Time-Step Constraints for Reaction-Diffusion Problems

Daniel Fortunato*
daniel.fortunato@tufts.edu

Abstract

Reaction-diffusion equations naturally arise in many biological, physical, chemical, and ecological contexts. Fisher's equation is the simplest reaction-diffusion equation. It models a population growing logistically while diffusing in space and admits traveling wave solutions. We consider finite difference schemes for Fisher's equation, which depend on the size of the time step Δt used. We can discretize Fisher's equation using explicit methods (like forward Euler or midpoint) or implicit methods (like backward Euler or Crank-Nicolson). For the explicit methods, a time step constraint appears as the result of a CFL condition. For backward Euler, there is no time step constraint. However, to solve the nonlinear system of equations with Newton's method or fixed-point iteration, the constraint reappears as a convergence constraint. If instead we use multigrid to solve the nonlinear system of equations, the constraint comes back as a convergence constraint for both the correction scheme (CS) and the full approximation scheme (FAS). If in the relaxation scheme for FAS we solve the nonlinear equations exactly—which the simplicity of Fisher's equation allows us to do—then the constraint appears once again as an accuracy constraint. Crank-Nicolson is unconditionally stable and second-order in time, so discretizing Fisher's equation using Crank-Nicolson and then using FAS to solve the system of equations relaxes the accuracy constraint somewhat.

*Tufts University, 2013

Contents

1 Introduction

Reaction-diffusion equations possess interesting properties that make them unique to study from both a numerical and an analytical point of view. Logistic population growth in the presence of spatial diffusion causes solutions to such equations to look like traveling waves, spreading out like ripples through the population. The physical applications of reaction-diffusion equations are far-reaching; such equations can describe many of the dynamics found in nature, from chemical reactions, to biological processes, to ecological patterns, to geological events. Thus, understanding the limits to numerically solving these types of equations is of utmost importance to many scientists.

Fisher's equation is a good model equation to study in order to understand these limits. It is the simplest example of a reaction-diffusion equation. It describes how a population acts in the presence of logistic growth and spatial diffusion. Specific applications of Fisher's equation also arise when modeling the spread of dominant gene alleles in a population of a particular species. If a mutation occurs in a gene of one organism, and the population reproduces logistically, then Fisher's equation describes how the gene mutation will spread throughout the population.

Solutions to Fisher's equation look like traveling waves. In Section 2 of the paper, we will derive some properties of the wave-like solution, including the minimum speed of the wave and the steepness of the wavefront.

Constraints on the time step required to solve the equation depend on the methods used to solve it. In Section 3, we will derive time step constraints on each term of Fisher's equation separately when solving the equation with explicit methods, and then compare the constraints numerically to the overall constraint when both terms are present. In Section 4, we will derive similar constraints for solving the logistic equation implicitly, and again compare them numerically to the full Fisher equation. Section 5 describes our numerical results using the multigrid method to solve Fisher's equation.

2 Fisher's Equation

Fisher's equation describes the propagation of gene alleles in a population of animal species. The spread of a gene mutation is modeled by a diffusion term and reaction term in the following partial differential equation (PDE):

$$u_t = \varepsilon u_{xx} + ru(1-u) \tag{$*$}$$

with $0 < u < 1$, $r > 0$, and $\varepsilon > 0$.

2.1 Traveling Wave Solutions and Stability

Let's look for traveling wave solutions to $(*)$. A function $u(x,t)$ is a traveling wave if there exists a reference frame moving with speed c such that $V(z) = u(x,t)$ with $z = x - ct$ (or $z = x + ct$ for motion in the opposite direction). Writing $V(z) = u(x,t)$ with $z = x - ct$ yields the second-order ordinary differential equation (ODE)

$$-cV' = \varepsilon V'' + rV(1-V).$$

We can write this as a system of two first-order ODEs:

$$\begin{aligned} V' &= -W \\ W' &= -\frac{c}{\varepsilon}W + \frac{r}{\varepsilon}V(1-V) \end{aligned} \tag{2.1}$$

Let's analyze this system by looking at nullclines in the V-W plane. Setting $V' = 0$ and $W' = 0$, (2.1) becomes

$$\begin{aligned} W &= 0 \\ W &= \frac{r}{c}V(1-V) \end{aligned}$$

Thus the nullclines intersect at the points $(V_1, W_1) = (0, 0)$ and $(V_2, W_2) = (1, 0)$. The Jacobian of (2.1) is given by

$$J = \begin{bmatrix} 0 & -1 \\ \frac{r}{\varepsilon}(1 - 2V) & -\frac{c}{\varepsilon} \end{bmatrix}$$

So at the two points of intersection we have

$$J\Big|_{(V_1,W_1)} = \begin{bmatrix} 0 & -1 \\ \frac{r}{\varepsilon} & -\frac{c}{\varepsilon} \end{bmatrix}$$

and

$$J\Big|_{(V_2,W_2)} = \begin{bmatrix} 0 & -1 \\ -\frac{r}{\varepsilon} & -\frac{c}{\varepsilon} \end{bmatrix}$$

To determine the stability of the points, we compute the eigenvalues of the Jacobian at each point. For (V_1, W_1), the eigenvalues are

$$\lambda_{\pm} = \frac{-c \pm \sqrt{c^2 - 4r\varepsilon}}{2\varepsilon}$$

and so (V_1, W_1) is a stable node provided that $c^2 - 4r\varepsilon > 0$, or $c > 2\sqrt{r\varepsilon}$. For (V_2, W_2), the eigenvalues are

$$\lambda_{\pm} = \frac{-c \pm \sqrt{c^2 + 4r\varepsilon}}{2\varepsilon}$$

and so (V_2, W_2) is a saddle point.

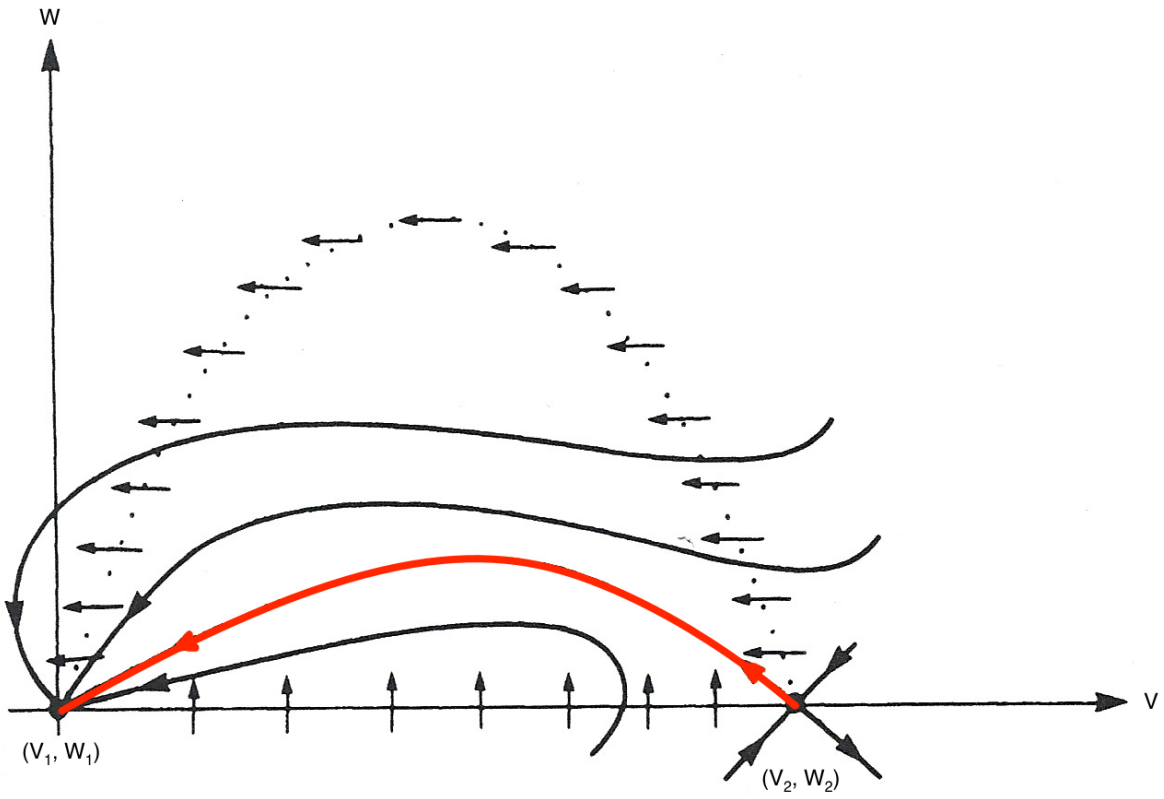


Figure 1: The V-W plane. The heteroclinic trajectory is marked in red. This is the tracjectory from $(V_2, W_2) = (1, 0)$ to $(V_1, W_1) = (0, 0)$, and is the only trajectory with a meaningful biological interpretation. This figure is adapted from [3].

