Benchmarking of a Quasi-Linear Convection/Diffusion Problem in MATLAB

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Abstract. We present a benchmark project for a second order quasi-linear convection/diffusion problem. We solved the PDE problem with simple-iterative scheme with three methods, namely; Central difference, Directed difference, and Exponential fitting schemes. We saw that with a value of $a(x) = 0$, central and directed difference schemes yield the same results. We analyzed the numerical error behavior for different values of nodal number N, and numerical diffusion factor ε. We found that the Exponential fitting scheme results in poor accuracy, whereas C-D difference schemes exhibits a better accuracy, overall. We also found that the best accuracy may be acquired by high nodal number N, which doesn't increase the iteration number but may increase the computation time, and low ε value, which increases the accuracy and decreases the iteration number.

Keywords: MATLAB, Quasi-Linear, Convection-Diffusion, PDE, Finite Difference Method, Computational Physics.

1. Introduction:

While solving PDE systems using FDM, it is straightforward to generate a simulation for linear systems. However, in real physical systems, the PDE systems are not in a linear form and require special treatment. To solve such non-linear systems, the system is first linearized and then iterations are made while solving the linearized system using the matrix solvers. In this project, we present a benchmarking for a quasi-linear convection/diffusion system.

2. The Description of the Problem

While solving partial differential equations in computational environments with FDM, it is crucial to get the coefficient matrix of the primary variable. Then, using the known matrix operations, the system of equations is solved and the solution is mapped onto the grid points. In general, the strong form of second order convection/diffusion problem is,

$$-\varepsilon u''_{(x)} - a_{(x)}u'_{(x)} + b_{(x)}g(u_{(x)}) = f_{(x)} \quad in \ \ \Omega \tag{1}$$

Here, $u_{(x)}$ is the primary function of interest, $f_{(x)}$ is the source function, ε is the diffusivity coefficient, $g(u_{(x)})$ is the nonlinear term which is a function of $u_{(x)}$, $a_{(x)}$ and $b_{(x)}$ are the coefficients depending on the problem. The boundary conditions subject to equation (1) are,

$$\begin{aligned} \xi_0 u_{(c)} - \eta_0 \varepsilon u'_{(c)} = \varphi \ \ in \ \ \partial\Omega \\ \xi_1 u_{(d)} - \eta_1 \varepsilon u'_{(d)} = \psi \ \ in \ \ \partial\Omega \end{aligned} \tag{2}$$

where the ξ terms represent the Dirichlet type boundary condition at boundary points (c,d), η terms represent the Neumann type boundary conditions. The mixture of two conditions arise the Robin boundary value problem. In our case, the problem is described by the partial differential system with Dirichlet boundary conditions as follows,

$$\begin{aligned} -\varepsilon u''_{(x)} + u_{(x)} + u^2_{(x)} = exp(-2x/\sqrt{\varepsilon}) \ \ in \ \ \Omega \\ u_{(0)} = 1, \quad u_{(1)} = exp(-1/\sqrt{\varepsilon}) \quad in \ \ \partial\Omega \end{aligned} \tag{3}$$

Where the problem domain is one dimensional, and in $x \in (0, 1)$. Compared to the general expression in relation 1, we have $a_{(x)} = 0,$, and $b_{(x)}$ to be determined by the linearized system, and the source function is as given in the RHS. The known analytical solution to be compared for the benchmark analysis is,

$$u_{(x)} = exp(-x/\sqrt{\varepsilon}) \tag{4}$$

2.1. Linearization of the System

One of the methods of linearizing systems is manipulating the system in a way that there is no non-linear terms in the LHS of the main PDE description. In that case, the terms with non-linear coefficients are moved towards the RHS, adding up to the primary source function.

$$-\varepsilon \frac{d^2 u^{(n+1)}}{dx^2} - a_{(x)} \frac{du^{(n+1)}}{dx} + b_{(x)} u^{(n+1)} + g(u^n) = f(x) \tag{5}$$

Where the superscripts represent the iteration number. The above equation with the coefficients in our case, $a_{(x)} = 0$, $b_{(x)} = 1$, and $g(u^n) = (u^n)^2$, yields,

$$-\varepsilon \frac{d^2 u^{(n+1)}}{dx^2} + u^{(n+1)} = f(x) - (u^n)^2 \tag{6}$$

2.2. Mapping the Problem onto the Finite Difference Scheme

In the FDM, a continuous problem is mapped onto the discrete set of points. The derivative operators of any kind are evaluated in those grids, and solved for the primary function of interest. In our case, the discretized version of the continuous problem yields,

$$\frac{-\varepsilon}{h^2}\left(\gamma_i - \frac{a_{(x_i)}h}{2\varepsilon}\right)u^h_{i-1} + \left(\frac{2\varepsilon\gamma_i}{h^2} + b_{(x_i)}\right)u^h_i - \frac{\varepsilon}{h^2}\left(\gamma_i + \frac{a_{(x_i)}h}{2\varepsilon}\right)u^h_{i+1} = f_{(x_i)}$$
$$u_{(x_1)} = 1, \quad u_{(x_n)} = exp(-1/\sqrt{\varepsilon}) \tag{7}$$

where γ is the artificial diffusion factor, and corresponds to different approximation schemes of the differential operators, subscript for the i^{th} variable of the space domain, superscript for the time level h. The different γ factors to the corresponding functions are given below.

