University of Reading

School of Mathematics, Meteorology and Physics

NUMERICAL SCHEMES FOR A NON-LINEAR DIFFUSION PROBLEM

by

Kylie Osman

August 2005

Contents

4.1 U

List of Figures

1 Introduction

1.1 An Introduction to Non-Linear Diffusion

Non-linear diffusion is characterised by the partial differential equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D(u)\frac{\partial u}{\partial x}\right). \tag{1.1}$$

where $D(u)$ is the diffusion coefficient. When $D(u) = u^n$, this equation is also known as the Porous Medium Equation (PME),

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(u^n\frac{\partial u}{\partial x}\right). \tag{1.2}$$

1.1.1 Gas Diffusion through a Porous Medium

he PME can be derived by considering the diffusion of a gas through a porous medium under the action of Darcy's law relating the velocity to the pressure gradient. he flow of gas is characterised in terms of pressure, p; density, u and velocity, v. he gas can be assumed to obey the conservation of mass equation

$$\rho\frac{\partial u}{\partial t} + \frac{\partial}{\partial t}(uv) = 0, \tag{1.3}$$

where ρ is the constant porosity of the medium. he gas also obeys Darcy's law

$$\mu v = -\kappa\frac{\partial p}{\partial t} \tag{1.4}$$

which is an empirical law for the dynamics of the flow through a porous medium. Here, μ is the viscosity of the gas and κ is the permeability of the medium; both these are assumed to be constant. he gas is assumed to be ideal so

$$p = p_0 u^{\lambda}, \tag{1.5}$$

where p_0 is the reference pressure and λ

radiation in detail but is expensive to solve numerically, whether by Monte Carlo methods or by some deterministic method such as Sn or Pn.

In cases when the mean free path of a photon is much smaller than a computational cell then an approximation can be made to the transport equation which yields the diffusion equation. In this approximation causality is no longer significant although in low opaque environments a radiation wave can exceed the speed of light and care must be taken when the approximation is applied. However, in a genuinely diffusive regime, it provides an adequate description of the radiation transport.

In the diffusion approximation, the diffusion coefficient is not a simple constant or linear function, but depends on the type of material and the density and temperature of the media being traversed. he dependence on temperature is roughly proportional to the 4th power and so the diffusion equation is highly non-linear. Hence to solve the diffusion equation with linear solvers the timestep must either be small so that the system is effectively linearised or an iterative scheme devised that takes into account the non-linear nature of the coefficient [10].

In practice, the temperature dependence is not evaluated via a polynomial function, but taken from tables derived from theory and experiment. Intermediate values are interpolated. In this case the derivative of the coefficient must be evaluated numerically if it is involved in the solving iteration.

I shall first be considering the case when the diffusion coefficient is known analytically to be u^4. he partial differential equation becomes

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(u^4 \frac{\partial u}{\partial x}\right). \tag{1.6}$$

I shall later look at using a table to evaluate $D(u)$.

1.2 Overview of the Report

In chapter two, I shall give the derivation of the self-similar solution for equation (1.6). his gives a family of analytic solutions which can be used to compare the errors in different methods. he self-similar solution also acts as an attractor for general solutions.

In chapter three, I shall look at three different static mesh methods used to solve the partial differential equation in conservation form, based on the standard Crank-Nicolson scheme. First, I will linearise the equation in u^{n+1} and use a standard solver. I will then look at two iterative ways of solving the full non-linear equations, using first Picard iteration and then the Newton-Raphson method.

In chapter four, I will look at solutions of the PDE with $n = 4$ in non-conservation form, as in

$$\frac{\partial u}{\partial t} = u^4 \frac{\partial^2 u}{\partial x^2} + 4u^3 \left(\frac{\partial u}{\partial x} \right)^2 ,$$

which comes from (1.2) by direct differentiation. In this form, I will use the Crank-Nicolson scheme and compare methods using upwind and central differences for the last term.

In chapter five I will look at a case where the diffusion coefficient $D(u)$ in (1.1) is not known analytically but is tabulated for a series of values of u. I will investigate two ways that can be used to extend the above methods for use in this case. First, I will simply use linear interpolation to find the value $D(u)$ for a value u not present in the table. Second, I will use a least squares minimisation to fit a function to the tabular data and then use this function to evaulate the different methods.

In chapter six I will look at a moving mesh method for solving the problem. Here, the area under the graph between consecutive grid-points is kept

2 A Self-Similar Solution

2.1 Scale Invariance

First we seek a coordinate transform under which the partial differential equation (1.6) is invariant. Consider the scaling transformation

$$u = \lambda^{\gamma} \hat{u} \qquad t = \lambda \hat{t} \qquad x$$

Integrating equation (1.6) gives

$$\int_a^b \frac{\partial u}{\partial t} dx = \int_a^b \frac{\partial}{\partial x} \left(u^4 \frac{\partial u}{\partial x} \right) dx.$$

his simplifies to become

$$\frac{d}{dt} \int_a^b u dx = u^4 \frac{\partial u}{\partial x} \bigg|_a^b .$$

2.2 Self-Similar Solutions

A time dependent phenomenon is called self-similar if the spatial distributions of its properties at different times can be obtained from one another by a similarity transform [8].

Note from (2.1) that

$$\lambda = \frac{u^{\frac{1}{\gamma}}}{\hat{u}^{\frac{1}{\gamma}}} = \frac{t}{\hat{t}} = \frac{x^{\frac{1}{\beta}}}{\hat{x}^{\frac{1}{\beta}}}.$$

We now introduce two new variables

$$\phi = \frac{u}{t^{\lambda}} = \frac{\hat{u}}{\hat{t}^{\lambda}}$$

and

$$y = \frac{x}{t^{\beta}} = \frac{\hat{x}}{\hat{t}^{\beta}}.$$

Note that these two variables are independent of λ and are invariant under the transformation (2.1).

Now take ϕ to be a function of y and transform the PDE (1.6) into the variables ϕ and y to obtain an ODE. First, transform the left hand side of the PDE into ϕ and y.

