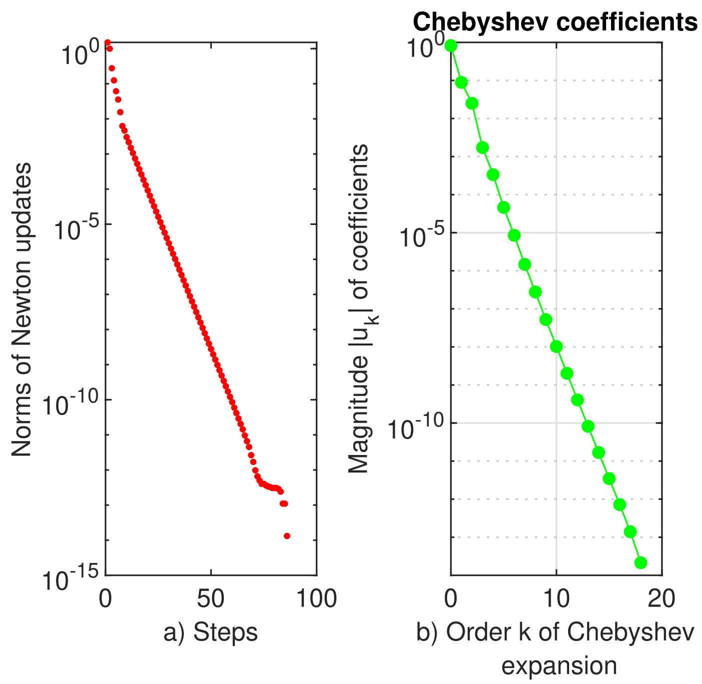


**Figure 8.** (**a**) The norm of the Newton's updates when Chebfun computes the solution $u(x, 2/5)$. (**b**) The Chebyshev coefficients of solution to problem (15) with $\nu = 2/5$.

The behavior (almost linear decrease to the machine precision level) of the Chebyshev coefficients of the solution suggests a still exponential convergent process (see the b) panel in Figure 8).

One remark is suitable at this stage. For lower values of Poison parameter (membrane made of stiffer materials) Chebfun simply failed.

### 3.7. *A nonlinear (super-linear) singular problem*

Our observations from many numerical experiments lead us to the conclusion that singularity is more difficult to manage than non-linearity for Chebfun. In order to strengthen this assertion we consider another example.

Thus, in [18] the authors are concerned the singular and non-linear problem:

$$\begin{cases} u''(x) + (u^{-\alpha}(x) + 1)(1 - (-u(x)')^{\gamma}) = 0,\ 0 < x < 1, \\ u'(0) = 0 = u(1),\ \alpha > 0,\ \gamma > 0. \end{cases} \tag{16}$$

Three solutions of this problem are displayed in the panel a) of Figure 9.

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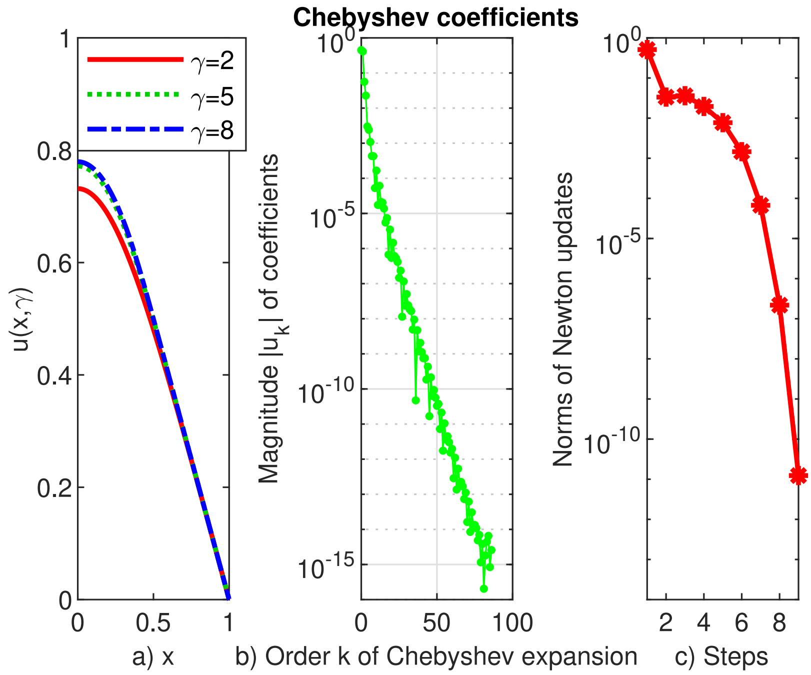


**Figure 9.** (**a**) Three solutions $u(x,\gamma)$ to the problem (16) when $\alpha := 1$. (**b**) This panel shows that when $\gamma := 8$ the Chebyshev coefficients of solution decrease almost linearly close to the machine precision with a slope a little bit larger than $-1$. (**c**) Newton updates are illustrated for the same value of $\gamma$.

For higher values of $\alpha$ than 1, Chebfun could not solve the problem even though the tolerance was considerably lower. This is not the case for the exponent $\gamma$.

For the highest value of $\gamma$ the convergence rate remains exponential and the Newton's method has an order close to two. These result from panels b) and c) of the same figure.

