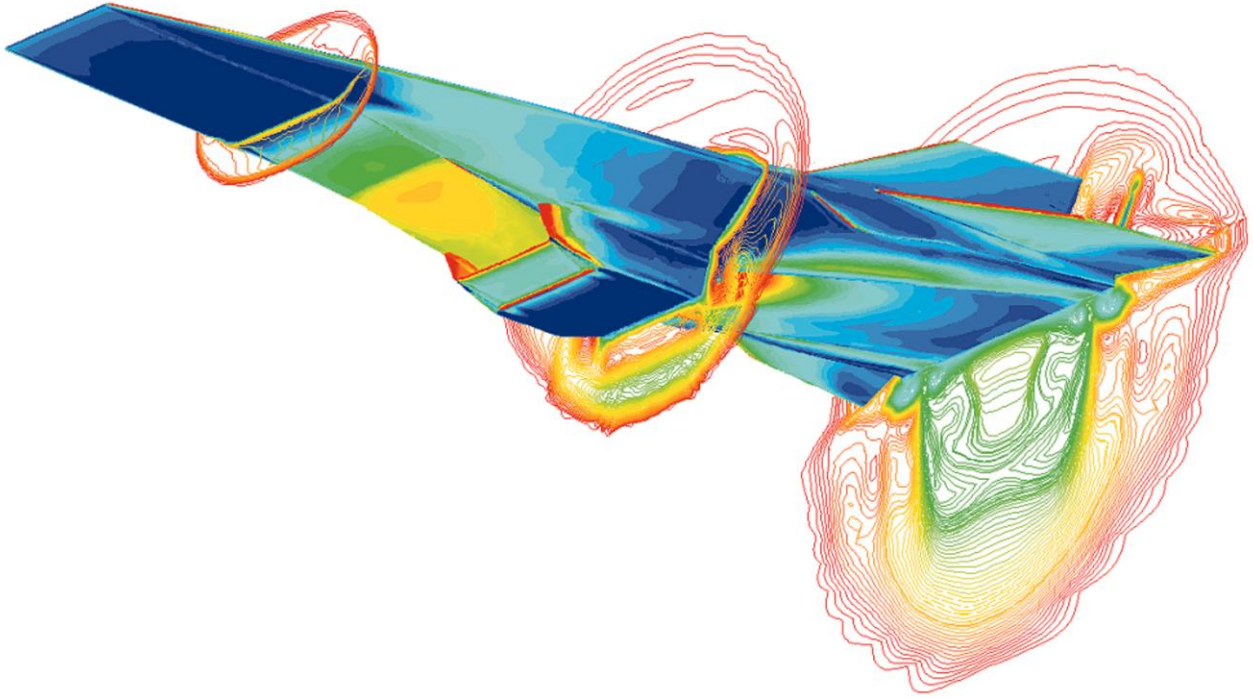
Difference Equations

SEBASTIAN THOMAS



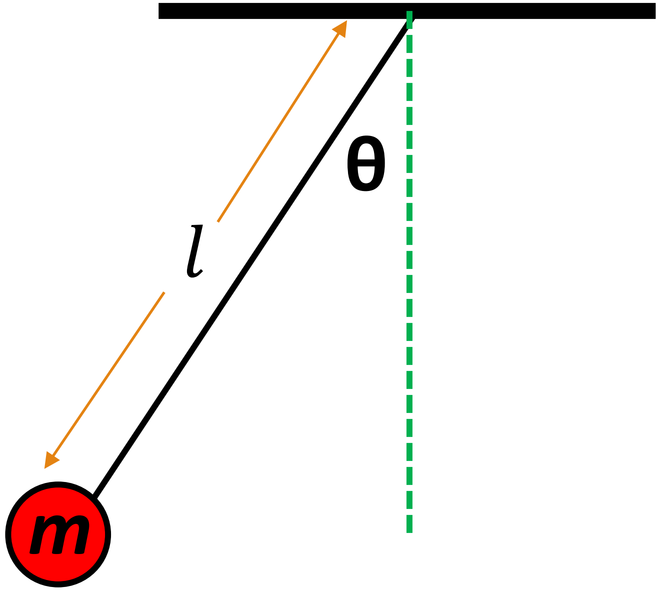
Differential Equations

The 'source code' of the universe is written in the language of differential equations i.e mathematical relationships between derivatives

Name	Describes
Schrödinger's Equation	Evolution of a QM wave function
Newton's 2nd Law	Motion of macroscopic objects
Navier-Stokes Equation	Behavior of Fluids
Einstein's Field Equations	Geometry of spacetime

Differential Equations

Not all differential equations have analytical solutions!

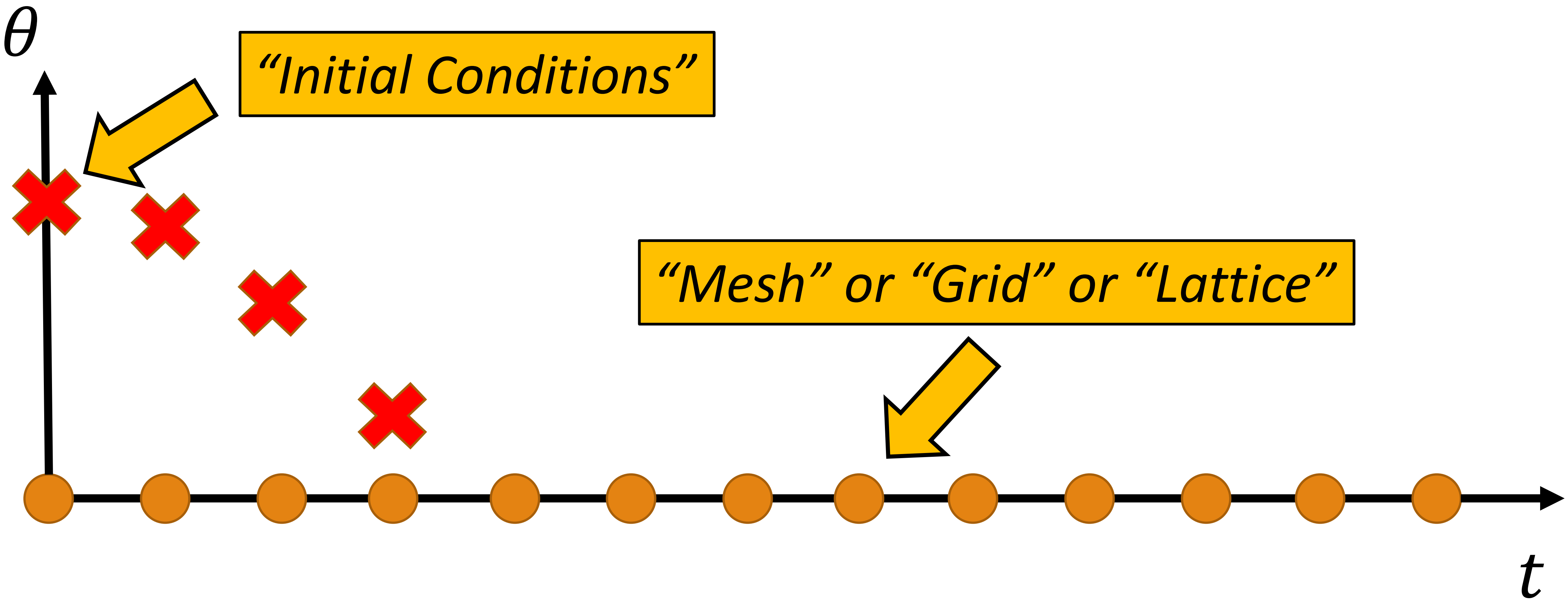


$$ml^2 \frac{d^2\theta}{dt^2} = -mgl\sin(\theta)$$

$\sin(\theta) \approx \theta$

$$ml^2 \frac{d^2\theta}{dt^2} = -mgl\theta$$

$$ml^2 \frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} = -mgl\sin(\theta)$$

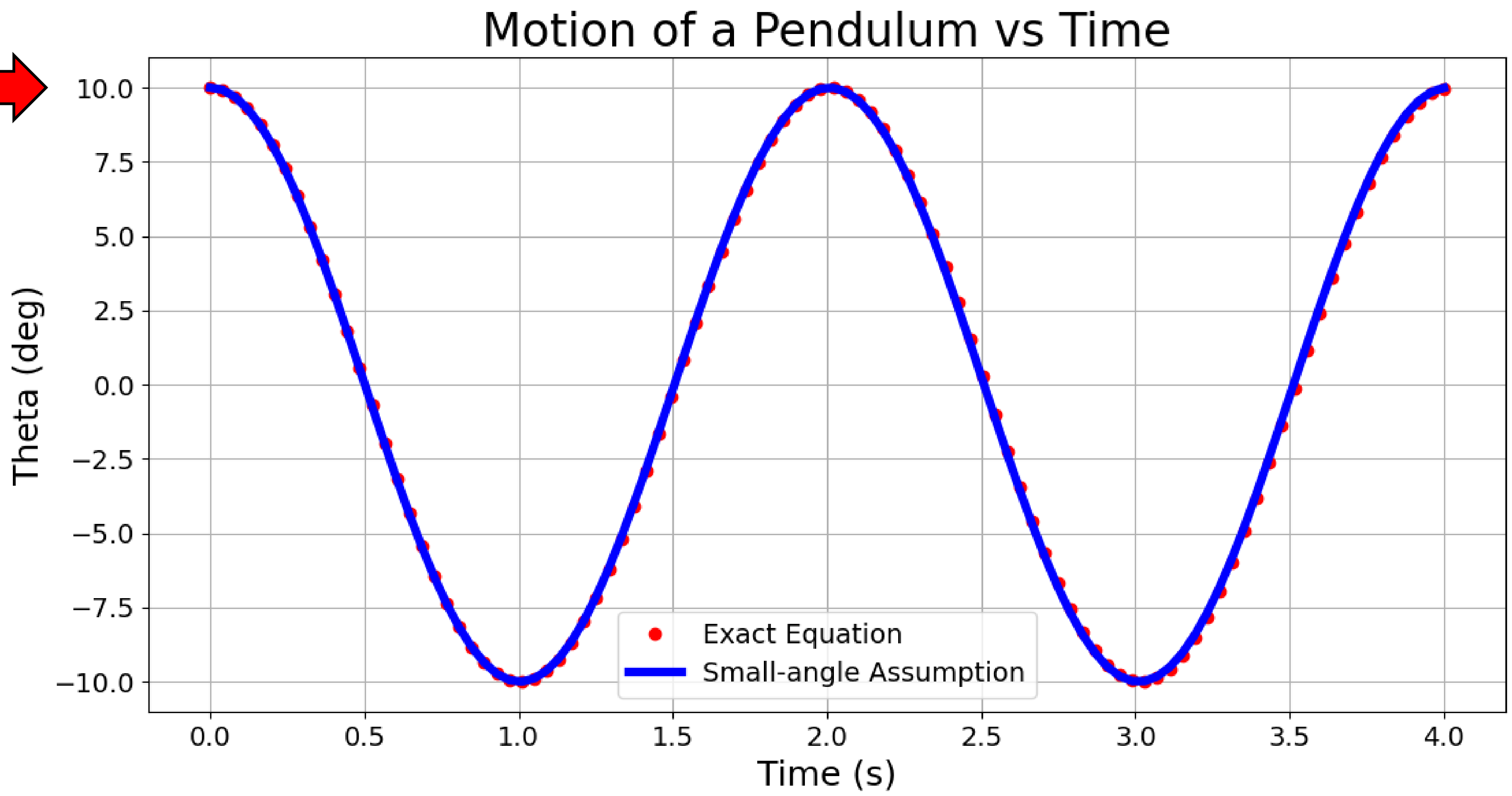


$$ml^2 \frac{d^2\theta}{dt^2} = -mgl\sin(\theta)$$

VS

$$ml^2 \frac{d^2\theta}{dt^2} = -mgl\theta$$

$\theta_0 = 10^{o}$

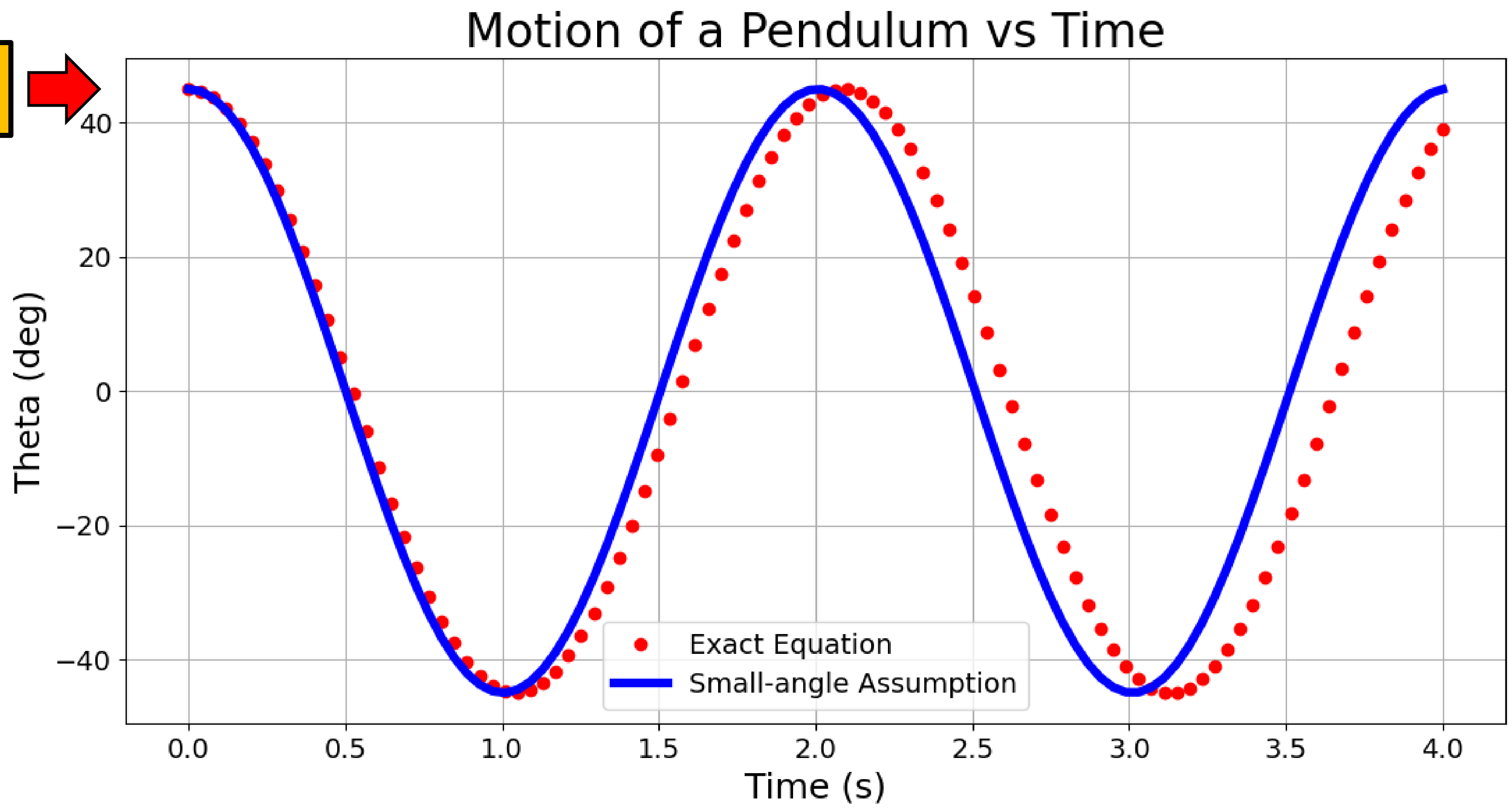


$$ml^2 \frac{d^2\theta}{dt^2} = -mgl\sin(\theta)$$

VS

$$ml^2 \frac{d^2\theta}{dt^2} = -mgl\theta$$

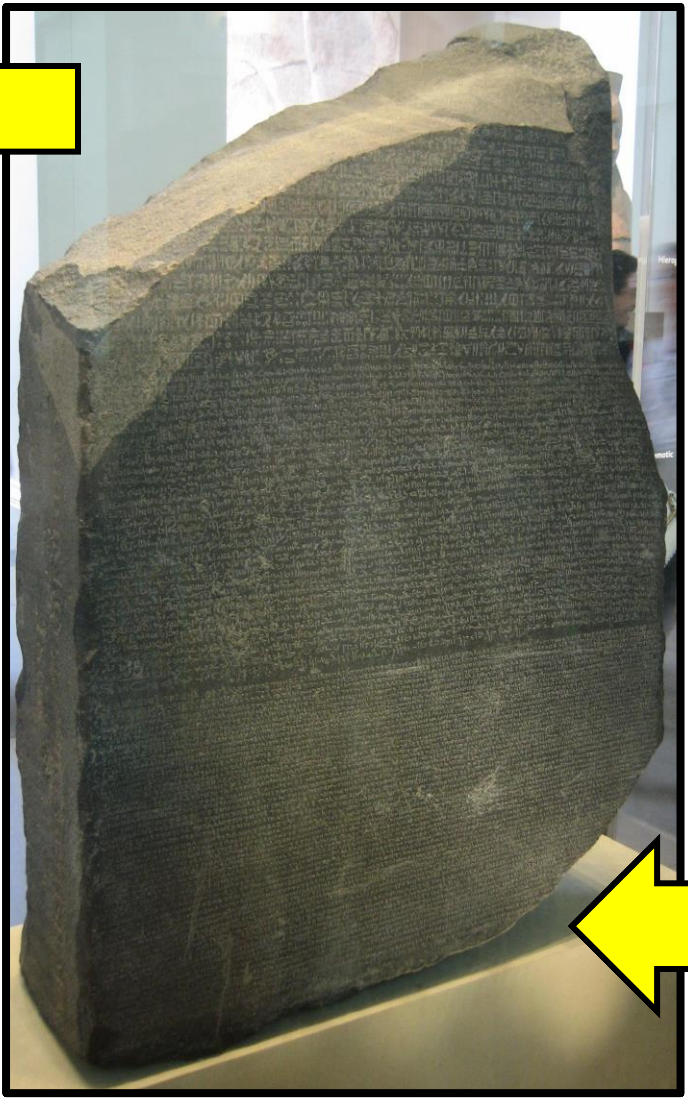
$\theta_0 = 45^o$



Some differential equations have no analytical solutions

Create a "mesh"