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \frac{\partial}{\partial t}(\phi t^{\gamma}) \\
&= t^{\gamma}\frac{\partial \phi}{\partial t} + \phi\gamma t^{\gamma-1} \\
&= t^{\gamma}\frac{d\phi}{dy}\frac{\partial y}{\partial t} + \phi\gamma t^{\gamma-1} \\
&= t^{\gamma}\frac{d\phi}{dy}\left(\frac{-\beta x}{t^{\beta+1}}\right) + \phi\gamma t^{\gamma-1} \\
&= -\frac{\beta y}{t}t^{\gamma}\frac{d\phi}{dy} + \phi\gamma t^{\gamma-1} \\
&= -\beta t^{\gamma-1}y\frac{d\phi}{dy} + \gamma\phi t^{\gamma-1}
\end{aligned}$$

Now transform the right hand side into ϕ and y.

$$
\begin{aligned}
\frac{\partial}{\partial x}\left(u^4 \frac{\partial u}{\partial x}\right) &= \frac{\partial y}{\partial x}\frac{d}{dy}\left(\phi^4 t^{4\gamma}\frac{\partial y}{\partial x}\frac{\partial u}{\partial \phi}\frac{d\phi}{dy}\right) \\
&= \frac{1}{t^\beta}\frac{d}{dy}\left(\phi^4 t^{4\gamma} t^{\gamma-\beta}\frac{d\phi}{dy}\right) \\
&= t^{5\gamma-2\beta}\frac{d}{dy}\left(\phi^4 \frac{d\phi}{dy}\right)
\end{aligned}
$$

Substituting these into equation (1.6) gives

$-$

Rearranging gives

$$\int \phi^3 d\phi = -\frac{1}{6} \int y dy.$$

his integrates to give

$$\frac{\phi^4}{4} = -\frac{1}{6} \left(\frac{y^2}{2} - d \right),$$

where d is a constant of integration. his simplifies to

$$\phi = \left(\frac{2}{3} \right)^{\frac{1}{4}} \left(d - \frac{y^2}{2} \right)^{\frac{1}{4}}.$$

where d is constant. Since ϕ has to be positive we obtain

ϕ [illegible]

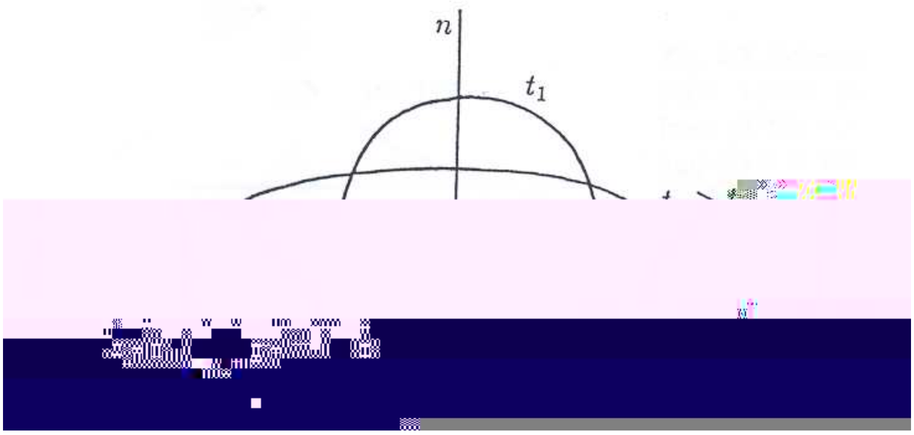


Figure 1: Self-Similar Solution at times t_1 and t_2

2.3 The Self-Similar Solution as an Attractor

Comparison theory says that if we have two solutions u, w to the problem with $u \geqslant w$ at t_0 then $u \geqslant w$ for all time, giving an ordering of solutions [4].

he self-similar solution is of particular interest due to the following convergence result from [5].

"Let $u(x,t) \geqslant 0$ be an arbitrary solution of equation (1.6) with integral I and centre of mass x_0. hen if $\bar{u}(x;t;A)$ is the self-similar solution with the same integral and centre of mass, then for all t_0 we have

$$t^{\frac{1}{3}} \parallel u - \bar{u} \parallel_{L_1} \rightarrow 0 \qquad \text{as} \qquad t \rightarrow \quad .$$

Equivalently, the PDE (1.6) has as a global attractor the solution of the ODE (2.7) with the same first integral." his means that a solution with arbitrary initial data will be squeezed between two discrete self-similar solutions. Diagram 2 from [4] show this for an initial solution that fits between self-similar solutions with $A = 0.9$ and $A = 2.3$. he figures in this diagram are plotted in a reference space ξ.

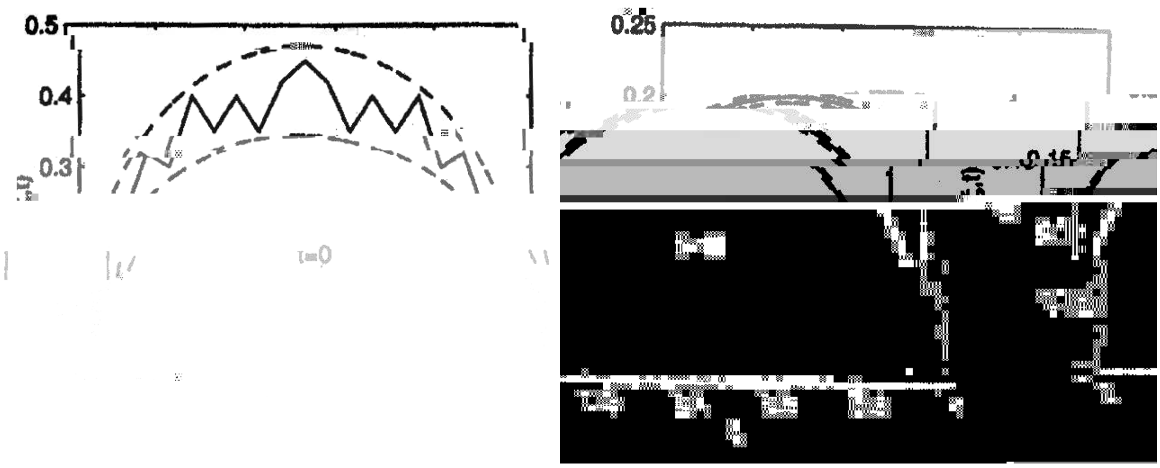


Figure 2: Convergence of the Solution in the Computational Domain

3 Solutions on a Stationary Mesh - Conservation Form

he partial differential equation will be first solved numerically using finite

3.1 Crank-Nicolson with Explicit Treatment of u^4

In this section, the non-linear term of the equation will be taken at time level n. his results in the semi-implicit scheme

