NSFD Schemes for the Heat Equation

Miles Smith, 2023

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Structure

1. Introduce the Heat Equation
2. Analytic Solution
3. Numerical Solutions
4. NSFD Approach
5. Current Progress and Next Steps

Introduction to the Heat Equation

The Heat Equation In $\mathbb{R}^1$:

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

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α represents thermal diffusivity

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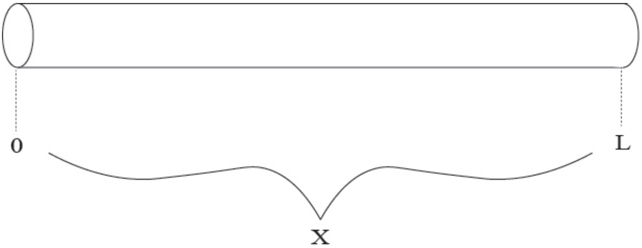
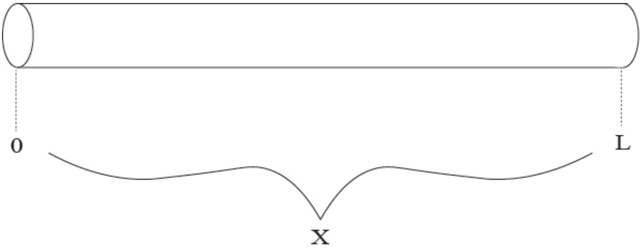
Solution

Heat Flow: How heat spreads out over time

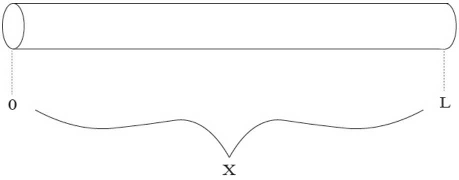
What 1-D Means



What 1-D Means



Question: If this rod starts out with some initial heat distribution, how does heat flow out of it over time? (What's the rod's heat in 1 second?)



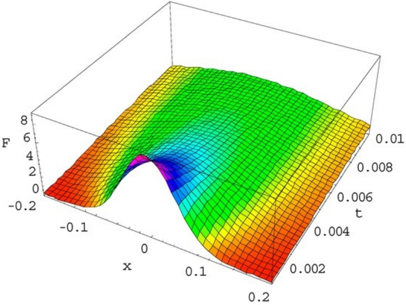
Question: how does heat flow over time?

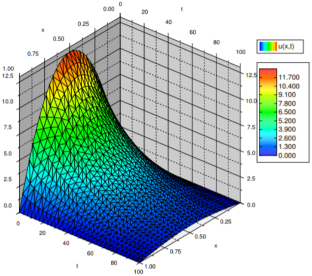
To Answer...

Initial heat distribution (IC): $u(x,0) = f(x)$

Heat at end-points (BC): $u(0,t) = ?\quad u(L,t) = ?$

Heat Equation Visualization





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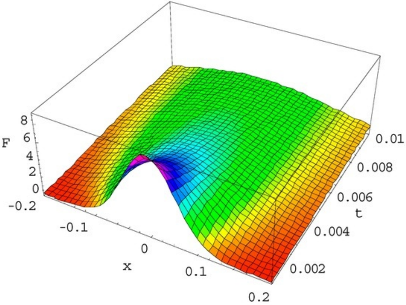

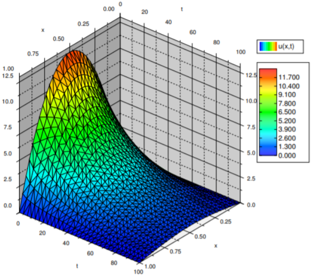

Here, $u(x,0)$ is the initial heat distribution
and $u(0,t) = u(L,t) = 0$

True Analytic Solution

Methods

Fourier Series (traditional)

Green's Function

Dirac-delta function for fundamental solution

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Let $u(0,t) = u(L,t) = 0$
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Methods

Fourier Series (traditional)
Green's Function
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Let $u(0,t) = u(L,t) = 0$
and $u(x,0) = f(x)$

The Answer...

$$u(x,t) = \sum_{n=1}^{\infty} b_n \cdot \sin\left(\frac{n\pi x}{L}\right) \cdot e^{-\left(\frac{\alpha n\pi}{L}\right)^2 t}$$

$$b_n = \frac{2}{L}\int_0^L f(x) \cdot \sin\left(\frac{n\pi x}{L}\right) dx$$

True Analytic Solution

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$$b_n = \frac{2}{L}\int_0^L f(x) \cdot \sin\left(\frac{n\pi x}{L}\right) dx$$

Problem: This is complicated... and what if $f(x)$ is complicated and makes it difficult to integrate?

