Exploring Approximations for the Diffusion Equation

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Introduction

- Heat as a function of 1-dimensional space and time: $u(x,t)$
- Notation for u evaluated at discretized points in space and time

$$u(x_i, t_n) = u_i^n$$

- The heat equation, a second order partial differential equation

$$\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}$$

- Three approximation strategies
  - Euler's method
  - Improved Euler's method
  - Implicit Time Stepping

Euler's Method

$$u_i^{n+1} \approx u_i^n + \frac{k\Delta t}{\Delta x^2}\left[u_{i+1}^n - 2u_i^n + u_{i-1}^n\right]$$

- This can be derived using Taylor series expansions in each variable

Improved Euler's method

- Approximate the slopes at the endpoints of each time interval
  - $\widetilde{K}_{i+1}$ is found using an approximation for u_i^{n+1}
- Use the average of these slopes to linearly approximate the solution over the interval

$$u_i^{n+1} = u_i^n + \Delta t \left[\frac{K_i + \widetilde{K}_{i+1}}{2} \right]$$

- $K_i \approx$ slope at u_i^n
- $\widetilde{K}_{i+1} \approx$ slope at u_i^{n+1}

- Pieces to the approximation
  - $K_i = \frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{k}{\Delta x^2}\left[u_{i-1}^n - 2u_i^n + u_{i+1}^n\right]$
  - $\tilde{u}_i^{n+1} = u_i^n + \frac{k\Delta t}{\Delta x^2}\left[u_{i-1}^n - 2u_i^n + u_{i+1}^n\right]$
  - $\widetilde{K}_{i+1} = \frac{u_i^{n+2} - u_i^{n+1}}{\Delta t} = \frac{k}{\Delta x^2}\left[\tilde{u}_{i-1}^{n+1} - 2\tilde{u}_i^{n+1} + \tilde{u}_{i+1}^{n+1}\right]$

Implicit Time Stepping

- Benefits
  - Increased stabilty of approximation
  - Able to handle larger diffusivity constants
- Drawbacks
  - Need to solve a linear system $Ax = b$

- Setting up the approximation
  - Use the Taylor's series expansion, but the RHS of our final approximation expression is in terms of u_x^{n+1} rather than u_x^n.

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{k}{\Delta x^2}\left[u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}\right]$$

$$u_i^n = u_i^{n+1} - \frac{k\Delta t}{\Delta x^2}\left[u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}\right]$$

$$u_i^n = u_i^{n+1}\left[1 + 2r\right] - r\left[u_{i-1}^{n+1} + u_{i+1}^{n+1}\right] \qquad , r = \frac{k\Delta t}{\Delta x^2}$$

  - We are using the value at the *next* time step

- Fix n (time) and let i (space) float over all of the interior points of our rod
  - Boundary conditions $u(x_1, t)$ and $u(x_N, t)$ are known for all t
  - Interior points

$$
\begin{aligned}
u_2^n &= u_2^{n+1}\left[1+2r\right] - r\left[u_1^{n+1} + u_3^{n+1}\right] \\
u_3^n &= u_3^{n+1}\left[1+2r\right] - r\left[u_2^{n+1} + u_4^{n+1}\right] \\
u_4^n &= u_4^{n+1}\left[1+2r\right] - r\left[u_3^{n+1} + u_5^{n+1}\right] \\
&\cdot \\
&\cdot \\
u_{N-2}^n &= u_{N-2}^{n+1}\left[1+2r\right] - r\left[u_{N-3}^{n+1} + u_5^{N-1}\right] \\
u_{N-1}^n &= u_{N-1}^{n+1}\left[1+2r\right] - r\left[u_{N-2}^{n+1} + u_N^{n+1}\right]
\end{aligned}
$$

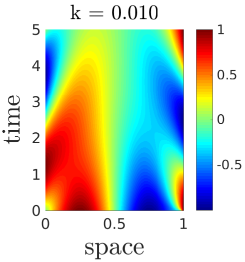
We move our known terms u_1^{n+1} and u_N^{n+1} to the RHS.