Function values at 'a' and neighboring points



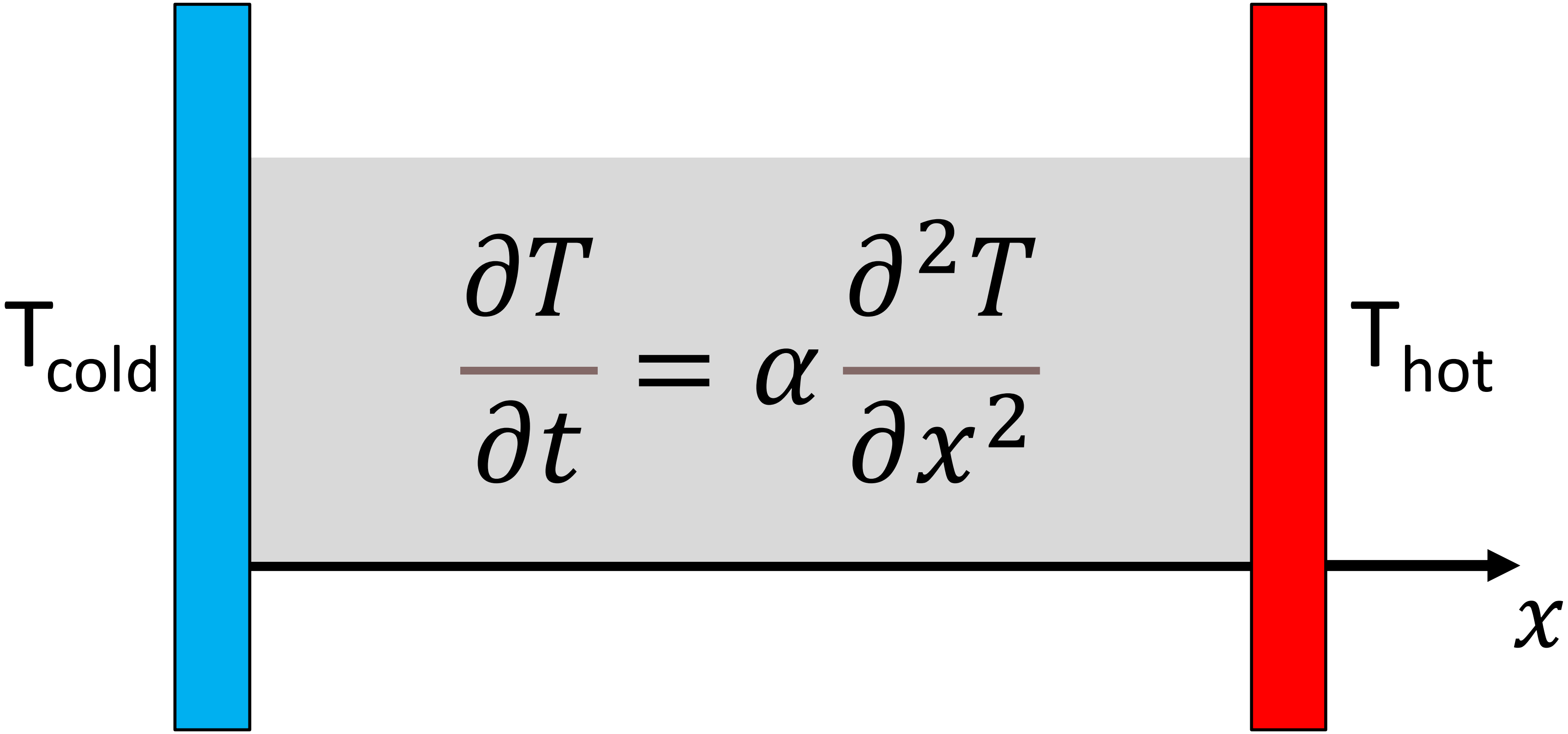
Taylor Series

Approximate derivatives at 'a'

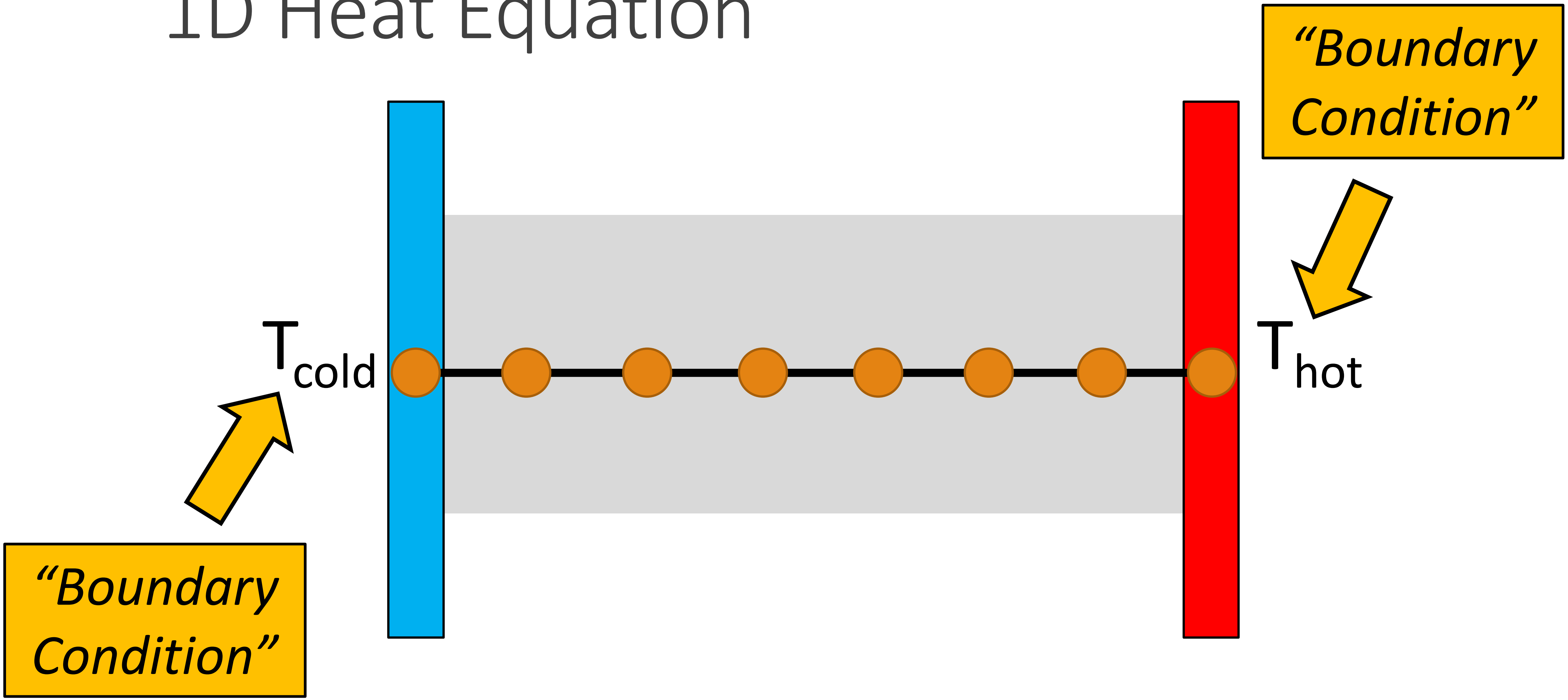
Approximate differential equation at point 'a'