General Problem

Let $L = 1,\ T = 1$

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BC: $u(0,t) = u(L,t) = 0$
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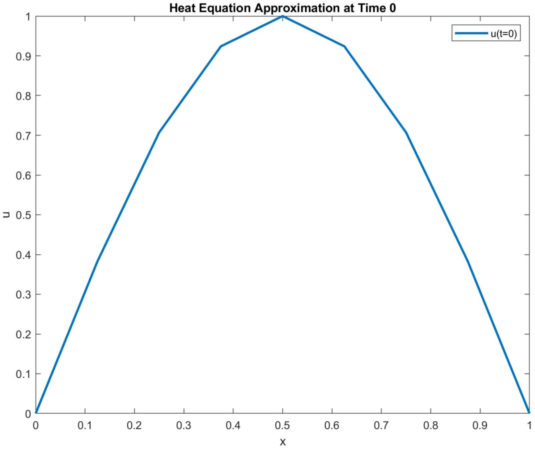
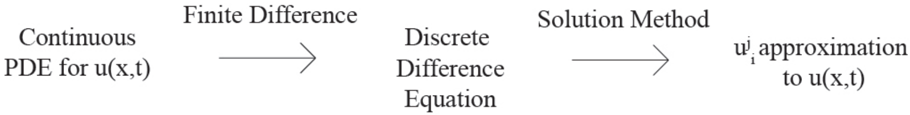


Numerical Solutions to the Heat Equations

Continuous PDE for u(x,t) $\xrightarrow{\text{Finite Difference}}$ Discrete Difference Equation $\xrightarrow{\text{Solution Method}}$ u^j_i approximation to u(x,t)

Numerical Solutions to the Heat Equations



Solution Methods:

- Explicit Euler
- Implicit Euler
- Crank-Nicolson
- Thomas Algorithm

Numerical Set-Up: (2) Finite Difference

Recall:

$$\frac{df(x)}{dx} \approx \frac{f(x+h) - f(x)}{h}$$

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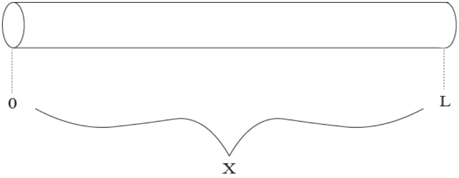

If $L = 1$, and we want to find the change in heat around $x = .5$ at $t = 0$ with respect to *time*.

Numerical Set-Up: (2) Finite Difference

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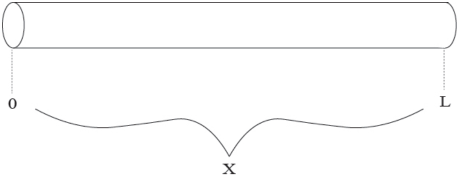

If $L = 1$, and we want to find the change in heat around $x = .5$ at $t = 0$ with respect to *time*. Then,

$$u_t(.5, 0) \approx \frac{u(.5, 0 + \Delta t) - u(.5, 0)}{\Delta t}$$

Numerical Set-Up: (2) Finite Difference

If both x and t go from 0 to 1, and we want to break them into discrete chunks...

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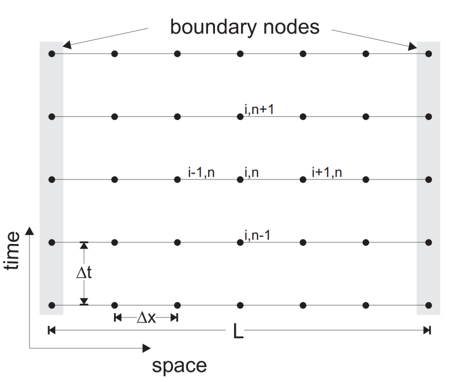
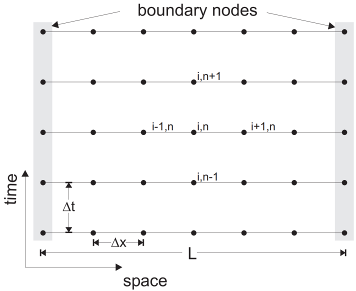
Finite Difference Mesh

$$\partial t \longrightarrow \Delta t \qquad \partial x \longrightarrow \Delta x$$



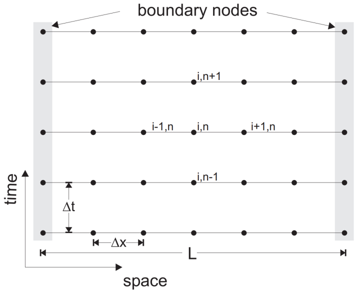
This mesh includes appoximations of heat, Δx and Δt apart, for all values of x and t.

