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NUMERICAL INVESTIGATION OF THE POINT-IMPLICIT SCHEME FOR THE 1-D HEAT EQUATION.

Vishal Jadhav
Department of Aerospace Engineering, IIT Madras
Student
Email: visujadhav@gmail.com

Dr. Santanu Ghosh
Department of Aerospace Engineering , IIT Madras
Asst. Professor
Email: sghosh1@iitm.ac.in

ABSTRACT

A point-implicit scheme has been used to solve the 1-D heat equation with and without source terms with Dirichlet boundary conditions. The point-implicit scheme is formulated by approximating the implicit operator, such that resulting finite difference equation does not involve the inversion of matrix at each iteration. The formulation is unconditionally stable for the Heat equation without source and with a negative source (sink), but shows conditional stability when (positive) source terms are included. Results compared with the Euler explicit method indicate that the point implicit schemes require 40% less time steps to arrive at the steady state solution. However, for computations with same value of $r = \alpha\frac{\Delta t}{\Delta x^2}$, explicit scheme requires less number of time steps to reach steady state. Hence computation cost is saved compared to a fully implicit scheme.

***Keywords*:** point-implicit, explicit, heat equation

NOMENCLATURE

Δt time step, s
Δx grid spacing, m
r $(= \alpha\Delta t/\Delta x^2)$.
α thermal diffusivity.
a source coefficient
δ $(=a\Delta t)$

INTRODUCTION

In development of computer codes for solving partial differential equations of the hyperbolic or parabolic type, which require (or are suitable for) a time-marching scheme for obtaining the solution, the choice of the time integration method used is an interesting dilemma. The general choices are the explicit formulation, which results in clean codes with low per-time-step cost, or the implicit formulation, which results in bulkier code with high cost per iteration but allows for use of arbitrarily high time steps in most cases. The time step restriction for the explicit methods stems from satisfying the CFL (Courant-Friedrichs-Lewy) condition in wave propagation problems, whereas fully implicit methods are generally unconditionally stable, implying that a time step of the user's choice can be used without worrying about solution divergence. If obtaining a steady-state solution is the objective, then typically implicit method is the winner In this paper, a point implicit scheme for computing the steady state numerical solution of heat equation [1, 2] with and without a source term is formulated using a finite difference method. Previous examples of the use of point-implicit schemes for the Navier-Stokes equations includes the work by Gnoffo [3] and Kadigolu et al [4]. Results are compared with the simple explicit scheme. The general problem statement can be mathematically expressed as follows:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + au \tag{1}$$

Here u is the temperature, α is thermal diffusivity, and a is source coefficient with dimensions of t^{-1}. For heat equation without source, a will be zero. This equation is solved numerically subjected to following condition:

Initial Condition : $u(x,0) = 0 \qquad 0 < x < 1$
Boundary Condition : $u(0,t) = 1$, $u(1,t) = 0$

Steady state solution is determined using explicit and point implicit time marching techniques, and the effects of grid spacing Δx, r, and a non-dimensional source strength δ, on number of iterations required to reach a converged solution, which is used as a comparison criteria, are studied.

METHODOLOGY

Consider the Euler or the Navier-Stokes Equations written in conservation form,

$$\frac{\partial \vec{U}}{\partial t} + \vec{\nabla}.\vec{F} = 0 \tag{2}$$

where $\vec{U}$ is the vector of conservative variables and $\vec{F}$ is the vector of fluxes. If we consider a scalar equation in similar form, then using a finite difference method, the differential equation solved at each node $'i'$ is given by

$$\frac{\partial U_i}{\partial t} + \left(\vec{\nabla}.\vec{F}\right)_i = 0 \tag{3}$$

The residual at node $'i'$ in that case is give by,

$$Res_i \equiv \frac{dU_i}{dt} \tag{4}$$

In practice, residual at a node is calculated using the divergence term in Eqn. 2. The definition for the global residual or L_2 norm of residual can then be given as [5],

$$||Res||_2 \equiv \sqrt{\frac{1}{N}\sum_{i=1}^{N} Res_i^2} \tag{5}$$

where N is the total number of nodes. For any solution variable s, the L_2 error is similarly defined as [5]

$$Error_{L_2} = \left[\frac{\sum_{i=1}^{N}\left(s_i - s_i^{exact}\right)^2}{N}\right]^{1/2} \tag{6}$$

For the current study, which solves the heat equation using the finite difference method, solution convergence criteria is based on the reduction of residuals. The solution is considered converged if $Res_{L_2} < 1e-14$ within 100000 iterations. This results in cases in which convergence is not reached within the maximum iterations allowed, although the residuals decreases with iterations, as will be observed in the results presented later. This is due to the restrictions imposed on the number of iterations computed for each run in this case, and does not indicate a diverging solution.

