Experiments with Reaction-Diffusion equations

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Abstract

The reaction-diffusion equations describe the behaviour of several systems where diffusion of material competes with the production of the same material. These equations are widely used for systems consisting of many interactive components such as chemical reactions and an infectious disease as we are going to look at in this paper.

1. Introduction

In this paper we will consider parabolic PDEs called reaction-diffusion-equations. The PDE is time-dependent, and the scheme that is used to solve the PDE is therefore based on forward and backward Euler. The first part of the paper contain a stability and consistency analysis of the method on a linear PDE, which also is justified numerically. In the last part of the paper we will look at a model for epidemiology using the SIR model.

2. Theory

The reaction-diffusion equations are given by

$$u_t = \mu u_{xx} + f(u), \tag{1}$$

where the diffusion constant μ is some positive constant, and the reaction term $f(u)$ is assumed to be nonstiff.

Let h be the constant step size in x-direction and k in t-direction, so that $x_{m+1} = x_m + h$ and $t_{n+1} = x_n + k$. Now discretize equation (1) using forward and backward Euler, together with a central difference in space.

$$\begin{aligned} \frac{1}{k}\nabla_t U_m^{n+1} &= \frac{1}{h^2}\delta_x^2 U_m^{n+1} + f(U_m^n) \\ U_m^{n+1} - U_m^n &= r(U_{m+1}^{n+1} - 2U_m^{n+1} + U_{m-1}^{n+1}) + kf(U_m^n), \end{aligned} \tag{2}$$

where $r = \mu\frac{k}{h^2}$ and U_m^n is the approximation to the solution $u_m^n = u(x_m, t_n)$ evaluated in the point (x_m, t_n). Consider the approximation of the PDE in (1)

on a rectangle $[0,1] \times [0,T]$. We will use Dirichlet boundary conditions such that $U(0,t) = U(1,t) = 0$.

The following is a modification of the Crank Nicholsen scheme,

$$\begin{aligned} U_m^* &= U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kf(U_m^n) \\ U_m^{n+1} &= U_m^* + \frac{k}{2}(f(U_m^*) - f(U_m^n)). \end{aligned} \tag{3}$$

We will now express the scheme defined in (15), in matrix-vector form $AU^{n+1} = BU^n$, where A and B depend on the step sizes. Let S be a symmetric matrix, $S = tridiag\{1, -2, 1\}$, and $f(u) = au$ for some constant a. When sorting the terms and replacing δ_x^2 with S we get,

$$\underbrace{(I - \frac{r}{2}S)}_{A} U^* = \underbrace{(I + \frac{r}{2}S + kaI)}_{B} U^n. \tag{4}$$

Insert $U^* = A^{-1}BU^n$ into the second part of equation (15) and we have a *two-level-method* of the form

$$U^{n+1} = \underbrace{(A^{-1}B + \frac{ka}{2}A^{-1}B - \frac{ka}{2}I)}_{C} U^n = CU^n. \tag{5}$$

The matrix C written out is

$$C = (I - \frac{r}{2}S)^{-1}(I + \frac{r}{2}S + ka)(1 + \frac{ka}{2}) - \frac{ka}{2}I. \tag{6}$$

Theorem 2.1 (Stability of the reaction-diffusion equation). *Let*

$$u_t = \mu u_{xx} + f(u) \tag{7}$$

be solved by a scheme of the form

$$U^{n+1} = CU^n \tag{8}$$

with stepsizes h in x-direction and k in t-direction on a rectangle $[0,1]\times[0,T]$. Then the scheme (8) is conditionally stable for $k\,|a| < 1$.

Proof of Theorem 2.1 :. Let S be a symmetric, tridiagonal matrix as defined earlier. Then we have the diagonalization $S = P\Lambda P^T$ where $P^T P = I$ and Λ is the diagonal matrix consisting of the eigenvalues λ_m of S. Substitute the diagonalization for S into the equation for (6)

$$C = P\Big(\underbrace{(I - \frac{r}{2}\Lambda)^{-1}(I + \frac{r}{2}\Lambda + kaI)(1 + \frac{ka}{2}) - \frac{ka}{2}I}_{\Delta}\Big)P^T \tag{9}$$

From the equation above we know that C is symmetric. We can also show this by observing $C = C^T$. In order to show that the scheme in (8) is stable, we

now need to find the spectral radius of C. We know that $\rho(C) = \max_m \mid \lambda_m \mid$, where λ_m are the eigenvalues of C.

