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Comparison between Newton's and Picard's methods for the nonlinear heat transfer modeling

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Abstract. The nonlinear heat equation has large applications in several areas, such as Engineering, Biology, and Medicine. In this paper, we compare Newton's and Picard's methods to numerically solve the one-dimensional nonlinear heat equation, where the thermal conductivity depends on the temperature of the medium. First, we discretize the equation in time using the implicit Euler method, obtaining a sequence of nonlinear boundary value problems with the sweep in time performed by standard Time-Stepping method. For the spatial derivative that is also dependent on the temperature gradient, we use the Finite Difference Method. The nonlinear systems obtained are linearized using Newton's and Picard's methods. Based on the numerical tests we compare the number of iterations and the computational times to solve the systems using each of the solution methods and list their advantages and disadvantages for this type of problem.

Keywords: Nonlinear Fourier, Time-Stepping, Number of Linearizations, Computational Time.

1 Introduction

Problems involving heat transfer have been studied in several application areas, especially those beginning with Fourier's Law, where heat flow is proportional to the temperature gradient.

In [1] the temperature dependence of thermal conductivity in semiconductors was solved with the Fourier equation, applying the finite difference method (FDM) and using Newton's method for linearization of the nonlinear systems. They obtained good results and the method used proved to be stable for the problem analyzed. [2] solved the Fourier equation using random thermal conductivity coefficients and used the Multigrid method to speed up convergence.

Newton's method is a typical method for solving nonlinear problems where the iterative process generates a sequence of points that at each iteration approaches the solution. The convergence is quadratic provided the choice of the initial estimate is appropriate [1]. On the other hand, Picard's method is known as the method of successive approximations, that is, it linearizes the system and then solves the resulting equations of the system. Among its main advantages are ease of implementation, maintenance of the symmetry of the system of equations, and a lower computational cost for each iteration. But such a method can have convergence problems in highly nonlinear cases, as reported by [3], The one, two, and three-dimensional finite element method involving both steady and transient states was used to solve the multidimensional saturated variable flow problem.

The solution of highly nonlinear problems was also the object of studies in [4] and [5], where they used Newton's and Picard's methods and a modification to Picard's method for Richards' equation.

[6] compared linearization methods, L-scheme, Newton's, and Modified Picard, for coupled multiphase flow and reactive transport in porous media. [7] compared such methods proposed by [6] for the one-dimensional problem of two-phase flow in a rigid porous medium, using the finite volume method for the spatial and implicit Euler for the temporal discretizations. For solving the generated linear systems they used the lexicographic coupled Gauss-Seidel solver, accelerating convergence with the Multigrid method and W-cycle.

In this work we discretize the one-dimensional nonlinear heat equation using the finite difference method (FDM) for the spatial and implicit Euler for the temporal discretizations. And for the linearizations, we use Newton's and Picard's methods. After that, we perform a study to indicate the advantages and disadvantages of each of the methods.

2 Mathematical and Numerical model

For [8], heat transfer is the transit of energy due to a temperature difference in the medium, and when this difference exists, one body gives off heat to the other. This heat exchange generates a rate classified as the thermal conductivity coefficient, which in general, in realistic problems, depends on the temperature itself.

Thus, the one-dimensional heat equation that will be treated in this paper, as described in [1] is

$$\rho c_p \frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(k(u)\frac{\partial u}{\partial x}\right) + f = 0, \tag{1}$$

in the spatial interval $x \in [a, b]$ and time $t \in (0, t_f]$, where ρ is the density, c_p is the pressurization heat capacity, and k is the thermal conductivity. Note that ρ and c_p are constant values, but k depends on the temperature u.

The boundary and initial conditions are given, respectively by:

$$u(a,t) = u_a, \quad u(b,t) = u_b, t > 0, \tag{2}$$

and

$$u(x,0) = u_0(x), x \in [a,b], \tag{3}$$

where $u(x,t)$ and $f(x,t)$ represent respectively, the temperature and the source term at position x and time t.

Rewriting the Equation (1) and using the chain rule, we have

$$\rho c_p \frac{\partial u}{\partial t} = \partial_u k(u)\left(\frac{\partial u}{\partial x}\right)^2 + k(u)\frac{\partial^2 u}{\partial x^2} + f, \tag{4}$$

where ∂_u represents the partial derivative with respect to variable u.

Analytical solutions are not always easy to find, so numerical modeling can be used. We will adopt here a uniform mesh over the spatial domain where each point $u(x_i)$ will be denoted by u_i with x_i given by

$$x_i = a + (i-1)h, \qquad i = 1, 2, ..., N, \tag{5}$$

where $h = \frac{b-a}{N-1}$ is the spacing between the nodes in the spatial mesh, with N being the number of nodes.

