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Exponentially fitted IMEX methods for advection-diffusion problems

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Abstract

The paper is devoted to the numerical solution of advection-diffusion problems of Boussinesq type, by means of adapted numerical methods. The adaptation occurs at two levels: along space, by suitably semidiscretizing the spatial derivatives through finite differences based on exponential fitting; along time integration, through an adapted IMEX method based on exponential fitting itself. Stability analysis is provided and numerical examples showing the effectiveness of the approach, also in comparison with the classical one, are given.

Keywords: Advection-diffusion problems; finite differences; exponential fitting; IMEX methods; stability analysis.

1. Boussinesq equation of hydrodynamics

Let us consider the following Boussinesq equation [15, 24]

$$\frac{\partial h}{\partial t} = \frac{K}{S} \left(h \frac{\partial^2 h}{\partial x^2} + \left(\frac{\partial h}{\partial x} \right)^2 - \vartheta \frac{\partial h}{\partial x} \right).$$

Such a problem governs one-dimensional groundwater flows on a sloping impervious base, where h denotes the height of the watertable, S is the drainable porosity, K is the hydraulic conductivity and ϑ is the slope of the impervious base. In particular, if h shows a small deviation from the weighted depth, Boussinesq equation assumes the following form

$$\frac{\partial h}{\partial t} = \gamma \frac{\partial^2 h}{\partial x^2} - \nu \frac{\partial h}{\partial x},$$

i.e. it results to be a linear-diffusion equation, where γ is the angle between the beach face and the horizontal datum and $v = K\theta/S$. As in [22], we are interested in solving the problem for $(x, t) \in [0, +\infty) \times [0, +\infty)$ and equipping it by the following initial condition

$$h(x, 0) = h_0(x),$$

and moving boundary condition

$$h(X(t), t) = f(t), \quad t > 0,$$

being $X(t)$ the parametric formulation of the moving boundary, depending on time. Therefore, $h_0(x)$ gives the analytic expression of the initial watertable, while $X(t)$, i.e. the abscissa of the moving boundary, following [22], can be regarded as

$$X(t) = \frac{f(t)}{\tan(\gamma)}.$$

In summary, we are interested in the following linear advection-diffusion problem:

$$\begin{aligned} h_t(x, t) &= \gamma h_{xx}(x, t) - v h_x(x, t), & x > 0, t > 0, \\ h(x, 0) &= h_0(x), & x \geq 0, \\ h(X(t), t) &= f(t), & t \geq 0. \end{aligned} \quad (1.1)$$

As proved in [14], if problem (1.1) is subject to a periodic boundary condition dictated by

$$f(t) = \exp(i\omega t), \quad (1.2)$$

where i is the imaginary unit, the solution exhibits the following form

$$h(x, t) = \exp(\alpha x + i(\beta x + \omega t)),$$

with $\alpha, \beta \in \mathbb{R}$. Taking into account the hydrodynamical features of the problem, the authors in [22] were able to determine suitable values of α and β , leading to the following final profile of the solution of (1.1)

$$h(x, t) = \exp\left[\left(\frac{v}{2D} - \mu\right)x\right] \exp[i(\omega t - \rho x)], \quad (1.3)$$

being

$$\mu = \frac{1}{2D} \sqrt{2 \sqrt{\omega^2 + \frac{v^4}{16D^2}} + \frac{v^2}{2}}.$$

In above formula, D is a constant depending on the transmissivity and the porosity S , ω provides the temporal frequency and ρx is the phase. Thus, since in presence of periodic boundary conditions dictated by (1.2) problem (1.1) shows a solution of the form (1.3), it is worth designing a numerical scheme that takes into account such a qualitative behavior, as described in the remainder of the manuscript.

1.1. Following known qualitative behaviors of the solutions: the role of adapted numerical methods

Numerical methods adapted to specific problems are usually intended as an efficient alternative to general purpose methods, which are designed in order to exactly solve (within round-off error) problems with polynomial solutions. Adapted methods are instead meant to exactly solve (within round-off error) problems whose solutions exhibit a non-polynomial qualitative behavior, a-priori known: we mention, for instance, periodic behaviors, oscillations and exponential decays or growths. In such cases, classical methods may result to be quite inefficient because they would need a very small value of the stepsize to reach a certain accuracy, while it would be useful employing fitted formulae shaped on suitably chosen functions, e.g. exponential and trigonometrical functions according to the solution of the problem and its features. On all above considerations exponential fitting technique relies (see [13, 17] and references therein), based on the idea of designing a space of approximants spanned by suitable chosen basis functions, forming the so-called fitting space.

As aforementioned, the basis functions follow the same qualitative behavior of the solution of the problem, and, therefore, they are oscillatory with a certain frequency if the solution is oscillatory, or exponentially decay with a certain rate if the solution is of decaying exponential type. The values of the frequencies or decay rates are clearly present in the basis functions and, of course, unknown; accurately detecting their values is a necessary step in applying adapted methods which is normally based on minimizing or annihilating the principal error term [6, 8] or trying to exploit theoretical a-priori known informations on the problem as in [5]. Thus, an effective employ of exponentially fitting methods relies on suitably choosing the fitting space and accurately estimating the unknown parameters.