From note by Brynjulf [1], we know that the eigenvalues of S are

$$\lambda_m = -4\sin^2\phi_m \qquad \phi_m = \frac{m\pi}{2(M+1)} \qquad m = 1, ..., M$$

Write the matrix Δ in element form

$$\begin{aligned} \Delta_m &= \Big(\frac{1+\frac{r}{2}\lambda_m + ka}{1-\frac{r}{2}\lambda_m}\Big)\Big(1+\frac{ka}{2}\Big) - \frac{ka}{2} \\ &= \Big(\frac{1-2r\sin^2\phi_m + ka}{1+2r\sin^2\phi_m}\Big)\Big(1+\frac{ka}{2}\Big) - \frac{ka}{2}. \end{aligned} \tag{10}$$

We know from the diagonalization that the elements of Δ in (10) are the eigenvalues of the matrix C.

$$\begin{aligned} \rho(C) &= \max_m |\Delta_m| \\ &= \max_m \left| \frac{1-2r\sin^2\phi_m + ka}{1+2r\sin^2\phi_m}(1+\frac{ka}{2}) - \frac{ka}{2} \right| \\ &= \max_m \left| \Big(\frac{1-2r\sin^2\phi_m}{1+2r\sin^2\phi_m}\Big)\Big(1+\frac{ka}{2}\Big) + ka\Big(1+\frac{ka}{2}-\frac{1}{2}\Big) \right| \end{aligned} \tag{11}$$

We notice that the denominator ≥ 1, and the first part of the nominator $(1-2r\sin^2\phi_m) \leq 1$ for all $m = 1, .., M$. This is because $0 \leq 2r\sin^2\phi_m \leq 2r$. Let $\sin^2\phi_m = 0$, and substitute 1 for the first part of the nominator and the denominator.

$$\begin{aligned} \rho(C) &\leq \left| 1 + \frac{ka}{2} + ka(1+\frac{ka}{2}-\frac{1}{2}) \right| \\ &\leq \left| 1 + ka + \frac{(ka)^2}{2} \right| \\ &\leq 1 + k\,|a| + \frac{(ka)^2}{2} \end{aligned} \tag{12}$$

We now assume $k\,|a| < 1$, a reasonable assumption as we want the stepsize k to be as small as possible. This implies that $(ka)^2 < k\,|a|$.

$$\rho(C) \leq 1 + k\,|a| \tag{13}$$

We have now showed that (8) is stable as long as $k\,|a| < 1$

□

Theorem 2.2 (Consistency of the reaction-diffusion equation). *Let*

$$u_t = \mu u_{xx} + f(u) \tag{14}$$

be solved by a scheme of the form

$$\begin{aligned} U_m^* &= U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kf(U_m^n) \\ U_m^{n+1} &= U_m^* + \frac{k}{2}(f(U_m^*) - f(U_m^n)). \end{aligned} \tag{15}$$

where $r = \mu\frac{k}{h^2}$ and $f(u) = au$ for some constant a. Then the differenece method is consistent of order 2.

Proof of Theorem 2.2 :. Write the equations with $f(u) = au$,

$$\begin{aligned} u_m^* &= u_m^n + \frac{r}{2}(\delta_x^2 u_m^* + \delta_x^2 u_m^n) + kau_m^n \\ u_m^{n+1} &= u_m^* + \frac{ka}{2}(u_m^* - u_m^n). \end{aligned} \tag{16}$$

then the local truncation error can be written as,

$$k\tau_m^n = u_m^{n+1} - (u_m^* + \frac{ka}{2}(u_m^* - u_m^n)) \tag{17}$$

Then write U_m^* out recursively,

$$u_m^* = u_m^n + \frac{r}{2}(\delta_x^2(u_m^n + \frac{r}{2}(\delta_x^2(u_m^n + ... + kau_m^n) + \delta_x^2 u_m^n) + kau_m^n) + \delta_x^2 u_m^n) + kau_m^n \tag{18}$$

