Numerical experiments with the Bratu equation in one, two and three dimensions

Janusz Karkowski

Received: 14 December 2011 / Revised: 3 July 2012 / Accepted: 3 July 2012 /
Published online: 16 April 2013
© The Author(s) 2013. This article is published with open access at Springerlink.com

Abstract The non-linear Bratu equation is solved numerically in one, two and three dimensions. The numerical results are obtained with help of three different numerical methods namely pseudospectral method, finite difference method and radial basis functions method. All methods give approximately the same results. One-dimensional case is used for testing numerical methods as the analytical solution is known in this case. In two dimensions, the existing results are generalized to larger area of eigenvalues. Three-dimensional case is solved for the first time and this is the most important result of the paper.

Keywords Non-linear pde · Bifurcation problem · RBF functions

1 Introduction

The aim of the present paper is to solve numerically the Bratu equation (see below) in three space dimensions. This equation coupled with appropriate boundary conditions is used to model the temperature distribution in combustion models (Bebernes and Eberly 1989). The three-dimensional model was considered in investigations on the suns core temperatures, see Chandrasekhar (1967); Buckmire (2003). The Bratu model stimulates also a thermal reaction process in a rigid material where the process depends on the balance between chemically generated heat and heat transfer by conduction (Wazwaz 2005; Noor and Mohyud-Din 2007a,b). We have chosen three different methods to achieve our goal: pseudospectral method, finite difference method and radial basis functions (RBF) method. Let us note that the RBF method we have used is original as it generalizes the classical approach on the boundary (see Sect. 3.4 for details). These methods are first intensively tested in the one-dimensional case in which

Communicated by Antonio Silva Neto.

J. Karkowski (✉)
M. Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4,
30-059 Kraków, Poland
e-mail: januszk@th.if.uj.edu.pl

the analytical solution is known. This case was also investigated numerically with help of many different methods: spline-based treatment (Abukhaled et al. 2012), (modified) variational iteration method (Jin 2010; Mohyud-Din 2008), Adomian's decomposition method (Wazwaz 2005; Syam and Hamdan 2006), the Lie-group shooting method (Abbasbandy et al. 2011), one-point pseudospectral collocation (Boyd 2011) and others. Our methods work fine and are in good agreement with analytical formulae and numerical results. The two-dimensional case is more complicated and analytical solutions are not known. It was studied numerically (Boyd 1986; Misirli and Gurefe 2011; Kapania 1990) and we verify and generalize the existing results. The three-dimensional case is examined, to our knowledge, for the first time and our results are novel. It is much more difficult than one- and two-dimensional cases. It requires parallel computations to save time, and the starting point of the linearization method must be very carefully chosen to achieve convergence of the whole procedure—this will be discussed later. Let us also stress that the qualitative behaviour of the three-dimensional bifurcation curve is very different from that in one and two dimensions.

The paper is organized as follows. In Sect. 2 we describe the Bratu problem in detail. Section 3 is devoted to numerical methods. We review the Newton's method used to linearize our problem and the details of the numerical procedures mentioned above. Numerical results concerning all three examined cases are presented in Sect. 4. Section 5 involves short conclusions.

2 Bratu equation

The Bratu equation in n dimensions is the non-linear eigenvalue problem of the form

$$\Delta\varphi(x_1, x_2, \dots, x_n) + \lambda \exp(\varphi(x_1, x_2, \dots, x_n)) = 0,$$

in the n -cube $|x_i| \leq 1$ ($i = 1, 2, \dots, n$), where Δ is the n -dimensional Laplace operator

$$\Delta = \sum_{i=1}^n \left(\frac{\partial}{\partial x^i} \right)^2,$$

and the following boundary conditions are imposed

$$\varphi(x_1, x_2, \dots, x_n) = 0 \quad \text{for } |x_i| = 1.$$

In the present paper, we solve numerically the above equation for $n = 1, 2, 3$. That is we examine how many solutions exist for a given eigenvalue $\lambda > 0$ and compute these solutions with the help of different numerical techniques. We have used the simple finite difference method, the pseudospectral method and the RBF method.

