# 5.3 Numerical Solutions to PDEs

# Differentials expressed as finite differences

From the Taylor series

- $u(x+\Delta x) = u(x) + u'(x)\Delta x + O(\Delta x^2)$

Therefore

- $u'(x) = \frac{u(x+\Delta x)-u(x)}{\Delta x}$ $+ \underbrace{\frac{O(\Delta x^2)}{\Delta x}}_{O(\Delta x)}$

On a discrete grid

$$u'_{m+1} = \frac{u_{m+1} - u_m}{\Delta x} + O(\Delta x)$$

# Discrete 2$^{nd}$ order differentials

Writing Taylor series

- $u(x+\Delta x) = u(x) + u'(x)\Delta x + \frac{\Delta x^2}{2!}u''(x) + \frac{\Delta x^3}{3!}u'''(x) + O(\Delta x^4)$

$+$

- $u(x-\Delta x) = u(x) - u'(x)\Delta x + \frac{\Delta x^2}{2!}u''(x) - \frac{\Delta x^3}{3!}u'''(x) + O(\Delta x^4)$

Adding these together

- $u''(x) = \frac{u(x+\Delta x)-2u(x)+u(x-\Delta x)}{(\Delta x)^2}$ $+ O(\Delta x^2)$

$$u_m'' = \frac{u_{m+1} - 2u_m + u_{m-1}}{(\Delta x)^2}$$

# Discrete Heat Equation

m – SPACE (x)

n – TIME (t)

$$\frac{\partial T}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2}$$

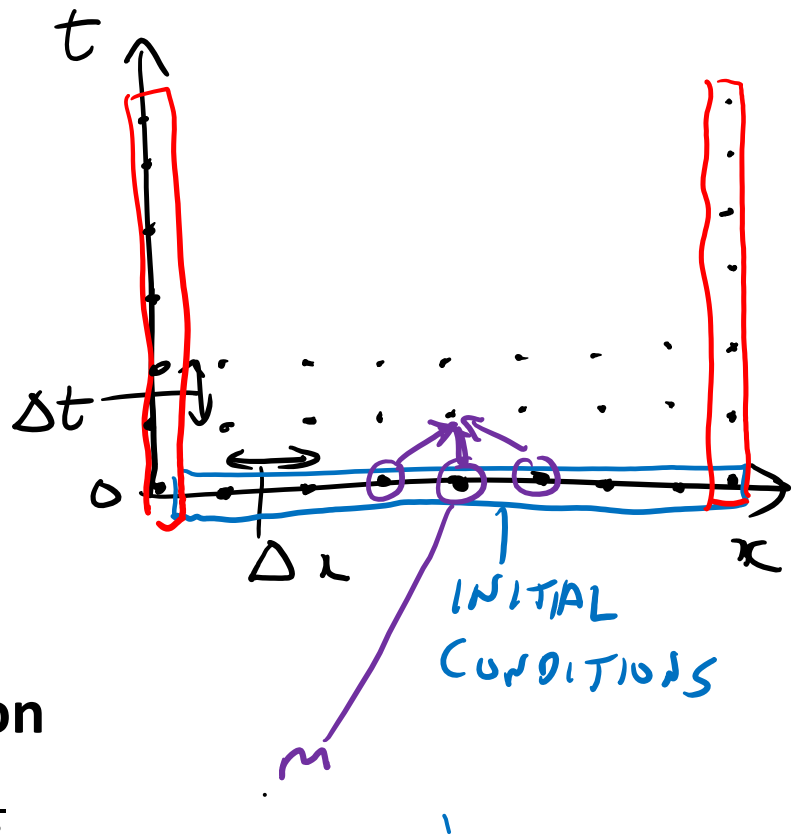
The heat equation is a parabolic 2nd order PDE, solved by ***marching forward in time***