where the dots represent terms with r of order > 2. We then insert the expression for u_m^* into equation (21). Then Taylor expand the different terms:

$$\begin{aligned} u_m^n &= u \\ u_m^{n+1} &= u + ku_t + \frac{k^2}{2}tt + O(k^3) \\ \delta_x^2(u_m^n) &= h^2 u_{xx} + \frac{h^4}{12}u_{4x} \\ \delta_x^4(u_m^n) &= h^4 u_{4x} + \frac{h^6}{6}u_{6x} + \frac{h^8}{u_{8x}}. \end{aligned} \tag{19}$$

Use (14) to rewrite the timederivatives,

$$\begin{aligned} u_t &= \mu u_{xx} + au \\ u_{tt} &= (u_t)_t \\ &= (\mu u_{xx} + au)_t \\ &= \mu^2 u_{4x} + 2\mu a u_{xx} + a^2 u. \end{aligned} \tag{20}$$

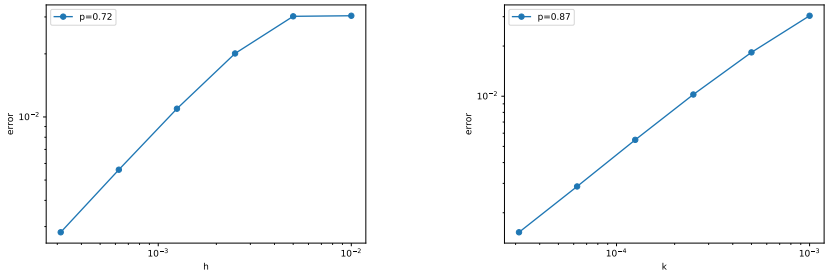

Figure 1: Left : Convergence plot for $h \to 0$. **Right** :Convergence plot for $k \to 0$

When writing out all the terms in equation (21) with their corresponding Taylor expansion, a lot of the terms cancel each other out, thus we are left with,

$$k\tau_m^n = -\frac{h^2 k\mu}{12}u_{4x} - \frac{\mu k^3 a}{4}u_{4x} - \frac{\mu k^3 a^2}{4}u_{xx} - \frac{\mu^2 k^3 a}{4}u_4 x + O(h^2 k + k^4) \quad (21)$$

Dividing both sides of the equation by k to achieve,

$$\tau_m^n \leq D(h^2 + k^2), \quad (22)$$

where D is some positive constant independent of h and k. Thus $\tau_m^n \to 0$ as $k, h \to 0$ and the scheme is consistent.

□

From Lax' equivalence theorem in the note by Brynjulf [1]. We know that a consistent scheme is convergent if and only if it is stable. The reaction-diffusion equation under the criteria $k\,|a| < 1$, is both stable and consistent. Thus we expect the equation to be convergent of order 2. Hence the global error will decrease as $k, h \to 0$.

3. Numerical experiments

To verify the theory we implemented the test function

$$u = \sin(\pi x)e^t, \quad (23)$$

with $\mu = \frac{1}{\pi^2}$, $a = 2$ and Dirichlet boundary conditions.

$$u(0,t) = 0 \qquad\qquad u(1,t) = 0.$$

From (22) and Lax' equivalence theorem we expect the convergence order for our method to be $p = 2$ for both increasing time steps k and space steps h.

Figure 1 is a result of the error $e = U^n - u(x, t_n)$ for different step sizes h when k is fixed and opposite. Note that we measured the error e for the last

time steps $t_n = T$ as this is where we expect the greatest error. The convergence rate is the slope, which in this case is unlike what we expected. This indicates that the script is not working correctly. Unfortunately we have not been able to find exactly what is wrong, but we think that it is something wrong in the implementation of the boundary conditions for the numerical solution.

4. Modelling spread of diseases with SIR models

As we are writing this report the COVID-19 virus, recently recognized as a pandemic by World Health Organization, is spreading across the globe. Modern techniques allow us to model such infectious diseases and predict their spread, making life-saving preparations possible. Additionally, models can help determine the effect of measures to halt the spread of the disease as well as where to begin vaccination programs. In this section we investigate the spread of diseases based on the SIR-model.

