1 Z-Transform Relation to Fourier Transform

In this problem we study how the grid scaled Z-transform of the discretized solution approaches the Fourier transform of the continuous solution as the space increment $h \to 0$. Recall that if $u_j = U(jh)$, the Z-transform $\hat{u}(\xi)$ is related to the Fourier transform $\hat{U}(\kappa) = \int_{-\infty}^{\infty} U(x)e^{-ix\kappa}dx$ via

$$h\hat{u}(h\kappa) = \sum_{m=-\infty}^{\infty} \hat{U}\left(\kappa - \frac{2\pi}{h}m\right).$$

Suppose that for $\kappa \in \mathbb{R}$, $\hat{U}(\kappa)$ satisfies

(a) $\left|\hat{U}(\kappa)\right| \le \frac{C_r}{1+|\kappa|^r}$,

(b) $\left|\hat{U}(\kappa)\right| \le Ce^{-\rho|\kappa|}$,

where $r \ge 2$, $C_r \ge 0$, $C > 0$ and $\rho > 0$ are constants. Show that for $|\kappa| \le \pi/h$, $\left|h\hat{u}(h\kappa) - \hat{U}(\kappa)\right|$ is bounded by

(a) $\frac{C_r h^r}{4\pi^{r-2}}$

(b) $\frac{2Ce^{-\rho\pi/h}}{1-e^{-2\rho\pi/h}}$.

Solution:

(a) First, note the fact that $\left|k \pm \frac{2\pi}{h}m\right| \ge \frac{2\pi m-\pi}{h}$ and $\sum_{m=1}^{\infty} \frac{1}{(2m-1)^2} = \frac{\pi^2}{8}$. Using these facts, we achieve the first upper bound as follows:

$$\begin{aligned}
\left|h\hat{u}(h\kappa) - \hat{U}(\kappa)\right| &= \left|\sum_{m=-\infty}^{\infty} \hat{U}\left(\kappa - \frac{2\pi}{h}m\right) - \hat{U}(\kappa)\right| \\
&= \left|\sum_{m\neq 0} \hat{U}\left(\kappa - \frac{2\pi}{h}m\right)\right| \\
&\le \sum_{m\neq 0} \left|\hat{U}\left(\kappa - \frac{2\pi}{h}\right)\right| \\
&\le \sum_{m\neq 0} \frac{C_r}{1+\left|\kappa - \frac{2\pi}{h}m\right|^r} \\
&\le \sum_{m=1}^{\infty} \frac{2C_r}{1+\left(\frac{2\pi m-\pi}{h}\right)^r} \\
&= \sum_{m=1}^{\infty} \frac{2C_r h^r}{1+\pi^r(2m-1)^r} \\
&\le \frac{2C_r h^r}{\pi^r} \sum_{m=1}^{\infty} \frac{1}{(2m-1)^r} \\
&\le \frac{2C_r h^r}{\pi^r} \sum_{m=1}^{\infty} \frac{1}{(2m-1)^2} \\
&= \boxed{\frac{C_r h^r}{4\pi^{r-2}}}.
\end{aligned}$$

(b) For the second upper bound, we start with the initial simplifications from the previous part as follows:

$$\begin{aligned}
\left|h\hat{u}(h\kappa) - \hat{U}(\kappa)\right| &\leq \sum_{m\neq 0} \left|\hat{U}\left(\kappa - \frac{2\pi}{h}\right)\right| \\
&\leq \sum_{m\neq 0} Ce^{-\rho|\kappa - 2\pi m/h|} \\
&\leq 2C\sum_{m=1}^{\infty} e^{-\rho(2\pi m-\pi)/h}) \\
&= 2Ce^{\rho\pi/h}\sum_{m=1}^{\infty}\left(e^{-2\rho\pi/h}\right)^m \\
&= \frac{2Ce^{\rho\pi/h}}{1-e^{-2\rho\pi h}}e^{-2\rho\pi/h} \\
&= \boxed{\frac{2Ce^{-\rho\pi/h}}{1-e^{-2\rho\pi h}}}
\end{aligned}$$

2 Circulant Matrix Properties

A circulant matrix is constant along diagonals with entries that "wrap around":

$$A_{jk} = \begin{Bmatrix} r_{k-j} & k \geq j, \\ r_{N+k-j} & k < j \end{Bmatrix}.$$

For convenience, we will index our matrices starting at zero. Show that $AU = U\Lambda$, with

$$U_{jk} = e^{2\pi ijk/N}, \quad \begin{pmatrix} 0 \leq j \leq N-1 \\ 0 \leq k \leq N-1 \end{pmatrix}, \quad \begin{pmatrix} \lambda_0 & & \\ & \ddots & \\ & & \lambda_{N-1} \end{pmatrix}$$

and $\lambda_k = \sum_{\ell=0}^{N-1} r_\ell e^{2\pi i\ell k/N}$.

