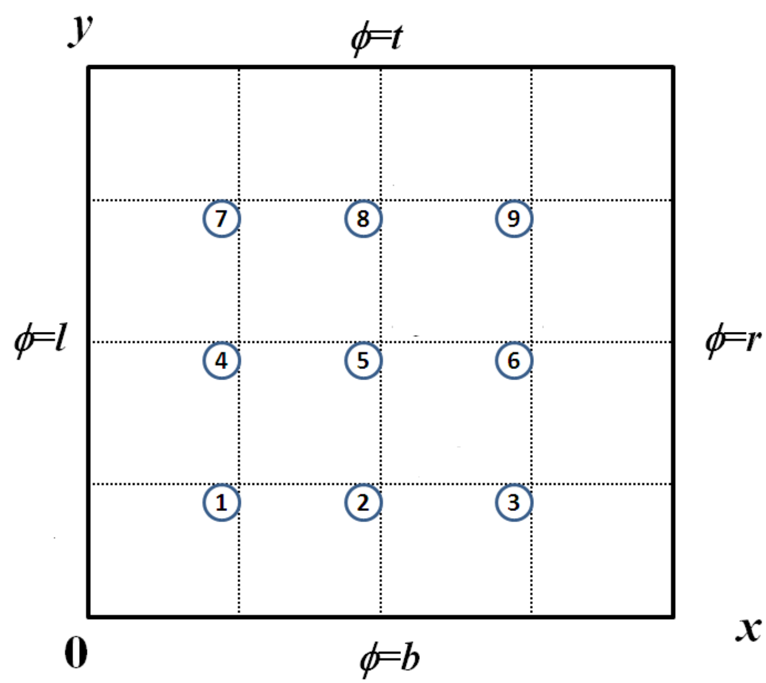
Laplace Equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0$$

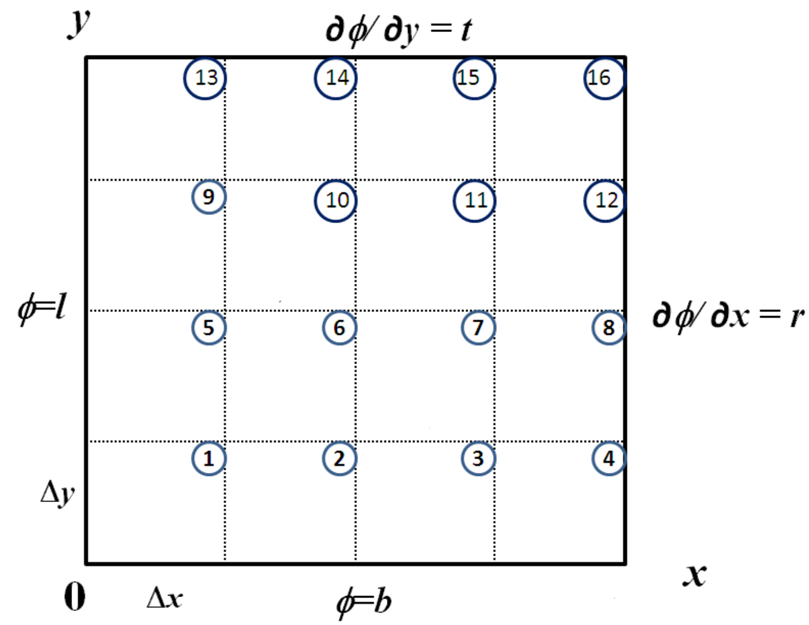


$$\frac{\phi_{i-1,j} - 2\phi_{i,j} + \phi_{i+1,j}}{\Delta x^2} + \frac{\phi_{i,j-1} - 2\phi_{i,j} + \phi_{i,j+1}}{\Delta y^2} = 0$$

Laplace Equation: Boundary Conditions

- Neumann, e.g.,

$$\frac{\phi_{i-2,j} - 4\phi_{i-1,j} + 3\phi_{i,j}}{2\Delta x} = r$$



- Robin, $\partial\phi/\partial x = k\,(\phi - \phi_0)$

$$\frac{\phi_{i-2,j} - 4\phi_{i-1,j} + 3\phi_{i,j}}{2\Delta x} = k\left(\phi_{i,j} - \phi_0\right)$$