Solve

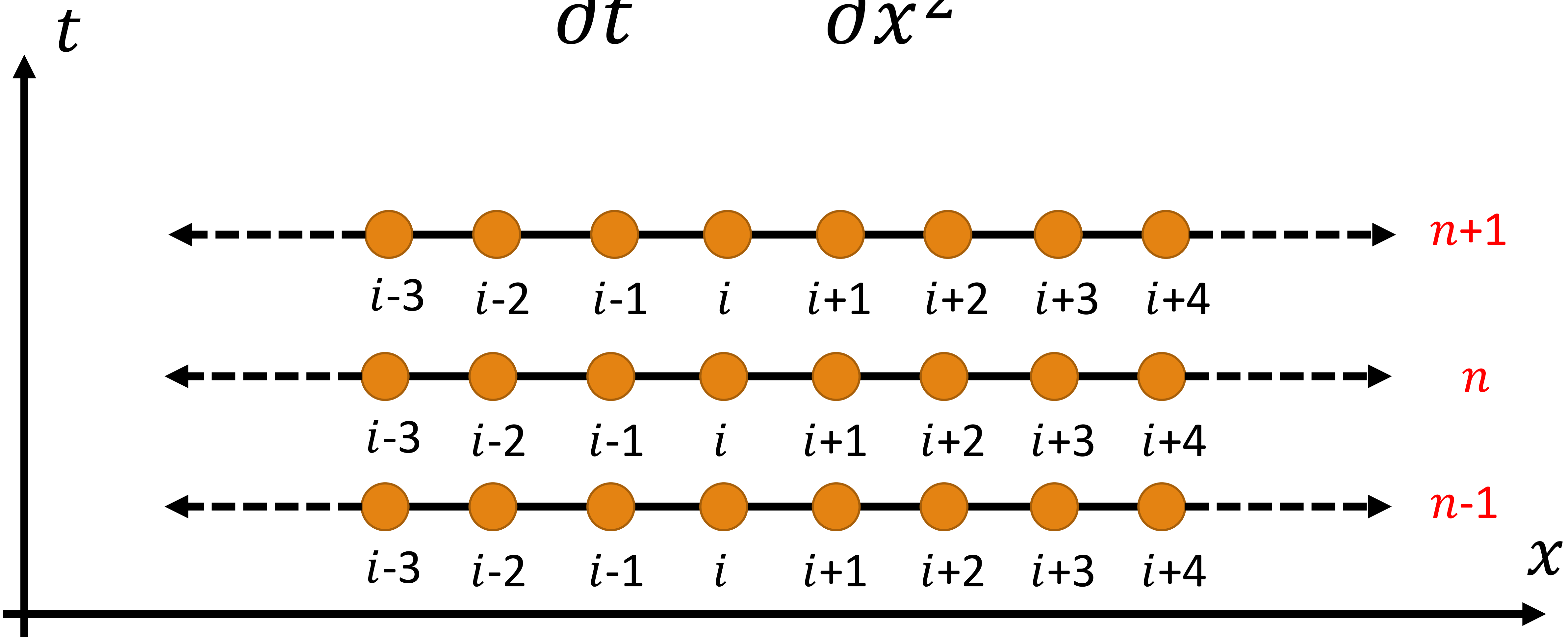
1D Heat Equation



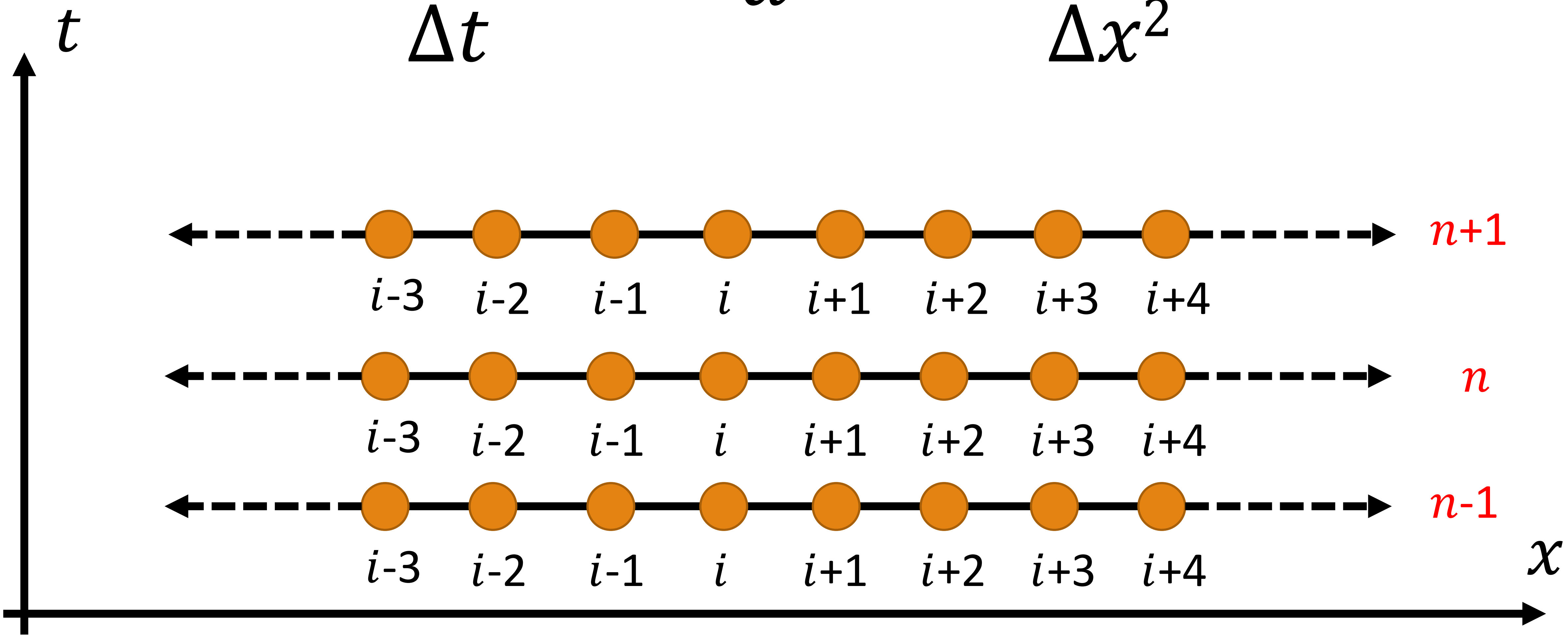
1D Heat Equation



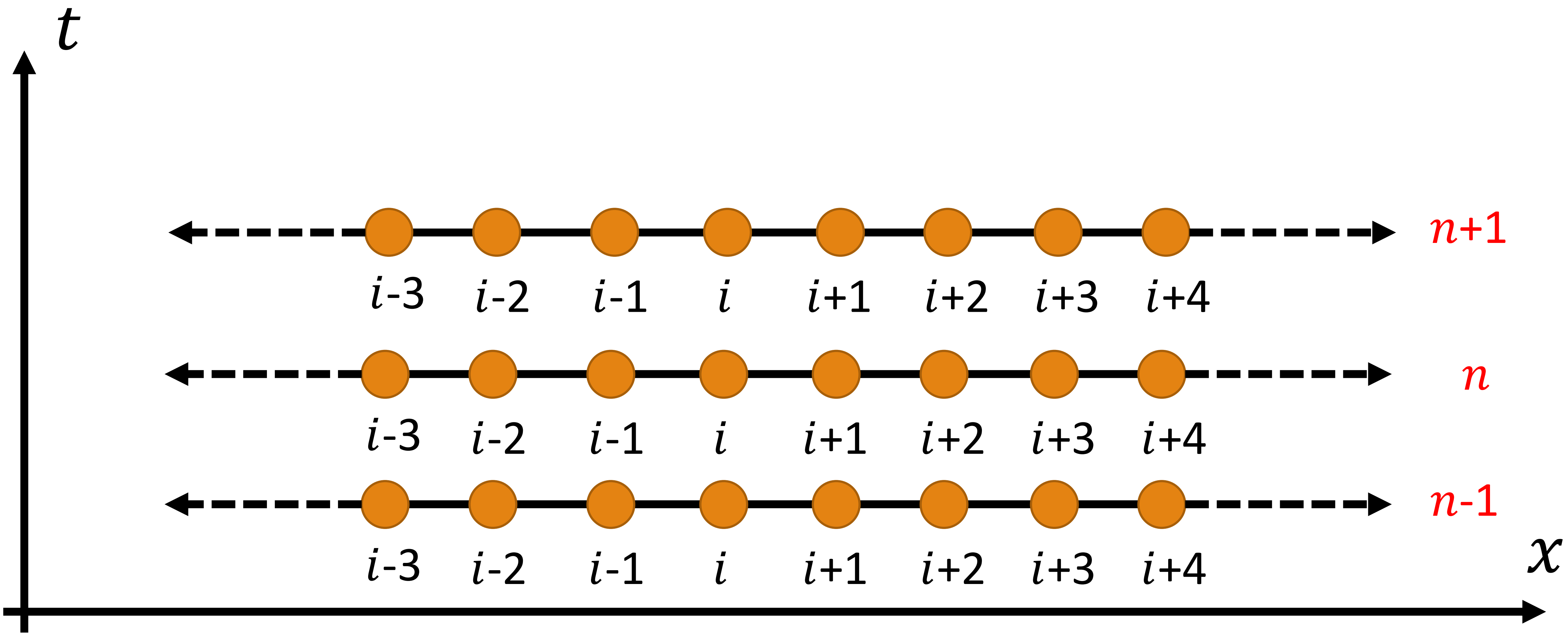
$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$

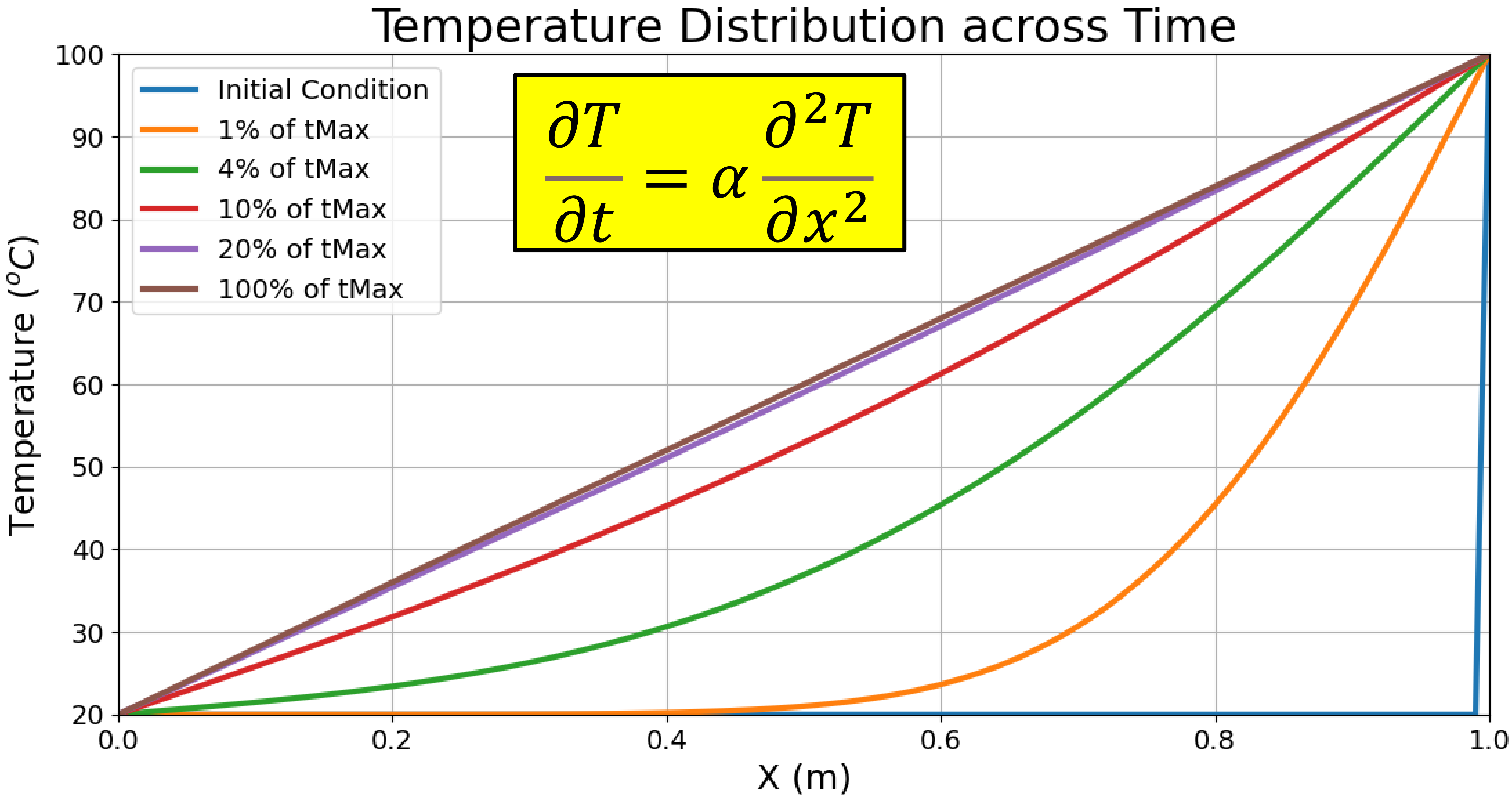


$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$



$$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)$$





Temperature Distribution across Time
Initial Condition
1% of tMax
4% of tMax
10% of tMax
20% of tMax
100% of tMax
$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2}$$
Temperature (^oC)
X (m)
100
90
80
70
60
50
40
30
20
0.0
0.2
0.4
0.6
0.8
1.0

Code Extension

1. Rerun the code with different timestep sizes
2. Replace the second-order accurate spatial scheme with a fourth-order spatial scheme

Explicit vs Implicit Methods

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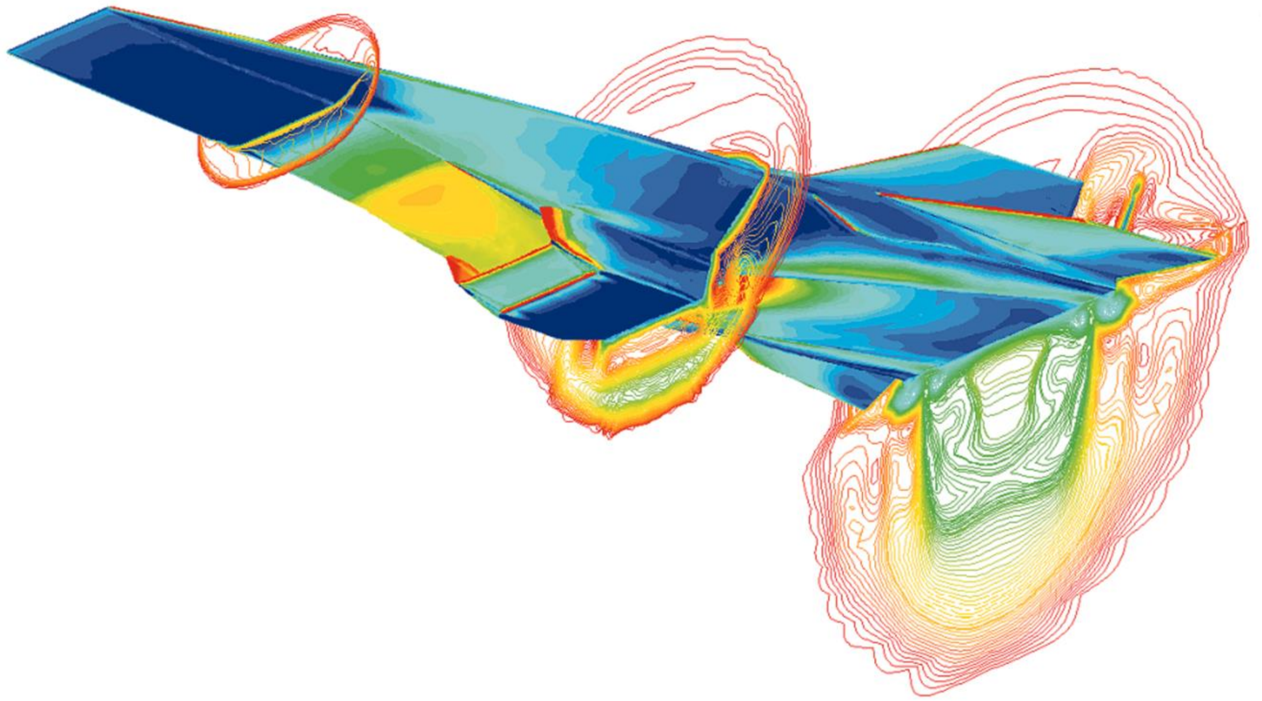
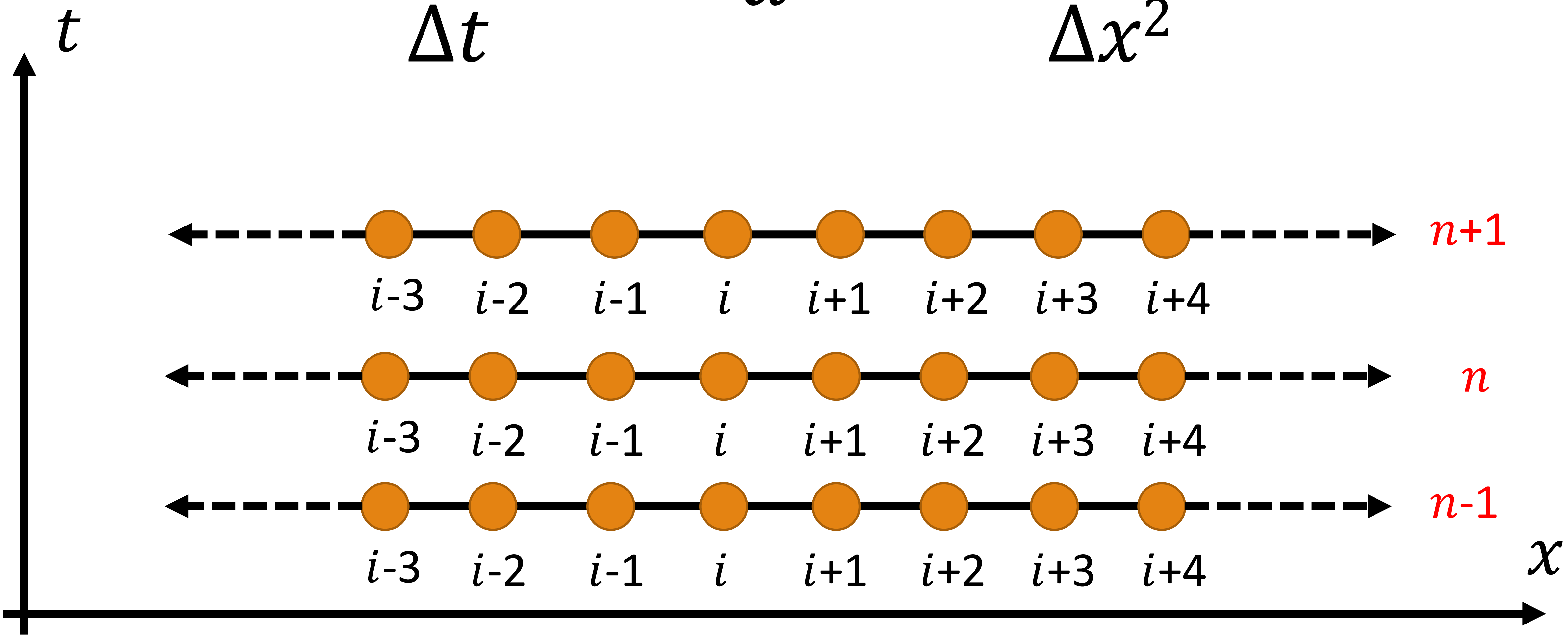
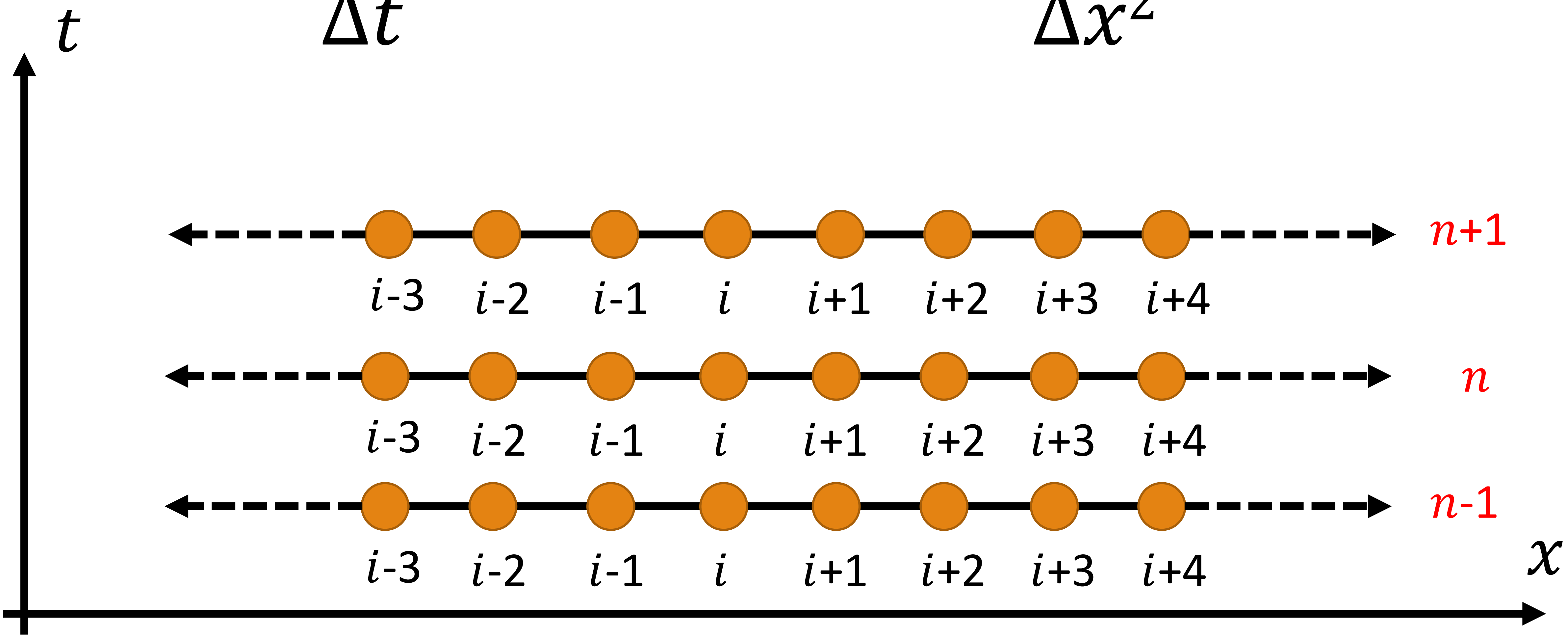