### *3.8. A singularly perturbed nonlinear problem*

In [19] the authors analyze the following problem:

$$\begin{cases} \varepsilon u'' + \exp(u)u' - \frac{\pi}{2}\sin\left(\frac{\pi x}{2}\right)\exp(2u) = 0,\ 0 < x < 1,\ 0 < \varepsilon << 1, \\ u(0) = u(1) = 0. \end{cases} \quad (17)$$

Five solutions of this problem are reported in Figure 10. They correspond to

$$\varepsilon := 10^{-1}, \ldots, 10^{-5}$$

and confirm that there exists a sharp *boundary layer* at the right of $x = 0$.

In order to reach the lowest value $\varepsilon := 10^{-5}$ we have used continuation with respect to this parameter and we have loosen the tolerance to $10^{-10}$. As a result, the convergence of the Newton method is no longer quadratic but is reduced to something around the unit.

It is very important to underline that for $\varepsilon := 10^{-1}$ Chebfun uses a solution of length 97 and for $\varepsilon := 10^{-5}$ it uses a much larger solution of length 2508. The Newton's method resolved the first case mentioned above using 7 iterations while for the later case it resolved the problem only in four iterations. The order of the Newton method is close to two, but the Chebyshev coefficients of the solution decrease only to the level $10^{-11}$.

We have not found numerical results in the literature to compare with ours. Some other listed problems in [19] have been solved by Chebfun without any difficulty.

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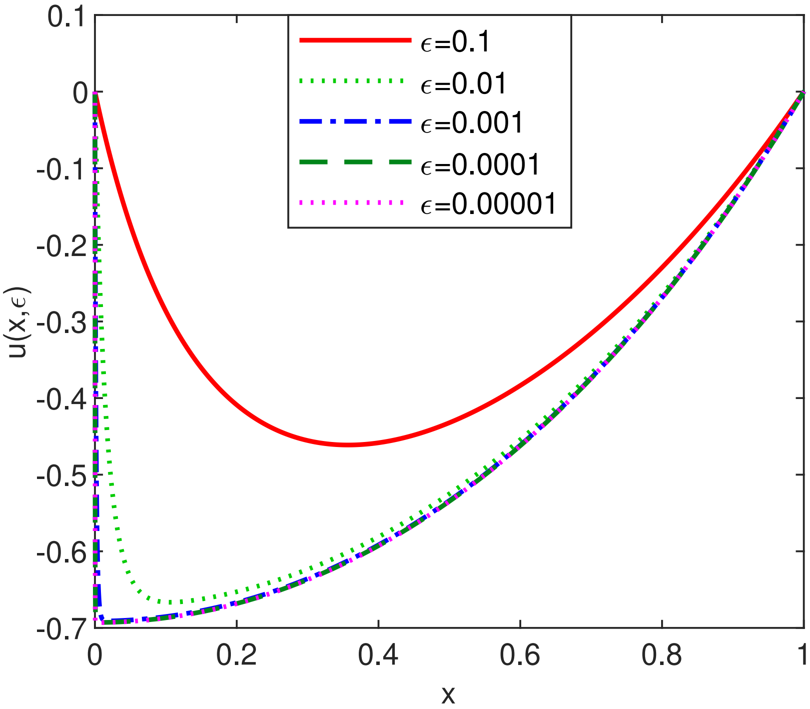


**Figure 10.** Five solutions to problem (17) for various values of the parameter $\epsilon$.

The exact solution to (17) has the form:

$$u(x,\varepsilon) = \widehat{u}(x,\varepsilon) + O(\varepsilon), \quad \widehat{u}(x,\varepsilon) := -\ln((1+\cos(\frac{\pi x}{2}))(1-\frac{1}{2}\exp(\frac{-x}{2\varepsilon}))). \tag{18}$$

When $\varepsilon := 10^{-5}$, the $inf\ norm$ of the error

$$u_{Chebfun}(x,\varepsilon) - \widehat{u}(x,\varepsilon)$$

reaches the value of order $10^{-5}$ which emphasizes the accuracy of the computations.

## 4. Discussion

*Chebfun is not a universal panacea!*

There are nonlinear and singular problems for which no matter how much we have reduced tolerance, i.e., *bvpTol*, Chebfun fails. An example is the problem (13). This seems to be the most difficult problem in the multitude of our numerical experiments.

The exponential accuracy is proved by the rate the Chebyshev coefficients of solutions decay. Again the problem (13) is in the worst situation. The rate of convergence is only algebraic. A slightly better situation is found relative to the singular problem (15). Otherwise in all other cases the problems are solved with exponential accuracy.

Another advantage of Chebfun compared to conventional ChC is the lack of rounding-off plateau in the analysis of solution coefficients. This is due to the way Chebfun truncates.

The main conclusion of the paper is that, up to date, collocation in form of Chebfun provides the most accurate solution in solving genuinely nonlinear and/or singular BVPs.

However, in order to see more clearly the effects of some singularities and even non-linearities on Chebfun's performances, we believe that further numerical experiments will have to be conducted. Some of them are in progress.

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**Sample Availability:** Samples of the Chebfun codes are available from the author by request.

## Abbreviations

The following abbreviations are used in this manuscript:

| | |
|---|---|
| BVP | Boundary Value Problem |
| ChC | the conventional Chebyshev collocation method |
| Chebfun | is a software system in object-oriented MATLAB;<br>it extends many MATLAB operations on vectors and matrices to functions and operators |
| 1D | one-dimensional |
| tilde | asymptotic equivalence |

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