Advection-Diffusion Equation

- Mass transport in moving fluids
- We consider only 1-D, homogeneous case

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$$

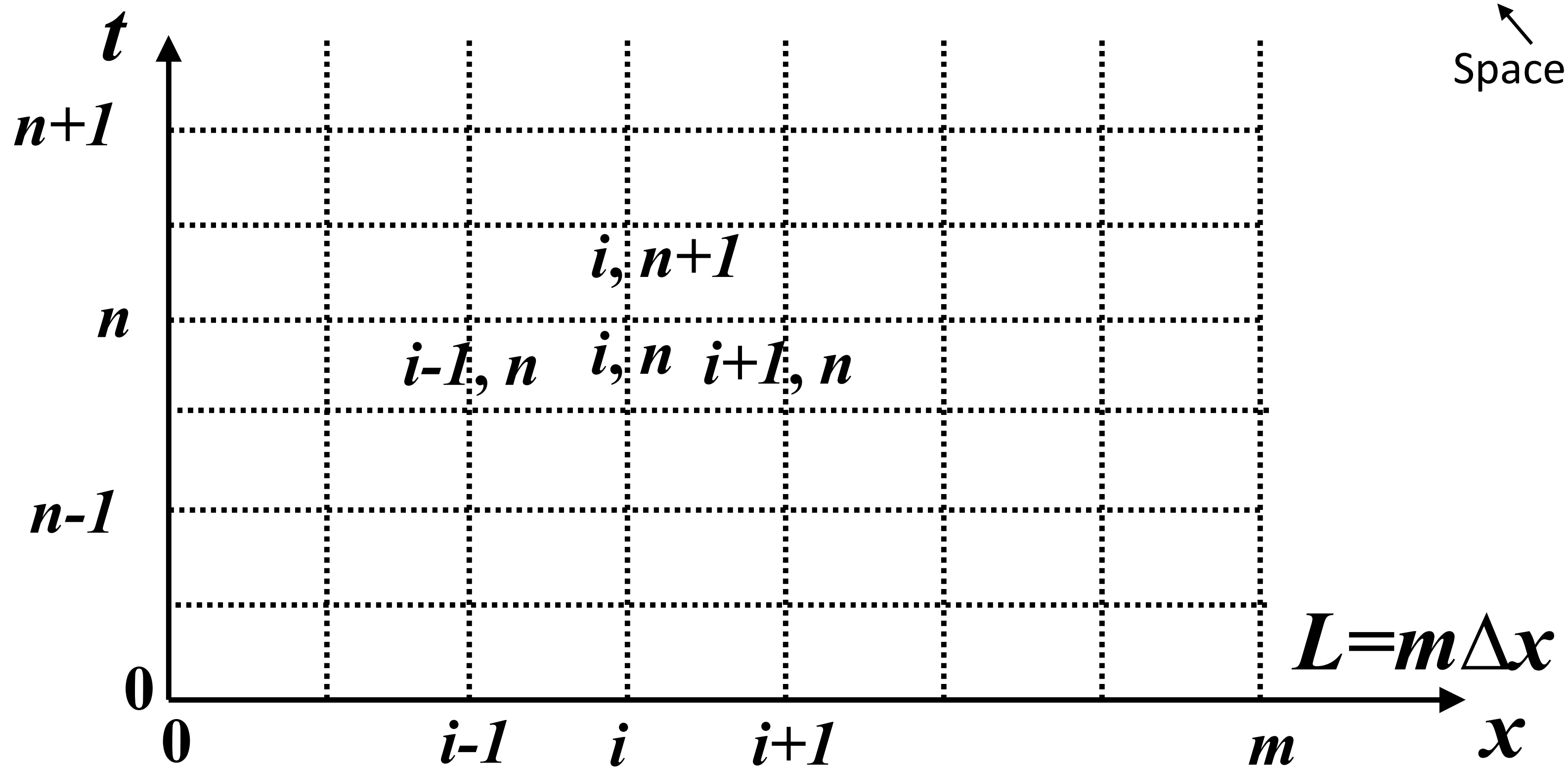
- u is velocity and D, diffusion coefficient
- In general, these could depend on x
- We will consider them to be constant
- The objective is to find the value of c at all points and at all times

Advection-Diffusion Equation

- When u=0, we get the Diffusion equation
- When D=0, we get pure advection or first-order wave equation
- Parabolic equation: Horizontal characteristic lines, need boundary conditions at all times and the initial condition must be at "the beginning"
- We cannot march back in time!