$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$



$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}}{\Delta x^2}$$

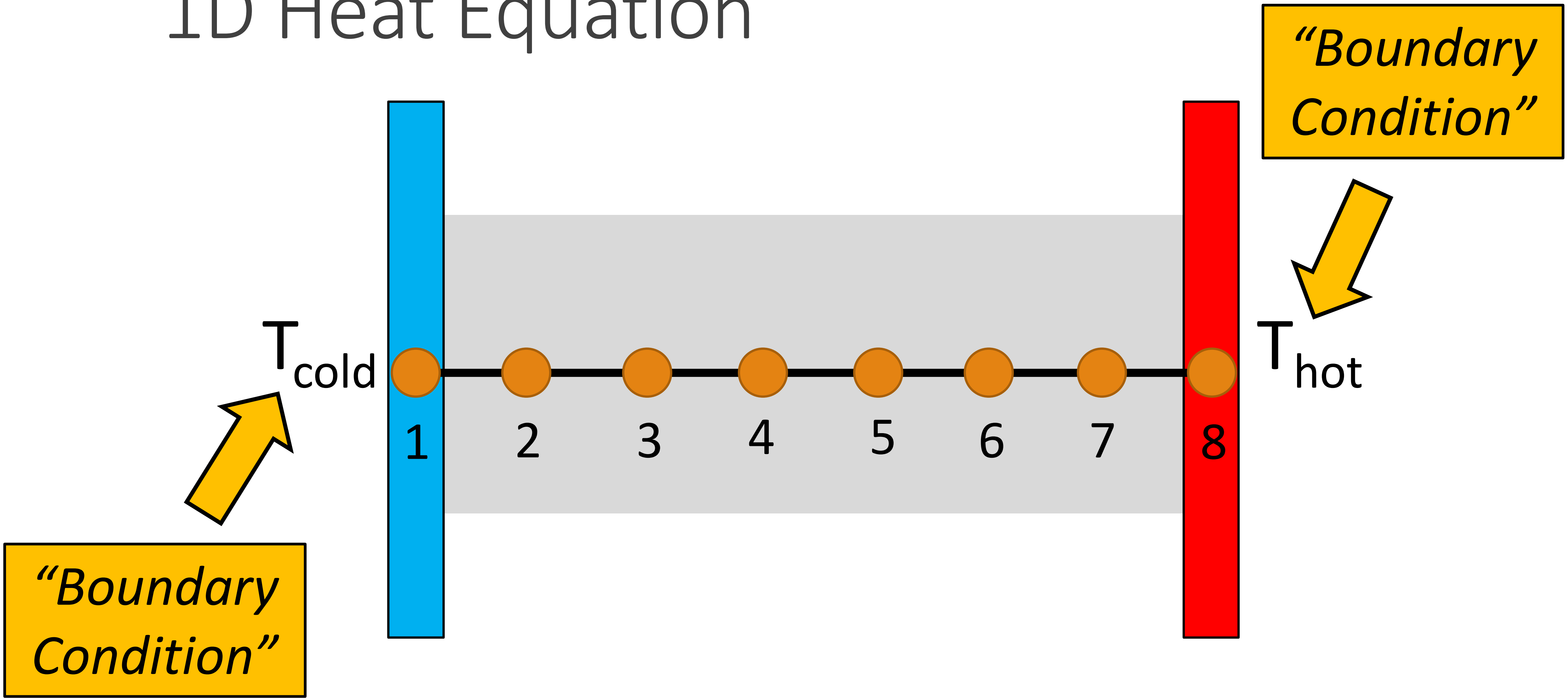


$$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}\right)$$

$$-KT_{i-1}^{n+1} + (1 + 2K)T_i^{n+1} - KT_{i+1}^{n+1} = T_i^n$$

Implicit method updates have multiple '*coupled*' unknowns

1D Heat Equation



$$-KT_{i-1}^{n+1} + (1+2K)T_i^{n+1} - KT_{i+1}^{n+1} = T_i^n$$

When $i = 2$: $-KT_1^{n+1} + (1+2K)T_2^{n+1} - KT_3^{n+1} = T_2^n$

When $i = 3$: $-KT_2^{n+1} + (1+2K)T_3^{n+1} - KT_4^{n+1} = T_3^n$

When $i = 4$: $-KT_3^{n+1} + (1+2K)T_4^{n+1} - KT_5^{n+1} = T_4^n$

When $i = 5$: $-KT_4^{n+1} + (1+2K)T_5^{n+1} - KT_6^{n+1} = T_5^n$

When $i = 6$: $-KT_5^{n+1} + (1+2K)T_6^{n+1} - KT_7^{n+1} = T_6^n$

When $i = 7$: $-KT_6^{n+1} + (1+2K)T_7^{n+1} - KT_8^{n+1} = T_7^n$

$$
\begin{bmatrix}
1+2K & -K & 0 & 0 & 0 & 0 \\
-K & 1+2K & -K & 0 & 0 & 0 \\
0 & -K & 1+2K & -K & 0 & 0 \\
0 & 0 & -K & 1+2K & -K & 0 \\
0 & 0 & 0 & -K & 1+2K & -K \\
0 & 0 & 0 & 0 & -K & 1+2K
\end{bmatrix}
\begin{bmatrix}
T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \\ T_6^{n+1} \\ T_7^{n+1}
\end{bmatrix}
=
\begin{bmatrix}
T_2^{n}+KT_1 \\ T_3^{n} \\ T_4^{n} \\ T_5^{n} \\ T_6^{n} \\ T_7^{n}+KT_8
\end{bmatrix}
$$

Von Neumann Stability

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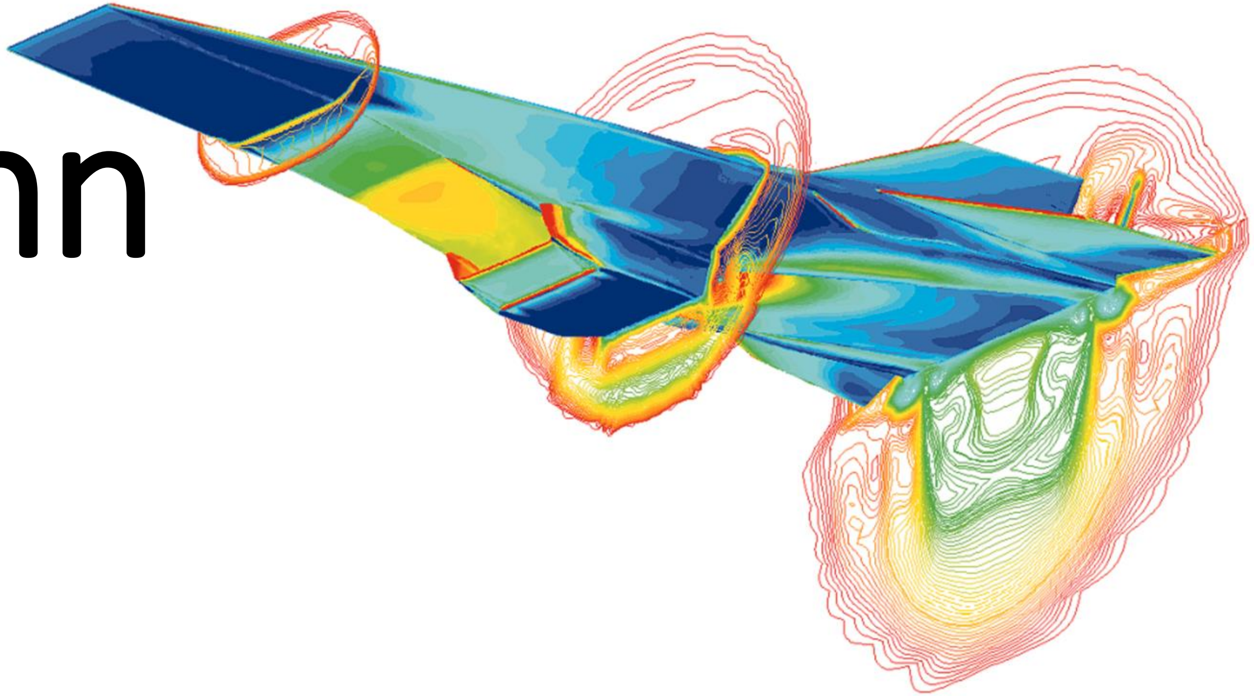


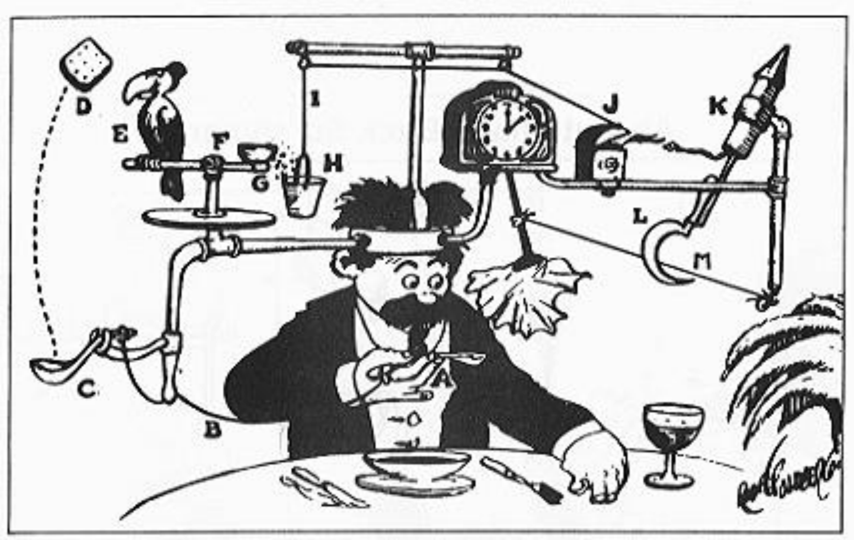
Explicit

$$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)$$

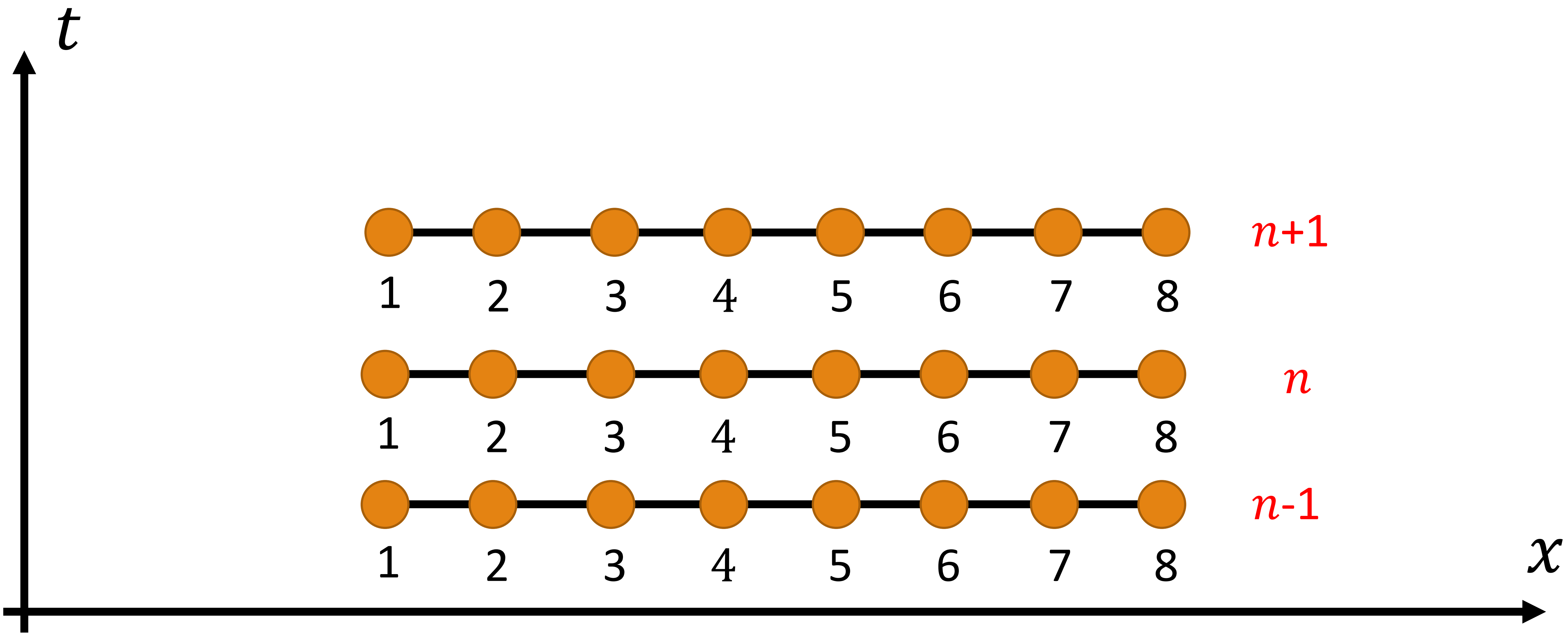
Why go through the effort of creating an implicit scheme when the explicit approach is so much easier?

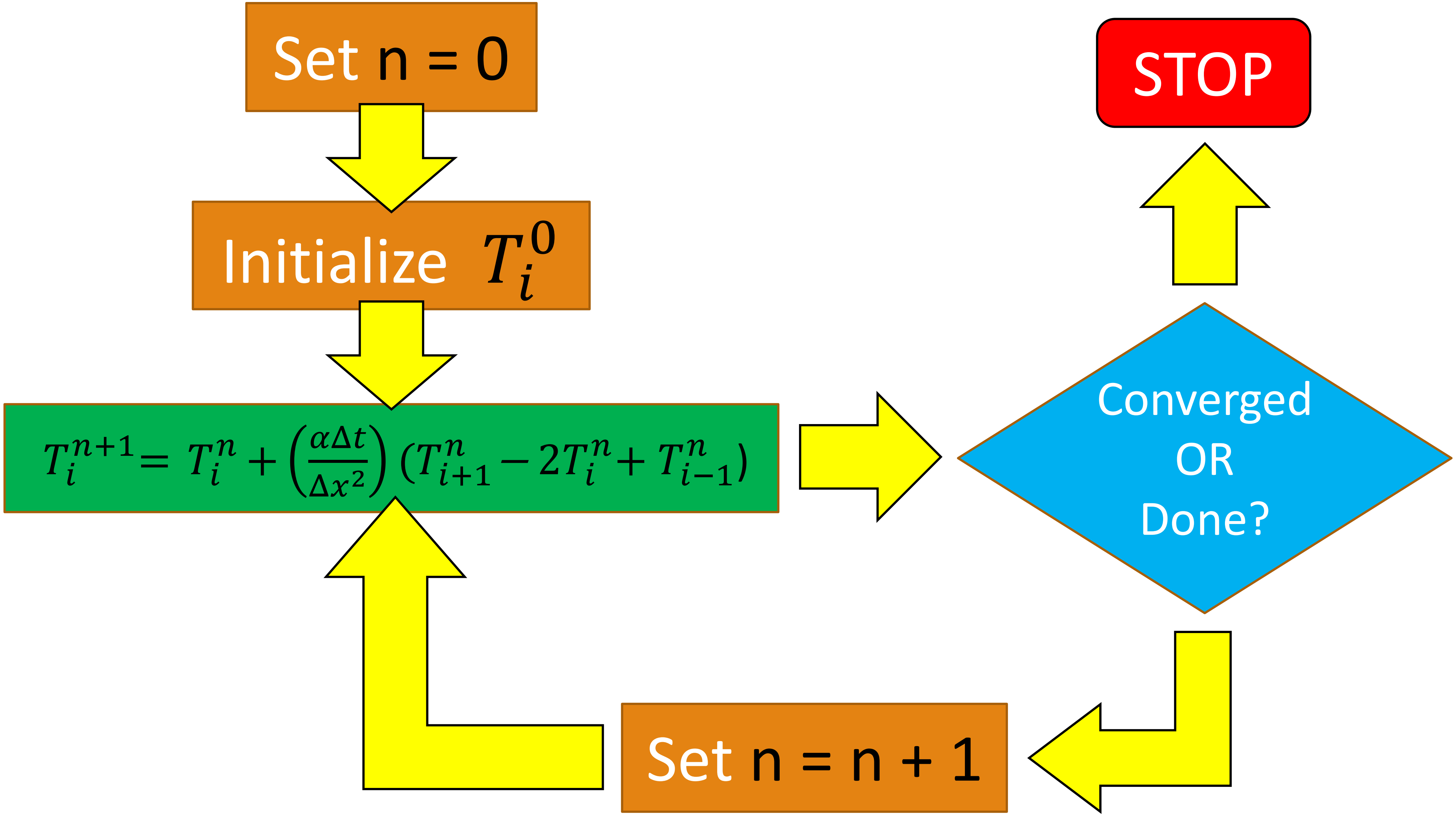
Implicit

$$\begin{bmatrix} 1+2K & -K & 0 & 0 & 0 & 0 \\ -K & 1+2K & -K & 0 & 0 & 0 \\ 0 & -K & 1+2K & -K & 0 & 0 \\ 0 & 0 & -K & 1+2K & -K & 0 \\ 0 & 0 & 0 & -K & 1+2K & -K \\ 0 & 0 & 0 & 0 & -K & 1+2K \end{bmatrix} \begin{bmatrix} T_2^{n+1} \\ T_3^{n+1} \\ T_4^{n+1} \\ T_5^{n+1} \\ T_6^{n+1} \\ T_7^{n+1} \end{bmatrix} = \begin{bmatrix} T_2^n + KT_1 \\ T_3^n \\ T_4^n \\ T_5^n \\ T_6^n \\ T_7^n + KT_8 \end{bmatrix}$$



$$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)$$




Set n = 0
Initialize T_i^0
$T_i^{n+1} = T_i^n + \left(\frac{\alpha \Delta t}{\Delta x^2}\right)\left(T_{i+1}^n - 2T_i^n + T_{i-1}^n\right)$
Converged
OR
Done?
STOP
Set n = n + 1

