# TMA4212 - PROJECT 2

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Abstract. In this paper, we propose a finite difference method to solve the reaction-diffusion equation. We prove that our method is convergent of order two for linear reaction terms and confirm this with computations. We apply our method to the SIR model in epidemiology and show some simulations with interesting parameter choices.

## 1. Introduction

In this paper we will study the numerical solution of the reaction-diffusion equation

$$u_t = \mu u_{xx} + f(u) \tag{1.1}$$

This is linear parabolic differential equation, which can be used to model diffusion processes augmented by, or counteracted by, a reaction process. For instance, (1.1) can be used to model the change in concentration of a chemical substance $u$ in solution over time.

The term $\mu u_{xx}$ represents the diffusion process, where $\mu > 0$ is a constant parameter governing the rate of the spread. The reaction term $f(u)$ is modelling any type of change in a system that is not due to diffusion in space. Our method of solution will be a finite difference scheme on a domain discretized in space and time.

In the second part, we apply our method to the SIR-model in epidemiology, augmented with diffusion.

## 2. Discretization and implementation

To study the nature of the reaction diffusion equation(1.1), we first solve a initial/boundary value Dirichlet problem on a chosen space-time domain $\Omega_T$. For the first implementation, we consider the unit interval in space, and all times up until a end time $T$.

$$\Omega_T = [0,1] \times [0,T] = (x,t) : 0 \leq x \leq 1, 0 \leq t \leq T$$

We want implement a solver of (1.1) on $\Omega_T$ which enables us to solve problems with boundary and initial conditions of the form

$$\begin{aligned} u(x,0) &= g(x), & 0 \leq x \leq 1 \\ u(0,t) &= h_0^d(t), & t > 0 \\ u(1,t) &= h_1^d(t), & t > 0 \end{aligned} \tag{2.1}$$

Where $g(x), h_0^d(t)$, and $h_1^d(t)$ are functions supplying the initial, and boundary, data.

We discretize the domain by imposing a regular grid with $M$ steps in the spatial, and $N$ steps in the temporal direction. This yields stepsizes of $h = \frac{1}{M}$ and $k = \frac{T}{N}$

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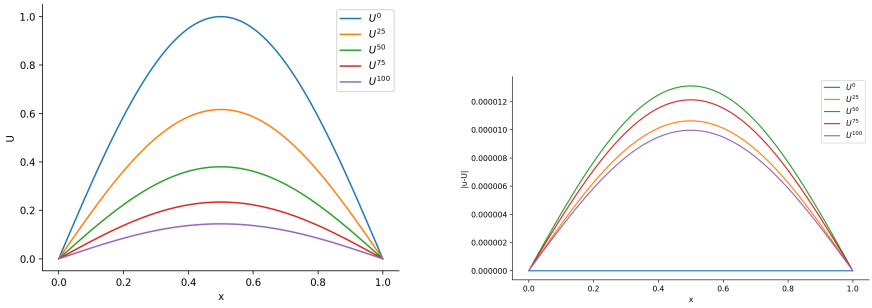


FIGURE 1. Solution of (3.1) given parameters $a = 3$, $\mu = 0.5$, with ending time $T = 1$ and initial value $g(x) = \sin \pi x$. The grid is chosen with $M = 100$ steps in space, and $N = 100$ in time. Numerical solution $U^n$ for a selection of times $t_n = nk$ plotted on the left, discretization error plotted on the right.

We define $r = \mu \frac{k}{h^2}$ and employ the following modification of the Crank-Nicolson method

$$U_m^* = U_m^n + \frac{r}{2}(\delta_x^2 U_m^* + \delta_x^2 U_m^n) + kf(U_m^n)$$
$$U_m^{n+1} = U_m^* + \frac{k}{2}(f(U_m^*) - f(U_m^n)) \tag{2.2}$$

as our discretization of (1.1). Here $U_m^n$ indicates the numerical solution in the point $(x_m, t_n) = (mh, nk)$, and $U_m^*$ is an intermediate computational step. We assume $f$ to be non-stiff.

## 3. A Dirichlet problem on the unit interval

As an instructive example, and to be able to study the error of the scheme, we consider a set of initial and boundary values for which we know the analytical solution.

