Numerical Solutions to PDEs

Lecture Notes #10 — Parabolic PDEs
Overview — Exact Solutions and Boundary Conditions

Peter Blomgren,
⟨blomgren.peter@gmail.com⟩

Department of Mathematics and Statistics
Dynamical Systems Group
Computational Sciences Research Center
San Diego State University
San Diego, CA 92182-7720

http://terminus.sdsu.edu/

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Outline

1. Parabolic PDEs
   - Introduction: Model, the 1D Heat Equation
   - Systems and Boundary Conditions
2. Finite Difference Schemes
   - Mostly Old News

Parabolic PDEs

Our simplest model for parabolic PDEs is the one-dimensional heat equation

$$\begin{aligned} u_t &= b\, u_{xx} \\ u(0,x) &= u_0(x) \end{aligned}$$

where

- $b \geq 0$ — the heat conductivity must be non-negative.
- In the simplest case b is a constant, but we can allow $b(t,x) \geq 0$.

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Parabolic PDEs

Parabolic PDEs show up in modeling of gas and fluid flow, economic modeling (the Black-Scholes equation, with a negative b), and diffusion processes — think pharmaceuticals spreading in the body, epidemiological studies (animal-of-the-year flu?), etc.

As with the one-way wave equation in the hyperbolic case, we can learn a lot from studying the 1D heat equation and numerical solutions thereof for the parabolic case.

The 1D Heat Equation

Some Fourier "Magic"

We Fourier transform (in the spatial coordinates) the 1D heat equation (with constant b), and get a friendly ODE:

$$\widehat{u}_t = -b\omega^2 \widehat{u}, \quad \widehat{u}(0,\omega) = \widehat{u}_0(\omega).$$

The solution, in the Fourier domain, is given by

$$\widehat{u}(t,\omega) = e^{-b\omega^2 t}\, \widehat{u}_0(\omega),$$

and by the Fourier inversion formula we get

$$u(t,x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega x} e^{-b\omega^2 t} \widehat{u}_0(\omega)\, d\omega,$$

in the physical domain.

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The 1D Heat Equation

The factor $e^{-b\omega^2 t}$ shows that $u(t,x)$ is obtained from $u_0(x)$ by damping the high-frequency content of u_0.

Hence, the solution operator for a parabolic equation is a **dissipative operator**.

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By using the Fourier transform formula

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in the previous expression for $u(t,x)$ we get

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The 1D Heat Equation

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in the previous expression for $u(t,x)$ we get

$$u(t,x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\omega x} e^{-b\omega^2 t} \left[\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega y} u_0(y)\, dy \right] d\omega$$

Next, we interchange the order of integration $dy \leftrightarrow d\omega$.

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The 1D Heat Equation

$$
\begin{aligned}
u(t,x) &= \frac{1}{\sqrt{4\pi}} \int_{-\infty}^{\infty} \left(\frac{\mathbf{1}}{\sqrt{\pi}} \int_{-\infty}^{\infty} \mathbf{e}^{\mathbf{i}\omega(\mathbf{x}-\mathbf{y})} \mathbf{e}^{-\mathbf{b}\omega^2\mathbf{t}}\, \mathbf{d}\omega \right) u_0(y)\, dy \\
&= \frac{1}{\sqrt{4\pi \mathbf{bt}}} \int_{-\infty}^{\infty} \mathbf{e}^{-(\mathbf{x}-\mathbf{y})^2/4\mathbf{bt}}\, u_0(y)\, dy.
\end{aligned}
$$

This expresses $u(t,x)$ as a weighted average of u_0, with a Gaussian weight function

$$
G(t,x,y) = \frac{e^{-(x-y)^2/4bt}}{\sqrt{4\pi bt}}.
$$

It has the property that $\forall t > 0$

$$
\frac{1}{\sqrt{4\pi bt}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4bt}\, dy = 1.
$$

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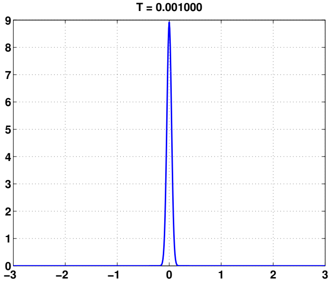
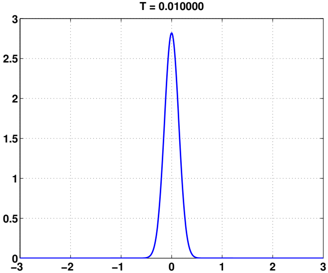
The 1D Heat Equation