Recurrence Relations

$$F_{n+2} = F_{n+1} + F_n$$

$$x_{n+1} = r^* x_n(1\text{-}x_n)$$

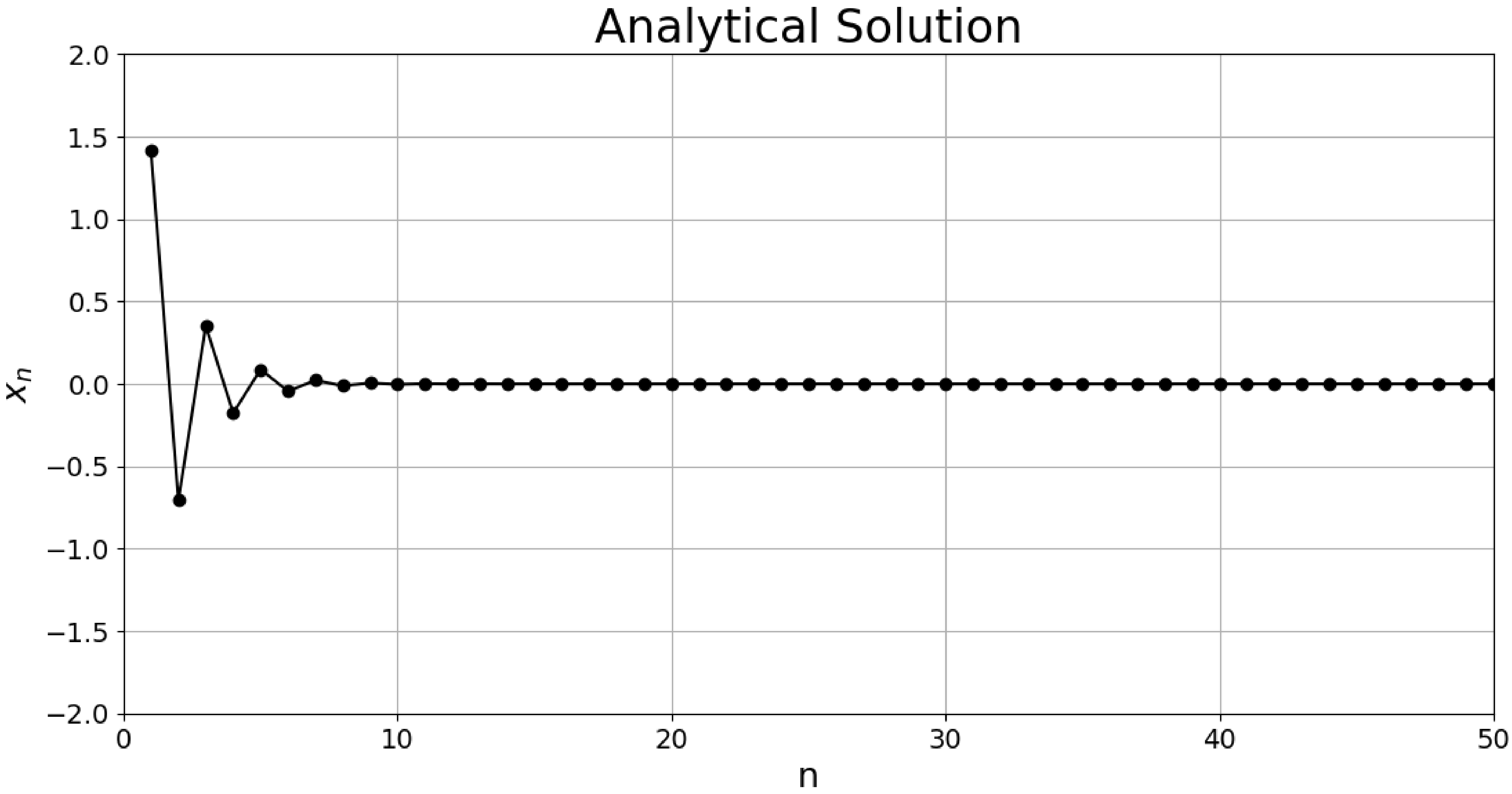
$$x_{n+2} = \frac{5}{2}x_{n+1} + \frac{3}{2}x_n$$

$$x_n = a(-2)^{-n} + b(3)^n$$

$$x_0 = \sqrt{2}$$
$$x_1 = -0.5\sqrt{2}$$

a	$\sqrt{2}$
b	0

$$x_n = \sqrt{2}(-2)^{-n}$$


Analytical Solution
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
x_n
0
10
20
30
40
50
n

Representing a number on a finite precision machine often requires truncation which introduces roundoff error

$$x_{n+2} = \frac{5}{2} x_{n+1} + \frac{3}{2} x_n$$

$$x_n = a(-2)^{-n} + b(3)^n$$

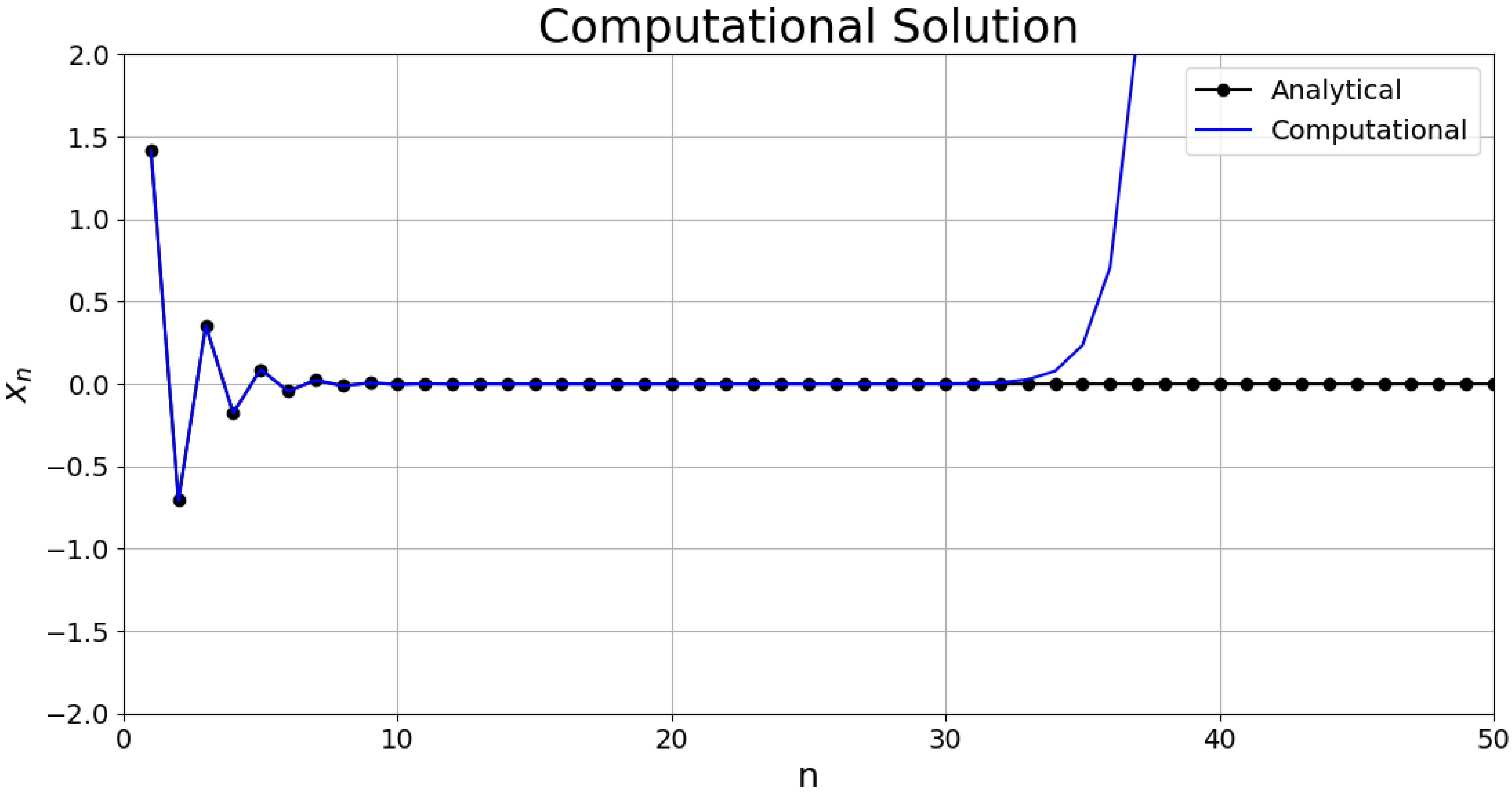
$\sqrt{2}$ = 1.4142135623730950488016887242096980785696718753769480731766797379907324784621…

$$x_0 = \sqrt{2} + \varepsilon_0$$
$$x_1 = -0.5\sqrt{2} + \varepsilon_1$$

$$a(-2)^{-0} + b(3)^0 = \sqrt{2} + \varepsilon_0$$
$$a(-2)^{-1} + b(3)^1 = -0.5\sqrt{2} + \varepsilon_1$$

a	$\left(\sqrt{2}+\varepsilon_0\right)-\left(\frac{\varepsilon_0+2\varepsilon_1}{7}\right)$
b	$\left(\frac{\varepsilon_0+2\varepsilon_1}{7}\right)$

$$x_n = a(-2)^{-n} + b(3)^n$$


Computational Solution
Analytical
Computational
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
10
20
30
40
50
n
x_n

$$\frac{T_i^{n+1} - T_i^n}{\Delta t} = \alpha \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

T	Approximate solution on a machine with finite precision
E	Exact solution of the difference equation
ε	Roundoff error, E - T

$$\frac{(E_i^{n+1} - \varepsilon_i^{n+1}) - (E_i^n - \varepsilon_i^n)}{\Delta t} = \alpha \frac{(E_{i+1}^n - \varepsilon_{i+1}^n) - 2(E_i^n - \varepsilon_i^n) + (E_{i-1}^n - \varepsilon_{i-1}^n)}{\Delta x^2}$$

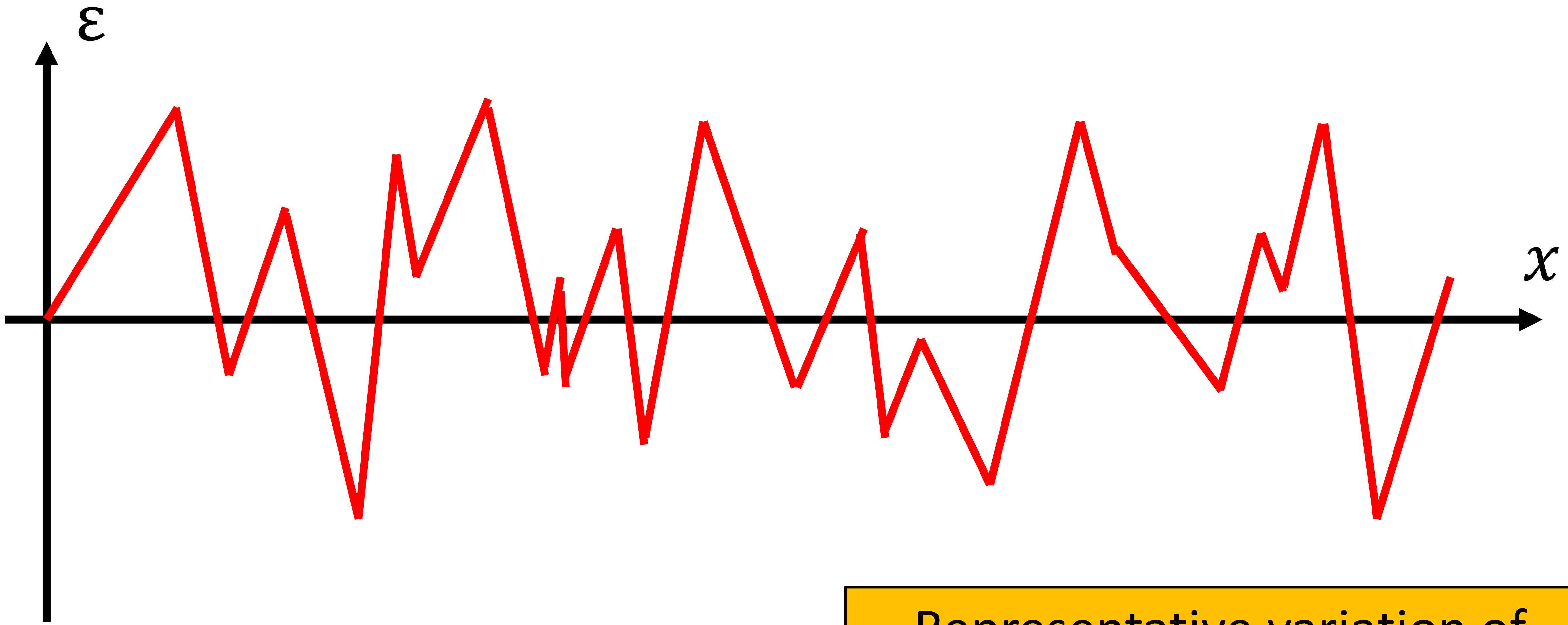
$$\frac{E_i^{n+1} - E_i^n}{\Delta t} - \frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \alpha \frac{E_{i+1}^n - 2E_i^n + E_{i-1}^n}{\Delta x^2} - \alpha \frac{\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n}{\Delta x^2}$$

$\boxed{E}$ Exact solution of the difference equation

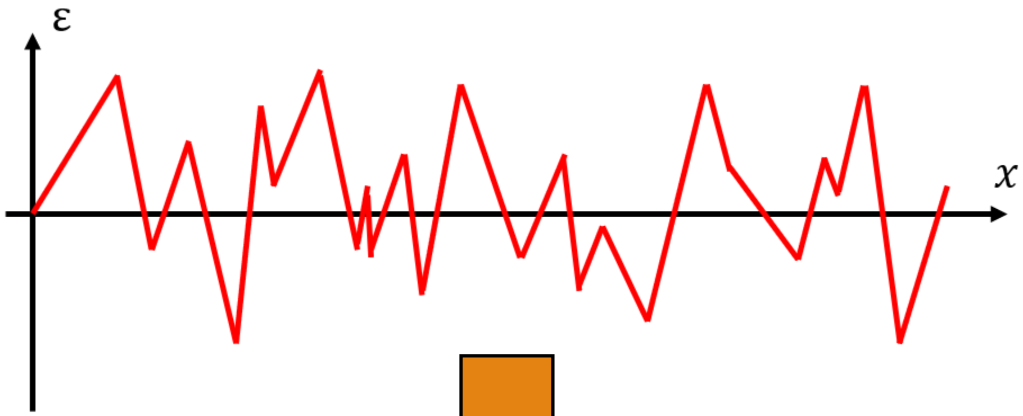
$$\boxed{\frac{E_i^{n+1} - E_i^n}{\Delta t} = \alpha \frac{E_{i+1}^n - 2E_i^n + E_{i-1}^n}{\Delta x^2}}$$

