Non-smooth data and stronger stability concepts

The previous analysis of consistency and stability builds on regularity of the solution: smoothness of sufficient order is needed to compute the truncation error. The most important applications in finance lack this regularity, as a result of non-smooth data. Moreover, solution and error are measured in certain norms, so at the very least the data have to lie locally in L_∞ or L_2. For Dirac initial data, even this is not the case. Fortunately, the smoothing properties of the PDE usually mean that these effects are seen only at isolated points in time, and it is perfectly possible to compare the exact and numerical solutions at a given time away from the singular points.

A prime case in point is the initial-value problem for the heat equation on the real line, with solution

$$u(x,t) = \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{\infty} u_0(y) \mathrm{e}^{-(x-y)^2/2t} \, \mathrm{d}y.$$

For reasonably well-behaved initial data u_0, the solution is infinitely smooth at any time $t > 0$. An interesting angle is given by the Fourier representation of u,

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \widehat{u_0}(k) \mathrm{e}^{-\frac{1}{2}k^2 t} \mathrm{e}^{ikx} \, \mathrm{d}k, \tag{5.46}$$

where $\widehat{u_0}$ is the Fourier transform of u_0. The wave components e^{ikx} of wave number k are dampened by $\mathrm{e}^{-\frac{1}{2}k^2 t}$, i.e. decay exponentially in time and increasingly fast for high k. This corresponds to the intuition that diffusion smoothens out highly oscillatory components rapidly.

In comparison, for the θ-central difference scheme, the damping factor is

$$R_\theta(\Delta x, \Delta t; k) = \frac{1 - 2(1-\theta)\Delta t/\Delta x^2 \sin^2(k/2)}{1 + 2\theta \Delta t/\Delta x^2 \sin^2(k/2)}. \tag{5.47}$$

There is also time exponential decay by R_θ^m after m timesteps, if $|R_\theta(\Delta x, \Delta t; k)| < 1$. We now scrutinize this in more detail for the Crank-Nicolson scheme. Given a consistency order of two in both space and time, one would like to pick $\Delta t = O(\Delta x)$. It is therefore practically relevant to analyse the behaviour as $\Delta t/\Delta x^2 \to \infty$, and one gets

$$R_{\frac{1}{2}}(\Delta x, \Delta t; k) \to -1 \quad \text{for} \quad \Delta t/\Delta x^2 \to \infty,$$

such that high frequency components maintain their amplitude persistently for fine meshes.

So refining the stability condition $|R_\theta(\Delta x, \Delta t; k)| < 1$, we want this to be true uniformly for all k, i.e.

$$|R_\theta(\Delta x, \Delta t; k)| < q \leq 1 \quad \forall\, 0 < k_0 \leq |k| \leq \pi,\ \Delta x, \Delta t \geq 0, \tag{5.48}$$

with Δt chosen in relation to Δx and k_0 a small number. The low frequencies $|k| \leq k_0$ correspond to the smooth component of the solution. Rearranging (5.47), (5.48) is guaranteed for $(1-2\theta+\epsilon)\Delta t \leq \Delta x^2$ for some small ϵ. This is automatically satisfied for $\theta > 1/2$. However, notably for the Crank-Nicolson scheme $\theta = 1/2$, there is a restriction $\Delta t = O(\Delta x^2)$ which compromises the efficiency of the scheme.

For implicit Euler, $\theta = 1$,

$$R_1(\Delta x, \Delta t; k) \to 0 \quad \text{for} \quad \Delta t/\Delta x^2 \to \infty \tag{5.49}$$

such that "high" frequencies with $k\Delta x = O(1)$ are dampened rapidly over timesteps. This comes at the expense of reduced accuracy for low wave-numbers. The implicit scheme is in a sense too diffusive. In contrast, the Crank-Nicolson scheme is not diffusive enough, which gives unrealistic solutions for non-smooth data.