Visualizing the Gaussian, $G(t, x, y = 0)$





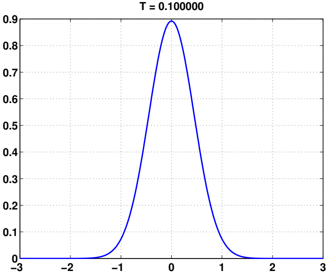


Figure: The Gaussian weight function at time $t = 0.001, 0.01, 0.1$. ($y = 0$, $b = 1$ are fixed).

Thought Experiment: What happens as $t \searrow 0$?

The 1D Heat Equation

Given the representation

$$u(t,x) = \frac{1}{\sqrt{4\pi bt}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4bt}\, u_0(y)\, dy,$$

we make the following observations:

- $u(t,x)$ is infinitely differentiable in t and x for $t > 0$.
- If $u_0(x) \geq 0$, then $u(t,x) \geq 0$.

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The 1D Heat Equation

Some Solutions

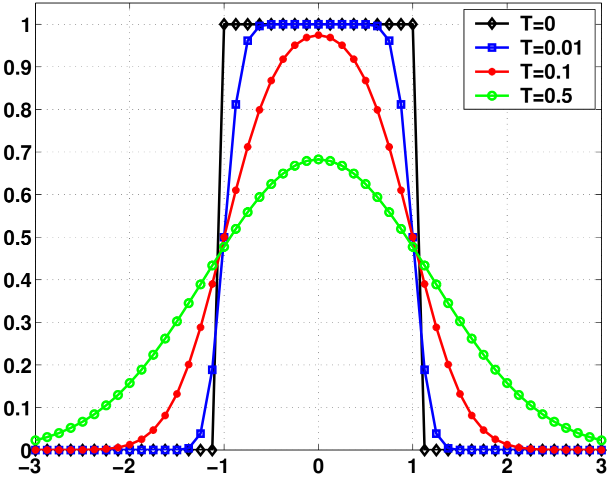

Figure: The exact solution(s) for the heat equation with initial condition 1 for $|x| \leq 1$ and 0 otherwise. We clearly see how the heat spreads out; this corresponds quite well with our physical intuition.

Parabolic Systems and Boundary Conditions

A system of the form

$$\bar{\mathbf{u}}_t = B\bar{\mathbf{u}}_{xx} + A\bar{\mathbf{u}}_x + C\bar{\mathbf{u}} + F(t,x),$$

where $\bar{\mathbf{u}}$ is a vector, and A, B, and C are matrices is **parabolic** if

$$\text{Real}(\lambda_i(B)) > 0.$$

B does not have to be positive definite, nor symmetric, nor must the eigenvalues be real; there are no restrictions on A and C.

Parabolic IVPs and Well-Posedness

Recall:

Definition (Well-Posed IVP)

The initial value problem for the first-order partial differential equation $Pu = 0$ is well-posed if for any time $T \geq 0$, there exists a constant C_T such that any solution $u(t,x)$ satisfies

$$\int_{-\infty}^{\infty} |u(t,x)|^2 \, dx \leq C_T \int_{-\infty}^{\infty} |u(0,x)|^2 \, dx,$$

for $0 \leq t \leq T$.

Parabolic IVPs and Well-Posedness

Theorem (Well-Posed Parabolic IVPs)

The initial value problem for the system

$$\bar{\mathbf{u}}_t = B\bar{\mathbf{u}}_{xx} + A\bar{\mathbf{u}}_x + C\bar{\mathbf{u}} + F(t,x),$$

is well-posed, and actually a stronger estimate holds: For each $T > 0$ *there is a constant* C_T *such that*

$$\int_{-\infty}^{\infty} |\bar{\mathbf{u}}(t,x)|^2\,dx + \int_0^t \int_{-\infty}^{\infty} |\bar{\mathbf{u}}_x(s,x)|^2\,dx\,ds \leq C_T \left[\int_{-\infty}^{\infty} |\bar{\mathbf{u}}(0,x)|^2\,dx + \int_0^t \int_{-\infty}^{\infty} |F(s,x)|^2\,dx\,ds \right]$$

for $0 \leq t \leq T$.