Referring to problem (1.1), we propose an adapted numerical scheme based on two separate steps: the first one consists in the spatial semidiscretization of the operator by a proper modification of the method of lines, while the second one deals with a suitable time integration, taking into account the nature of the resulting semidiscretized system. In particular, since the resulting system of ODEs

exhibits stiff components (arising from the diffusion term) and non-stiff ones (arising from the advection term), it is more natural to differently treat them, by means of implicit-explicit (IMEX) numerical methods that implicitly integrate the stiff terms and explicitly the other ones, following the classical idea [1, 23].

The manuscript is organized as follows: Section 2 introduces the spatial semidiscretization of the problem, by means of exponentially fitted finite differences, adapted to both the diffusion and the advection terms; Section 3 shows the development of an adapted IMEX time solver for the semidiscrete problem, while Section 4 analyzes its stability properties; Section 5 is devoted to the illustration of numerical results showing the effectiveness of the approach; some conclusions are given in Section 6.

2. Spatial semidiscretization of the problem

As announced in the previous section, we aim to solve problem (1.1) by first providing a spatial semidiscretization that takes into account the nature of the solution. First of all, let us better clarify the selection of the numerical domain: taking into account that the dynamics evolves in an unbounded domain with free boundary, i.e. $[0, \infty) \times [0, \infty)$, the actual domain of integration is chosen as follows

$$\mathcal{D} = [0, X(T)] \times [0, T], \quad (2.4)$$

where T is a large enough real number such that any further increase would not affect the solution at all. Thus, problem (1.1) reformulated in $[0, X(T)] \times [0, T]$ assumes the form

$$\begin{aligned} h_t(x, t) &= \gamma h_{xx}(x, t) - \nu h_x(x, t), & (x, t) &\in (0, X(T)) \times (0, T], \\ h(x, 0) &= h_0(x), & x &\in [0, X(T)], \\ h(0, t) &= h(X(T), t) = f(t), & t &\in [0, T]. \end{aligned} \quad (2.5)$$

Following the method of lines (see [12, 19, 20] and references therein), we consider the following spatially discretized domain

$$\mathcal{D}_{\Delta x} = \{(x_i, t) : x_i = i\Delta x, \quad i = 0, \dots, N-1, \quad \Delta x = X(T)/(N-1)\},$$

where Δx is the spatial integration step. Then, problem (1.1) in $\mathcal{D}_{\Delta x}$ is equivalent to the following initial value problem

$$\begin{aligned} h'_0(t) &= f'(t), \\ h'_i(t) &= \gamma\Gamma_2 - \nu\Gamma_1, \quad 1 \leq i \leq N-2, \\ h'_{N-1}(t) &= f'(t), \\ h_i(0) &= h_0(x_i), \quad 0 \leq i \leq N-1, \end{aligned} \tag{2.6}$$

where Γ_2 is a finite difference approximating the second spatial derivative in (2.5), and Γ_1 is a finite difference for the approximation of the first spatial derivative in (2.5). Inspired by [5, 7], we approximate the first and second spatial derivatives by the following finite differences

$$\begin{aligned} \Gamma_2 &= \frac{\alpha_0 h(x_{n-1}, t) + \alpha_1 h(x_n, t) + \alpha_2 h(x_{n+1}, t)}{\Delta x^2}, \\ \Gamma_1 &= \frac{\beta_0 h(x_{n-1}, t) + \beta_1 h(x_n, t)}{\Delta x}, \end{aligned} \tag{2.7}$$

and compute $\alpha_0, \alpha_1, \alpha_2, \beta_0$ and β_1 in order to make Γ_2 and Γ_1 exact on exponential functions, motivated by the qualitative behaviour of the solution (1.3).

2.1. Discretization of the diffusion term

We first provide the expression of the discretized diffusion term Γ_2 , given by the first equation in (2.7), i.e. we compute the unknown coefficients $\alpha_0, \alpha_1, \alpha_2$. This aim is achieved by taking into account the parametrization (1.3) of the solution of the problem (1.1): indeed, such a parametrization indicates that the solution is of the form

$$\exp(\alpha x) \exp(i(\beta x + \omega t)),$$

or, equivalently,

$$\exp((\alpha + i\beta)x) \exp(i\omega t),$$

which suggest us the employ of the following fitting space for the approximation of the second order spatial derivative

$$\mathcal{F} = \{1, \exp(\zeta x), x \exp(\zeta x)\},$$

with $\zeta \in \mathbb{C}$. In summary, we are looking for the following approximant

$$h_{xx}(x_n, t) \approx \Gamma_2 = \frac{\alpha_0 h(x_{n-1}, t) + \alpha_1 h(x_n, t) + \alpha_2 h(x_{n+1}, t)}{\Delta x^2},$$

imposing its exactness on \mathcal{F} . For the computation of the coefficients of Γ_2 , we introduce the following linear operator

$$\mathcal{L}[\Delta x]h(x, t) = h_{xx}(x, t) - \frac{\alpha_0 h(x - \Delta x, t) + \alpha_1 h(x, t) + \alpha_2 h(x + \Delta x, t)}{\Delta x^2}.$$