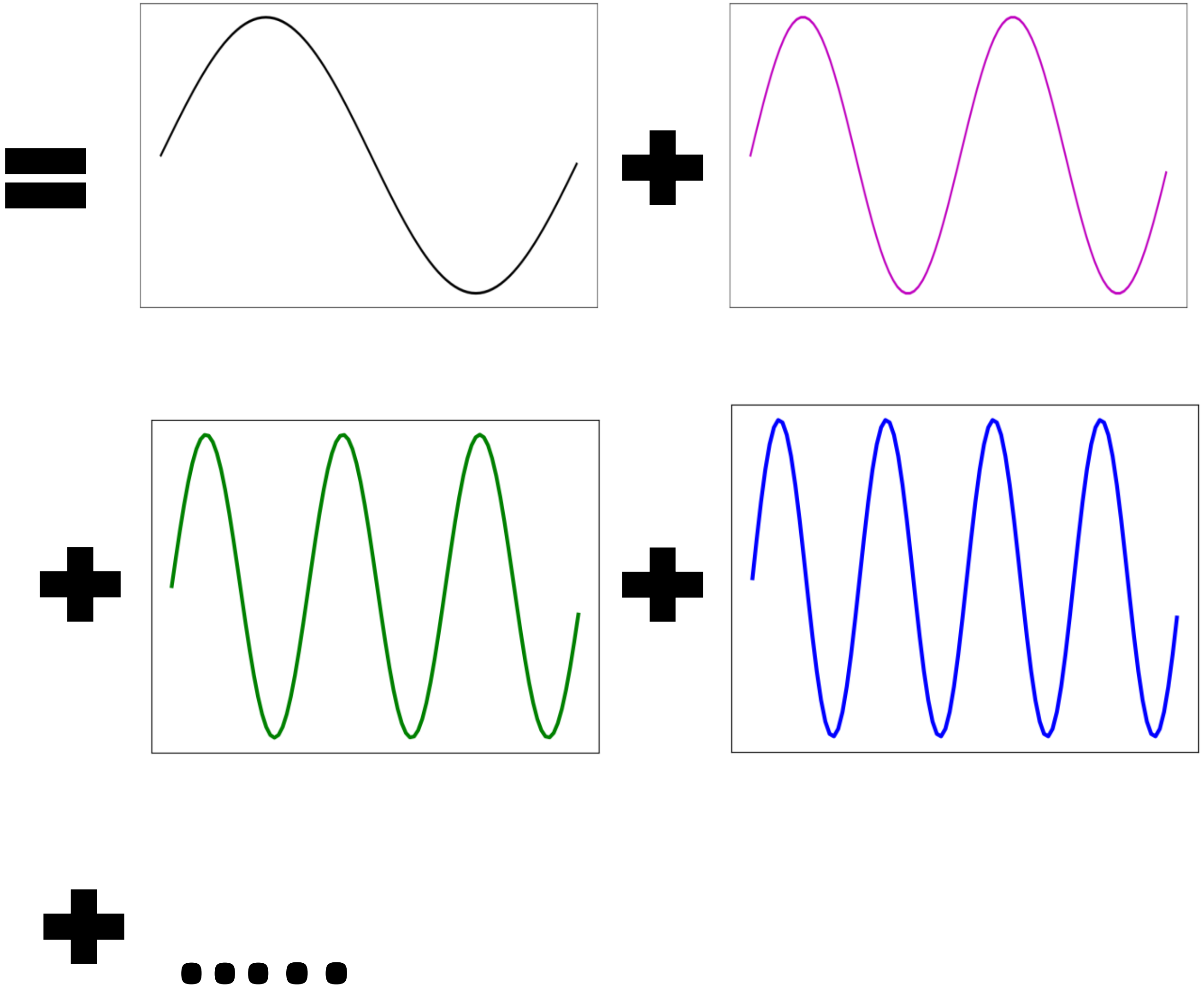
$$\boxed{\frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \alpha \frac{\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n}{\Delta x^2}}$$

The roundoff error satisfies the difference equation!



Representative variation of roundoff error across the mesh





$$\boldsymbol{\varepsilon}^n = \sum_1^{\infty} A_k e^{jkx}$$

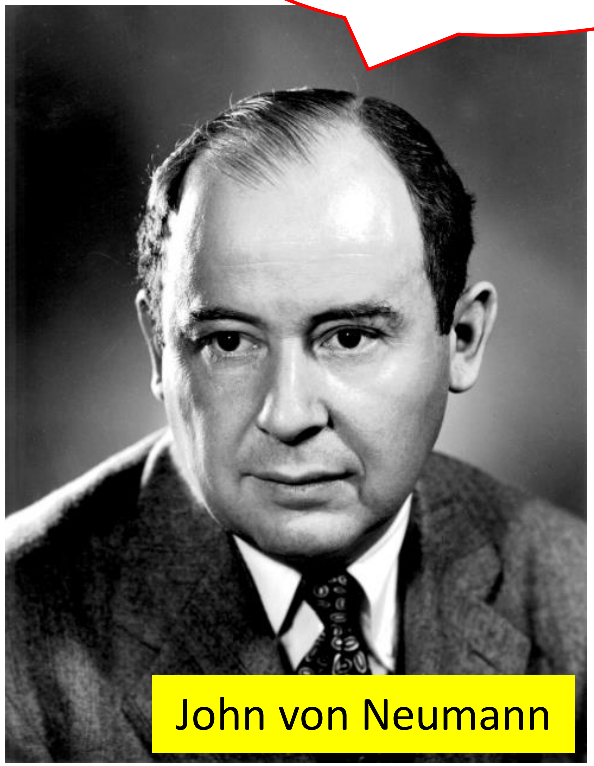
Any variation can be decomposed into an infinite series of sinusoids

$$\varepsilon^n = \sum_1^\infty A_k e^{jkx}$$

$$\varepsilon^n = A_k e^{jkx}$$

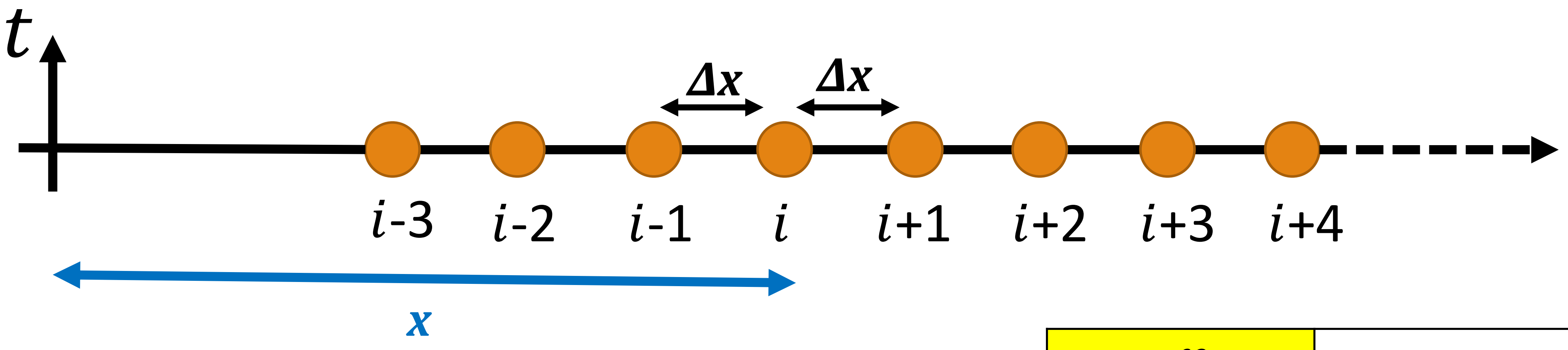
$$\varepsilon^{n+1} = (A_k e^{jkx}) e^{a\Delta t}$$

"Make sure the amplification factor stays below ONE!"



Consider just one component of the Fourier decomposition

$$\boxed{\frac{\varepsilon_i^{n+1} - \varepsilon_i^n}{\Delta t} = \alpha \frac{\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n}{\Delta x^2}}$$



ε_i^n	$A_k e^{jkx}$
ε_{i-1}^n	$A_k e^{jk(x-\Delta x)}$
ε_{i+1}^n	$A_k e^{jk(x+\Delta x)}$
ε_i^{n+1}	$(Ake^{jkx})e^{a\Delta t}$

A straightforward derivation to show that stability requires $(\alpha\Delta t/\Delta x^2) <= 1/2$

Numerical Error

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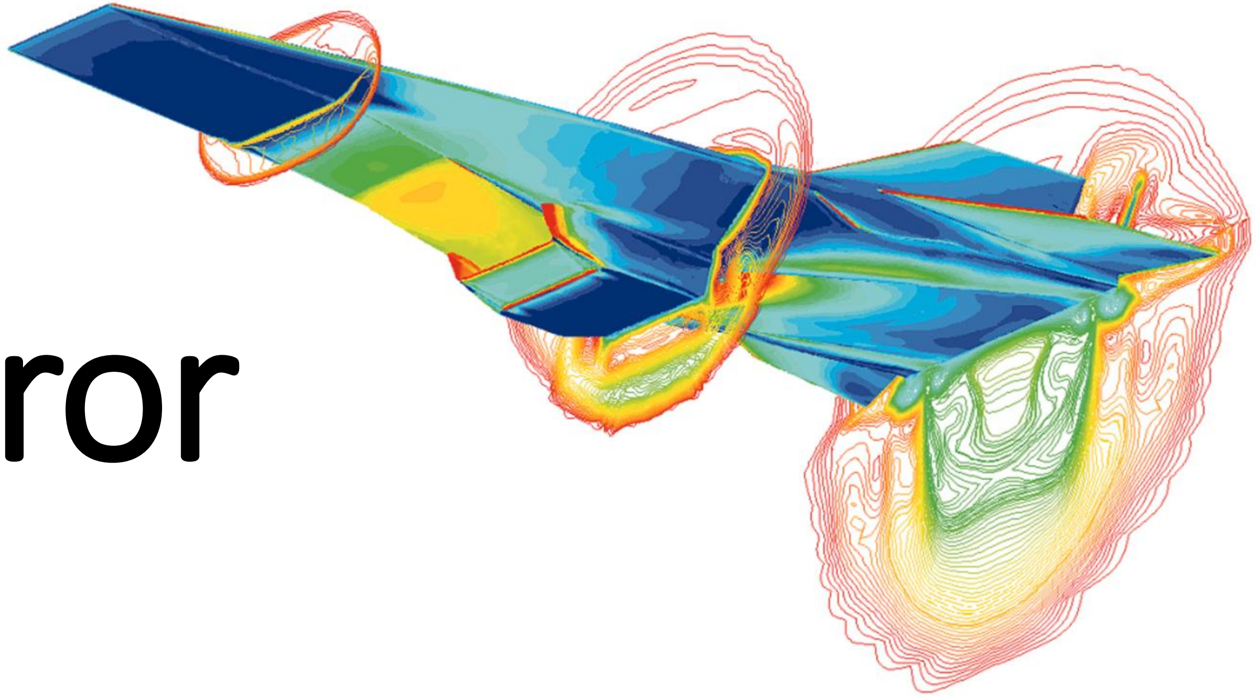
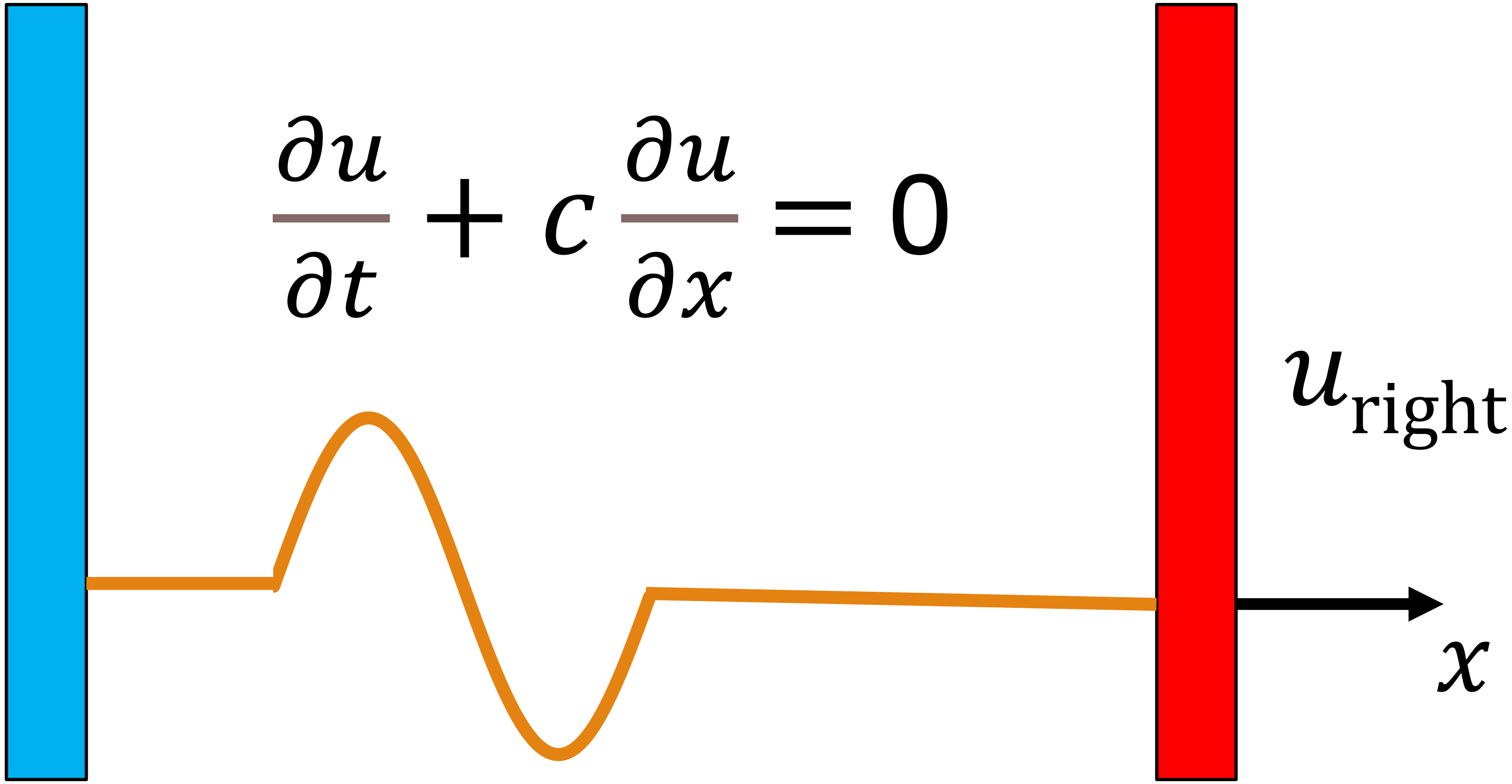


