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High-efficiency implicit scheme for solving first-order partial differential equations

Alicia Cordero [a,*], Renso V. Rojas-Hiciano [b], Juan R. Torregrosa [a], Maria P. Vassileva [c]

[a] *Multidisciplinary Mathematics Institute, Universitat Politècnica de València, Camino de Vera, 46022, Valencia Spain*

[b] *Escuela de Ciencias Naturales y Exactas, Pontificia Universidad Católica Madre y Maestra, Sarasota Ave., 10109 Santo Domingo D.N., Dominican Republic*

[c] *Ciencias Básicas y Ambientales, Instituto Tecnológico de Santo Domingo, Los Próceres, 10602 Santo Domingo D.N., Dominican Republic*

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ABSTRACT

We present three new approaches for solving first-order quasi-linear partial differential equations (PDEs) with iterative methods of high stability and low cost. The first is a new numerical version of the method of characteristics that converges efficiently, under certain conditions. The next two approaches initially apply the unconditionally stable Crank–Nicolson method, which induces a system of nonlinear equations. In one of them, we solve this system by using the first optimal schemes for systems of order four (Ermakov's Hyperfamily). In the other approach, using a new technique called JARM decoupling, we perform a modification that significantly reduces the complexity of the scheme, which we solve with scalar versions of the aforementioned iterative methods. This is a substantial improvement over the conventional way of solving the system. The high numerical performance of the three approaches is checked when analyzing the resolution of some examples of nonlinear PDEs.

1. Introduction

Partial differential equations (PDEs) first appeared in the context of mathematical modeling of phenomena in Continuum Physics [1–4]. They play a crucial role in the modeling of complex real-world phenomena and allow modeling numerous physical problems, fluid mechanics, elasticity, aerodynamics, waves of any type, convection, diffusion, heat distribution, potential, economic problems (Black–Scholes Models), electromagnetic fields (Maxwell's Equations), Astronomy, Electricity, among others.

Their solution, in most cases, can only be carried out numerically. This often leads to algorithms that require solving large systems of nonlinear equations.

A first-order PDE is said to be quasi-linear with two independent variables $(x, y) \in \mathbb{R}^2$ and unknown function $u : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$, $u = u(x, y)$, if it can be written as follows

$$A(x, y, u)u_x + B(x, y, u)u_y = C(x, y, u), \tag{1}$$

where A, B y C are functions of any of the indicated variables. In case A and B do not depend on u, and $C(x, y) = E(x, y)u$, we say that it is linear.

A first-order ordinary differential equation (ODE), with unknown function $u : D \subset \mathbb{R} \to \mathbb{R}, t \in \mathbb{R}$, can be written as

$$\frac{du(t)}{dt} = c(u(t), t),$$

* Corresponding author.
E-mail address: acordero@mat.upv.es (A. Cordero).

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where c is a function of u and t.

To solve first-order PDEs, the method of characteristics and the finite difference scheme are often used [5].

Theorem 1 (*[6]*). *The general solution of quasi-linear partial differential equation (1) is*

$$f(\phi, \psi) = 0,$$

where f is an arbitrary function of $\phi(x, y, u)$ and $\psi(x, y, u)$ and both $\phi = c_1$ and $\psi = c_2$, where c_1, and c_2 are constants, are solution curves of the characteristic equations

$$\frac{dx}{A} = \frac{dy}{B} = \frac{du}{C}.$$

The solution curves $\phi(x, y, u) = c_1$ and $\psi(x, y, u) = c_2$ are called families of characteristic curves of the PDE.

The following result guarantees the existence and uniqueness of the solution of a quasi-linear PDE (1), under certain conditions.

Proposition 2 (*Cauchy Problem for Quasi-Linear Equations, [7]*). *Given the quasi-linear partial differential equation (1), suppose $x_0(s), y_0(s)$ and $u_0(s)$ are continuously differentiable functions of s on the interval [0,1]. Moreover, $A(x, y, u)$, $B(x, y, u)$ and $C(x, y, u)$ are of class $C^1(D)$, with D a domain in the (x, y, u)-space, containing the initial curve*

$$\Gamma : x = x_0(s), \quad y = y_0(s), \quad u = u_0(s),$$

and satisfying the condition

$$y_0'(s)A\left(x_0(s), y_0(s), u_0(s)\right) - x_0'(s)B\left(x_0(s), y_0(s), u_0(s)\right) \neq 0.$$

Then, there exists a unique solution $u = u(x, y)$ of (1) in a neighborhood of $x = x_0(s)$, $y = y_0(s)$, and the solution satisfies the initial condition

$$u_0(s) = \left(x_0(s), y_0(s)\right), s \in [0, 1].$$

One of the simplest first-order equations is the so-called linear transport equation:

$$u_t + cu_x = 0, \tag{2}$$

with initial condition $u(x, 0) = u_0(x)$, and $c \in \mathbb{R}$, which meets the properties: time-dependent, conservative, does not evolve to a steady state; therefore, it is hyperbolic, according to the criterion for general PDEs, proposed by Heath in [8].

We can understand the behavior of hyperbolic PDEs in more detail by studying the characteristic curves, which are paths in the xt-plane, denoted by $(x(t), t)$, in which the solution is constant. For (2) we have $x(t) = x_0 + ct$, since

$$\begin{aligned}\frac{d}{dt}u(x(t), t) &= u_t(x(t), t) + u_x(x(t), t)\frac{dx(t)}{dt} \\ &= u_t(x(t), t) + cu_x(x(t), t) \\ &= 0.\end{aligned} \tag{3}$$

Therefore $u(x(t), t) = u(x(0), 0) = u_0\left(x_0\right)$, i.e., the initial condition is carried along the characteristics.

It is important to emphasize that each different choice of x_0 gives a different characteristic curve.

As we have seen in Theorem 1 and Proposition 2, the systems of characteristic equations have important implications for the direction of the information flow and for the boundary conditions.

More generally, if the PDE is not homogeneous, then the situation is a bit more complicated for each characteristic curve. Let us consider

$$u_t + cu_x = f(x, t, u(x, t)), \tag{4}$$

and $x(t) = x_0 + ct$. Then,

$$\begin{aligned}\frac{d}{dt}u(x(t), t) &= u_t(x(t), t) + u_x(x(t), t)\frac{dx(t)}{dt} \\ &= u_t(x(t), t) + cu_x(x(t), t) \\ &= f(x(t), t, u(x(t), t)).\end{aligned}$$

In this case, the solution is no longer constant in $(x(t), t)$, but we have reduced a PDE to a set of ODEs, so that:

$$u(x(t), t) = u_0\left(x_0\right) + \int_0^t f(x(t), t, u(x(t), t))dt. \tag{5}$$

We can also find characteristics for variable coefficient advection, $c(x(t), t)$. It is easy to prove that the characteristic curve of $u_t + c(x, t)u_x = 0$ is given by

$$\frac{dx(t)}{dt} = c(x(t), t).$$

In this case, we have to solve an ODE to obtain the curve $(x(t), t)$ in the xt-plane, then, the curves present a nonlinear behavior, unlike the homogeneous transport equation. The characteristics also apply to nonlinear hyperbolic PDEs, such as the Burger equation, among others. The characteristic curves are a way to solve the quasi-linear equation (4), and we can do it by numerical techniques for ODEs, but one of the most widespread method at present is the one we present in the next section, of finite differences. The idea is to approximate the derivative, through numerical differences and then we can get closer to the solution, depending on the order of said approximation. The approximate solution is finally obtained by solving a system of nonlinear equations.