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}=$$

$$\frac{\theta}{\Delta x^2}\left(\left(\frac{u_{j+1}^n+u_j^n}{2}\right)^4\left(u_{j+1}^{n+1}-u_j^{n+1}\right)-\left(\frac{u_j^n+u_{j-1}^n}{2}\right)^4\left(u_j^{n+1}-u_{j-1}^{n+1}\right)\right)$$

$$+\frac{(1-\theta)}{\Delta x^2}\left(\left(\frac{u_{j+1}^n+u_j^n}{2}\right)^4\left(u_{j+1}^n-u_j^n\right)-\left(\frac{u_j^n+u_{j-1}^n}{2}\right)^4\left(u_j^n-u_{j-1}^n\right)\right). \tag{3.1}$$

After rearranging, this becomes

$$u_{j-1}^{n+1}\left(-\nu\theta\left(\frac{u_j^n+u_{j-1}^n}{2}\right)^4\right)+u_j^{n+1}\left(1+\nu\theta\left(\left(\frac{u_{j+1}^n+u_j^n}{2}\right)^4+\left(\frac{u_j^n+u_{j-1}^n}{2}\right)\right)\right)+$$

$$u_{j+1}^{n+1}\left(-\nu\theta\left(\frac{u_{j+1}^n+u_j^n}{2}\right)^4\right)=u_j^n+$$

$$\nu(1-\theta)\left(\left(\frac{u_{j+1}^n+u_j^n}{2}\right)^4\left(u_{j+1}^n-u_j^n\right)-\left(\frac{u_j^n+u_{j-1}^n}{2}\right)^4\left(u_j^n-u_{j-1}^n\right)\right). \tag{3.2}$$

his is solved as a matrix equation $A\mathbf{u}^{n+1}=\mathbf{b}$ with A being the matrix of coefficients of the components of the vector $\mathbf{u}^{n+1}$ and $\mathbf{b}$ being a vector of the right hand side of equation (3.2). his can easily be solved using any standard method. In this case, A is tridiagonal and we use the homas algorithm [11].

3.1.1 Stability and Accuracy

he stability of this method can be examined using Fourier analysis. Consider the diffusion coefficient u^4 to be frozen and replace it with a constant.

he PDE now becomes

$$\frac{\partial u}{\partial t} = \sigma \frac{\partial^2 u}{\partial x^2},$$

where σ is constant.

he scheme to be analysed is simply

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = \frac{\sigma}{\Delta x^2} \left(\theta \left(u_{j+1}^{n+1} - 2u_j^{n+1} - u_{j-1}^{n+1} \right) + (1-\theta) \left(u_{j+1}^n - 2u_j^n - u_{j-1}^n \right) \right). \tag{3.3}$$

Substituting $u_j^n = a_n e^{ikj\Delta x}$ into the equation (3.3), multiplying through by Δt and dividing through by $e^{ijk\Delta x}$ gives

$$a_{n+1} - a_n = \nu \left((1-\theta) a_n + \theta a_{n+1} \right) \left(e^{ik\Delta x} - 2 + e^{-ik\Delta x} \right),$$

where $\nu = \frac{\sigma \Delta t}{\Delta x^2}$.

his then becomes

$$a_{n+1} = \left(\frac{1 - 4\nu(1-\theta) \sin^2\left(\frac{k\Delta x}{2}\right)}{1 + 4\nu\theta \sin^2\left(\frac{k\Delta x}{2}\right)} \right) a_n.$$

For stability, we require that $|a_{n+1}| \leqslant |a_n|$. For this, we need

$$-1 - 4\nu\theta \sin^2\left(\frac{k\Delta x}{2}\right) \leqslant 1 - 4\nu(1-\theta)\sin^2\left(\frac{k\Delta x}{2}\right) \leqslant 1 + 4\nu\theta \sin^2\left(\frac{k\Delta x}{2}\right).$$

he right hand part of this inequality always holds. Moreover, for $\theta \geqslant \frac{1}{2}$, the left hand side of the equation is always $\leqslant 0$ so the inequality holds and the scheme is unconditionally stable.

If $\theta < \frac{1}{2}$, then the scheme will be stable only if $\nu(1-2\theta)\sin^2\left(\frac{k\Delta x}{2}\right) \leqslant \frac{1}{2}$. he worst possible case is when $\sin^2\left(\frac{k\Delta x}{2}\right) = 1$. his gives Fourier stability for $\nu \leqslant \frac{1}{2(1-2\theta)}$.

If θ is taken to be equal to $\frac{1}{2}$ then the method is known as the Crank-Nicolson method. his method is stable for all ν and is second order accurate in both space and time. he stability can be exploited to use large timesteps (with the order of the space and time steps being equal) and since it is second order accurate in time, good accuracy will still be obtained.

σ is obtained by freezing u^4 so the maximum value it can take is the maximum value of u^4. Due to the maximum principle, this is equal to the maximum value of u^4 in the initial data. Hence the maximum possible value of ν is $\frac{\Delta t}{\Delta x^2}\max_i u_i^4$.

3.1.2 A Maximum Principle

he theta method of equation (3.1) with $0 \leqslant \theta \leqslant 1$ and

$$\nu(1-\theta) \leqslant \frac{1}{2} \tag{3.4}$$

yields u_j^n satisfying

$$u_{min} \leqslant u_j^n \leqslant u_{max}$$

where

$$u_{min} := \min\{u_0^m, 0 \leqslant m \leqslant n; u_j^0, 0 \leqslant j \leqslant J; u_J^m, 0 \leqslant m \leqslant n\},$$

and

$$u_{max} := \max\{u_0^m, 0 \leqslant m \leqslant n; u_j^0, 0 \leqslant j \leqslant J; u_J^m, 0 \leqslant m \leqslant n\}$$

are the minimum and maximum values of u on the initial line and the boundaries [2].