The simplest model assumes that every individual in a population belongs to one of the classes susceptible (S), infected (I) or removed (R). We will consider a scaled model where the functions $S()$, $I()$ and $R()$ represent fractions of the total population P. Specifically, at any time t_n, $S(t_n)$ is the fraction of the population that can get infected by the disease, $I(t_n)$ is the fraction of the population that is infected by the disease and $R(t_n)$ is the fraction of the population that neither is infected or can get infected, typically either immune or dead. Furthermore, we consider a closed system in which the population P is constant, and hence the relations

$$\begin{aligned} P &= S(t) + I(t) + R(t) = constant \\ P_t &= S_t + I_t + R_t = 0 \end{aligned} \tag{24}$$

hold for all $0 \leq t \leq \inf$.

Looking at a single location under the assumption that all individuals are equally likely to run into each other, we can model the spread with the following nonlinear set of differential equations called the SIR model

$$\begin{aligned} \frac{dS}{dt} &= -\beta SI \\ \frac{dI}{dt} &= \beta SI - \gamma I \\ \frac{dR}{dt} &= \gamma I. \end{aligned} \tag{25}$$

Here β is the infection rate from S to I and γ is the transition rate from I to R, intuitively representing the rate of which infected individuals recover or die. We observe that the equations sum to 0 as expected. This system is easily solved explicitly by using methods like forward Euler.

4.1. Expanding the model to space

The simple SIR model we have discussed so far assumes all individuals in the population are at the same location and are equally likely to infect each other. While this assumption might be a sufficient approximation for a small, closed population, it will in most cases be a crude over-simplification. A much more realistic model is obtained by letting the SIR components be functions of both time and position, and only allowing spatial interactions between neighbouring points. These interactions can be modelled with a diffusion term, allowing high concentrations to "leak" to nearby locations. Murray [2] proposes the modified SIR model

$$\begin{aligned} \frac{\partial S}{\partial t} &= -\beta SI + \mu_S \Delta S \\ \frac{\partial I}{\partial t} &= \beta SI - \gamma I + \mu_I \Delta I \\ \frac{\partial R}{\partial t} &= \gamma I, \end{aligned} \tag{26}$$

where Δ is the Laplace operator such that in two spatial dimensions we have $\Delta u = (u_{xx} + u_{yy})$. Furthermore, μ_S and μ_I represent how fast susceptible and infected individuals move around, respectively.

We introduce a spatial domain $\Omega \subset R^2$ with boundary $\partial\Omega$. In order to keep our previous requirement of a closed system, we need to impose that no individuals can cross the boundary of our domain. Thus, we enforce Neumann boundary conditions on the form

$$S_t|_{\partial\Omega} = I_t|_{\partial\Omega} = R_t|_{\partial\Omega} = 0. \tag{27}$$

4.2. Numerical Scheme

We want to model the functions $S(x, y, t)$, $I(x, y, t)$ and $R(x, y, t)$, given some initial functions $S_0(x, y) = S(x, y, 0)$, $I_0(x, y) = I(x, y, 0)$ and $R_0(x, y) = R(x, y, 0)$. The equations for S, I and R in (26) are reaction-diffusion equations (with $\mu_R = 0$), and can be solved numerically using the modified Crank-Nicolson scheme in (15). We introduce a square grid

$$x_l = lh, \quad l = 0, ..., M-1, \quad \text{and} \quad y_m = mh, \quad m = 0, ..., M-1,$$

with constant step size $h = 1/M$ in both x- and y-direction. Central differences in two dimensions with equal step size can be rewritten using the classic 5-point formula $\delta_x^2 U_p + \delta_y^2 U_p = U_w + U_e + U_s + U_n - 4U_p$. To represent the 5-point formula, we introduce the symmetric matrix $A = (a_{ij}) \in \mathbb{R}^{M^2 \times M^2}$ which has *only* zero entries except for the tridiagonal band $\{1, -4, 1\}$ along its main diagonal, as well as ones at its $m'th$ upper and lower diagonal.