Observe that for the solution to have a meaningful biological interpretation, the following conditions must be satisfied:

$$V(z) \to 1 \text{ as } z \to -\infty \tag{2.2a}$$
$$V(z) \to 0 \text{ as } z \to +\infty \tag{2.2b}$$
$$0 < V(z) < 1 \text{ for all } z \tag{2.2c}$$

A function V satisfying these conditions has a shape of a moving wavefront. Condition (2.2a) says that the mutated gene has become dominant in the left part of the domain, and condition (2.2b) says that the mutated gene has not yet reached the right part of the domain. There is only one nontrivial bounded trajectory that satisfies these conditions. This is the heteroclinic trajectory (marked in red in the figure above) in the V-W phase plane, emanating from $(V_2, W_2) = (1, 0)$ and going to $(V_1, W_1) = (0, 0)$. It satisfies these conditions provided that $c > 2\sqrt{r\varepsilon}$. So the minimum wave speed must be

$$c_{\min} = 2\sqrt{r\varepsilon}$$

2.2 Steepness of the Traveling Wave

Let's see if we can compute the steepness of the traveling wavefront explicitly, in terms of r and ε. With the steepness of the wave known, we can compute a reasonable size for the spatial step Δx needed to resolve the wavefront.

$$\begin{aligned} W' &= \frac{1}{\varepsilon}(rV(1-V) - cW) \\ &= \frac{1}{\varepsilon}(rV(1-V) - 2\sqrt{r\varepsilon}W) \\ &= \frac{r}{\varepsilon}V(1-V) - 2\sqrt{\frac{r}{\varepsilon}}W \end{aligned}$$

In the V-W plane, $W' = 0$ at $V = \frac{1}{2}$.

$$\begin{aligned} & W' = \frac{r}{\varepsilon}V(1-V) - 2\sqrt{\frac{r}{\varepsilon}}W = 0 \\ \Leftrightarrow \quad & W = \frac{1}{2}\sqrt{\frac{\varepsilon}{r}}\left(\frac{r}{\varepsilon}\right)\frac{1}{4} \\ \Leftrightarrow \quad & W = \frac{1}{8}\sqrt{\frac{r}{\varepsilon}} \end{aligned}$$

So the steepness of the traveling front at $z = 0$ in Fisher's equation is given by $V'(0) = W(0) = \frac{1}{8}\sqrt{\frac{r}{\varepsilon}}$.

3 Stability Constraints of Explicit Time Differencing

We first examine the constraints imposed on the time step when solving the equation using an explicit scheme, such as forward Euler or the midpoint method. We treat each term of Fisher's equation separately to derive the constraints analytically, and then compare them numerically to the actual constraint when both terms are present in the equation.

3.1 Diffusive Time-Step Constraint

We first consider the diffusion term: $u_t = \varepsilon u_{xx}$. Let's analyze the constraint on Δt when solving this equation using the midpoint method.

Proposition 3.1. *The diffusive time step constraint for the midpoint method is*

$$\Delta t \leq \frac{1}{2}\frac{\Delta x^2}{\varepsilon}.$$

Proof. The midpoint method is given by

$$\begin{aligned} u_{k+1/2} &= u_k + \frac{\Delta t}{2}Au_k \\ u_{k+1} &= u_k + \Delta t A\left(u_k + \frac{\Delta t}{2}Au_k\right) \\ &= \left(I + \Delta t A + \frac{\Delta t^2}{2}A^2\right)u_k \end{aligned}$$

Here A is given by

$$A = \frac{\varepsilon}{\Delta x^2}\begin{bmatrix} 1 & -2 & 1 \end{bmatrix}$$

where the notation inside the brackets denotes the entries along the sub-, main, super-diagonals of A, and all other entries in A are zero. Then A^2 is

$$A^2 = \frac{\varepsilon^2}{\Delta x^4}\begin{bmatrix} 1 & -4 & 6 & -4 & 1 \end{bmatrix}$$

and

$$I + \Delta t A + \frac{\Delta t^2}{2} A^2 = \begin{bmatrix} \frac{1}{2}\lambda^2 & -2\lambda^2 + \lambda & 3\lambda^2 - 2\lambda + 1 & -2\lambda^2 + \lambda & \frac{1}{2}\lambda^2 \end{bmatrix}$$
$$= \begin{bmatrix} \frac{\lambda^2}{2} & \lambda(1-2\lambda) & (\lambda-1)^2 + 2\lambda^2 & \lambda(1-2\lambda) & \frac{\lambda^2}{2} \end{bmatrix}$$

Suppose $(u_k)_j = (-1)^j$. Then

$$((I + \Delta t A + \frac{\Delta t^2}{2} A^2) u_k)_j = (3\lambda^2 - 2\lambda + 1 - 2\lambda(1-2\lambda) + \lambda^2)(-1)^j$$
$$= (8\lambda^2 - 4\lambda + 1)(-1)^j$$
$$= ((2\lambda - 1)^2 + 4\lambda^2)(-1)^j$$

If $\lambda = \frac{1}{2}$ then this quantity is still $(-1)^j$, but if $\lambda > \frac{1}{2}$ then this quantity is greater than $(-1)^j$ and some mode blows up. Since the discrete maximum principle holds if $\Delta t \leq \Delta x^2 / 2\varepsilon$, the claim holds. □

Now let's do the same analysis for the forward Euler method.

Proposition 3.2. *The diffusive time step constraint for forward Euler is*

$$\Delta t \leq \frac{1}{2} \frac{\Delta x^2}{\varepsilon}.$$

Proof. First, if $\Delta t \leq \frac{1}{2} \frac{\Delta x^2}{\varepsilon}$, then the discrete maximum principle holds for the diffusion equation. Second, suppose

$$u_{k,\ell} = (-1)^k.$$

Then using the forward Euler method,

$$u_{k,\ell+1} = (1 - 2\lambda) u_{k,\ell} + \lambda(u_{k+1,\ell} + u_{k-1,\ell})$$
$$= (-1)^k (1 - 4\lambda)$$

where $\lambda = \frac{\varepsilon \Delta t}{\Delta x^2}$. So if $\lambda > \frac{1}{2}$, or $\Delta t > \frac{1}{2} \frac{\Delta x^2}{\varepsilon}$ then some mode of $u_{k,\ell}$ blows up. Thus, the diffusive time step constraint for forward Euler is

$$\Delta t \leq \frac{1}{2} \frac{\Delta x^2}{\varepsilon}.$$

□

3.2 Reactive Time-Step Constraint

Now we consider the reaction term: $u_t = ru(1-u)$. Let's analyze the constraint on Δt when solving this equation using the midpoint method.

