Derivation of non-standard finite difference schemes for differential equations

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Abstract

In this document, we illustrate the construction process of non-standard finite difference schemes for an ordinary and partial differential equations, by making the discrete scheme satisfy a known solution to the differential equation. We start by deriving the methods presented by Mickens, et al. and go on to derive a new nsfd scheme for the heat equation. We also explore the application of the non-standard finite difference operators we deduce to more general equations.

1 Introduction

The method of finite differences is a popular numerical technique for modeling the solutions to ordinary and partial differential equations. In most practical cases, we are interested in modeling equations to which we cannot readily find analytical solutions. However, it is often the case that these equations have related but simpler counterparts to which we can derive analytical solutions. Consider for example, the IVP:

$$\frac{du}{dt} = -\lambda u \quad ; \quad u(0) = u_0 \tag{1.1}$$

The solution is $\tilde{u}(t) = u_0 e^{-\lambda t}$. Hence, we have that:

$$\left(\frac{d}{dt} + \lambda\right)\tilde{u}(t) = 0$$

Let us now discretize the problem on the time interval $0 < t < T$ and use finite difference to construct a discrete approximation to the operator. If we use N points such that $t_0 = 0, t_N = T$, then the step size $h = \frac{T}{N} = t_{k+1} - t_k$ and the discrete time derivative operator is given by $\frac{d}{dt}_{(\mathrm{fd})} u = \frac{u_{k+1} - u_k}{h}$. When applied to (1.1), we get the scheme:

$$u_{k+1} = (1 - \lambda h) u_k$$

Notice that when h is large, this scheme may not even converge to zero as $k \to \infty$ as the analytical solution $\tilde{u}(t)$ does. Moreover,

$$\left(\frac{d}{dt}_{(\mathrm{fd})} + \lambda\right)\tilde{u} \neq 0$$

It is clear that the standard finite difference scheme does not properly model a fundamental property of (1.1) (at least when the step size h is not very small). With the knowledge of the analytical solution, we can easily find an exact, non-standard finite difference scheme for (1.1). We can then apply the modified operator we obtained from this scheme to more complicated equations, which may not have easily derived analytical solutions. We start our discussion by recounting results developed by Mickens et al and Cole et al [3, 2, 1] and then apply the idea to the heat equation pde.

2 Applying nsfd to ODEs

Given $\tilde{u} = u_0 e^{-\lambda t}$ as the solution to (1.1), we see that the difference equation $u_{k+1} = u_k e^{-\lambda h}$ is the discrete analogue of the exact solution. Notice that $u_1 = u_0 e^{-\lambda h}, u_2 = u_0 e^{-2\lambda h}, \ldots, u_{k+1} = u_0 e^{-(k+1)\lambda h}$. If we define our non-standard finite difference operator via:

$$\frac{d}{dt}_{(\text{nsfd})} = \frac{u_{k+1} - u_k}{\phi(h)}$$

where $\phi(h)$ is a more general function of h than h, we can derive an exact finite difference scheme by comparing the nsfd scheme to the exact scheme:

$$\frac{u_{k+1} - u_k}{\phi(h)} = -\lambda u_k \implies u_{k+1} = (1 - \lambda\phi(h))\, u_k \quad \text{and} \quad u_{k+1} = e^{-\lambda h} u_k$$

Setting $(1 - \lambda\phi(h)) = e^{-\lambda h}$, we get $\phi(h) = \frac{1-e^{-\lambda h}}{\lambda}$. The scheme

$$\frac{d}{dt}_{(\text{nsfd})} u_k = -\lambda u_k$$

is exact for (1.1). The non-standard finite difference operator satisfies:

$$\left(\frac{d}{dt}_{(\text{nsfd})} + \lambda \right) \tilde{u} = 0$$

We can easily see this by expanding:

$$\begin{aligned} \frac{(1-e^{-\lambda h})}{\lambda} \left[\frac{u_0 e^{-\lambda t_{k+1}} - u_0 e^{-\lambda t_k}}{\frac{(1-e^{-\lambda h})}{\lambda}} + \lambda u_0 e^{-\lambda t_k} \right] &= u_0 e^{-\lambda t_{k+1}} - u_0 e^{-\lambda t_k} + (1 - e^{-\lambda h}) u_0 e^{-\lambda t_k} \\ &= u_0 e^{-\lambda t_{k+1}} - u_0 e^{-\lambda h} e^{-\lambda t_k} = 0 \end{aligned}$$

where we have used $e^{-\lambda h} e^{-\lambda t_k} = e^{-\lambda(t_k + h)} = e^{-\lambda t_{k+1}}$.

