Numerical Integration of Differential Equations, PART B
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Finite Difference Method for Integration of PDE's

These notes will consider integration of the following parabolic PDE using the finite difference method.

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

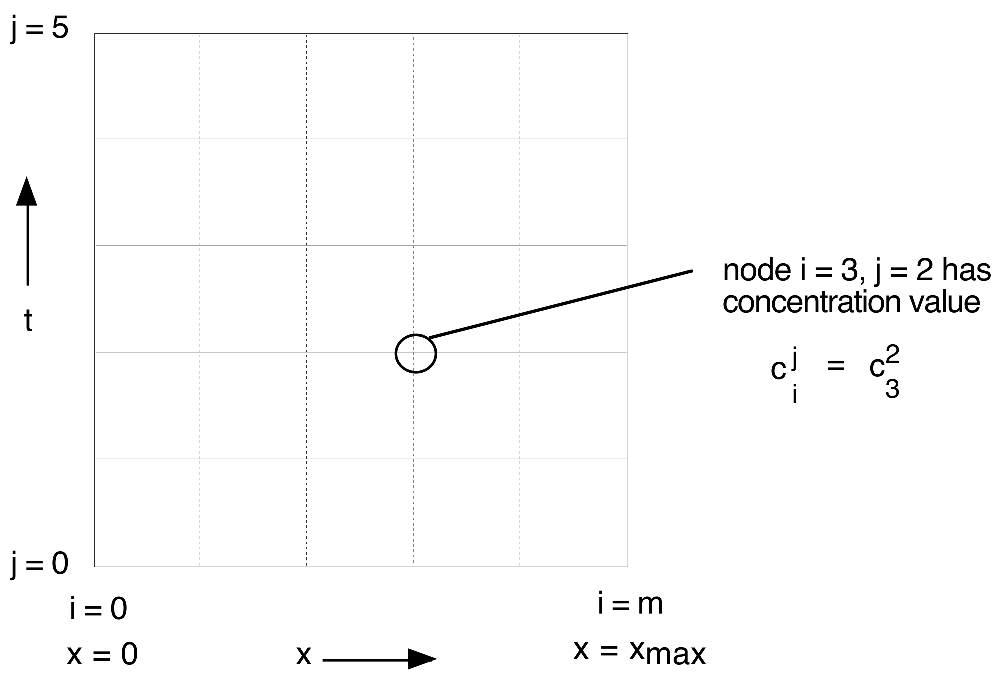
Note that this mass diffusion equation has an analogous form for heat conduction, with temperature, T, replacing concentration, c, and thermal diffusivity, $\alpha = k_t / \rho C_p$, replacing the mass diffusivity D.

Since there is variation with time we need an initial condition and since there is a second derivative with respect to position we need two boundary conditions.

Initial Condition: $c(x,0) = K_1$
Boundary condition at $x = 0$, $c(0,t) = K_2$
Boundary condition at $x = x_{max}$

$$\left.\frac{\partial c}{\partial x}\right|_{x = x_{max}} = 0$$

Imagine that spatial position x and time t are represented by a grid, with each node of the grid representing a point in x and a point in time. The spacing of the nodes along the x direction is Δx and the spacing of the nodes along the t direction is Δt. We use the subscript i to indicate which x location we are at and the superscript j to indicate which t location we are at on the grid.



The first derivative of c with respect to x is approximated by the “finite difference” approximation

$$\frac{\partial c}{\partial x} \approx \frac{c_{i+1} - c_i}{\Delta x}$$

The second derivative of c with respect to x is approximated by the following “centered finite difference derivative”:

$$\frac{\partial^2 c}{\partial x^2} \approx \lim_{\Delta x \to 0} \left[\frac{\left.\frac{\partial c}{\partial x}\right|_{i+1} - \left.\frac{\partial c}{\partial x}\right|_{i}}{\Delta x} \right] \approx \frac{\frac{c_{i+1} - c_i}{\Delta x} - \frac{c_i - c_{i-1}}{\Delta x}}{\Delta x}$$

$$\frac{\partial^2 c}{\partial x^2} \approx \frac{c_{i+1} - 2\,c_i + c_{i-1}}{(\Delta x)^2}$$

The time derivative is approximated by the following “forward finite divided difference” which is equivalent to using Euler’s method to integrate in time:

$$\frac{\partial c}{\partial t} \approx \frac{c_i^{j+1} - c_i^j}{\Delta t}$$

The finite difference approximation to our PDE is:

$$\frac{c_i^{j+1} - c_i^j}{\Delta t} = D\,\frac{c_{i+1}^j - 2\,c_i^j + c_{i-1}^j}{(\Delta x)^2}$$

Rearranging, we have the result for the concentration c at the next time step, j+1, as a function of concentrations at the current time step j:

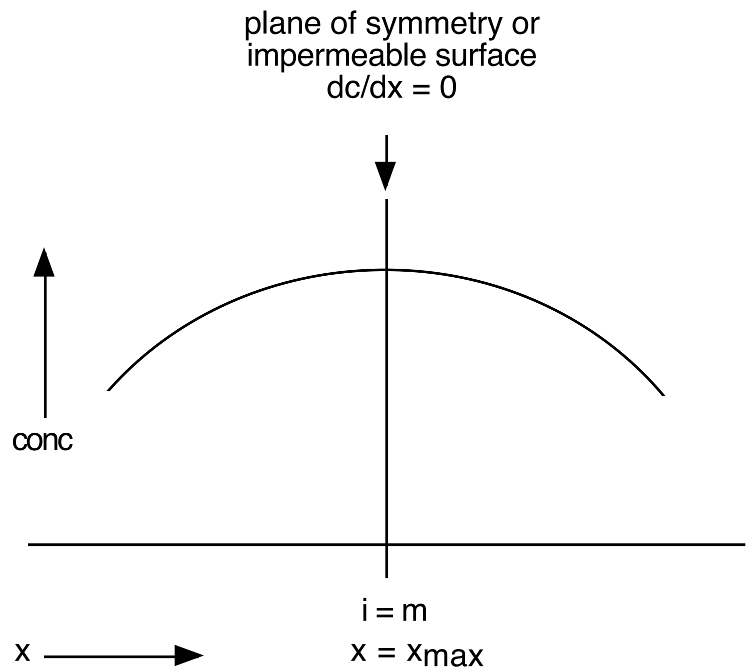
$$c_i^{j+1} = c_i^j + \lambda\left(c_{i+1}^j - 2\,c_i^j + c_{i-1}^j\right)$$

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

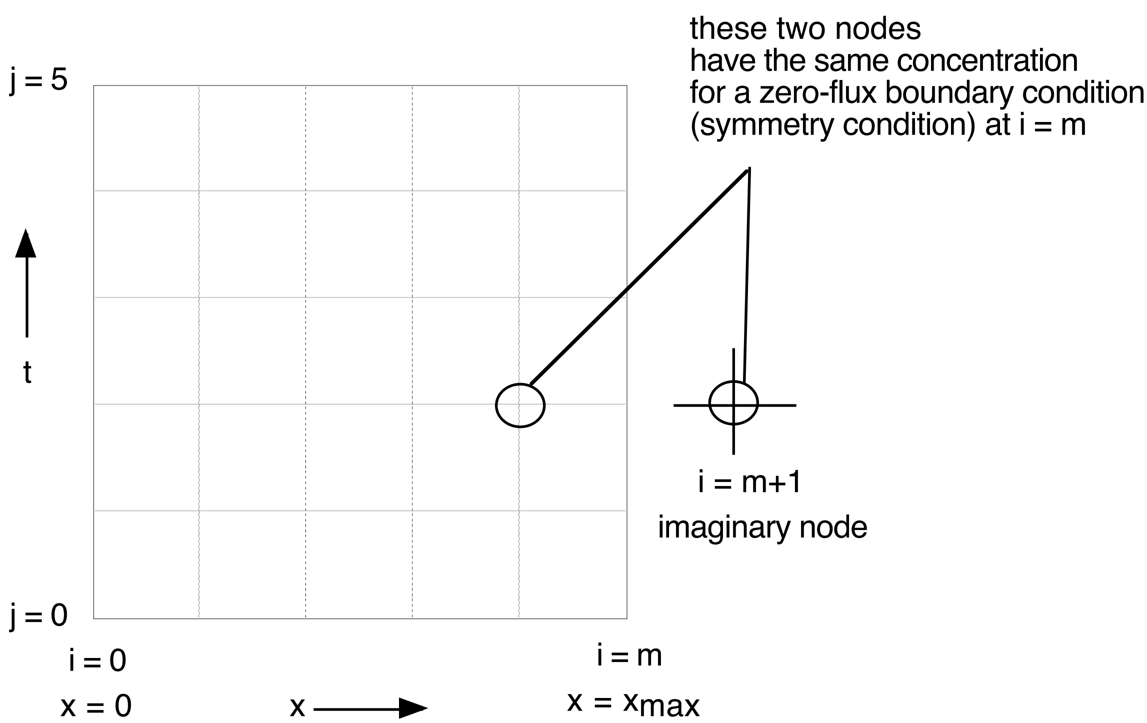
The above equation can be applied at all the internal nodes, that is, all nodes except those at the boundaries: node i = 0 representing position x = 0 and node i = m representing $x = x_{max}$.

At x = 0, the boundary condition above specifies that c_0 equals the constant K_2.

At $x = x_{max}$, the boundary condition above is the “zero flux” boundary condition. This type of boundary condition is also encountered at planes of symmetry:



We can formulate the difference equation for the node at i = m, $x = x_{max}$, by referencing an imaginary node at an imaginary grid location i = m + 1, where this imaginary node has the same concentration c as the node at i = m – 1. This would be the case for a concentration profile that is symmetrical about the plane at $x = x_{max}$, i = m.



Modifying the difference approximation for an internal node so that it applies to the node at i = m, we get:

$$c_m^{j+1} = c_m^j + \lambda\left(c_{m+1}^j - 2\,c_m^j + c_{m-1}^j\right)$$

$$c_m^{j+1} = c_m^j + \lambda\left(2c_{m-1}^j - 2\,c_m^j\right)$$

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

Stability and convergence criterion

In order to obtain a stable, non oscillatory and converging solution, the grid spacings Δt and Δx must be selected in order to meet the following criterion:

$$\lambda \leq 0.25$$

You will probably need to have more nodes - a finer grid spacing - than shown in the illustrations above.