Point Implicit Scheme For Heat Equation

The point implicit scheme applied to Eqn. 1 results in the discretized form of the equation shown in Eqn. 7.

$$\frac{U_i^{n+1} - U_i^n}{\Delta t} = \alpha \frac{U_{i+1}^n - 2U_i^{n+1} + U_{i-1}^n}{\Delta x^2} + aU_i^{n+1} \tag{7}$$

It is to be noted that eqn. 7 is not a consistent discretization for the unsteady heat equation, but will approach the proper representation of the steady-state problem at large values of t.

Rearranging terms and writing $\alpha\Delta t/\Delta x^2$ as r , and $a\Delta t$ as δ, we get the difference equation as,

$$U_i^{n+1} = U_i^n + \frac{\left[r\left(U_{i+1}^n - 2U_i^n + U_{i-1}^n\right) + \delta U_i^n\right]}{(1 + 2r - \delta)} \tag{8}$$

Instead of solving Eqn. 1 for particular values of α and a, non-dimensional parameters $r = \left(\alpha\Delta t/\Delta x^2\right)$, $\delta = a\Delta t$, and $Sc = \delta/r$ are varied. For a fixed value of $\alpha = 1.22e-02$, different values of Sc and r are selected and iterations are performed. Distinct values of Sc selected are 0 (for no source term), -0.01, -0.1, -1.0 (for negative source coefficients), and 0.01, 0.1, 1.0 (for positive source coefficients). Iterations are performed for different uniform grids wherein the number of grid points (GP) used are $\{11,21,41,81,161\}$. The range of r is $0.001 - 100000$. In order to keep a cap on the number of cases, the change in r across simulations is not kept a constant, but varied, as the order of magnitude of r varies. Thus for $r < 1$, $\Delta r = 0.01$, whereas for $r \approx O(100)$, $\Delta r = 10$ (see Table 1).

TABLE 1: Increment of r for different ranges of r

Range	Δr
0.001-0.01	0.001
0.01-1.0	0.01
1.0-10	0.1
10-100	1
100-1000	10
1000-10000	1000
10000-100000	10000

RESULTS AND DISCUSSION

Heat equation with ($Sc \neq 0$) and without ($Sc = 0$) source is solved using explicit and point implicit schemes. In all cases, the number of iterations corresponding to converged solution (if obtained) is determined for each value of r, and number of iterations vs r is plotted for both explicit and point implicit scheme.

Heat Equation Without Source

Iterations for this case are performed by keeping $Sc = 0$ and varying r using different grids. Figure 1 shows plots of number of iterations (for converged solution) vs. r, for explicit and point implicit scheme applied to heat equation without source with $\alpha = 1.22e-02$. It can be observed, that for both point implicit and explicit schemes, with increase in r, the number of iterations to convergence decreases. This is expected, as a higher value of r implies a higher value of Δt, for fixed values of α and Δx (grid).

For the convergence criteria considered in this study, converged solution is not obtained till r reaches certain value (denoted as r_{min}), for a given grid. For $r < r_{min}$, it is observed (not shown) that reduction in residuals is too slow and it does not reach a value of $1e-14$ after 10^5 iterations. The value of r_{min} increases with increase in number of grid points for both explicit and point implicit scheme. For explicit scheme, after a particular value of r (denoted as r_{max}), residuals shoot up to very high value and converged solution is not obtained. For all grids, value of r_{max} obtained is 0.5 using explicit scheme. For a given value of r ($r < r_{max}$), number of iterations required to reach convergence using the point implicit scheme is higher than that required for the explicit scheme. However, there exists a particular value of r (the value varies with grid resolution) for which the number of iterations required to attain convergence using point implicit scheme is less than the minimum number of iterations required for explicit scheme.