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Parabolic IVPs and Well-Posedness

The bound in the theorem is stronger than the one in the definition since it gives a **bound on the derivative of u with respect to x** in addition to a bound on u. The bound on u_x implies that the solution to the system is infinitely differentiable for $t > 0$.

The proof of the theorem is quite straight-forward using the Fourier transform (+ Parseval's Theorem) — *quick handwaving:*

$$\begin{aligned}
\widehat{u}_t &= \left(-\omega^2 B + i\omega A + C\right)\widehat{u} \\
\widehat{u}(t,\omega) &= e^{-(\omega^2 B + i\omega A + C)t}\,\widehat{u}_0(\omega) \\
|\widehat{u}(t,\omega)| &\leq K e^{(a-b\omega^2)t}\,|\widehat{u}_0(\omega)| \\
\int_{-\infty}^{\infty} |\widehat{u}(t,\omega)|^2\,d\omega &\leq K_T \int_{-\infty}^{\infty} |\widehat{u}_0(\omega)|^2\,d\omega \\
\int_0^t \int_{-\infty}^{\infty} \omega^2 |\widehat{u}(s,\omega)|^2\,d\omega\,ds &\leq K_T^* \int_{-\infty}^{\infty} |\widehat{u}_0(\omega)|^2\,d\omega, \quad t \leq T.
\end{aligned}$$

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Boundary Conditions for Parabolic Systems

A parabolic system with d equations defined on a finite interval requires d boundary conditions at **each boundary**, common forms include

$$\begin{aligned} T_0 \vec{u}(t,\xi) &= \vec{b}_0 \\ T_1 \vec{u}_x(t,\xi) + T_2 \vec{u}(t,\xi) &= \vec{b}_1 \end{aligned}$$

where $\xi \in \partial\Omega$, thus specifying the temperature, or the relation between the flux and temperature at the boundary.

Note: $T_0 \in \mathbb{R}^{d_0 \times d}$, T_1, $T_2 \in \mathbb{R}^{(d-d_0)\times d}$.

E.g. a perfectly insulated refrigerator would have

$$u_x(t,\xi) = 0.$$

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Boundary Conditions for Parabolic Systems

Boundary conditions are said to be **well-posed** if the solution of the PDE depends continuously on the boundary data; expressed in terms of the matrices T_0, T_1, and B, we must require that the $d \times d$ matrix

$$T = \begin{bmatrix} T_0 \\ T_1 B^{-1/2} \end{bmatrix}$$

is non-singular.

When $T_0 = I_{d \times d}$ we have **Dirichlet boundary conditions** (specified temperatures), and when $T_1 = I_{d \times d}$ and $T_2 = 0$ we have **Neumann boundary conditions** (specified temperature fluxes).

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A Note of "Square Roots" of Matrices

- A positive semi-definite matrix, M has a unique positive semi-definite square root, $R = M^{1/2}$; a diagonalizable matrix has a square-root (defined for an appropriate branch of the scalar square root) $R_2 = M^{1/2}$:
- When $M = X\Lambda X^{-1} \stackrel{\text{SPD}}{=} Q\Lambda Q^T$, either let $R = QSQ^T$, then (using the SVD)

$$R^2 = (QSQ^T)^2 = QSQ^TQSQ^T = QSSQ^T = QS^2Q^T = M,$$

or let $R_2 = XDX^{-1}$ (using the eigenvalue/eigenvector decomposition)

$$R_2^2 = (XDX^{-1})^2 = XDX^{-1}XDX^{-1} = XDDX^{-1} = XD^2X^{-1} = M,$$

showing that

$$S = \Lambda^{1/2}, \quad \text{and therefore} \quad R = Q\Lambda^{1/2}Q^T,$$

or

$$D = \Lambda^{1/2}, \quad \textit{and} \quad R_2 = X\Lambda^{1/2}X^{-1}$$

- $\exists$ other approaches.