We evaluate $\mathcal{L}[\Delta x]1$, $\mathcal{L}[\Delta x]\exp(\zeta x)$, $\mathcal{L}[\Delta x]x\exp(\zeta x)$ and, due to the invariance in translation of the operator, we refer to the values gained in correspondence of $x = 0$ and annihilate them, obtaining the following linear system of equations

$$\begin{cases} \alpha_0 + \alpha_1 + \alpha_2 = 0 \\ \alpha_0 \exp(-z) + \alpha_1 + \alpha_2 \exp(z) = z^2 \\ -\alpha_0 \exp(-z) + \alpha_2 \exp(z) = 2z \end{cases}$$

with $z = \zeta \Delta x$. The solution of such system is given by

$$\begin{aligned} \alpha_0 &= -\frac{ze^z(2 - 2e^z + ze^z)}{(e^z - 1)^2}, \\ \alpha_1 &= \frac{z(2 - 2e^{2z} + z + ze^{2z})}{(e^z - 1)^2}, \\ \alpha_2 &= -\frac{z(2 - 2e^z + z)}{(e^z - 1)^2}. \end{aligned} \tag{2.8}$$

Of course, it is evident that such coefficients are no longer constant, as in the classical polynomial case, but are functions of z . In general, $z \neq 0$ because $\Delta x \neq 0$ and the ζ is generally non-zero (at least for non-degenerate cases), ensuring that the denominators in (2.8) are non-zero. Nevertheless, when z tends to 0, the variable coefficients (2.8) tend to the classical values

$$\alpha_0 = \alpha_2 = 1, \quad \alpha_1 = -2. \tag{2.9}$$

Hence, the exponentially fitted formula retains the same order of accuracy of the corresponding classical one, which is equal to 2.

2.2. Discretization of the advection term

We now discretize the advection term by the approximant Γ_1 given by the second equation in (2.7). As aforementioned, the choice of the fitting space is dictated by the parametrization of the solution (1.3) and is given by

$$\mathcal{G} = \{1, \exp(\zeta x)\},$$

with $\zeta \in \mathbb{C}$. We now compute

$$h_x(x_n, t) \approx \Gamma_1 = \frac{\beta_0 h(x_{n-1}, t) - \beta_1 h(x_n, t)}{\Delta x},$$

imposing its exactness on \mathcal{G} . We introduce the following linear operator

$$\mathcal{M}[\Delta x]h(x, t) = h_x(x, t) - \frac{\beta_0 h(x - \Delta x, t) + \beta_1 h(x, t)}{\Delta x}.$$

We evaluate $\mathcal{M}[\Delta x]1$, $\mathcal{M}[\Delta x]\exp(\zeta x)$ and annihilate the values gained in correspondence of $x = 0$, obtaining the linear system

$$\begin{cases} \beta_0 + \beta_1 = 0 \\ \beta_0 \exp(-z) + \beta_1 = z \end{cases}$$

with $z = \zeta \Delta x$. The solution of such system is given by

$$\begin{aligned} \beta_0 &= \frac{z}{e^{-z} - 1}, \\ \beta_1 &= -\frac{z}{e^{-z} - 1}. \end{aligned} \tag{2.10}$$

Also in this case, when z tends to 0, the variable coefficients (2.10) tend to the classical values

$$\beta_0 = 1, \quad \beta_1 = -1 \tag{2.11}$$

and, therefore, the exponentially fitted formula retains the same order of accuracy of the corresponding classical one, which is equal to 1.

Remark 2.1. *It is important to highlight that previous approaches on the numerical solution of partial differential equations by exponentially fitted methods have already been considered in the literature, though characterized by different basis functions. For instance (see [16, 18] and references therein), for the convection-diffusion problem*

$$-\varepsilon \Delta u + a \nabla u + bu = f, \quad 0 < \varepsilon \ll 1,$$

the following fitting space has been considered

$$\left\{ 1, x, \dots, x^p, \exp\left(\frac{1}{\varepsilon} \int a\right), x \exp\left(\frac{1}{\varepsilon} \int a\right), \dots, x^{p-1} \exp\left(\frac{1}{\varepsilon} \int a\right) \right\}, \tag{2.12}$$

which is, differently from our case, more closely related to the problem rather than to its solution. This is visible from the arguments of the exponentials in (2.12), which generally do not match those of the solution of the problem.