An exact finite difference scheme of (1.1) may not be of much interest, since it is based on the analytical solution which is easy to derive. However, the non-standard finite difference operator which we derived, can be applied to related, but more complicated equations. Consider, for example:

$$\frac{du}{dt} = \cos(u) u \quad ; \quad u(0) = u_0 \tag{2.1}$$

While the equation looks simple, an analytical solution is not readily available. We can however, analyze the behavior of the solution. For instance, $\frac{du}{dt} \to 0$ as $u \to \frac{\pi}{2}$. The standard finite difference scheme given by $u_{k+1} = u_k + h\cos(u_k)u_k$ gives poor results when h is not small enough, for example with $h = 1$, as illustrated in Figure 1. On the other hand, we can appy the non-standard finite difference operator we derived for (1.1) for (2.1). To do this, notice that if we have an approximation u_k for $u(t_k)$ at iteration k, then we can set $\cos(u_k) = -\alpha$ and apply the scheme with the nsfd $\frac{d}{dt}_{(\text{nsfd})}$ operator we derived; where the operator is now iteration dependent:

$$u_{k+1} = u_k + \frac{1 - e^{\cos(u_k)h}}{-\cos(u_k)} \cos(u_k)u_k$$

where we apply the above update as long as $|\cos(u_k)|$ is far enough from zero. As we show in Figure 1, the nsfd scheme gives better performance than the standard finite difference method for higher values of h.

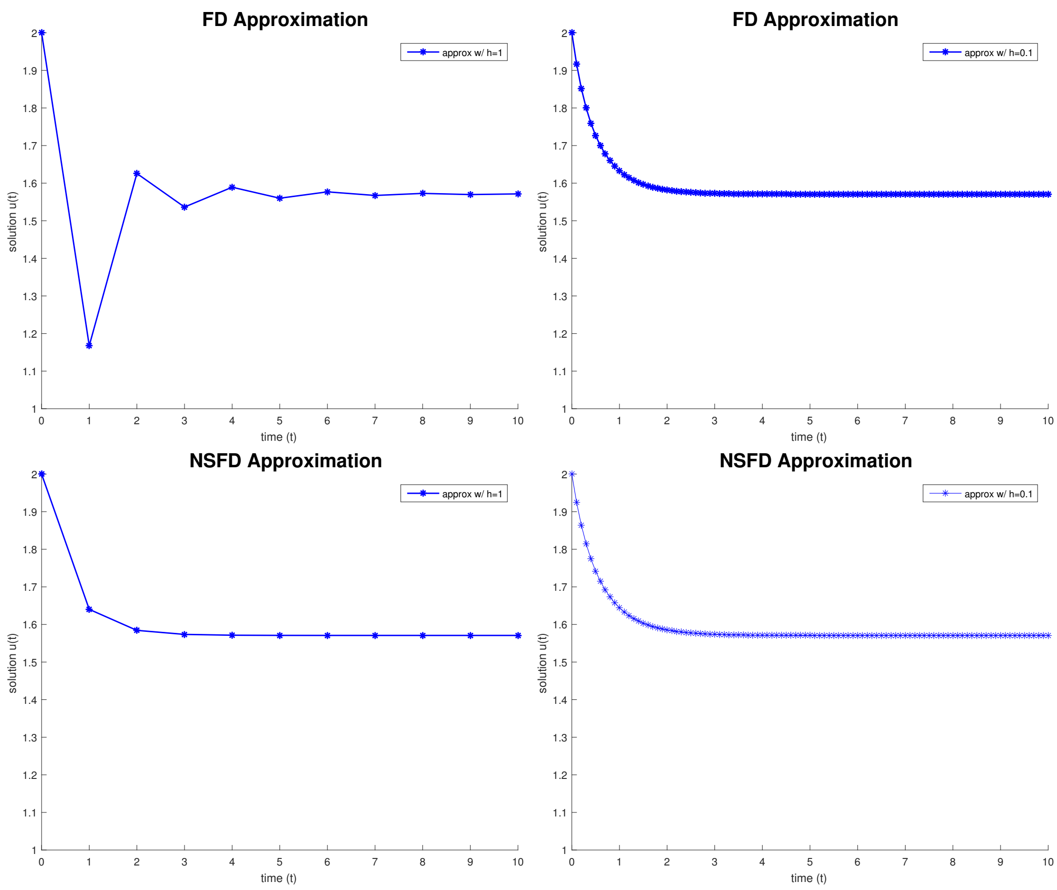

Figure 1: Comparision of fd and nsfd schemes with step size $h = 1$ and $h = 0.1$ for (2.1).