$$\begin{aligned} \gamma = 1 \quad (Central\ Difference) \\ \gamma = 1 + 0.5|R_i| \quad (Directed\ Difference) \\ \gamma = 0.5R_i \coth(0.5R_i) \quad (Exponential\ Fitting) \end{aligned} \tag{8}$$

where $R_i = a_{(x_i)}h/\varepsilon \equiv$ *Local Reynold's number*.

Note that in our problem, $R_i = a_{(x_i)} = 0$, hence, central and directed difference schemes yield the same result. Furthermore, $\gamma = 0.5$ for the exponential fitting scheme. To gather the solution for the discrete linear system described in Equation 7, we describe it in a matrix form as follows,

$$\begin{bmatrix} B_1 & -C_1 & 0 & . & . & 0 \\ -A_2 & B_2 & -C_2 & 0 & . & . \\ 0 & -A_3 & B_3 & . & . & . \\ . & 0 & . & . & . & . \\ . & . & . & . & . & 0 \\ . & . & . & . & B_{N-1} & -C_{N-1} \\ 0 & . & . & 0 & -A_N & B_N \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ . \\ . \\ . \\ u_N \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ . \\ . \\ . \\ f_N \end{bmatrix} \tag{9}$$

Which is a tridiagonal sparse matrix, and has special algorithms to generate and solve in numerical environments, since problems with a high number of nodal elements require a vast amount of memory and computation sources. The coefficients in relation 5 are simplified by the notation set of (A_i, B_i, C_i) in the domain $(2, N-1)$, which are shown in the relation below.

$$
\begin{aligned}
A_i &= \frac{\varepsilon}{h^2}\left(\gamma_i - \frac{a_{(x_i)}h}{2\varepsilon}\right) \\
B_i &= \left(\frac{2\varepsilon\gamma_i}{h^2} + b_{(x_i)}\right) \\
C_i &= \frac{\varepsilon}{h^2}\left(\gamma_i + \frac{a_{(x_i)}h}{2\varepsilon}\right)
\end{aligned} \tag{10}
$$

Note that, for the central-directed schemes and the exponential fitting schemes, the values of the coefficient matrix yield,

$$
\begin{aligned}
&Central - Directed\ Schemes: \quad A_i = \frac{\varepsilon}{h^2},\ B_i = \frac{\varepsilon}{h^2} + 1,\ C_i = \frac{\varepsilon}{h^2} \\
&Exponential\ Fitting\ Scheme: \quad A_i = \frac{\varepsilon}{2h^2},\ B_i = \frac{\varepsilon}{2h^2} + 1,\ C_i = \frac{\varepsilon}{2h^2}
\end{aligned} \tag{11}
$$

3. Solution in MATLAB

We solved the problem described in section 1, in MATLAB environment. The test configurations are divided into two parts. In the first part, we held the ε coefficient constant with a value of 0.01, and with a varying nodal point density of N = (10, 20, 40, 80). In the second part, we take the point density constant with a value of N = 40 and apply the simulation with varying ε value of $(1, 10^{-1}, 10^{-2}, 10^{-3})$. In both parts, we applied the conditions for $\gamma = 1$, since the numerical Reynold's number is zero, hence, the central and directed schemes reduce to the same condition. We also applied the same conditions for the exponential fitting scheme with γ value of 0.5.

4. Data and Error Analysis

In this section, we investigated the errors in terms of root mean square error, and maximum norms. The error types taken into consideration were the convergence error $\|e_1\|$, which is the difference between the last two iteration values, and the numerical error$\|e_2\|$, which is the difference between the analytical and numerical results. The relations we used to calculate the errors are given below.

$$
\|e_2\|_2 = \left[\frac{1}{N^2}\sum_{i=1}^{N}(u_{(x_i)} - u_i)^2\right]^{1/2} \tag{12}
$$

$$
\|e_1\|_\infty = \max_{1\le i\le N} |u_{(x_i)}^{n+1} - u_i^n| \tag{13}
$$

$$
\|e_2\|_\infty = \max_{1\le i\le N} |u_{(x_i)} - u_i| \tag{14}
$$

$$
\gamma_i > 0.5|R_i| \equiv 0 \tag{15}
$$

$$\|L^h(u)^h - (Lu)'h\|_\infty \le C\left(\max_{1\le i\le N-1} |1-\gamma_i| + h^2\right) \tag{16}$$

Note that the numerical schemes for this problem are inherently stable which condition is described in (14), since for the central and directed schemes $\gamma \equiv 1 > 0 \equiv 0.5|R_i|$, and for the exponential fitting scheme, $\gamma \equiv 0.5 > 0 \equiv 0.5|R_i|$.