3. Adapted IMEX Euler method

We now focus our attention on the time integration of the spatially semidiscretized system (2.6). In order to highlight a proper time integrator for this problem, we recast it in the following matrix form

$$\mathbf{h}'(t) = A(z)\mathbf{h}(t) + B(z)\mathbf{h}(t),$$

where

$$A(z) = \frac{1}{\Delta x^2} \begin{bmatrix} 0 & 0 & 0 & \dots & 1 \\ \gamma\alpha_0 & \gamma\alpha_1 & \gamma\alpha_2 & & \\ & \gamma\alpha_0 & \gamma\alpha_1 & \gamma\alpha_2 & \\ & & \ddots & \ddots & \ddots \\ & & & \gamma\alpha_0 & \gamma\alpha_1 & \gamma\alpha_2 \\ 1 & & & & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N \times N},$$

$$B(z) = \frac{1}{\Delta x} \begin{bmatrix} 0 & 0 & \dots & 0 \\ -v\beta_0 & -v\beta_1 & & \\ & -v\beta_0 & -v\beta_1 & \\ & & \ddots & \ddots \\ & & & -v\beta_0 & -v\beta_1 \\ & & & 0 & 0 \end{bmatrix} \in \mathbb{R}^{N \times N}, \quad (3.13)$$

and

$$\mathbf{h}'(t) = \begin{bmatrix} h'_0(t) \\ h'_1(t) \\ \vdots \\ h'_{N-1}(t) \end{bmatrix}, \quad \mathbf{h}(t) = \begin{bmatrix} h_0(t) \\ h_1(t) \\ \vdots \\ h_{N-2}(t) \\ f'(t) \end{bmatrix}.$$

The first summand, depending on the matrix $A(z)$, belongs to the diffusion term, thus it is notoriously stiff [1, 11] and requires an implicit solver in the time integration, while the part belonging to the advection term, i.e. the summand depending on $B(z)$, can be treated by an explicit time integrators. Thus, it

looks worthwhile solving this problem by an implicit-explicit (IMEX) time solver [1, 3, 4, 11] which creates a good compromise among accuracy, stability and computational cost. With respect to the fully discretized domain

$$\mathcal{D}_{\Delta x, \Delta t} = \{(x_i, t_j) : x_i = i\Delta x, \quad t_j = j\Delta t, \quad i = 0, \dots, N-1, \quad j = 0, 1, \dots, M-1\}, \quad (3.14)$$

being $\Delta x = X(T)/(N-1)$ and $\Delta t = T/(M-1)$, we integrate (2.6) in time with the following adapted IMEX-Euler scheme

$$\mathbf{h}^{j+1} = \varepsilon_0 \mathbf{h}^j + \varepsilon_1 (\Delta t A(z) \mathbf{h}^{j+1} + \Delta t B(z) \mathbf{h}^j), \quad j = 0, \dots, M-2, \quad (3.15)$$

where $\mathbf{h}^j = \mathbf{h}(t_j)$. The adapted version of the IMEX-Euler method we aim to introduce, coherently with the space discretization discussed in Section 2, is carried out by taking into account the character in time of the solution (1.3), which shows an exponential behaviour of complex parameter. Hence, we compute the unknown coefficients ε_0 , ε_1 and ε_2 by imposing the exactness of the time integrator (3.15) on the fitting space

$$\mathcal{H} = \{1, \exp(i\omega t)\}.$$

We introduce the following linear operator

$$\mathcal{L}[\Delta t] \mathbf{h}(t) = \mathbf{h}(t + \Delta t) - \varepsilon_0 \mathbf{h}(t) - \varepsilon_1 (\Delta t A(z) \mathbf{h}(t + \Delta t) + \Delta t B(z) \mathbf{h}(t))$$

and, by means of Taylor series arguments around (x, t) and neglecting $O(\Delta t^2)$ terms, we recast it as

$$\widetilde{\mathcal{L}}[\Delta t] h(t) = \mathbf{h}(t + \Delta t) - \varepsilon_0 \mathbf{h}(t) - \varepsilon_1 \Delta t \mathbf{h}'(t).$$

We observe that \mathcal{L} and $\widetilde{\mathcal{L}}$ differ for $O(\Delta t^2)$, which does not compromise the accuracy of the resulting IMEX-Euler method, having order 1.

We evaluate

$$\mathcal{L}[\Delta x] \mathbf{1}, \quad \mathcal{L}[\Delta x] \mathbf{e}(x, t),$$

being $\mathbf{1} = [1, \dots, 1]^\top \in \mathbb{R}^N$ and $\mathbf{e}(x, t) = \exp(i\omega t) \mathbf{1}$ and, due to the invariance in translation of the operator, we refer to the values gained in correspondence of $t = 0$ and annihilate them, obtaining the following linear system of equations

$$\begin{cases} 1 - \varepsilon_0 = 0 \\ \exp(i\omega) - \varepsilon_0 - i\omega \varepsilon_1 = 0 \end{cases}$$

with $w = \omega\Delta t$. The solution of such system is given by

$$\begin{aligned}\varepsilon_0 &= 1, \\ \varepsilon_1 &= -\frac{i(e^{iw} - 1)}{w}.\end{aligned}\tag{3.16}$$

Also in this situation, $w \neq 0$ because $\Delta t \neq 0$ and the ω is generally non-zero (at least for non-degenerate cases), ensuring that the denominators in (3.16) are non-zero. Moreover, as expected, when w tends to 0, the variable coefficients (3.16) tend to the classical values

$$\varepsilon_0 = \varepsilon_1 = 1.\tag{3.17}$$

of the coefficients of the IMEX-Euler method based on algebraic polynomials. Hence, the exponentially fitted formula retains the same order of accuracy of the corresponding classical one, which is equal to 1.