In the following, we analyse this more precisely and then propose modifications which address this problem. For many of the data encountered in financial engineering, the irregularities are localised and appear in the form of kinks or discontinuities of an otherwise smooth function, or as Dirac components. This allows us to study these effects in isolation, given the linearity of the equations, and we can think of decomposing the data into smooth components and specific singularities of the above type. We start with the most severe, Dirac distributions. We have seen that they come up naturally in models for probability densities.

5.3.1 Dirac initial data and θ-schemes

We focus on the IBVP

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{1}{2}\frac{\partial^2 u}{\partial x^2}, \quad x \in \mathbb{R},\ t > 0, \\ u(\cdot, 0) &= \delta. \end{aligned}$$

A Dirac distribution as initial data is not even square integrable and the previous analysis of the error uniformly in time breaks down. We will instead use exact formulae for the analytic and finite difference solutions to the heat equation at a fixed finite time, which are known in this specific case, and compare the two to compute the discretisation error. This is clearly a stylized problem but we argue that the qualitative behaviour is similar in more general situations: in the presence of drift, boundary conditions, and even variable coefficients. This is because accuracy and stability are determined *locally* and we can therefore imagine "freezing" the coefficients at a constant level in a neighbourhood of the point of interest. Similarly, the effect of boundary conditions can be analyzed separately to this question. Finally, stability is influenced predominantly by the highest order term in the equation, which here is the second order diffusion term.

So, for a one-step finite difference scheme to the heat equation, recall from (4.16) in 4.3.2 that there is a Fourier representation

$$u_n^m = \int_{-\pi}^{\pi} R(\Delta x, \Delta t; k)^m \widehat{u}^0(k) \mathrm{e}^{ink}\, \mathrm{d}k. \tag{5.50}$$

In particular, for

$$u_n^0 = \frac{1}{\Delta x}\delta_{n0},$$

a discrete approximation to the Dirac distribution as in (2.16), it follows from (4.15) that

$$\widehat{u}^0(k) = \Delta x \sum_{n=-\infty}^{\infty} u_n^0 \mathrm{e}^{-ink} = 1.$$

Note that $u^0 \in l_2$, somewhat breaking the analogy with the continuous problem where $u(\cdot,0) = \delta \notin L_2$. From $|u^0|_2 = 1/\Delta x$ it is clear however that the limit $\Delta x \to 0$ is in some sense singular. The inversion formula (4.14) is easily verified here as

$$u_n^0 = \frac{1}{2\pi\Delta x}\int_{-\pi}^{\pi} \widehat{u}^0(k)\mathrm{e}^{ink}\,\mathrm{d}k = \frac{1}{2\pi\Delta x}\int_{-\pi}^{\pi} \mathrm{e}^{ink}\,\mathrm{d}k = \frac{1}{\Delta x}\delta_{n0}.$$

From (4.16),

$$u_n^m = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{1}{\Delta x} R(\Delta x, \Delta t; k)^m \mathrm{e}^{ink}\,\mathrm{d}k = \frac{1}{2\pi}\int_{-\pi/\Delta x}^{\pi/\Delta x} \widehat{u}^m(k)\mathrm{e}^{ikx_n}\,\mathrm{d}k.$$

This compares to the known analytical solution in the form

$$u(x_n, t_m) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \widehat{u}(t_m, k)\mathrm{e}^{ikx_n}\,\mathrm{d}k = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}k^2 m\Delta t}\mathrm{e}^{ikx_n}\,\mathrm{d}k.$$