From Equation (4), with time step $\tau = \frac{t_f}{M}$, where M is the number of time steps, and using the implicit Euler method for time discretization, we have

$$\rho c_p \frac{u_i^{n+1} - u_i^n}{\tau} = \partial_u k_i^{n+1}\left(\frac{\partial u_i^{n+1}}{\partial x}\right)^2 + k_i^{n+1}\frac{\partial^2 u_i^{n+1}}{\partial x^2} + f_i^{n+1}, \tag{6}$$

where $n+1$ is the current time step, i denotes the position in space and k_i^{n+1} denotes $k(u_i^{n+1})$. The spatial discretization of the derivatives involved in Equation (6) will be given by the FDM, with Central Difference Scheme (CDS) of second order. Therefore, we have

$$\frac{\partial u^{n+1}}{\partial x} = \frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2h} \qquad \text{and} \qquad \frac{\partial^2 u^{n+1}}{\partial x^2} = \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{h^2}. \tag{7}$$

Substituting Equation (7) into Equation (6), we have

$$\rho c_p \left(\frac{u_i^{n+1} - u_i^n}{\tau} \right) = \partial_u k_i^{n+1} \left(\frac{u_{i-1}^{n+1} - u_{i+1}^{n+1}}{2h} \right)^2 + k_i^{n+1} \left(\frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{h^2} \right) + f_i^{n+1}. \tag{8}$$

3 Linearization Methods

The nonlinearity of the heat equation can be handled using several methods. In this work, we use Newton's and Picard's linearization methods.

3.1 Newton's Method

Newton's iteration scheme can be thought of as a parallel chord method with an update, that is, we use the tangent of the function as the iteration matrix and update this slope matrix at each iteration. Newton's scheme has quadratic convergence, this is secured as long as the initial estimate is close to the solution [9]. For the implementation of Newton's method [1] we will introduce a column vector $\mathbf{G}^{n+1} = [G_1^{n+1}, G_2^{n+1}, ..., G_N^{n+1}]^T$ with the components:

$$G_1^{n+1} = u_1^{n+1} - u_a, \quad G_N^{n+1} = u_N^{n+1} - u_b, \tag{9}$$

$$G_i^{n+1} = \rho c_p \left(\frac{u_i^{n+1} - u_i^n}{\tau} \right) - \partial_u k_i^{n+1} \left(\frac{u_{i-1}^{n+1} - u_{i+1}^{n+1}}{2h} \right)^2 - k_i^{n+1} \left(\frac{u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}}{h^2} \right) - f_i^{n+1}, \tag{10}$$

for $i = 2, 3, \ldots, N-1$.

The system of nonlinear equations given in Equation (10) and the boundary conditions, Equation (9), are written as one equation

$$\mathbf{G}^{n+1}(\mathbf{u}^{n+1}) = 0, \tag{11}$$

where

$$\mathbf{u}^{n+1} = [u_1^{n+1}, u_2^{n+1}, ..., u_N^{n+1}]^T. \tag{12}$$

Introducing the iterative process by $\mathbf{u}^{n+1,\nu+1}$, where $\nu + 1$ is current iteration, and starting by some initial guess $\mathbf{u}^{n+1,0}$, the nonlinear system Equation (11) can be solved by the

$$\mathbf{u}^{n+1,\nu+1} = \mathbf{u}^{n+1,\nu} - \left(\mathbf{L}^{n+1,\nu} \right)^{-1} \mathbf{G}^{n+1}(\mathbf{u}^{n+1,\nu}), \quad \nu = 0, 1, 2, ... \tag{13}$$

where $\mathbf{L}^{n+1,\nu}$ is the Jacobian matrix of $\mathbf{G}^{n+1}$ with respect to $\mathbf{u}^{n+1,\nu}$. So:

$$\mathbf{L}^{n+1,\nu} = \frac{\partial \mathbf{G}^{n+1}}{\partial \mathbf{u}^{n+1}} \left(\mathbf{u}^{n+1,\nu} \right). \tag{14}$$

3.2 Picard Method

It is possible to derive a simpler method from the fixed point problem, which is called successive replacement or Picard, which has among its characteristics the ease of implementation, conservation of the symmetry of the system of equations and lower computational cost for each iteration [10], but may present convergence problems in highly nonlinear problems [3]. According to [9], the Picard iterative technique presents itself as a robust fixed-point method that is globally convergent with a linear or sublinear rate.