Proposition 3.3. *The reactive time step constraint for the midpoint method is*

$$\Delta t < 2/r.$$

Proof. The midpoint method is given by

$$u_{k+1/2} = u_k + \frac{\Delta t}{2} r u_k (1 - u_k)$$
$$u_{k+1} = u_k + \Delta t r u_{k+1/2} (1 - u_{k+1/2})$$

Now write u_{k+1} as a function of u_k:

$$u_{k+1} = u_k + \Delta t r \left(u_k + \frac{\Delta t}{2} r u_k (1 - u_k) \right) \left(1 - u_k - \frac{\Delta t}{2} r u_k (1 - u_k) \right)$$

That is,

$$u_{k+1} = g(u_k)$$

where

$$g(u) = u + 2\gamma\left(u + \gamma u(1-u)\right)\left(1 - u - \gamma u(1-u)\right)$$

with $\gamma = r\Delta t/2$. g has a fixed point at $u = 1$. Let's check if this fixed point is stable.

$$g(u) = (1 + 2\gamma + 2\gamma^2)u - (2\gamma + 6\gamma^2 + 2\gamma^3)u^2 + (4\gamma^2 + 4\gamma^3)u^3 - 2\gamma^3 u^4$$

$$g'(u) = (1 + 2\gamma + 2\gamma^2) - (4\gamma + 12\gamma^2 + 4\gamma^3)u + (12\gamma^2 + 12\gamma^3)u^2 - 8\gamma^3 u^3$$

Plugging in $u = 1$, we get

$$\begin{aligned} g'(1) &= (1 + 2\gamma + 2\gamma^2) - (4\gamma + 12\gamma^2 + 4\gamma^3) + (12\gamma^2 + 12\gamma^3) - 8\gamma^3 \\ &= 2\gamma^2 - 2\gamma + 1 \\ &= 2\gamma(\gamma - 1) + 1 \end{aligned}$$

So the fixed point is stable if $0 < \gamma < 1$ and unstable if $\gamma > 1$. That is, the fixed point is stable if $r\Delta t/2 < 1$, so

$$\Delta t < \frac{2}{r}.$$

This is the reactive time-step constraint.

□

Let's compare this with the time step constraint for forward Euler.

Proposition 3.4. *The reactive time step constraint for forward Euler is*

$$\Delta t < 1/r.$$

Proof. The forward Euler method is given by

$$u_{k+1} = u_k + r\Delta t\, u_k(1 - u_k).$$

Suppose $0 \leq u_k < 1$. We wish to find the conditions under which $u_{k+1} < 1$. Let $\gamma = r\Delta t$. Then our question is when is

$$\gamma u_k^2 - (1 + \gamma)u_k + 1 > 0.$$

The solutions of $\gamma u_k^2 - (1 + \gamma)u_k + 1 = 0$ are 1 and $1/\gamma$. If $1/\gamma > 1$, then $u_{k+1} < 1$ is guaranteed, but if $1/\gamma < 1$, then not. So the conditions under which $u_{k+1} < 1$ for all times is $\gamma < 1$, or

$$\Delta t < \frac{1}{r}.$$

□

3.3 Overall Constraint

We now seek to compare the time step constraints derived for each term with the actual time step constraint for solving Fisher's equation. First, let's look at using forward Euler. We expect the constraint required to solve Fisher's equation with forward Euler to be $\min(\Delta x^2/2\varepsilon, 1/r)$. When the diffusive constraint begins to become not satisfied, but the reactive constraint is still satisfied, our solution suffers from numerical error.

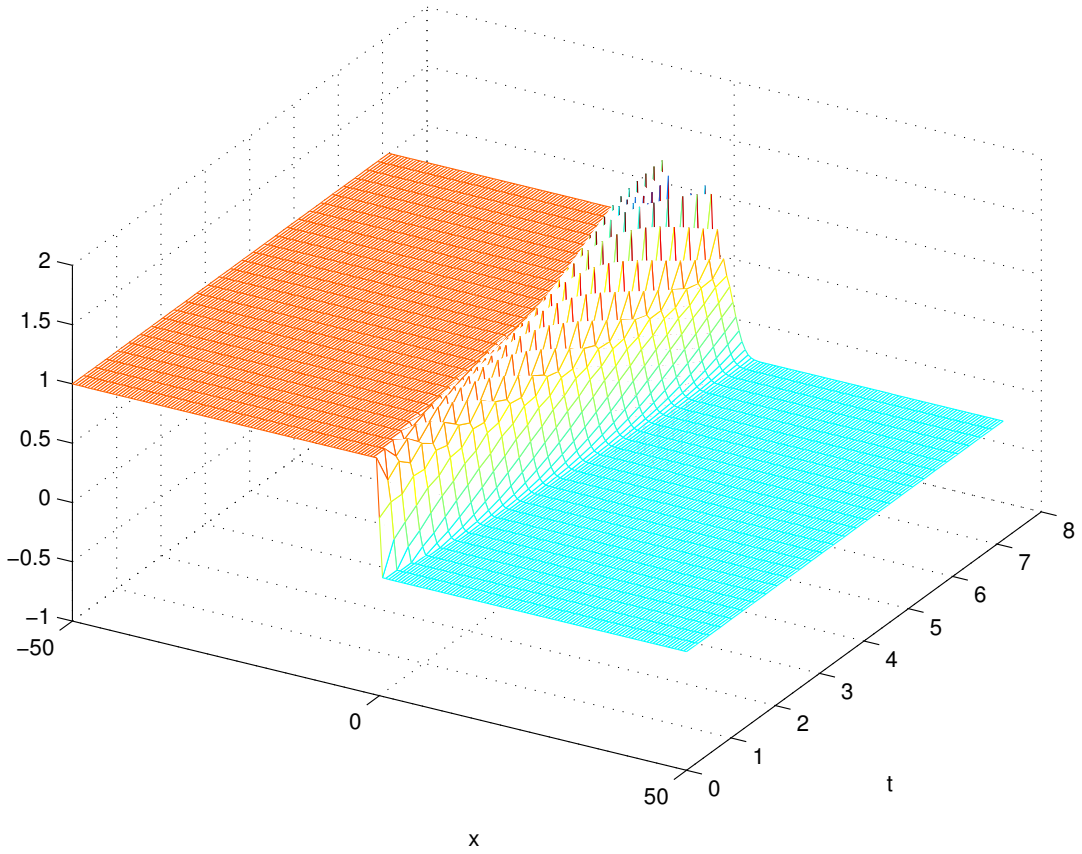


Figure 2: $\varepsilon = 0.5, r = 1$. Forward Euler. The diffusive constraint is not satisfied: $\Delta t = 0.51\Delta x^2/\varepsilon$.

When the reactive constraint is not satisfied, we get a similar picture.

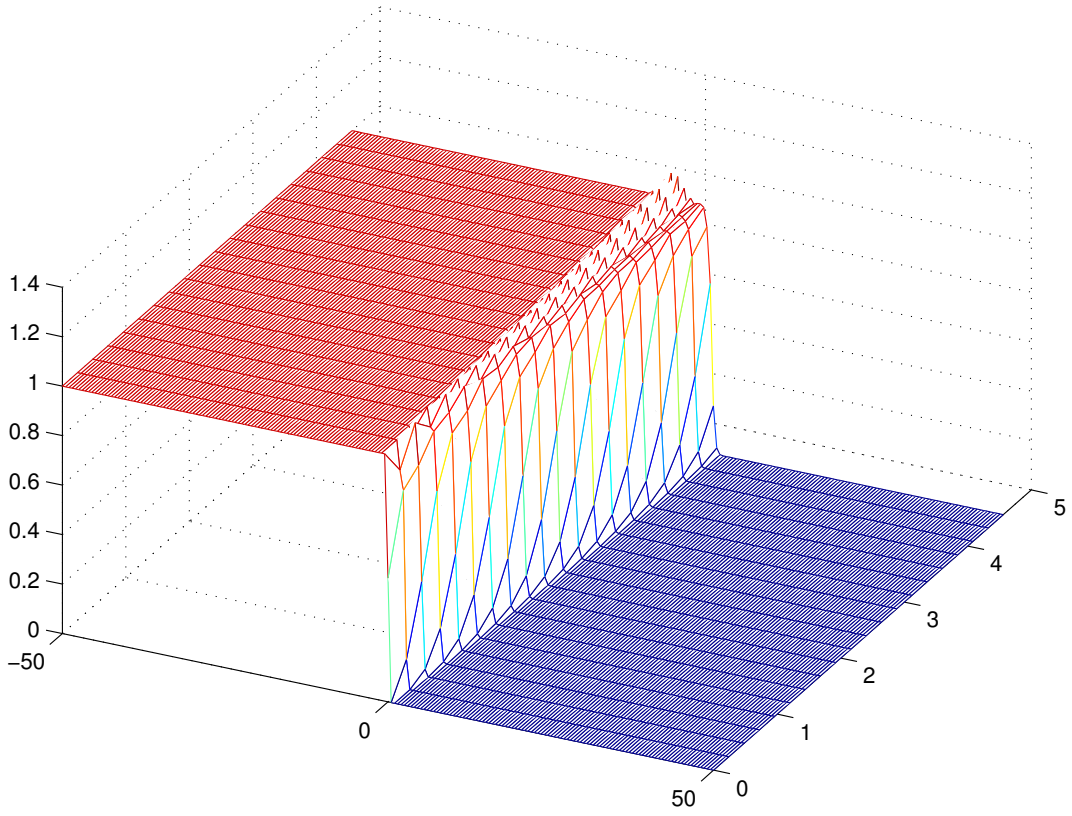


Figure 3: $\varepsilon = 0.25, r = 5$. Forward Euler. The reactive constraint is not satisfied: $\Delta t = 1.2/r$.

