A brief Report on the article [BAW 10]"Higher order global solution and normalized flux for singularly perturbed reaction-diffusion problems "

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Abstract: The authors consider a one dimensional singularly perturbed reaction–diffusion equation. A modified Shishkin mesh is introduced and a higher order compact finite difference solution on this mesh is presented. Piecewise cubic interpolants for both the exact solution and discrete solution are formulated. Thanks to the modfied Shishkin mesh, the authors proved that the convergence is uniform in the sense that the convergence accuracy is the same for any value of the diffusion parameter ε. More precise, the convergence order analysis contains two principle results. The first result states that the method is, almost, of fourth convergence order. The second result states that the normalized flux of the piecewise cubic interpolant of the discrete solution approximates the normalized flux of the piecewise cubic interpolant of the exact solution by order three, almost everywhere, and by order four at mid–points of the mesh. The theoretical results are confirmed by numerical examples.

Key words and phrases:singularly perturbed reaction–diffusion equation; normalized flux; finite difference scheme; higher order compact finite difference scheme; piecewise cubic interpolants

Subject Classification: 65L10

what i have learned from this article

1. principle references: the article [ROO 08, FAR 00] is well cited in the literature of "numerical methods for singularly perturbed reaction–diffusion equation".
2. area where singularly perturbed problems (SPPs: SPPs arise in several branches of engineering sciences: Fluid dynamics (which include linearized Navier–Stokes equation at high Reynolds number, Quantum mechanics, Elasticity, Chemical reactor theory, Gaz porous electrodes theory, Drift–Diffusion equation of semi–conductor device modeling...
3. boundary layers for small parameter: for $\varepsilon << 1$, problem [31]–[32] has two boundary layers (this statement needs more explanation, I think) of thikhness $0\left(\sqrt{\varepsilon}\ln(1/\varepsilon)\right)$ near the boundaries $x = 0, 1$.

4. classical finite difference methods for singularly perturbed problems: classical finite difference methods using uniform meshes does not give a satisfactory (as said the authors of [BAW 10]) approximation (what meant by "satisfactory"), see [FAR 00, ROO 08] and references therein, near the boundary layers.

5. practical case where the flux is importan: in some practical case, the computation of the exact solution and its flux is important, see blow

6. good reference in splines: it is mentioned that [BOO 78] is a good reference in splines.

7. hoc scheme: the so called (HOC) higher order compact finite difference scheme is introduced in [GRA 01]

1 An overview on some standard numerical methods for singularly perturbed equations

Let us consider the following simple example (which is given in [FEI 04, Pages 342–344]):

$$-\varepsilon u''(x) + \nu\, u'(x) = 1,\ x \in \Omega = (0,1), \qquad [1]$$

with

$$u(0) = u(1) = 0, \qquad [2]$$

where $\varepsilon > 0$ and $\nu \neq 0$ are two constants. The solution of [1]–[2] is defined by

$$u(x) = \frac{1}{\nu}\left\{x - \frac{\exp(\nu\, x/\varepsilon) - 1}{\exp(\nu\,/\varepsilon) - 1}\right\},\ x \in [0,1]. \qquad [3]$$

If $\varepsilon \to 0$ and $\nu > 0$, then $u(x) \to x/\nu$ for $x \in [0,1)$. The limit function is the solution of

$$\nu\, u'(x) = 1,\ x \in (0,1) \text{ and } u(0) = 0. \qquad [4]$$

1.1 Standard linear finite element methods and Gibs phenomenon

Let us apply the linear finite element method to approximate [1]–[2]. We then consider the uniform mesh $\mathcal{T}_h = \{K_i; i = 0, \ldots, N\}$ with $K_i = [x_i, x_{i+1}]$ and $x_{i+1} - x_i = h$. The approximate solution u_h as well as the test functions are in the space:

$$\mathcal{V}_h = \left\{\varphi_h \in \mathcal{C}(\overline{\Omega}); \varphi_h|_{K_i} \in \mathcal{P}_1,\ \forall\, K_i \in \mathcal{T}_h,\ \varphi_h(0) = \varphi_h(1) = 0\right\}. \qquad [5]$$