Finite Difference Schemes for Parabolic Equations

Our previous definitions, given in the context of finite difference schemes for hyperbolic equations, of convergence, consistency, stability, and accuracy were general enough that they **apply without modification to finite difference schemes for parabolic equations.**

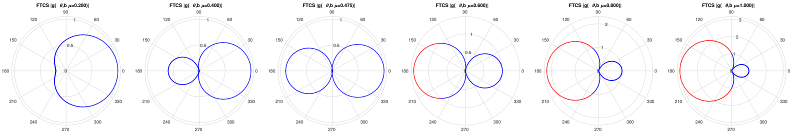
We start by considering the forward-time central-space scheme for the heat equation

$$\frac{v_m^{n+1} - v_m^n}{k} = b\,\frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2}.$$

We get the amplification factor using our old trick $v_m^n \rightsquigarrow g^n e^{im\theta}$

$$\frac{g(\theta) - 1}{k} = b\,\frac{e^{i\theta} - 2 + e^{-i\theta}}{h^2}.$$

Conditional Stability of Forward-Time Central-Space [EXPLICIT]



With $\mu = \frac{k}{h^2}$, we get

$$\underbrace{g(\theta) = 1 - 4b\mu \sin^2\left(\frac{\theta}{2}\right)}_{\text{dissipative of order 2, when } 0 < b\mu < \frac{1}{2}}$$

so that $|g(\theta)| \leq 1$ as long as $b\mu \leq \frac{1}{2}$.

Dissipation is desirable for parabolic equations since this implies that the numerical solution will become smoother as t increases, mimicking the behavior of the PDE.

The stability condition, expressed in terms $\mu = \frac{k}{h^2}$, is generic for the parabolic "universe" of finite difference schemes; μ plays the role of $\lambda = \frac{k}{h}$ for hyperbolic problems.

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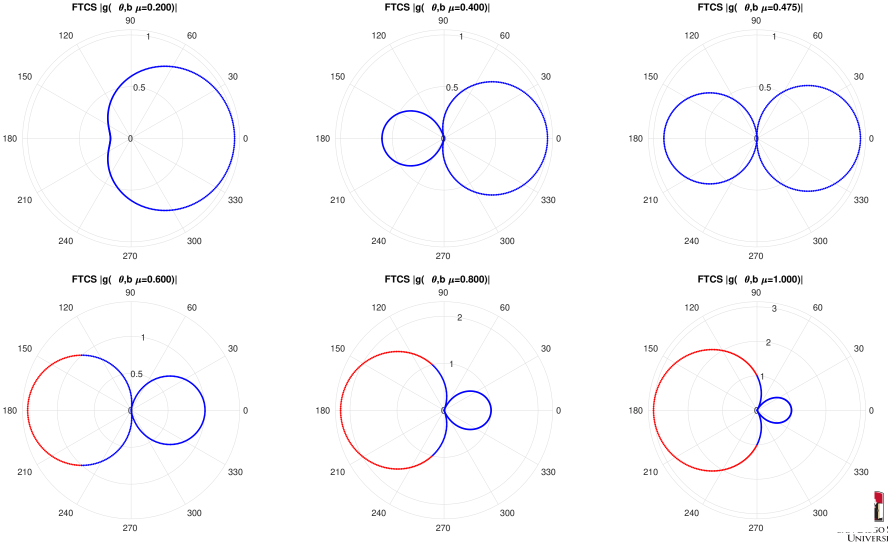
Conditional Stability of Forward-Time Central-Space [Explicit] 2 of 2



Some Forward-Time Central-Space Solutions

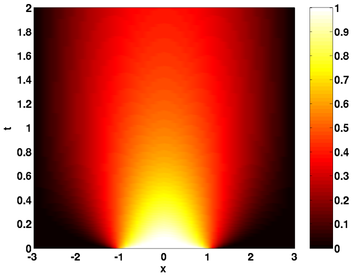
On the next slide(s) we see solutions to ($b = 1$)

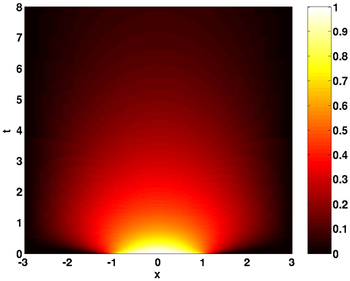
$$\begin{aligned} u_t &= u_{xx}, \quad x \in [-3,3],\; t \in [0,T] \\ u(0,x) &= \begin{cases} 1 & |x| \leq 1 \\ 0 & |x| > 1 \end{cases} \end{aligned}$$

We have $h = \frac{1}{8}$, and $k = 0.005$, so that $\mu = 0.32 < 0.5$. The solutions are shown for 3 different time-intervals $[0,2]$, $[0,8]$, and $[0,16]$.