So the overall constraint for forward Euler is indeed the minimum of the constraint for the diffusive term and the constraint for the reactive term.

Now let's see if the same is true for the midpoint method. Again, we expect the time step required to solve Fisher's equation to be $\min(\Delta x^2/2\varepsilon, 2/r)$. If the diffusive constraint is not satisfied and the reactive constraint satisfied, then the computed solution overflows. On the other hand, if the diffusive constraint is satisfied but the reactive constraint not satisfied, the computed solution has large errors, as in Figure 4. However, errors are introduced into the computed solution even for some values of Δt below $2/r$. Errors appear for $\Delta t \approx 1.3/r$ and beyond. So the overall constraint is even more stringent than the reactive constraint.

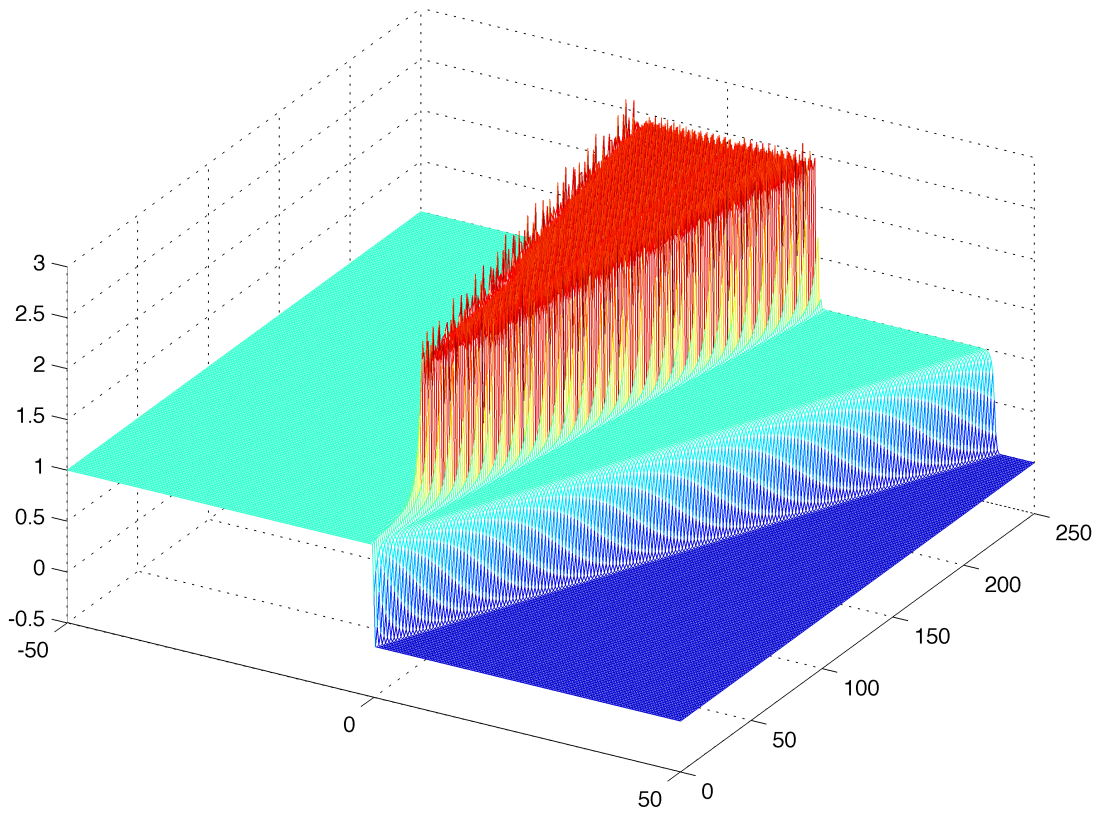


Figure 4: $\varepsilon = 0.01, r = 1$. Midpoint Method. Here the diffusive and reactive constraints are satisfied, but $\Delta t = 1.3/r$.

3.4 Comparison of Constraints

To see which of these constraints is more stringent, suppose that we wish to resolve the wave front so that a few grid points (say, 4) lie on the profile of the wave. That is, the wave front is neither over- nor under-resolved. We can find what Δx should be since we know the steepness of the wave. We need

$$\frac{1}{4\Delta x} = \frac{1}{8}\sqrt{\frac{r}{\varepsilon}}$$

or

$$\Delta x = 2\sqrt{\frac{\varepsilon}{r}}.$$

For this value of Δx, the diffusive time step constraint Δt_{diff} becomes

$$\Delta t_{\text{diff}} \leq \frac{1}{2}\frac{\Delta x^2}{\varepsilon} = \frac{1}{2}\frac{4\varepsilon/r}{\varepsilon} = \frac{2}{r}$$

and the reactive time step constraint Δt_{reac} is unchanged:

$$\Delta t_{\text{reac}} \leq \frac{2}{r}.$$

So Δt_{diff} and Δt_{reac} are approximately equal for a reasonably resolved wave front.

In general, if we resolve the wave profile with n grid points, then Δx is given by

$$\Delta x = \frac{8}{n}\sqrt{\frac{\varepsilon}{r}}.$$

If we choose to over-resolve the profile, say with 8 grid points this time, then $\Delta x = \sqrt{\frac{\varepsilon}{r}}$. So $\Delta t_{\text{diff}} = \frac{1}{2r} < \frac{2}{r} = \Delta t_{\text{reac}}$. Conversly, if we under-resolve the profile, say with 1 grid point, then $\Delta x = 8\sqrt{\frac{\varepsilon}{r}}$. So $\Delta t_{\text{diff}} = \frac{32}{r} > \frac{2}{r} = \Delta t_{\text{reac}}$.

4 Implicit Methods

We now examine what happens to the time step constraint if we use implicit discretization instead of explicit. Since the diffusive and reactive time step constraints are roughly equal—for a reasonable choice of Δx—by the analysis in Section 3.4, implicitly discretizing only the diffusion term won't help overcome the constraint. We must use implicit schemes on both terms.

4.1 Implicit Discretization of the Logistic Equation

As before, we consider the logistic equation

$$u_t = ru(1-u), \qquad u(0) = u_0$$

with $r > 0$ and $0 < u_0 < 1$. An implicit method such as backward Euler gets rid of the time step constraint, but the constraint reappears when using an iterative method like fixed-point iteration or Newton's method to solve the nonlinear equations in each time step.

Proposition 4.1. *The equation*

$$u_{k+1} = u_k + r\Delta t\, u_{k+1}(1-u_{k+1}). \tag{4.1}$$

defines the backward Euler method for the logistic equation.

(a) No time step constraint is introduced when using backward Euler to solve the logistic equation. That is, for any $r > 0$ and $u_k \in (0,1)$, $u_{k+1} \in (0,1)$ with no condition on Δt.

(b) Fixed point iteration for (4.1) locally converges to the solution if and only if

$$\Delta t \le \frac{1}{r}.$$

(c) Newton's method for (4.1) locally converges to the solution starting with initial guess $u_k \in (0,1)$ if and only if

$$\Delta t \le \frac{1}{r}.$$

Proof. Let $\gamma = r\Delta t$.