We would like to examine a linear PDE, so we choose the reaction function as the general linear term $f(u) = au$, where $a \in \mathbb{R}$ is an arbitrary constant.

$$u_t = \mu u_{xx} + au \tag{3.1}$$

Let $h_0^d(t) = h_1^d(t) = 0$ and $g(x) = \sin(\pi x)$ be the inital and boundary data as defined in (2.1). By the standard method of separation of variables, we find that the analytical solution of (3.1) is

$$u(x,t) = \sin(\pi x) e^{(a - \pi^2 \mu)t} \tag{3.2}$$

Implementing our finite difference scheme, we solve the initial/boundary value problem, and get the results in Figure 1.

If we assume that the error grows polynomially in the stepsize of both time and space; $||e||_\infty = \max_{0 \le t_n \le T} \max_{0 \le x_m \le 1} |u(x_m, t_n) - U_m^n| = Ch^p + Dk^q$, we can compare the errors of solutions for different stepsizes $h_i$ to get the following estimates for the orders $p$ and $q$ of the method.

$$p \approx \frac{\log ||e(h_i)||_\infty - \log ||e(h_j)||_\infty}{\log h_i - \log h_j} \qquad q \approx \frac{\log ||e(k_i)||_\infty - \log ||e(k_j)||_\infty}{\log k_i - \log k_j} \tag{3.3}$$

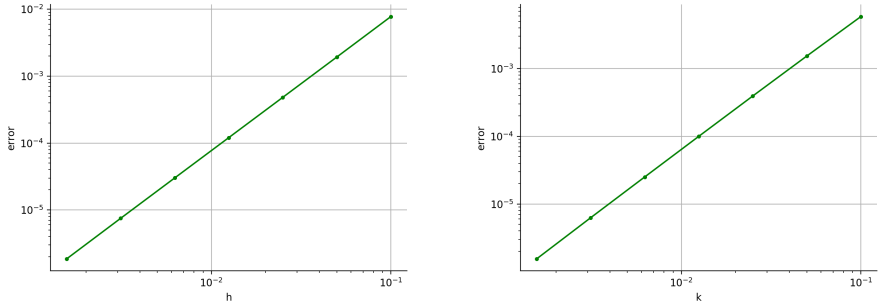


FIGURE 2. Discretization error for different stepsizes in space and time. When one step size is varied, the other is fixed. Axes are logarithmically scaled.

Taking the difference of our numerical and analytical solution, we get the error plot in Figure 2. From the slope of the plot, we can infer that $p = q = 2$ and the error decreases quadratically with the step size, both in space and in time.

## 4. Error analysis of the Dirichlet problem

In light of the findings of our implementation, we now perform a complete error analysis of the scheme (2.2), as applied to the homogenous Dirichlet problem given by our linear reaction-diffusion equation (3.1).

4.1. **Consistency.** We investigate the consistency of the method on a linear pde by setting $f(u) = au$ for some arbitrary $a \in \mathbb{R}$. In this linear case, the equation for $U_m^*$ becomes

$$U_m^* = (1 + ka + \frac{r}{2}\delta_x^2)U_m^n + \frac{r}{2}\delta_x^2 U_m^* = \mathcal{L}U_m^n + \frac{r}{2}\delta_x^2 U_m^*. \tag{4.1}$$

By recursively expanding this expression, it becomes clear that

$$\begin{aligned} U_m^* &= \sum_{l=0}^{\infty} (\frac{r}{2}\delta_x^2)^l \mathcal{L}U_m^n \\ &= \sum_{l=0}^{\infty} (\frac{r}{2}\delta_x^2)^l ((1+ka)U_m^n + \frac{r}{2}\delta_x^2 U_m^n) \\ &= (1+ka)\sum_{l=0}^{\infty} (\frac{r}{2}\delta_x^2)^l U_m^n + \sum_{l=1}^{\infty} (\frac{r}{2}\delta_x^2)^l U_m^n \end{aligned}$$

$$U_m^* = (2+ka)\sum_{l=0}^{\infty} (\frac{r}{2}\delta_x^2)^l U_m^n - U_m^n. \tag{4.2}$$

With the linear $f(u) = au$, the formula for $U_m^{n+1}$ in (2.2) becomes

$$U_m^{n+1} = (1 + a\frac{k}{2})U_m^* - a\frac{k}{2}U_m^n. \tag{4.3}$$

**Lemma 4.1.** *The method* (2.2) *applied to the solution of the reaction-diffusion equation with a linear reaction function has local truncation error bounded by* $|\tau_m^n| \leq C_h h^2 + C_k k^2$, *assuming* $\mu\frac{k}{2} < 1$.