It is important to note that when we work in a regular domain (in general, rectangle, cube, …) of unknown function in PDE (1), the results provided by the finite difference methods are satisfactory. Hymers in [9] deepened in the study of finite differences applied to differential equations and Boole in [10] does the same concentrating an important part of his work in the application to PDEs.

We partition the interval containing the variable t into m equispaced subintervals with step size k, and do the same with x, a step size h and n subintervals, then $t_j = t_0 + jk,\ j = 0, 1, 2, \dots, m$ and $x_i = x_0 + ih,\ i = 0, 1, 2, \dots, n$. We denoted the value of unknown function in each node by $u_{i,j} = u\left(x_i, t_j\right)$.

A common path followed by some researchers [11] consists of developing a finite difference approximation for the homogeneous transport equation is to consider the Courant, Friedrichs and Lewy condition, which we denote hereafter by CFL. This is a necessary condition for the convergence of a finite difference approximation of the hyperbolic problem.

Applying first-order finite differences, the resulting explicit schemes need convergence conditions, and the implicit method obtained by using the symmetric differences is unstable.

It is said that a numerical scheme is consistent with a PDE if its truncation error tends to zero when $h, k \to 0$. For example, any first-order (or higher) scheme is consistent.

The solution of first-order PDEs has been studied and some conditions in the numerical case have been established by Lax in [12] to guarantee the convergence, if finite differences are used. In addition, the solution of the transport equation was studied (see [11]) by applying the method of characteristics and the finite difference method. The former was approached considering the homogeneous case and the non-homogeneous case. In the latter method, two explicit schemes in the time variable were considered. Lax's Theorem on consistency is established as follows.

Theorem 3. *(Lax [12]). For a consistent finite difference approximation of a linear evolutionary problem, stability of the scheme is necessary and sufficient for convergence.*

On the other hand, the Crank–Nicolson method (CN) is second order and, moreover, unconditionally stable. It does not need convergence conditions. CN induces a system of nonlinear equations that we must solve, which can be written in the form $F(x) = 0$, where $F : D \subset \mathbb{R}^n \to \mathbb{R}^n$, is a function defined on an open convex domain D.

In general, these types of systems cannot be solved analytically or exactly, so iterative methods are used to obtain an approximate solution to these problems. The most used iterative scheme is Newton's method (N2S), of order 2, whose iterative expression is given by

$$x^{(k+1)} = x^{(k)} - \left[F'\left(x^{(k)}\right)\right]^{-1} F\left(x^{(k)}\right), \quad k = 0, 1, \dots, \tag{6}$$

where $F' \in \mathscr{L}\left(\mathbb{R}^n, \mathbb{R}^n\right)$ is the Jacobian matrix of function F.

Recently, the authors have presented in [13] a new parametric class of iterative schemes, Ermakov's Hiperfamily, with a particular subclass, KLAM4S$_\lambda$, that improves Newton's scheme as in the order of convergence as in the set of convergent initial estimates, and whose extension to systems in [14] is the first optimal method of order four for solving nonlinear systems:

$$x^{(k+1)} = y^{(k)} - \frac{1}{1 - \lambda v_k}\left[F'(x^{(k)})\right]^{-1}\left(F(y^{(k)}) + 2v_k F(x^{(k)})\right), \quad k = 0, 1, \dots \tag{7}$$

$v_k = \frac{\left\|F(y^{(k)})\right\|^2}{\left\|F(x^{(k)})\right\|^2}, \lambda \in \mathbb{R}$.

We use both schemes in all numerical tests, in their scalar or vectorial version, as appropriate, in order to compare them.

In Section 2, we present a new approach to solve first-order PDEs, the numerical feature method, in which we solve the corresponding system of ODEs with an implicit/implicit scheme. Numerical results are presented applying optimal scheme (7). This scheme shows superior performance in cost and efficiency with respect to Newton's method.

Similarly, in Section 3, we apply the optimal iterative scheme (7) for solving the systems of nonlinear equations formed by solving PDEs discretizing with CN in the most efficient and least cost way, as far as we know.

Finally, in Section 4, we introduce a new contribution: after applying the unconditionally stable Crank–Nicolson method, we simplify the resulting system, with a decoupling strategy and finally we apply optimal KLAM$_5$ method [13]. Furthermore, we compare the numerical behavior against linearization. The improvement introduced in this section substantially outperforms in the sense of computational effort, time and accuracy the usual way of solving nonlinear PDEs with implicit methods.

2. Numerical method of characteristics for first-order PDEs

2.1. Homogeneous case

Let us now address the one-dimensional linear transport equation, which has the form

$$u_t + c\, u_x = 0,$$

where $c \in \mathbb{R}$, and the initial condition is verified

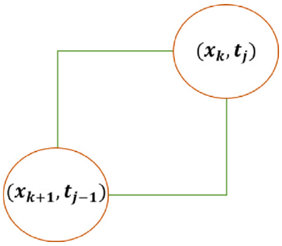


Fig. 1. Pair of nodes with slope 1 satisfying the characteristic equations.

$$u(x,0) = u_0(x). \tag{8}$$

The application of the method of characteristic curves of Theorem 1 involves solving the following system of ordinary differential equations with parameter c:

$$\begin{cases} \dfrac{dx}{dt} = c, \\ \dfrac{du}{dt} = 0. \end{cases} \tag{9}$$

By solving the first equation we observe that it is a set of straight lines parallel to $x = c\,t$. Then, the solution of the system (9) is the set of all lines with slope c intersecting the plane curve $u_0(x)$. Therefore, the solution is a cylindrical surface, that corresponds to geometric space of all the displaced points of $u_0(x)$ in the direction of $x = c\ t$.

Suppose we want to find the numerical solution. First, we choose the regular enclosure $R = \{(x,t) \mid 0 \le x \le 2,\ 0 \le t \le 1\}$. For meshing, we divide the spatial variable interval into $2n+1$ equispaced nodes, forming the vector

$$X = (x_0,\ x_1,\ x_2,\ \dots,\ x_{n-1},\ x_n\ \dots, x_{2n}),$$

where $x_0 = 0$, $x_k = x_0 + k\ \Delta x = k\ \Delta x$, $\Delta x = \frac{1}{2n}$ for $k = 1, 2, \dots, 2n$.

We can note that the slope from (x_k, t_j) to (x_{k+1}, t_{j-1}) is

$$\frac{\Delta x}{c\Delta t}.$$

In such a case, if we make $\Delta x = c\Delta t$, then the straight line containing the points (x_k, t_j) and (x_{k+1}, t_{j-1}) will have slope equal to 1, which satisfies the system of characteristic curves (9) with $c = 1$.

Then, since u is constant in this curve, we have $u(x_k, t_j) = u(x_{k+1}, t_{j-1})$, that is, $u_{k,j} = u_{k+1,j-1}$, as illustrated in Fig. 1.

Similarly, it is immediate to observe that the slope of any pair of nodes (x_k, t_j) and (x_{k+m}, t_{j-m}) with $m = 0, \dots, n$, is

$$\frac{\Delta x}{\Delta t},$$

which will be equal to 1, if the two step sizes are equal.

Fig. 2 shows several nodes located on a straight line parallel to the secondary diagonal. In these the slope is 1, then the value of u is constant along each straight line at all its nodes, as indicated in the characteristic equations. Extending the above analysis, since u is constant along this curve, we have $u(x_k, t_j) = u(x_{k+m}, t_{j-m})$, that is, $u_{k,j} = u_{k+m,j-m}$.