(a) u_{k+1} is obtained from u_k by solving the quadratic equation

$$\gamma u_{k+1}^2 + (1-\gamma)u_{k+1} - u_k = 0$$

for u_{k+1}. Assume that $u_k \in (0,1)$. The two solutions are

$$u_{k+1}^{\pm} = \frac{\gamma - 1 \pm \sqrt{(1-\gamma)^2 + 4\gamma u_k}}{2\gamma}.$$

We claim that $u_{k+1}^+ < 1$. To see this, note that $u_{k+1}^+ < 1$ if and only if

$$\begin{aligned} & \gamma - 1 + \sqrt{(1-\gamma)^2 + 4\gamma u_k} < 2\gamma \\ \Leftrightarrow \quad & \sqrt{(1-\gamma)^2 + 4\gamma u_k} < \gamma + 1 \\ \Leftrightarrow \quad & \gamma^2 - 2\gamma + 1 + 4\gamma u_k < \gamma^2 + 2\gamma + 1 \\ \Leftrightarrow \quad & u_k < 1 \end{aligned}$$

and so the claim holds.

(b) Fixed point iteration is given by

$$v_0 = u_k, \qquad v_{j+1} = \varphi(v_j), \qquad j = 0, 1, 2, \ldots$$

where

$$\varphi(v) = u_k + r\Delta t\, v(1-v).$$

The derivative of $\varphi(v)$ with respect to v is $r\Delta t(1-2v)$. For u_{k+1}^+ to be a stable fixed point, we need $|r\Delta t(1-2u_{k+1}^+)| \le 1$. This holds for all $u_k \in (0,1)$ if and only if $\Delta t \le 1/r$.

(c) We can rewrite (4.1) as

$$\gamma u_{k+1}^2 + (1-\gamma)u_{k+1} - u_k = 0.$$

Consider Newton's method to solve this for u_{k+1}, starting with initial guess u_k. The left-hand side of this equation is a function of u_{k+1} with a local minimum at $u^* = (\gamma-1)/(2\gamma)$. Note that $u_{k+1}^- < u^* < u_{k+1}^+$, so Newton's method, starting with an initial guess of u_k, will converge to u_{k+1}^+ if and only if $u_k > u^*$. But since this must hold for any $u_k \in (0,1)$, we must have that $u^* \le 0$. This means $(\gamma-1)/(2\gamma) \le 0$ or $\Delta t \le 1/r$.

□

4.2 Numerical Experiments for the Full Fisher Equation

The constraints we have derived above were only for the reaction term when viewed in isolation. We hope that the theoretical constraints will give us insight into the real constraint when both terms are present. So let's check to see if the constraint on the reactive term from the previous section gives rise to the same constraint when solving the full Fisher equation implicitly.

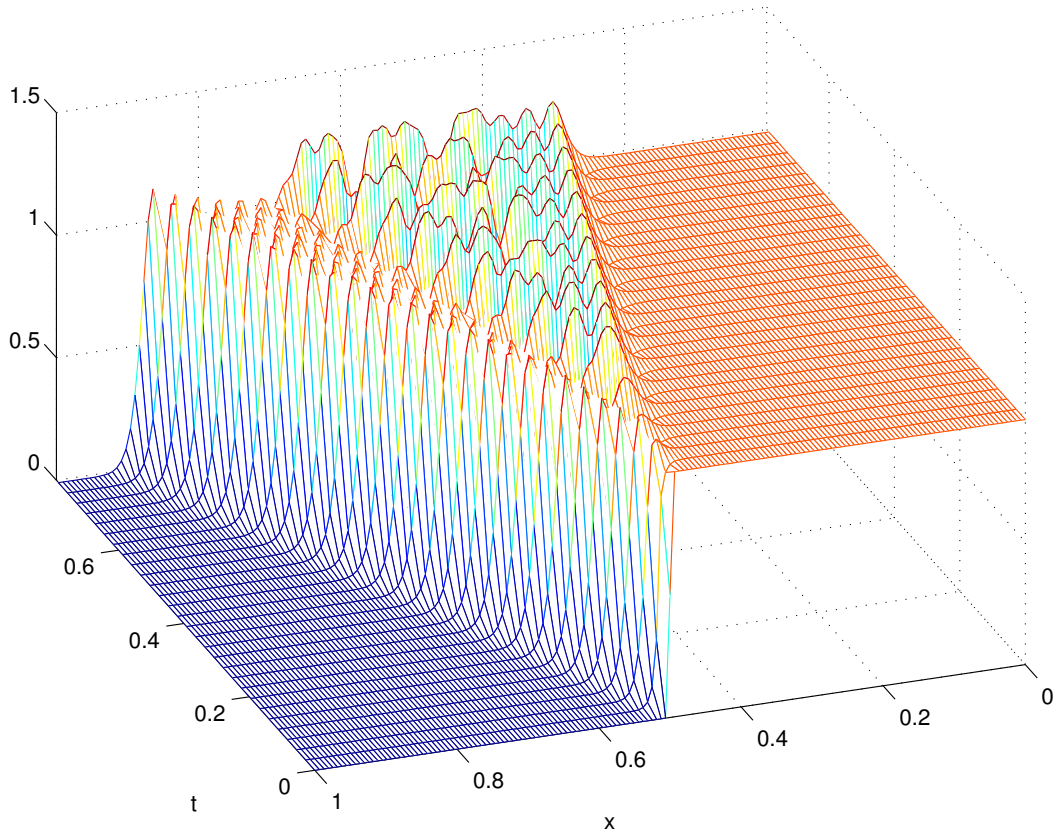


Figure 5: The reactive constraint is not satisfied. Here $\Delta t = 2.8/r$.

The constraint is not as stringent as our results above suggest, but nonetheless it is still there. We numerically found the value of Δt at which errors start to blow up to be roughly $\Delta t \approx 2/r$. This makes sense—the presence of the diffusion term has the effect of smearing out some of the error amplification that the reaction term introduces.

5 Fully Implicit Discretization with Multigrid

As we have discovered in the previous two sections, neither explicit nor implicit methods get rid of the time-step constraint needed to solve Fisher's equation. We now examine if the same is true for the correction or full approximation multigrid schemes. That is, we use the multigrid method to solve the system of nonlinear equations in each time step that arise from implicit discretization.

Let

$$A\mathbf{u} = \mathbf{f}$$

with $\mathbf{u}, \mathbf{f} \in \mathbb{R}^n$, $A \in \mathbb{R}^{n \times n}$ denote a system of (linear or nonlinear) algebraic equations. Let $\mathbf{u}$ denote the exact solution of this system and $\mathbf{v}$ denote an approximation to the exact solution. (The j-th component of a vector $\mathbf{u}$ is denoted by u_j.) The error $\mathbf{e}$ is given by $\mathbf{e} = \mathbf{u} - \mathbf{v}$, and the residual $\mathbf{r}$ is given by $\mathbf{r} = \mathbf{f} - A\mathbf{v}$. If A is linear, it then follows that $A\mathbf{e} = \mathbf{r}$; this is called the residual equation. We can use the residual equation to solve for the error $\mathbf{e}$, and then compute a new approximation from $\mathbf{u} = \mathbf{v} + \mathbf{e}$.

5.1 The Multigrid Method

We begin by defining the general two-grid procedure, as described in [2]. Let Ω^h be a regular uniform grid with mesh spacing $h > 0$. The notation of a superscript h denotes the grid on which the vector or matrix is defined.

- Relax ν_1 times on $A^h\mathbf{u}^h = \mathbf{f}^h$ on Ω^h with initial guess $\mathbf{v}^h$.
- Compute new approximation $\mathbf{v}^h$ from 5.3 or 5.4.
- Relax ν_2 times on $A^h\mathbf{u}^h = \mathbf{f}^h$ on Ω^h with initial guess $\mathbf{v}^h$.

5.2 Gauss-Seidel Relaxation

A relaxation method is an iterative method for solving systems of equations. In our experiments we use a red-black implementation of the Gauss-Seidel relaxation method to solve the equations in each time step. That is, we first sweep through the odd points in the grid and solve for the unknown at each point, using newly computed data as soon as it becomes available, and then sweep through the even points, again using newly computed data immediately.