Remark 3.1. *Of course the application of the adapted numerical scheme requires the computation of the parameters z and w in (2.8), (2.10) and (3.16). Parameter estimation in exponentially fitted methods usually requires optimization techniques having as objective function the leading term of the local discretization error or solving nonlinear systems of equations in order to annihilate such error term [6, 8, 10]. In our case, we can efficiently approach the problem of computing the unknown parameters by exploiting the expression given by (1.3), suggesting us to define*

$$\begin{aligned}z &= \left(\frac{\nu}{2D} - \mu - i\rho\right)\Delta x, \\ w &= i\omega\Delta t.\end{aligned}$$

The case of parameter estimation when a parametrization of the solution of the problem is not known is object of [9], in the case of reaction-diffusion problem.

4. Stability analysis

We now aim to analyze the stability properties of our numerical scheme. While accuracy properties are mostly highlighted by the constructive issues themselves, stability deserves an independent analysis, which also clarifies the relationship between the classical method (i.e. classical finite differences for the spatial semidiscretization and classical IMEX-Euler time integration) and the adapted one (i.e.

adapted finite differences for the spatial semidiscretization and exponentially fitted IMEX-Euler method for the time integration).

Following the idea in [21], we aim to prove stability by controlling the propagation of the error caused by an incoming perturbation. To do this, we perturb the solution \mathbf{h}^j as follows

$$\widetilde{\mathbf{h}}^j = \mathbf{h}^j + \delta^j,$$

and study the behaviour of the error

$$E^j = \mathbf{h}^j - \widetilde{\mathbf{h}}^j.$$

Consequently, the following stability result occurs.

Theorem 4.1. *For the IMEX-Euler method (3.15) for the semidiscrete problem (2.6), the following stability inequality occurs*

$$\|E^{j+1}\|_{\infty} \leq \|M\|_{\infty} \|E^j\|_{\infty}, \quad (4.18)$$

where

$$M = \Lambda (\varepsilon_0 I + \varepsilon_1 \Delta t B(z)), \quad (4.19)$$

being $\Lambda = (I - \varepsilon_1 \Delta t A(z))^{-1}$ and I the identity matrix in $\mathbb{R}^{N \times N}$.

Proof: We first recast the IMEX-Euler method (3.15) in the following compact form

$$\mathbf{h}^{j+1} = \Lambda (\varepsilon_0 \mathbf{h}^j + \varepsilon_1 \Delta t B(z) \mathbf{h}^j),$$

obtaining by collecting the approximations in the same step point at each hand side. Similarly, we get the following expression of the perturbed method

$$\widetilde{\mathbf{h}}^{j+1} = \Lambda (\varepsilon_0 \widetilde{\mathbf{h}}^j + \varepsilon_1 \Delta t B(z) \widetilde{\mathbf{h}}^j),$$

Therefore, the corresponding error associated to the introduced propagation is given by

$$E^{j+1} = \mathbf{h}^{j+1} - \widetilde{\mathbf{h}}^{j+1} = \Lambda (\varepsilon_0 I + \varepsilon_1 \Delta t B(z)) E^j,$$

and passing to its norm gives the thesis. \square

Thus, according to Theorem 4.1, for the stability analysis it is sufficient to analyze the inequality

$$\|M\|_{\infty} < 1 \quad (4.20)$$

with M given by (4.19). Let us specialize this inequality for both the classical and adapted cases:

- for the classical case, covered by Theorem 4.1 when z and w tend to zero, we know that $\varepsilon_0 = \varepsilon_1 = 1$ and the matrix $B(z)$ reduces to

$$\tilde{B} = \frac{1}{\Delta x} \begin{bmatrix} 0 & 0 & \dots & 0 \\ -\nu & \nu & & \\ & -\nu & \nu & \\ & & \ddots & \ddots \\ & & & -\nu & \nu \\ & & & 0 & 0 \end{bmatrix},$$

and the matrix $A(z)$ is equal to

$$\tilde{A} = \frac{1}{\Delta x^2} \begin{bmatrix} 0 & 0 & 0 & \dots & 1 \\ \gamma & -2\gamma & \gamma & & \\ & \gamma & -2\gamma & \gamma & \\ & & \ddots & \ddots & \ddots \\ & & & \gamma & -2\gamma & \gamma \\ & & & & 0 & 1 \end{bmatrix}.$$

Since $\|\tilde{B}\|_\infty = 2|\nu|/\Delta x$, then

$$\|M\|_\infty \leq \|(I - \Delta t \tilde{A})^{-1}\| \left(1 + 2 \frac{\Delta t}{\Delta x} |\nu|\right).$$

Hence, it is sufficient to check, for stability purposes, that

$$\|(I - \Delta t \tilde{A})^{-1}\| \left(1 + 2 \frac{\Delta t}{\Delta x} |\nu|\right) < 1;$$

- for the adapted case, the infinity norm of the matrix $B(z)$ in (3.13) is equal to $|\nu|(|\beta_0| + |\beta_1|)/\Delta x$. Thus,

$$\|M\|_\infty \leq \|(I - \varepsilon_1 \Delta t A(z))^{-1}\| \left(1 + 2|\nu \varepsilon_1| \frac{\Delta t}{\Delta x} \left| \frac{z}{\exp(-z) - 1} \right| \right)$$

and it is sufficient to secure, for stability purposes, that

$$\|(I - \varepsilon_1 \Delta t A(z))^{-1}\| \left(1 + 2|\nu \varepsilon_1| \frac{\Delta t}{\Delta x} \left| \frac{z}{\exp(-z) - 1} \right| \right) < 1.$$

Examples of these bounds are provided in the following section.