Note also that, from relation (16), we expect that the error for the central-directed differences schemes will be lower than the numerical error produced during the exponential fitting scheme. To see clearly, The expected numerical error in the C-D differences schemes,

$$\|e_{(C-D)}\| \equiv \|L^h(u)^h - (Lu)'h\|_\infty \le Ch^2 \tag{17}$$

Whereas for the exponential fitting scheme, the expected numerical error is,

$$\|e_{(E)}\| \equiv \|L^h(u)^h - (Lu)'h\|_\infty \le C(0.5 + h^2) \tag{18}$$

The error and the iteration values for the C-D scheme are given in Tables 1 and 2, and for the Exponential scheme are given Tables 3 and 4. On the other hand, the numerical errors as described in relations (12-13-14) are illustrated in Figure 1, for all schemes.

Table 1: Central-Directed data by varying N values.

N	$\|e_1\|_\infty$	$\|e_2\|_\infty$	$\|e\|_2$	i
10	$7.354\ 10^{-5}$	$1.300\ 10^{-2}$	$5.316\ 10^{-2}$	9
20	$4.353\ 10^{-5}$	$3.137\ 10^{-3}$	$2.686\ 10^{-2}$	9
40	$3.282\ 10^{-5}$	$7.656\ 10^{-4}$	$1.326\ 10^{-2}$	9
80	$3.056\ 10^{-5}$	$1.929\ 10^{-4}$	$6.699\ 10^{-3}$	9

Table 2: Central-Directed data by varying ε values.

ε	$\|e_1\|_\infty$	$\|e_2\|_\infty$	$\|e\|_2$	i
1	$2.240\ 10^{-5}$	$1.147\ 10^{-6}$	$3.587\ 10^{-5}$	5
0.1	$4.152\ 10^{-5}$	$8.370\ 10^{-5}$	$2.312\ 10^{-3}$	8
0.01	$3.282\ 10^{-5}$	$7.656\ 10^{-4}$	$1.325\ 10^{-2}$	9
0.001	$8.232\ 10^{-5}$	$7.040\ 10^{-3}$	$7.002\ 10^{-2}$	9

Table 3: Exponential data by varying N values.

N	$\|e_1\|_\infty$	$\|e_2\|_\infty$	$\|e\|_2$	i
10	$9.384\ 10^{-5}$	$6.834\ 10^{-2}$	$2.629\ 10^{-2}$	9
20	$3.745\ 10^{-5}$	$8.331\ 10^{-2}$	$3.391\ 10^{-2}$	10
40	$7.266\ 10^{-5}$	$8.871\ 10^{-2}$	$3.611\ 10^{-2}$	9
80	$6.457\ 10^{-5}$	$9.014\ 10^{-2}$	$3.677\ 10^{-2}$	9

Table 4: Exponential data by varying ε values.

ε	$\|e_1\|_\infty$	$\|e_2\|_\infty$	$\|e\|_2$	i
1	$7.384\ 10^{-5}$	$5.332\ 10^{-2}$	$3.882\ 10^{-2}$	6
0.1	$4.380\ 10^{-5}$	$8.989\ 10^{-2}$	$6.121\ 10^{-2}$	7
0.01	$7.266\ 10^{-5}$	$8.871\ 10^{-2}$	$3.611\ 10^{-2}$	9
0.001	$6.060\ 10^{-5}$	$7.761\ 10^{-2}$	$1.765\ 10^{-2}$	10