- The continuous function is mapped onto a grid

Using the discrete finite difference forms of the differentials

$$\frac{\partial T}{\partial t} = \frac{T_{m,n+1} - T_{m,n}}{\Delta t}$$

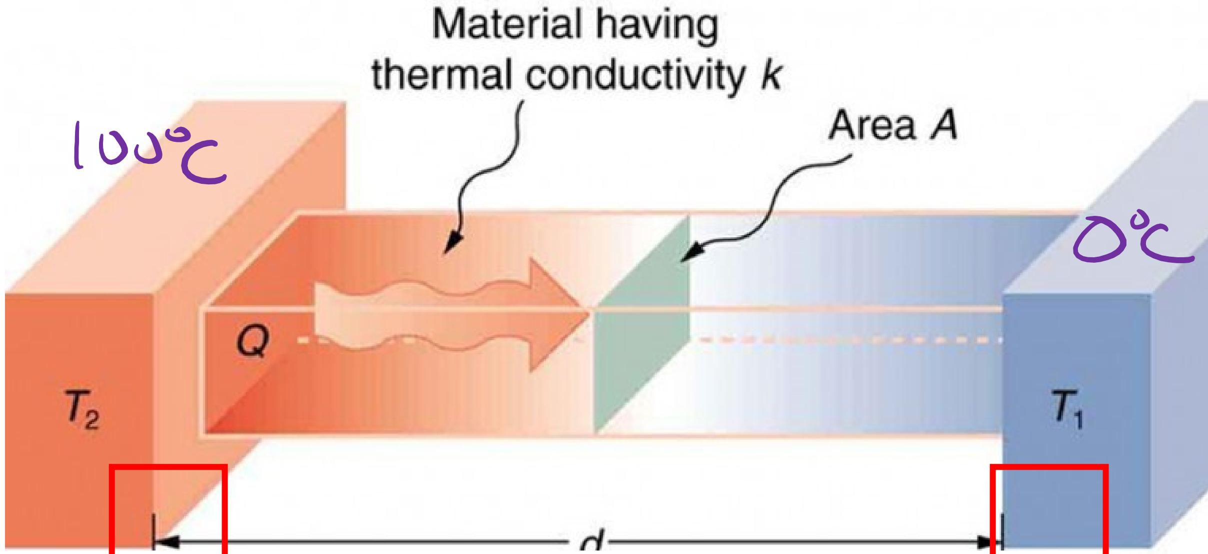
$$\frac{\partial^2 T}{\partial x^2} = \frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{(\Delta x)^2}$$




- This gives the Forward in Time (Explicit) **Finite Differen~~t~~ce Equation**
- $T_{m,n+1} = \lambda T_{m+1,n} + T_{m,n}(1 - 2\lambda) + \lambda T_{m-1,n}$ where $\lambda = D\,\frac{\Delta t}{(\Delta x)^2}$

# Heat Equation Example

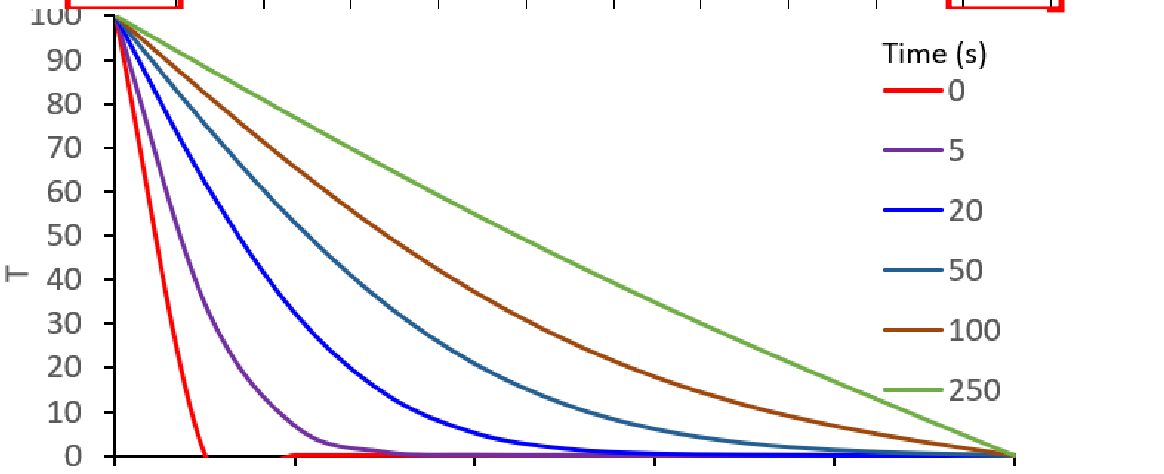
- Consider a straight, well insulated metal rod with its ends in good thermal contact with heat reservoirs of temperature $T_1$ and $T_2$ with $\lambda = 0.2$
- BC: $T(0,t) = 100°\mathrm{C},\ T(d,t) = 0°\mathrm{C}$
- IC: $T(x,0) = 0°\mathrm{C},\ T(0,0) = 100°\mathrm{C}$