$$A = \begin{bmatrix} -4 & 1 & \dots & 1 & & & & & \\ 1 & -4 & 1 & \dots & 1 & & & & \\ & & \ddots & & & \ddots & & & \\ 1 & \dots & 1 & -4 & 1 & \dots & 1 & & \\ & 1 & \dots & 1 & -4 & 1 & \dots & 1 & \\ & & \ddots & & & \ddots & & & \ddots \end{bmatrix}$$

To incorporate the Neumann boundary conditions into our model, we introduce ghost cells and use the first order central differences to obtain the following update to the 5-point formula along the south boundary: $\delta_x^2 U_p + \delta_y^2 U_p = U_w + U_e + 2U_n - 4U_p$ on $\partial\Omega_S$. This procedure is repeated for all boundaries. The boundary conditions can then be directly incorporated in A, through some individual handling of all edges. Furthermore, we flatten the matrices S, I and R and get the following Crank-Nicolson updates on vector form, using time step size k (note that vector products are *element-wise*):

$$\begin{aligned} S^* &= S^n + \frac{\mu_S k}{2h^2} A(S^* + S^n) - k\beta I^n S^n \\ S^{n+1} &= S^* + \frac{k}{2}(-\beta I^* S^* + \beta I^n S^n) \\ I^* &= I^n + \frac{\mu_I k}{2h^2} A(I^* + I^n) + k(\beta I^n S^n - \gamma I^n) \\ I^{n+1} &= I^* + \frac{k}{2}(\beta I^* S^* - \gamma I^* - \beta I^n S^n + \gamma I^n) \\ R^{n+1} &= R^n + \gamma I^n. \end{aligned} \tag{28}$$

The first half-steps are implicit and solved as systems of equations, while the second half-steps are solved explicitly.

The rest of the report is dedicated to looking at the effect different measures have on the spread of the disease. We do not try to draw any conclusions, just toy around with our model.

4.3. Reducing β

Reducing the β in our SIR model means to reduce the probability of a sick individual infecting a susceptible individual given that they are in the same location. This includes hygienic measures such as proper hand washing, as well as social measures such as social distancing. Figure 2 shows the effect of reducing β to one third at $t = 30$.

4.4. Reducing μ

In this experiment we enforce regulations on the movement behaviour of the individuals. The left hand plot in Figure 3 shows a run where the movement coefficients μ_S and μ_I are halved at $t = 30$. In the experiment corresponding

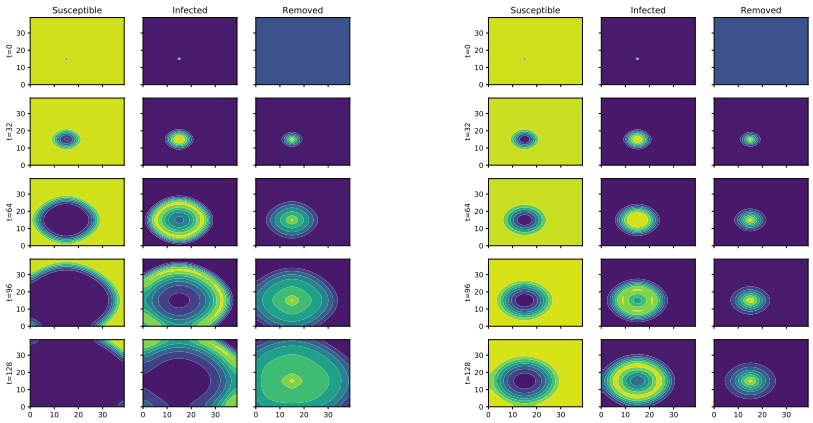

Figure 2: Solutions to the SIR model over 160 time steps on a 40×40 grid. Starting parameters are $\beta = 3.0$, $\gamma = 0.5$, $\mu_S = 1.0$ and $\mu_I = 0.6$. **Left** : In this run the parameters stay unchanged. We observe that from a small starting point, the infection spreads through the whole domain. **Right** : The same experiment as in the left image, except that after 30 iterations β is reduced from 3.0 to 1.0. The spread clearly slows significantly down when β is reduced.