In the simple, one-dimensional case, the Bratu equation reduces to

$$\frac{\partial^2}{\partial x^2} \varphi(x) + \lambda \exp(\varphi(x)) = 0, \tag{1}$$

in the interval $|x| \leq 1$, with boundary conditions

$$\varphi(\pm 1) = 0.$$

This case lets us test our computational methods, as the analytical solution is known up to some numerical constant $z(\lambda)$ which can be obtained from the transcendental equation (Boyd 2011)

$$z = \cosh\left(\sqrt{\frac{\lambda}{2}}z\right).$$

This equation has two real branches meeting at the limit point $\lambda_{\text{limit}} = 0.8784576797812903015$, $z_{\text{limit}} = 1.8101705806989772753$, above which there are no solutions. The exact solution of Eq. (1) reads

$$\varphi(x; \lambda) = 2 \log \left(\frac{z}{\cosh\left(z\sqrt{\frac{\lambda}{2}}x\right)} \right).$$

Thus $\varphi(x; \lambda)$ has also two branches meeting at the bifurcation point.

The analytical solution of the two-dimensional Bratu-equation is not known and the numerical study of it (Boyd 1986) shows also the existence of two branches which were (partly) computed only approximately. The present paper is, to our knowledge, the first (numerical) study of the three-dimensional case.

3 Numerical methods

3.1 Newton's linearization method

Let us first discuss a more general problem of the form

$$L\varphi = F(\varphi),$$

where L is some linear operator (Laplace operator in our case) and F a non-linear function ($-\lambda \cdot \exp$ for the Bratu equation). Assume that we know φ_n : the n -th approximation to the solution of our problem. We seek the next $(n + 1)$ -th approximation in the form

$$\varphi_{n+1} = \varphi_n + \delta\varphi_n,$$

where $\delta\varphi_n$ is a small correction. Linearizing our problem we get the following equation for the $\delta\varphi_n$

$$(L - F'(\varphi_n))\delta\varphi_n = F(\varphi_n) - L\varphi_n. \quad (2)$$

Because

$$L\varphi_n = F(\varphi_{n-1}) + F'(\varphi_{n-1})\delta\varphi_{n-1},$$

we finally obtain

$$(L - F'(\varphi_n))\delta\varphi_n = F(\varphi_n) - F(\varphi_{n-1}) - F'(\varphi_{n-1})(\varphi_n - \varphi_{n-1}). \quad (3)$$

This is a linear problem with the linear operator $L - F'(\varphi_n)$ and the source term on the right hand side of the above formula. The procedure requires the starting pair (φ_0, φ_1) — φ_0 should be carefully chosen and satisfy the desired boundary conditions, φ_1 in turn can be calculated from Eq. (2) for $n = 0$. In the case of the Bratu problem, the Eq. (3) takes the form

$$(\Delta + \lambda \exp(\varphi_n))\delta\varphi_n = -\lambda(\exp(\varphi_n) - \exp(\varphi_{n-1}) - \exp(\varphi_{n-1})(\varphi_n - \varphi_{n-1})). \quad (4)$$

It must be solved on the area $[-1, 1]^{\text{dim}}$ with zero boundary conditions and the whole procedure is stopped when the norm $|\delta\varphi_n|$ is less than some small positive constant ϵps .