*Proof.* By Taylor expansion around $u_m^n$, we know that

$$u_m^{n+1} = u_m^n + ku_t + \frac{1}{2}k^2u_{tt} + C_1k^3$$

for some $C_1 \in \mathbb{R}$. By assuming continuous partial derivatives up to at least order 4 and using the definition of the reaction-diffusion equation,

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

and $u_m^{n+1}$ can be rewritten as

$$u_m^{n+1} = u_m^n + k(\mu u_{xx} + au) + \frac{1}{2}k^2(\mu^2u_{4x} + 2a\mu u_{xx} + a^2u) + C_1k^3.$$

By using (4.3) and (4.2), with the first three summands in the series written explicitly,

$$\begin{aligned} U_m^{n+1} =& (2 + 2ka + k^2\frac{a^2}{2})\sum_{l=0}^{\infty}(\frac{r}{2}\delta_x^2)^lU_m^n - (1 + ka)U_m^n \\ =& (1 + ka + k^2\frac{a^2}{2})U_m^{n+1} + r(1 + ka + k^2\frac{a^2}{4})\delta_x^2U_m^{n+1} \\ &+ \frac{1}{2}r^2(1 + ka + k^2\frac{a^2}{4})\delta_x^4U_m^n + \sum_{l=3}^{\infty}(\frac{r}{2}\delta_x^2)^lU_m^n. \end{aligned} \tag{4.4}$$

Looking at the series in the above expression, we find

$$\sum_{l=3}^{\infty}(\frac{r}{2}\delta_x^2)^lU_m^n = \sum_{l=3}^{\infty}(\frac{r}{2})^lh^{2l}(\partial_{(2l)x}U_m^n + C_lh^2) = \sum_{l=3}^{\infty}(\mu\frac{k}{2})^l(\partial_{(2l)x}U_m^n + C_lh^2)$$

where $C_l = u_{(4l)x}(\xi, t_n)$ for some $\xi \in (x_m - lh, x_m + lh)$, a term representing difference between $(\delta_x^2)^l$ and exact $2l$-times differentiation. If we set $K = \sup_{l,\xi}|u_{(2l)x}(\xi, t_n)|$, where $\xi$ is in our space domain,

$$|\sum_{l=3}^{\infty}(\frac{r}{2}\delta_x^2)^lU_m^n| \leq k^3(K(\frac{\mu}{2})^3\sum_{l=0}^{\infty}(\mu\frac{k}{2})^l + K(\frac{\mu}{2})^3h^2\sum_{l=0}^{\infty}(\mu\frac{k}{2})^l) \leq Ak^3 + Bk^3h^2$$

for some constants $A, B > 0$, assuming $\mu\frac{k}{2} < 1$.

Regrouping terms from (4.4), we match the taylor expansion for $u_m^{n+1}$,

$$\begin{aligned}U_m^{n+1} - u_m^{n+1} =& U_m^n - u_m^n \\ &+ r\delta_x^2 U_m^n + kaU_m^n - k\partial_t u_m^n \\ &+ \frac{1}{2}r^2\delta_x^4 U_m^n + rka\delta_x^2 U_m^n + k^2\frac{a^2}{2}U_m^n - \frac{1}{2}k^2\partial_{tt}u_m^n \\ &+ rk^2\frac{a^2}{4}\delta_x^2 U_m^n + \frac{1}{2}r^2(ka + k^2\frac{a^2}{4})\delta_x^4 U_m^n + \sum_{l=3}^{\infty}(\frac{r}{2}\delta_x^2)^l U_m^n + C_1k^3\end{aligned}$$