On slide 19 the solution is computed with boundary conditions $u(t,\pm 3) = 0$. On slide 20 the solution is computed with boundary conditions which match the exact solution in an infinite domain (this is quite artificial, but allows us to compare the solutions, see slide 21.)

FT-CS Solutions to the Heat Equation





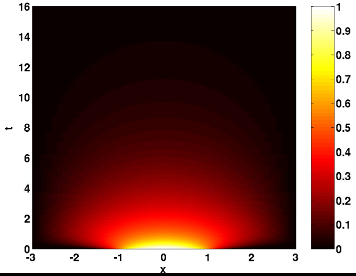


Figure: Solutions to the heat equation for ranges $T \in [0, 2]$, $T \in [0, 8]$, and $T \in [0, 16]$.

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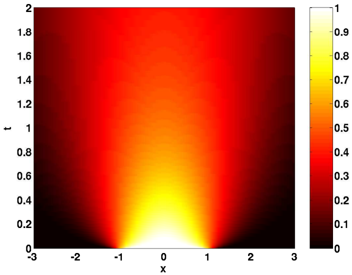
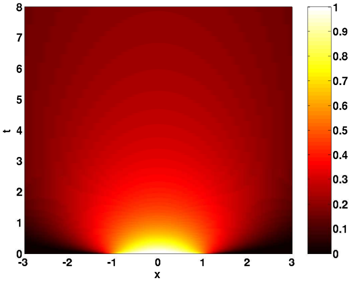
FT-CS Solutions to the Heat Equation





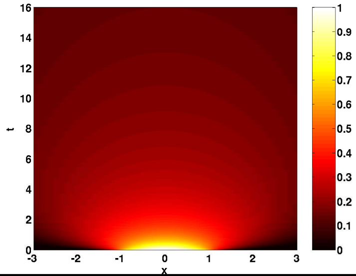


Figure: Comparison of the numerical and exact solution in the "infinite-domain" case; shown for $T = 2$, $T = 8$, and $T = 16$.

FT-CS Solutions to the Heat Equation

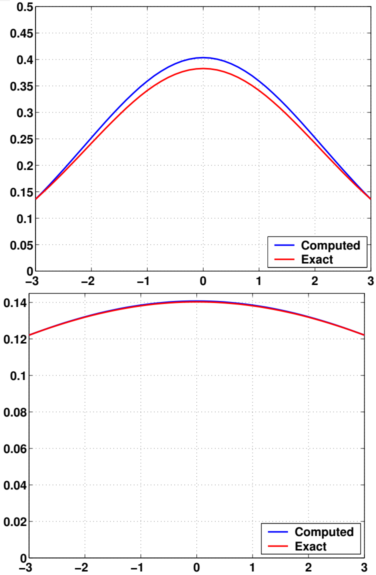


Figure: Comparison of the computed and exact solutions to the heat equation for $T = 2$, $T = 8$, and $T = 16$.

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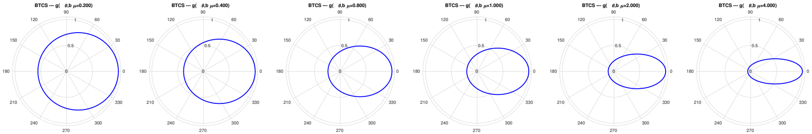
Unconditional Stability of Backward-Time Central-Space [Implicit]



Backward-time central-space applied to $u_t = bu_{xx} + f$ gives:

$$\frac{v_m^{n+1} - v_m^n}{k} = b\,\frac{v_{m+1}^{n+1} - 2v_m^{n+1} + v_{m-1}^{n+1}}{h^2} + f_m^{n+1}.$$

The amplification factor is

$$g(\theta) = \frac{1}{1 + 4b\mu \sin^2\left(\frac{\theta}{2}\right)}.$$

This implicit scheme is order-(1,2) and is unconditionally stable. When $\mu \geq c > 0$, it is also dissipative of order 2.