The solution to the transport equation is

$$U(x,t) = [u_0(x_0)\ \ u_0(X_1)\ \ \dots\ \ u_0(X_n)]^T, \tag{10}$$

where

$$X_i = (x_i,\ x_{i+1},\ \dots,\ x_{n+i}),$$

for $i = 0,\ 1,\ \dots,\ n$. Table 1 shows the developed form of the solution (10).

2.2. Non-homogeneous case (symmetrical)

Consider the Cauchy problem for the nonlinear transport equation

$$u_x + u_t = f(u), \tag{11}$$

with initial condition $u(x,0) = u_0(x)$.

Applying the method of characteristics, we must solve the system of ordinary differential equations

$$\begin{cases} \dfrac{dx}{dt} = 1, \\ \dfrac{du}{dt} = f(u). \end{cases} \tag{12}$$

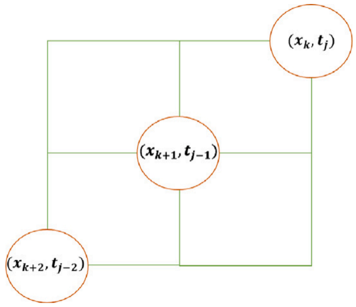


Fig. 2. The set of nodes located at any of the parallels to the secondary diagonal satisfies the characteristic equations.

Table 1
Structure of the solution matrix for the transport equation with $c = 1$.

(x_k, t_j)	t_0	t_1	t_2	t_3	t_4	$\dots$	t_n
x_0	$u_0(x_0)$	$u_0(x_1)$	$u_0(x_2)$	$u_0(x_3)$	$u_0(x_4)$	$\dots$	$u_0(x_n)$
x_1	$u_0(x_1)$	$u_0(x_2)$	$u_0(x_3)$	$u_0(x_4)$	$u_0(x_5)$	$\dots$	$u_0(x_{n+1})$
x_2	$u_0(x_2)$	$u_0(x_3)$	$u_0(x_4)$	$u_0(x_5)$	$u_0(x_6)$	$\dots$	$u_0(x_{n+2})$
x_3	$u_0(x_3)$	$u_0(x_4)$	$u_0(x_5)$	$u_0(x_6)$	$u_0(x_7)$	$\dots$	$u_0(x_{n+3})$
x_4	$u_0(x_4)$	$u_0(x_5)$	$u_0(x_6)$	$u_0(x_7)$	$u_0(x_8)$	$\dots$	$u_0(x_{n+4})$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$		$\vdots$
x_n	$u_0(x_n)$	$u_0(x_{n+1})$	$u_0(x_{n+2})$	$u_0(x_{n+3})$	$u_0(x_{n+4})$	$\dots$	$u_0(x_{2n})$

Note that, in this case, $u_0(x)$ does not need to be constant along the characteristic curves.

We now concentrate on a particular case. When solving the second equation, if we find that $u_0'(x) = f(u(x_0, t))$, then the solution graph is again a cylinder. In other words, in case it is satisfied that $u(a, 0) = u(0, a),\ a \in \mathbb{R}$ or that $\lim_{i\to\infty} |u(x_i, 0) - u(0, t_i)| = 0$, then the surface S corresponding to the function $u(x, t)$ is a cylinder with orthogonal generatrices with respect to the plane $t = x$. Then, the PDE (11) can be written as

$$u_x - u_t = 0. \tag{13}$$

Then the mesh is constructed similarly as in the homogeneous case, whose numerical solution is given by the matrix (10). Each row is obtained by shifting each component in the previous row by one unit to the right.

2.3. Numerical tests

Each calculation was performed using Matlab R2022b with variable precision arithmetics with a 200-digit mantissa to minimize rounding errors.

Problem 1. Nonlinear transport equation

We consider a particular case of the nonlinear, nonhomogeneous transport equation. This equation models physical phenomena, referring to the motion of different entities, such as quantity of motion, mass or energy, through a medium, solid or fluid, with particular conditions existing within the medium and is expressed as follows

$$u_t + u_x = -2u^2. \tag{14}$$

The boundary conditions on $u(x, t)$ are imposed as $u(0, t) = \frac{1}{1+t}, u(1, t) = \frac{1}{2+t}$, being $0 \le t \le 1$, along the initial condition: $u(x, 0) = \frac{1}{1+x}$ for $0 \le x \le 1$.

We first form the system of ODEs generated by applying the method of characteristics, then solve it by applying implicit/implicit scheme with trapezoidal rule, and finally solve the system of nonlinear equations resulting from applying finite differences to the PDE, applying Newton's method for nonlinear systems and optimal fourth-order method (7). In this way, we determine the effectiveness and competitiveness of such schemes.

Now, applying the method of characteristics we obtain.

$$\begin{cases} \dfrac{dx}{dt} = 1, \\ \dfrac{du}{dt} = -2u^2. \end{cases} \tag{15}$$

With the first equations we impose that $\Delta x = \Delta t$.

From the second equation we form a system of $n = 500$ equations, taking as step size $\Delta t = 1/(n-1)$ we obtain our initial approximation, applying the initial condition, $u(x, 0) = \frac{1}{1+x}$ for $0 \le x \le 1$.

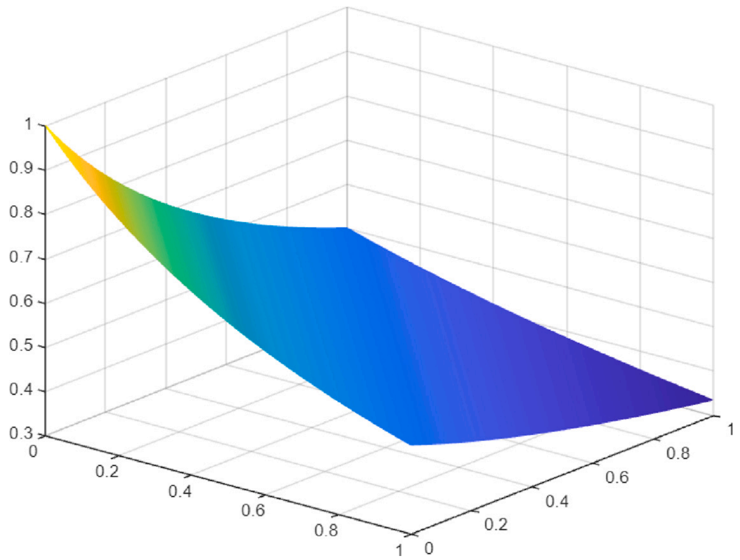


Fig. 3. Numerical approximation of the solution of the nonlinear and nonhomogeneous transport equation $u_t + u_x = -2\,u^2$ with the method of numerical features.

Now we must solve numerically the system obtained by applying the implicit/implicit scheme with trapezoidal rule:

$$\begin{aligned} &u_1 - 1 = 0, \\ &u_i - u_{i-1} + \Delta t\,(u_i^2 + u_{i-1}^2) = 0,\ i = 2, 3 \ldots, 500. \end{aligned} \tag{16}$$

The maximum number of iterations considered is 50 and the stopping criterion is $\left\|x^{(k+1)} - x^{(k)}\right\| < 10^{-100}$ or $\left\|F(x^{(k+1)})\right\| < 10^{-100}$, where F is the vectorial function that describes the nonlinear system. Then, we form the corresponding mesh, considering the domain

$$D = \{(x,t)\,|\,(x,t) \in [0,1] \times [0,1]\},$$

with step size partition

$$\Delta t = \Delta x = \frac{1}{n-1},$$

for the respective domains. The second differential equation of the system has been solved by applying the new iterative schemes. It is observed that this solution corresponds to the initial condition $u_0(x)$, therefore the solution of the PDE is a cylindrical surface symmetric with respect to $t = x$.