$$T_{m,n+1} = \lambda T_{m+1,n} + T_{m,n}(1-2\lambda) + \lambda T_{m-1,n}$$

| t | | x: m = 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | n = 0 | 100.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 0.2 | 1 | 100.0 | | | | | | | | | | 0.0 |
| 0.4 | 2 | 100.0 | | | | | | | | | | 0.0 |
| 0.6 | 3 | 100.0 | | | | | | | | | | 0.0 |
| 0.8 | 4 | 100.0 | | | | | | | | | | 0.0 |
| 1.0 | 5 | 100.0 | | | | | | | | | | 0.0 |
| 1.2 | 6 | 100.0 | | | | | | | | | | 0.0 |

| | m= 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| n= 0 | 100.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| 1 | 100.0 | 20.0 | 0.0 | 0.0 | 0.0 |
| 2 | 100.0 | 32.0 | 4.0 | 0.0 | 0.0 |
| 3 | 100.0 | 40.0 | 8.8 | 0.8 | 0.0 |



# Backward (Implicit) Finite Difference Method

- Forward (explicit) method is fast and simple but unstable if $\lambda > 0.5$
- Backward in time method is implicitly stable
- 2nd order space derivative is now evaluated at n+1 rather than n
- $\underline{\frac{T_{m,n+1}-T_{m,n}}{\Delta t}} \approx D\,\frac{T_{m+1,n+1}-2T_{m,n+1}+T_{m-1,n+1}}{(\Delta x)^2}$ EVALUATED AT NEXT TIME STEP n+1
- $T_{m,n} = -\lambda T_{m+1,n+1} + T_{m,n+1}(1+2\lambda) - \lambda T_{m+1,n+1}$ where $\lambda = D\,\frac{\Delta t}{(\Delta x)^2}$

| | $m = 0$ | 1 | 2 | 3 |
|---|---|---|---|---|
| $n = 0$ | **100.0** | **0.0** | **0.0** | **0.0** |
| 1 | **100.0** | $\times -\lambda$ | $\times(1+2\lambda)$ | $\times -\lambda$ |
| 2 | **100.0** | | | |
| 3 | **100.0** | | | |

- Linear algebra algorithms used to solve the resulting simultaneous equations
- Implicit methods slower than explicit but stable

$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial x^2}$$

$x$ CONSTANT

$m$ "

$t$ CONSTANT

$n$ "

$T(x,t) \longrightarrow T_{m,n}$

CONTINUOUS

DISCRETE

$x$ INDEX $x_m$

$t$ INDEX $t_n$

$$\frac{T_{m,n+1} - T_{m,n}}{\Delta t} = D \, \frac{T_{m+1,n} - 2T_{m,n} + T_{m-1,n}}{(\Delta x)^2}$$

$$T_{m,n+1} = \lambda T_{m+1,n} + (1-2\lambda) T_{m,n} + \lambda T_{m-1,n}$$

FORWARD IN TIME SOLUTION

$$\lambda = \frac{\Delta t}{(\Delta x)^2} D$$

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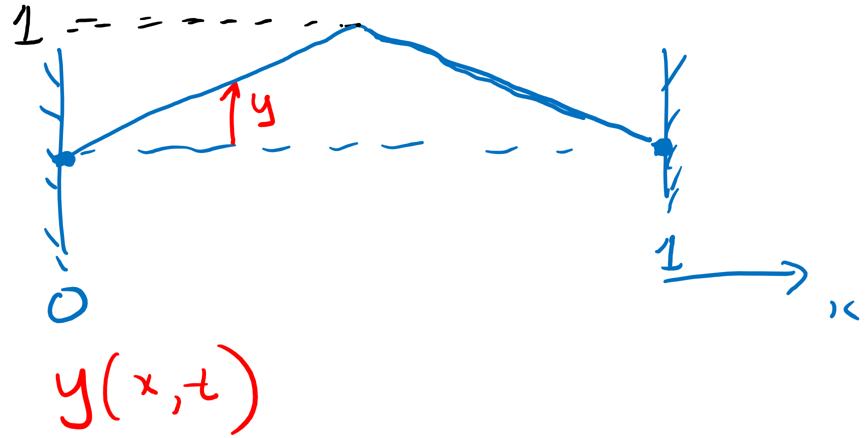
| METHOD | | | | |
|---|---|---|---|---|
| FORWARD | $\left.\frac{\partial^2 T}{\partial x^2}\right\vert_n$ | EXPLICIT | FAST | UNSTABLE $\lambda > 0.5$ |
| BACKWARD | $\left.\frac{\partial^2 T}{\partial x^2}\right\vert_{n+1}$ | IMPLICIT | SLOW | STABLE INHERENTLY |