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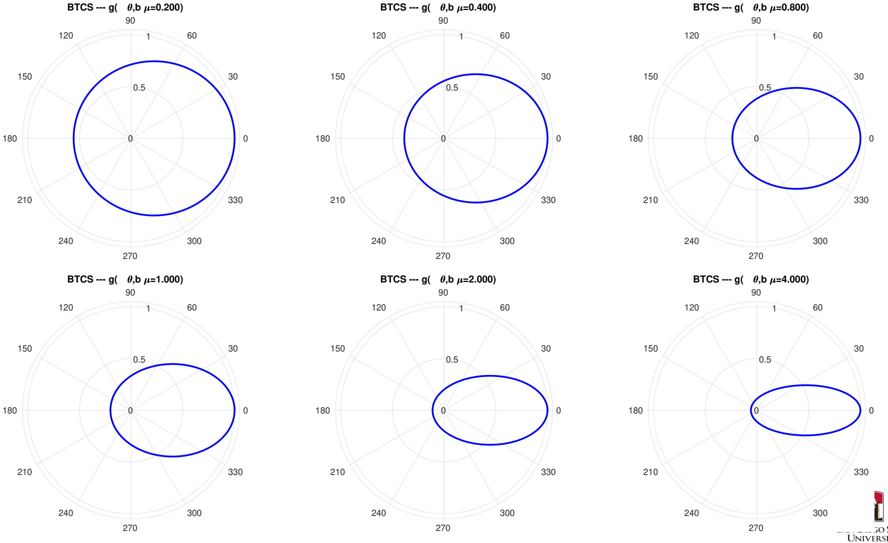
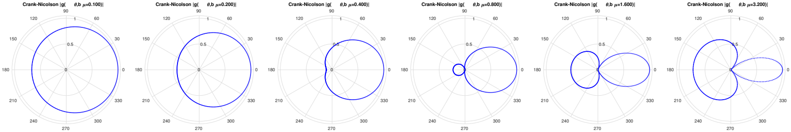
Unconditional Stability of Backward-Time Central-Space [IMPLICIT]



Unconditional Stability of Crank-Nicolson [IMPLICIT] 1 of 2



The Crank-Nicolson scheme applied to $u_t = bu_{xx} + f$ is given by

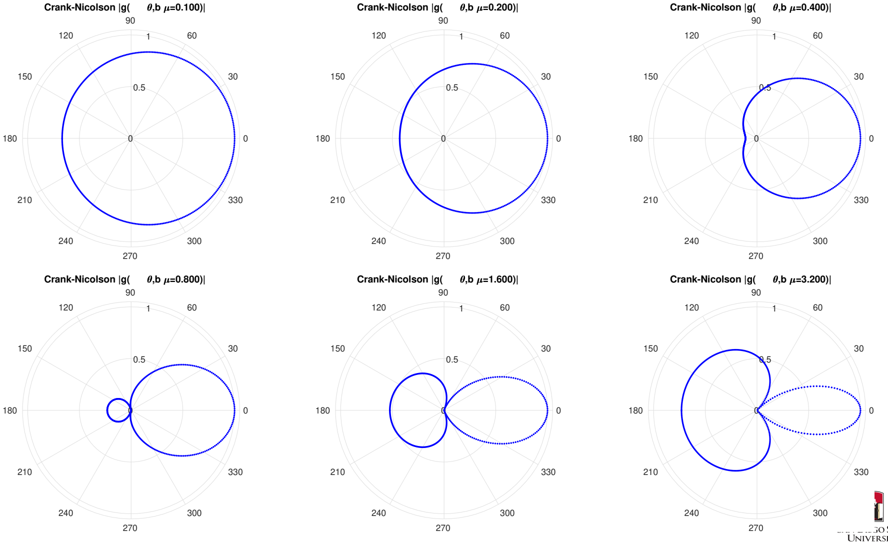
$$\frac{v_m^{n+1} - v_m^n}{k} = \frac{b}{2}\left[\frac{v_{m+1}^{n+1} - 2v_m^{n+1} + v_{m-1}^{n+1}}{h^2} + \frac{v_{m+1}^{n} - 2v_m^{n} + v_{m-1}^{n}}{h^2}\right] + \frac{1}{2}\left[f_m^{n+1} + f_m^n\right].$$

