

2nd-order derivative: $\frac{\partial^2 T}{\partial x^2}$

3-point formula

$$a T_{j-1}'' + b T_j'' + c T_{j+1}'' = (a + b + c) T_j'' + (-a + c) \frac{\partial T}{\partial x}(x_j, t_n) \Delta x + (a + c) \frac{\partial^2 T}{\partial x^2}(x_j, t_n) \frac{\Delta x^2}{2} + (-a + c) \frac{\partial^3 T}{\partial x^3}(x_j, t_n) \frac{\Delta x^3}{6} + O(\Delta x^4)$$

when $a = c = \frac{1}{2}, b = 0 \Rightarrow$

$$\frac{\partial^2 T}{\partial x^2}(x_j, t_n) = \frac{T_{j+1}'' - 2 T_j'' + T_{j-1}''}{\Delta x^2} + O(\Delta x^2)$$

... Centered-difference method (2nd-order approximation)

First-order derivative: $\frac{\partial T}{\partial x}(x_j, t_n)$

<i>Discretization method</i>	<i>Algebraic formula</i>	<i>Truncation error (leading term)</i> $T_{xx} = \frac{\partial^2 T}{\partial x^2}$
forward difference	$\frac{T_{j+1}^n - T_j^n}{\Delta x}$	$\frac{\Delta x}{2} T_{xx} + \dots$
backward difference	$\frac{T_j^n - T_{j-1}^n}{\Delta x}$	$-\frac{\Delta x}{2} T_{xx} + \dots$
3 point centered difference	$\frac{T_{j+1}^n - T_{j-1}^n}{2 \Delta x}$	$\frac{\Delta x^2}{6} T_{xxx} + \dots$
5 point centered difference	$\frac{-T_{j+2}^n + 8T_{j+1}^n - 8T_{j-1}^n + T_{j-2}^n}{12 \Delta x}$	$-\frac{\Delta x^4}{30} T_{xxxx} + \dots$

Second-order derivative: $\frac{\partial^2 T}{\partial x^2}(x_j, t_n)$

<i>Discretization method</i>	<i>Algebraic formula</i>	<i>Truncation error (leading term)</i> $T_{xx} = \frac{\partial^2 T}{\partial x^2}$
3 point centered difference	$\frac{T_{j+1}^n - 2 T_j^n + T_{j-1}^n}{\Delta x^2}$	$\frac{\Delta x^2 T_{xxxx}}{12} + \dots$
5 point centered difference	$\frac{-T_{j+2}^n + 16 T_{j+1}^n - 30 T_j^n + 16 T_{j-1}^n - T_{j-2}^n}{12 \Delta x^2}$	$-\frac{\Delta x^4 T_{xxxxx}}{90} + \dots$

High-order approximation
vs.
Low-order approximation

Should we always use high-order approximation?

→ Answer is **"No"**.

Two reasons:

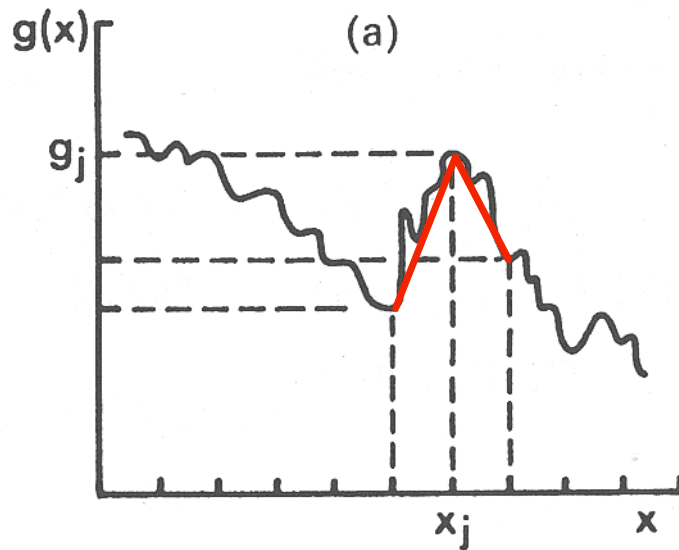
High-order approximation

=> needs **more grid-point information** than low-order approximation to convert differential to difference (**less economical**)