Table 2, shows minimum number of iterations obtained for explicit and point-implicit scheme for heat equation without source term, with $\alpha = 1.22e-02$, for different grids. For explicit scheme, column $r_{min.NOI}$ indicates value of r for which number of iterations required to get converged solution is minimum and column NOI represents number of iterations corresponding to $r_{min.NOI}$. As point implicit scheme exhibits unconditional stability, and the number of iterations decreases with increase in r, notion of $r_{min.NOI}$ is not be applicable for this case. Instead, NOI are given in Table 2 for maximum value of r(=100000) used in this study. It can be observed that for each grid, $NOI_{pt.imp} \approx 0.6NOI_{exp}$. Solutions obtained with explicit and point implicit schemes for $r = 0.04, \alpha = 1.22e-02$, and 21 grid points are compared with the exact solution in, Fig. 2); both the numerical solutions matches very well with exact solution. Error norm obtained in this case is $7.57e-14$ for both explicit and point implicit schemes.

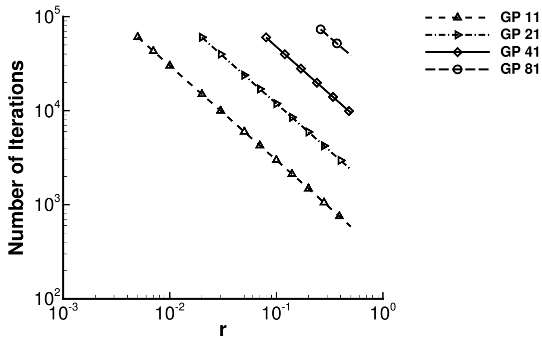
TABLE 2: Minimum number of iterations without source; $\alpha = 1.22e-02$

	Explicit		Point Implicit	
GP	$r_{min.NOI}$	NOI	r	NOI
11	0.5	591	100000	348
21	0.5	2396	100000	1409
41	0.5	9713	100000	5647
81	0.5	38485	100000	22511
161	-	-	100000	89194

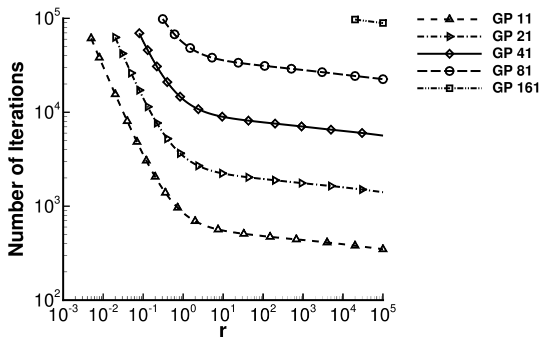
Heat Equation With Source

For each value of Sc, r is varied with the value of α fixed. The variation in the number of iterations required to achieve convergence with r is noted for both explicit and point implicit schemes.

Heat Equation With Negative Source Term Figures 3 and 4 plot number of iterations (required for convergence) against r for heat equation with negative source coefficient having $\alpha = 1.22e-02$, using explicit and point implicit schemes respectively. It can be seen that for each value of Sc, converged solution is obtained with both explicit and point implicit scheme, but for explicit scheme, maximum value of r is less than or equal to 0.5 and varies with value of Sc. An interesting point to note



(a) Explicit scheme



(b) Point implicit scheme

FIGURE 1: Number of iteration vs. r without source.