$$\begin{aligned}U_m^{n+1} - u_m^{n+1} =& U_m^n - u_m^n \\ &+ k(\frac{\mu}{h^2}\delta_x^2 U_m^n + aU_m^n) - k(\mu\partial_{xx}u_m^n + au_m^n) \\ &+ \frac{1}{2}k^2(\frac{\mu^2}{h^4}\delta_x^4 U_m^n + 2a\frac{\mu}{h^2}\delta_x^2 U_m^n + a^2 U_m^n) - \frac{1}{2}k^2(\mu^2\partial_{4x}u_m^n + 2a\mu\partial_{xx}u_m^n + a^2u_m^n) \\ &+ rk^2\frac{a^2}{4}\delta_x^2 U_m^n + \frac{1}{2}r^2(ka + k^2\frac{a^2}{4})\delta_x^4 U_m^n + \sum_{l=3}^{\infty}(\frac{r}{2}\delta_x^2)^l U_m^n + C_1k^3\end{aligned}$$

$$|U_m^{n+1} - u_m^{n+1}| \leq kEh^2 + k^2Fh^2 + Gk^3 + Ak^3 + Bk^3h^2 + C_1k^3$$

where $E$ and $F$ are constants bounding the truncation error of the approximations for $\partial_t u_m^n$ and $\partial_{tt}u_m^n$ respectively and $Gk^3$ gives a bound for $rk^2\frac{a^2}{4}\delta_x^2 U_m^n + \frac{1}{2}r^2(ka + k^2\frac{a^2}{4})\delta_x^4 U_m^n$.

Thus, by using the definition of $\tau_m^n$ and assuming exact solution in $U_m^n$, we get

$$\begin{aligned}|k\tau_m^n| = |U_m^{n+1} - u_m^{n+1}| &\leq kEh^2 + k^2Fh^2 + Gk^3 + Ak^3 + Bk^3h^2 + C_1k^3 \\ |\tau_m^n| &\leq C_h h^2 + C_k k^2\end{aligned}$$

□

4.2. **Stability and convergence.** Having established consistency of the discretization, we wish to use the powerful Lax' equivalence theorem to prove convergence. For this, we need stability.

**Lemma 4.2.** *The method* (2.2) *applied to the solution of the reaction-diffusion equation* (3.1) *with Dirichlet conditions* $h_0^d(t) = h_1^d(t) = 0$ *is unconditionally stable on the entire domain* $\Omega_T$.

*Proof.* We prove stability using a standard von Neumann analysis argument. Assume that the numerical solution has a fourier expansion of the form

$$U_m^n = \sum_{\beta=-\infty}^{\infty} A_\beta \xi^n e^{i\beta x_m}, \qquad A_\beta = \frac{1}{2\pi}\int_{-\infty}^{\infty} g(x)e^{-i\beta x}dx$$

To show stability, we consider an arbitrary term in the series

$$U_m^n = \xi^n e^{i\beta x_m}$$

which we insert into the first term of our method (2.2) and get

$$\xi^* e^{i\beta x_m} = \xi^n e^{i\beta x_m} + \frac{r}{2}(\xi^* e^{i\beta(x_m+h)} - 2\xi^* e^{i\beta x_m} + \xi^* e^{i\beta(x_m-h)}) + ka\xi^n e^{i\beta x_m}$$

Which after solving for $\xi^*$ and applying a trigonometric identity, yields

$$\xi^* = \xi^n \frac{1 - 2r\sin^2\frac{\beta h}{2} + ka}{1 + 2r\sin^2\frac{\beta h}{2}}$$

Now, inserting (4.2) into the second term of our method returns

$$\xi^{n+1}e^{i\beta x_m} = \xi^* e^{i\beta x_m} + \frac{ka}{2}\left(\xi^* e^{i\beta x_m} - \xi^n e^{i\beta x_m}\right)$$

Inserting the expression for $\xi^x$ and solving for $\xi$

$$\xi = \frac{1 - 2r\sin^2\frac{\beta h}{2} + ka}{1 + 2r\sin^2\frac{\beta h}{2}}\left(1 + \frac{ka}{2}\right) - \frac{ka}{2}$$

$$\begin{aligned}|\xi| &\leq |1 + \frac{ka}{2}|\left|\frac{1 - 2r\sin^2\frac{\beta h}{2}}{1 + 2r\sin^2\frac{\beta h}{2}}\right| + \left|\frac{ka}{1 + 2r\sin^2\frac{\beta h}{2}}\right| + \left|\frac{k^2a^2}{1 + 2r\sin^2\frac{\beta h}{2}}\right| \\ &\leq 1 + \frac{k|a|}{2} + k|a| + k^2|a|^2 \leq 1 + \frac{3}{2}k|a| + kT|a|^2 \leq 1 + Ck\end{aligned}$$

Where $C = \frac{3}{2}|a| + T|a|^2$ In the last step we use that the stepsize $k$ cannot exceed the size of the entire time interval, and thus $k^2|a|^2 \leq kT|a|^2$.