Picard's method is usually used in the initial iterations of a general strategy for solving systems of nonlinear equations, to enable the convergence of faster methods, such as Newton's method, discussed earlier. This is because the method has a large radius of convergence, but has a low rate of convergence, so it is interesting to combine the method with faster methods that have a low radius of convergence. [3] [4].

Linearization using Picard's method, is computationally classified by [3] [5] [11][12] as simple to implement, and computationally cheaper. Still, it is not as accurate because the approximation is made by a linear and a nonlinear part, [7], and where is used the Gaussian elimination or Gauss-Seidel methods as solvers.

Isolating the variable u_i^{n+1} at Equation (8), and generating the iterative process, we have Picard's method given by

$$u_i^{n+1,\nu+1} = \frac{u_i^n}{A} + \frac{A\chi k_0}{4h^2}\partial_u k_i^{n+1,\nu}\left(u_{i+1}^{n+1,\nu} - u_{i-1}^{n+1,\nu+1}\right)^2 + \frac{Ak_0}{h^2}k_i^{n+1,\nu}\left(u_{i+1}^{n+1,\nu} - 2u_i^{n+1,\nu} + u_{i-1}^{n+1,\nu+1}\right) + Af_i^{n+1}, \quad (15)$$

where $A = \frac{\tau}{\rho c_p}$, $\nu + 1$ is the current iteration and u_i^n represents the converged solution at the previous time step.

Note that when we have the positions in space i and $i-1$, we use the results of iteration ν, while at position $i+1$, we use $\nu + 1$.

4 Results

This work aimed at comparing Newton's and Picard's methods for the model described in [1], in other words, we consider a thin homogeneous rod along the x axis in the interval $x \in [1, 3]$, with no heat sources and no radiation. The density ρ and the heat capacity c_p are unit constants and the thermal conductivity is given by

$$k(u) = \kappa_0 e^{(\chi u)}, \quad (16)$$

where κ_0 and χ are physical constants associated with greater or lesser nonlinearity. Consider the boundary conditions expressed by

$$u(1, t) = 2, \quad u(3, t) = 1, t > 0, \quad (17)$$

and the initial condition given by

$$u(x, 0) = 2 - \frac{x-1}{2} + (x-1)(x-3), \quad x \in [1, 3]. \quad (18)$$

The numerical simulations were performed with Matlab software, version R2015a. The verification of the code for Picard's method was done by comparing it with the results presented by [1] for Newton's method, and tested for the points $M = N = 2^p + 1$, with $p \in \mathbb{Z}$ ranging from 5 to 12. We will present the results for the case $p = 12$, since the other cases presented similar results. In Equations (10) (15), respectively, for Newton's and Picard's methods, $\partial_u(k_i^{n+1,\nu}) = \chi\kappa_0\, e^{(u_i^{n+1,\nu})}$. We will use the variation for κ_0 being the values $10^{-3}, 10^{-2}$ and 10^{-1}; and χ being the values $-9.0, -7.0, -5.0, -3.0$ and -1.0. We use as a stopping criterion for solving the system of linear equations resulting from the linearization process, the l_2 norm of the difference between the solutions of two consecutive iterations, with a tolerance of 10^{-8}, according to [1].

In Table 1, the comparison between the methods was made by the number of mean linearizations at each time step, until the tolerance was reached. We can observe that with Newton's method, the number of linearizations

remains roughly stable for any value of κ_0 and χ, while with Picard's method this number increases with increasing κ_0 and χ. This behavior can be confirmed by measuring the computational time (t_{CPU}) required to obtain the numerical solution in both methods, as shown in Figure 1.

Table 1. Several mean linearizations of Newton's and Picard's methods considering a mesh with N = M = 4097 points, for various values of κ_0 and χ.

κ_0	10^{-3}			10^{-2}			10^{-1}		
χ	-9.0	-5.0	-1.0	-9.0	-5.0	-1.0	-9.0	-5.0	-1.0
Newton's	2.0	2.0	2.0	2.0	2.0	2.0	2.0	2.1	2.6
Picard's	3.0	7.0	36.9	10.7	51.1	315.8	72.7	332.6	1994.8

We can notice that Picard's method, Figure 1, has lower t_{CPU} in most cases compared to Newton's method, despite performing a larger number of linearizations. Notice the cases that $\kappa_0 = 10^{-1}$ and $\chi = -3.0$ or $\chi = -1.0$, the Newton's method is more efficient than Picard's method. This fact was also observed by [3] [6], where the authors showed that Picard's method is more efficient when you have low nonlinearities.