Multiplying both sides of [1] by $\varphi \in \mathcal{C}^1(\overline{\Omega})$, with $\varphi(0) = \varphi(1) = 0$, we get

$$\int_0^1 (\varepsilon\, u'(x)\varphi'(x) + \nu\, u'(x)\varphi(x))dx = \int_0^1 \varphi(x)dx,\ \forall \varphi \in \mathcal{C}^1(\overline{\Omega}),\ \varphi(0) = \varphi(1) = 0. \qquad [6]$$

The approximate finite element solution is then defined by: find $u_h \mathcal{V}_h$ such that

$$\int_0^1 (\varepsilon\, u_h'(x)\varphi_h'(x) + \nu\, u_h'(x)\varphi_h(x))dx = \int_0^1 \varphi_h(x)dx,\ \forall \varphi \in \mathcal{V}_h. \qquad [7]$$

This is equivalent to the following linear system:

$$-\frac{\varepsilon}{h^2}(u_{i+1} - 2u_i + u_{i-1}) + \frac{\nu}{2h}(u_{i+1} - u_{i-1}) = 1, \quad [8]$$

with

$$u_0 = u_{N+1} = 0. \quad [9]$$

Note that [8] is also a finite difference scheme by approximating:

1. $u''(x_i)$ by
$$\frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}. \quad [10]$$

2. $u'(x_i)$ by the central quotient
$$\frac{u(x_{i+1}) - u(x_{i-1})}{2h}. \quad [11]$$

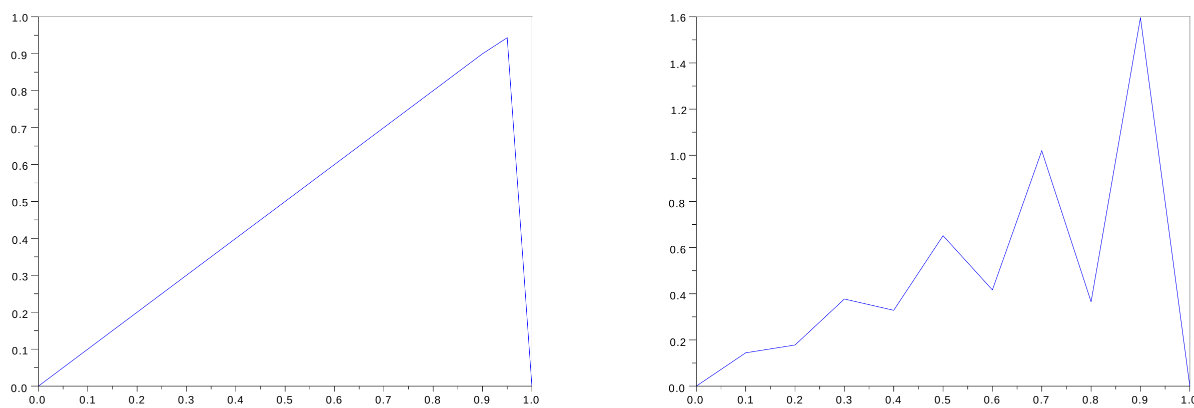

Figure 1: Left graph of the function u, right the finite difference solution [8]–[9] with $h = 1/10$; both simulations are in $\varepsilon = 10^{-2}$ and $\nu = 1$

The linear equations [8]–[9] can be written as

$$\mathcal{A}U = 1, \quad [12]$$

where $\mathcal{A}$ is a $N \times N$ matrix and 1 in the r.h.s. of [12] is the vector of $\mathbb{R}^N$ whose components are equal to 1. The matrix $\mathcal{A}$ is nonsymmetric, but for $h < 2\varepsilon/|\nu|$ it is *diagonally dominant* (In the sense $\sum_{j=1,j\neq i}^{N} |a_{ij}| \leq |a_{ii}|$ for all $i = 1, \ldots, N$ with strict inequality for at least one i.) and *irreducibly*. These previous stated properties of $\mathcal{A}$ guarantees good properties of the approximate solution. But, for $h \geq 2\varepsilon/|\nu|$, the approximate solution do not make sense because of *spurious oscillations* shown in the right Figure 1. This means that the *Gibbs phenomenon* arises here. We see here that *mesh Péclet number* defined by

$$Pe = \frac{h\nu}{2\varepsilon} \quad [13]$$

must satisfy the condition

$$Pe < 1 \qquad [14]$$

in order to avoid the *Gibbs phenomenon*.