Advection-Diffusion Equation

- Assume Dirichlet B.C. at x=0 and L: $c(t,0)=1$, $c(t,L)=0$; , and zero initial condition: $c(0,x)=0$
- Uniform grid, space Δx and time, Δt: c_i^n



Advection-Diffusion Equation: Discretization

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$$

- Forward difference for time and central for space

$$\frac{c_i^{n+1} - c_i^n}{\Delta t^n} + u_i^n \frac{c_{i+1}^n - c_{i-1}^n}{2\Delta x_i} = D_i^n \frac{c_{i+1}^n - 2c_i^n + c_{i-1}^n}{\Delta x_i^2}$$

- Assumption: uniform step size, constant velocity and dispersion

$$c_i^{n+1} = \left(\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^n + \left(1 - \frac{2D\Delta t}{\Delta x^2}\right)c_i^n + \left(-\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^n$$

Advection-Diffusion Equation: Discretization

$$c_i^{n+1} = \left(\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2} \right) c_{i-1}^n + \left(1 - \frac{2D\Delta t}{\Delta x^2} \right) c_i^n + \left(-\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2} \right) c_{i+1}^n$$

- Not applicable at i=0 and i=m
- Not needed, since c is given
- Explicit, nodal values at any time step directly from those at previous time step
- For better stability, we could use implicit

$$\frac{c_i^{n+1} - c_i^n}{\Delta t} + u \frac{c_{i+1}^{n+\theta} - c_{i-1}^{n+\theta}}{2\Delta x} = D \frac{c_{i+1}^{n+\theta} - 2c_i^{n+\theta} + c_{i-1}^{n+\theta}}{\Delta x^2}$$

where, $c_i^{n+\theta} = (1-\theta) c_i^n + \theta c_i^{n+1}$

Time-Weighting

- θ denotes the weight assigned to the "unknown" time step
- Sometimes, the weighting factor θ is replaced by 1-μ, with μ being the weight assigned to the "known" time step
- We will use μ: $c_i^{n+1-\mu} = \mu c_i^n + (1-\mu) c_i^{n+1}$
- For μ=1, explicit; μ≠1, implicit (μ=0, fully-implicit; μ=1/2, Crank-Nicolson which has a higher order accuracy)

Courant and Peclet Numbers

- The discretized nodal equation is

$$(1-\mu)\left(-\frac{u\Delta t}{2\Delta x}-\frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^{n+1}+\left(1+\frac{2(1-\mu)D\Delta t}{\Delta x^2}\right)c_i^{n+1}+(1-\mu)\left(\frac{u\Delta t}{2\Delta x}-\frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^{n+1}=$$

$$\mu\left(\frac{u\Delta t}{2\Delta x}+\frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^{n}+\left(1-\frac{2\mu D\Delta t}{\Delta x^2}\right)c_i^{n}+\mu\left(-\frac{u\Delta t}{2\Delta x}+\frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^{n}$$

- We use the Courant number, $C=\dfrac{u\Delta t}{\Delta x}$ and

  the Grid Peclet number, $P_g=\dfrac{u\Delta x}{D}$
  (the Peclet no. based on domain length is given by $P_e=\dfrac{uL}{D}$)

Courant and Peclet Numbers

- Cournt no. represents the number of grid-lengths travelled in one time step
- Peclet number represents the relative influence of advection and dispersion
- The nodal equation becomes

$$-(1-\mu)\left(\frac{C}{2}+\frac{C}{P_g}\right)c_{i-1}^{n+1}+\left(1+\frac{2(1-\mu)C}{P_g}\right)c_i^{n+1}+(1-\mu)\left(\frac{C}{2}-\frac{C}{P_g}\right)c_{i+1}^{n+1}=$$

$$\mu\left(\frac{C}{2}+\frac{C}{P_g}\right)c_{i-1}^{n}+\left(1-\frac{2\mu C}{P_g}\right)c_i^{n}+\mu\left(-\frac{C}{2}+\frac{C}{P_g}\right)c_{i+1}^{n}$$