Using this maximum principle we can deduce stability and hence convergence. For any ν which satisfies the stability condition (3.4), the approximations given by equation (3.1) with consistent initial and Dirichlet boundary data converge uniformly if the initial data are smooth enough for the truncation error to tend to zero as Δt and Δx are decreased, whilst keeping ν constant [2].

he condition used in the above theorem, $\nu(1-\theta) \leqslant \dfrac{1}{2}$ is much more restrictive than that obtained using Fourier stability analysis, $\nu(1-2\theta) \leqslant \dfrac{1}{2}$. For example, the Crank-Nicolson scheme is always stable but only if $\nu \leqslant 1$ does it satisify the maximum principle which is then used to deduce stability and convergence. If the boundary conditions are $u_0^n = u_J^n = 0$ then we want

$$\left|u_j^n\right| \leqslant K \max_{0 \leqslant i \leqslant J} \left|u_i^0\right| \quad \forall j, n$$

to be satisfied with $K = 1$ for a maximum principle to hold. However, for Fourier stability any value of K is accepted in this bound. he weaker condition $\nu(1-2\theta) \leqslant \dfrac{1}{2}$ is then adequate [2].

Hence the maximum priciple can be viewed as an alternative way of obtaining stability conditions but it may derive conditions that are only sufficient.

3.2 Crank-Nicolson with Semi-Implicit Treatment of u^4

3.2.1 Picard Iteration

Here, the non-linear term of the implicit section of equation is taken at time level $n + \frac{1}{2}$. It is known that for the Crank-Nicolson method, the diffusion coefficient, here u^4, produces better accuracy if taken at time level $n + \frac{1}{2}$. At the start of each time step, u^4 is taken at time level n and the problem is iterated to find a provisional value of u^{n+1}. hen $u^{n+\frac{1}{2}}$ is calculated as $\dfrac{u^{n+1} + u^n}{2}$ and the process repeated. When the solution for u^{n+1} has converged, the time step is advanced and the next time step commenced. he scheme is

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} =$$

$$\frac{\theta}{\Delta x^2}\left(\left(\frac{u_{j+1}^{n+\frac{1}{2}} + u_j^{n+\frac{1}{2}}}{2}\right)^4 \left(u_{j+1}^{n+1} - u_j^{n+1}\right) \left(\frac{u_j^{n+\frac{1}{2}} + u_{j-1}^{n+\frac{1}{2}}}{2}\right)^4 \left(u_j^{n+1} - u_{j-1}^{n+1}\right)\right)$$

$$+\frac{(1-\theta)}{\Delta x^2}\left(\left(\frac{u_{j+1}^n + u_j^n}{2}\right)^4 \left(u_{j+1}^n - u_j^n\right) - \left(\frac{u_j^n + u_{j-1}^n}{2}\right)^4 \left(u_j^n - u_{j-1}^n\right)\right).$$

he equations can be solved using Picard iteration with the matrix equation being solved as before.

3.2.2 Newton-Raphson Iteration

Here, the non-linear part of the implicit section of the method is taken at time level $n + 1$.

Let

$$F_j\left(\mathbf{u}^{n+1}\right) = 0 = u_j^{n+1} - u_j^n -$$

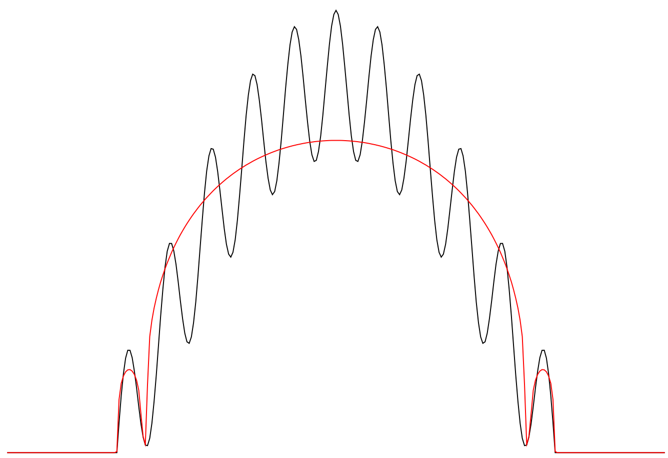
$$\frac{\Delta t}{\Delta x^2}\left(\left(\frac{u_{j+1}^{n+1}+u_j^{n+1}}{2}\right)^4\left(u_{j+1}^{n+1}-u_j^{n+1}\right)-\left(\frac{u_j^{n+1}+u_{j-1}^{n+1}}{2}\right)^4\left(u_j^{n+1}-u_{j-1}^{n+1}\right)\right).$$

o solve the equation $\mathbf{F}\left(\mathbf{u}^{n+1}\right)=\mathbf{0}$, this method iterates

$$\begin{aligned} \mathbf{J}(\mathbf{u}^{n+1})^p\delta\mathbf{u} &= -\mathbf{F}(\mathbf{u}^{n+1})^p \\ \left(\mathbf{u}^{n+1}\right)^{p+1} &= \left(\mathbf{u}^{n+1}\right)^p + \delta\mathbf{u} \end{aligned} \tag{3.5}$$

where p is the iteration count and $\mathbf{J}$ is the jacobian matrix $\dfrac{\partial\mathbf{F}(\mathbf{u})}{\partial\mathbf{u}}$. he Jacobian is evaluated by analytically finding the derivatives of $\mathbf{F}(\mathbf{u})$ and coding these into the fortran. he Jacobian is tridiagonal so the equation can be solved using the homas algorithm as before.