1D (One-Way) Wave Equation

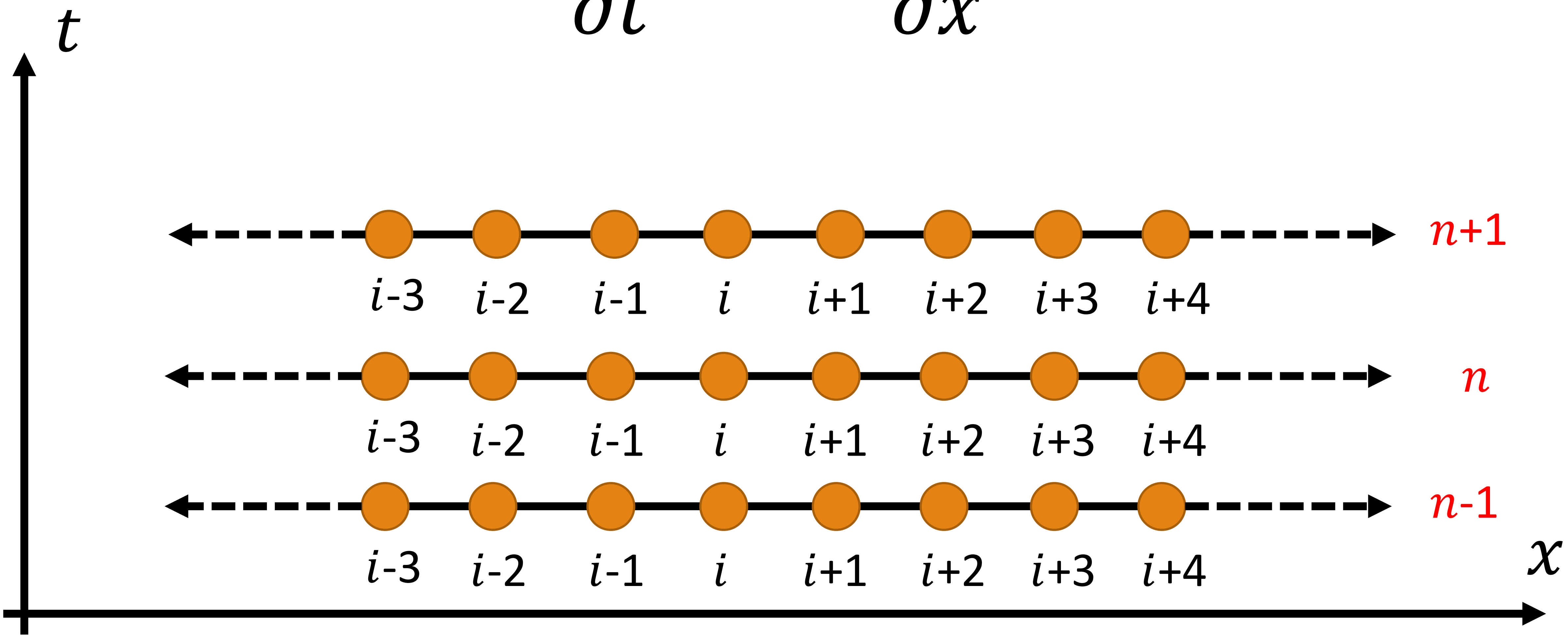
f(x-ct)

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

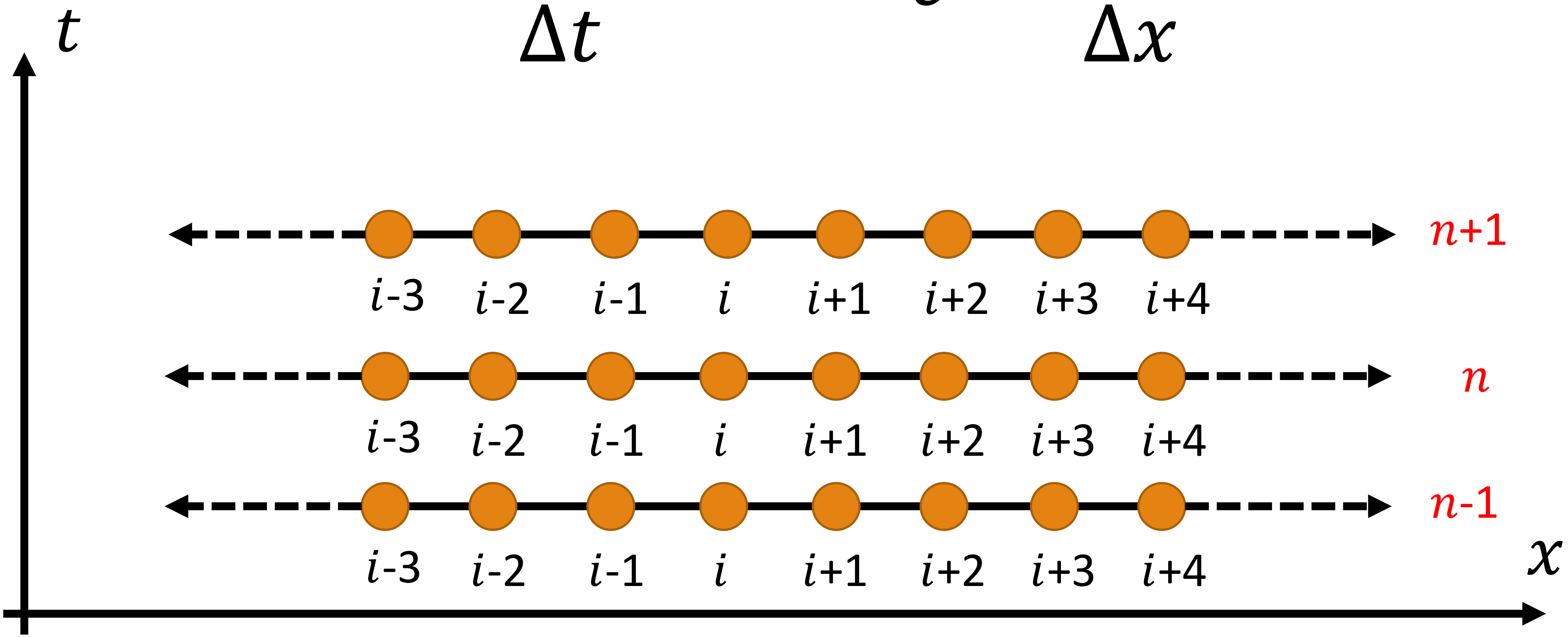
$$u_{\text{left}} = 0 \qquad u_{\text{right}} = 0$$



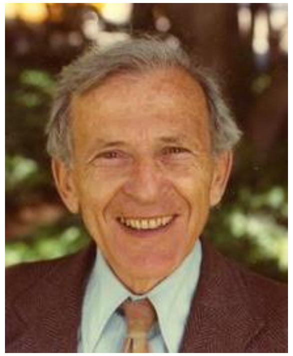
$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}$$



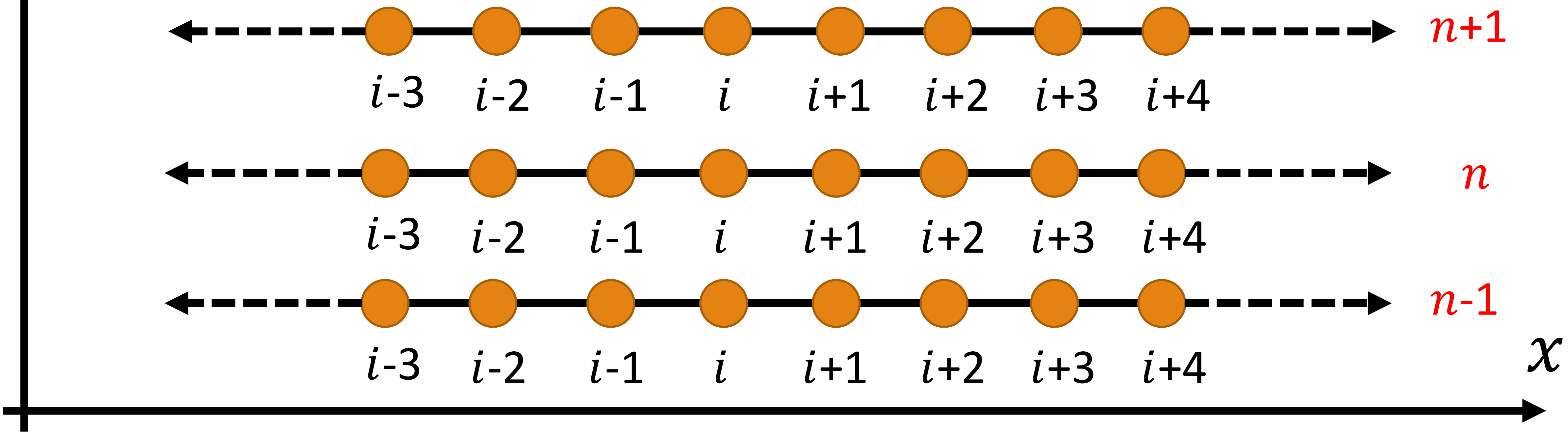
$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c\frac{u_i^n - u_{i-1}^n}{\Delta x}$$



$$u_i^{n+1} = u_i^n - \underbrace{\left(\frac{c\Delta t}{\Delta x}\right)}_{\text{CFL Number}} \left(u_i^n - u_{i-1}^n\right)$$



t



$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c\frac{u_i^n - u_{i-1}^n}{\Delta x}$$

A straightforward derivation to show that stability requires CFL <= 1

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = -c\frac{u_i^n - u_{i-1}^n}{\Delta x}$$

$$u_{i-1}^n = u_i^n - \frac{\partial u}{\partial x}\Delta x + \frac{\partial^2 u}{\partial x^2}\frac{(\Delta x)^2}{2!} - \frac{\partial^3 u}{\partial x^3}\frac{(\Delta x)^3}{3!} + \ldots$$

$$u_i^{n+1} = u_i^n + \frac{\partial u}{\partial t}\Delta t + \frac{\partial^2 u}{\partial t^2}\frac{(\Delta t)^2}{2!} + \frac{\partial^3 u}{\partial t^3}\frac{(\Delta t)^3}{3!} + \ldots$$

$$\boxed{\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}}$$

Equation we set out to solve

$$\boxed{\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + c\frac{\partial^2 u}{\partial x^2}\frac{(\Delta x)}{2!}(1 - \mathrm{CFL})}$$

Equation we are *actually* solving (i.e the modified equation)

$$\frac{\partial u}{\partial t} = -c\,\frac{\partial u}{\partial x} + c\,\frac{\partial^2 u}{\partial x^2}\frac{(\Delta x)}{2!}(1\text{-CFL})$$

Assume solution is summation of terms like $(A_k e^{jk\mathbf{x}})e^{\alpha t}$

$$\alpha(A_k e^{jk\mathbf{x}})e^{\alpha t} = -cjk(A_k e^{jk\mathbf{x}})e^{\alpha t} + c(jk)^2(A_k e^{jk\mathbf{x}})e^{\alpha t}\,\frac{(\Delta x)}{2!}(1 - CFL)$$

$$\alpha = -cjk\ - ck^2\frac{(\Delta x)}{2!}(1 - CFL)$$

$$\mathrm{u(x,t)} = A_k e^{jk(\mathbf{x}\text{-}ct)}\mathrm{e}^{-(1-\mathrm{CFL})(ck^2)\Delta x/2}$$

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + R\frac{\partial^n u}{\partial x^n}$$

Assume solution is summation of terms like $(A_k e^{jk\mathbf{x}})e^{\alpha t}$

$$\alpha(A_k e^{jk\mathbf{x}})e^{\alpha t} = -cjk(A_k e^{jk\mathbf{x}})e^{\alpha t} + R(jk)^n(A_k e^{jk\mathbf{x}})e^{\alpha t}$$

$$\alpha = -cjk + R(jk)^n$$

$$\mathrm{u}(\mathrm{x},\mathrm{t}) = A_k \mathrm{e}^{jk(x-[c\pm(Rk^{\mathrm{n}})]t)}$$

$$\mathrm{u}(\mathrm{x},\mathrm{t}) = A_k e^{jk(\mathbf{x}-ct)}\mathrm{e}^{\pm(Rk^{\mathrm{n}})}$$

Wave speeds are going to be 'wrong'
(*DISPERSIVE* ERROR)

$$\alpha = -cjk + R(jk)^n$$

$$u(x,t) = A_k e^{jk(x-[c\pm(Rk^n)]t)}$$

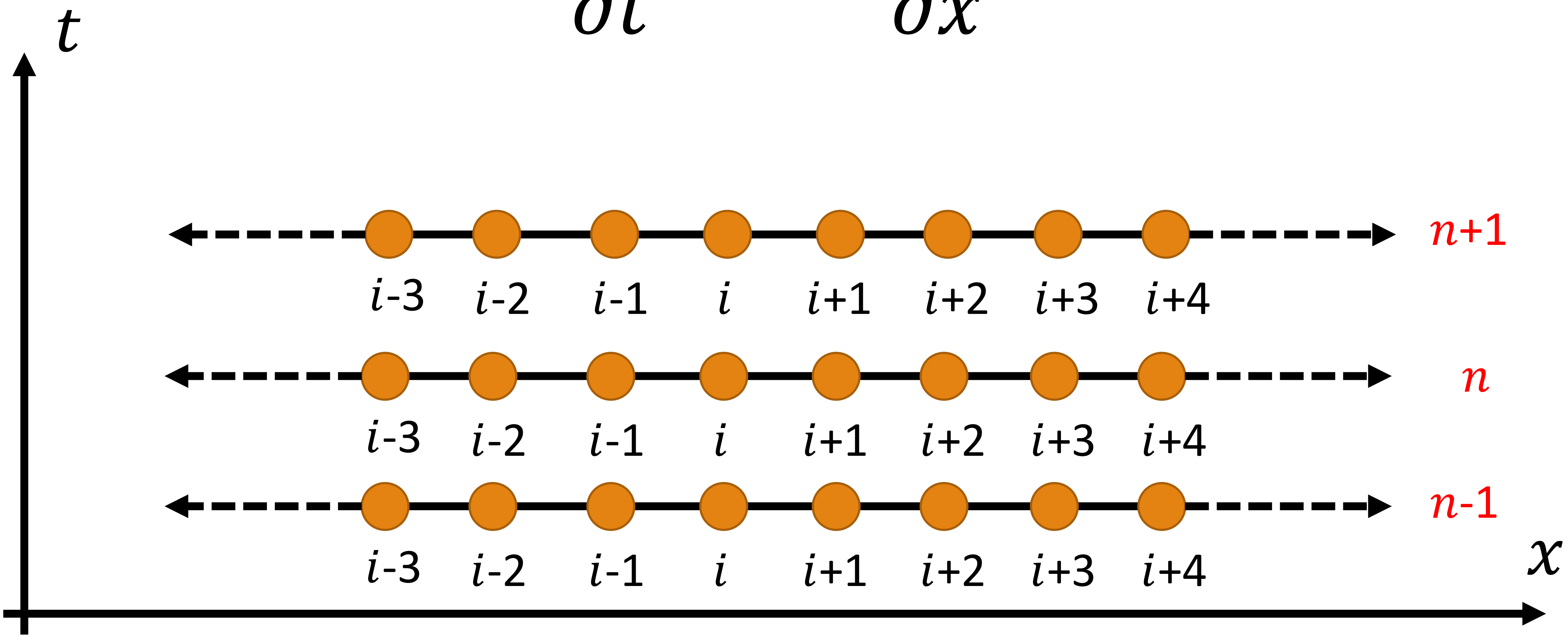
$$u(x,t) = A_k e^{jk(x\text{-}ct)} e^{\pm(Rk^n)}$$

Wave amplitudes are going to be 'wrong'
(*DISSIPATIVE* ERROR)

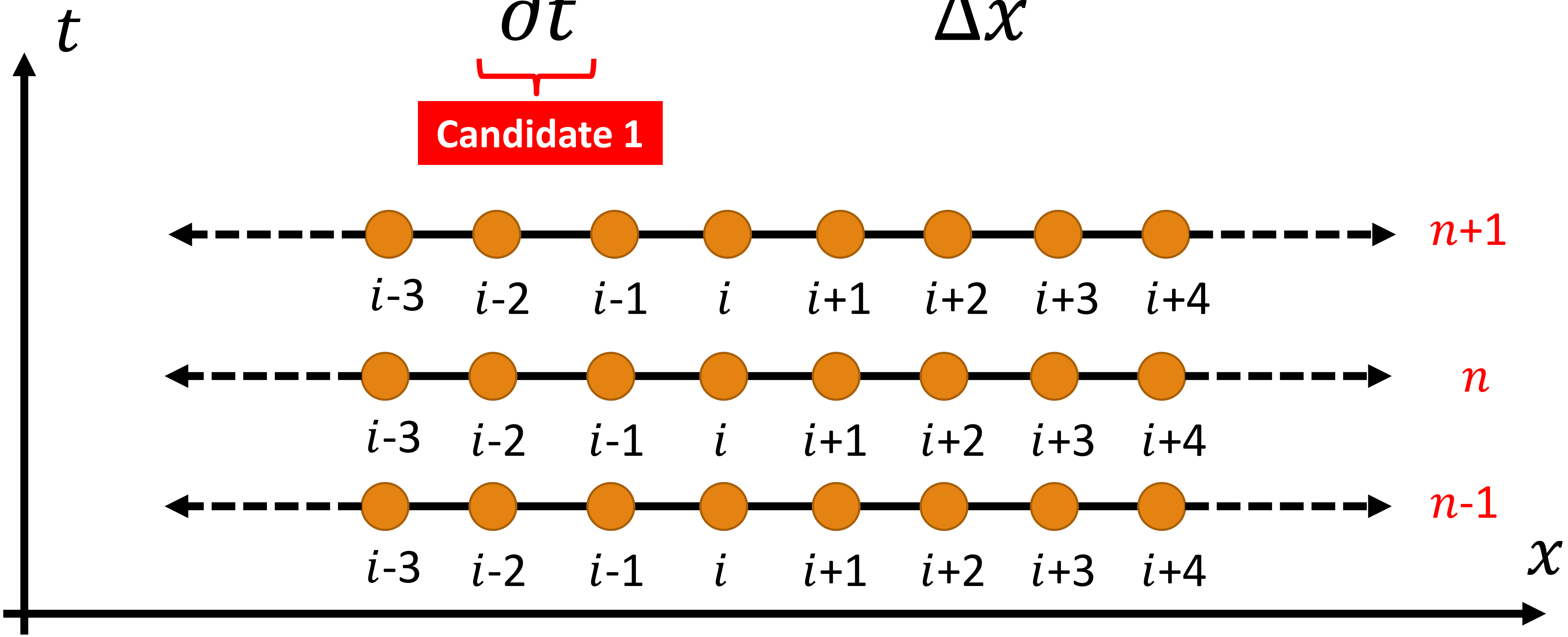
MacCormack's Method

An example of a predictor-corrector method that produces 'dispersive error'