3.2 Finite difference method

In this method each interval $[-1, 1]$ is divided into n subintervals of equal length $h = 2/n$. The grid in each dimension consists of $n + 1$ equidistant points $x_0, x_1, \dots, x_n$ and the second derivative of the function u is approximated by

$$\frac{\partial^2}{\partial x^2} u(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2},$$

where $h = x_{i+1} - x_i$. Thus, for instance in three dimensions we have

$$\begin{aligned} \Delta u(i, j, k) = & \frac{u(i+1, j, k) - 2u(i, j, k) + u(i-1, j, k)}{h^2} \\ & + \frac{u(i, j+1, k) - 2u(i, j, k) + u(i, j-1, k)}{h^2} \\ & + \frac{u(i, j, k+1) - 2u(i, j, k) + u(i, j, k-1)}{h^2}, \end{aligned}$$

where i, j, k are the node numbers in x, y, z direction, respectively. Inserting this formula into Eq. (4) we obtain the symmetric, sparse system of linear equations for $\delta\varphi_n(i, j, k)$. There are several excellent numerical packages solving such systems—in our practice we have used IBM Watson Sparse Matrix Package (WSMP) https://researcher.ibm.com/researcher/view_project.php?id=1426 and the Parallel Direct Sparse Solver (PARDISO) included in INTEL MKL library <http://software.intel.com/en-us/articles/intel-mkl/>. Let us stress that these packages work fine in multiprocessor (multicore) environment.

3.3 Pseudospectral method

In this method, we choose the Chebyshev points of the second kind to form the grid in the interval $[-1, 1]$. These points are given by

$$x_j = \cos\left(\frac{j\pi}{n}\right), \quad j = 0, 1, \dots, n.$$

The second derivative in the given node is approximated by the second derivative of the Lagrange polynomial interpolant in that point. The appropriate formula is linear in the node values of the function $u(i)$ and is usually written with help of the differentiation matrix (Berrut et al. 2005; Berrut and Trefethen 2004)

$$\frac{\partial^2}{\partial x^2} u(i) = \sum_{j=0}^n D^{(2)}(i, j) u(j),$$

where $D^{(2)}$ is the second differentiation matrix with elements

$$D^{(2)}(i, j) = \begin{cases} 2D^{(1)}(i, j) \left(D^{(1)}(i, i) - \frac{1}{x_i - x_j} \right), & i \neq j, \\ -\sum_{k \neq i} D^{(2)}(i, k), & i = j, \end{cases}$$

and $D^{(1)}$ is the first differentiation matrix

$$D^{(1)}(i, j) = \begin{cases} \frac{w_j/w_i}{x_i - x_j}, & i \neq j, \\ -\sum_{k \neq i} D^{(1)}(k, i), & i = j. \end{cases}$$

Table 1 Some commonly used RBFs

RBF	$f(r)$
Piecewise polynomial (R_n)	$ r ^n, \quad n \text{ odd}$
Thin plate spline (TPS_n)	$ r ^n \ln r, \quad n \text{ even}$
Multiquadric (MQ)	$\sqrt{1 + (\varepsilon r)^2}$
Inverse multiquadric (IMQ)	$\frac{1}{\sqrt{1 + (\varepsilon r)^2}}$
Inverse quadratic (IQ)	$\frac{1}{1 + (\varepsilon r)^2}$
Gaussian (GS)	$\exp(-(\varepsilon r)^2)$

The so-called barycentric weights w_j are given by

$$w_j = (-1)^j \delta_j, \quad \delta_j = \begin{cases} \frac{1}{2}, & j = 0 \text{ or } j = n, \\ 1, & \text{otherwise.} \end{cases}$$

Applying the pseudospectral method to the Eq. (4), we obtain a sparse, unsymmetric system of linear equations, which can also be solved by WSMP or PARDISO package as these packages include unsymmetric solvers as well.