5. Numerical experiments

We now present the numerical evidence originated by applying the IMEX-Euler scheme (3.15) to the advection-diffusion problem (1.1), with the following values of the parameter

$$\gamma = -5, \quad \nu = -2, \quad D = 3, \quad \rho = 10,$$

in correspondence of several values of the frequency ω . The domain chosen for the integration is given by the square $(x, t) \in [0, 100] \times [0, 100]$, which is discretized in space and in time with different values of the stepsizes Δx and Δt . The compared solvers are the following:

- **IEclass**, obtained by coupling the spatial semidiscretization based on classical finite differences (2.7) with coefficients (2.9) and (2.11) with the classical IMEX-Euler time integration, giving rise to (3.15) with coefficients (3.17);
- **IEef**, obtained by coupling the spatial semidiscretization based on adapted finite differences (2.7) with coefficients (2.8) and (2.10) with the classical IMEX-Euler time integration, giving rise to (3.15) with coefficients (3.16).

The results here reported are oriented in two directions: first of all, confirming the effectiveness of the approach **IEef** based on adapted methods as well as providing a comparison between **IEclass** and **IEef** in terms of stability, at the same computational cost. Figures 1 and 2 show the profile of the real part of the numerical solution for $\omega = -2$, obtained by the two aforementioned solvers with stepsizes $\Delta x = 1/10$ and $\Delta t = 1$. An unstable behaviour of **IEclass** is clearly visible, while **IEef** is able to correctly reproduce the profile of the solution. We observe that such stable and unstable behaviors observed in Figures 1–3 are coherent with the result highlighted in Theorem 4.1: indeed, the value of $\|M\|_\infty$ is equal to 1 for the classical case **IEclass**, while for **IEef** it is equal to 0.0302. The solution obtained with **IEef** is also zoomed in Figure 3, which better highlights the shape of the oscillations.

6. Conclusions

We have introduced an alternative approach for the numerical solution of advection diffusion problems (1.1) by means of adapted methods which take into

account the qualitative behaviour of the solution. The approach here presented is based on spatial semidiscretization of the advection and diffusion terms by exponentially fitted finite differences and the time integration of the resulting system of ODEs by an exponentially fitted IMEX-Euler solver. This novel approach, in comparison with its classical counterpart based on algebraic polynomials, provides a more stable method, as theoretically proved in Section 4 and confirmed by the numerical experiments in Section 5. Further development of this research will be oriented to introducing adapted numerical methods for other evolutionary operators and problems, by emphasizing on the analysis of stability and accuracy properties in comparison with existing approaches, and on an efficient and accurate parameter estimation.

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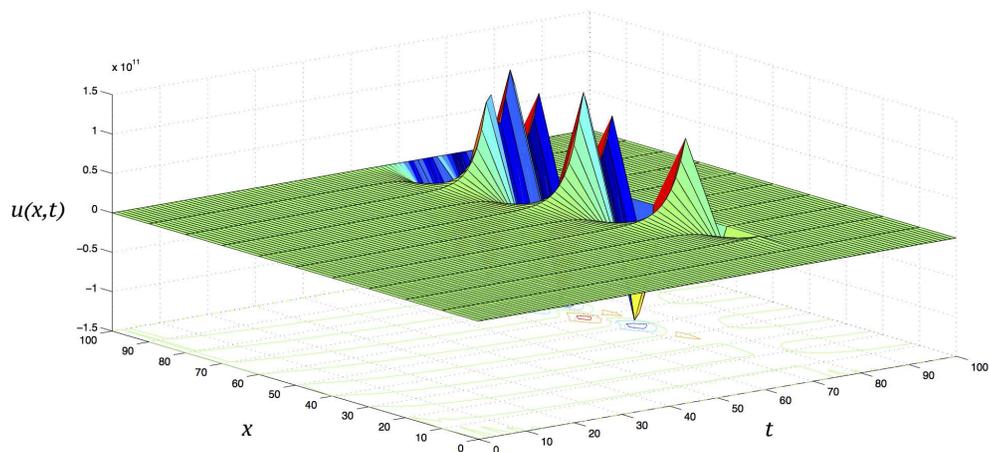


Figure 1: Real part of the numerical solution of (1.1) with $\omega = -2$ computed by IEclass solver, with $\Delta x = 1/10$ and $\Delta t = 1$.