For the θ-scheme, specifically, from (4.11),

$$\widehat{u}^m(k\Delta x) = R_\theta(\Delta x, \Delta t; \Delta x k)^m = \left(\frac{1 - 2(1-\theta)\Delta t/\Delta x^2 \sin^2(k\Delta x/2)}{1 + 2\theta\Delta t/\Delta x^2 \sin^2(k\Delta x/2)}\right)^m, \tag{5.51}$$

which has to be measured against

$$\widehat{u}(t_m, k) = \exp(-\tfrac{1}{2}k^2 m\Delta t). \tag{5.52}$$

From $(1 + x/m)^m \to \exp(x)$ for $m \to \infty$, it looks reasonably promising that the difference between (5.51) and (5.52) can be computed up to a certain order of Δt and Δx by Taylor expansion, as long as $k\Delta x$ is "small". We look at this regime first. For "large" k, the analytical solution goes to 0 exponentially fast and we have to make sure the timestepping scheme dampens these components at least to some order in $\Delta t, \Delta x$ as well (see the introductory comments). This is analysed in the subsequent section.

Low wavenumber range

We Taylor-expand in Δt and Δx the expression

$$\begin{aligned}\log(\widehat{u}^m(k\Delta x)) &= m\log(1 - 2(1-\theta)\Delta t/\Delta x^2 \sin^2(k\Delta x/2)) - m\log(1 + 2\theta\Delta t/\Delta x^2 \sin^2(k\Delta x/2)) \\ &= -\frac{1}{2}\,t\,k^2 + \frac{1}{24}\,t\,\Delta x^2\,k^4 + \frac{1}{8}(\theta^2 - (1-\theta)^2)\,t\,\Delta t\,k^4 - \frac{1}{4}(\theta^3 + (1-\theta)^3)\,t\,\Delta t^2\,k^6 \\ &\qquad + O(\Delta x^3 k^6) + O(\Delta t^3 k^8).\end{aligned}$$

As expected, the error is of second order in Δt exactly if $\theta = 1/2$, otherwise of first order. In the first case, we want to pick $\Delta t \sim \Delta x$ to balance leading order error terms in Δt and Δx^2, otherwise $\Delta t \sim \Delta x^2$. For the first remainder term to go to zero for $\Delta x \to 0$, we need

$k = o(\Delta x^{-1/2})$, for the second $k = o(\Delta t^{-3/8})$. Depending on whether $\Delta t \sim \Delta x^2$ or $\Delta t \sim \Delta x$, the first or second condition will be stringent.

Taking the exponential and Taylor-expanding again,

$$\begin{aligned} \widehat{u}^m(k\Delta x) &= \exp(-\tfrac{1}{2}k^2 t)\left(1 + \Delta t(2\theta - 1)\widehat{a}_1^m(k) + \Delta t^2 \widehat{a}_2^m(k) + \Delta x^2 \widehat{a}_3^m(k)\right. \\ &\qquad \left. + O(\Delta x^3 k^6) + O(\Delta t^3 k^8)\right), \quad (5.53) \end{aligned}$$

with suitably defined $\widehat{a}_1^m$, $\widehat{a}_2^m$, $\widehat{a}_3^m$.

Medium to high wavenumber range

Now looking at the behaviour for larger k, the first observation is that R_θ is decreasing in k. We argued earlier in 4.3.2 that for u^0 in l_2, i.e. square summable initial data, with $|u^0|_2$ bounded independent of Δx, the condition

$$(1 - 2\theta)\frac{\Delta t}{\Delta x^2} \leq 1$$

guarantees stability and consequently convergence. The above prerequisites on u^0 are not met here. In this case, we have to make sure that high wavenumber components are dampened sufficiently. Now we look at a number of key cases more closely.

For the fully implicit scheme, it still holds that $0 < R < 1$ for all $k \neq 0$. Because this term comes up so often, we introduce $f(y) = \sin^2(y/2)/(y/2)^2$ with $y \in [-\pi, \pi]$ and then $f(y) \in [4/\pi^2, 1]$. This implies

$$\widehat{u}^m(k\Delta x) = (1 + \tfrac{1}{2}k^2 \Delta t f(k\Delta x))^{-m} \to \exp(-\tfrac{1}{2}k^2 t f(k\Delta x)) \quad \text{for } m \to \infty, \qquad (5.54)$$

where $f(k\Delta x)$ is $O(1)$. In the range $\Delta x^{-p} \leq k \leq \pi/\Delta x$ for any $0 < p < 1$ the convergence to 0 is faster than Δx^r for any order $r > 0$.