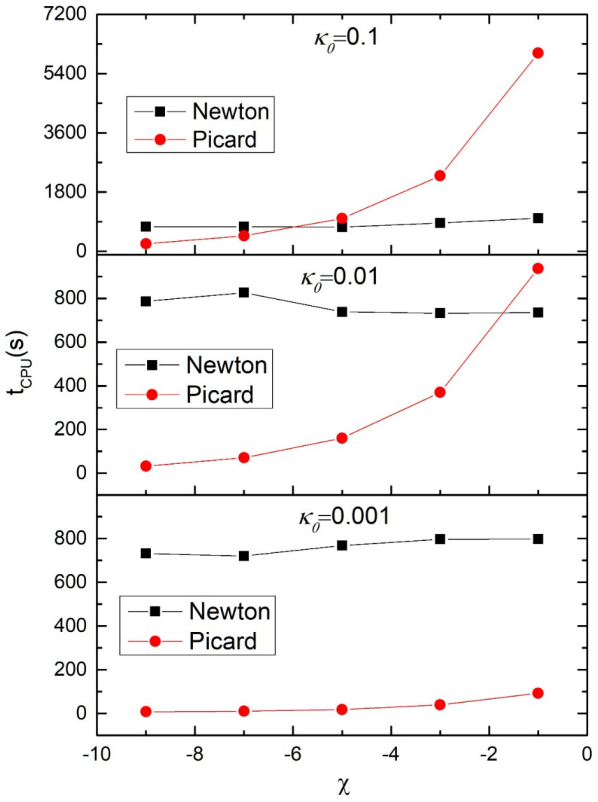

Figure 1. Computational time used by Newton's and Picard's methods, considering a mesh with N = M = 4097 points, for various values of κ_0 and χ.

5 Conclusions

In this work, the one-dimensional heat transfer equation with thermal conductivity depending on the temperature itself was considered. This equation was solved numerically using the implicit Euler Method for the temporal discretization and the FDM with CDS-type approximation for the spatial discretization. Newton's and Picard's linearizations were compared. The results showed the efficiency of Picard's compared to Newton's methods when dealing with problems with a low degree of nonlinearity. In the information collected, we observe that the number

of linearizations for Newton's method remains roughly constant and much lower than Picard's method, but when computational time is taken into account, Newton's method loses its efficiency.

References

[1] S. M. Filipov and I. Faragó. Implicit Euler time discretization and FDM with Newton method in nonlinear heat transfer modeling, 2018.
[2] P. Kumar, C. Rodrigo, F. Gaspar, and C. Oosterlee. On local Fourier analysis of multigrid methods for PDEs with jumping and random coefficients. *SIAM Journal on Scientific Computing*, vol. 41, pp. A1385–A1413, 2019.
[3] C. Paniconi, A. A. Aldama, and E. F. Wood. Numerical evaluation of iterative and noniterative methods for the solution of the nonlinear Richards equation. *Water Resources Research*, vol. 27, n. 6, pp. 1147–1163, 1991.
[4] M. Celia, E. Bouloutas, and R. Zarba. A general mass-conservative numerical-solution for the unsaturated flow equation. *Water Resources Research - WATER RESOUR RES*, vol. 26, pp. 1483–1496, 1990.
[5] R. L. Zarba. *A numerical investigation of unsaturated flow*. PhD thesis, Massachusetts Institute of Technology, 1988.
[6] D. Illiano, I. Pop, and F. Radu. Iterative schemes for surfactant transport in porous media. *Computational Geosciences*, vol. 25, pp. 1–18, 2021.
[7] M. Oliveira, M. Pinto, C. Rodrigo, F. Gaspar, and S. Franco. L-scheme and modified Picard with multigrid method for a 1D two-phase problem in rigid porous media with analytical solution, 2021.
[8] F. Incropera. *Fundamentals of heat and mass transfer*. LTC, 2008.
[9] G. Golub and J. Ortega. *Scientific Computing and Differential Equations: An Introduction to Numerical Methods*. ACADEMIC PressINC, 1991.
[10] R. Quevedo. Numerical implementation for 3D transient flow analysis in dams (*in portuguese*). *Pontifícia Universidade Católica do Rio de Janeiro PUC-RJ, Master in Civil Engineering*, 2008.
[11] W. L. Briggs, V. E. Henson, and S. F. McCormick. *A Multigrid Tutorial*. SIAM, Philadelphia, 2nd edition, 2000.
[12] K. Huang, B. Mohanty, F. Leij, and M. T. v. Genuchten. Solution of the nonlinear transport equation using modified picard iteration. *Advances in Water Resources*, vol. 21, n. 3, pp. 237–249, 1996.