From Owren [1], we get that $|\xi| \leq 1 + Ck$ is a necessary and sufficient criterion for stability given that the follwing points are satisfied:

(1) The differential equation has constant coefficients and one dependent variable.
(2) We are given a pure initial value problem.
(3) We apply a 2-level difference formula.

Criterion (1) and (3) are evident. For (2) we observe that our Dirichlet conditions can be made equivalent to a pure initial value problem. Since $u_t(0,t) = u_t(0,t) = 0$, the boundary points $(0,t)$ and $(1,t)$ are fixed points for all $t > 0$. Thus, we can extend the initial value function $u(x,0) = g(x)$ to periodically cover the entire real line, setting $g(x+p) = g(x)$ where $p \in \mathbb{Z}$. This new extended initial condition will preserve the Dirichlet conditions on the unit interval, since $g(x)$ has to be chosen as compatible with $h_0^d$ and $h_1^d$. Thus our Dirichlet problem satisfies (2), and the method is found to be unconditionally stable on $\Omega_T$. □

Having established both consistency and stability, we get convergence.

**Theorem 4.3.** *The method* (2.2) *applied to the solution of the reaction-diffusion equation* (3.1) *with Dirichlet conditions* $h_0^d(t) = h_1^d(t) = 0$ *is convergent, and the error obeys the following inequality, where* $C, D$ *are positive real constants.*

$$||e||_\infty \leq Ch^2 + Dk^2$$

*Proof.* Lax' equivalence theorem states that a consistent difference scheme is convergent if and only if it is stable. Hence, since the scheme is both constistent by Lemma 4.1, and stable by Lemma 4.2, the method is convergent.

Furthermore, we have

$$||e||_\infty \leq K \max_{(x_m,t_n)\in\Omega_T} |\tau_m^n| \overset{\text{Lemma 4.1}}{\leq} Ch^2 + Dk^2$$

The first inequality follows from an error estimate for a general convergent scheme on page 59 of Owren [1]. $K$ is a positive constant. This concludes the proof. □

With this theorem, we have concluded our error analysis. We have established that the method we implemented in the previous section is convergent and of order 2 in both space and time, as could be expected from the experimental error in Figure 2.

## 5. Application: Epidemic

5.1. **Model.** With the method we derived earlier, we use the Susceptible, Infectious, Removed (SIR) model augmented with diffusion to simulate the development of an epidemic in time and one spatial dimension. A population of constant size $N$ is divided into the categories $S$, $I$ and $R$, such that $N = S(t)+I(t)+R(t)$ at all times. The removed population refers to individuals who are removed from the interactions, by either dying or recovering and gaining immunity, and are therefore disregarded. The populations are further broken down in space by looking at local densities instead of populations, given by $s(x,t)$ and $i(x,t)$ with $S(t) = \int s(x,t)dx$ and $I(t) = \int i(x,t)dx$.

The movements of the populations are assumed to behave like diffusion, with diffusion parameters $\mu_s$ and $\mu_i$ for the susceptible and infectious populations respectively. The rate of susceptible individuals becoming infected in a given point is assumed to be proportional to the product of susceptible and infectious densities and the rate of removal of the infected population is assumed proportional to the infected density. This gives us the model

$$\begin{aligned} s_t &= \mu_s \Delta s - \beta i s \\ i_t &= \mu_i \Delta i + \beta i s - \gamma i \end{aligned} \tag{5.1}$$

where $\mu_s$, $\mu_i$, $\beta$ and $\gamma$ are constants describing the how infectious the pathogen is and how long it takes to die or recover from the illness.