An identical line of reasoning shows that for *any* θ, as long as $0 \leq R$, i.e. if $2(1 - \theta)\Delta t/\Delta x^2 \leq 1$, the convergence in the large wave number range is exponential. This guarantees e.g. convergence of the Crank-Nicolson scheme for $\Delta t \leq \Delta x^2$.

If $R \geq 0$ is not ensured, then there is a zero of R where

$$\tfrac{1}{2}(1 - \theta)\Delta t k^2 f(k\Delta x) = 1,$$

which appears at

$$k_0 = O(\Delta t^{-1/2}).$$

From the previous reasoning, we are covered for $k \leq k_0$. If we can ensure that

$$|R_\theta| \leq q < 1 \qquad (5.55)$$

for $k \geq k_0$, then surely in this range

$$|\widehat{u}^m(k)| \leq q^{-t/\Delta t} = o(\Delta t^r) = o(\Delta x^r)$$

for all $r > 0$.

The inequality (5.55) is given for $\theta > 1/2$ for all combinations of Δt and Δx, but *not* for the Crank-Nicolson scheme, $\theta = 1/2$, where $R_{1/2}(\Delta x, \Delta t; k) \to -1$ for $k \to \pm\pi$, $\Delta t/\Delta x^2 \to \pm\infty$.

Putting it all together

Summing up, if

$$1/2 < \theta \leq 1 \quad \text{or} \quad 2\Delta t \leq \Delta x^2 \text{ for } 0 \leq \theta \leq 1/2, \tag{5.56}$$

the approximation error is

$$u(x_n, t_m) - u_n^m = \frac{1}{2\pi} \int_{|k|>\pi/\Delta x} \mathrm{e}^{-\frac{1}{2}k^2 t_m} \mathrm{e}^{ikx_n} \, \mathrm{d}k + \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \left(\widehat{u}(k, t_m) - \widehat{u}^m(k\Delta x)\right) \mathrm{e}^{ikx_n} \, \mathrm{d}k,$$

where

$$\Big| \int_{|k|>\pi/\Delta x} \mathrm{e}^{-\frac{1}{2}k^2 t_m} \mathrm{e}^{ikx_n} \, \mathrm{d}k \Big| \leq \int_{|k|>\pi/\Delta x} \mathrm{e}^{-\frac{1}{2}k^2 t_m} \, \mathrm{d}k = o(\Delta x^r)$$

for all $r > 0$ and

$$\begin{aligned} \int_{-\pi/\Delta x}^{\pi/\Delta x} \left(\widehat{u}(k, t_m) - \widehat{u}^m(k\Delta x)\right) \mathrm{e}^{ikx_n} \, \mathrm{d}k \; &= \; \Delta t(2\theta - 1) a_1^m(x_n) + \Delta t^2 a_2^m(x_n) + \Delta x^2 a_3^m(x_n) \quad (5.57) \\ &\quad + O(\Delta x^3) + O(\Delta t^3), \end{aligned}$$

where

$$a_j^m(x) = \frac{1}{2\pi} \int_{-\pi/\Delta x}^{\pi/\Delta x} \widehat{a}_j^m(k) \mathrm{e}^{-\frac{1}{2}k^2 t_m} \mathrm{e}^{ikx} \, \mathrm{d}k.$$

In short,

$$u(x_n, t_m) - u_n^m = (1 - 2\theta) O(\Delta t) + O(\Delta t^2) + O(\Delta x^2), \tag{5.58}$$

provided the stronger "stability"[1] constraint (5.56) is satisfied.