3 Applying nsfd to PDEs

The nsfd idea, as we have presented it, can be applied also to partial differential equations. Below we illustrate the application to the wave and heat equations, which results in minimial modifications to the respective classical difference schemes, but gives better numerical performance.

3.1 Wave equation

Consider the $1-D$ wave equation problem with common boundary and initial conditions:

$$\begin{aligned} & u_{tt} - v^2 u_{xx} = 0 \quad ; \quad 0 < x < L \quad ; \quad 0 < t < T \\ & u(0,t) = U_0 \quad ; \quad u(L,t) = U_L \quad ; \quad 0 < t < T \\ & u(x,0) = f(x) \quad ; \quad u_t(x,0) = g(x) \quad ; \quad 0 < x < L \end{aligned} \tag{3.1}$$

We proceed to discretize this using standard finite differences, using the operators:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2}_{\text{fd}}(x_i, t_j) &= \frac{u(x_i, t_{j+1}) - 2u(x_i, t_j) + u(x_i, t_{j-1})}{l^2} \\ \frac{\partial^2 u}{\partial x^2}_{\text{fd}}(x_i, t_j) &= \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} \end{aligned} \tag{3.2}$$

with h, l being, respectively, the spatial and time variable step sizes. Upon plugging into (3.1), we obtain the scheme:

$$u_{i,j+1} = 2(1 - s_i)u_{i,j} + s_i u_{i+1,j} + s_i u_{i-1,j} - u_{i,j-1} \tag{3.3}$$

with $s_i = \left(\frac{l}{h}\right)^2 v_i^2$; defined so that a non-constant wave speed can also be used. To implement the initial conditions in (3.1), we can use the center difference formula:

$$u_{i,1} - u_{i,-1} = 2g(x_i)l,$$

which allows us to replace the fictitious values $u_{i,-1}$.

For the purpose of deriving a non-standard finite difference scheme as proposed in [2], we look at a plain wave solution of the differential equation in (3.1):

$$\tilde{u}(x,t) = e^{i(kx - wt)}$$

Here $k = \frac{2\pi}{\lambda}$, with λ the wavelength of the wave, and $w = 2\pi f$ the angular frequency. The speed of the wave is given by $v = \lambda f = \frac{w}{k}$. Notice that $\tilde{u}$ satisfies (3.1). Since $\tilde{u}_{tt} = -w^2 e^{ikx} e^{-iwt}$ and $\tilde{u}_{xx} = -k^2 e^{ikx} e^{-iwt}$, it follows that:

$$\left(\frac{\partial^2}{\partial t^2} - v^2 \frac{\partial^2}{\partial x^2}\right) \tilde{u} = -w^2 e^{ikx} e^{-iwt} + v^2 k^2 e^{ikx} e^{-iwt} = 0$$

where we use that $v^2 k^2 = \frac{w^2}{k^2} k^2 = w^2$. When we apply the standard finite differences discretized operators, however, we get that:

$$\left(\frac{\partial^2}{\partial t^2}_{\text{fd}} - v^2 \frac{\partial^2}{\partial x^2}_{\text{fd}}\right) \tilde{u} \neq 0$$

As in the case of the ODE example we considered, we would like to find non-standard finite difference operators in place of the standard ones, such that $\tilde{u}$ solves the resulting equation. Based on (3.2), we define:

$$\begin{aligned} \vec{d}_x^2 f(x,t) &= f(x+h,t) - 2f(x,t) + f(x-h,t) \\ \vec{d}_t^2 f(x,t) &= f(x,t+l) - 2f(x,t) + f(x,t-l) \end{aligned}$$