5.3 Correction Scheme

If A is linear, it is guaranteed that $A(0) = 0$, and so the solution is a fixed point of the procedure. The correction scheme (CS) is guaranteed to converge to the solution when this is the case:

- Define $\mathbf{r}^{2h} = I_h^{2h}(\mathbf{f}^h - A^h\mathbf{v}^h)$.
- Solve $A^{2h}\mathbf{e}^{2h} = \mathbf{r}^{2h}$ for $\mathbf{e}^{2h}$.
- Set $\mathbf{v}^h \leftarrow \mathbf{v}^h + I_{2h}^h\mathbf{e}^{2h}$.

I_h^{2h} is a fine-to-coarse transfer operator from the fine grid with mesh spacing h to the coarse grid with mesh spacing $2h$. Similarly, I_{2h}^h is a coarse-to-fine transfer operator. The operators can be implemented using linear interpolation for a coarse-to-fine transfer and restriction either by direct injection or full weighting for a fine-to-coarse transfer (see [2]).

5.4 Full Approximation Scheme

In general it may not be true that $A(0) = 0$. Then CS is not guaranteed to converge, and A must be nonlinear. The previous residual equation no longer holds, since $\mathbf{u} - \mathbf{v} = \mathbf{e}$ does not imply that $A\mathbf{u} - A\mathbf{v} = A\mathbf{e}$. The residual equation we must use now instead is $A\mathbf{u} - A\mathbf{v} = \mathbf{r}$. The full approximation scheme (FAS) multigrid method always has the solution as a fixed point, and is given by:

- Define $\mathbf{r}^{2h} = I_h^{2h}(\mathbf{f}^h - A^h\mathbf{v}^h)$ and $\mathbf{v}^{2h} = I_h^{2h}\mathbf{v}^h$.
- Solve $A^{2h}\mathbf{u}^{2h} - A^{2h}\mathbf{v}^{2h} = \mathbf{r}^{2h}$ for $\mathbf{u}^{2h}$.
- Set $\mathbf{v}^h \leftarrow \mathbf{v}^h + I_{2h}^h(\mathbf{u}^{2h} - \mathbf{v}^{2h})$.

5.5 Analysis for the Logistic Equation

What happens if we use CS or FAS to solve the logistic equation? Strictly speaking, one cannot apply a multigrid scheme to the logistic equation, since it is only one question in one unknown. It useful to think of solving the logistic equation in this way though, since we can derive a theoretical bound on the time step.

FAS for the logistic equation simply means to directly solve the equation, and we can do it in one step since it's a quadratic. CS, on the other hand, is an iterative scheme. The logistic equation is given by

$$\frac{dx}{dt} = rx(1 - x)$$

or, upon implicit discretization,

$$\frac{x_{k+1} - x_k}{\Delta t} = r x_{k+1}(1 - x_{k+1}).$$

So

$$x_{k+1} - r\Delta t x_{k+1}(1 - x_{k+1}) = x_k.$$

Let

$$\begin{aligned}\varphi(x) &= x - r\Delta t x(1 - x) \\ &= x(1 - r\Delta t + r\Delta t x)\end{aligned}$$

So this says that $\varphi(x_{k+1}) = b$, where $b = x_k$. CS says to update x_{k+1} by

$$x_{k+1} \leftarrow x_{k+1} + \varphi^{-1}(b - \varphi(x_{k+1})).$$

Since $\varphi(0) = 0$, $\varphi^{-1}(b)$ is a fixed point of this iteration. Convergence requires that

$$\left| 1 + \frac{d}{dx}\varphi^{-1}\left(b - \varphi(x)\right) \right| < 1$$

or

$$\left| 1 - \frac{\varphi'(x)}{\varphi'(\varphi^{-1}\left(b - \varphi(x)\right))} \right| < 1$$

when evaluated at $x = \varphi^{-1}(b)$. At that point this becomes

$$\left| 1 - \frac{\varphi'(\varphi^{-1}(b))}{\varphi'(0)} \right| < 1.$$

Since $\varphi'(0) = 1 - r\Delta t$ and $\varphi'(\varphi^{-1}(b)) = 1 - r\Delta t + 2r\Delta t\varphi^{-1}(b)$, we obtain

$$\left| \frac{2r\Delta t\varphi^{-1}(b)}{1 - r\Delta t} \right| < 1$$

or

$$\left| \frac{2\varphi^{-1}(b)}{\frac{1}{r\Delta t} - 1} \right| < 1.$$

If all goes well, then $\varphi^{-1}(b)$ will eventually be 1, and so this constraint becomes

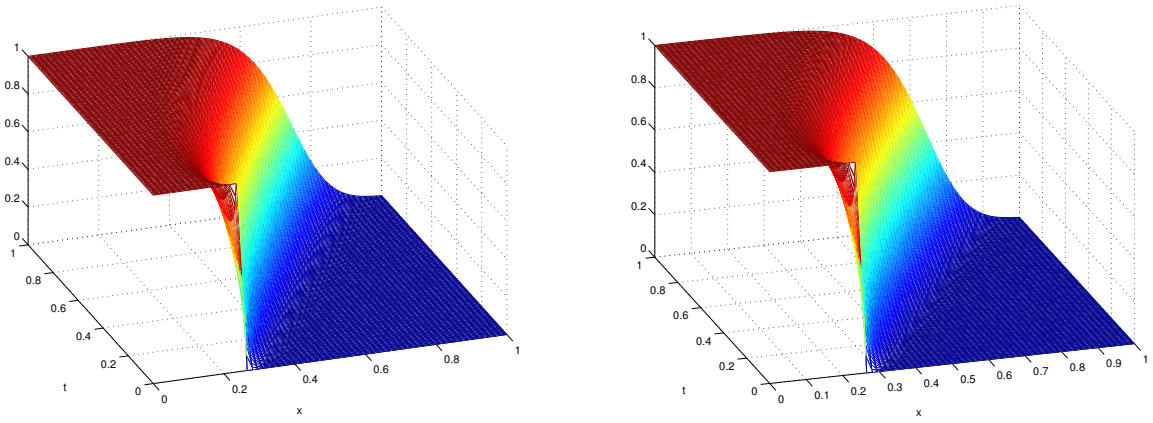
$$\Delta t < \frac{1}{3r}.$$

So a similar time step constraint is needed for CS to converge when solving the logistic equation. We expect this same constraint to appear when we solve the full Fisher equation with CS.

5.6 Numerical Results

We have computed solutions to Fisher's equation using both CS and FAS with multigrid W-cycles, having first discretized with backward Euler. It is worth noting that both schemes do indeed converge, but for different values of Δt. This is true because 0 is a solution to the equation with zero right-hand side. CS turns out to work slightly better than FAS for small values of Δt, whereas FAS computes a solution even for large Δt.

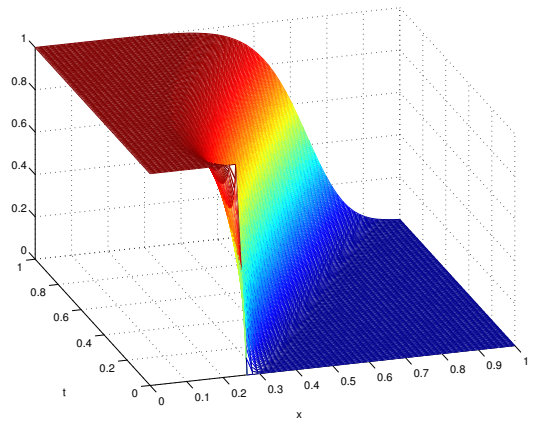
Note that we are interested in small ε and large r in these experiments. The reaction rate in many reaction-diffusion equations is very high, so testing the constraints for practical applications is our goal. The Hodgkin-Huxley PDEs [4] are one example of a reaction-diffusion equation for which the considerations of this paper could be applied.