In particular:

- As expected, the fully implicit scheme converges of first order in Δt and second order in Δx, unconditionally.
- Also, unsurprisingly, the explicit Euler scheme converges also of first order in Δt, but only if a timestep constraint $2\Delta t \leq \Delta x^2$ is fulfilled.
- A genuinely new phenomenon is encountered for the Crank-Nicolson scheme which is not unconditionally convergent in l_2 for Dirac initial data, even though it is unconditionally stable in the l_2 sense.

In the following, we will introduce notions of stability which classify exactly this behaviour. We will also present a few solutions to the practical problem of constructing a second order convergent scheme which works for non-smooth, especially Dirac, initial data.

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[1] The term stability constraint is not entirely accurate, because it is incorrect to say that the scheme is unstable if these are violated, rather the data and the solution lie outside the class of functions where the standard stability analysis is applicable.

5.3.2 Stronger stability of time-stepping schemes

The last section provided ample evidence that the stability of time-stepping schemes is characterised by the amplification or damping of highly oscillatory components. These are best singled out by studying the equations in Fourier space. We have in mind in the following time-stepping schemes for the heat equation with drift, as in (5.1). For the θ-central difference scheme, for instance, Exercise 2 in 5.4 shows that on an infinite grid,

$$\widehat{u}^m(k) = R(\Delta x, \Delta t; k)\widehat{u}^{m-1}(k) = R^m(\Delta x, \Delta t; k)\widehat{u}^0(k), \tag{5.59}$$

where

$$R(\Delta x, \Delta t; k) = \frac{1 - (1-\theta)[2\sigma^2\Delta t/\Delta x^2 \sin^2(k/2) + i\mu\Delta t/\Delta x \sin(k)]}{1 + \theta[2\sigma^2\Delta t/\Delta x^2 \sin^2(k/2) + i\mu\Delta t/\Delta x \sin(k)]}$$

is the amplification facor or symbol. One identifies the lengthy expression in $-[\ldots]$ as the eigenvalues of the spatial finite differences. For the equation without drift, the symbol reduces to (5.47), which is purely real, but generally we get an imaginary (phase) component. The domain of stability in Fourier space has to encompass all possible values of k. The corresponding eigenvalues $-[\ldots]$ are then characterised by negative real part, where the size depends on Δt and Δx but can be large. This motivates to investigate

$$R(z) = \frac{1 + (1-\theta)z}{1 - \theta z},$$

where $z \in \mathbb{C}^- = \{z \in \mathbb{C} : \, \mathrm{Re} z < 0\}$.

For a finite grid, recall the θ-scheme in matrix form

$$(I - \theta A)u^{m+1} = (I + (1+\theta)A)u^m \quad \Rightarrow \quad u^{m+1} = R(A)u^m = Q^{-1}(A)P(A)u^m, \tag{5.60}$$

where P, Q, R are appropriately defined (polynomial or rational) functions of the matrix A. For diagonalisable $A = BDB^{-1}$, a matrix function can be defined as $R(A) = BR(D)B^{-1}$ where $R(D)$ is the diagonal matrix with entries $R(d_{ii})$, where d_{ii} are the diagonal entries of D. (To see why this makes sense, picture the terms in a Taylor series for $R(A)$.) Writing

$$B^{-1}u^m = R(D)B^{-1}u^{m-1} = R(D)^m B^{-1}u^0$$

shows that stability is determined by the symbol R acting on the eigenvalues of A. For the central difference scheme, again for the heat equation with drift, the eigenvalues of A as per above are easily seen to be $\lambda_k = -\Delta t/\Delta x^2(\sigma^2 + \cos(k\xi)\sqrt{\sigma^4 - \Delta x^2\mu^2})$ with $\mathrm{Re}\lambda_k < 0$. They are real if $\sigma^2 \geq |\mu|\Delta x$.

The following classical notion of stability arises naturally.