At the start of each time step, u^4 is taken at time level n and Newton-Raphson is applied as in (3.5) to find u^{n+1}. When the solution for u^{n+1} has converged, the time step is advanced and the proces [illegible] d the pr [illegible]



4 Solutions on a Stationary Mesh - Non-Conservation Form

he partial differential equation will now be solved numerically in non-conservation form using finite differences applied using the theta method. Where ν is used in the following section, it is a constant and is equal to $\frac{\Delta t}{\Delta x^2}$.

he PDE (1.6) can be differentiated to give

$$\frac{\partial u}{\partial t} = u^4 \frac{\partial^2 u}{\partial x^2} + 4u^3 \left(\frac{\partial u}{\partial x} \right)^2 .$$

Finite differences can be applied to this eq

$$+\frac{(1-\theta)}{\Delta x^2}\left((u_j^n)^4\left(u_{j+1}^n-2u_j^n+u_{j-1}^n\right)+4(u_j^n)^3\left(u_{j+1}^n-u_j^n\right)^2\right)$$

At $x = 0$, either case can be used.

4.2 Central Differencing

Central differences are of a higher order than upwind differences but they take data from a wider area and so may use data on which the solution is not physically dependent. his may cause the solution to be less physical than the upwind solution. he central difference scheme is

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}=$$

$$\frac{\theta}{\Delta x^2}\left((u_j^n)^4\left(u_{j+1}^{n+1}-2u_j^{n+1}+u_{j-1}^{n+1}\right)+(u_j^n)^3\left(u_{j+1}^n-u_{j-1}^n\right)\left(u_{j+1}^{n+1}-u_{j-1}^{n+1}\right)\right)$$

$$+\frac{(1-\theta)}{\Delta x^2}\left((u_j^n)^4\left(u_{j+1}^n-2u_j^n+u_{j-1}^n\right)+(u_j^n)^3\left(u_{j+1}^n-u_{j-1}^n\right)^2\right).$$

4.3 Results

4.3.1 Evolution of Various Initial Conditions

Figure 8 shows the evolution of the solution with perturbed non-self-similar initial data

$$u=\begin{cases}\cos\left(\frac{\pi x}{2}\right)+0.2\cos\left(\frac{21\pi x}{2}\right) & \text{for } |x|<1\\ 0 & \text{for } |x|\geqslant 1\end{cases}$$

using the scheme with upwind differencing.

5 Solutions on a Stationary Mesh - A Tabular Non-Linearity

For some applications, the exact form of the diffusion coefficient, $D(u)$ in equation (1.1) the range of the table then linear extrapolation is carried out using the final two points in the table.

5.1.1 Conservation Form - Explicit Implementation of u^4

his scheme is easy to convert to use the tabular data. he scheme becomes

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} =$$

$$\frac{\theta}{\Delta x^2} \left(D_{LI} \left(\frac{u_{j+1}^n + u_j^n}{2} \right) \left(u_{j+1}^{n+1} - u_j^{n+1} \right) - D_{LI} \left(\frac{u_j^n + u_j^n}{} \right. \right.$$

$$+\frac{1-\theta}{\Delta x^2}\Bigg(D_{LI}\Bigg(u^n_{j+1}+$$

he equation $\mathbf{F}\left(\mathbf{u}^{n+1}\right) = 0$ can now be solved exactly as in Section 3.2.2, using this new implementation of the Jacobian.

5.1.4 Non-Conservation Form - Upwind Finite Differencing

his is slightly more complicated to alter to use the tabular data since the scheme requires that $D_{LI}(u)$ is differentiated. However, an approximation to the derivative is easily achieved using an upwinded numerical derivative.

he scheme is given in equations (5.2) and (5.3) for the cases $x > 0$ and $x < 0$ respectively.

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} =$$

$$\frac{\theta}{\Delta x^2}\left(D_{LI}\left(u_j^n\right)\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right) + \left(u_j^{n+1} - u_{j-1}^{n+1}\right)\left(D_{LI}\left(u_j^n\right) - D_{LI}\left(u_{j-1}^n\right)\right)\right)$$

$$+\frac{1-\theta}{\Delta x^2}\left(D_{LI}\left(u_j^n\right)\left(u_{j+1}^{n} - 2u_j^{n} + u_{j-1}^{n}\right) + \left(u_j^{n} - u_{j-1}^{n}\right)\left(D_{LI}\left(u_j^n\right) - D_{LI}\left(u_{j-1}^n\right)\right)\right) \tag{5.2}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} =$$

$$\frac{\theta}{\Delta x^2}\left(D_{LI}\left(u_j^n\right)\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right) + \left(u_{j+1}^{n+1} - u_{j}^{n+1}\right)\left(D_{LI}\left(u_{j+1}^n\right) - D_{LI}\left(u_{j}^n\right)\right)\right)$$

$$+\frac{1-\theta}{\Delta x^2}\left(D_{LI}\left(u_j^n\right)\left(u_{j+1}^{n} - 2u_j^{n} + u_{j-1}^{n}\right) + \left(u_{j+1}^{n} - u_{j}^{n}\right)\left(D_{LI}\left(u_{j+1}^n\right) - D_{LI}\left(u_{j}^n\right)\right)\right) \tag{5.3}$$

5.1.5 Non-Conservation Form - Central Differencing

As with the above method, this requires an approximation of the derivative of $D_{LI}(u)$. he scheme becomes

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} =$$

$$\frac{\theta}{4\Delta x^2}\left(D_{LI}\left(u_j^n\right)\left(u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}\right) + \left(u_{j+1}^{n+1} - u_{j-1}^{n+1}\right)\left(D_{LI}\left(u_{j+1}^n\right) - D_{LI}\left(u_{j-1}^n\right)\right)\right)$$

$$+\frac{1-\theta}{4\Delta x^2}\left(D_{LI}\left(u_j^n\right)\left(u_{j+1}^{n} - 2u_j^{n} + u_{j-1}^{n}\right) + \left(u_{j+1}^{n} - u_{j-1}^{n}\right)\left(D_{LI}\left(u_{j+1}^n\right) - D_{LI}\left(u_{j-1}^n\right)\right)\right).$$

5.2 Least Squares Minimisation

In this method, a polynomial function is fitted to the data in the table and this function is used in the place of $D(u)$ in the schemes. he polynomial chosen to be fitted is $Ku^4 + L$. his has been chosen since it is known that for the physical examples considered in chapter one, the function $D(u)$ is generally u^4. his analysis could easily be ex u

It is now required to minimise these deviations. he condition for R^2 to be a minimum and

$$K = \frac{n\sum_{i=1}^{n} u_i^4 D_i - \sum_{i=1}^{n} u_i^4 \sum_{i=1}^{n} D_i}{n\sum_{i=1}^{n} u_i^8 - \left(\sum_{i=1}^{n} u_i^4\right)^2}.$$

he exact values of K and L are now easily calculated in the fortran program.

his diffusion coefficient can easily be applied to all the methods in the previous two chapters, simply by replacing $D(u) = u^4$ by $Ku^4 + L$ and replacing $\frac{\partial D}{\partial u} = 4u^3$ with $4Ku^3$.