By applying the new approach, we obtain the solution shown in Fig. 3.

Table 2 shows the results obtained by applying N2S and KLAM4S$_0$ to solve the system (16), in addition to the ACOC (ρ), it also shows the number of iterations (Iter) required, two error estimates, $\|x^{(k+1)} - x^{(k)}\|$ and $\|F(x^{(k+1)})\|$, the time required to reach the tolerance previously indicated, and the computational effort, that some authors [15] define as the total number of evaluations and operations in an iterative process. So we can calculate it using

$$Effort = Iter \times (d + op), \tag{17}$$

where $Iter, d$ and op indicate the number of iterations, total evaluation of function F and Jacobian matrix, and operations needed to solve the linear systems in each iteration, respectively.

In Table 2, we can see that KLAM4S$_0$ outperforms Newton in almost all categories, both in number of iterations, error, residual error. It is worth noting that Newton requires twice as much effort as KLAM4S$_0$. The theoretical order of convergence is preserved for each method.

Problem 2. Logistic transport equation

A non-homogeneous transport equation that allows the modeling of transport phenomena in various areas and disciplines is

$$u_t + u_x = -2u(1-u), \tag{18}$$

with boundary conditions $u(0,t) = \frac{1}{1+e^t}$, $u(1,t) = \frac{1}{1+e^{t+1}}$ for all $t \geq 0$, in addition to the initial condition: $u(x,0) = \frac{1}{1+e^x}$, for $0 \leq x \leq 1$.

We proceed to solve the problem described by (18) similarly and with the same stopping criteria as the nonlinear transport equation in the previous section.

Table 2
Comparison of iterative schemes applied to Problem 1.

Method	Iter	$\|x^{(k+1)} - x^{(k)}\|$	$\|F(x^{(k+1)})\|$	ρ	Time	Effort ($\times 10^6$)
N2	8	6.979×10^{-131}	1.881×10^{-131}	2	14.96	337
KLAM4S$_0$	3	2.550×10^{-137}	1.303×10^{-276}	4	25.00	127

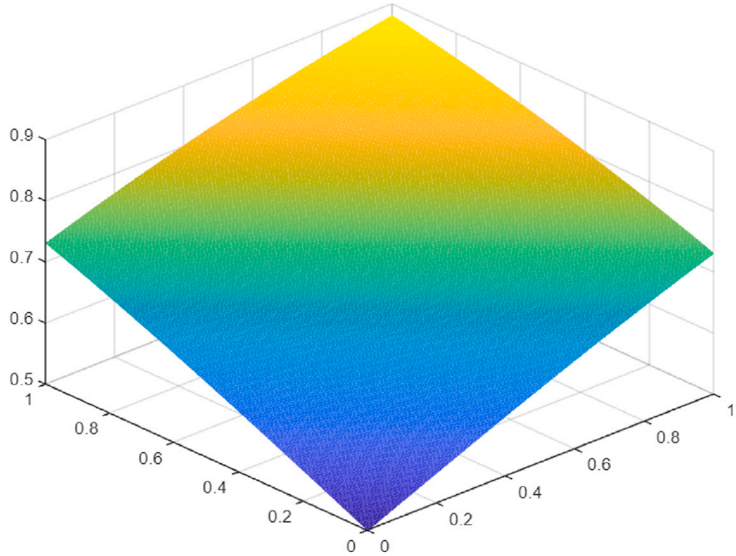


Fig. 4. Numerical solution of the Logistic Transport Equation $u_t + u_x = -2u(1-u)$ with the numerical characteristics method.

Applying the method of characteristics, we have the system:

$$\begin{cases} \dfrac{dt}{ds} = 1, \\ \dfrac{dx}{ds} = 1, \\ \dfrac{du}{ds} = -2u(1-u), \end{cases} \tag{19}$$

we discretize similarly to the previous problem. We must determine the numerical solution of the system of nonlinear equations of size 500:

$$\begin{aligned} & u_1 - 1/2 = 0, \\ & u_i - u_{i-1} + \Delta s\ \left(u_i(1-u_i) + u_{i-1}(1-u_{i-1})\right) = 0,\ i = 2, 3 \ldots, 500. \end{aligned} \tag{20}$$

The last differential equation of the system has been solved by applying implicit/implicit with trapezoidal rule.

The solution surface of the PDE is a cylinder symmetric with respect to the $t = x$ plane. By applying the new approach, the solution obtained is shown in Fig. 4 and Table 3.

3. Crank–Nicolson method with the first optimal methods of order 4 for nonlinear systems

The most of existing numerical methods to solve PDEs are finite differences of first-order for the time variable and of first or second order for the spatial variable. There are other methods of order 2, both in the temporal and spatial variables, such as Richardson's method. However, both it has serious stability problems.

A method that reaches the same second order in both variables, and does not have this problem, is the one proposed by John Crank and Phyllis Nicolson [16], based on the trapezoid rule. In several studies, Dahlquist in [17,18] has highlighted the stability, convergence and consistency properties of the trapezoid method, which point to it as an important scheme, it is unconditionally stable, so it is a very reliable method, because it is consistent and stable, therefore it is convergent.

3.1. Transformation and discretization of the problem

Suppose that the first-order partial differential equation in the one-dimensional case is

$$u_t = G\left(x, t, u, u_x\right). \tag{21}$$

Table 3
Comparison of iterative schemes applied to the Logistic Equation.

Method	Iter	$\|x^{(k+1)}-x^{(k)}\|$	$\|F(x^{(k+1)})\|$	ρ	Time	Effort ($\times 10^6$)
N2S	5	1.433×10^{-159}	1.435×10^{-159}	2	18.75	211
KLAM4S$_0$	3	4.478×10^{-156}	4.485×10^{-156}	4	23.60	127

Applying the trapezoid method to the problem (21), we have

$$u(x,t+\Delta t)=u(x,t)+\frac{\Delta t}{2}\left[G\left(x,t+\Delta t,u(x,t+\Delta t),u_x(x,t+\Delta t)\right)\right. \\ \left.+G\left(x,t,u(x,t),u_x(x,t)\right)\right], \tag{22}$$

where Δt is the temporary step.

Now, approximating the partial derivatives of u with respect to x with central differences, as in Section 1, we have

$$\begin{aligned} u(x,t+\Delta t)=&u(x,t)\\ &+\frac{\Delta t}{2}\left[G\left(x,t+\Delta t,u(x,t+\Delta t),\frac{u(x+\Delta x,t+\Delta t)-u(x-\Delta x,t+\Delta t)}{2\Delta x}\right)\right.\\ &\left.+G\left(x,t,u(x,t),\frac{u(x+\Delta x,t)-u(x-\Delta x,t)}{2\Delta x}\right)\right], \end{aligned} \tag{23}$$

where Δx is the spatial step.

Rewriting for each node, we have

$$\begin{aligned} u_{i,j+1}=u_{i,j}+\frac{k}{2}&\left[G\left(x_i,t_{j+1},u_{i,j+1},\frac{u_{i+1,j+1}-u_{i-1,j+1}}{2\Delta x}\right)\right.\\ &\left.+G\left(x_i,t_j,u_{i,j},\frac{u_{i+1,j}-u_{i-1,j}}{2\Delta x}\right)\right], \end{aligned} \tag{24}$$

for $i=0,1,2,\dots,nx$ and $j=0,1,2,\dots,nt$ in the general case, being nx and nt the amount of subintervals in the respective spatial and time variables.