Numerical Set-Up: (2) Finite Difference



Bottom line:

$$u^{j=1} = \begin{bmatrix} u_{i=1}^{j=1} & u_{i=2}^{j=1} & \dots & u_{i=7}^{j=1} \end{bmatrix}$$



Bottom line:

$$u^{j=1} = \begin{bmatrix} u_{i=1}^{j=1} & u_{i=2}^{j=1} & \dots & u_{i=7}^{j=1} \end{bmatrix}$$

$$u_{i=5}^{j=2} \approx u(x = .5, t = .2)$$

Numerical Set-Up: (2) Finite Difference

$$u_t(.5, 0) \approx \frac{u(.5, 0 + \Delta t) - u(.5, 0)}{\Delta t}$$

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Discretize Derivatives Using Finite Difference

$$\frac{\partial u}{\partial t} \approx \frac{u_i^{j+1} - u_i^j}{\Delta t}$$

and

$$\frac{\partial^2 u}{\partial x^2} \approx \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}$$

Numerical Set-Up: (3) Discrete Difference Equation

Bringing pieces together...

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = \alpha \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}$$

Numerical Set-Up: (3) Discrete Difference Equation

Bringing pieces together...

$$\frac{u_i^{j+1} - u_i^j}{\Delta t} = \alpha \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{\Delta x^2}$$

Rearranged:

Discrete Heat Equation

$$u_i^{j+1} = (1 - 2R)u_i^j + R\left(u_{i+1}^j + u_{i-1}^j\right)$$

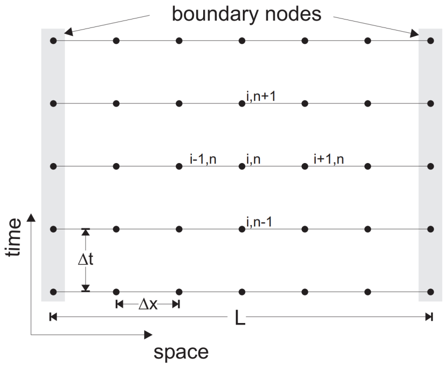
$$R = \frac{\Delta t \cdot \alpha}{\Delta x^2}$$

Numerical Set-Up: (4) Solution Methods

1. **Explicit Euler**
2. Implicit Euler

Solution Method: Explicit Euler

$$u_i^{j+1} = (1 - 2R)u_i^j + R\left(u_{i+1}^j + u_{i-1}^j\right)$$



Solution Method: Explicit Euler

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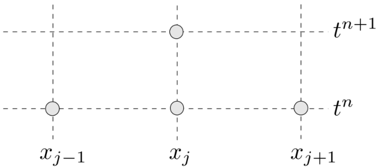
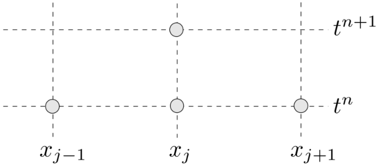


Solution Method: Explicit Euler

$$u_i^{j+1} = (1-2R)u_i^j + R\left(u_{i+1}^j + u_{i-1}^j\right)$$



$$u_3^4 = (1-2R)u_3^3 + R(u_4^3 + u_2^3) \approx u(x=.5, t=.05)$$

Solution Method: Explicit Euler

How do you create each time-step vector?