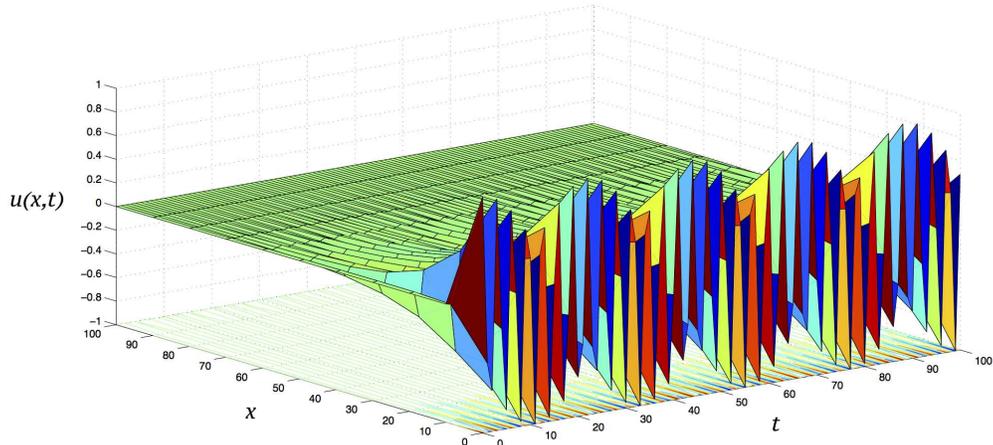


Figure 2: Real part of the numerical solution of (1.1) with $\omega = -2$ computed by IEef solver, with $\Delta x = 1/10$ and $\Delta t = 1$.

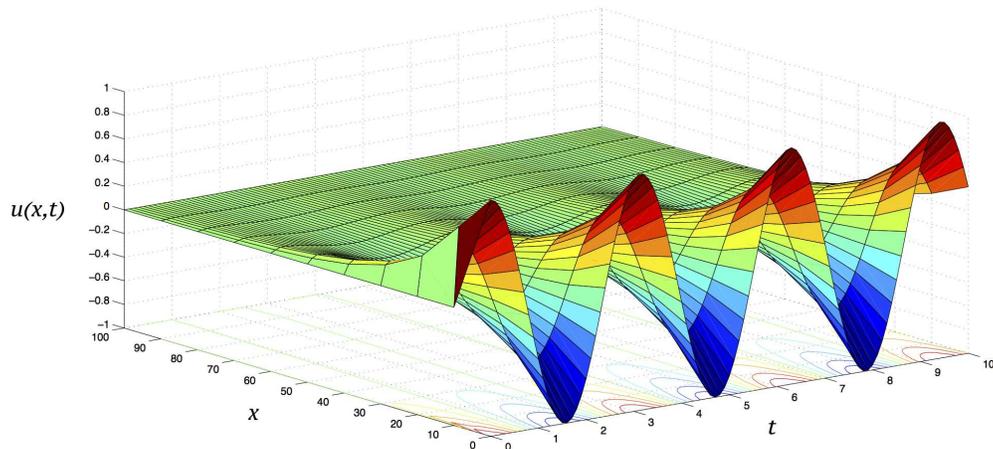


Figure 3: Real part of the numerical solution of (1.1) with $\omega = -2$ computed by IEef solver, with $\Delta x = 1/10$ and $\Delta t = 1$, zoomed for $(x, t) \in [0, 100] \times [0, 10]$.

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Fisciano, August 1, 2016

Dear Editor,

I submit to your attention the amended version of the manuscript "*Exponentially fitted IMEX methods for advection-diffusion problems*", by Angelamaria Cardone, Raffaele D'Ambrosio and Beatrice Paternoster, for possible publication in the special issue of J. Comput. Appl. Math. related to Numdiff 2015 conference.

This version of the manuscript has been carried out taking care of the precious comments of the reviewer, as I am going to describe in the remainder of this letter.

Reviewer 1

- *page 1, in the first formula there is s , but in the subsequent lines S appears (twice).*

Thank you, the typo is fixed: all the occurrences of S are now in capital letters.

- *page 2, line 11 : what does $\cot(\gamma)$ mean? Where does this come from?*

We wrote $1/\tan(\gamma)$ instead of $\cot(\gamma)$ and added a references to [22], where the details on this formulation of the moving boundary is explained in details.

- *page 3, line 3: multiple frequencies ... is ω_n a number or a vector? How should I interpret this?*

This part has been removed, because redundant (we are not dealing with sequences of moving boundaries).

- *page 3, line -6: oscillatory (instead of oscillate)*

Fixed.

- *page 5, line 12: where do Δ_1 and Δ_2 appear?*

We have removed Δ_1 and Δ_2 from the text.

- *page 6, line 3: I think there are several choices possible for the third fitting function. Why does one choose this one?*

Yes, many choices are possible. However, this is a quite common one (compare [13, 17] and references therein), because it highlights the exponential character of the fitting space.

- page 6, line 9: *there is a +-sign missing.*

Fixed.

- page 12, line 5: *infinity norm*

Fixed.

- page 12, line 6: *The infinity norm is equal to $(|\nu\beta_0| + |\nu\beta_1|)/\Delta x$, it is not equal to $|\nu\beta_0 + \nu\beta_1|$, so the constraint on $\|\Lambda\|$ changes.*

Fixed.