(Pure advection, $C/P_g=0$; Diffusion: $C=0$, $C/P_g=D\Delta t/\Delta x^2=D^*$)

- Tridiagonal system. Thomas algorithm

Predictor-Corrector method

- Predictor-corrector methods or R-K methods could also be used
- For example, Mid-point method:
  - At Δt/2:

$$c_i^{n+\frac{1}{2}} = \left(\frac{u\Delta t}{4\Delta x} + \frac{D\Delta t}{2\Delta x^2}\right)c_{i-1}^n + \left(1 - \frac{D\Delta t}{\Delta x^2}\right)c_i^n + \left(-\frac{u\Delta t}{4\Delta x} + \frac{D\Delta t}{2\Delta x^2}\right)c_{i+1}^n$$

  - And, at Δt:

$$c_i^{n+1} = c_i^n + \left(\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^{n+\frac{1}{2}} - \frac{2D\Delta t}{\Delta x^2}c_i^{n+\frac{1}{2}} + \left(-\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^{n+\frac{1}{2}}$$

Advection-Diffusion Equation: Example

- Given: c(0,x)=1−x/3, c(t,0)=1, c(t,3)=0 (c in kg/m^3; x in m, t in s); u= 1 m/s; D= 2 m^2/s
- Use: Δx=1 m; Δt=1 s
- Find: c after 1 s at x=1 m and 2 m
- C=1, P_g=0.5
- Explicit: $$c_i^{n+1} = C\left(\frac{1}{2}+\frac{1}{P_g}\right)c_{i-1}^n + \left(1-\frac{2C}{P_g}\right)c_i^n + C\left(-\frac{1}{2}+\frac{1}{P_g}\right)c_{i+1}^n$$

$$c_i^{n+1} = 2.5c_{i-1}^n - 3c_i^n + 1.5c_{i+1}^n$$

- At 1 s:

$$c_1^1 = 2.5c_0^0 - 3c_1^0 + 1.5c_2^0 = 2.5 - 2 + 0.5 = 1$$

$$c_2^1 = 2.5c_1^0 - 3c_2^0 + 1.5c_3^0 = 5/3 - 1 = 2/3$$

Advection-Diffusion Equation: Example

- Fully implicit (μ=0):

$$-\left(\frac{C}{2}+\frac{C}{P_g}\right)c_{i-1}^{n+1}+\left(1+\frac{2C}{P_g}\right)c_i^{n+1}+\left(\frac{C}{2}-\frac{C}{P_g}\right)c_{i+1}^{n+1}=c_i^n$$

$$-2.5c_{i-1}^{n+1}+5c_i^{n+1}-1.5c_{i+1}^{n+1}=c_i^n$$

- At 1 s:

$$-2.5c_0^1+5c_1^1-1.5c_2^1=c_1^0 \Rightarrow 5c_1^1-1.5c_2^1=19/6$$

$$-2.5c_1^1+5c_2^1-1.5c_3^1=c_2^0 \Rightarrow -2.5c_1^1+5c_2^1=1/3$$

- Solution: 0.7686, 0.4510

Advection-Diffusion Equation: Example

- Crank-Nicolson or Time-centered (μ=0.5):

$$-\frac{1}{2}\left(\frac{C}{2}+\frac{C}{P_g}\right)c_{i-1}^{n+1}+\left(1+\frac{C}{P_g}\right)c_i^{n+1}+\frac{1}{2}\left(\frac{C}{2}-\frac{C}{P_g}\right)c_{i+1}^{n+1}=\frac{1}{2}\left(\frac{C}{2}+\frac{C}{P_g}\right)c_{i-1}^{n}+\left(1-\frac{C}{P_g}\right)c_i^{n}+\frac{1}{2}\left(-\frac{C}{2}+\frac{C}{P_g}\right)c_{i+1}^{n}$$

$$-1.25c_{i-1}^{n+1}+3c_i^{n+1}-0.75c_{i+1}^{n+1}=1.25c_{i-1}^{n}-c_i^{n}+0.75c_{i+1}^{n}$$