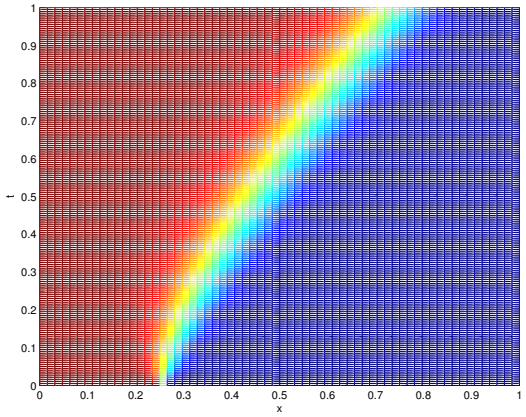
(a) CS (b) FAS

Figure 6: $\varepsilon = 0.01$, $r = 10$, $\Delta t = 0.005$.

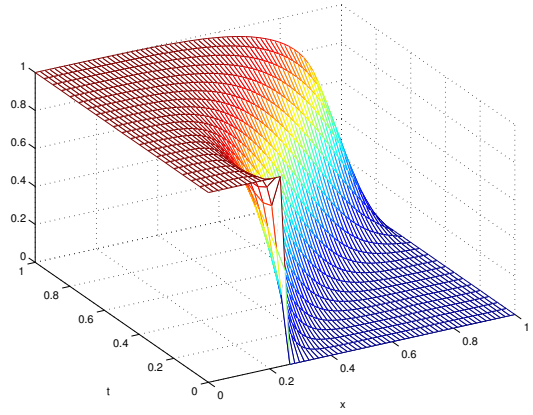
CS does not converge to a solution for large values of Δt. FAS, on the other hand, computes a reasonable picture even for large Δt. That is, it correctly captures the wave profile, but computes increasingly worse wave speeds as Δt gets larger.



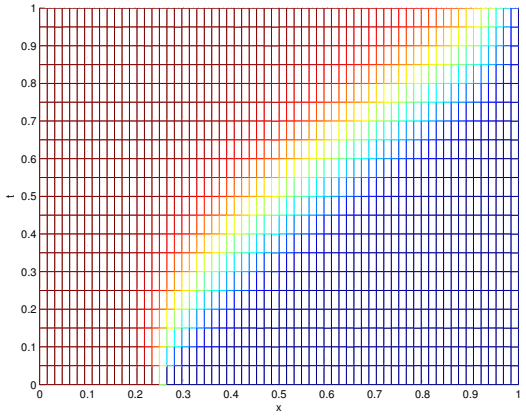
(a) $\Delta t = 0.005$



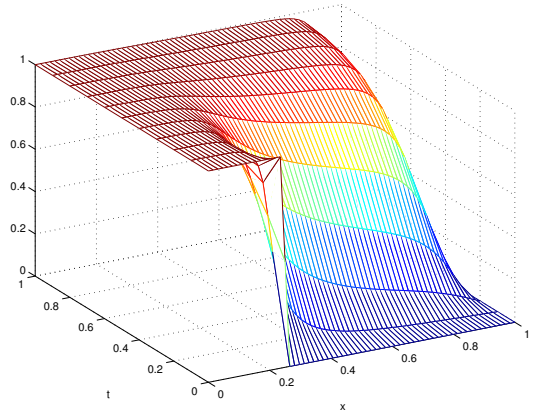
(b) Top view



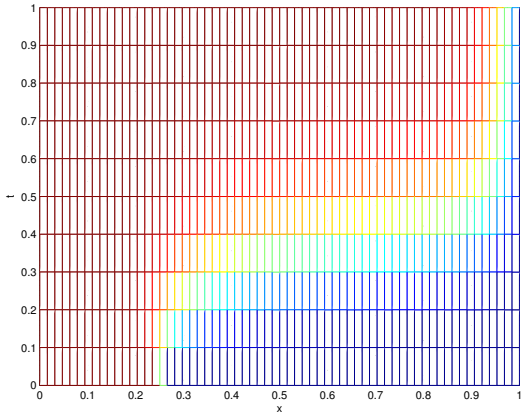
(c) $\Delta t = 0.05$



(d) Top view



(e) $\Delta t = 0.1$



(f) Top view

Figure 7: FAS with varying Δt. $N = 64$, $\varepsilon = 0.01$, $r = 10$. In (c), the wave speed is calculated to be slightly faster than it should be. In (e), the wave speed is completely wrong.

So, although FAS gets rid of the convergence constraint, there is still an accuracy constraint. We need the time step to be small to get the wave speed right. CS requires the time step to be small for convergence

to a solution, and this constraint turns out to be enough for accuracy to hold as well.

Next we discretize the equation using Crank-Nicolson instead of backward Euler, and then use FAS to solve the nonlinear equations in each time step. Since Crank-Nicolson is second-order in time, we expect that this method might more accurately capture the wave speed.

Figure 8 shows the results, using the same parameter values and time step sizes as Figure 7. In all three time step trials, the wave speed calculated using Crank-Nicolson is indeed more accurate than the one calculated from backward Euler. So using Crank-Nicolson with FAS loosens the accuracy constraint.

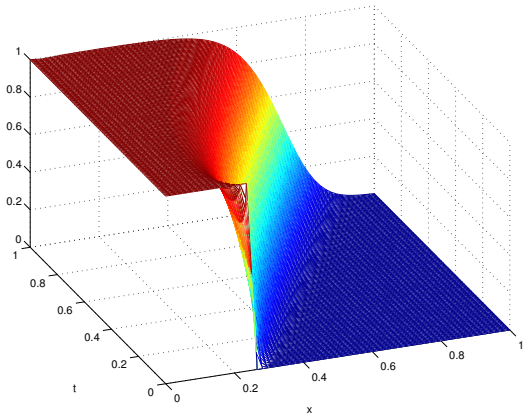
Table 1 shows approximate values of the accuracy constraint for different parameter values.

N	ε	r	FAS+BE	FAS+CN
64	0.01	1	0.1	0.1
64	0.01	10	0.05	0.1
64	0.1	10	0.05	0.05
32	0.01	10	0.01	0.1
32	0.1	10	0.01	0.01
32	0.01	20	0.001	0.1

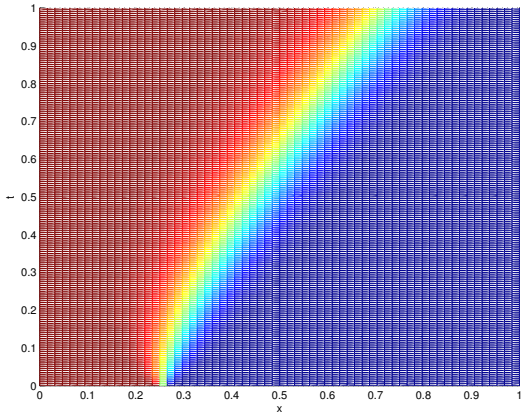
Table 1: Approximate values of Δt required to accurately calculate the wave speed for FAS, with different parameter values for N, ε, and r.

In both CS and FAS, each relaxation sweep involves solving a sequence of nonlinear equations. In the case of Fisher's equation, we can compute the solution to each equation directly, since each equation is a simple quadratic. However, for general reaction-diffusion equations the nonlinear equations which we must solve will not be so simple. Techniques such as Newton's method or fixed point iteration must be used, and the time-step constraint will become stringent once again, as a convergence constraint on these methods.

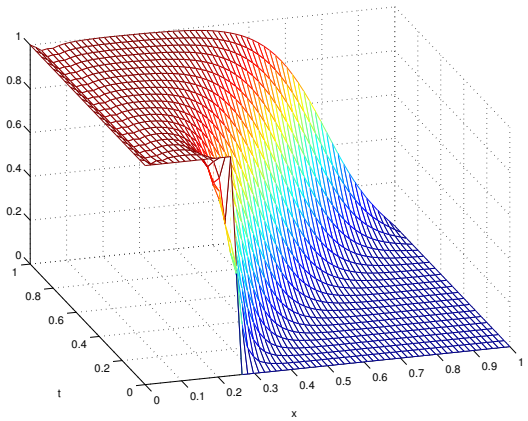
To see this, we perform an experiment. Instead of directly solving the quadratic equations each time we relax, we perform one step of Newton's method. If Δt is small—roughly anything below $\Delta t \approx 0.009$—then we get the correct solution, even when reaction is large.