5.3 Results

Ordinarily, the data in the table would be experimental data. For the purpose of this project however, this data is not available and the function u^4 has simply been used for $D(u)$. his allows the results from these schemes to be compared to the schemes in the previous two chapters which have u^4 programmed into them.

5.3.1 Least Squares Best Fit

In this case, the result is that $K = 1$ and $L = 0$ so the schemes are exactly the same as those in chapters three and four and the results are identical. he program will run slightly more slowly due to having to calculate K and L at the beginning but this difference is too small to be noticeable. o ensure this scheme works correctly, a new set of data for $D(u)$ have been calculated. For these, the function $D(u) = u^4 + 0.01 \times$ random, where random is a random number, has been used. Running this I obtain $K = 0.9982$ and $L = 0.0055$.

he results from this run are shown at the final time $t = 10$ in figure 10

Method	Δx	ime	Error
Analytic $D(u)$	0.01	$7.65s$	0.0618%
abular $D(u)$	0.01	$48.04s$	0.0580%
Analytic $D(u)$	0.25	$0.67s$	0.9125%
abular $D(u)$	0.25	$1.60s$	0.9163%

6 A Moving Mesh Method

6.1 Deriving a Moving Mesh Method for the Solution of the Non-Linear Diffusion Equation

With a moving mesh, it must be assumed that the grid points x_i are dependent on time. It can then be shown [1] that

$$\frac{d}{dt}\int_{x_{i-1}(t)}^{x_i(t)} u dx = \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial u}{\partial t} dx + \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u\frac{dx}{dt}\right) dx.$$

aking the original partial differential equation $\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(u^4\frac{\partial u}{\partial x}\right)$ and substituting for $\frac{\partial u}{\partial t}$ in the above equation gives

$$\begin{aligned}\frac{d}{dt}\int_{x_{i-1}(t)}^{x_i(t)} u dx &= \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u^4\frac{\partial u}{\partial x}\right) dx + \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u\frac{dx}{dt}\right) dx \\ &= \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u^4\frac{\partial u}{\partial x} + u\frac{dx}{dt}\right) dx.\end{aligned}$$

Now let $\frac{dx}{dt} = \frac{\partial \phi}{\partial x}$, where ϕ is a velocity potential. he above equation then becomes

$$\begin{aligned}\frac{d}{dt}\int_{x_{i-1}(t)}^{x_i(t)} u dx &= \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u^4\frac{\partial u}{\partial x} + u\frac{\partial \phi}{\partial x}\right) dx \\ &= \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u\left[u^3\frac{\partial u}{\partial x} + \frac{\partial \phi}{\partial x}\right]\right) dx \\ &= \int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u\frac{\partial}{\partial x}\left[\frac{u^4}{4} + \phi\right]\right) dx.\end{aligned}$$

Suppose that $\frac{dx}{dt}$ is such that $\frac{d}{dt}\int_{x_{i-1}(t)}^{x_i(t)} u dx = 0$.

hen

$$\int_{x_{i-1}(t)}^{x_i(t)} \frac{\partial}{\partial x}\left(u\frac{\partial}{\partial x}\left[\frac{u^4}{4} + \phi\right]\right) dx = 0. \tag{6.1}$$

A solution of (6.1) for which $\phi = 0$ when $u = 0$ which is

$$\frac{u^4}{4} + \phi = 0.$$

aking $\phi = -\frac{u^4}{4}$ and $\frac{dx}{dt} = \frac{\partial \phi}{\partial x}$, gives

$$\frac{dx}{dt} = -u^3 \frac{\partial u}{\partial x}$$

everywhere. his equation tells us how the grid points move such that the area under the graph of u between each pair of points remains constant for all time.

6.2 Implementing this Method

6.2.1 Integrating using Fourth Order Runge-Kutta [14]

ake an initial condition and a grid equally spaced over the domain of this initial condition. Calculate the inital areas under the graph of u between grid points using the trapezium rule,

$$A_i = \frac{1}{2}\left(x_i - x_{i-1}\right)\left(u(x_i) + u(x_{i-1})\right).$$

hese areas should remain fixed,approximately, for the rest of the problem. Integrate $\frac{dx}{dt} = -u^3 \frac{\partial u}{\partial x} = f(x)$ using fourth order Runge-Kutta.

$$\begin{aligned}
x_i^{n+1} - x_i^n &= \frac{\Delta t}{6}\left(K_1 + 2K_2 + 2K_3 + K_4\right) \\
K_1 &= f\left(x_i^n\right) \\
K_2 &= f\left(x_i^n + \frac{\Delta t}{2} K_1\right) \\
K_3 &= f\left(x_i^n + \frac{\Delta t}{2} K_2\right) \\
K_4 &= f\left(x_i^n + \Delta t K_3\right)
\end{aligned}$$

he derivative $\frac{\partial u}{\partial x}$ required in the function f can be calculated analytically provided the initial condition is differentiable. he solution given by the Runge-Kutta method gives the new grid points. he solution at these grid points can be constructed using the trapezium rule since the area between grid points has remained unchanged. he solution at the boundaries is known to be zero since the grid points are moving such that they always exactly cover the whole domain of the solution. Hence we have

$$u_i = \frac{2A_i}{x_i - x_{i-1}} - u_{i-1}. \tag{6.2}$$

his process must now be repeated each time step until the end time has been reached. However, we now do not have an analytic function for u and hence cannot find $\frac{\partial u}{\partial x}$ analytically. Instead, we use an upwind finite difference, given by

$$\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_i - u_{i-1}}{x_i - x_{i-1}} \qquad x_i > 0$$