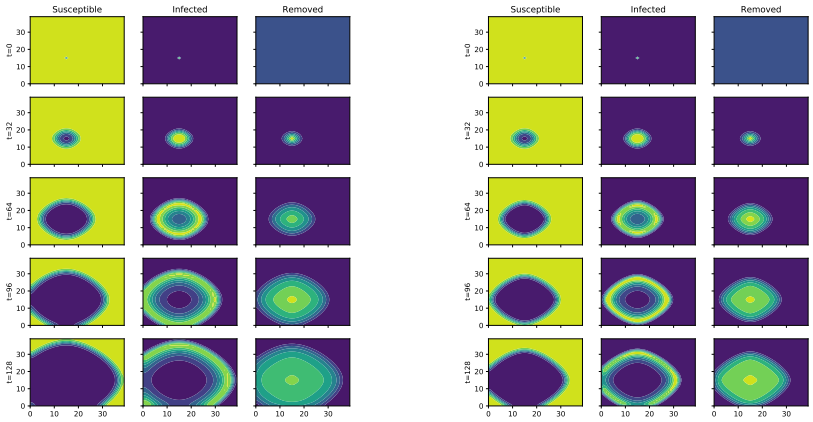

Figure 3: Solutions to the SIR model over 160 time steps on a 40×40 grid. Starting parameters are $\beta = 3.0$, $\gamma = 0.5$, $\mu_S = 1.0$ and $\mu_I = 0.6$. **Left** : At $t = 30$ the movement parameters are halved. **Right** : At $t = 30$ the movement parameter for susceptible individuals μ_S is halved, and the parameter for infected individuals μ_I is set to 0.

to the plot on the right hand side, total lock down of infected individuals was enforced, μ_I was set to 0. Note that susceptible individuals are still able to move to the location of the infected. Both cases clearly show a decrease in the infection rate, but the results seem less significant than reducing β, especially given that we are actually setting a coefficient to 0.

4.5. Stopping the pandemic

In this experiment we try both the measures we already discussed, and additionally enforce an extra weapon: increasing γ. Intuitively, increasing γ can correspond to increasing the death rate of the disease, but we are going to consider the more optimistic interpretation of isolation of the infected, such that they are no longer able to infect new individuals. In this run we increase γ to 10 to observe a instant halt in the spread of the disease.

References

[1] Brynjulf Owren, Note on finite difference methods, `http://www.math.ntnu.no/emner/TMA4212/2020v/notes/master.pdf`

[2] J.D. Murray *Mathematical Biology II: Spatial Models and Biomedical Applications*, 3th ed., Springer, 2003.

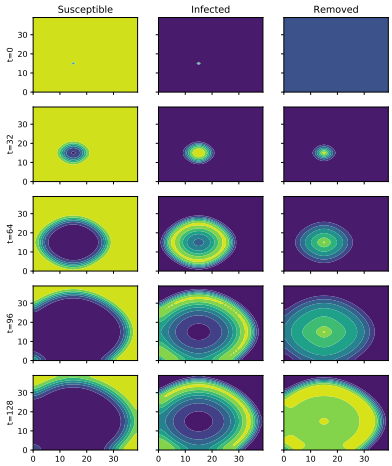

Figure 4: Solutions to the SIR model over 160 time steps on a 40×40 grid. Starting parameters are $\beta = 3.0$, $\gamma = 0.5$, $\mu_S = 1.0$ and $\mu_I = 0.6$. In this run, all measures against the spread of the disease are enforced at $t = 100$. β and μ are reduced and γ is increased. The spread clearly stops in its tracks.

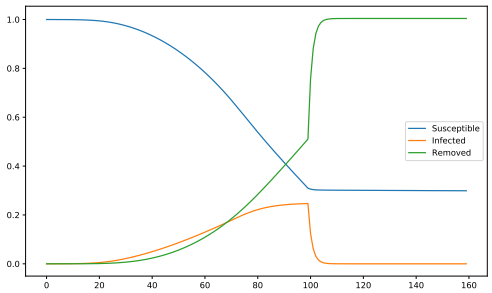

Figure 5: Sum of classes over the whole domain. Starting parameters are $\beta = 3.0$, $\gamma = 0.5$, $\mu_S = 1.0$ and $\mu_I = 0.6$. In this run, all measures against the spread of the disease are enforced at $t = 100$. β and μ are reduced and γ is increased.