Solution:

We proceed by showing that $(AU)_{jk} = (U\Lambda)_{jk}$. We compute the right hand side first:

$$\begin{aligned}(U\Lambda)_{jk} &= \lambda_k e^{2\pi ijk/N} \\ &= \sum_{\ell=0}^{N-1} r_\ell e^{2\pi i(\ell+j)k/N}.\end{aligned}$$

Now consider the left hand side:

$$\begin{aligned}(AU)_{jk} &= \sum_{\ell=0}^{N-1} A_{j\ell}U_{\ell k} \\ &= \sum_{\ell=0}^{N-1} A_{j\ell}e^{2\pi i\ell k/N}\end{aligned}$$

The value of $A_{j\ell}$ depends on the relationship between j and ℓ so we split up the sum into corresponding parts:

$$\begin{aligned}\sum_{\ell=0}^{N-1} A_{j\ell}e^{2\pi i\ell k/N} &= \sum_{\ell=0}^{j-1} A_{j\ell}e^{2\pi i\ell k/N} + \sum_{\ell=j}^{N-1} A_{j\ell}e^{2\pi i\ell k/N} \\ &= \sum_{\ell=0}^{j-1} r_{N+\ell-j}e^{2\pi i\ell k/N} + \sum_{\ell=j}^{N-1} r_{\ell-j}e^{2\pi i\ell k/N} \\ &= \sum_{\ell=N-j}^{N-1} r_\ell e^{2\pi i(\ell+j-N)k/N} + \sum_{\ell=0}^{N-j-1} r_\ell e^{2\pi i(\ell+j)k/N} \\ &= \sum_{\ell=N-j}^{N-1} r_\ell e^{2\pi i(\ell+j)k/N} + \sum_{\ell=0}^{N-j-1} r_\ell e^{2\pi i(\ell+j)k/N} \\ &= \sum_{\ell=0}^{N-1} r_\ell e^{2\pi i(\ell+j)k/N}.\end{aligned}$$

The expressions for $(AU)_{jk}$ and $(U\Lambda)_{jk}$ are indeed equal so we conclude that $AU = \Lambda U$.

3 Crank-Nicolson

Use the Crank-Nicolson scheme to solve the equation

$$u_t = \alpha u_{xx} - \beta u_x, \qquad \alpha = \frac{1}{512}, \quad \beta = \frac{33}{32} \tag{$\star$}$$

on the interval $[0,1]$ with periodic boundary conditions and initial conditions

$$u(x,0) = g(x), \quad g(x) = (\sin \pi x)^{100}.$$

Solution:

For the spatial discretizations, we replace the right-hand side of ($\star$) by $\alpha D_x^+ D_x^- u - \beta D_x^0 u$ and then use the trapezoidal rule in time. The trapezoidal rule is the approximation $(x_{n+1} - x_n)/h \approx (f_n + f_{n+1})/2$. Applying this method yields the following finite difference:

$$D_t^+ u^n = \frac{1}{2}(\alpha D_x^+ D_x^- u^n + \alpha D_x^+ D_x^- u^{n+1} - \beta D_x^\circ u^n - \beta D_x^\circ u^{n+1})$$

Consider $k \in \mathbb{R}, M \in \mathbb{Z}, h = \frac{1}{M}$, and operators A, B defined as follows:

$$\begin{aligned} Au_j &= u_{j+1} - u_{j-1} \\ Bu_j &= u_{j+1} - 2u_j + u_{j-1} \end{aligned}$$

We can then rewrite the finite difference as

$$\frac{u^{n+1} - u^n}{k} = \frac{\alpha}{2h^2}(Bu^n + Bu^{n+1}) - \frac{\beta}{4h}(Au^n - Au^{n+1}).$$

We then bring the u^{n+1} terms to one side to yield an implicit update step

$$\left(I + \frac{\beta k}{4h}A - \frac{\alpha k}{2h^2}B\right)u^{n+1} = \left(I - \frac{\beta k}{4h}A + \frac{\alpha k}{2h^2}B\right)u^n$$

The last part of the scheme construction is accounting for the periodic boundary conditions. We can do this by creating a ghost node u_{-1} where $u_{-1} = u_M = u_0$. The ghost node will then slightly change the update steps for u_0 and u_{M-1}. Note that the nodes for u_0 and u_M can be treated as the same. We redefine A and B correspondingly to act on $\mathbb{R}_h^M$ while accounting for the boundary conditions.