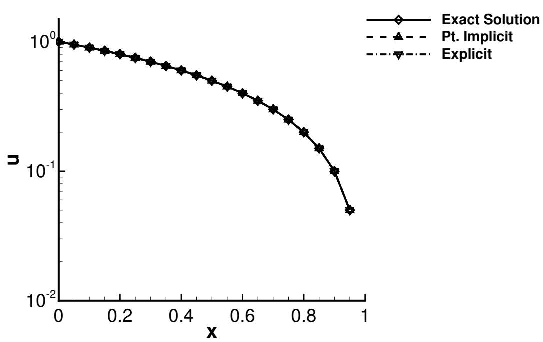
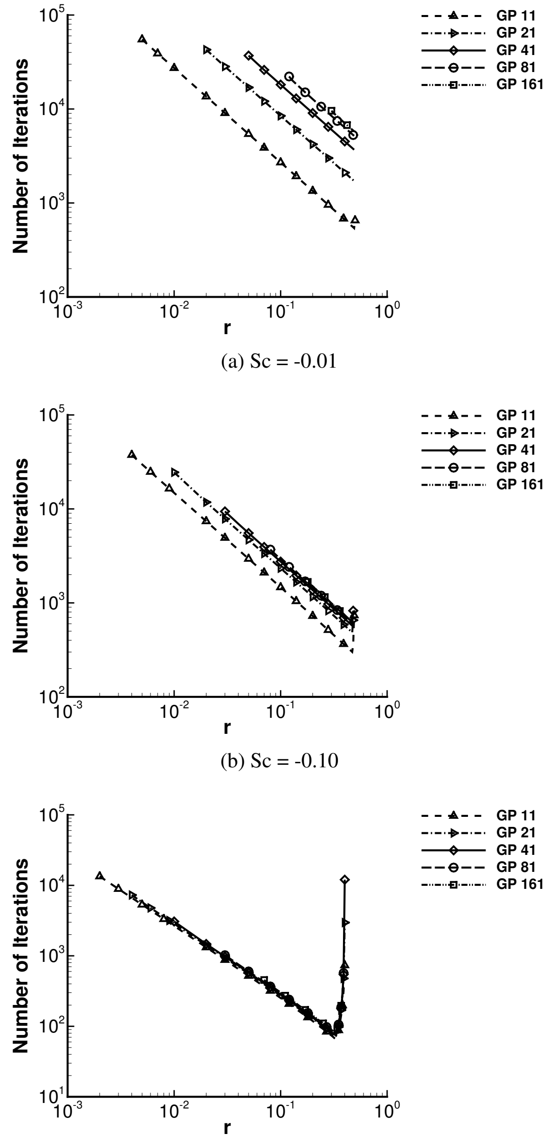


FIGURE 2: Exact and numerical solution comparison for $Sc = 0.00$, $\alpha = 1.22e-02$, $r = 0.04$, 21 grid points

is that for the explicit scheme, the number of iterations (to convergence) decreases with increase in r up to a specific value of r ($r_{min.NOI}$), and with further increase in $r(> r_{min.NOI})$, the number of iterations increases till the solution diverges for $r > r_{max}$. It should be noted that the value of $r_{min.NOI}$ does not change with number of grid points for given value of Sc, which is clearly observed in Fig. 3 for $Sc = -1.0$. For point implicit scheme, with all values of Sc, number of iterations decreases with increase in r, and converged solution can be obtained with any value of r .

Table 3 shows minimum number of iterations for heat equation with negative source with $\alpha = 1.22e-02$ for different values of Sc and grids considered in this study. For explicit scheme, $r_{min.NOI}$ remains constant for given value of Sc, irrespective of the grid resolution used. Also, $r_{min.NOI}$ in one case ($S_c = -1.0$) is less than r_{max}. Value of $r_{min.NOI}$ decreases with increase in absolute value of Sc. For a given grid resolution, minimum number of iterations decreases with increase in absolute value of Sc. Point implicit scheme in this case is unconditionally stable, hence concept of $r_{min.NOI}$ is not applicable here. In Table 3 the number of iterations corresponding to $r = 100000$ are mentioned for the point-implicit scheme, but it is to be noted that r can be further increased to get reduction in number of iterations. Minimum number of iterations obtained with point implicit scheme ($NOI_{pt.imp}$) is less than that with explicit scheme (NOI_{exp}). Also, it can be observed for each grid resolution, $NOI_{pt.imp} \approx 0.6 NOI_{exp}$.

Solution for $Sc = -0.01$ for both point implicit and explicit scheme is given in Fig. 5, with $r = 0.04$, 21 grid points and $\alpha = 1.22e-02$. It can be seen that the numerical solutions obtained with explicit and point implicit scheme are virtually identical although both of these show some difference with the exact solution. In this case the error norm is obtained as $9.68e-02$, for both point implicit and explicit scheme. For explicit and point implicit schemes, error norm does not changes with r for a given grid (not shown here).