Explicit For-Loop

```
a = @(t) 0;              %boundary condition x=0
b = @(t) 0;              %boundary condition x=L
g = @(x) sin(pi.*x);     %initial condition, t=0

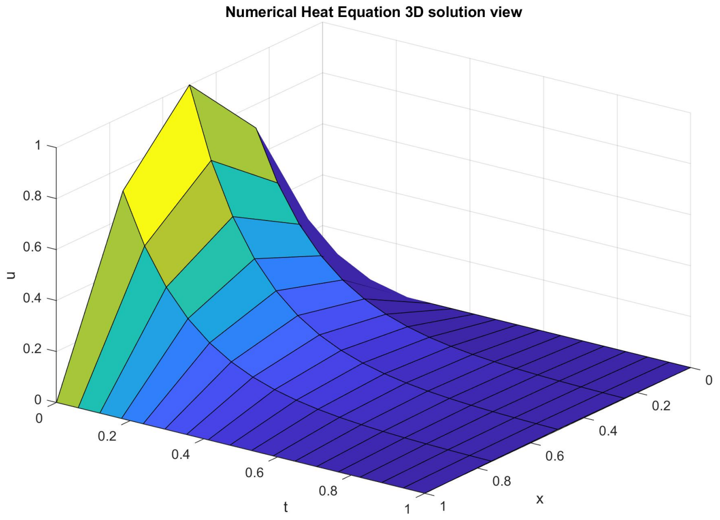
u=zeros(M+1, K+1);

u(1,:)=a(t'); %input BCs
u(end,:)=b(t');
u(:,1)=g(x); %input ICs

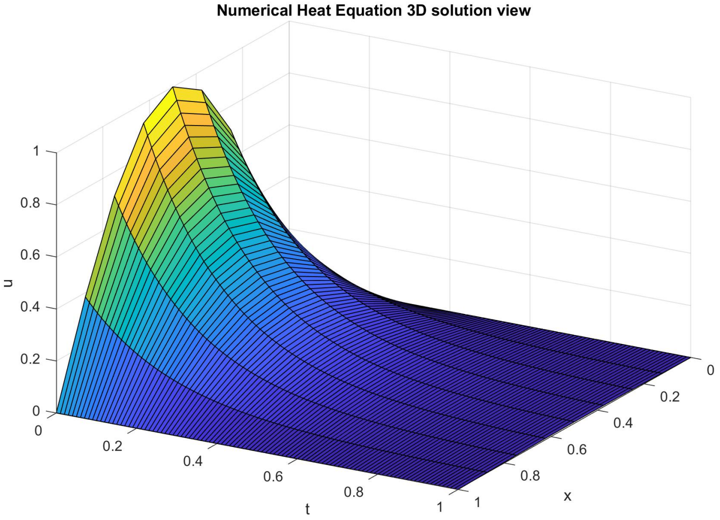
% Forward Difference Scheme
for j=1:K
    for i=2:M
        u(i, j+1) = (1-2*R)*u(i,j) + R*(u(i+1,j) + u(i-1,j));
    end
end
```

K and M are the number of steps for time and space, respectively

Explicit Euler Example: Simple Mesh



Explicit Euler Example: Refined Mesh



Approximate True Solution

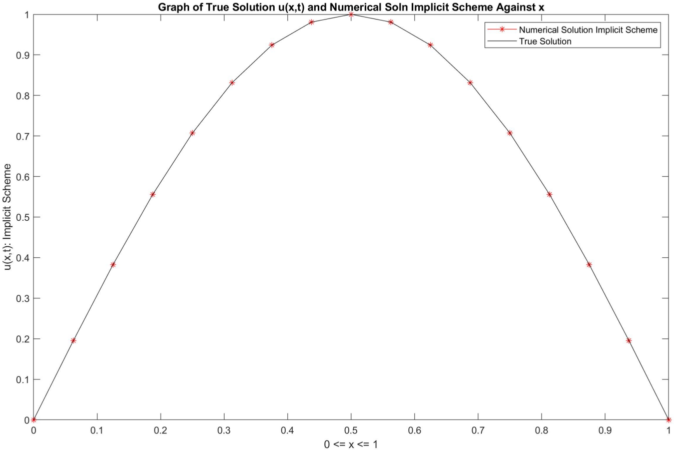
How do we know if our approximation is good?