Definition 5.3.1. A scheme (5.59) is called *absolutely stable (A-stable)* if

$$|R(z)| < 1 \quad \forall z \in \mathbb{C}^- = \{z \in \mathbb{C} : \, \mathrm{Re} z < 0\}. \tag{5.61}$$

The θ-scheme is A-stable for $\theta \geq \frac{1}{2}$.

Strong A-stability – fractional step schemes

We saw earlier that Crank-Nicolson does not dampen high wavenumber oscillations sufficiently, and this creates problems for non-smooth data. A stronger stability concept, which captures the required uniform damping across the spectrum, is the following.

Definition 5.3.2. A scheme (5.59) is called *strongly A-stable*, if it is A-stable and

$$\lim_{\mathrm{Re}z\to-\infty} |R(z)| < 1. \tag{5.62}$$

The θ-method is strongly A-stable for $\theta > \frac{1}{2}$, but the Crank-Nicolson scheme as borderline case is not. Recall that the Crank-Nicolson scheme of stepsize Δt can be seen as a combination of an explicit step ($\theta = 0$) of size $\Delta t/2$, followed by a fully implicit step ($\theta = 1$) of size $\Delta t/2$. This symmetry provides second order consistency, but lies just on the verge of stability. A natural generalisation are schemes which combine two or more, say k steps of θ-schemes with potentially different θ_j and potentially different step-size Δt_j, into one macro-step. For the scheme to be consistent, it is necessary that

$$\sum_{j=1}^{k} \Delta t_j = \Delta t, \tag{5.63}$$

and one easily sees that this is also sufficient. This leaves $2k-1$ degrees of freedom to play with to achieve higher than first order accuracy and strong stability. An analysis similar to the one leading onto (5.53) shows that the additional condition

$$\sum_{j=1}^{d} (2\theta_j - 1)\Delta t_j = 0 \tag{5.64}$$

leads to second order accuracy for constant coefficient problems. This shows immediately that it is not possible to pick all $\theta_j > 1/2$. Any number of Crank-Nicolson sub-steps is of course second order accurate, but not strongly stable. For strong stability, one has to ensure (5.61) and (5.62). Strictly, this fractional step scheme is not consistent with our earlier definitions of a symbol for a one-step scheme, but it is obvious that the definition

$$R(z) = \prod_{j=1}^{k} R_{\theta_j}(\Delta t_j/\Delta t z)$$

provides the necessary generalisation. Assuming A-stability, which of course has to be checked (Exercise 8 in 5.4), strong A-stability is given if

$$\prod_{j=1}^{k} \frac{(1-\theta_j)}{\theta_j} < 1.$$

We search in the parameter range $0 \le \Delta t_j \le \Delta t$ and $0 \le \theta_j \le 1$. This still leaves room for various choices.

The following scheme with $k = 3$ substeps has been proposed by Glowinski [Glowinski, 1985], with parameters chosen according to Table 5.1. The inuitive explanation why the scheme is

Table 5.1: Parameters for a fractional step θ-scheme.

i	Δt_i	θ_i
1	$(1-\sqrt{2}/2)\Delta t$	$2-\sqrt{2}$
2	$(\sqrt{2}-1)\Delta t$	$\sqrt{2}-1$
3	$(1-\sqrt{2}/2)\Delta t$	$2-\sqrt{2}$

of second order accurate is to note the symmetry of the substeps

$$t_m \;\rightarrow\; t_m+\Delta t_1 \;\rightarrow\; t_{m+1}-\Delta t_1 \;\rightarrow\; t_{m+1}$$

(and their θ-parameters) around $t+\Delta t/2$. It is left to Exercise 8 in 5.4 to show in detail that the resulting scheme is strongly A-stable and of second order accurate.

As an added bonus, $\theta_1\Delta t_1 = \theta_2\Delta t_2 = \theta_3\Delta t_3$, and therefore the implicit discretisation matrices $I-\theta_j\Delta t_j A$ are identical in each sub-step and therefore only one matrix has to be computed. Practically, if an implementation of the θ-scheme is available, this modification can be added on at almost no extra implementation cost, and guarantees second-order convergence for non-smooth data.

