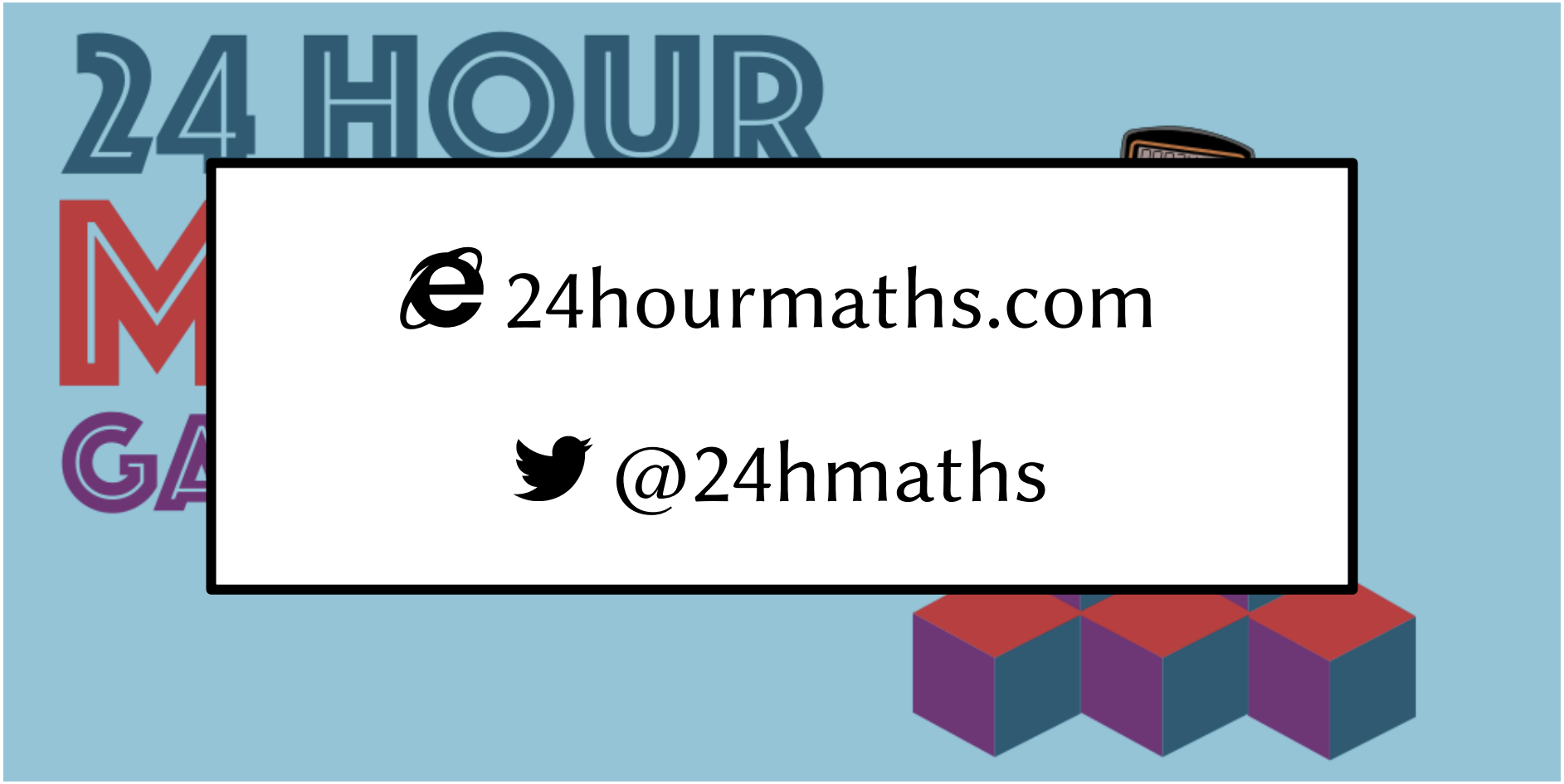
PHAS0102: Techniques of High-Performance Computing