Recognizing the pattern we build the linear system:

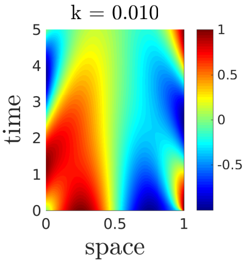
$$\begin{pmatrix} 1+2r & -r & 0 & 0 & . & . & 0 \\ -r & 1+2r & -r & 0 & 0 & . & 0 \\ 0 & -r & 1+2r & -r & 0 & . & 0 \\ . & & . & . & . & & . \\ . & & . & . & . & & . \\ . & & . & . & . & & . \\ 0 & 0 & . & . & -r & 1+2r & -r \\ 0 & 0 & . & . & 0 & -r & 1+2r \end{pmatrix} \begin{pmatrix} u_2^{n+1} \\ u_3^{n+1} \\ u_4^{n+1} \\ . \\ . \\ . \\ u_{N-2}^{n+1} \\ u_{N-1}^{n+1} \end{pmatrix} = \begin{pmatrix} u_2^n + ru_1^{n+1} \\ u_3^n \\ u_4^n \\ . \\ . \\ . \\ u_{N-2}^n \\ u_{N-1}^n + ru_N^{n+1} \end{pmatrix}$$

Comparing plots

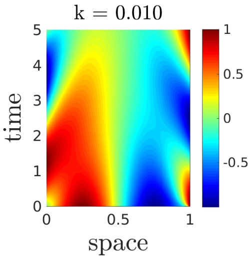
- We need the initial temperature profile of the rod and the temperatures for all points in time of the endpoints of the rod
  - We will give these values in our MatLab code
- Example 1
  - Length of rod, L: 1 meter
  - Number of points: 50
  - Total time, t_f: 5 seconds
  - Number of time points: 2000
  - Diffusivity constant: k
  - $r = k\frac{\Delta t}{\Delta x^2}$ $r < 0.50$ required
  - $u(1,:) = \sin\left(\frac{2\pi}{t_f}\ t\right)$ Left endpoint boundary conditions
  - $u(N,:) = \cos\left(\frac{2\pi}{t_f}\ t\right)$ Right endpoint boundary conditions
  - $u(:,1) = \sin\left(\frac{2\pi}{L}\right)\ x$ Initial conditions



Euler's



Improved Euler's



Implicit Time Stepping

Exploring Error

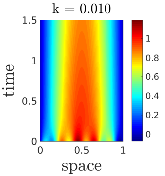
- Simplify IC and Boundary conditions so the we can solve for an explicit solution
  - IC
    $$u(x,0) = \sin(\pi x) + 0.2\sin(10\pi x)$$
  - Boundary conditions
    $$u(0,t) = u(1,t) = 0$$
  - Guess a solution to $u_t = ku_{xx}$

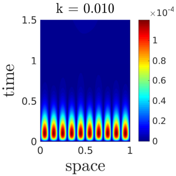
$$u(t,x) = e^{-\pi^2 kt}\sin(\pi x) + 0.2e^{-(10\pi)^2 kt}\sin(10\pi x)$$

$$
\begin{aligned}
u_t &= \frac{\partial}{\partial t}\Big[u(x,t)\Big] \\
&= \frac{\partial}{\partial t}\Big[e^{-\pi^2 kt}\sin(\pi x) + 0.2e^{-(10\pi)^2 kt}\sin(10\pi x)\Big] \\
&= -\pi^2 k e^{-\pi^2 kt}\sin(\pi x) + 0.2\left[-(10\pi)^2 k\right] e^{-(10\pi)^2 kt}\sin(10\pi x) \\
&= k\Big[-\pi^2 e^{-\pi^2 kt}\sin(\pi x) + 0.2\left[-(10\pi)^2 k\right] e^{-(10\pi)^2 t}\sin(10\pi x)\Big] \\
&= k\frac{\partial^2 u}{\partial x^2}\Big[e^{-\pi^2 kt}\sin(\pi x) + 0.2e^{-(10\pi)^2 kt}\sin(10\pi x)\Big] \\
&= k\frac{\partial^2 u}{\partial x^2}\Big[u(x,t)\Big] \\
&= ku_{xx}
\end{aligned}
$$

It is a solution! We can use this to measure the error in our approximations!

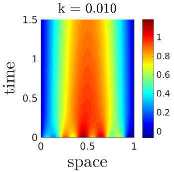
Plots with $M = 2000, N = 200, k = 0.01 \rightarrow r = 0.2972$