- At 1 s:

$$-1.25c_0^1+3c_1^1-0.75c_2^1=1.25c_0^0-c_1^0+0.75c_2^0\Rightarrow 3c_1^1-0.75c_2^1=2.083$$

$$-1.25c_1^1+3c_2^1-0.75c_3^1=1.25c_1^0-c_2^0+0.75c_3^0\Rightarrow -1.25c_1^1+3c_2^1=0.5$$

- Solution: 0.8217, 0.5090

Advection-Diffusion Equation: Example

- Mid-point method:
- Predictor:

$$c_i^{n+\frac{1}{2}} = \left(\frac{u\Delta t}{4\Delta x} + \frac{D\Delta t}{2\Delta x^2}\right)c_{i-1}^n + \left(1 - \frac{D\Delta t}{\Delta x^2}\right)c_i^n + \left(-\frac{u\Delta t}{4\Delta x} + \frac{D\Delta t}{2\Delta x^2}\right)c_{i+1}^n$$

$$c_i^{\frac{1}{2}} = 1.25c_{i-1}^0 - c_i^0 + 0.75c_{i+1}^0 \Rightarrow c_1^{\frac{1}{2}} = 0.8333; c_2^{\frac{1}{2}} = 0.5$$

- Corrector:

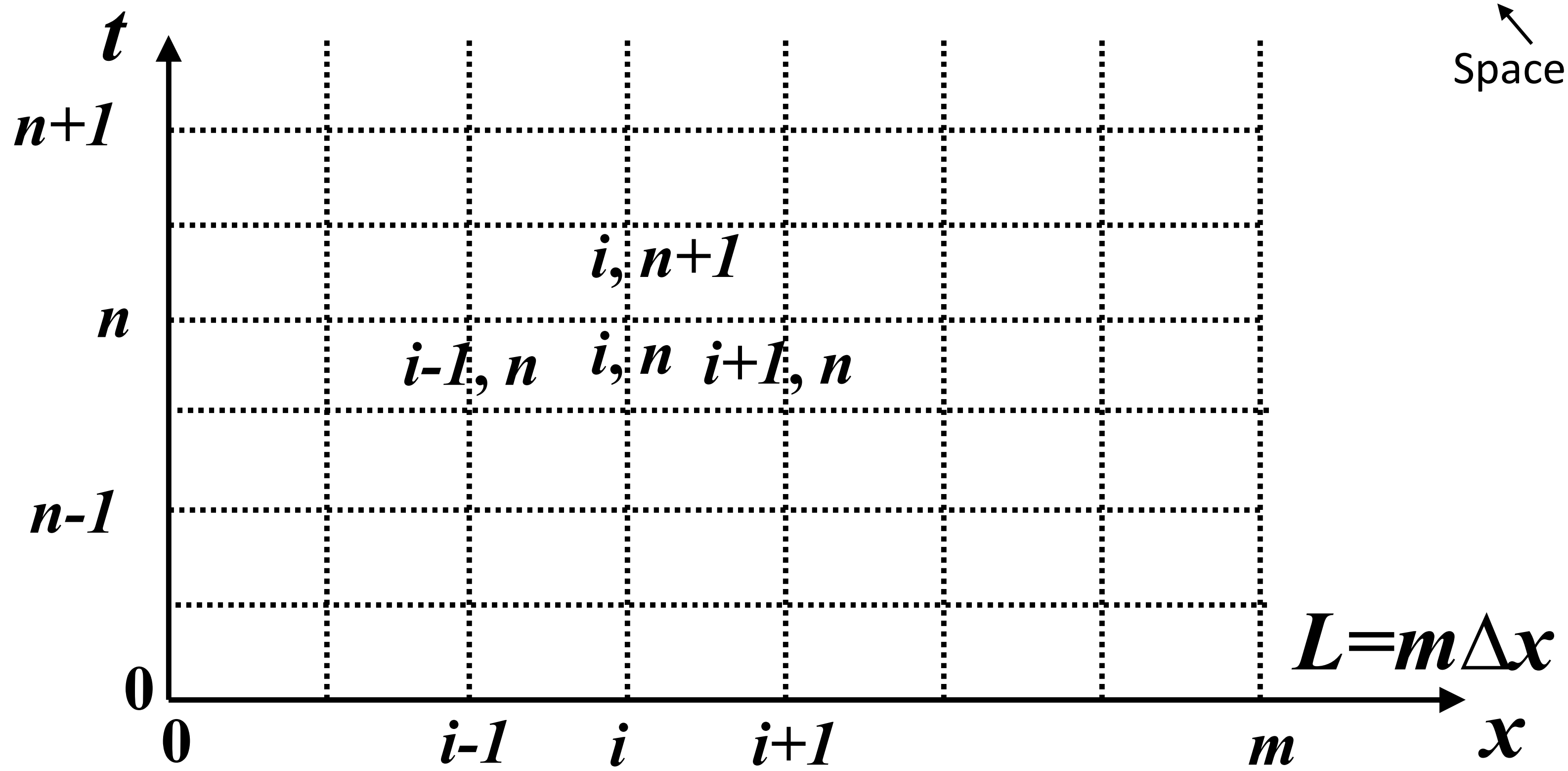
$$c_i^{n+1} = c_i^n + \left(\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^{n+\frac{1}{2}} - \frac{2D\Delta t}{\Delta x^2}c_i^{n+\frac{1}{2}} + \left(-\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^{n+\frac{1}{2}}$$