We proceed to evaluate the result of $\left(\frac{\vec{d}_t^2}{l^2} - v^2\frac{\vec{d}_x^2}{h^2}\right)\tilde{u}(x,t)$, with the goal of adjusting the differencing operators to achieve an exact scheme with respect to $\tilde{u}$:

$$\begin{aligned} \vec{d}_x^2\left[e^{i[kx-wt]}\right] &= e^{i[k(x+h)-wt]} + e^{i[k(x-h)-wt]} - 2e^{i[kx-wt]} = e^{i[kx-wt]}\left(e^{ikh}+e^{-ikh}\right) - 2e^{i[kx-wt]} \\ &= 2e^{i[kx-wt]}\left[\cos(kh)-1\right] \end{aligned}$$

$$\begin{aligned} \vec{d}_t^2\left[e^{i[kx-wt]}\right] &= e^{i[kx-w(t+l)]} + e^{i[kx-w(t-l)]} - 2e^{i[kx-wt]} = e^{i[kx-wt]}\left(e^{iwl}+e^{-iwl}\right) - 2e^{i[kx-wt]} \\ &= 2e^{i[kx-wt]}\left[\cos(wl)-1\right] \end{aligned}$$

Thus, with $\tilde{u}(x,t) = e^{i[kx-wt]}$, we get:

$$\begin{aligned} \left(\frac{\vec{d}_t^2}{l^2} - v^2\frac{\vec{d}_x^2}{h^2}\right)\tilde{u}(x,t) = 0 \quad &\Longrightarrow \quad \frac{2}{l^2}\tilde{u}(x,t)\left[\cos(wl)-1\right] - v^2\frac{2}{h^2}\tilde{u}(x,t)\left[\cos(kh)-1\right] = 0 \\ &\Longrightarrow \quad \tilde{u}(x,t)\left[\left[\cos(wl)-1\right] - v^2\frac{l^2}{h^2}\left[\cos(kh)-1\right]\right] = 0 \\ &\Longrightarrow \quad v^2\frac{l^2}{h^2} = \frac{\left[\cos(wl)-1\right]}{\left[\cos(kh)-1\right]} \end{aligned}$$

To make an exact scheme out of (3.3) with respect to $\tilde{u}$, we replace s_i by $p_i = \frac{[\cos(wl)-1]}{[\cos(k_i h)-1]}$ with $k_i = \frac{w}{v_i}$ to obtain the scheme:

$$u_{i,j+1} = 2(1-p_i)u_{i,j} + p_i u_{i+1,j} + p_i u_{i-1,j} - u_{i,j-1} \tag{3.4}$$

For constant velocity v, we can make use of D'Alembert's formula for the solution of the initial value problem in (3.1):

$$u(x,t) = \frac{1}{2}\left[f(x-vt) + f(x+vt)\right] + \frac{1}{2v}\int_{x-vt}^{x+vt} g(s)ds$$

In Figure 2, we plot the solutions to (3.1) using the nsfd and fd schemes with $v = 2, f(x) = \sin(2\pi x), g(x) = 0$ with step sizes $h = 0.0016$ and $l = 0.2h$ for $0 < x < 1$ and $0 < t < 1$. For constant velocity problems, the schemes give about the same results. For variable velocity problems, for example with $v(x) = |\cos(x)|+1$, we find more consistent solutions with the nsfd scheme, when the solution is evaluated at larger step sizes. In Figure 3, we show the approximation to $u(:,1)$ obtained with different step sizes with both schemes. Given the above velocity profile, we expect the amplitude of the wave to not blow up, but this is precisely the effect we observe for larger step sizes with the standard scheme. When the step size h is reduced, we get consistent results with both schemes. To see why this is the case, notice that the only difference between (3.3) and (3.4) is in the replacement of $s_i = \left(\frac{l}{h}\right)^2 v_i^2$ by

$$p_i = \frac{[\cos(wl) - 1]}{[\cos(k_i h) - 1]} = \frac{\sin^2\left(\frac{wl}{2}\right)}{\sin^2\left(\frac{k_i h}{2}\right)}$$

When $0 < h, l \ll 1$, we can use the Taylor series approximation $\sin(q) \approx q$ valid for small q, as well as the relation $k = \frac{w}{v}$, to obtain:

$$p_i \approx \frac{\left(\frac{wl}{2}\right)^2}{\left(\frac{kh}{2}\right)^2} = \frac{w^2 l^2}{k^2 h^2} = \frac{k^2 v^2 l^2}{k^2 h^2} = \frac{v^2 l^2}{h^2} = s_i$$

For small h, l, the stability criterion $s_i \leq 1$ is valid for both schemes.