True Solution Baseline

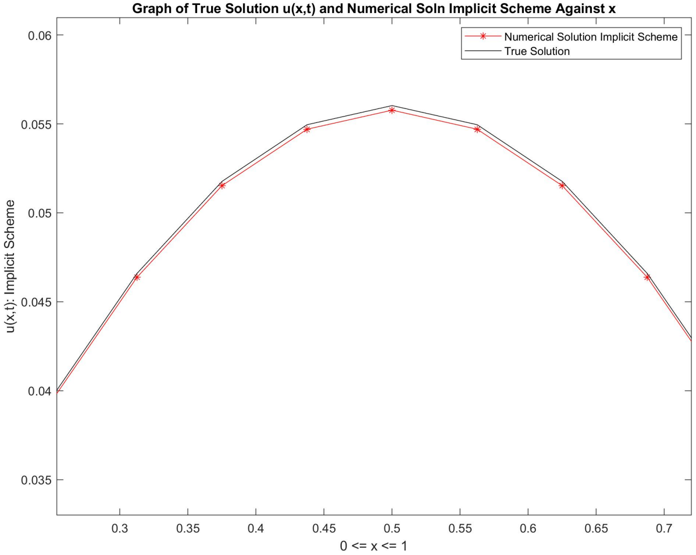
```
%loop for exact solution
u_true=zeros(M+1,K+1);

for j=1:K+1
    for i=1:M+1
        u_true(i,j) = sin(pi.*x(i))*exp(-D*pi^2*t(j));
    end
end
```

True versus Explicit Euler: First Time Step



True versus Explicit Euler: 300th Time Step



Explicit Method Analysis

Order of Convergence:

$$\mathcal{O}(\Delta x)^2 + \mathcal{O}(\Delta t)$$

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$$\mathcal{O}(\Delta x)^2 + \mathcal{O}(\Delta t)$$

$\mathcal{O}(\Delta t) \approx 1$, and $\mathcal{O}(\Delta x)^2 \approx 2$

The total order is *dominated* by Δt, so it should be closer to 1

Explicit Method Analysis

Conditionally Stable: Under the CFL condition

$$R = \frac{\Delta t \cdot \alpha}{\Delta x^2} < 1/2$$

Explicit Method Analysis

Conditionally Stable: Under the CFL condition

$$R = \frac{\Delta t \cdot \alpha}{\Delta x^2} < 1/2$$

Means: Δt has to be *much* smaller than Δx

Numerical Set-Up: (4) Solution Methods

1. Explicit Euler
2. **Implicit Euler**

Solution Method: Implicit Euler

$$u_i^{j+1} = (1 - 2R)u_i^j + R\left(u_{i+1}^j + u_{i-1}^j\right)$$

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$$u_i^{j+1} = (1-2R)u_i^j + R\left(u_{i+1}^j + u_{i-1}^j\right)$$

$$A \cdot \vec{x} = \vec{b}$$

Coefficient Matrix, A: A matrix representing the coefficients in the system of equations

Solution Method: Implicit Euler

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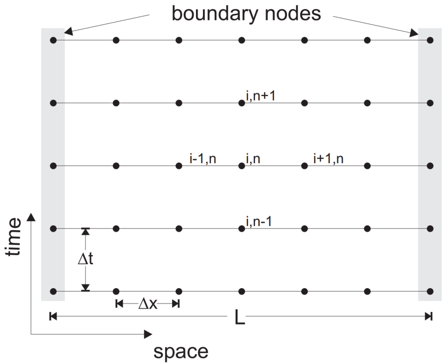
Coefficient Matrix, A: A matrix representing the coefficients in the system of equations

$$\vec{x} = A^{-1}\vec{b}$$

Solution Method: Implicit Euler



Solution Method: Implicit Euler

$$u_i^{j+1} = (1-2R)u_i^j + R\left(u_{i+1}^j + u_{i-1}^j\right)$$

$$\underbrace{\begin{bmatrix} 1-2R & R & 0 & 0 & 0 & \dots & 0 \\ R & 1-2R & R & 0 & 0 & \dots & 0 \\ 0 & R & 1-2R & R & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & R & 1-2R \end{bmatrix}}_{A} \cdot \begin{bmatrix} u_2^{j+1} \\ u_3^{j+1} \\ u_4^{j+1} \\ \vdots \\ u_M^{j+1} \end{bmatrix} = \begin{bmatrix} u_2^j \\ u_3^j \\ u_4^j \\ \vdots \\ u_M^j \end{bmatrix} + R \begin{bmatrix} u_1^j \\ 0 \\ \vdots \\ 0 \\ u_{M+1}^j \end{bmatrix}$$