Shameless self-promotion



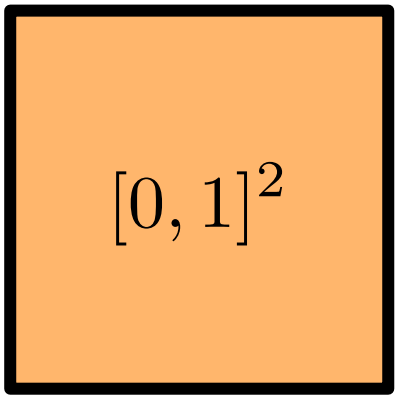
Assignment 2

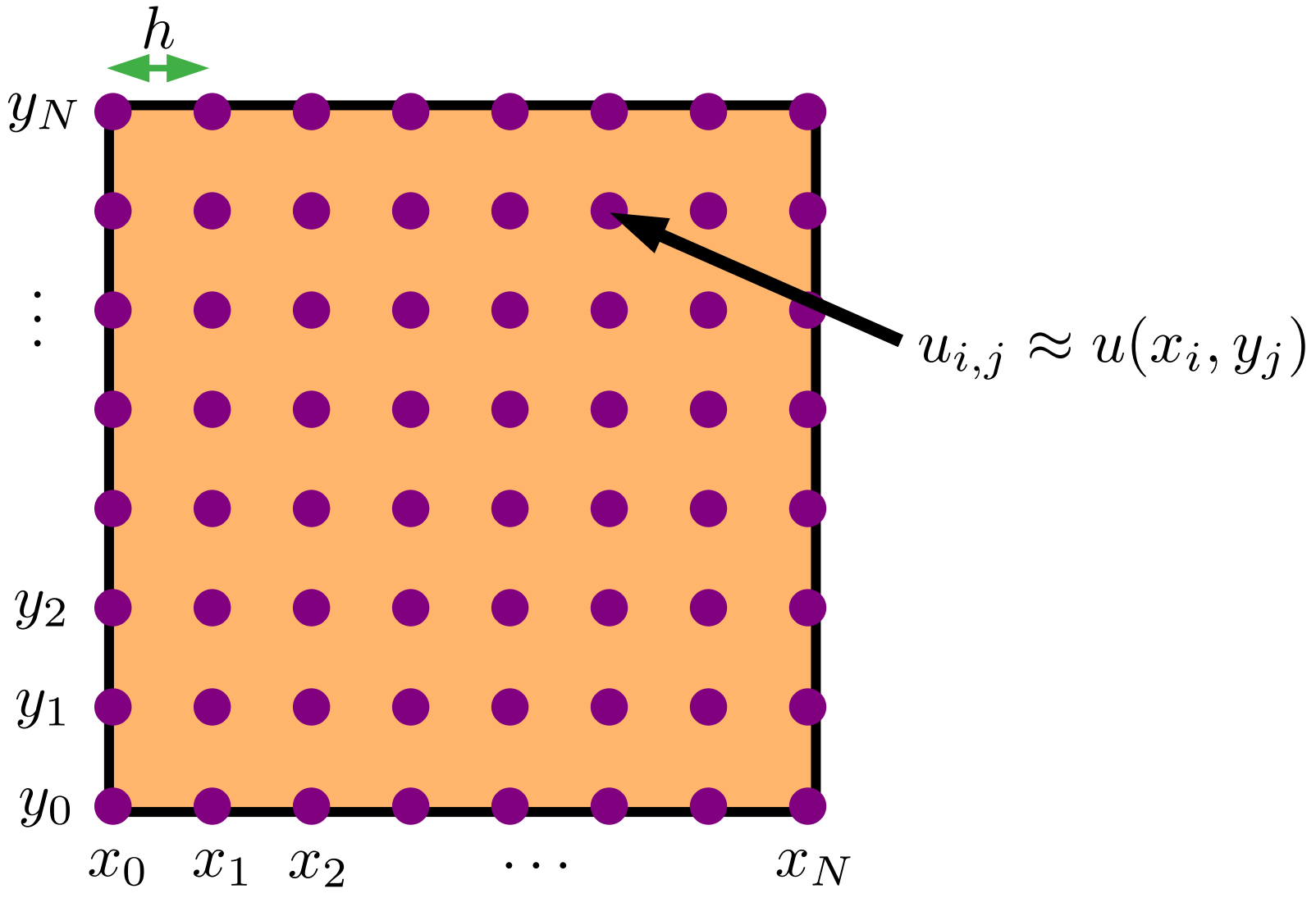
- On Moodle and mscroggs.co.uk/phas0102
- Deadline: 5pm on Thursday 3 November

Example problem

- Poisson problem

$$
\begin{aligned}
-\Delta u &= 1 && \text{in } [0,1]^2, \\
u &= 0 && \text{on the boundary}
\end{aligned}
$$




h
y_N
y_2
y_1
y_0
x_0 x_1 x_2 $\cdots$ x_N
$u_{i,j} \approx u(x_i, y_j)$

Finite differences

$$\frac{\mathrm{d}u}{\mathrm{d}x} \approx \frac{u_{i+1,j} - u_{i,j}}{h}$$

$$\frac{\mathrm{d}^2u}{\mathrm{d}x^2} \approx \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2}$$