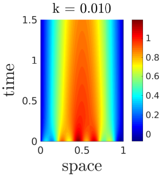


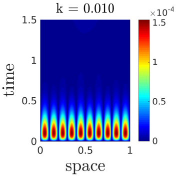


Exact solution

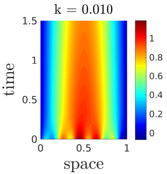
Euler's

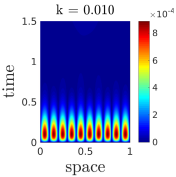






Improved Euler's

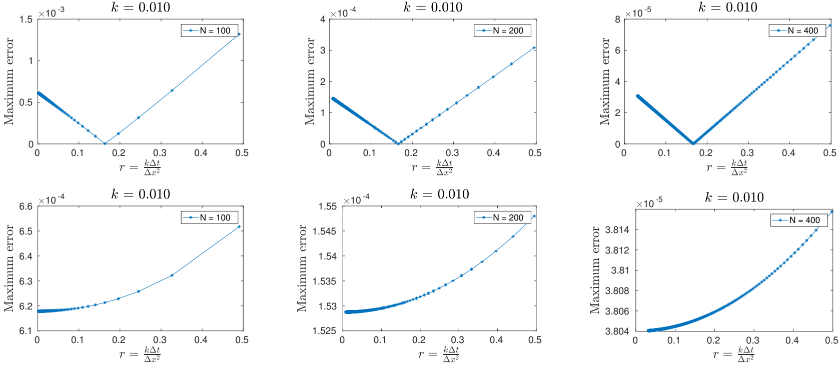




Implicit

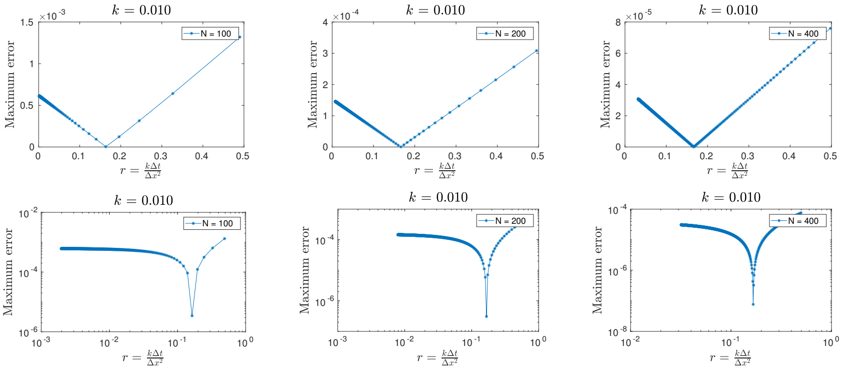
At which point in time should we sample the error across the rod?

- t large and $t \approx 0$ the error is nearly zero
- Error appears non-trivial at $t \approx 0.10$ seconds
- Experiment:
  - A given number of sample points in space
  - Range through different numbers of sample points in time
    - $r = \frac{k\Delta t}{\Delta x^2} \downarrow \quad \text{as } \Delta t \downarrow$



Implicit time stepping: The code ran forever

Log plot to get a closer look at Euler's method approximation



At some point just above $r = 0.10$ we see the error becoming very small!

Intersting...Why?

$$U_t = kU_{xx}$$

Approximation: $$\frac{U^{n+1} - U^n}{\Delta t} = k\frac{U_{j+1} - 2U_j - U_{j-1}}{\Delta x^2}$$

Recall the Taylor series expansion in one variable

$$u(x_j \pm \Delta x) = \sum_{k=0}^{N} (\pm\Delta x)^k f^{(k)}(x_j) + error\ term.$$

$$u(t^n \pm \Delta t) = \sum_{k=0}^{N} (\pm\Delta t)^k f^{(k)}(t^n) + error\ term.$$

x first...

$$
\begin{aligned}
U_{j+1} &= u(x_j + \Delta x) \\
&= u(x_j) + \Delta x U_x(x_j) + \frac{\Delta x^2}{2!} U_{xx}(x_j) + \frac{\Delta x^3}{3!} U_x xx(x_j) + \frac{\Delta x^4}{4!} U_{4x}(x_j) + \ldots.
\end{aligned}
$$

$$
\begin{aligned}
U_{j-1} &= u(x_j - \Delta x) \\
&= u(x_j) - \Delta x U_x(x_j) + \frac{\Delta x^2}{2!} U_{xx}(x_j) - \frac{\Delta x^3}{3!} U_x xx(x_j) + \frac{\Delta x^4}{4!} U_{4x}(x_j) + \ldots.
\end{aligned}
$$

$$
\frac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2} = U_{xx}(x_j) + 2\frac{\Delta x^2}{4!} U_{4x}(x_j) + \ldots.\Delta x^{large} \qquad (1)
$$

Now t...