In the case that $\mu_s = \mu_i$, (5.1) is the reaction-diffusion equation with reaction term $f(s,i) = \begin{pmatrix} -\beta i s & \beta i s - \gamma i \end{pmatrix}$, lending itself well to our method. If $\mu_s \neq \mu_i$, we can still transform (5.1) to reaction-diffusion form, by scaling our infected population to an alternate variable $\tilde{i}$ such that $\mu_s \tilde{i} = \mu_i i$ and scaling the reaction terms to match. In our implementation, we instead solve two reaction-diffusion equations where the reaction terms are dependent on both $s$ and $i$,

$$\begin{aligned} s_t &= \mu_s \Delta s + f_s(s,i) \\ i_t &= \mu_i \Delta i + f_i(s,i) \end{aligned}$$

and solve each of these systems individually with our method, using the latest steps from both. The reaction term in this model is not linear, but is still very simple, so we expect our method to work well on this model.

We use initial conditions for $s(x,0)$ and $i(x,0)$, and Neumann boundary conditions $\frac{\partial s}{\partial x} = \frac{\partial i}{\partial x} = 0$ at the boundaries to enforce that the populations stay in our domain.

5.2. **Simulations.** One important factor to consider when simulating epidemics is whether or not the hospitals in the region can cope with the increased number of patients. If the hospitals' capacity is exceeded, many extra casualties will follow, both because of victims of the epidemic not receiving the care they require and the fact that other casualties in the population will continue as normal, but not receive the care they would outside the epidemic. When plotting the progression of the epidemic, we therefore include a chosen hospital capacity, to better view the societal effects of changing various parameters of the epidemic. In all our simulations we use the unit interval $[0,1]$ in space and $[0,10]$ in time as our domain, with $M = 100$ steps in space and $N = 200$ steps in time. We use flat initial distributions of the susceptible

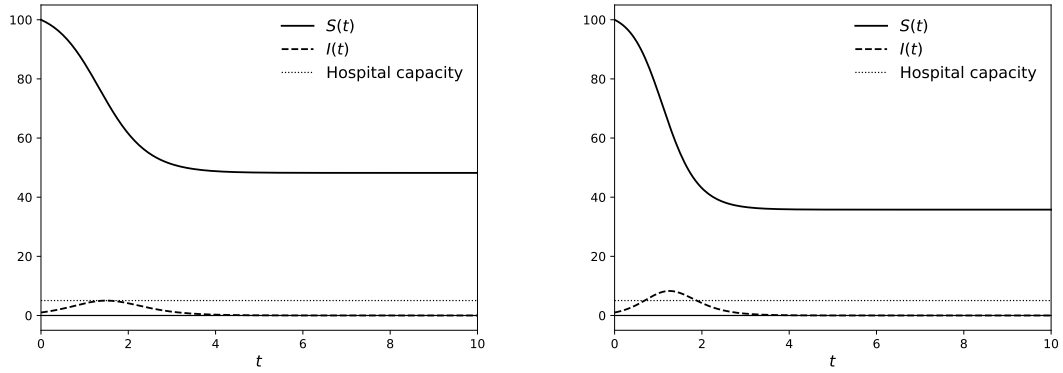


FIGURE 3. Two simulations of (5.1) with parameters $\beta = 7$ on the left, $\beta = 8$ on the right. Other parameters are equal, $\gamma = 5$, $\mu_s = 0.1$, $\mu_i = 0.02$

population, and for the infectious population a normalised product of $\sin^2(\pi x)$ and a normal distribution, to weigh the distribution more to the middle of the domain.

In figure 3 we show two simulations with similar parameters. The proportion of the total population that is infected at time 0 is 1% in both cases, and we set $\gamma = 5$. We assume in this population that the infectious population moves around much less than the susceptible population, so we set $\mu_s = 0.1$ and $\mu_i = 0.02$. The parameter we change is $\beta$, in the first simulation we use $\beta = 7$ and in the second simulation we use $\beta = 8$. We arbitrarily assume that the region's hospitals have capacity enough for 5% of the region's population to be infected and we see that in the first simulation the epidemic reaches this capacity almost exactly. In the slightly more infectious case in the second simulation, with $\beta = 8$, the hospitals' capacity is breached by quite a bit and stays that way for some time. This would likely result in many more casualties in the second simulation than in the first, both directly and indirectly.