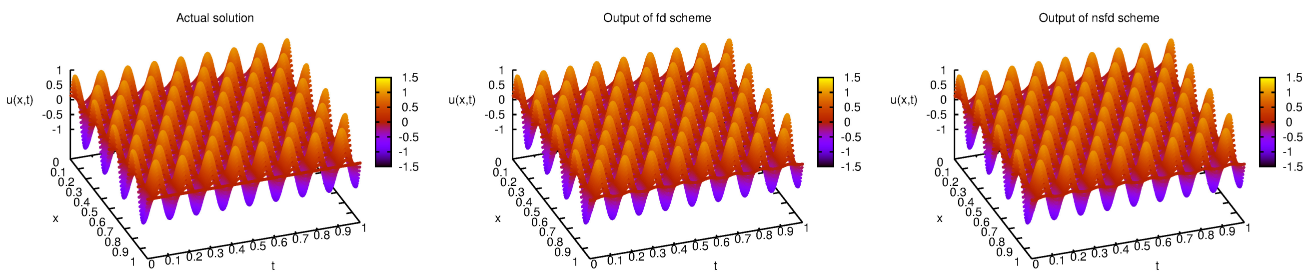

Figure 2: Exact, fd and nsfd scheme solutions to (3.1) with constant $v \in \mathbb{R}$.

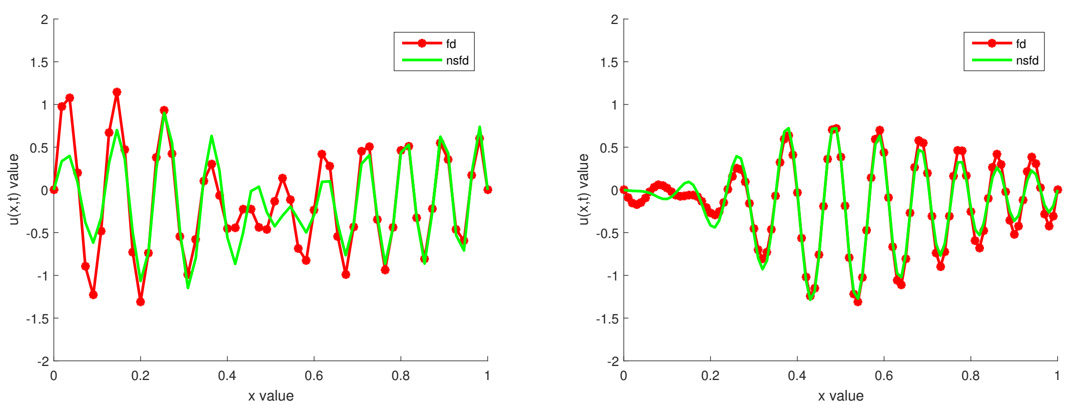

Figure 3: fd and nsfd scheme solution curves at $t = 1$ to (3.1) with non-constant $v(x) = |\cos(x)| + 1$, using larger ($h = 0.05$) and smaller ($h = 0.01$) step sizes (with $l = h^2$).

3.2 Heat equation

We consider the heat equation initial boundary value problem:

$$\begin{aligned} u_t &= ku_{xx}, \quad 0 < x < 1, \\ u(x,0) &= f(x), \quad 0 < x < 1, \\ u(0,t) &= u(1,t) = 0, \quad t > 0 \end{aligned} \tag{3.5}$$

with constant $k \in \mathbb{R}$. Via a transformation, we can extend this problem to nonzero boundary conditions. The difference scheme we will derive for (3.5) can then be applied also to the case of non-constant k, which is more interesting to model. For (3.5), separation of variables gives the solution as the superposition of solutions of the form

$$\tilde{u} = e^{-\pi^2 kt} \sin(\pi x)$$

A quick calculation shows that $\left[\frac{\partial}{\partial t} - k\frac{\partial^2}{\partial x^2}\right] \tilde{u} = 0$. However, as before, when we replace the continous derivative operators by finite differences, the solution $\tilde{u}$ is not satisfied. To form the well known explicit scheme, we use the forward in time and central in space difference operators:

$$\begin{aligned} \frac{\partial u}{\partial t}_{\text{fd}}(x_i, t_j) &= \frac{u(x_i, t_{j+1}) - u(x_i, t_j)}{l} \\ \frac{\partial^2 u}{\partial x^2}_{\text{fd}}(x_i, t_j) &= \frac{u(x_{i+1}, t_j) - 2u(x_i, t_j) + u(x_{i-1}, t_j)}{h^2} \end{aligned} \tag{3.6}$$

which results in the explicit finite diffence scheme:

$$u_{i,j+1} = u_{i,j} + \frac{kl}{h^2}\left(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}\right) \tag{3.7}$$

As for the wave equation, we would like to find non-standard finite difference operators in place of the standard ones, such that $\tilde{u}$ solves the resulting equation. Based on (3.6), we define:

$$\begin{aligned} \bar{d}_t f(x,t) &= f(x, t+l) - f(x,t) \\ \bar{d}_x^2 f(x,t) &= f(x+h, t) - 2f(x,t) + f(x-h, t) \end{aligned}$$

and proceed to evaluate $\left(\frac{\bar{d}_t}{l} - k\frac{\bar{d}^2{}_x}{h^2}\right) \tilde{u}(x,t)$.

$$\begin{aligned} \bar{d}_t\left[\tilde{u}(x,t)\right] &= \sin(\pi x)\left[e^{-\pi^2 k(t+l)} - e^{-\pi^2 kt}\right] = \sin(\pi x) e^{-\pi^2 kt}\left(e^{-\pi^2 kl} - 1\right) = \tilde{u}\left(e^{-\pi^2 kl} - 1\right) \\ \bar{d}_x^2\left[\tilde{u}(x,t)\right] &= e^{-\pi^2 kt}\left[\sin(\pi(x+h)) - 2\sin(\pi x) + \sin(\pi(x-h))\right] \\ &= e^{-\pi^2 kt}\left[\frac{1}{2i}\left(e^{i\pi(x+h)} - e^{-i\pi(x+h)}\right) - 2\sin(\pi x) + \frac{1}{2i}\left(e^{i\pi(x-h)} - e^{-i\pi(x-h)}\right)\right] \\ &= e^{-\pi^2 kt}\frac{1}{2i}\left[e^{i\pi x}e^{i\pi h} - e^{-i\pi x}e^{-i\pi h} - 4i\sin(\pi x) + e^{i\pi x}e^{-i\pi h} - e^{-i\pi x}e^{i\pi h}\right] \\ &= e^{-\pi^2 kt}\frac{1}{2i}\left[e^{i\pi x}\left(e^{i\pi h} + e^{-i\pi h}\right) - e^{-i\pi x}\left(e^{-i\pi h} + e^{i\pi h}\right) - 4i\sin(\pi x)\right] \\ &= e^{-\pi^2 kt}\frac{1}{2i}\left[2\cos(\pi h)\left(e^{i\pi x} - e^{-i\pi x}\right) - 4i\sin(\pi x)\right] = e^{-\pi^2 kt}\frac{1}{2i}\left[4i\cos(\pi h)\sin(\pi x) - 4i\sin(\pi x)\right] \\ &= 2e^{-\pi^2 kt}\sin(\pi x)\left[\cos(\pi h) - 1\right] = 2\tilde{u}\left[\cos(\pi h) - 1\right] \end{aligned}$$

Setting $\left(\bar{d}_t - \frac{kl}{h^2}\bar{d}^2{}_x\right)\tilde{u}(x,t) = 0$, we obtain:

$$\tilde{u}\left[e^{-\pi^2 kl} - 1\right] - \frac{2kl}{h^2}\tilde{u}\left[\cos(\pi h) - 1\right] = 0 \implies \left[e^{-\pi^2 kl} - 1\right] = \frac{2kl}{h^2}\left[\cos(\pi h) - 1\right]$$

Hence, the nsfd scheme follows if we make the following replacement in (3.7):

$$\frac{kl}{h^2} = \frac{1}{2}\left[\frac{e^{-\pi^2 kl} - 1}{\cos(\pi h) - 1}\right]$$