CRANK-NICOLSON $\longrightarrow$ MORE ACCURATE $\left.\frac{\partial^2 T}{\partial x^2}\right|_{n+\frac{1}{2}} = \frac{1}{2}\left( \left.\frac{\partial^2 T}{\partial x^2}\right|_n + \left.\frac{\partial^2 T}{\partial x^2}\right|_{n+1} \right)$

Jan 2021 Paper

**C.2** A wire of length $L = 1$ m and density per unit length $\mu = 0.01$ kg m$^{-1}$, is attached rigidly at both ends and placed under tension $T = 1$ N. At a position $x$ along the wire, it is displaced a distance $y(x,t)$ from equilibrium at time $t$. The motion of the wire is governed by the wave equation




$$\frac{\mu}{T}\frac{\partial^2 y}{\partial t^2} = \frac{\partial^2 y}{\partial x^2}$$

(a) The following is a Taylor expansion to third order for a function $u(x)$

$$u(x+\Delta x) = u(x) + \Delta x u'(x) + \frac{\Delta x^2}{2!}u''(x) + \frac{\Delta x^3}{3!}u'''(x) + O(\Delta x^4)$$

By considering $u(x+\Delta x)$ and $u(x-\Delta x)$, obtain an approximate expression for the second order derivative $u''(x)$. To what order of $\Delta x$ does the error in this expression depend?

$$u(x-\Delta x) = u(x) - \Delta x u'(x) + \frac{(\Delta x)^2}{2!}u''(x) - \frac{(\Delta x)^3}{3!}u'''(x) + O(\Delta x^4)$$

$$u(x+\Delta x) + u(x-\Delta x) = 2u(x) + (\Delta x)^2 u''(x) + O(\Delta x^4)$$

$$u''(x) = \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{(\Delta x)^2} + \underbrace{\frac{O(\Delta x^4)}{(\Delta x)^2}}_{O(\Delta x)^2}$$

(b) To obtain a solution to the wave equation, $y(x,t)$ can be represented on a grid $y_{m,n}$ and solved numerically. Show that the wave equation can be written as the following finite difference equation

$$\frac{\mu}{T}\frac{\partial^2 y}{\partial t^2}\bigg|_{x \text{ constant},\ m} = \frac{\partial^2 y}{\partial x^2}\bigg|_{t \text{ constant},\ n}$$