The corresponding amplification factor is

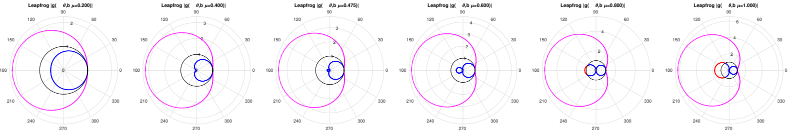
$$g(\theta) = \frac{1 - 2b\mu\sin^2\left(\frac{\theta}{2}\right)}{1 + 2b\mu\sin^2\left(\frac{\theta}{2}\right)}.$$

The Crank-Nicolson scheme is implicit, unconditionally stable, and order-(2,2) accurate; unlike its hyperbolic version, it is not conservative. When μ is constant it is dissipative of order 2.

Unconditional Stability of Crank-Nicolson [Implicit] 2 of 2



[UNSTABLE] The Leapfrog Scheme



The leapfrog scheme applied to $u_t = bu_{xx} + f$ is given by

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} = b\,\frac{v_{m+1}^n - 2v_m^n + v_{m-1}^n}{h^2} + f_m^n.$$

The corresponding amplification polynomial is

$$g(\theta)^2 + 8g(\theta)b\mu\sin^2\left(\frac{\theta}{2}\right) - 1,$$

with roots

$$g_\pm(\theta) = \pm\sqrt{1 + \left(4b\mu\sin^2\left(\frac{\theta}{2}\right)\right)^2} - 4b\mu\sin^2\left(\frac{\theta}{2}\right).$$

We see that $|g_-(\theta)| > 1$, for most values of θ, hence the leapfrog scheme is **unconditionally unstable**.

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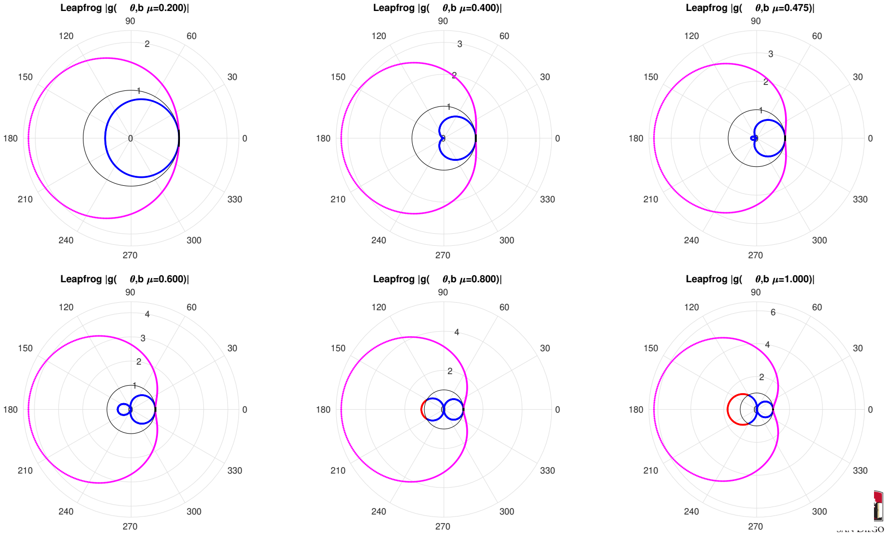
[UNSTABLE] The Leapfrog Scheme 2 of 2



Unconditional Stability of The Du Fort-Frankel Scheme [EXPLICIT] 1 of 3

The Du Fort-Frankel scheme is essentially the "fixed" leapfrog scheme [It uses a time-based "averaging fix" (in the spatial derivative) similar to the spatial average (in the time derivative) used in the hyperbolic setting FTCS $\rightsquigarrow$ LAX-FRIEDRICHS]

$$\frac{v_m^{n+1} - v_m^{n-1}}{2k} = b\,\frac{v_{m+1}^n - (\mathbf{v}_\mathbf{m}^{\mathbf{n+1}} + \mathbf{v}_\mathbf{m}^{\mathbf{n-1}}) + v_{m-1}^n}{h^2} + f_m^n.$$