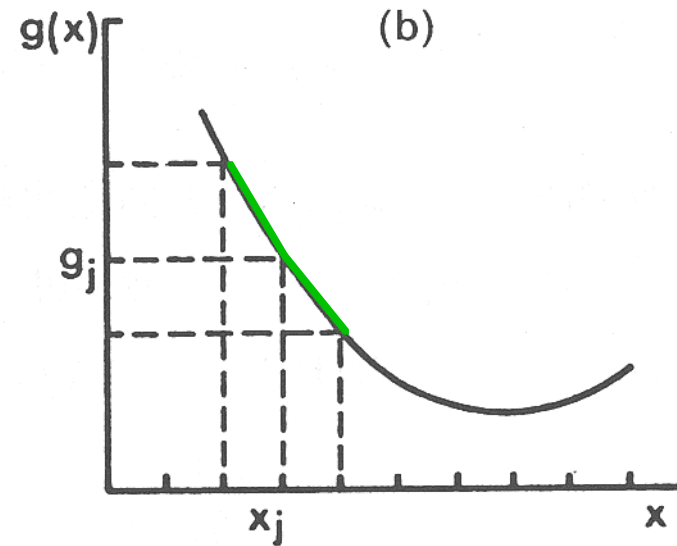
=> needs **more calculation steps** than low-order approximation, while having little advantage in accuracy when small grid spacing is used (**less efficient**)

↑ accumulate round error

Selection of appropriate grid spacing is important...



Bad selection
(smaller grid spacing is necessary)



Good selection
(grid spacing is appropriate)

Vectorization

High-speed calculation technique I

What is "vectorization"?

1-dimensional array

$$c_1 = a_1 + b_1$$

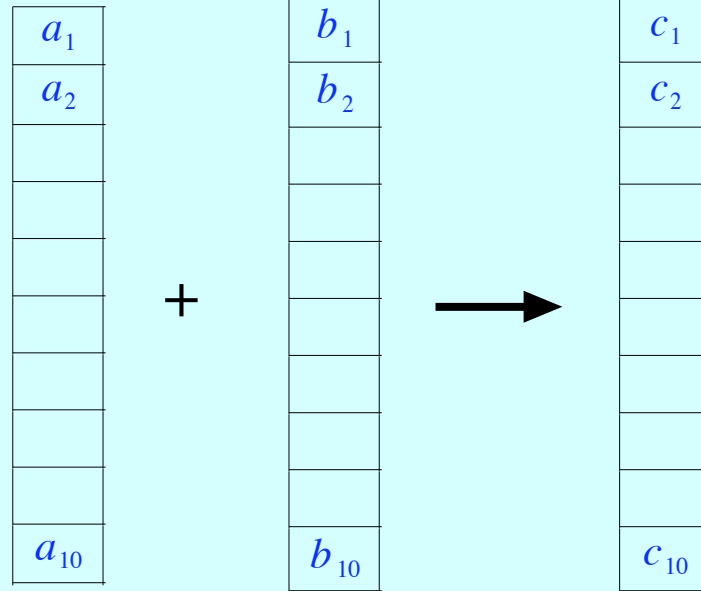
$$c_2 = a_2 + b_2$$

$\vdots$

$$c_{10} = a_{10} + b_{10}$$

Number of calculation step is

10



When it is vectorized,

$$c = a + b$$

Number of calculation step is

1

10 times faster

2-dimensional array...

$$c_{1,1} = a_{1,1} + b_{1,1}$$

$\vdots$

$$c_{10,10} = a_{10,10} + b_{10,10}$$

Number of calculation step is

100



When it is vectorized,

$$c = a + b$$

Number of calculation step is

1

100 times faster

3-dimensional array...