$$y(x,t) \longrightarrow y_{m,n}$$

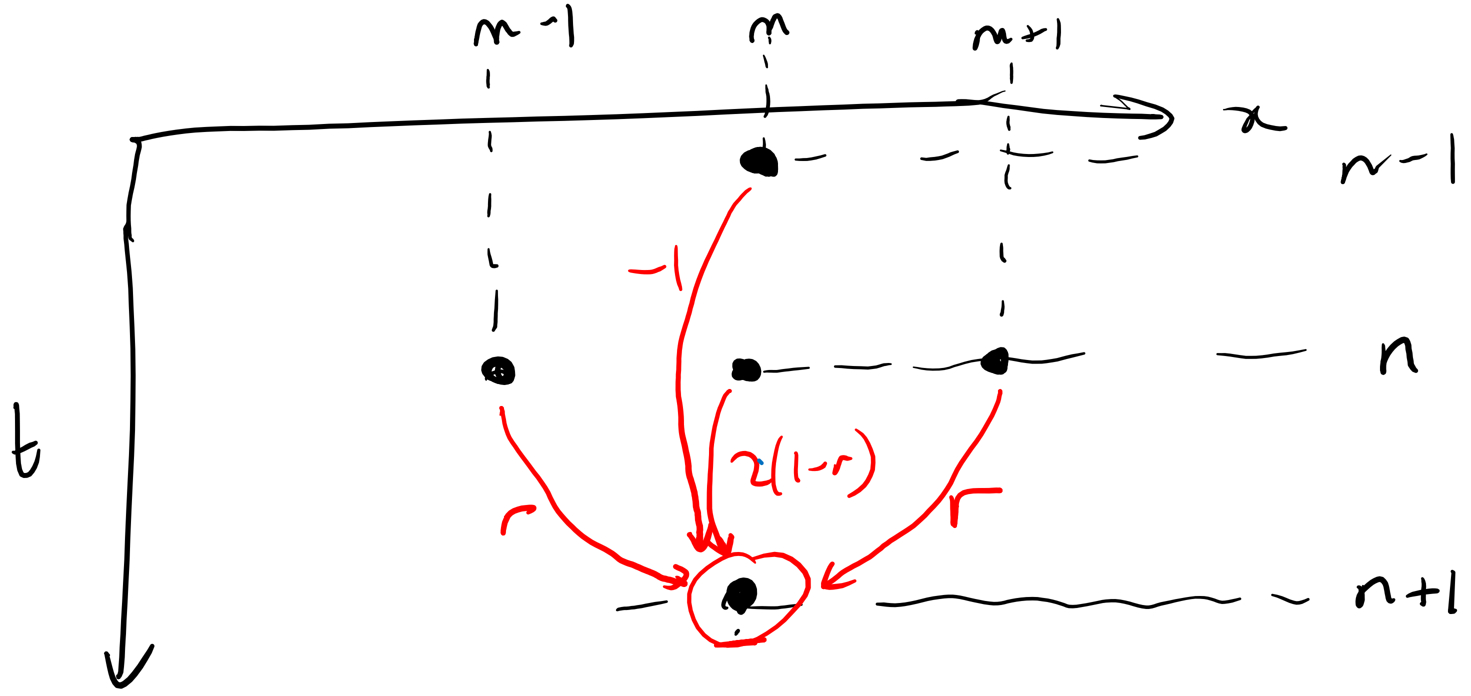
$$y_{m,n+1} = r(y_{m+1,n} + y_{m-1,n}) + 2y_{m,n}(1-r) - y_{m,n-1}$$

where $m, n$ are the grid indices for the variables $x, t$ and

$$r = \frac{T}{\mu}\left(\frac{\Delta t}{\Delta x}\right)^2$$

$$\frac{\mu}{T}\,\frac{y_{m,n+1} - 2y_{m,n} + y_{m,n-1}}{(\Delta t)^2} = \frac{y_{m+1,n} - 2y_{m,n} + y_{m-1,n}}{(\Delta x)^2}$$

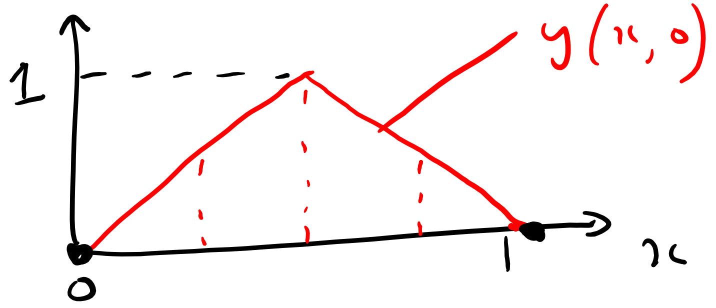
$$y_{m,n+1} - 2y_{m,n} + y_{m,n-1} = \underbrace{\frac{T}{\mu}\frac{(\Delta t)^2}{(\Delta x)^2}}_{r}\left(y_{m+1,n} - 2y_{m,n} + y_{m-1,n}\right)$$



m-1
m
m+1
x
t
n-1
n
n+1
-1
2(1-r)
r
r

(c) The wire is pulled a distance $y = 1$ from equilibrium at its midpoint and released from rest so that

$$y(x,0) = \begin{cases} 2x & \text{for } 0 < x < 1/2 \\ 2(1-x) & \text{for } 1/2 < x < 1 \end{cases}$$




A numerical solution based on the grid shown below (where $\Delta x = 0.25$, $\Delta t = 0.01$) can be obtained using these initial conditions by "marching forward in time". Explaining your methodology, fill the first 3 rows of this grid with the values of $y_{m,n}$ for $n = 0, 1, 2$.