As for the wave equation nsfd scheme, when $h, l \ll 1$, the nsfd substitution coincides with the standard finite difference scheme. We use the small $|q|$ Taylor series approximations $e^q \approx 1 + q$ and $sin(q) \approx q$ to obtain:

$$\frac{1}{2}\left[\frac{e^{-\pi^2 kl} - 1}{\cos(\pi h) - 1}\right] = \left[\frac{e^{-\pi^2 kl} - 1}{-2\sin^2\left(\frac{\pi h}{2}\right)}\right] \approx \frac{1}{2}\left[\frac{1 - \pi^2 kl - 1}{-\frac{\pi^2 h^2}{2}}\right] = \frac{kl}{h^2}$$

By this it follows that for small h, l, the stability constraint $\frac{kl}{h^2} \leq 1$ is satisfied in the nsfd scheme when $l \leq \frac{h^2}{2}$ just like in the original scheme. This also holds for large h, as long as h is chosen so that $|\cos(\pi h) - 1|$ is not very small.

In all cases we tested for constant $k \in \mathbb{R}$ in (3.5), we found the nsfd scheme performs as good or better than the fd scheme. In Figure 4, we illustrate the errors vs step size obtained for a particular example, with the initial condition, $u(x,0) = \sin(\pi x) + x$ for problem 1, with boundary conditons $u(0,t) = 0$ and $u(1,t) = 1$ and with the initial condition $u(x,0) = 12\sin(9\pi x) - 7\sin(4\pi x)$ and zero homogeneous boundary conditions for problem 2. The nsfd scheme can also be used for non-constant $k = k(x)$. In our experiments, for larger step sizes h, the nsfd scheme gave more consistent results.

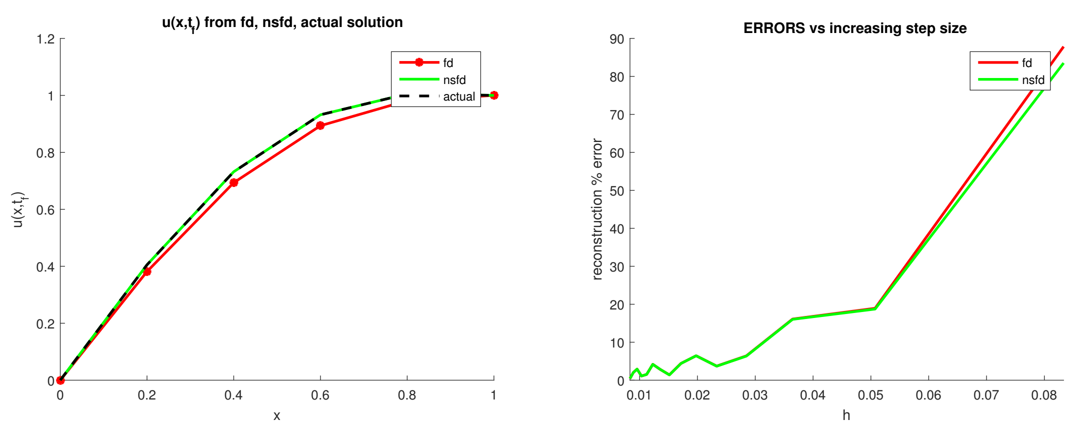

Figure 4: Solution to heat equation problem 1 with $h = 0.2$ and reconstruction errors vs step size h (with $l = \frac{h^2}{2}$) using the fd and nsfd schemes for heat equation problem 2.

4 Conclusions

In this document, we illustrated the derivation and use of non-standard finite difference schemes for ordinary and partial differential equations. In particular, we have illustrated how to obtain the non-standard finite difference scheme by forcing the differential operator equation to satisfy a known solution, rather than by the use of a set of rules to generalize the differential operator. We have then showed that the adjustments we derived can be used for more general equations (e.g. with non-constant terms) for which analytical solutions are not readily obtainable.

References

[1] James B Cole. High accuracy solution of maxwellś equations using nonstandard finite differences. Computers in Physics, 11(3):287–292, 1997. 2

[2] Ronald E Mickens. Nonstandard finite difference schemes for differential equations. The Journal of Difference Equations and Applications, 8(9):823–847, 2002. 2, 4

[3] Ronald E Mickens. Advances in the applications of nonstandard finite difference schemes. World Scientific, 2005. 2