1.2 Gibbs phenomenon and upwind finite difference scheme

An issue to avoid the Gibbs phenomenon is to chose an upwind finite difference scheme instead of the central finite difference scheme [8]–[9], that is to chose

$$-\frac{\varepsilon}{h^2}(u_{i+1} - 2u_i + u_{i-1}) + \frac{\nu}{h}(u_i - u_{i-1}) = 1, \qquad [15]$$

with

$$u_0 = u_{N+1} = 0. \qquad [16]$$

So, the upwind scheme [15]–[16] is performed thanks to

1. the approximation of $u''(x_i)$ by

$$\frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}. \qquad [17]$$

2. the approximation of $u'(x_i)$ by the central quotient

$$\frac{u(x_i) - u(x_{i-1})}{h}. \qquad [18]$$

Figure 2 represents, using Scilab, the finite difference solution [15]–[16] with $h = 1/10$. As we can see that the finite difference solution [15]–[16] is more reasonable than that of [8]–[9].

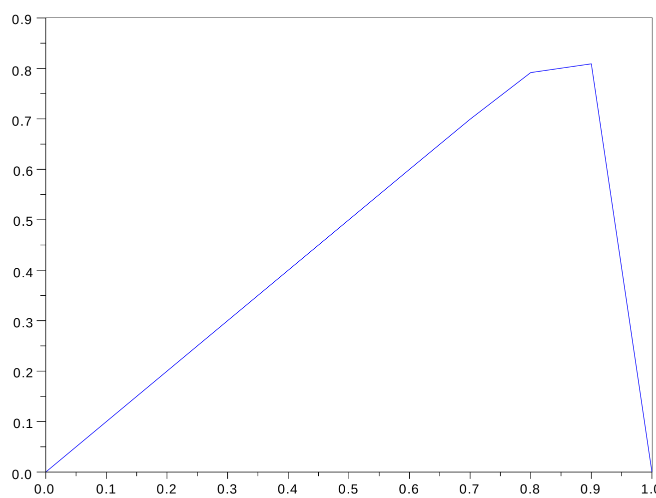

Figure 2: The upwind finite difference solution [15]–[16] with $h = 1/10; \varepsilon = 10^{-2}$ and $\nu = 1$

1.3 Standard linear finite element methods and convergence order

As usual, we use the technique of Cea Lemma to compute the convergence order. The key, for that target is the following equality:

$$a(u - u_h, v_h) = 0, \ \forall\, v_h \in \mathcal{V}_h. \qquad [19]$$

This implies that

$$a(u - u_h, u - u_h) = a(u - u_h, u - \pi\, u), \qquad [20]$$

where π is the usual interpolation operator defined from $\mathcal{C}(\overline{\Omega})$ into $\mathcal{V}_h$ and

$$a(u, v) = \int_0^1 (\varepsilon\, u'(x)v'(x) + \nu\, u'(x)v(x))dx. \qquad [21]$$

Equality [20] implies that

$$\alpha \,\|\, u - u_h\|_{1,\Omega}^2 \leq\, M \,\|\, u - u_h\|_{1,\Omega}\|\, u - \pi\, u\|_{1,\Omega}, \qquad [22]$$

which implies in turn, using the known result of the interpolation error

$$\alpha \,\|\, u - u_h\|_{1,\Omega} \leq\, CMh \max_{x\in\overline{\Omega}} |\, u''(x)|, \qquad [23]$$

where C is only depending on Ω, the constants α and M used in [22] are defined by

$$a(v, v) \geq \alpha \,\|\, v\|_{1,\Omega}^2, \ \forall\, v \in H_0^1(\Omega), \qquad [24]$$

and

$$a(u, v) \leq\, M\|\, u\|_{1,\Omega}\|\, v\|_{1,\Omega}, \ \forall\, u, v \in H_0^1(\Omega). \qquad [25]$$

Let us compute M, α, and $\max_{x\in\overline{\Omega}} |\, u''(x)|$

1. *computation of* α: using [21], the fact that $v(0) = v(1) = 0$, and the Poincaré inequality

$$\begin{aligned} a(v, v) &= \varepsilon \int_0^1 (v')^2(x)dx + \nu \int_0^1 v'(x)v(x))dx \\ &= \varepsilon \int_0^1 (v')^2(x)dx + \nu \int_0^1 (v^2)'(x)dx \\ &= \varepsilon \int_0^1 (v')^2(x)dx \\ &\geq \varepsilon\, C(\Omega)\|\, v\|_{1,\Omega}^2, \end{aligned} \qquad [26]$$

   where $C(\Omega)$ is only depending on Ω.