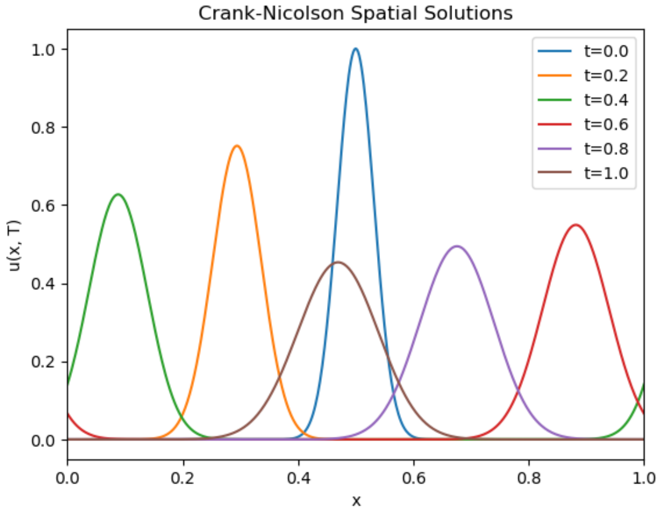
$$\begin{aligned} Au_0 &= u_1 - u_{M-1} \\ Au_{M-1} &= u_0 - u_{M-2} \\ Bu_0 &= u_1 - 2u_0 + u_{M-1} \\ Bu_{M-1} &= u_0 - 2u_{M-1} + u_{M-2} \end{aligned}$$

Shown below are the matrix representations of the operators $A, B \in \mathbb{R}_h^{M \times M}$.

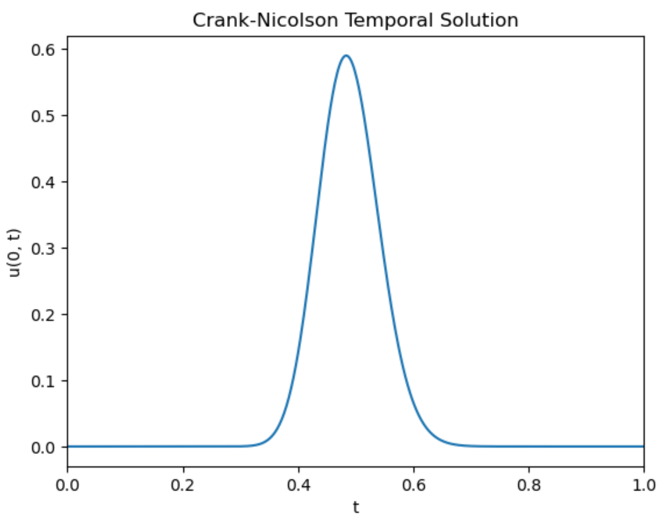
$$A = \begin{pmatrix} 0 & 1 & \cdots & 0 & -1 \\ -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & -1 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} -2 & 1 & \cdots & 0 & 1 \\ 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & -2 & 1 \\ 1 & 0 & \cdots & 1 & -2 \end{pmatrix}$$

We discuss results and analysis of the Crank-Nicolson scheme below.

(a) We first solve the PDE for various time steps on the entire interval $[0, 1]$. These solutions are plotted below. Observe that the solution is both translational and dissipative.



(b) We can gain further insights by looking at the solution trajectory over time for $u(0, t)$ where $0 \leq t \leq 1$. This is again plotted below. The translational effect is seen by the increasing and then decreasing value at $x = 0$.



(c) The amplification factor of the scheme is found via the Z-transform of the update step. We compute this below.

$$u^{n+1} = \underbrace{\left(I + \frac{\beta k}{4h} A - \frac{\alpha k}{2h^2} B\right)^{-1} \left(I - \frac{\beta k}{4h} A + \frac{\alpha k}{2h^2} B\right)}_{\mathcal{B}} u^n$$

$$\hat{u}^{n+1}(\xi) = \underbrace{\frac{1 - \frac{\beta k}{4h} G_A(\xi) + \frac{\alpha k}{2h^2} G_B(\xi)}{1 + \frac{\beta k}{4h} G_A(\xi) - \frac{\alpha k}{2h^2} G_B(\xi)}}_{G(\xi)} \hat{u}^n(\xi)$$