$$\left.\frac{\partial u}{\partial x}\right|_i = \frac{u_{i+1} - u_i}{x_{i+1} - x_i} \qquad x_i < 0. \tag{6.3}$$

he differential equation $\frac{dx}{dt} = -u^3 \frac{\partial u}{\partial x} = f(x)$ is then solved as before using fourth order Runge-Kutta. Where the function in the Runge-Kutta method needs to be evaluated at x values that are not exact grid points (for example, $x_i^n + \frac{\Delta t}{2} K_{1(i)}$ will not be on a grid point) then the value of u at this point should be found using linear interpolation on the values of u at the grid points on either side of this point. he value of $\frac{\partial u}{\partial x}$ should be found numerically as given in equation (6.3) but using $u(x_i^n + \frac{\Delta t}{2} K_{1(i)})$ and $u(x_{i-1}^n + \frac{\Delta t}{2} K_{1(i-1)})$ in the case where $x_i^n + \frac{\Delta t}{2} K_{1(i)} > 0$ and $u(x_i^n + \frac{\Delta t}{2} K_{1(i)})$

and x^1 are now known and the backward differentiation scheme can be used to find the values of x_i at all following time steps.

Since $f(x_i^{n+1})$ is not known, the scheme must be iterated as

$$(x_i^{n+1})^{p+1} - \frac{4}{3}x_i^n + \frac{1}{3}x_i^{n-1} = \frac{2}{3}\Delta t f((x_i^{n+1})^p).$$

Here, p is the iteration count and $(x^{n+1})^0$ is taken as x^n. he iteration is repeated until $|(x^{n+1})^{p+1} - (x^{n+1})^p|$ is within a specified range and we have convergence.

6.3 Results

6.3.1 Evolution of Various Initial Conditions

Figure 11 shows the evolution of the solution with non-self-similar initial data

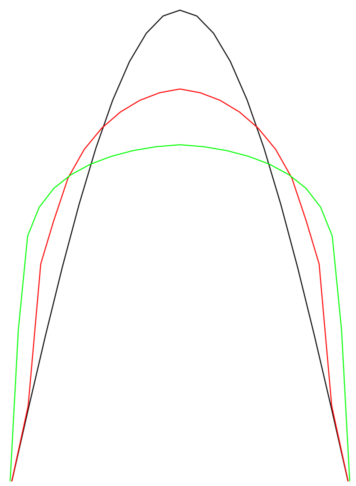
$$u = \begin{cases} \cos\left(\frac{\pi x}{2}\right) & \text{for } |x| < 1 \\ 0 & \text{for } |x| \geqslant 1 \end{cases}$$

using the fourth order Runge Kutta method to do the integration.

Figure 12 shows the evolution of the solution with self-similar initial data

$$u = \begin{cases} \left(1 - \frac{x^2}{3}\right)^{\frac{1}{4}} & \text{for } x^2 < 3 \\ 0 & \text{for } x^2 \geqslant 3 \end{cases}$$

using the second order backward differentiation method to do the integration.



6.3.2 The Self-Similar Solution as an Attractor for the Numerical Solution

As with the static mesh methods, the numerical solution should hopefully

6.3.3 Accuracy of the Numerical Solution

By using the analytic solution at time $t = 1$, the numerical evolution of this solution can be compared to the analytic evolution to find a percentage error in the numerical solution at final time. he initial condition is

$u = 1 - \left(x^2 \right.$

the numerical solution to depend on data on which the physical solution does not depend.

6.3.4 Conservation of the Integral

If the method used is conservative then it is expected that the integral of the solution will remain constant. It will probably not be equal to the analytic integral due to the discretisation in space. Using the initial condition $u = \cos\left(\frac{\pi x}{2}\right)$, the analytic integral is $\frac{2}{\pi}\left[\sin\left(\frac{\pi x}{2}\right)\right]_{-1}^{1} = \frac{4}{\pi} = 1.27324$.

Method			ime	Integral
Analytic				1.27324
Conservation Form	Explicit u^4		$t = 0$	1.27321
			$t = 10$	1.27321
	Implicit u^4	Picard	$t = 0$	1.27321
			$t = 10$	1.27321
		Newton	$t = 0$	1.27321
			$t = 10$	1.27321
Non-Conservation Form	Central Difference		$t = 0$	1.27321
			$t = 10$	1.05728
	Upwind Difference		$t = 0$	1.27321
			$t = 10$	1.23091
Moving Mesh	RK4		$t = 0$	1.27321
			$t = 10$	1.27321
	BDF2		$t = 0$	1.27321
			$t = 10$	1.27321

he static mesh methods all have $\Delta x = 0.01$ and the moving mesh method has an initial regular mesh with $\Delta x = 0.01$. he moving mesh method is based on the area under the solution curve remaining constant between each grid point so must conserve the integral of the solution. he numerical methods based on the PDE in conservation form are shown to be conservative, as expected.

7 Conclusions

For this dissertation, I have looked mainly at a number of different numerical schemes that can be used to solve the non-linear diffusion equation.

Initially, I investigated scale invariance and how it was used to obtain a family of self-similar solutions to the problem. his family of solutions acted as an attractor for more general solutions.

I have looked at different static mesh methods for solving the equation in both conservation form and non-conservation form. I also looked at a moving mesh method.

In conservation form, I used the Crank-Nicolson scheme with three different solvers. First, the equation was linearised in u^{n+1} and a standard solver used. he fully non-linear equation was then solved using Picard iteration and the Newton-Raphson method.

In non-conservation form, the equation was linearised in u^{n+1} and both up-wind and central differences were used in the scheme.

All the static mesh methods have also been applied to the case where the diffusion coefficient is not known analytically but is in the form of a table of values.

For the moving mesh method, the integral of the solution is kept constant between consecutive grid points throughout the entire calculation and this fact is used to form an ordinary differential equation which can be solved to give the new positions of the grid points at the next time step. his differential equation was solved in two different ways, using fourth order Runge-Kutta and using second order backward differentiation with the initial values given by second order Runge-Kutta.

All the methods carried the property of the analytic solution that a general solution should tend to the self-similar solution. Even an oscillatory initial condition remains sandwiched by two self-similar solutions for all methods.