3.4 RBF method

A RBF is a real-valued function whose value depends only on the distance from some point c , called a centre, so that

$$f(x, c) = f(|x - c|).$$

In this method, we choose the centres c_i , $i = 1, \dots, N$ lying in the computation area and the shape of the function f . The RBF method becomes very popular nowadays and is extensively studied both from theoretical and numerical point of view [see [Boyd \(2010a,b\)](#);

Fig. 1 One-dimensional bifurcation curve: λ versus $\phi(0)$

(a) Error values for the lower branch

(b) Error values for the upper branch

Fig. 2 Numerical errors: $\ln(\text{Err}_{\max})$ versus λ

Boyd and Gildersleeve (2011) and references therein]. Some of the most popular RBFs are given in Table 1. [see for instance Larsson and Fornberg (2003)]

Let us note that the RBFs shown in the Table 1 can depend on the shape parameter ε and we denote $r = \|x - c\|$. The simplest RBF interpolant is a linear combination of RBFs centred at the scattered points c_i

$$\varphi(x) = \sum_{i=1}^N w_i f(\|x - c_i\|),$$

(a) The lower branch numerical errors

(b) The upper branch numerical errors

Fig. 3 Numerical errors for different numbers of grid points: finite difference method

however, in our case we use a little bit more complicated interpolant, which has the form

$$\varphi(x) = \sum_{i=1}^N w_i f(\|x - c_i\|) + \sum_{i=1}^{N_B} w'_i \Delta f(\|x - c_i\|), \quad (5)$$

where the second sum is over all centres lying on the boundary. The reason is that we want our Laplace equations to be valid also at the boundary centres where the (Dirichlet) boundary conditions must be fulfilled as well. Thus, we need two RBFs for each boundary centre. This

Fig. 4 Two-dimensional bifurcation curve: λ versus $\phi(0, 0)$

is a modified method of Fedoseyev et al. (2002) in which the additional centres are lying outside the boundary.

Let us now apply the RBF interpolant for $\delta\varphi_n$ to the Bratu problem. We must solve Eq. (4) subject to zero boundary conditions. We require this equation to be strictly valid at all centres and boundary conditions must be fulfilled at boundary centres. We have

$$\Delta\delta\varphi(x) = \sum_{i=1}^N w_i \Delta f(\|x - c_i\|) + \sum_{i=1}^{N_B} w'_i \Delta^2 f(\|x - c_i\|),$$

Fig. 5 Two-dimensional numerical solution for $\lambda = 1.5$

and insert this formula into (4). Thus, we obtain N linear equations for $N + N_B$ unknowns w_i , $i = 1, \dots, N$ and w'_i , $i = 1, \dots, N_B$. The remaining N_B equations we get from the boundary conditions. They read

$$\delta\varphi_n(c_k) = \sum_{i=1}^N w_i f(\|c_k - c_i\|) + \sum_{i=1}^{N_B} w'_i \Delta f(\|c_k - c_i\|) = 0, \quad k = 1, \dots, N_B.$$

As a result we must solve the dense linear system for $N + N_B$ variables. The previously mentioned numerical packages WSMP and PARDISO are not suitable for this case as they have been derived for sparse linear systems and we have used Parallel Linear Algebra Software for Multicore Architectures (PLASMA) package <http://icl.cs.utk.edu/plasma/> which turned out to be excellent for solving dense linear systems on multicore processors.

Fig. 6 Three-dimensional bifurcation curve: λ versus $\phi(0, 0, 0)$

4 Numerical results

4.1 The one-dimensional case

As was mentioned earlier the analytical solution is known in this case, so we compare our numerical results with this solution. Let us first show two real branches of the solutions meeting at the bifurcation point

$$\lambda_{\text{bif}} = 0.8784576797812903015.$$

They are presented in Fig. 1.

It is interesting to show the errors of the numerical solutions depending on the eigenvalue λ . The error is defined as

$$\text{Err}_{\max} = \max_x ||\phi(x) - \phi_{\text{num}}(x)||,$$

and we present the logarithm of the errors for our three numerical methods in Fig. 2. The number of grid points is 2,000 for the finite difference method, 25 for the pseudospectral method and 200 for the RBF method. It is evident that the best results we have obtained with the pseudospectral method (with the exception of the area of small λ for the upper (right) branch).

To be complete we present also the dependence of the numerical error on the number on grid points. Figure 3 presents this dependence for the finite difference method.