3.2. Discretized particular problem

In our particular case, the non-homogeneous transport equation, we have

$$\begin{aligned} &u_t(x,t)+c\,u_x(x,t)=f(u),\quad 0\le x\le L,\quad t\ge 0\\ &u(0,t)=g_1(t),u(L,t)=g_2(t),t>0,;\quad u(x,0)=ci(x),x\in[0,L], \end{aligned} \tag{25}$$

then $G\left(u,x,t,\frac{\partial u}{\partial x}\right)=-c\,u_x(x,t)+f(u)$.

Given the spatial $h=\frac{L}{nx}$ and temporal $k=\frac{T}{nt}$ steps, we define the nodes $x_i=0+ih, i=0,1,2,\dots,nx-1,nx$ and $t_j=0+jk, j=0,1,\dots,nt-1,nt$.

Now, applying Crank Nicolson's method with the (24) scheme, problem (25) is discretized as

$$u_{i,j+1}=u_{i,j}+\frac{k}{2}\left(\frac{-c\left(u_{i+1,j+1}-u_{i-1,j+1}+u_{i+1,j}-u_{i-1,j}\right)}{2h}+f(u_{i,j+1})+f(u_{i,j})\right), \tag{26}$$

where $\quad i=1,\dots,nx-1,\ j=1,\dots,nt-1.$

If $c=1,\ k=h$, we will have

$$u_{i,j+1}=u_{i,j}+\frac{u_{i-1,j+1}-u_{i+1,j+1}+u_{i-1,j}-u_{i+1,j}}{4}+\frac{h}{2}f\left(u_{i,j+1}\right)+\frac{h}{2}f\left(u_{i,j}\right),$$

so,

$$4u_{i,j+1}=4u_{i,j}+u_{i-1,j+1}-u_{i+1,j+1}+u_{i-1,j}-u_{i+1,j}+2hf\left(u_{i,j+1}\right)+2hf\left(u_{i,j}\right),$$

and, finally, when clearing the three values still to be calculated, which are those of the instant $j+1$ in (26), and reorganizing, we obtain

$$-u_{i-1,j+1}+4u_{i,j+1}-2hf\left(u_{i,j+1}\right)+u_{i+1,j+1}=u_{i-1,j}+4u_{i,j}+2hf\left(u_{i,j}\right)-u_{i+1,j}. \tag{27}$$

3.3. Numerical resolution using Crank–Nicolson and iterative schemes

The nonlinear PDE model that we consider to perform all the numerical tests is the nonlinear transport equation (14):

$$u_t+u_x=-2u^2,$$

whose boundary conditions are $u(0,t)=\frac{1}{1+t},\ u(1,t)=\frac{1}{2+t}$. for all $t\ge 0$, together with the initial condition as: $u(x,0)=\frac{1}{1+x}$, for $0\le x\le 1$.

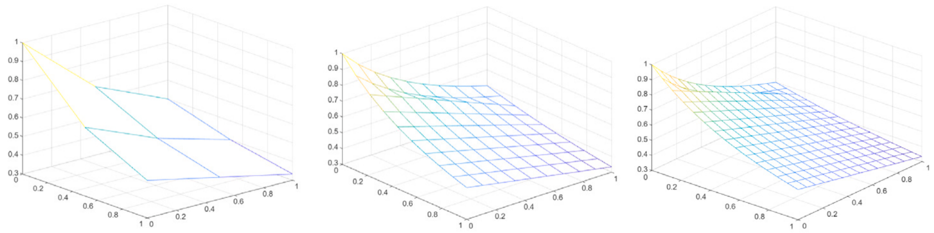

(a) 3×3 (b) 10×10 (c) 15×15

Fig. 5. Numerical approximation of the solution $u_t + u_x = -2u^2$ with the Crank–Nicolson method and optimal schemes.

In the nonlinear transport equation, $f(u) = -2u^2$. Then, applying the Crank–Nicolson type method, from the nonlinear system (27), we have

$$-u_{i-1,j+1} + 4u_{i,j+1} + 4h\,(u_{i,j+1})^2 + u_{i+1,j+1} = u_{i-1,j} + 4u_{i,j} - 4h(u_{i,j})^2 - u_{i+1,j}, \tag{28}$$

which is nonlinear, where the indices $i = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, n$ and $h = k = 1/n$.

To approximate numerically $u(x,t)$, we form as many systems of nonlinear equations as the number of subintervals in the time variable, and therefore we use iterative methods to solve these nonlinear systems.

In each case, we take as initial estimate, for each instant, a vector with values between the boundary conditions and the approximation of the solution at the previous instant, then we solve the nonlinear system (28) with optimal scheme KLAM4S$_\lambda$ for vectorial problems. We use $\lambda = -5$ which is one of the methods with the best stability conditions, based on the analysis performed in the scalar case [13].

Then, we solve the same nonlinear systems using Newton's method, and compare these results to determine whether high convergence order techniques offer a substantial improvement in approximating the solution of these problems.

The maximum number of iterations considered is 50 and the stopping criterion is $\|x^{(k+1)} - x^{(k)}\| < 10^{-100}$ or $\|F(x^{(k+1)})\| < 10^{-100}$. Each calculation is performed using Matlab R2022b with variable precision arithmetic with a 200-digits mantissa to minimize rounding errors.

In Tables 4, we consider the number of iterations (Iter), the error between two successive iterations ($\|x^{(k+1)} - x^{(k)}\|$), the residual error ($\|F(x^{(k+1)})\|$), the computing time (Time-CPU or Time) in seconds, the total effort (Effort) in each of the n systems and finally the relative true error (EVRE), that is $\frac{\|u_{i,n}-u(x,1)\|}{\|u(x,1)\|}$, comparing the obtained solution with the analytical solution at the nodes.

The robustness of our new schemes is evident from Tables 4 and Fig. 5. We obtain the behavior of our method for systems, taking various values of h and k, with systems of size $n \times n$, with $n = 3$, $n = 10$ and $n = 15$. The true relative error (EVRE) is at the level of thousandths and hundredths. Our methods applied to systems perform much better than N2S. This is because the computational cost, as demonstrated in [14], outperforms all iterative schemes for systems known so far.

4. New strategy: Crank–Nicolson and new JARM decoupling

Definition 4. Given two nonlinear systems of equations $S_1 : F(x) = 0$ and $S_2 : G(x) = 0$, we say that they are 'quasi-equivalent' if when solving them numerically, even by different methods, starting from the same initial estimate, we obtain the same solution, i.e. $\lim_{n\to\infty} \|F(x_n) - G(x_n)\| = 0$.

Solving the nonlinear system resulting from applying the Crank–Nicolson method requires the use of iterative schemes that can be very expensive, in cases where the system is more complex or larger. So it is reasonable to design simpler quasi-equivalent systems that are simpler to solve, allowing us to approximate the solution.

Definition 5. The nonlinear system (28) can be linearized, according to the strategy proposed by Langtangen in [19], by approximating the quadratic term, $(u_{i,j+1})^2$, with the product $u_{i,j}u_{i,j+1}$, where $u_{i,j}$ is known and $u_{i,j+1}$ the element to be known. We call this strategy the 'Langtangen linearization'. In this way, we transform the problem into a quasi-equivalent linear system that we solve with a direct method.

In this manuscript, we present a new approach, starting from a similar idea:

Definition 6. If in each system of (28), for time t_{j+1} we approximate the values $u_{i-1,j+1}$ and $u_{i+1,j+1}$ by $u_{i-1,j}$ and $u_{i+1,j}$, respectively. We obtain a decoupled system, which we assume as quasi-equivalent of size n that we can solve individually, applying a method for nonlinear equations. We call this new approach 'JARM decoupling'.