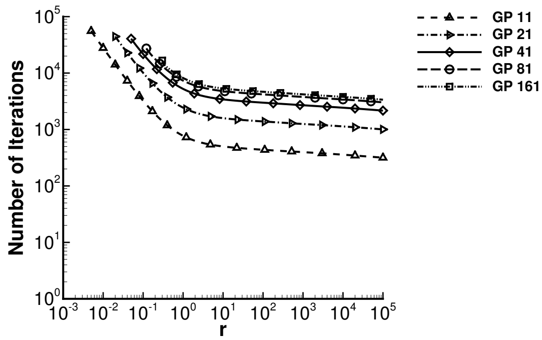


(a) Sc = -0.01

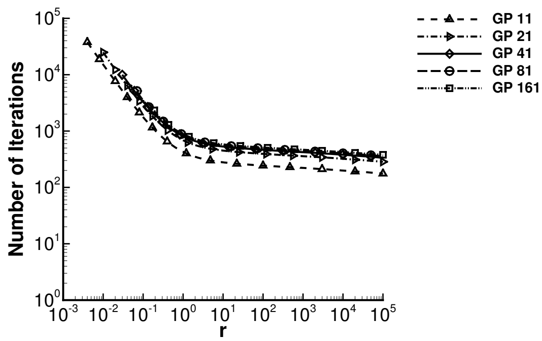
(b) Sc = -0.10

(c) Sc = -1.00

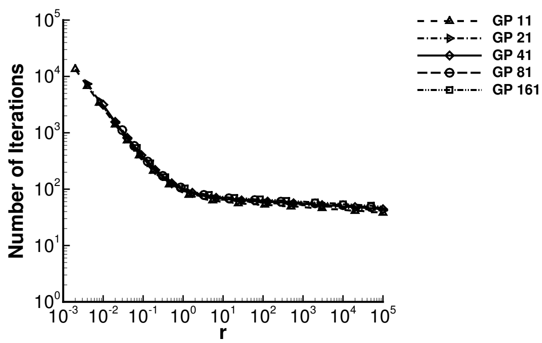
FIGURE 3: Number of iteration vs. r for explicit scheme with negative source coefficient; $\alpha = 1.22e-02$, $r = 0.04$.



(a) Sc = -0.01



(b) Sc = -0.10



(c) Sc = -1.00

FIGURE 4: Number of iteration vs. r for point implicit scheme with negative source coefficient; $\alpha = 1.22e-02$, $r = 0.04$.

Heat Equation With Positive Source Term For $Sc = 0.01$ converged solution is obtained for 11 and 21 grid points only, and for 41, 81, and 161 grid points, converged solution is not obtained as residuals shoot up with every iteration for all values of r for both explicit and point implicit scheme. For $Sc = 0.1, 1.0$ converged solution is not obtained for any grid as residual was found to be diverging for any value of r.

Figure. 6 and 7 shows the number of iteration vs. r for different grids and values of Sc, for explicit and point implicit scheme respectively. It can be seen that for explicit scheme, number of iterations (to convergence) decrease with increase in r, except for 11 grid points, where near $r = 0.5$, the number of iterations increase with increase in $r(< r_{max})$. For point implicit scheme, number of iterations required for convergence decreases with increase in r for grids on which converged solution is achieved.

TABLE 3: Minimum number of iterations with negative source; $\alpha = 1.22e-02$

	Explicit		Point Implicit	
GP	$r_{min.NOI}$	NOI	r	NOI
Sc=-0.01				
11	0.49	540	100000	317
21	0.49	1714	100000	1005
41	0.49	3689	100000	2161
81	0.49	5184	100000	3029
161	0.49	5789	100000	3375
Sc=-0.10				
11	0.47	301	100000	176
21	0.47	486	100000	285
41	0.47	573	100000	336
81	0.47	603	100000	358
161	0.47	624	100000	379
Sc=-1.00				
11	0.33	66	100000	38
21	0.33	72	100000	42
41	0.33	74	100000	44
81	0.33	77	100000	46
161	0.33	79	100000	49

Table 4 shows minimum number of iterations for explicit and point implicit scheme for heat equation with positive source having $\alpha = 1.22e-02$. For explicit scheme and $Sc = 0.01$, value of $r_{min.NOI} = 0.5$ for both 11 and 21 grid points. For point implicit scheme concept of $r_{min.NOI}$ is not applicable in this case as with increase in r, number of iterations corresponding to converged solution decreases. Minimum number of iterations obtained with explicit scheme (NOI_{exp}) are much higher than that obtained with point implicit scheme ($NOI_{pt.imp}$) for cases in which converged solution is obtained. Also, for $Sc = 0.01$, $NOI_{pt.imp} \approx 0.6 NOI_{exp}$ is satisfied for 11 and 21 grid points.

Solution for $Sc = 0.01$, $r = 0.04$, and $\alpha = 1.22e-02$ obtained for 21 grid points is mentioned in Fig. 8. Numerical solution obtained with explicit and point implicit scheme are same and matches approximately with exact solution. Error norm of $2.67e-01$ is obtained in this case for both explicit and point implicit scheme. Error norm for converged solution does not change with r for all grid (not shown here).