L-stable schemes – fully implicit start-up

A different type of scheme is more directly taylored to the important situation where non-smoothness arises only from initial data. We then know that the diffusion equation provides for smoothness of the solution after infinitesimally small time. This is seen e.g. from the formula (5.46) which shows the decay of high wavenumbers which may be present in the initial data u_0. In the class of θ-schemes, only the fully implicit scheme $\theta = 1$ has the same asymptotic behaviour for small grid sizes, as we saw in (5.49). This motivates an even stronger notion of stability.

Definition 5.3.3. A method is called *L-stable*, if it is A-stable and

$$\lim_{\mathrm{Re}\, z\to-\infty} R(z) = 0.$$

The θ-method is L-stable only for $\theta = 1$, i. e. the fully implicit method.

The idea to combine the smoothing property of an L-stable scheme to deal with non-smooth initial data, with the accuracy of a higher order A-stable scheme to take over the smooth solution, was proposed by Rannacher [Rannacher, 1984]. The underlying principle is that a small fixed (!) number of lower order steps does not reduce the order of convergence, while it smoothens the solution enough to eliminate spurious oscillations.

The following variant, now often referred to as Rannacher start-up, has proved useful in practice. Using the Crank-Nicolson scheme as basis, the first say l timesteps are replaced by $2l$ fully implicit steps of half the stepsize. A detailed analysis for the advection-diffusion equation with Dirac initial data is found in [Carter and Giles, 2007] and [Giles and Carter, 2006].

Essentially similar to (5.51), but now accounting for the modified start-up phase, the Fourier transform of the finite difference solution can be written as

$$\widehat{u}^m(k) = R_{\frac{1}{2}}(\Delta x, \Delta t; k)^{m-l} R_1(\Delta x, \Delta t/2; k)^{2l}\widehat{u}^0(k), \tag{5.65}$$