Note: A is a *Tridiagonal Matrix*

Solution Method: Implicit Euler

Since out boundary condition is always 0,

$$\begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ u_3^{j+1} \\ \vdots \\ u_M^{j+1} \end{bmatrix} = A^{-1} \cdot \begin{bmatrix} u_1^{j} \\ u_2^{j} \\ u_3^{j} \\ \vdots \\ u_M^{j} \end{bmatrix}$$

$$A = \begin{bmatrix} 1-2R & R & 0 & 0 & 0 & \dots & 0 \\ R & 1-2R & R & 0 & 0 & \dots & 0 \\ 0 & R & 1-2R & R & 0 & \dots & 0 \\ \vdots & & & & & & \vdots \\ 0 & 0 & 0 & 0 & 0 & R & 1-2R \end{bmatrix}$$

```
% Data structures for the linear tridiagonal system
A = zeros(N_x-1, N_x-1);

    for i=1:N_x-1
    A(i,i)=1-2*lambda; % diagonal
    end

for i=2:N_x-1
    A(i,i-1)=lambda; %subdiagonal
end

for i=1:N_x-2
    A(i,i+1)=lambda; %superdiagonal
end
```

Implicit Code

```
v=zeros(N_x-1,1);        %BC
for j=1:N_t-1
% Solve triagonal system
v(1,1)=0;                    %BC at start
v(N_x-1,1)=0;                %BC at end

u(:,j+1)=A\(u(:,j)+lambda*v);    %x = A^-1 * b
end
```