4.2 The two-dimensional case

This case was examined long ago by [Boyd \(1986\)](#). We present in Fig. 4 the Boyd's bifurcation curve obtained both by numerical and approximated analytical methods and compare it with our purely numerical bifurcation curve obtained by three different numerical

Fig. 7 Three-dimensional sections of the numerical solutions for $\lambda = 2.25$: $\phi(x, y, 0)$ versus (x, y)

methods described above. Let us stress that our curve obeys larger area although the upper branch slightly differs for different numerical methods especially for small values of the eigenvalue λ (Fig. 4).

We have obtained our numerical results for the following numbers of grid points: 25×25 for pseudospectral method, 100×100 for finite difference method and 1,850 for rbf method. An example of the two-dimensional numerical φ -surface (both for lower (left) and upper (right) branch) is presented in Fig. 5

4.3 The three-dimensional case

The most important aim of the numerical study of this case was to get the bifurcation curve of the solutions in the largest possible area. As in the previous cases we applied three numerical

Fig. 8 Bifurcation curves for one, two and three dimensions

methods: the pseudospectral method with $25 \times 25 \times 25$ grid points, the finite difference method with $100 \times 100 \times 100$ grid points and the RBF method with about 9,200 grid points plus 2,400 grid points on the boundary (see Sect. 3.4 for details). All three methods worked fine for the lower branch but for the upper branch they failed for λ approximately equal to 1.3. Therefore, the neighbourhood of this point required very careful investigations. After doing them it turned out that the qualitative behaviour of the bifurcation curve in three dimensions is quite different than in one and two dimensions. We have found two new bifurcation points: $\lambda_2 \approx 1.321$ (local minimum) and $\lambda_3 \approx 1.556$ (local maximum). The first bifurcation point $\lambda_1 \approx 2.475$ is the global maximum of our bifurcation curve which is presented in Fig. 6. Thus, starting from $\lambda \approx 0.0$ we have two solutions for a given λ (up to $\lambda = \lambda_2$). For $\lambda = \lambda_2$ and $\lambda = \lambda_3$, three solutions are present and between these values four solutions exist. Above λ_3 , we have two solutions up to $\lambda = \lambda_1$ and for λ greater than this value there are no solutions at all. Let us note that obtaining upper branches of the three-dimensional bifurcation curve was a difficult numerical task as this process was very sensitive to the choice of the starting point of the Newton's procedure (see Sect. 3.1).

We present also two examples of the solutions for $\lambda = 2.25$, one from the lower branch and the second from the first upper branch. Figure 7 shows their sections by the hyperplane $z = 0$.

5 Conclusions

In the present paper, we have presented numerical solutions of the Bratu equation in one, two and three dimensions. Our results in the one dimension show that the numerical procedures we have applied work fine and our numerics agrees with analytical formulae with high precision. Therefore, it was tempting to apply them in higher dimensions. In the two-dimensional case, the numerical results we have obtained confirm qualitatively the shape of the bifurcation

curve presented by Boyd, but our bifurcation curve covers a wider range (it is valid also for small values of the eigenvalue λ in the upper branch).

The three-dimensional case is numerically much more complicated. The lower branch of the bifurcation curve was rather easy to obtain numerically, but for the upper branch the numerical procedures failed for $\lambda \approx 1.3$. The reason of such behaviour became clear for us after very careful investigation of the neighbourhood of this point. It turned out that two new bifurcation points exist (the local minimum and the local maximum) and the qualitative behaviour of the three-dimensional bifurcation curve is quite different than in one and two dimensions (see Fig. 6). Let us add that finding the additional branches of the bifurcation curve was a very hard task. First, we had to get one point of a given branch. Then, we obtained other points by changing infinitesimally the parameter $\lambda \rightarrow \lambda + \delta\lambda$ and taking the solution for λ as the starting point of the Newton's procedure (see Sect. 3.1) that yielded the solution for $\lambda + \delta\lambda$. We repeated this procedure for all values of λ on the given branch. It is worth mentioning that the pseudospectral method seems to be the quickest in three dimensions. Our results are summarized in Fig. 8, where the all three bifurcation curves are presented.