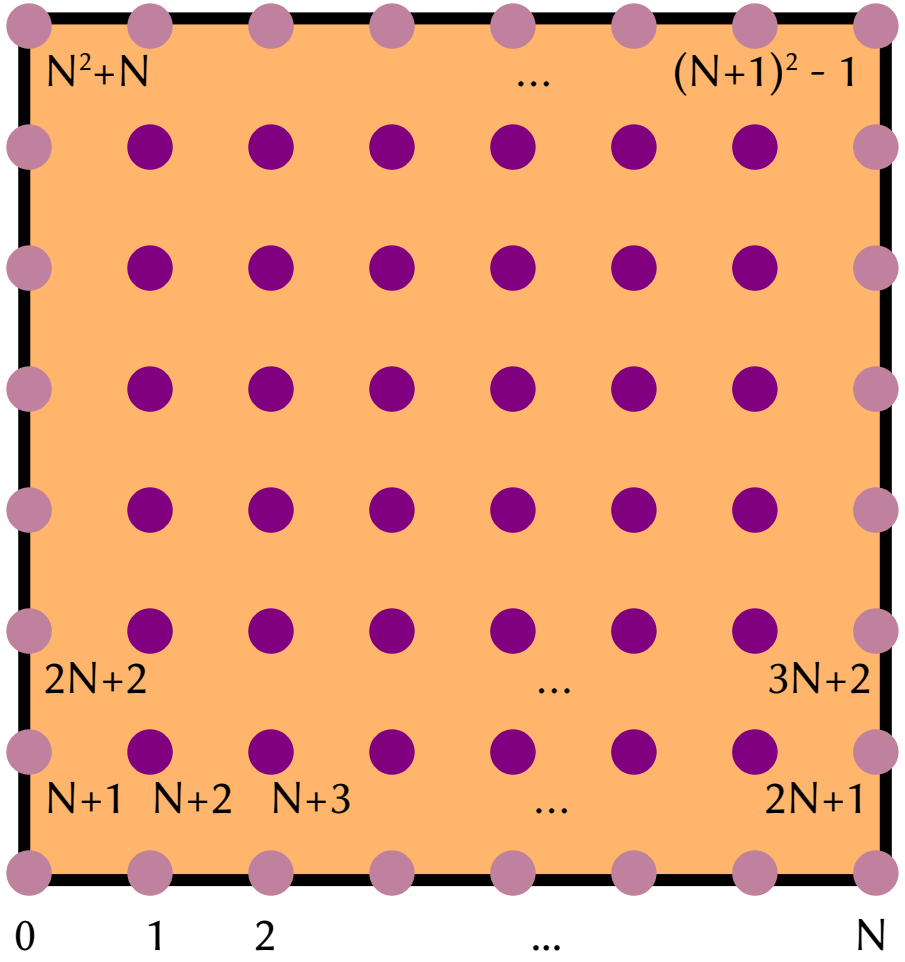
$$\Delta u = \frac{\mathrm{d}^2u}{\mathrm{d}x^2} + \frac{\mathrm{d}^2u}{\mathrm{d}y^2} \approx \frac{u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i+1,j} + u_{i,j+1}}{h^2}$$

$$-\Delta u = 1$$

$$\frac{4u_{i,j} - u_{i-1,j} - u_{i,j-1} - u_{i+1,j} - u_{i,j+1}}{h^2} = 1$$

$$u = 0 \text{ on the boundary}$$

$$u_{i,j} = 0 \text{ on the boundary}$$



$$\frac{4u_{i,j} - u_{i-1,j} - u_{i,j-1} - u_{i+1,j} - u_{i,j+1}}{h^2} = 1$$

$$u_{i,j} = 0 \text{ on the boundary}$$

$$u_{i,j} \to j(N+1) + i$$

[live code demo]

Sparse matrix storage

- We would like to not have to store all the 0s in the matrix in memory.
- Ideas?

COO (coordinate) format

- Store two lists of integers and one list of data:
  - First integer list is rows
  - Second integer list is columns
  - Data list is values in (row, column)
- eg
  - [0, 1]
  - [1,0]
  - [0.5, 0.7]

$$\begin{pmatrix} 0 & 0.5 \\ 0.7 & 0 \end{pmatrix}$$

- COO is the easiest format to use to create a sparse matrix

CSR (compressed sparse rows) format

- Store two lists of integers and one list of data:
  - First integer list is columns
  - Second integer list is when row changes
  - Data list is values in (row, column)
- eg
  - [0, 1]
  - [1]
  - [0.5, 0.7]

$$\begin{pmatrix} 0 & 0.5 \\ 0.7 & 0 \end{pmatrix}$$

- CSR uses less storage space, and is used by many sparse solvers.

CSC (compressed sparse columns) format

- This is the same as CSR, but with the role of rows and columns swapped.

[live code demo]

Other formats

- There are lots of other sparse matrix formats, including:
  - LIL (list of lists)
  - DOK (dictionary of keys)
  - DIA (diagonal storage)
  - BSR (block sparse rows)