Here $G_A(\xi)$ and $G_B(\xi)$ are the Z-transforms of A and B, and $G(\xi)$ is the amplification factor.

$$\begin{aligned} G_A(\xi) &= e^{i\xi} - e^{-i\xi} = 2i\sin\xi \\ G_B(\xi) &= e^{i\xi} - 2 + e^{-i\xi} = 2\cos\xi - 2 = -4\sin^2\frac{\xi}{2} \end{aligned}$$

Putting these terms together, we can explicitly write the amplification factor.

$$\boxed{G(\xi) = \frac{1 - \frac{2\alpha k}{h^2}\sin^2\frac{\xi}{2} - \frac{\beta k}{2h} i\sin\xi}{1 + \frac{2\alpha k}{h^2}\sin^2\frac{\xi}{2} + \frac{\beta k}{2h} i\sin\xi}}$$

Now define variables $a = \frac{2\alpha k}{h^2}\sin^2\frac{\xi}{2}$ and $b = \frac{\beta k}{2h}\sin\xi$. Note that $a, b \in \mathbb{R}$ and $a \geq 0$. We then plug the expressions for $G_A(\xi)$ and $G_B(\xi)$ into the earlier expression to upper bound the amplification factor.

$$\begin{aligned} |G(\xi)| &= \left|\hat{u}^{n+1}(\xi)\right| \\ &= \frac{|1-a-bi|}{|1+a+bi|} \\ |1-a-bi| &= |1-a+bi| \\ &= |1+a+bi| \\ |G(\xi)| &\leq \frac{\cancel{|1+a+bi|}}{\cancel{|1+a+bi|}} \\ &= 1 \end{aligned}$$

Furthermore, $G(0) = 1$, so the upper bound is achievable on the finite interval and $\|\mathcal{B}\|_{\ell_h^2} = \|G\|_\infty = 1$. Since 1 is an upper bound for $\|\mathcal{B}\|_{\ell_h^2}$, and in fact an equality, we conclude that the scheme is **unconditionally stable**.

(d) Consider the equation $v(x,t) = u(x+\beta t, t)$. Consider the partial v_x.

$$\begin{aligned} v_t(x,t) &= \beta u_x(x+\beta t, t) + u_t(x+\beta t, t) \\ &= \beta v_x(x,t) + u_t(x+\beta t, t) \\ &= \beta v_x(x,t) + \alpha u_{xx}(x+\beta t, t) - \beta u_x(x+\beta t, t) \\ &= \cancel{\beta v_x(x,t)} + \alpha v_{xx}(x,t) - \cancel{\beta v_x(x,t)} \\ &= \alpha v_{xx}(x,t) \end{aligned}$$

This yields the following PDE: $\boxed{v_t = \alpha v_{xx}, \quad v(x,0) = g(x)}$. The definition of $v(x,t)$ is just a shift of the x coordinate by a scalar multiple of t so it will also have periodic boundary conditions.

(e) We now derive an exact formula for $v(x,t)$. First, we expand $g(x)$ in terms of its Fourier coefficients.

$$\begin{aligned} g(x) &= (\sin\pi x)^{100} \\ &= \left(\frac{1}{2i}\right)^{100}\left(e^{\pi i x} - e^{-\pi i x}\right)^{100} \\ &= \frac{1}{2^{100}}\sum_{k=0}^{100}\binom{100}{k}(-1)^{100-k}e^{2\pi i k x}e^{-100\pi i x} \\ &= \frac{1}{2^{100}}\sum_{k=-50}^{50}\binom{100}{k+50}(-1)^k e^{2\pi i k x} \end{aligned}$$

Thus, the Fourier coefficients of $g(x)$ are $c_k = \binom{100}{k+50}(-1)^k 2^{-100}$ for $-50 \leq k \leq 50$. Observe that the PDE is separable so basis elements of the solution space will be of the form $v_k(x,t) = T_k(t)X_k(t)$. By observation of the initial condition and the periodicity of $v(x,t)$, we can write the general form as

$$v(x,t) = \sum_{k=-50}^{50} c_k T_k(t) e^{2\pi ikx}$$

where each c_k is the coefficient of a basis element. We apply the PDE to an arbitrary kth term to calculate T_k since each term is in the solution space.

$$\begin{aligned} \cancel{c_k} T_k'(t) \cancel{e^{2\pi ikx}} &= \cancel{c_k} \alpha T_k(t)(-4\pi^2 k^2) \cancel{e^{2\pi ikx}} \\ T_k'(t) &= (-4\alpha\pi^2 k^2) T_k(t) \end{aligned}$$