2. *computation of* M: using the Cauchy Schwarz inequality, the fact that $\left(\int_0^1 (u')^2(x)dx\right)^{\frac{1}{2}} \leq \|\, v\|_{1,\Omega}$ to get, assuming that $\varepsilon << 1$

$$\begin{aligned} a(u, v) &= \int_0^1 (\varepsilon\, u'(x)v'(x) + \nu\, u'(x)v(x))dx \\ &\leq \varepsilon\|\, u\|_{1,\Omega}\|\, v\|_{1,\Omega} + \nu\|\, u\|_{1,\Omega}\|\, v\|_{L^2(\Omega)} \\ &\leq (\varepsilon + \nu)\|\, u\|_{1,\Omega}\|\, v\|_{1,\Omega} \\ &\leq (1 + \nu)\|\, u\|_{1,\Omega}\|\, v\|_{1,\Omega}. \end{aligned} \qquad [27]$$

3. *computation of* $u''(x)$: using expression [3] to get

$$u''(x) = -\frac{\nu}{\varepsilon^2}\frac{\exp(\nu\, x/\varepsilon)}{\exp(\nu\,/\varepsilon)-1},\ \forall\, x \in (0,1). \qquad [28]$$

So, an estimate for u'' can be provided as, since $0 < \exp(\nu\, x/\varepsilon) \le \exp(\nu\,/\varepsilon)$:

$$\max_{x\in[0,1]} |\, u''(x)| \le \frac{\nu}{\varepsilon^2\,(\exp\,(\nu\,/\varepsilon)-1)}. \qquad [29]$$

Gathering [26]–[29] with [23] to get

$$\begin{aligned} \|\, u - u_h\|_{1,\Omega} &\le C(\Omega)\frac{M}{\alpha} h \max_{x\in\overline{\Omega}} |\, u''(x)| \\ &\le C(\Omega)\frac{\nu(1+\nu)}{\varepsilon^3\,(\exp\,(\nu\,/\varepsilon)-1)} h. \end{aligned} \qquad [30]$$

So, estimate [30] depends adversly on ε which is not so good when ε is small.

2 Motivation and some literature

The work [BAW 10] is interested with the following singularly perturbed reaction–diffusion equation:

$$\mathcal{L}\, u(x) = -\varepsilon u(x) + b(x)u(x) = f(x),\ x \in D = (0,1), \qquad [31]$$

with the following Dirichlet boundary condition:

$$u(0) = A,\ u(1) = B, \qquad [32]$$

where ε is a *small* parameter, b and f are *smooth* functions. We assume that, for some $\beta > 0$, $b(x) \ge \beta$, for all $x \in \overline{D}$.

It is known that, under above assumptions, problem [31]–[32] has a unique solution satisfying $u \in \mathcal{C}^2(D) \cap \mathcal{C}(\overline{D})$ (see [ROO 08]).

SPPs arise in several branches of engineering sciences: Fluid dynamics (which include linearized Navier–Stokes equation at high Reynolds number, Quantum mechanics, Elasticity, Chemical reactor theory, Gaz porous electrodes theory, Drift–Diffusion equation of semi–conductor device modeling...

For $\varepsilon << 1$, problem [31]–[32] has two boundary layers of thikhness $0\,(\sqrt{\varepsilon}\ln(1/\varepsilon))$ near the boundaries $x = 0, 1$. Classical finite difference methods using uniform meshes does not give a satisfactory (as said the authors of [BAW 10]) approximation (what meant by "satisfactory"), see [FAR 00, ROO 08] and references therein. We need then to use a special numerical methods giving a uniform convergence, i.e., methods for which the convergence is same everywhere in the domain D and for any value ε (convergence order is independent of the parameter ε).