8 Further Work

he most successful method considered here is the Newton-Raphson method. However, this req

(b) Compute the preconditoned Krylov vector, $J\tilde{M}^{-1}\mathbf{v}$, using a multigrid cycle to approximate the solution to $A\mathbf{y}_n = \mathbf{v}_n$.

(c) Perform the matrix-vector multiply through the operation $\mathbf{w}_n = \dfrac{F(\mathbf{u} + \epsilon \mathbf{y}_n) - F(\mathbf{u})}{\epsilon}$.

(d) Complete the Krylov iteration, $\mathbf{v}_{n+1} = \dfrac{\mathbf{w}_n}{||\mathbf{w}_n||_2}$ and compute convergence. If converged, exit, otherwise $n := n + 1$ and go to (b).

3. Compute the update to the full nonlinear problem.

4. Check for nonlinear convergence. If converged, exit; otherwise, $k := k + 1$ and go to 2.

his method proves to be more accurate than the standard Crank-Nicolson method with Picard iteration. Figure 15 from [7] shows the propogation of a one dimensional radiation heat wave (also referred to as a Marshak wave [15]). he system was run using four different solvers, backward Euler with Picard iteration, Crank-Nicolson with Picard iteration, backward Euler with Newton-Krylov iteration and Crank-Nicolson with Newton-Krylov iteration. It is obvious from this graph that the solutions using Newton-Krylov iteration are much closer to the exact solution than those using Picard iteration.

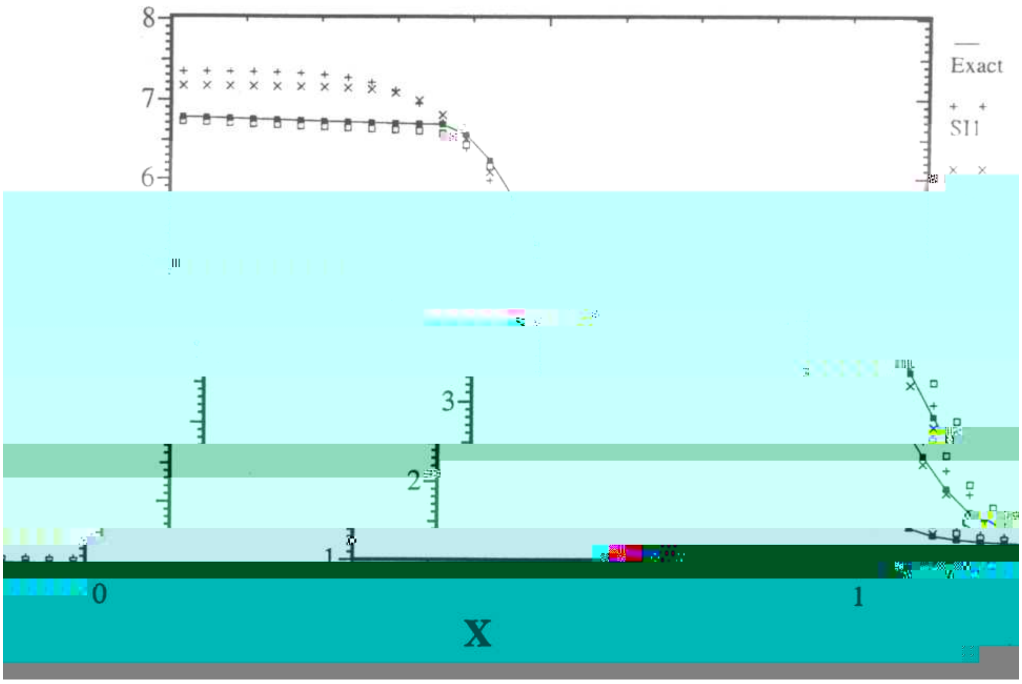


Figure 15: he one-dimensional Marshak wave problem used to demonstrate the accuracy of various non-linear iterative techniques.

References

[1] D.J. ritton. *Physical Fluid Dynamics.* Oxford Science Publications, 1988.

[2] K.W.Morton & D.F.Mayers. *Numerical Solution of Partial Differential Equations.* Cambridge University Press, 1994.

[3] J.D.Murray. *Mathematical Biology.* Springer Verlag, 1989.

[4] C.J.Budd & M.D.Piggott. *Geometric Integration and its Applications*, Handbook of Numerical Analysis Vol XI (2003), 35-135.

[5] C.J.Budd, G.J.Collins, W.Huang & R.D.Russell. *Self-Similar Numerical Solutions of the Porous-Medium Equation using Moving Mesh Methods*, Phil. rans. R. Soc. Lond. A (1999) 357, 1047-1077.

[6] P.J.Capon. *Adaptive Stable Finite Element Methods for the Compressible Navier-Stokes Equation.* PhD hesis, University of Leeds, 1995.

[7] W.J.Rider, D.A.Knoll & G.L.Olson. *A Mulitgrid Newton-Krylov Method for Multimaterial Equilibrium Radiation Diffusion*, Journal of Computational Physics (1999) 152, 164-191.

[8] G.I.Barenblatt. *Scaling, Self-Similarity and Intermediate Asymptotics.* Cambridge University Press. 1996.

[9] http://mathworld.wolfram.com/LeastSquaresFitting.html

[10] [illegible]

[12] B.V.Wells. *A Moving Mesh Finite Element Method for the Numerical Solution of Partial Differential Equations and Systems.* PhD hesis, Univeristy of Reading, 2004.

[13] Y.Saad. *Iterative Methods for Sparse Linear Systems.* PWS Publishing Co., Boston, 1996.

Available online at: http://www-users.cs.umn.edu/~saad/books.html

[14] K.W.Blake. *Moving Mesh Methods for Nonlinear Parabolic Partial Differential Equations.* PhD hesis, University of Reading, 2001.

[15] S.L.Lee, C.S.Woodward, F.Graziani. *Analyzing Radiation Diffusion using Time-Dependent Sensitivity-Based Techniques.* March 13 2003.

Available online at: http://www.llnl.gov/CASC/nsde/pubs/diffusion_sens.pdf