Next we observe that the Crank–Nicolson scheme with JARM decoupling is less expensive than the Crank–Nicolson scheme with Langtangen linearization if each nonlinear equation in the first scheme converges with 10 iterations and the system has size $n > 8$. In this analysis, we consider 10 iterations because in numerical tests of methods for equations, convergence occurs in a smaller number of iterations.

Table 4
Comparison of iterative schemes applied to the nonlinear transport equation with the Crank–Nicolson method with different mesh sizes.

Method	Iter	$\|x^{(k+1)} - x^{(k)}\|$	$\|F(x^{(k+1)})\|$	Time	Effort	EVRE
			3×3			
N2S	6	1.876×10^{-66}	7.039×10^{-132}	0.2492	174	0.006667
KLAM4S$_{-5}$	3	6.669×10^{-30}	2.176×10^{-117}	0.2628	123	0.006667
			10×10			
N2S	6	5.805×10^{-70}	1.041×10^{-139}	0.5902	3240	0.015035
KLAM4S$_{-5}$	4	2.658×10^{-62}	4.895×10^{-187}	0.7498	2600	0.015035
			15×15			
N2S	6	6.563×10^{-74}	7.772×10^{-139}	0.8882	9510	0.018754
KLAM4S$_{-5}$	4	7.102×10^{-64}	2.769×10^{-192}	1.0856	7300	0.018754

The cost of solving a linear system of size n with LU factorization is $\frac{1}{3}(n^3 - n) + n^2$. Also, it requires solving each linear system by iteration in Newton's method, which needs, in the scalar case, two evaluations and a quotient, then, with 10 iterations of the n nonlinear equations, we will have a maximum cost of $30n$. It can be checked that

$$\frac{1}{3}(n^3 - n) + n^2 > 30n \Rightarrow n > 8.$$

Then, the cost of the Crank–Nicolson scheme with JARM decoupling is lower. Next we solve the model equation and applying the Crank–Nicolson with Langtangen linearization.

4.1. *Numerical tests applying Crank–Nicolson with Langtangen linearization*

From the system (28) and with Langtangen's linearization we obtain the linear system

$$-u_{i-1,j+1} + 4u_{i,j+1} + 4h\,(u_{i,j})\,(u_{i,j+1}) + u_{i+1,j+1} = u_{i-1,j} + 4u_{i,j} - 4h(u_{i,j})^2 - u_{i+1,j}, \tag{29}$$

where $i = 1, 2, \dots, n$ and $j = 1, 2, 3, \dots, n$ which in tridiagonal matrix form is $A\,u^{(j+1)} = B$, where

$$A = \begin{bmatrix} r_{1,j} & 1 & & & & & \\ -1 & r_{2,j} & 1 & & & \mathbf{O} & \\ & & \ddots & & & & \\ & & -1 & r_{i,j} & 1 & & \\ & & & & \ddots & & \\ & \mathbf{O} & & & -1 & r_{n-1,j} & 1 \\ & & & & & -1 & r_{n,j} \end{bmatrix}, \quad u^{(j+1)} = \begin{bmatrix} u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ u_{i,j+1} \\ \vdots \\ u_{n-1,j+1} \\ u_{n,j+1} \end{bmatrix},$$
$$B = \begin{bmatrix} u_{0,j+1} + u_{0,j} + \bar{r}_{1,j} - u_{2,j} \\ u_{1,j} + \bar{r}_{2,j} - u_{3,j} \\ \vdots \\ u_{k-1,j} + \bar{r}_{i,j} - u_{i+1,j} \\ \vdots \\ u_{n-2,j} + \bar{r}_{n-1,j} - u_{n,j} \\ u_{n-1,j} + \bar{r}_{n,j} - u_{n+1,j} - u_{n+1,j+1} \end{bmatrix}, \tag{30}$$

where $r_{i,j} = 4(1 + h\,u_{i,j})$ and $\bar{r}_{k,j} = 4(1 - h\,u_{i,j})u_{i,j}$, that we solve by Crout's direct method.

As you can see in Fig. 6, linearization works best when taking small systems. In this case the EVRE is smaller. However, it is less accurate with smaller step sizes, because the solution presents greater oscillation as n increases.

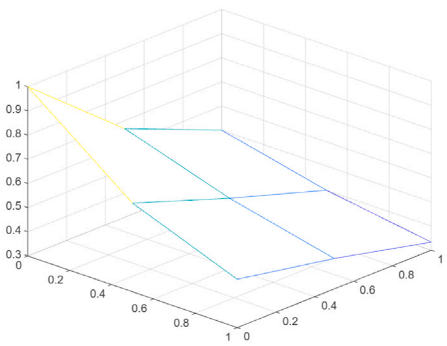
Fig. 7 shows Crank–Nicolson + KLAM4S$_0$ with lower computational effort, higher accuracy and high precision. By applying the new optimal methods for systems, with a single iteration, we have better approximation to the true value with lower computational cost. It is worth noting that applying the new methods, we obtain a fast error adjustment giving rise to a smooth solution.

4.2. *Crank–Nicolson with new JARM decoupling*

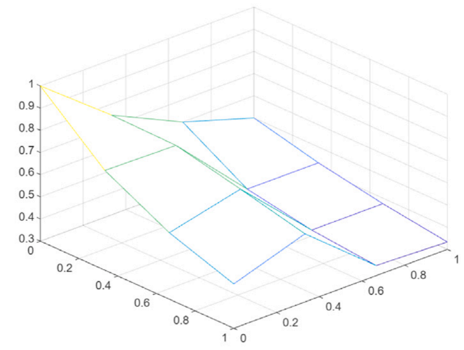
Based on Lagtangen's idea in [19] we propose a system that we assume as quasi-equivalent to (28), but significantly reduces the computational cost when compared to any strategy known so far, with better performance. We apply to the system (28) the JARM decoupling (Definition 6). In this way, we have for each spatial node a nonlinear equation with one unknown $u_{i,j+1}$,

$$2h\,(u_{i,j+1})^2 + 2u_{i,j+1} = u_{i-1,j} + 2u_{i,j} - 2h(u_{i,j})^2 - u_{i+1,j}, \tag{31}$$

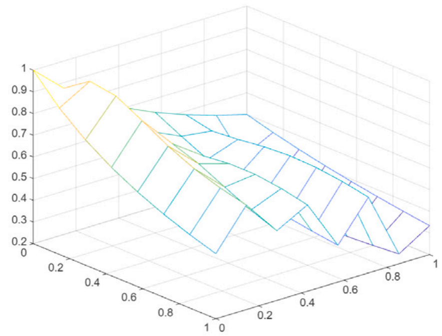
$i = 1, 2, 3, \dots, n$, $j = 1, 2, \dots, n$, that we can solve at each level by applying an iterative method for the scalar case, as Newton, KLAM$_0$ or KLAM$_{-5}$.