Implicit Code

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v=zeros(N_x-1,1);       %BC
for j=1:N_t-1
% Solve triagonal system
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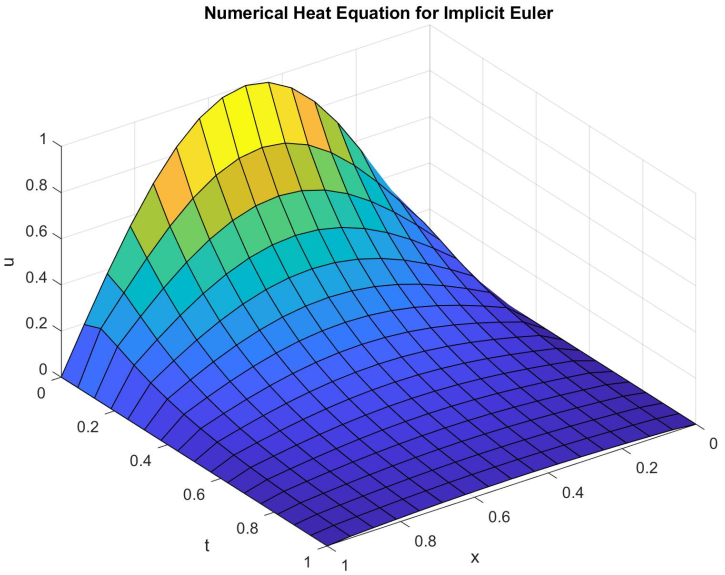
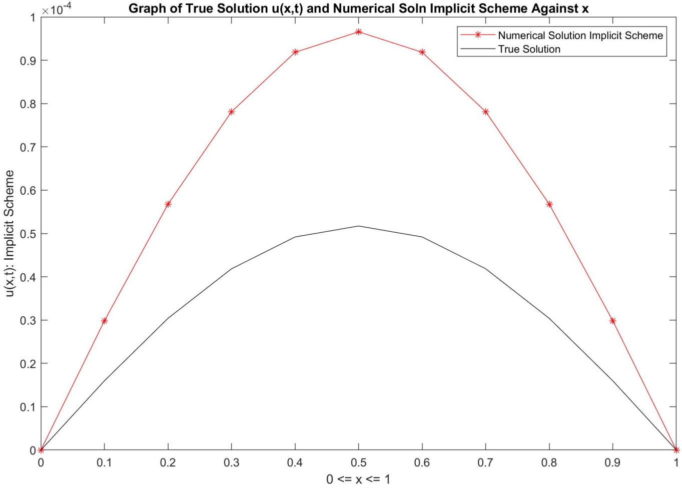
```

Implicit Graph



True versus Implicit Euler



Implicit Method Analysis

Unconditionally Stable: *always works*

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L^1, L^2, L^∞ Error for Implicit Scheme for the Heat Equation: For fixed Δx and when Δt is cut in half.

Δx	Δt	L^1 Error	L^2 Error	L^∞ Error
0.01000	0.01000	$2.42598905e-03$	$2.69481799e-04$	$3.81104814e-05$
0.01000	0.00500	$1.08459172e-03$	$1.20477760e-04$	$1.70381282e-05$
0.01000	0.00250	$5.13610852e-04$	$5.70525148e-05$	$8.06844401e-06$
0.01000	0.00125	$2.50928217e-04$	$2.78734099e-05$	$3.94189542e-06$
0.01000	0.000625	$1.25033217e-04$	$1.38888410e-05$	$1.96417873e-06$

Implicit Method Analysis: Order

$$\mathcal{O}(\Delta x)^2 + \mathcal{O}(\Delta t) \approx 1$$

Δx	Δt	Δt Ratio	L^∞ Error	Ratio of Errors	Order
0.01000	0.01000	$\sim$	$3.81104814e-05$	$\sim$	$\sim$
0.01000	0.00500	0.50000	$1.70381282e-05$	$1.70381282e-05/3.81104814e-05 = 0.44707$	1.1614
0.01000	0.00250	0.50000	$8.06844401e-06$	$8.06844401e-06/1.70381282e-05 = 0.47355$	1.0784
0.01000	0.00125	0.50000	$3.94189542e-06$	$3.94189542e-06/8.06844401e-06 = 0.48855$	1.0334
0.01000	0.000625	0.50000	$1.96417873e-06$	$1.96417873e-06/3.94189542e-06 = 0.49828$	1.0049

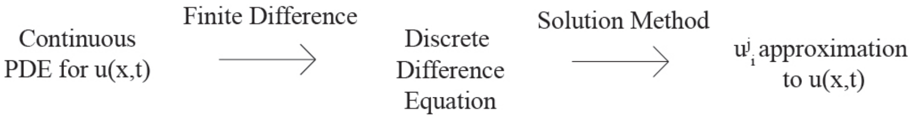
$$log_2(0.44707)/log_2(0.5) = 1.1614$$

$$log_2(0.47355)/log_2(0.5) = 1.0784$$

$$log_2(0.48855)/log_2(0.5) = 1.0334$$

$$log_2(0.49828)/log_2(0.5) = 1.0049$$

NSFD Approach



Change Finite Difference Scheme: Then, see how explicit and implicit change as a result