??

| | m | 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|---|
| n | t \ x | 0.0 | 0.25 <br> 0.5 | 0.50 <br> 1 | 0.75 | 1.0 |
| 0 | 0.00 | 0 | 0.5 | 1 | 0.5 | 0 |
| 1 | 0.01 | 0 | 0.5 | 0.84 | 0.5 | 0 |
| 2 | 0.02 | 0 | 0.47 | 0.57 | 0.47 | 0 |

As the wire is originally at rest you may assume that $y_{m,-1} = y_{m,0}$

INITIAL CONDITIONS

1. $y(x, 0)$
2. $\left.\dfrac{\partial y}{\partial t}\right|_{t=0} = 0$

BOUNDARY CONDITIONS

1. $y(0, t) = 0$
2. $y(1, t) = 0$

$$r = \frac{T}{\mu}\left(\frac{\Delta t}{\Delta x}\right)^2 = \frac{1}{0.01}\left(\frac{0.01}{0.25}\right)^2$$

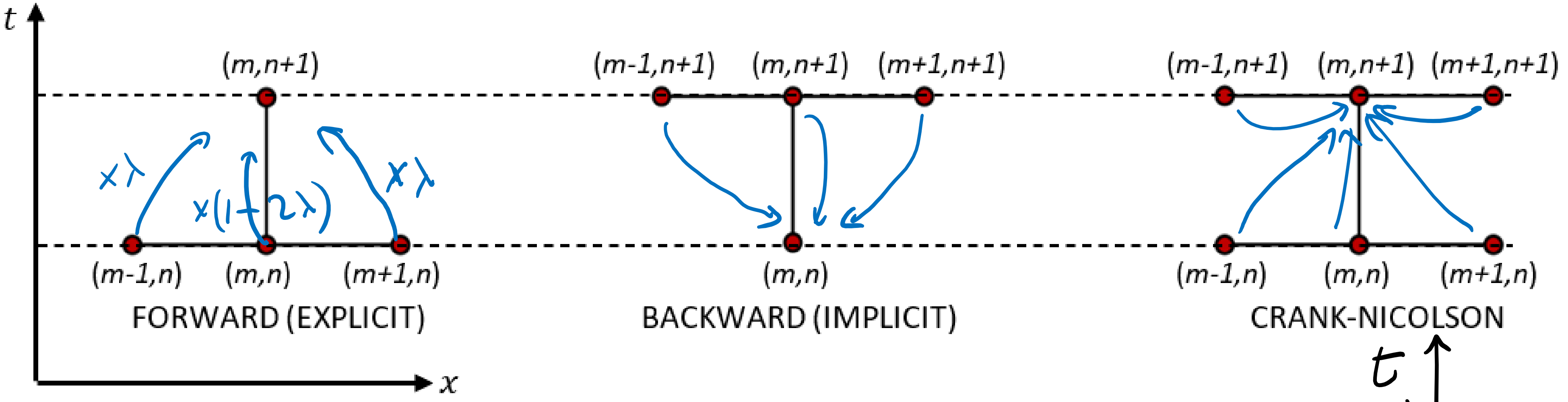
$$r = 0.16$$

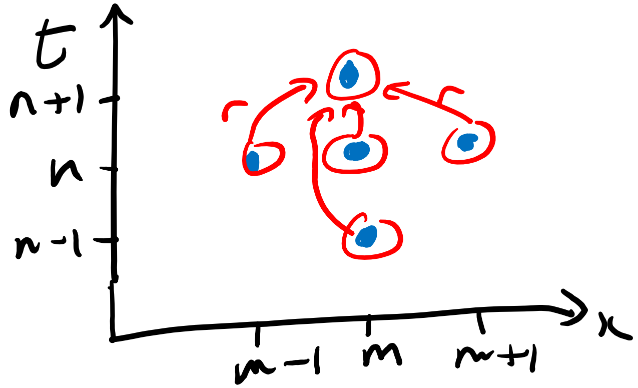
$$y_{1,1} = 0.16(0 + 1) + \underbrace{2(1 - 0.16)}_{1.68}(0.5) - 0.5$$
$$= 0.5$$

$$y_{2,1} = 0.16(0.5 + 0.5) + (1.68)(1) - 1$$
$$= 0.84$$

# Stencils

- Stencils show how grid values are determined by surrounding points
- For P**arabolic equations** such as Heat and Schrodinger Equation




- For **Hyperbolic equations** such as the wave equation
- $v^2 \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial t^2}$

$u(x,t) \longrightarrow u_{m,n}$ ($m \leftarrow x$, $n \leftarrow t$)

$$v^2 \frac{u_{m+1,n} - 2u_{m,n} + u_{m-1,n}}{(\Delta x)^2} = \frac{u_{m,n+1} - 2u_{m,n} + u_{m,n-1}}{(\Delta t)^2}$$