The corresponding amplification polynomial is

$$[1 + 2b\mu]g(\theta)^2 - [4b\mu\cos(\theta)]g(\theta) - [1 - 2b\mu],$$

with roots

$$g_\pm(\theta) = \frac{2b\mu\cos(\theta) \pm \sqrt{1 - 4b^2\mu^2\sin^2(\theta)}}{1 + 2b\mu}.$$

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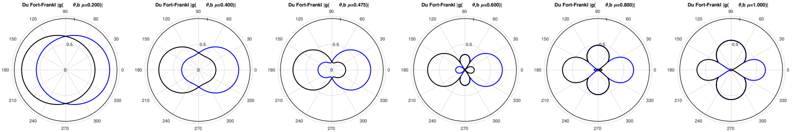
Unconditional Stability of The Du Fort-Frankel Scheme [EXPLICIT] 2 of 3



When $1 - 4b^2\mu^2 \sin^2(\theta) \geq 0$, we get

$$|g_\pm(\theta)| \leq \frac{2b\mu|\cos(\theta)| + \sqrt{1 - 4b^2\mu^2\sin^2(\theta)}}{1+2b\mu} \leq \frac{2b\mu+1}{1+2b\mu} = 1$$

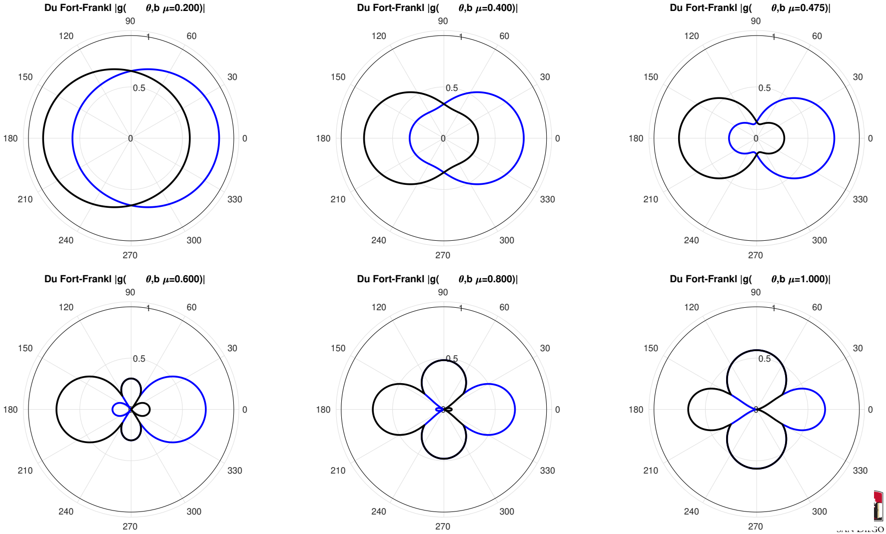
and when $1 - 4b^2\mu^2 \sin^2(\theta) < 0$, we get

$$|g_\pm(\theta)|^2 \leq \frac{(2b\mu\cos(\theta))^2 + 4b^2\mu^2\sin^2(\theta) - 1}{(1+2b\mu)^2} = \frac{4b^2\mu^2 - 1}{4b^2\mu^2 + 4b\mu + 1} < 1$$

Thus, this explicit scheme is **unconditionally stable**. The one caveat is that it is only consistent if k/h tends to zero as h and k go to zero.

The caveat is a generic property for finite difference schemes applied to parabolic problems, as expressed in the theorem on the following slide.

Unconditional Stability of The Du Fort-Frankel Scheme [Explicit] 3 of 3



Convergence of Explicit Schemes

Theorem (Convergence of Explicit Schemes)

An explicit, consistent scheme for the parabolic system

$$\bar{\mathbf{u}}_t = B\bar{\mathbf{u}}_{xx} + A\bar{\mathbf{u}}_x + C\bar{\mathbf{u}} + F(t,x)$$

is convergent only if k/h tends to zero as k and h tend to zero.

Recall (for hyperbolic problems):

Theorem

There are no explicit, unconditionally stable, consistent finite difference schemes for hyperbolic systems of partial differential equations.