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x}$$

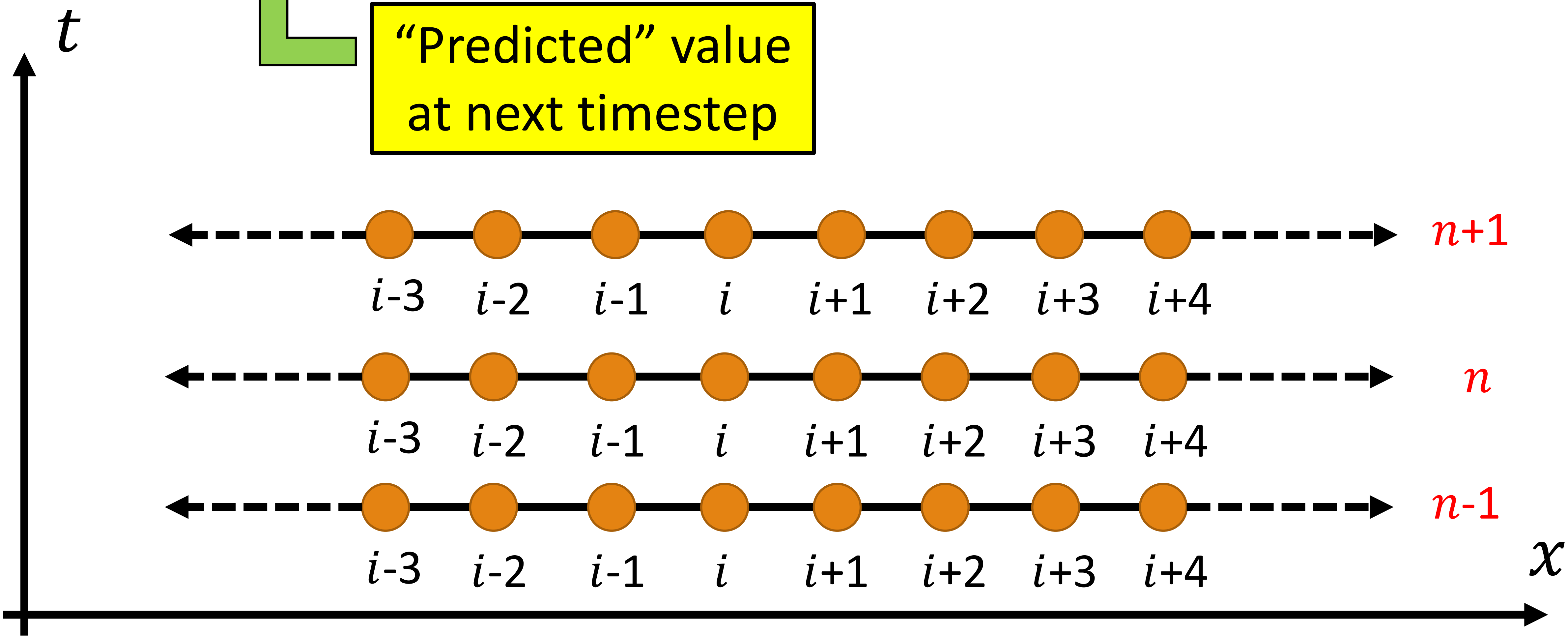


$$\underbrace{\frac{\partial u}{\partial t}}_{\text{Candidate 1}} = -c\,\frac{u_i^n - u_{i-1}^n}{\Delta x}$$

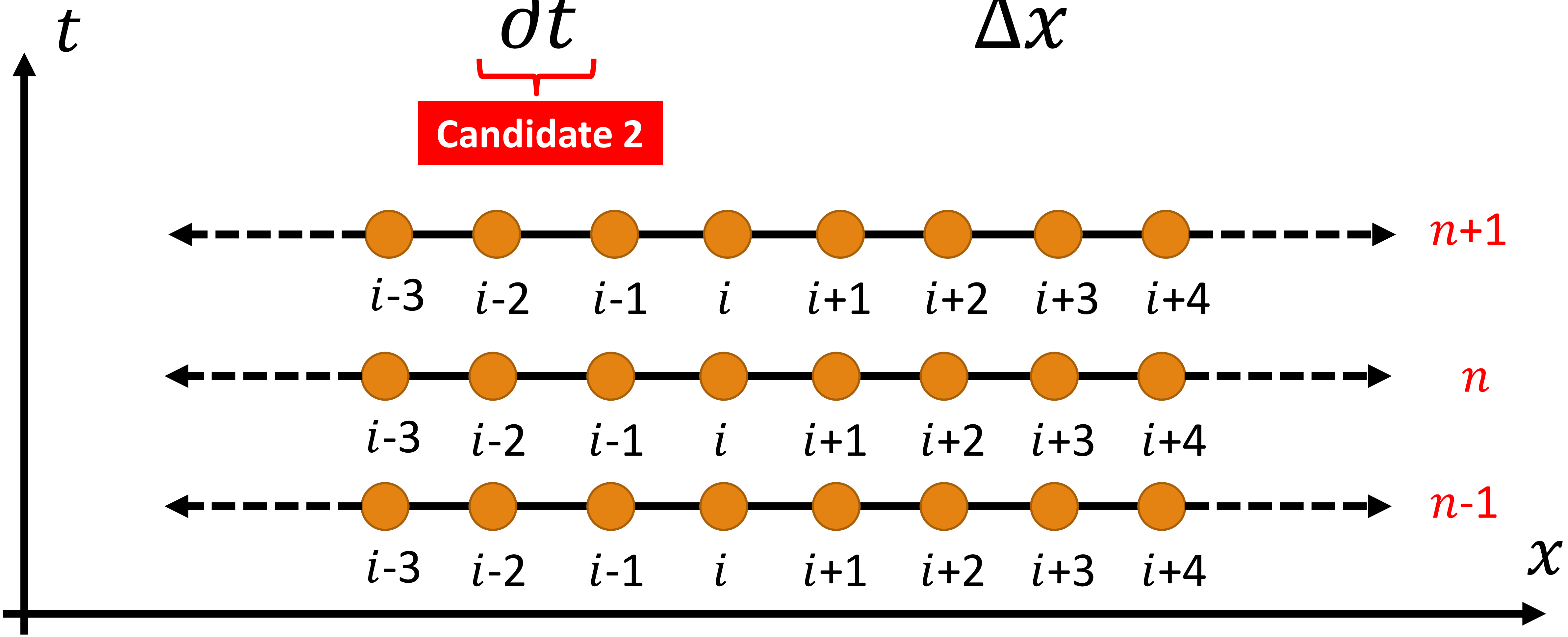


$$\tilde{u}_i^{n+1} = u_i^n - \left(\frac{c\Delta t}{\Delta x}\right)\left(u_i^n - u_{i-1}^n\right)$$

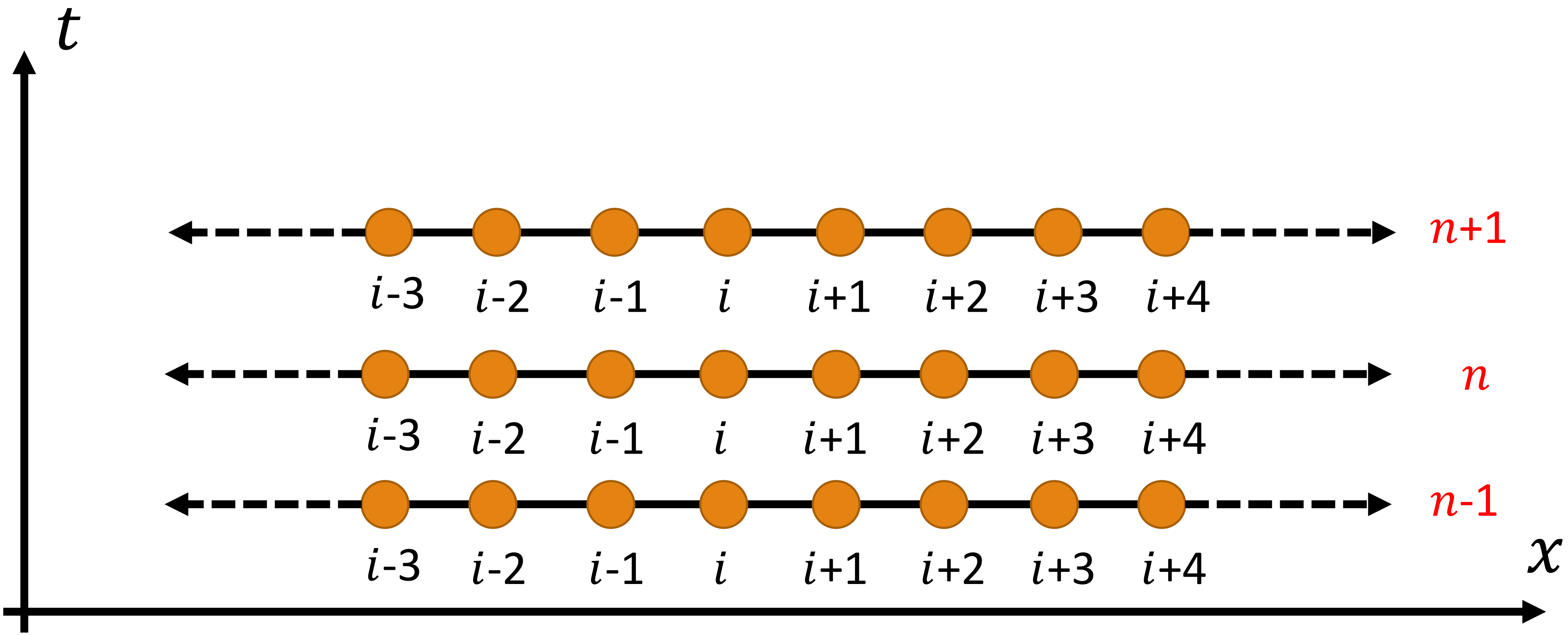
"Predicted" value at next timestep



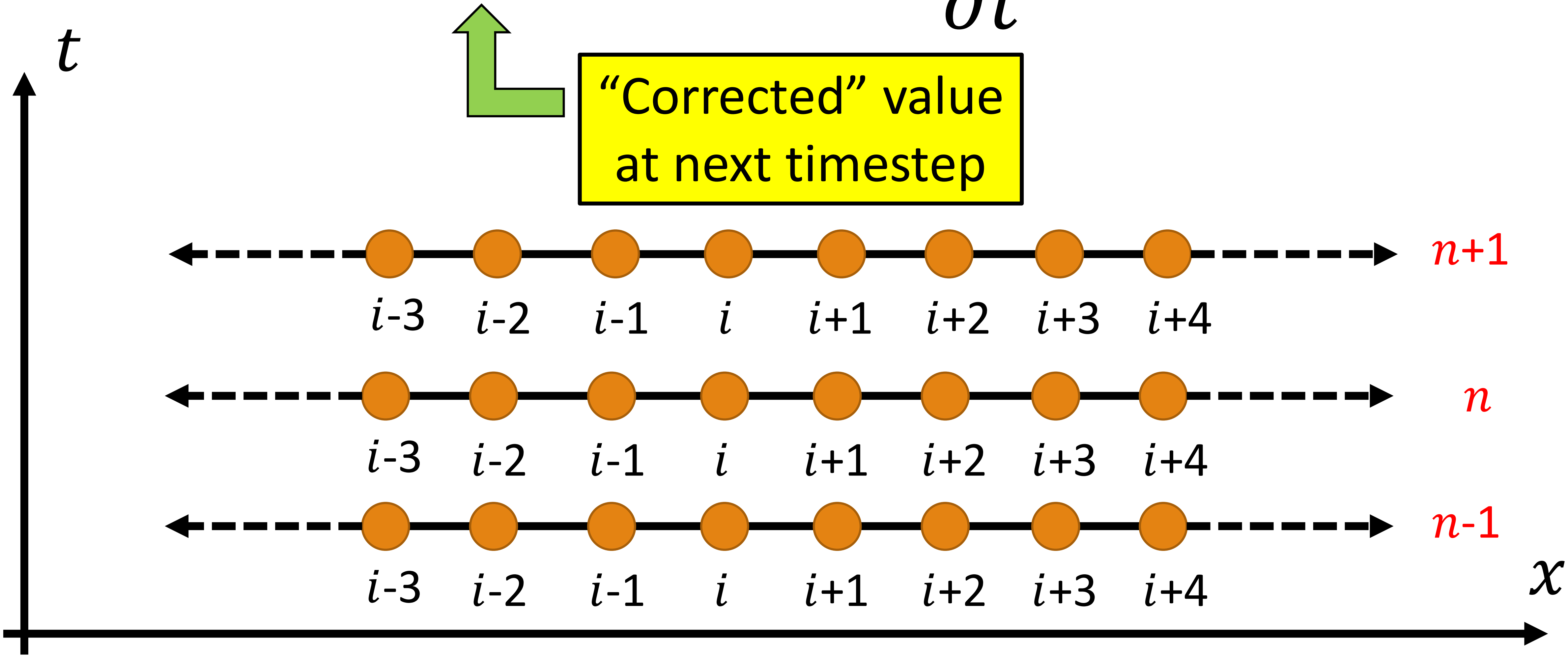
$$\underbrace{\frac{\partial u}{\partial t}}_{\text{Candidate 2}} = -c\,\frac{\tilde{u}_{i+1}^{n+1} - \tilde{u}_{i}^{n+1}}{\Delta x}$$



$$\left(\frac{\partial u}{\partial t}\right)_{\mathrm{av}} = \frac{1}{2}\left\{\left(\frac{\partial u}{\partial t}\right)_{\mathrm{c1}} + \left(\frac{\partial u}{\partial t}\right)_{\mathrm{c2}}\right\}$$



$$u_i^{n+1} = u_i^n + \left(\frac{\partial u}{\partial t}\right)_{\text{av}} \Delta t$$



$$u_i^{n+1} = u_i^n + \left(\frac{\partial u}{\partial t}\right)_{\mathrm{av}} \Delta t$$

$$\frac{1}{2}\left\{\left(\frac{\partial u}{\partial t}\right)_{\mathrm{c1}} + \left(\frac{\partial u}{\partial t}\right)_{\mathrm{c2}}\right\}$$

$$-c\,\frac{u_i^n - u_{i-1}^n}{\Delta x}$$

$$-c\,\frac{\tilde{u}_{i+1}^{n+1} - \tilde{u}_i^{n+1}}{\Delta x}$$

$$\tilde{u}_i^{n+1} = u_i^n - \left(\frac{c\Delta t}{\Delta x}\right)\left(u_i^n - u_{i-1}^n\right)$$

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \frac{c(\Delta x)^2}{6}\frac{\partial^3 u}{\partial x^3} - \frac{c^3(\Delta t)^2}{6}\frac{\partial^3 u}{\partial x^3} + \text{H.O.T}$$

MacCormack's method is second order accurate in time and space!

$$\frac{\partial u}{\partial t} = -c\frac{\partial u}{\partial x} + \frac{c(\Delta x)^2}{6}\frac{\partial^3 u}{\partial x^3}\left[1 - (CFL)^2\right] + \text{H.O.T}$$

Dispersive quality of MacCormack will vanish when CFL = 1