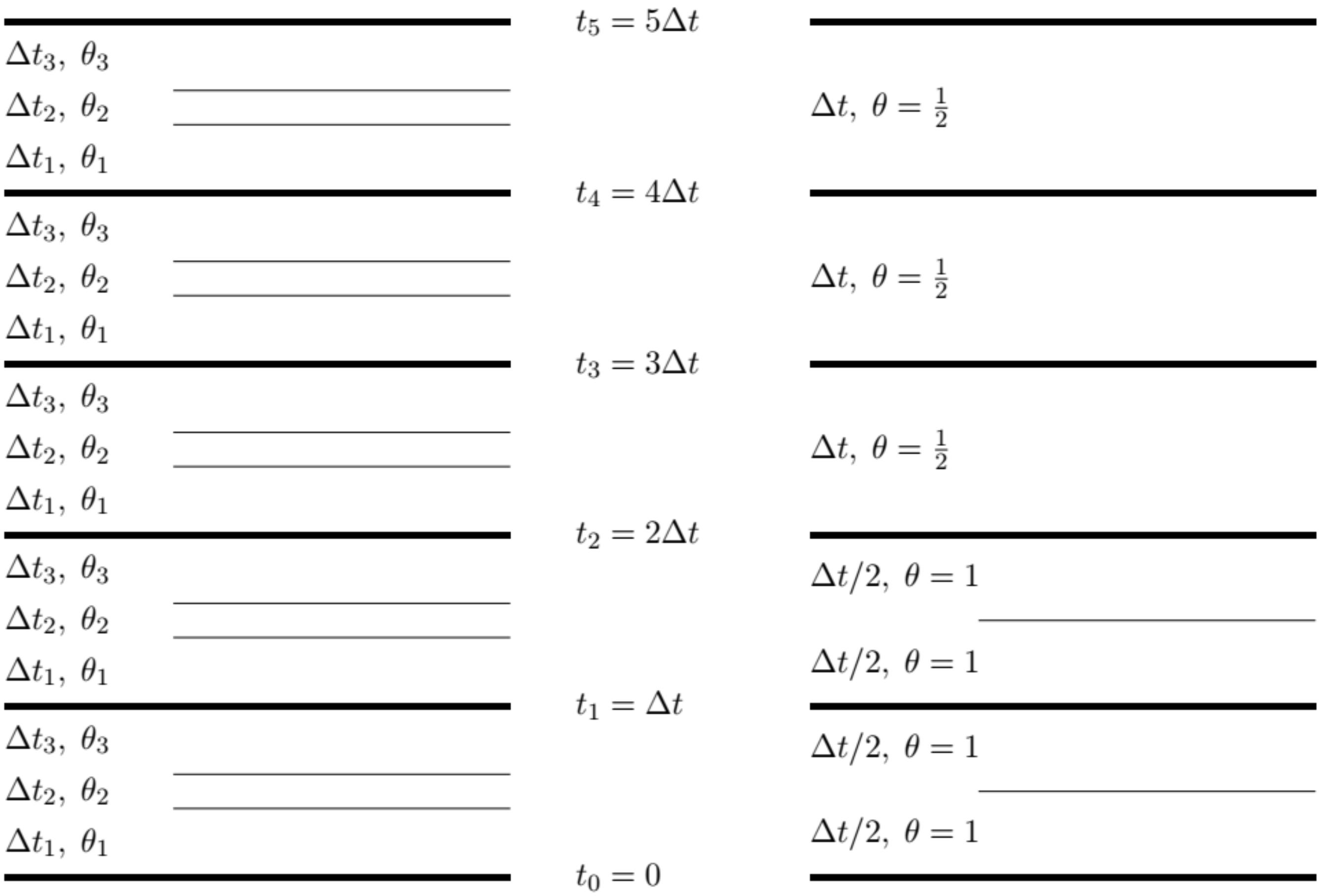

Figure 5.1: Schematic plot of the fractional-step θ-scheme (left) and Crank-Nicolson with "Rannacher start-up". In the first, *each* timestep is a sequence of three steps of θ-schemes with different θ_j and Δt_j, $j = 1, 2, 3$. In the latter, only the first four steps are implicit Euler steps ($\theta = 1$) of size $\Delta t/2$, all subsequent steps are Crank-Nicolson steps ($\theta = 1/2$) of size Δt.

where R_1 and $R_{1/2}$ are again the symbols of the fully implicit and Crank-Nicolson methods. Writing again

$$u_n^m = \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{\Delta x} R_{\frac{1}{2}}(\Delta x, \Delta t; k)^{m-l} R_1(\Delta x, \Delta t/2; k)^{2l} \mathrm{e}^{ink} \, \mathrm{d}k,$$

a careful analysis as in [Giles and Carter, 2006] shows that

- for small k, $|k|/\Delta x < \Delta x^{-p}$, $0 < p < 1/3$, the difference between the analytical solution (5.52) and numerical solution (5.65) is $O(\Delta x^2) + O(\Delta t^2)$, by Taylor expansion;
- for medium k, $\Delta x^{-p} < |k|/\Delta x < \Delta x^{-q}$, $1/2 < q < 1$, analytical and numerical solution are negligible;

- for large k, $\Delta x^{-q} < |k|/\Delta x$, the analytical solution is still negligible, but at least $l = 2$ fully implicit steps are needed to dampen these high frequency components in the numerical solution to below order Δx^2. Recall this is the range where Crank-Nicolson runs into problems.

Indeed it turns out that this is the optimal choice and restores second order convergence for Dirac initial data. A practical advantage of this particular setup is that the system matrices for Crank-Nicolson, and implicit Euler of half the stepsize, are identical, so similarly to the fractional step scheme only one matrix has to be computed.