Limiting the movements of the population through quarantines and similar measures is a tool available to fight epidemics. To investigate the effects of movement in our model we make two simulations. In the first the population moves fairly freely, with $\mu_s = 0.05$ and $\mu_i = 0.025$, and in the second movements are very limited, having $\mu_s = 0.02$ and $\mu_i = 0$. In both simulations we have $\beta = 8$, $\gamma = 5$ and 1% of the population starts as infected. We again assume the hospitals have capacity for 5% of the region to be infected. As we see in figure 5, the simulation with freer movement breaks our chosen hospital capacity, while the simulation with movement restrictions stays under the capacity. In figure 4 we see that the infected population is very localised in the simulation with movement restrictions, which can make it easier to protect at-risk parts of the population. This shows that in our model, restricting movement can be an effective tool to fight the epidemic.

## 6. Conclusion

In this paper, we have proposed a finite difference scheme to solve the reaction-diffusion equation. (1.1) We have shown that it is convergent of order two in both space and time for linear reaction terms and confirmed this with computations. We have applied this method to the SIR model in epidemiology and made simulations showing the effects of varying some of the parameters in the model.

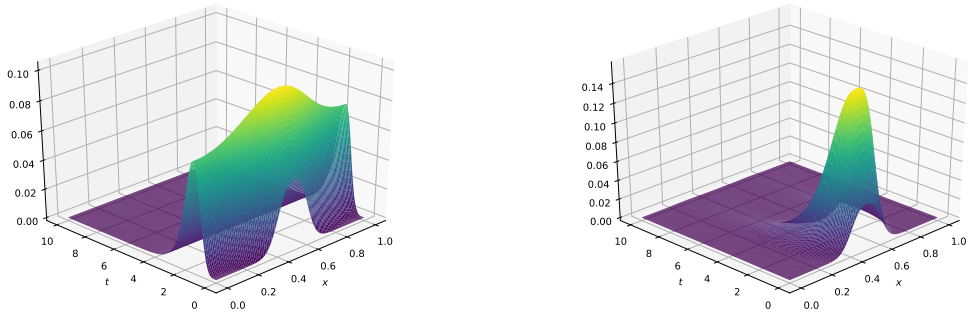


FIGURE 4. Time and space evolution of the infected population in two simulations of (5.1) with interesting parameters. $\mu_s = 0.05, \mu_i = 0.025$ on the left, $\mu_s = 0.02, \mu_i = 0$ on the right. Other parameters are equal, $\beta = 8$ $\gamma = 5$.

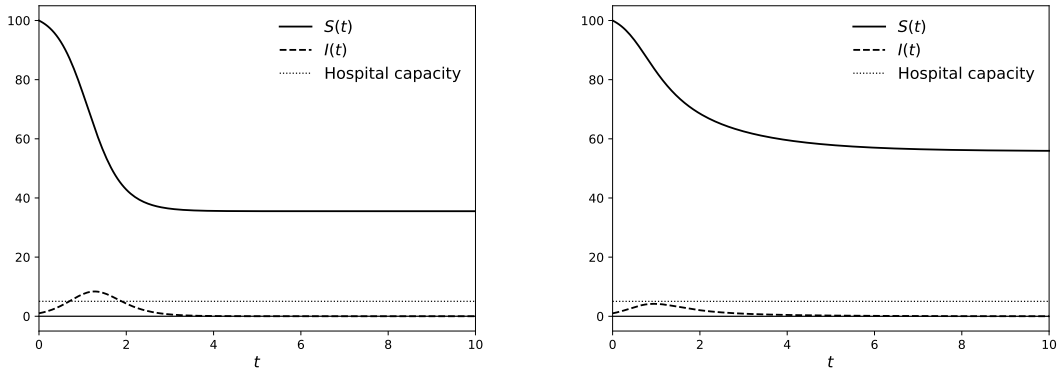


FIGURE 5. Two simulations of (5.1) with parameters $\mu_s = 0.05, \mu_i = 0.025$ on the left, $\mu_s = 0.02, \mu_i = 0$ on the right. Other parameters are equal, $\beta = 8$ $\gamma = 5$.

## REFERENCES

[1] Brynjulf Owren. *TMA4212 Numerical solution of partial differential equations with finite difference methods*. NTNU, 2017.