If we take the ansatz $T_k(t) = e^{\lambda_k t}$, we see that $\lambda_k = -4\alpha\pi^2 k^2$. Thus, the exact solution for $v(x,t)$ expressed in terms of the Fourier coefficients c_k is

$$\boxed{v(x,t) = \sum_{k=-50}^{50} c_k e^{-4\alpha\pi^2 k^2 t} e^{2\pi ikx}}$$

From our discussion earlier, we know $u(x,t) = v(x - \beta t, t)$, so we can recover the solution to original PDE.

$$\boxed{u(x,t) = \sum_{k=-50}^{50} c_k e^{-(4\alpha\pi^2 k^2 + 2\beta\pi ik)t} e^{2\pi ikx}}$$

While we could compute c_k explicitly with the exact formula found earlier, this can be computationally challenging due to floating point errors. Instead, we demonstrate an alternative approximate method. First, sample $g(x)$ on a uniform grid with $M = 128$ grid-points and apply the DFT. The DFT yields coefficients

$$\tilde{g}_k = \sum_{j=0}^{M-1} g_j e^{-2\pi ikx_j}$$

where $x_j = j/M$ are the uniform sample positions. The coefficients $\tilde{g}_j$ relate to c_k by the following inverse transform:

$$g_j = \frac{1}{M} \sum_{k=0}^{M-1} \tilde{g}_k e^{2\pi ikx_j}.$$

However, we need coefficients between -50 and 50. This can be done by shifting the indices cyclically. Here we assume M is even. Then,

$$\begin{aligned} g_j &= \frac{1}{M} \sum_{k=0}^{M-1} \tilde{g}_k e^{2\pi ikj/M} \\ &= \frac{1}{M} \sum_{k=0}^{M-1} \tilde{g}_k e^{2\pi i(k-M)j/M} \\ &= \frac{1}{M} \sum_{k=-M/2}^{-1} \tilde{g}_{k+M} e^{2\pi ikj/M} + \frac{1}{M} \sum_{k=0}^{M/2-1} \tilde{g}_k e^{2\pi ikj/M} \end{aligned}$$

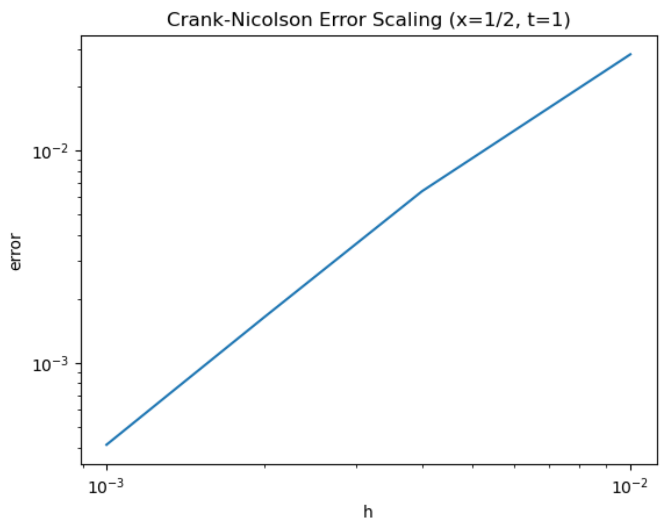
Finally, we can match terms to get approximations for the Fourier coefficients.

$$\boxed{c_k = \begin{cases} \tilde{g}_{k+M}/M, & -M/2 \leq k \leq -1 \\ \tilde{g}_k/M, & 0 \leq k \leq M/2 - 1 \end{cases}}$$

Note that we only need $-50 \leq k \leq 50$ so $M = 128 > 50 \times 2$ is sufficiently large. We also compute the exact solutions for c_k as a baseline by using the combinatorial formula described earlier. With the given selection for M, the corresponding relative error is less than 10^{-15}.

(f) We can now compute $u(x,t)$ directly by using the exact form in part (e) and the DFT approximations of c_k. As an example, $\boxed{u(1/2, 1) = 0.41023088876098807}$.

(g) We can now use our solution for $u(1/2, 1)$ in part (f) to compute the error of the Crank-Nicolson method and show its order of accuracy. Let the error be $e_h = |u_h(1/2, 1) - u(1/2, 1)|$ where $u_h(x,t)$ is the numerical solution from Crank-Nicolson with the refinement path $k = h$. The truncation error of the method is $O(k^2 + h^2)$ so we expect $O(h^2)$ error.



The line plot above has a slope of ≈ 2 verifies the expected second order convergence.