Open Access This article is distributed under the terms of the Creative Commons Attribution License which permits any use, distribution, and reproduction in any medium, provided the original author(s) and the source are credited.

References

- Abbasbandy S, Hashemi MS, Liu CS (2011) The Lie-group shooting method for solving the Bratu equation. *Commun Nonlinear Sci Numer Simul* 16(11):4238–4249
- Abukhaled M, Khuri S, Sayfy A (2012) Spline-based numerical treatments of Bratu-type equations. *Palestine J Math* 1:63–70
- Bebernes J, Eberly D (1989) Mathematical problems from combustion theory. In: *Applied mathematical sciences*, vol 83. Springer, New York
- Berrut JP, Baltensperger R, Mittelmann HD, de Bruin MG, Mache DH, Szabados J (eds) (2005) Recent developments in barycentric rational interpolation. In: *Trends and Applications in Constructive Approximation*, ser. International Series of Numerical Mathematics, vol 151. Birkhäuser, Basel, pp 27–51
- Berrut JP, Trefethen LN (2004) Barycentric Lagrange interpolation. *SIAM Rev* 46(3):501–517
- Boyd JP (1986) An analytical and numerical study of the two-dimensional Bratu equation. *J Sci Comput* 1(2):183
- Boyd JP (2010a) Error saturation in Gaussian radial basis functions on a finite interval. *J Comput Appl Math* 234:1435–1441
- Boyd JP (2010b) Six strategies for defeating the Runge phenomenon in Gaussian radial basis functions on a finite interval. *Comput Math Appl* 60:3108–3122
- Boyd JP (2011) One-point pseudospectral collocation for the one-dimensional Bratu equation. *Appl Math Comput* 217:5553–5565
- Boyd JP, Gildersleeve KW (2011) Numerical experiments on the condition number of the interpolation matrices for radial basis functions. *Appl Numer Math* 61:443–459
- Buckmire R (2003) Investigations of nonstandard Mickens-type finite-difference schemes for singular boundary value problems in cylindrical or spherical coordinates. *Numer Methods Partial Differ Equ* 19(3):380–398
- Chandrasekhar S (1967) *An introduction to the study of stellar structure* dover
- Fedoseyev AI, Friedman MJ, Kansa EJ (2002) Improved multiquadric method for elliptic partial differential equations via PDE collocation on the boundary. *Comput Math Appl* 43(3–5):439–455
- Jin L (2010) Application of modified variational iteration method to the Bratu-type problems. *Int J Contemp Math Sci* 5(4):153–158
- Kapania RK (1990) A pseudo-spectral solution of 2-parameter Bratus equation. *Comput Mech* 6(1):55–63
- Larsson E, Fornberg B (2003) A numerical study of some radial basis function based solution methods for elliptic PDEs. *Comput Math Appl* 46:891–902

- Misirli E, Gurefe Y (2011) Exp-function method for solving nonlinear evolution equations. *Math Comput Appl* 16(1):258–266
- Mohyud-Din ST (2008) Variational iteration method for solving initial and boundary value problems of Bratu-type. *Appl Math* 3(1):89–99
- Noor MA, Mohyud-Din ST (2007a) An efficient method for fourth order boundary value problems. *Comput Math Appl* 54:1101–1111
- Noor MA, Mohyud-Din ST (2007b) Variational iteration technique for solving higher order boundary value problems. *Appl Math Comput* 189:1929–1942
- Syam MI, Hamdan A (2006) An efficient method for solving Bratu equations. *Appl Math Comput* 176(2–5):704–713
- Wazwaz AM (2005) Adomians decomposition method for a reliable treatment of the Bratu-type equations. *Appl Math Comput* 166:652–663