In the study of some physical phenomena, if we consider a substance in a solution with a flux satisfying Fick's law, where the distribution is given by a diffusion equation, and the initial concentration of an admixture at the boundaryof the body is known, it is interesting to obtain a good approximation for both the exact solution and its normalized flux. This problem appears in the context of environmental sciences in determining the pollution entering the environment from manufacturing sources. The diffusion Fourier number, which is proportional to the diffusion coefficient of the substance, can be sufficiently small. Then a diffusion boundary layer can appear in narrow neighborhoods of the boundary of the domain. (it is useful to detail these information; i think it are condensed)!!

The basic idea of using Lagrange's interpolation to find the global solution and the normalized lux was provided in [MIL 96].

In [SUR 97], a cubic splines were used to solve nonlinear reaction–diffusion problem, and the uniform convergence of the method is shown. Nevertheless, the proof of the theoretical results is incomplete and is unclear. In [SUR 04], a quadratic spline was used to solve semilinear reaction–diffusion problems, proving second order of uniform convergence at the mesh points and also the uniform convergence for the global solution and the normalized flux. In [STA 05], a scheme is proposed to approximate the global solution of singularly perturbed problems and it proves that the theoretical convergence order at mesh points is $\min(h^2, \varepsilon^2)$ and for the global approximate solution is $\min(h, \varepsilon)$; furthermore, no numerical results were presented to support the theory. Recently in [CLA 10], the authors presented a hybrid scheme combining central difference and piecewise cubic interpolants, and they obtained a second order convergent method for both the global solution and the global normalized flux.

3 Aim of the paper and description of the main results

The aim of the article [BAW 10] is to obtain a higher order convergent global solution and global normalized flux for the reaction–diffusion problem [31]–[32] by following ideas of [CLA 10].

To obtain higher order globally convergent solution and normalized flux, the authors of [BAW 10] combined a finite difference scheme of higher order compact (HOC) type together with classical piecewise cubic interpolant. More precise, the global approximate solution is a piecewise cubic interpolant which concides with the numerical solution (HOC) of at the mesh points.

4 Definition of the scheme and outlines of the analysis

It is well known, see [MIL 96] that the solution of [31]–[32] satisfies

$$|\, u(x)| \le C(1+\varepsilon^{-k/2}e(x,\beta,\varepsilon)),\; 0\le k\le j+1, \qquad [33]$$

where

$$e(x,\beta,\varepsilon)) = \exp\left(-\sqrt{\beta}\xi/\sqrt{\varepsilon}\right) + \exp\left(-\sqrt{\beta}(1-\xi)/\sqrt{\varepsilon}\right), \qquad [34]$$

and j depends on the smoothness of data b and f.

Next, we describe in brief the finite difference scheme and an outline for its analysis.

1. mesh: a modified Shishkin mesh is considered.

2. scheme: (HOC) higher order finite difference scheme, see [GRA 01], is considered on the modified Shishkin mesh. This HOC solution will be refereed to as the discrete solution $U^h = (U_i)_i$

3. piecewise cubic for the exact solution: a picewise cubic interpolant for the exact solution, denoted by $\mathcal{S}$, with some momentum values $M_i = u''(x_i)$, for all mesh point x_i

4. normalized flux: the normalized flux is $\sqrt{\varepsilon}\mathcal{S}'$.

5. piecewise cubic for the discrete solution: a picewise cubic interpolant, denoted by $\mathcal{S}_h$, for the discrete solution with some momentum values $\overline{M}_i = (b_i U_i - f_i)/\varepsilon$, for all mesh point x_i (it is useful to note that $(b_i u(x_i) - f(x_i))/\varepsilon = u''(x_i)$).

6. normalized flux for the discrete solution: the normalized flux for the discrete solution is $\sqrt{\varepsilon}\mathcal{S}'_h$.

7. Errors: the following estimates hold:

$$\sup_{x\in[x_i,x_{i+1}]} |\mathcal{S}(x) - \mathcal{S}_h(x)| \le Ch^4(1+\varepsilon^2 \max\left(e(x_i,\beta,\varepsilon), e(x_{i+1},\beta,\varepsilon)\right), \qquad [35]$$

and a similar estimate for $\sup_{x\in[x_i,x_{i+1}]} |\sqrt{\varepsilon}\mathcal{S}'(x) - \sqrt{\varepsilon}\mathcal{S}'_h(x)|$.

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