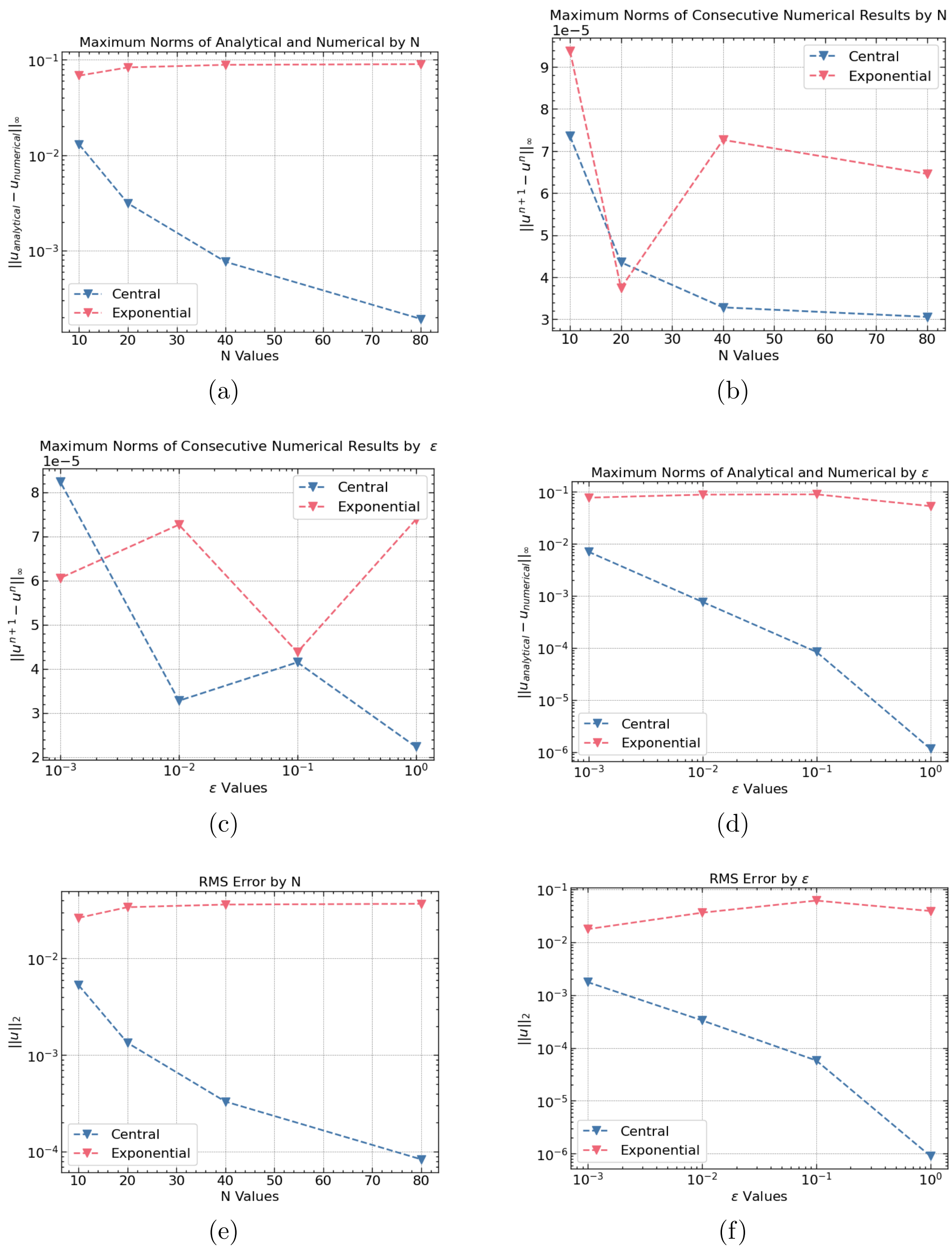

Figure 1: Distribution of RMS and normal errors by control parameters, N and ε. ***(a)*** shows the maximum norms between the analytical and numerical results, ***(b)*** shows the maximum norms between the last two iterations, by varying N values. ***(c)*** shows the maximum norms between the analytical and numerical results, ***(b)*** shows the maximum norms between the last two iterations, by varying ε values. ***(e)*** and ***(f)*** show the RMS error between the analytical and numerical results by varying N and ε, respectively.

5. Conclusion

We simulated the quasi-linear convection/diffusion problem as described in equation (3) by FDM in MATLAB, using Thomas Matrix Algorithm to solve the linearized system shown in equations (6) and (7), and described by the matrix system (9). We firstly held the ε value constant and increased the grid density. For the Central-Directed schemes, we found that decreasing the grid spacing increases the accuracy, while keeping the iteration number constant. Secondly, we held the grid density constant and decreased the ε value and saw that the error all types of errors increased as we decreased the ε. Furthermore, the iteration to get a converging solution increases as we decrease ε, which requires more computation power and time. For the Exponential scheme, on the other hand, despite the expectations from the relation (18), we hardly see a considerable amount of decrease in the numerical error. As illustrated in Figure 1, the exponential scheme resulted in poor numerical accuracy when compared to the C-D schemes. Even though the exponential scheme seems to exhibit a more accurate behavior for smaller ε values, the precision must be analyzed by further decreasing the ε value. As a result, for the problems described in the form of relation 3, we conclude that the best accuracy may be acquired with Central-Directed schemes by taking relatively high ε values such as 1, and relatively high nodal point numbers, for the Central-Directed schemes.