- page 13: *numerical experiments: in order to fully understand why there is instability, I think it is necessary to compute the value of $\|\tilde{\Lambda}\|$ and $\|\Lambda\|$ for the chosen values and compare these with the constraints. What are the values of $\|\tilde{\Lambda}\|$ and $\|\Lambda\|$ in this case?*

(Answer to both reviewers) Following the remark on stability by both reviewers, we have significantly amended Section 4 and also the corresponding counterpart in the numerical experiments. Indeed, Theorem 4.1 now gives a direct sufficient condition on stability, making this result (and the whole section) more conclusive. The rest of the section specializes Theorem 4.1 to the adapted and classical cases. Moreover, in the section on numerical experiments we have given examples of the values of the bounds, given an experimental confirmation of the theoretical results. Thanks a lot to the reviewers for their precious suggestions;

- pages 15, 16 and 17 : *is it necessary to include the Figures 4, 5, 6 and 7?*

Following the remark of the reviewer, we have removed the pictures, since they only confirm what already happened for $\omega = -2$.

Reviewer 2

1. *First of all, the formulation of the problem is not quite clear to me. What is the role of the moving boundary, and how do the authors deal with this? This should be explained.*

The considered problem, i.e. Boussinesq equation leading to the advection-diffusion problem (1.1), has been taken from the existing literature and we made much more reference to the manuscript [22], where the problem

is formulated in terms of a moving boundary condition; however, this fact does not affect at all the numerical scheme, that works well also in case of time-independent bounds on the space interval. Clearly, in the numerical experiments, we have fixed our bounds, as visible from the assertion on the domain used for the discretization (line +6 of Section 5).

2. *Exponential fitting is an old technique to discretize advection-diffusion equations; see e.g. K.W. Morton, Numerical Solution of Convection-Diffusion Problems, Chapman & Hall, London, 1996 and the many references therein. References to the relevant literature should be included.*

References [16, 18] has been added and Remark 2.1 has also been included in the amended manuscript, better highlighting the frame into the existing literature.

3. *Usually, in exponentially fitting the advection-diffusion operator is taken as one operator, in this paper the authors treat the diffusive and advective terms separately. Please explain. The choice of the fitting space F is not clear to me, why include a term like $x \exp(\zeta x + i\omega t)$? Moreover, for the spatial discretization the time-dependent part is irrelevant and could be left out. It cancels in the derivation of the coefficients α_0 , α_1 and α_2 .*

The advection term is, in general non-stiff, while the diffusion term is generally source of stiffness (this is clear in the literature, compare for instance [23] and references therein: this issue clearly motivates the employ of implicit-explicit method, treating the advection explicitly and the diffusion implicitly. As it regards the use of mixed terms, e.g. $x \exp(\zeta x)$, this is a classical choice (also in the case of PDEs, as highlighted in Remark 2.1). We have also removed the time-dependent parts in the fitting spaces adopted in Sections 2.1 and 2.2.

4. *For time integration the authors derive an exponentially fitted IMEX scheme, which is interesting.*

Thanks a lot for your appreciation.

5. *The result of the stability analysis is not very conclusive. The authors should at least give a time step restriction (if any) for stability.*

(Answer to both reviewers) Following the remark on stability by both reviewers, we have significantly amended Section 4 and also the corresponding counterpart in the numerical experiments. Indeed, Theorem 4.1 now gives a direct sufficient condition on stability, making this result (and the whole section) more conclusive. The rest of the section specializes Theorem 4.1 to the adapted and classical cases. Moreover, in the section on numerical experiments we have given examples of the values of the bounds, given an experimental confirmation of the theoretical results. Thanks a lot to the reviewers for their precious suggestions.

6. *My major concern is how to choose the parameters z and w . The choice of z and w on page 13 depends of knowledge of the exact solution, which we usually don't have. A clear description how to determine z and w should be added.*

Please refer to Remark 3.1. We highlight that the case of the numerical solution by adapted methods to problem whose parametrization of the solution is not a priori known, is object of [9], where the treatise is focused on reaction-diffusion systems generating periodic wavefronts.

7. *The numerical results are not very convincing. How does the method compare to other methods, what about accuracy and computational costs?*

Section 5 on numerical experiments has been simplified a lot in its treatise. Indeed, the experiments are now clearly referred to the novel Section 4 on stability. Moreover, there is a comparison between classical the finite difference numerical scheme (IEclass) and the proposed exponentially fitted version (IEef). As highlighted in the text, the superiority of IEef is visible, since IEclass looks unstable.

8. *The axes of all figures are not labelled.*

Axis labels added in Figures 1–3.

9. *The formulation is rather sloppy, with a lot of repetition. Moreover, the english should be improved.*

We spent our efforts to improve both the presentation and the English. As it regards possible repetition, the section on stability has been improved and specialized, as well as we have removed too many numerical experiments going to the same direction and giving the same conclusions.

We have also added a further acknowledgment session containing our grateful appreciation of the comments provided by the anonymous referees.

Thank you very much for your time and attention.

Sincerely yours,
the corresponding author
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