Unity Approximations: Averaging

$$u_i^{j+1} = (1 - 2R)u_i^j \times 1_0 + R(u_{i+1}^j + u_{i-1}^j) \times 1_1$$

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2-point Average:

$$\frac{u_A^j + u_B^j}{2u_C^j}, \quad A, B, C \in \{i, i+1, i-1\}$$

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2-point Average:

$$\frac{u_A^j + u_B^j}{2u_C^j}, \quad A, B, C \in \{i, i+1, i-1\}$$

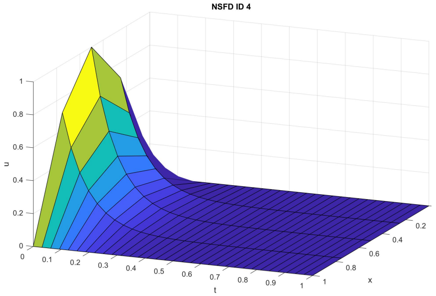
3-point Average:

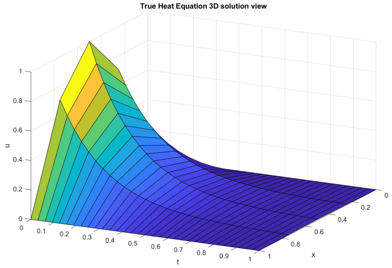
$$\frac{u_A^j + u_B^j + u_C^j}{3u_D^j}, \quad A, B, C, D \in \{i, i+1, i-1\}$$

2-pt Avg Technique at 1_0

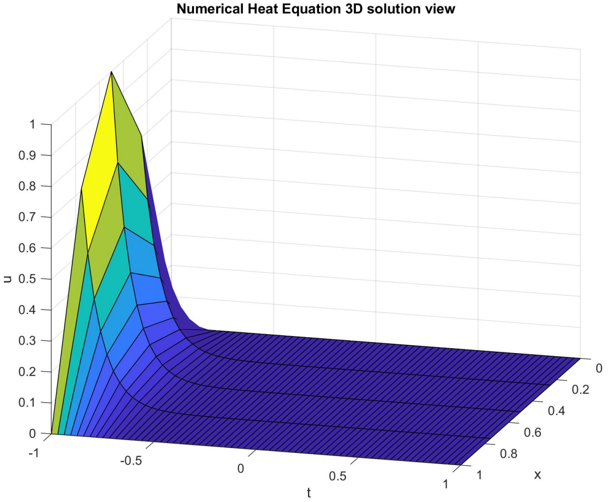
ID	A	B	C	$u_i^{j+1} =$
1	i	i + 1	i - 1	$\dfrac{(1-2R)\,u_i^j\left(u_i^j+u_{i+1}^j\right)}{2u_{i-1}^j}+R\left(u_{i+1}^j+u_i^j\right)$
3	i + 1	i	i - 1	$\dfrac{(1-2R)u_i^j\left(u_i^j+Ru_{i+1}^j\right)}{2u_{i-1}^j}+R/2$
4	i + 1	i - 1	i	$\dfrac{u_{i+1}^j+u_{i-1}^j}{2}$
6	i - 1	i + 1	i	$\dfrac{u_{i-1}^j+u_{i+1}^j}{2}$

NSFD ID 4: Explicit Euler

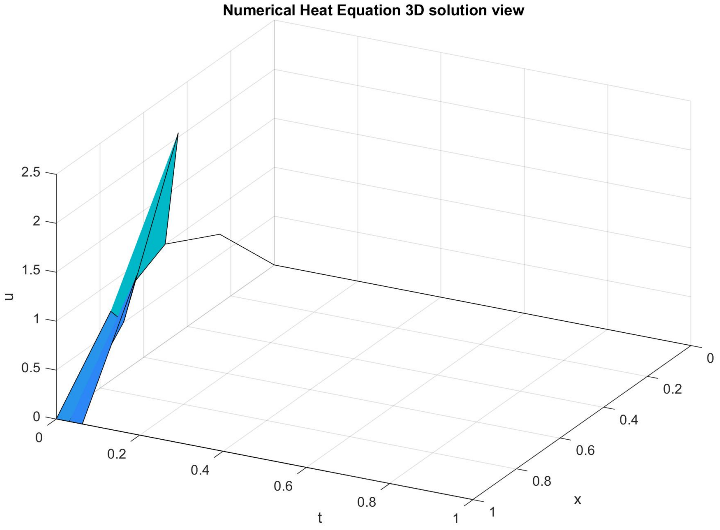




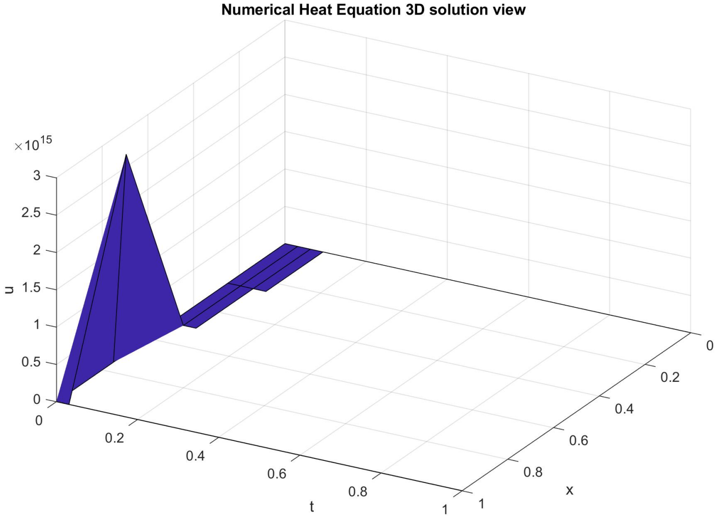
NSFD ID 16 (3pt Avg): Explicit Euler



NSFD ID 17 (3pt Avg): Explicit Euler



NSFD ID 25 (3pt Avg): Explicit Euler



Implicit NSFD Schemes

Goal: Create the A matrix

2-point Average:

$$\frac{u_A^X + u_B^Y}{2u_C^Z}, \quad A, B, C \in \{i, i+1, i-1\} \quad X, Y, Z \in \{j, j+1, j-1\}$$

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When $j = 1$, $u_i^1 =$ function in terms of u_i^0

When $j = 2$, $u_i^2 =$ function in terms of u_i^1

Then can find the matrix A such that

$$A \cdot u^{j+1} = u^j$$

Next Steps

1. More Averages
2. Build out Implicit NSFDs
3. Find orders and compare against Implicit SFDs

Thank you!

Questions?