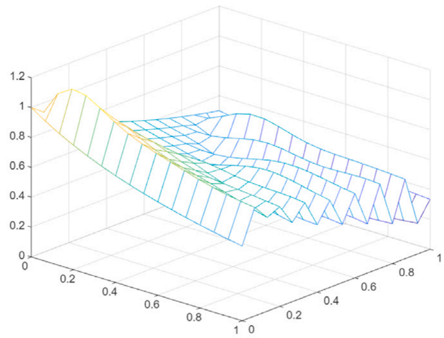
(a) $n = 3$ (EVRE=0.0103, Time=0.06, Eff.=17)



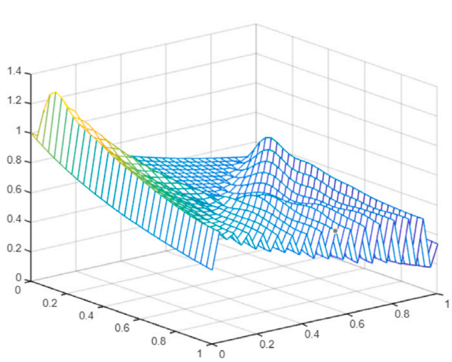
(b) $n = 4$ (EVRE=0.0774, Time=0.11, Eff.=36)



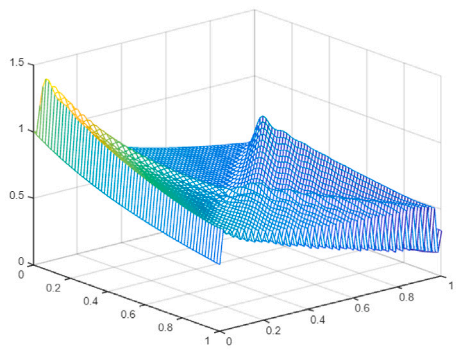
(c) $n = 8$ (EVRE=0.1524, Time=0.49, Eff.=232)



(d) $n = 16$ (EVRE=0.2462, Time=2.07, Eff.=1,616)



(e) $n = 32$ (EVRE=0.3700, Time=7.3, Eff.=11,936)



(f) $n = 64$ (EVRE=0.5384, Time=28.87, Eff.=91,456)

Fig. 6. Langtangen linearization + Crout for discretizations in regular enclosures.

However, it is possible to be more demanding, applying a Gauss–Seidel type strategy, updating the values just calculated at each position, that is $u_{i-1,j+1}$ found in the previous equation, then instead of working with the system (31), we can work with the system

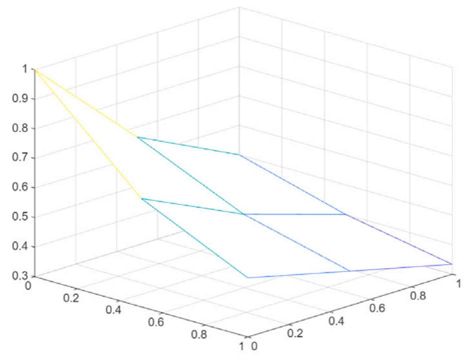
$$4u_{i,j+1} + 4h\,(u_{i,j+1})^2 = u_{i-1,j+1} + u_{i-1,j} + 4u_{i,j} - 4h(u_{i,j})^2 - 2u_{i+1,j} \tag{32}$$

where $i = 1, 2, 3, \dots, n$ and $j = 1, 2, \dots, n$.

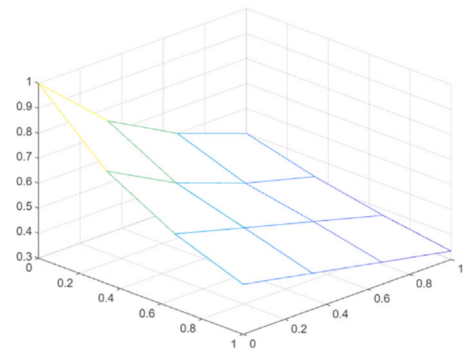
As can be seen in Table 5, KLAM_0 and KLAM_{-5} are very competitive, and even, they use less time and less effort, to reach the tolerance. Our methods have the best performance.

The results in Tables 5 and Fig. 8 show the remarkable superiority of the new decoupling approach over Langtangen linearization, with respect to the criteria computational effort, relative true error and Execution Time.

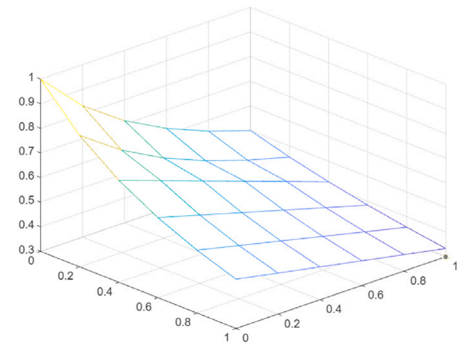
In Tables 4, 5, 6, 7 and 8 we present the results after 50 runs with each method, so that the CPU-Time indicated in each case is the average obtained.



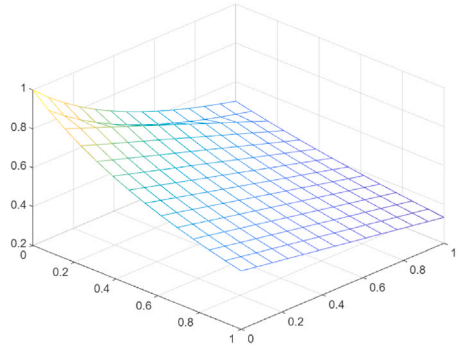
(a) $n = 3$ (EVRE=0.00667, Time=0.1000, Eff.=41)



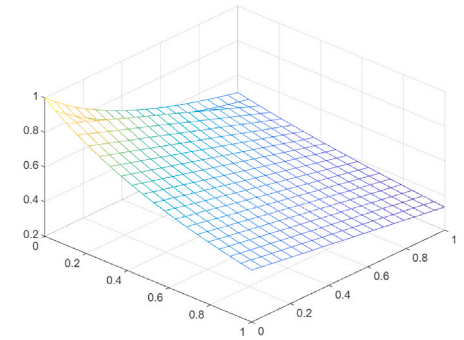
(b) $n = 4$ (EVRE=0.008567, Time=0.15, Eff.=76)



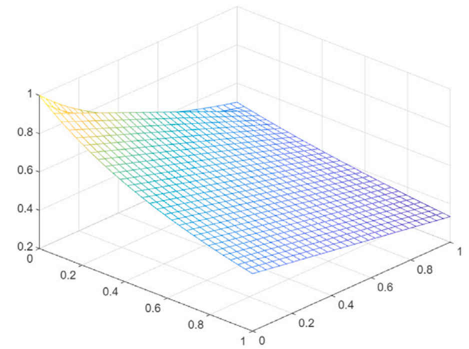
(c) $n = 6$ (EVRE=0.011187, Time=0.2000, Eff.=190)



(d) $n = 14$ (EVRE=0.018071, Time=0.45, Eff.=1526)



(e) $n = 20$ (EVRE=0.021848, Time=0.69, Eff.=3900)



(f) $n = 30$ (EVRE=0.026993, Time=0.79, Eff.=11750)

Fig. 7. Crank–Nicolson and implicit/implicit with KLAM4S$_{-5}$ iteration converging in one iteration: high accuracy and low cost.

Fig. 9 details information about the performance of the Crank–Nicolson scheme with decoupling on systems of sizes 3, 4, 8, 16, 32 and 64, namely, true relative error (EVRE), execution time and effort. Then it is appreciated that this technique shows excellent results: high stability, precision, accuracy and low computational cost.

In Tables 4–5, it can see a comparison of computational cost (sum of functional and product/quotient evaluations) applying iterative methods for systems is almost unnecessary: it is cheaper to solve a decoupled nonlinear system equation by equation, than to solve a coupled system of the same size.

5. Conclusions

In this manuscript, we apply optimal iterative schemes to solve the nonlinear transport equation. The numerical characteristics method works very well. The system clearly marks that the solution is a cylinder, because the curves of x with respect to t are parallel lines, however it is a starting point. We continue developing and deepening this path, analyzing different cases.

Table 5
Comparison of iterative schemes applied to the nonlinear transport equation with the Crank–Nicolson method with JARM decoupling and different mesh sizes.