$$U^{n+1} = u(t^n + \Delta t) = u(t^n) + \Delta t U_t(t^n) + \frac{\Delta t^2}{2!} U_{tt}(t^n) + \frac{\Delta t^3}{3!} U_{ttt}(t^n) + \ldots . \Delta t^{large}$$

$$\frac{U^{n+1} - U^n}{\Delta t} = U_t(t^n) + \frac{\Delta t}{2!} U_{tt}(t^n) + \frac{\Delta t^2}{3!} U_{ttt}(t^n) + \ldots . \Delta t^{large} \tag{2}$$

$$(2) = k(1)$$

$$\frac{U^{n+1} - U^{n}}{\Delta t} = k\left[\frac{U_{j+1} - 2U_{j} + U_{j-1}}{\Delta x^{2}}\right]$$

$$U_t(t^n) + \frac{\Delta t}{2!}U_{tt}(t^n) + \frac{\Delta t^2}{3!}U_{ttt}(t^n) + \ldots. = k\left[U_{xx}(x_j) + 2\frac{\Delta x^2}{4!}U_{4x}(x_j) + \ldots.\right]$$

$$U_t = kU_{xx} - \frac{\Delta t}{2}U_{tt} - \frac{\Delta t^2}{6}U_{3t} + k\frac{\Delta x^2}{12}U_{4x} + \ldots. \qquad (3)$$

$$U_t = kU_{xx} - error$$

$$\frac{\partial}{\partial t}\left[U_t = kU_{xx}\right] \longrightarrow U_{tt} = kU_{xxt}$$

$$\frac{\partial^2}{\partial x^2}\left[kU_{xx} = U_t\right] \longrightarrow kU_{4x} = U_{txx}$$

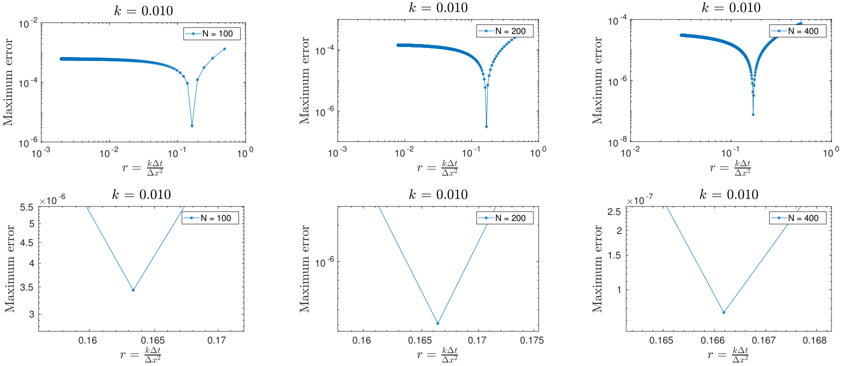
So,

$$U_{tt} = k^2 U_{4x}$$

$$U_t = kU_{xx} - \frac{\Delta t}{2}\left[k^2 U_{4x}\right] - \frac{\Delta t^2}{6} U_{3t} + k\frac{\Delta x^2}{12} U_{4x} + \ldots.$$

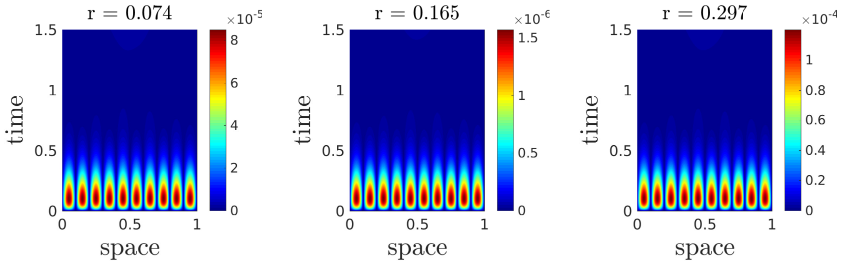
$$U_t = kU_{xx} + U_{4x}\left[k\frac{\Delta x^2}{12} - k^2\frac{\Delta t}{2}\right] - \frac{\Delta t^2}{6} U_{3t} + \ldots..$$

$$
\begin{aligned}
0 &= k\frac{\Delta x^2}{12} - k^2\frac{\Delta t}{2} \\
0 &= \frac{\Delta x^2}{6} - k\Delta t \\
k\Delta t &= \frac{\Delta x^2}{6} \\
\frac{k\Delta t}{\Delta x^2} &= \frac{1}{6} \\
r &= \frac{1}{6}.
\end{aligned}
$$



$k = 0.010$
N = 100
Maximum error
$r = \frac{k\Delta t}{\Delta x^2}$
$k = 0.010$
N = 200
Maximum error
$r = \frac{k\Delta t}{\Delta x^2}$
$k = 0.010$
N = 400
Maximum error
$r = \frac{k\Delta t}{\Delta x^2}$
$k = 0.010$
N = 100
$\times 10^{-6}$
Maximum error
$r = \frac{k\Delta t}{\Delta x^2}$
$k = 0.010$
N = 200
Maximum error
$r = \frac{k\Delta t}{\Delta x^2}$
$k = 0.010$
N = 400
$\times 10^{-7}$
Maximum error
$r = \frac{k\Delta t}{\Delta x^2}$

Error with different r values



Remarks

Thank you Juan

Thank you Professor Platte

Acknowledgments