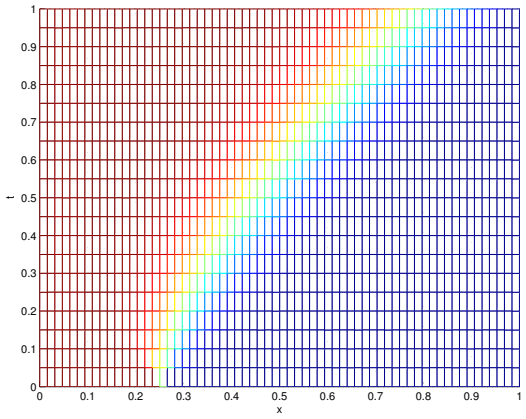
(a) $\Delta t = 0.005$



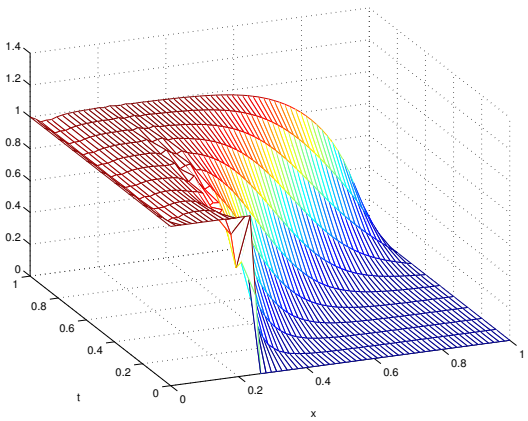
(b) Top view



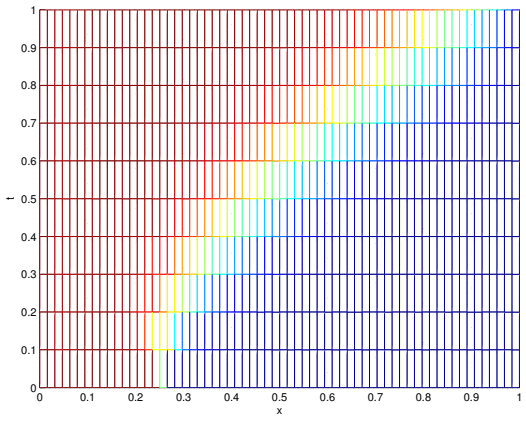
(c) $\Delta t = 0.05$



(d) Top view



(e) $\Delta t = 0.1$



(f) Top view

Figure 8: Crank-Nicolson method using FAS to solve the system of nonlinear equations at each time step, for varying Δt. $N = 64$, $\varepsilon = 0.01$, $r = 10$. In (c), the wave speed is quite accurate. In (e), the wave speed is slightly faster than it should be. Compare this to Figure 7.

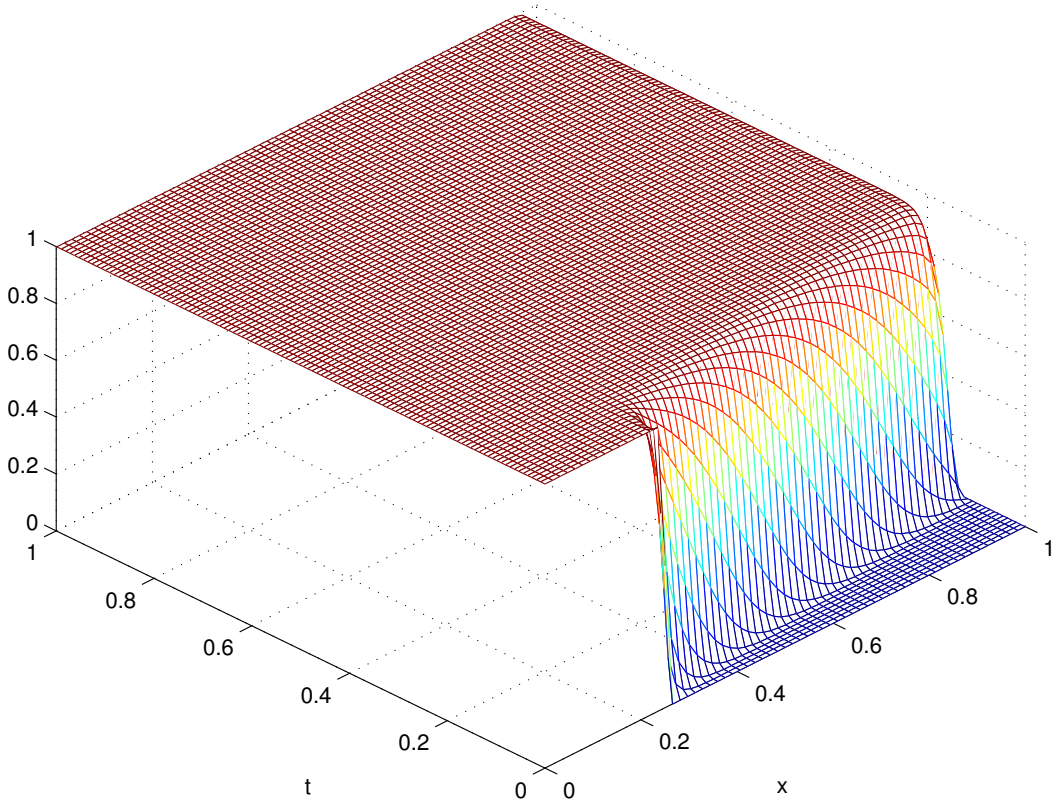


Figure 9: FAS using one step of Newton's method on each of the scalar nonlinear equations that we have to solve during a relaxation sweep. $\varepsilon = 0.0025$, $r = 100$, $\Delta t = 0.009$.

However, when $\Delta t \approx 0.01$, the relaxation step introduces errors into the approximate solution that yield complex numbers after directly solving the quadratic equation on the coarsest grid.

Table 2 summarizes the constraints on Δt required for CS and FAS with Newton's method to converge, for some different values of N, ε, and r.

N	ε	r	CS	FAS + Newton
64	0.01	1	0.25	1
64	0.01	10	0.03	0.01
64	0.01	100	0.006	0.01
64	0.1	1	0.2	1
64	0.1	10	0.02	0.01
64	0.1	100	0.002	0.01
32	0.01	1	0.3	1
32	0.01	10	0.05	0.1
32	0.01	100	0.007	0.009
32	0.1	1	0.3	1
32	0.1	10	0.02	0.01
32	0.1	100	0.005	0.01

Table 2: Approximate values of Δt required for convergence for CS and FAS with one step of Newton's method for relaxation, with different parameter values for ε and r. Note that there is no convergence constraint for FAS, since it always converges.

6 Discussion and Future Work

Both the accuracy constraints and convergence constraints for multigrid computed in the previous section are comparable to the constraints derived for the other methods in this paper. Most are on the order of $1/r$, and in many cases are much less than that. Thus, we haven't overcome the time step constraint with much success by implicitly discretizing Fisher's equation and then solving the nonlinear system with multigrid. Moreover, the nonlinearity in Fisher's equation is simple compared to nonlinearities in other reaction-diffusion equations. This simplicity allowed us to exactly solve the nonlinear equations in each relaxation sweep—something which is either impossible or unreasonably expensive to do in the general case.

A method which may provide solace from the ever-present time step constraint is exponential time differencing. Further investigation is required to understand if an accuracy constraint reappears when using this method as well.

Of course, it may not even be possible to overcome the constraint. We need $\Delta x/\Delta t$ to be at least as large as the wave speed, which is $2\sqrt{r\varepsilon}$. If we choose a reasonable Δx, as in Section 3.4, so that $\Delta x = 2\sqrt{\varepsilon/r}$, then $\Delta x/\Delta t \geq 2\sqrt{r\varepsilon}$ becomes

$$\Delta t \leq \frac{2\sqrt{\varepsilon/r}}{2\sqrt{r\varepsilon}} = \frac{1}{r}.$$

So the constraint may in fact be an intrinsic property of the problem.

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[4] A. L. Hodgkin and A. F. Huxley, *A quantitative description of membrane current and its application to conduction and excitation in nerve*, J. Physiol. (London), 117 (1952), pp. 500–544.