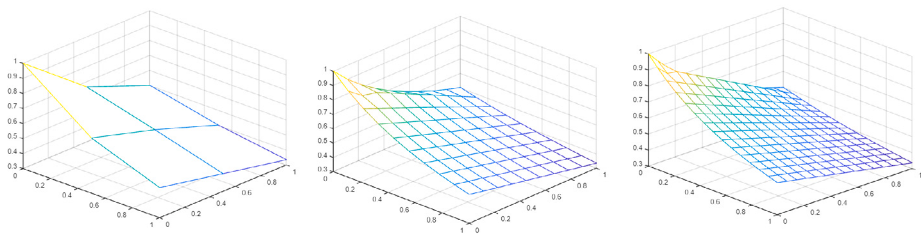
Method	Iter	$\|x^{(k+1)} - x^{(k)}\|$	$\|F(x^{(k+1)})\|$	Time	Effort	EVRE
			3 × 3			
N2	6	5.059 $\times 10^{-77}$	2.559 $\times 10^{-153}$	0.085600	36	0.006667
$KLAM_0$	3	4.113 $\times 10^{-35}$	1.498 $\times 10^{-138}$	0.050000	27	0.006667
$KLAM_{-5}$	3	1.400 $\times 10^{-56}$	0	0.054600	27	0.006667
			10 × 10			
N2	6	1.317 $\times 10^{-82}$	3.854 $\times 10^{-165}$	0.157600	120	0.006887
$KLAM_0$	3	1.133 $\times 10^{-37}$	1.612 $\times 10^{-150}$	0.126600	90	0.006887
$KLAM_{-5}$	3	7.035 $\times 10^{-61}$	0	0.130800	90	0.006887
			15 × 15			
N2	6	1.691 $\times 10^{-90}$	4.087$\times 10^{-181}$	0.233200	180	0.006920
$KLAM_0$	3	1.584 $\times 10^{-41}$	1.811 $\times 10^{-166}$	0.198400	135	0.006920
$KLAM_{-5}$	3	5.351 $\times 10^{-67}$	0	0.201600	135	0.006920

Table 6
Relative true error comparison.

Method, n	3	4	8	16	32	64
Linearization	0.010370	0.010370	0.152400	0.246200	0.370000	0.538400
Decoupling	0.006670	0.006803	0.006920	0.006944	0.006930	0.006944

Table 7
Comparison of computational cost (linearization vs. decoupling).

Method, n	3	4	8	16	32	64
Linearization	17	21	232	1,616	11,936	91,456
Decoupling	21	28	56	112	224	448



(a) 3 × 3 (b) 10 × 10 (c) 15 × 15

Fig. 8. Numerical solution of $u_t + u_x = -2u^2$ with the Crank–Nicolson method and JARM decoupling with the indicated meshes.

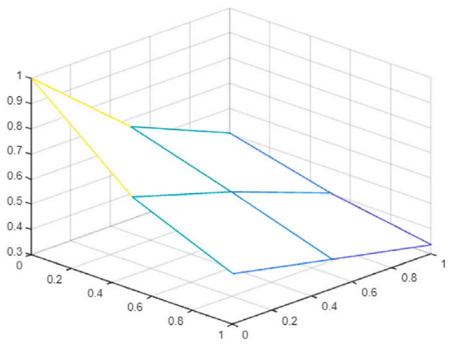
Table 8
Time comparison (linearization vs. decoupling).

Method, n	3	4	8	16	32	64
Linearization	0.06	0.11	0.15	0.25	7.30	28.87
Decoupling	0.04	0.04	0.10	0.23	0.87	2.70

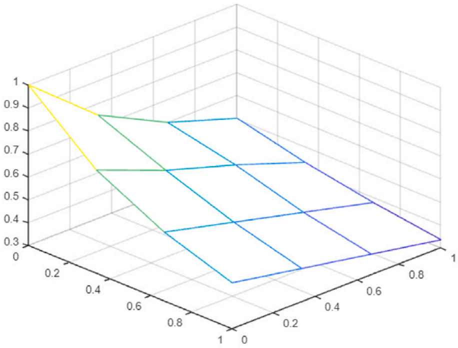
Then, when discretizing with the unconditionally stable Crank–Nicolson method, and applying our optimal methods, we corroborate that we outperform Newton's method in computational cost, time, approximate error and residual error and order of convergence.

The linearization proposed by Langtangen significantly reduces the computational cost, but as evidenced by the numerical behavior, it sacrifices the stability of the Crank–Nicolson method, although it maintains a true absolute relative error of the order of tenths, for different system sizes.

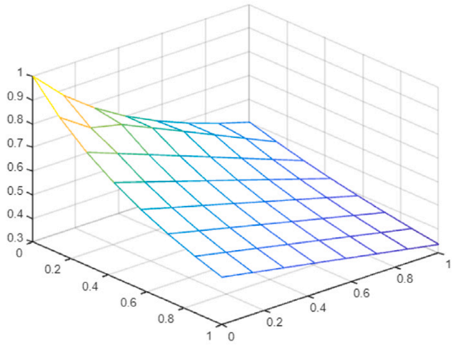
The new approach, JARM decoupling, is an important contribution of this work, because it preserves nonlinearity. Furthermore, it simplifies the computational cost and maintains stability and convergence. The solution it provides us is better than all the other proposals, with a true relative error that remains in the order of thousandths, for all the sizes studied.



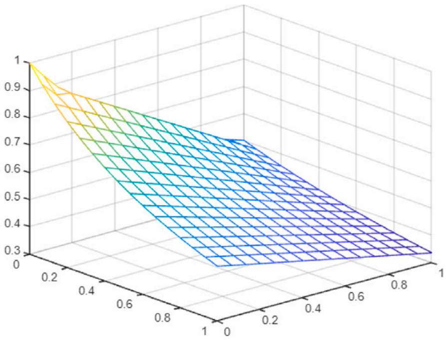
(a) $n = 3$ (EVRE=0.00667, Time=0.04, Eff.=21)



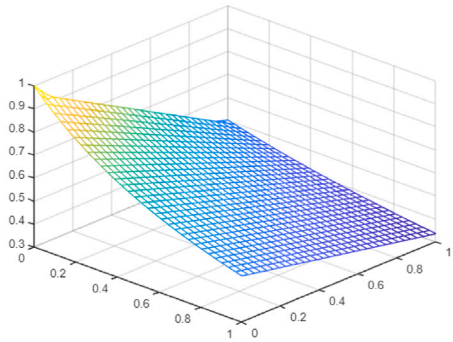
(b) $n = 4$ (EVRE=0.006803, Time=0.04, Eff.=28)



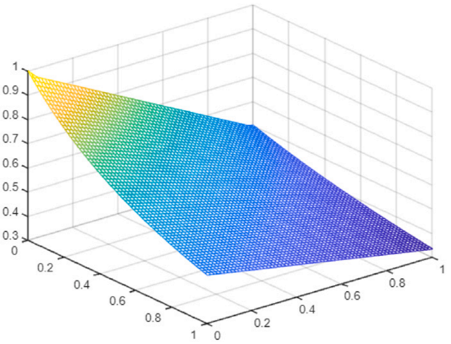
(c) $n = 8$ (EVRE=0.006920, Time=0.10, Eff.=56)



(d) $n = 16$ (EVRE=0.006944, Time=0.23, Eff.=112)



(e) $n = 32$ (EVRE=0.006939, Time=0.87, Eff.=224)



(f) $n = 64$ (EVRE=0.006944, Time=2.7, Eff.=448)

Fig. 9. Crank–Nicolson results with JARM decoupling + $KLAM_0$ in one iteration: improvement in accuracy and effort over known schemes.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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