- $u_{m,n+1} = r\left(u_{m+1,n} + u_{m-1,n}\right) + 2u_{m,n}(1-r) - u_{m,n-1}$ where $r = \left(\frac{v\Delta t}{\Delta x}\right)^2$

# Elliptical PDEs – Relaxation Techniques

- E.g. Laplace/Poisson's Equation

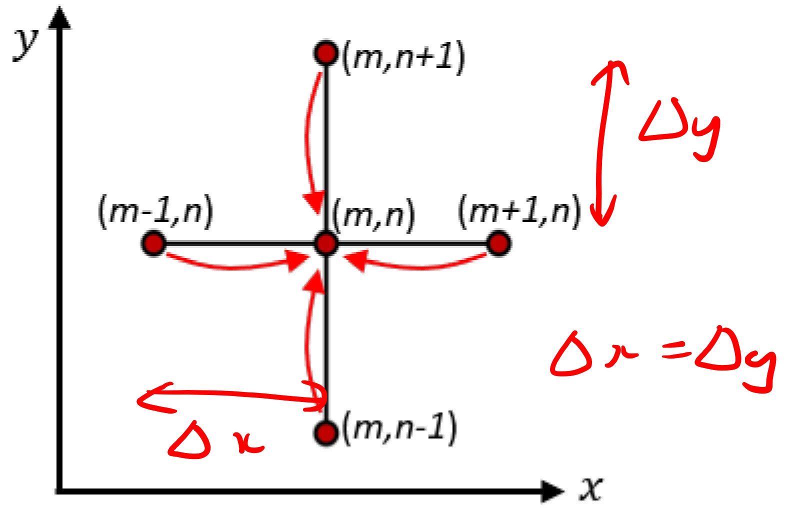
NO TIME DEPENDENCE

$V(x,y) \longrightarrow V_{m,n}$

x y

- $\dfrac{\partial^2 V(x,y)}{\partial x^2} + \dfrac{\partial^2 V(x,y)}{\partial y^2} = 0$

- $\dfrac{V_{m,n-1} - 2V_{m,n} + V_{m,n+1}}{(\Delta x)^2} + \dfrac{V_{m+1,n} - 2V_{m,n} + V_{m-1,n}}{(\Delta y)^2} = 0$




- If $\Delta x = \Delta y$
- $V_{m,n} = \frac{1}{4}\left(V_{m,n-1} + V_{m,n+1} + V_{m+1,n} + V_{m-1,n}\right)$

# Relaxation Techniques

- All grid points are calculated. This is repeated many times (iterations) until convergence

**Iteration 0**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| -100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -100 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 0 | 0 |

**Iteration 1**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 33.3 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 33.3 | 0 |
| -33 | 0 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 0 | -33 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -100 | -25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | -25 | -100 |
| -33 | 0 | 25 | 25 | 25 | 25 | 25 | 25 | 25 | 0 | -33 |
| 0 | 33.3 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 33.3 | |

**Iteration 2**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 33.3 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 33.3 | 0 |
| -33 | 0 | 31.3 | 37.5 | 37.5 | 37.5 | 37.5 | 37.5 | 31.3 | 0 | -33 |
| -100 | -31 | 0 | 6.25 | 6.25 | 6.25 | 6.25 | 6.25 | 0 | -31 | -100 |
| -100 | -38 | -6.3 | 0 | 0 | 0 | 0 | 0 | -6.3 | -38 | -100 |
| -100 | -38 | -6.3 | 0 | 0 | 0 | 0 | 0 | -6.3 | -38 | -100 |
| -100 | -38 | -6.3 | 0 | 0 | 0 | 0 | 0 | -6.3 | -38 | -100 |
| -100 | -38 | -6.3 | 0 | 0 | 0 | 0 | 0 | -6.3 | -38 | -100 |
| -100 | -38 | -6.3 | 0 | 0 | 0 | 0 | 0 | -6.3 | -38 | -100 |
| -100 | -31 | 0 | 6.25 | 6.25 | 6.25 | 6.25 | 6.25 | 0 | -31 | -100 |
| -33 | 0 | 31.3 | 37.5 | 37.5 | 37.5 | 37.5 | 37.5 | 31.3 | 0 | -33 |
| 0 | 33.3 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 33.3 | 0 |