$$c_{1,1,1} = a_{1,1,1} + b_{1,1,1}$$

⋮

$$c_{10,10,10} = a_{10,10,10} + b_{10,10,10}$$

Number of calculation step is

1000



When it is vectorized,

$$c = a + b$$

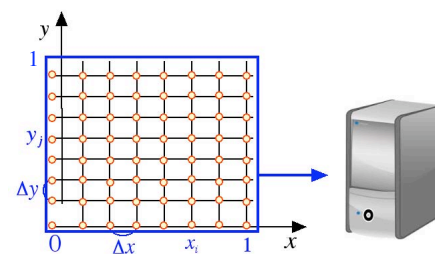
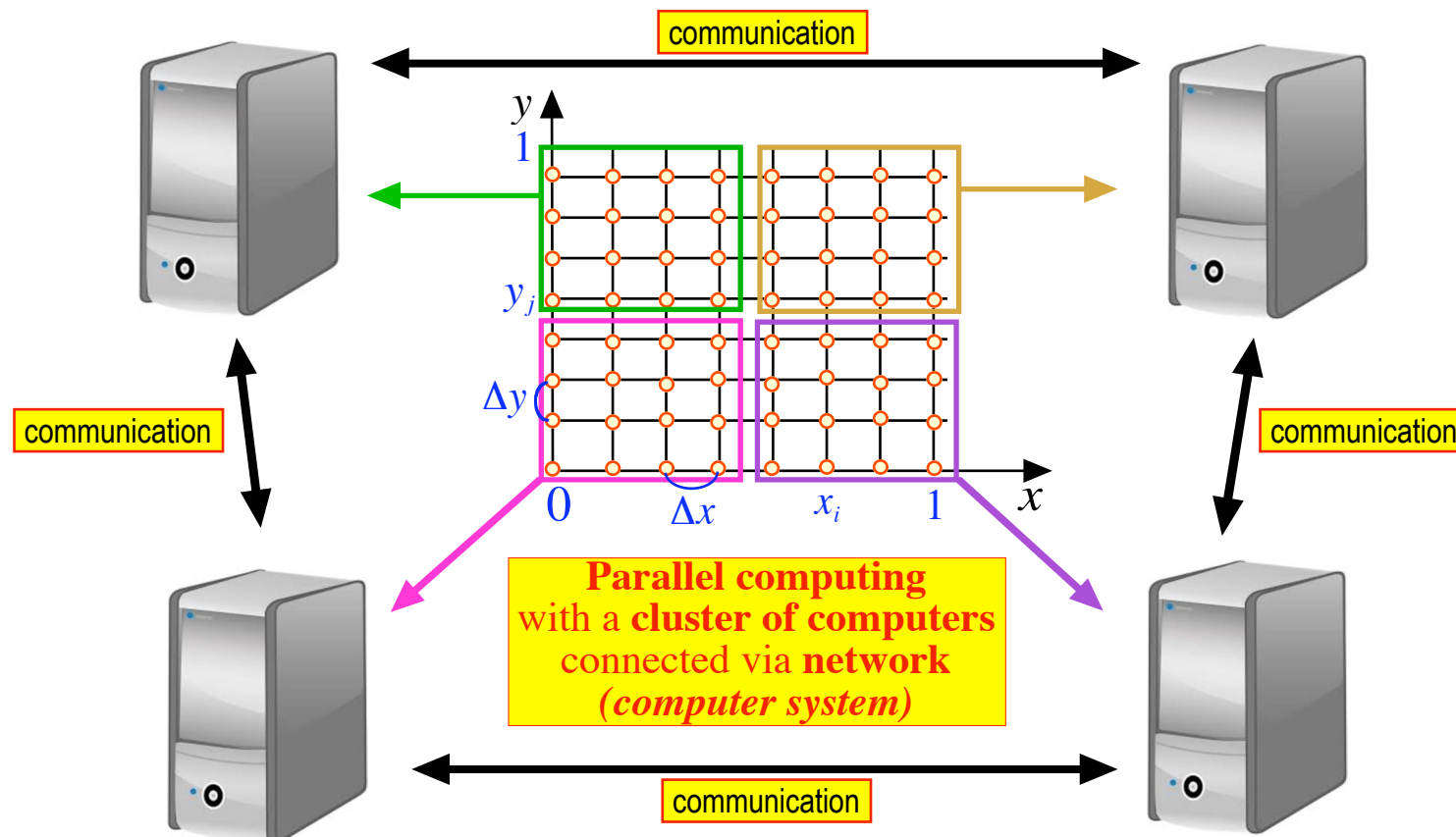
Number of calculation step is

1

1000 times faster

Parallelization

High-speed calculation technique II



Non-parallel computing
with a single computer



Supercomputer system for parallel computing