$$c_i^1 = c_i^0 + 2.5c_{i-1}^{\frac{1}{2}} - 4c_i^{\frac{1}{2}} + 1.5c_{i+1}^{\frac{1}{2}} \Rightarrow c_1^1 = 0.5833; c_2^1 = 0.4167$$

Advection-Diffusion Equation: Neumann B.C.

- Assume Dirichlet B.C. at x=0 and Neumann at L: $c(t,0)=1$, $\partial c/\partial x(t,L)=0$; , and zero initial condition: $c(0,x)=0$
- Uniform grid, space Δx and time, Δt: c_i^n

Time
Space



Neumann B.C. – Explicit Method

$$c_i^{n+1} = \left(\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i-1}^n + \left(1 - \frac{2D\Delta t}{\Delta x^2}\right)c_i^n + \left(-\frac{u\Delta t}{2\Delta x} + \frac{D\Delta t}{\Delta x^2}\right)c_{i+1}^n$$

- Not applicable at i=0 (not needed)
- Use a ghost node (m+1)
- Approximate the derivative by central difference $\quad \dfrac{c_{m+1}^n - c_{m-1}^n}{2\Delta x_i} = 0$
- The equation at node m:

$$c_m^{n+1} = \frac{2D\Delta t}{\Delta x^2}c_{m-1}^n + \left(1 - \frac{2D\Delta t}{\Delta x^2}\right)c_m^n$$

Neumann B.C.: Example

- Given: $c(0,x)=1-x/3$, $c(t,0)=1$, $\partial c/\partial x(t,3)=0$; $u=1$ m/s; $D=2$ m^2/s
- Use: $\Delta x=1$ m; $\Delta t=1$ s
- Find: c after 1 s at $x=1$ m and 2 m
- $C=1$, $P_g=0.5$
- Explicit:

$$c_i^{n+1} = C\left(\frac{1}{2}+\frac{1}{P_g}\right)c_{i-1}^n + \left(1-\frac{2C}{P_g}\right)c_i^n + C\left(-\frac{1}{2}+\frac{1}{P_g}\right)c_{i+1}^n$$

$$c_i^{n+1} = 2.5c_{i-1}^n - 3c_i^n + 1.5c_{i+1}^n$$

- At 1 s:

$$c_1^1 = 2.5c_0^0 - 3c_1^0 + 1.5c_2^0 = 2.5 - 2 + 0.5 = 1$$

$$c_2^1 = 2.5c_1^0 - 3c_2^0 + 1.5c_3^0 = 5/3 - 1 = 2/3$$

$$c_3^1 = 4c_2^0 - 3c_3^0 = 8/3 - 1 = 5/3$$

Large Error