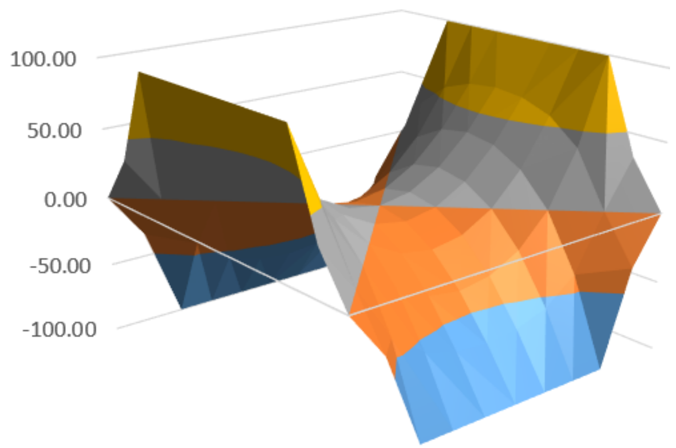
**Iteration 20**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0.00 | 33.33 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 33.33 | 0.00 |
| -33.33 | 0.00 | 39.12 | 56.51 | 64.33 | 66.61 | 64.33 | 56.51 | 39.12 | 0.00 | -33.33 |
| -100 | -39.12 | 0.00 | 22.70 | 34.40 | 38.00 | 34.40 | 22.70 | 0.00 | -39.12 | -100 |
| -100 | -56.51 | -22.70 | 0.00 | 12.78 | 16.89 | 12.78 | 0.00 | -22.70 | -56.51 | -100 |
| -100 | -64.33 | -34.40 | -12.78 | 0.00 | 4.21 | 0.00 | -12.78 | -34.40 | -64.33 | -100 |
| -100 | -66.61 | -38.00 | -16.89 | -4.21 | 0.00 | -4.21 | -16.89 | -38.00 | -66.61 | -100 |
| -100 | -64.33 | -34.40 | -12.78 | 0.00 | 4.21 | 0.00 | -12.78 | -34.40 | -64.33 | -100 |
| -100 | -56.51 | -22.70 | 0.00 | 12.78 | 16.89 | 12.78 | 0.00 | -22.70 | -56.51 | -100 |
| -100 | -39.12 | 0.00 | 22.70 | 34.40 | 38.00 | 34.40 | 22.70 | 0.00 | -39.12 | -100 |
| -33.33 | 0.00 | 39.12 | 56.51 | 64.33 | 66.61 | 64.33 | 56.51 | 39.12 | 0.00 | -33.33 |
| 0.00 | 33.33 | 100 | 100 | 100 | 100 | 100 | 100 | 100 | 33.33 | 0.00 |

**Iteration 20 – Iteration 19**

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 0.00 | 0.00 | 0.01 | 0.03 | 0.06 | 0.07 | 0.06 | 0.03 | 0.01 | 0.00 | 0.00 |
| 0.00 | -0.01 | 0.00 | 0.04 | 0.08 | 0.09 | 0.08 | 0.04 | 0.00 | -0.01 | 0.00 |
| 0.00 | -0.03 | -0.04 | 0.00 | 0.05 | 0.07 | 0.05 | 0.00 | -0.04 | -0.03 | 0.00 |
| 0.00 | -0.06 | -0.08 | -0.05 | 0.00 | 0.02 | 0.00 | -0.05 | -0.08 | -0.06 | 0.00 |
| 0.00 | -0.07 | -0.09 | -0.07 | -0.02 | 0.00 | -0.02 | -0.07 | -0.09 | -0.07 | 0.00 |
| 0.00 | -0.06 | -0.08 | -0.05 | 0.00 | 0.02 | 0.00 | -0.05 | -0.08 | -0.06 | 0.00 |
| 0.00 | -0.03 | -0.04 | 0.00 | 0.05 | 0.07 | 0.05 | 0.00 | -0.04 | -0.03 | 0.00 |
| 0.00 | -0.01 | 0.00 | 0.04 | 0.08 | 0.09 | 0.08 | 0.04 | 0.00 | -0.01 | 0.00 |
| 0.00 | 0.00 | 0.01 | 0.03 | 0.06 | 0.07 | 0.06 | 0.03 | 0.01 | 0.00 | 0.00 |
| 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

Laplace Solution for quadrupole field




- Faster convergence can be obtained using over-relaxation (see notes)