CONCLUSION

A point implicit scheme applied to the heat equation shows that it is unconditionally stable for heat equation without a source term and with a negative source term, whereas it is conditionally stable for heat equation with a positive source term. Comparison with an explicit scheme shows that the minimum number of iterations required for convergence with point-implicit

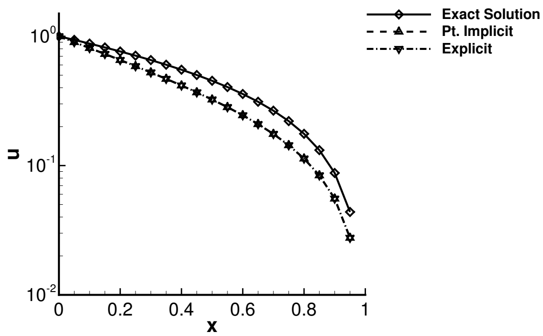
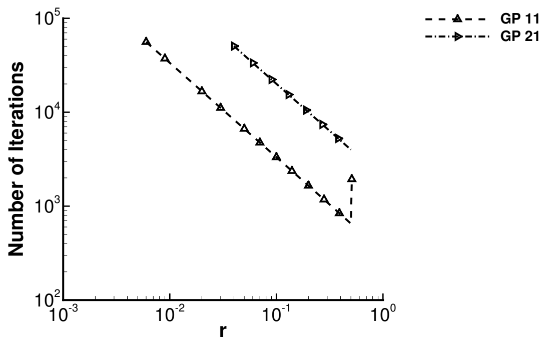
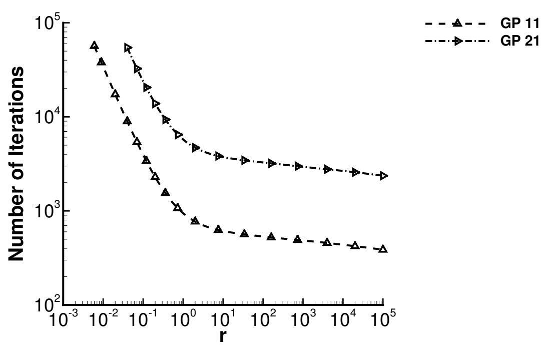


FIGURE 5: Exact and numerical solution comparison for $Sc = -0.01$, $\alpha = 1.22e-02$, $r = 0.04$, 21 grid points



(a) Sc = 0.01

FIGURE 6: Number of iteration vs. r for explicit scheme with positive source coefficient; $\alpha = 1.22e-02$, $r = 0.04$.



(a) Sc = 0.01

FIGURE 7: Number of iteration vs. r for point implicit scheme with negative source coefficient; $\alpha = 1.22e-02$, $r = 0.04$.

scheme is about 60% of the number of iterations required for the explicit scheme. Hence, approximately 40%+ reduction in number of iterations can be achieved with point implicit scheme. Considering the fact that the simple explicit and point-implict schemes have almost identical computational cost it can be inferred that if steady-state solution of the heat equation is to be obtained using time-marching schemes, point implicit scheme outperforms explicit scheme.

TABLE 4: Minimum number of iterations with positive source; $\alpha = 1.22e-02$

	Explicit		Point Implicit	
GP	$r_{min.NOI}$	NOI	r	NOI
Sc=0.01				
11	0.5	653	100000	387
21	0.5	3996	100000	2367

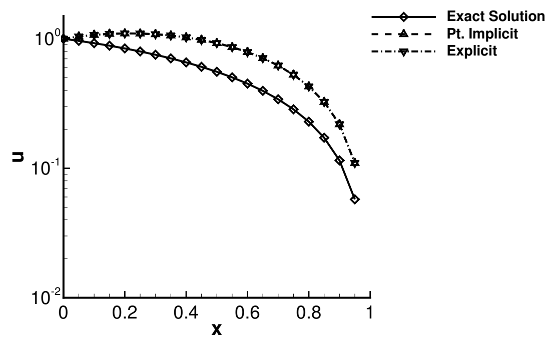


FIGURE 8: Exact and numerical solution comparison for $Sc = 0.01$, $\alpha = 1.22e-02$, $r = 0.04$, 21 grid points

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