DISCRETIZATION OF THE FLOW EQUATIONS

As we already have seen, finite difference approximations of the partial derivatives appearing in the flow equations may be obtained from Taylor series expansions. We shall now proceed to derive approximations for all terms needed in reservoir simulation.

Spatial discretization

Constant grid block sizes

We showed that the approximation of the second derivative of pressure may be obtained by forward and backward expansions of pressure:

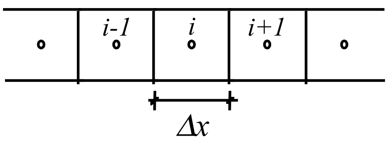
$$P(x+\Delta x,t) = P(x,t) + \frac{\Delta x}{1!}P'(x,t) + \frac{(\Delta x)^2}{2!}P''(x,t) + \frac{(\Delta x)^3}{3!}P'''(x,t) + \ldots..$$

$$P(x-\Delta x,t) = P(x,t) + \frac{(-\Delta x)}{1!}P'(x,t) + \frac{(-\Delta x)^2}{2!}P''(x,t) + \frac{(-\Delta x)^3}{3!}P'''(x,t) + \ldots..$$

to yield

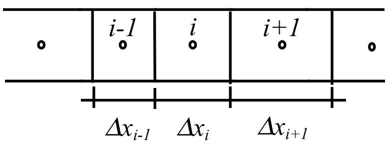
$$(\frac{\partial^2 P}{\partial t^2})_i^t = \frac{P_{i+1}^t - 2P_i^t + P_{i-1}^t}{(\Delta x)^2} + O(\Delta x^2),$$

which applies to the following grid system:



Variable grid block sizes

A more realistic grid system is one of variable block lengths, which will be the case in most simulations. Such a grid would enable finer description of geometry, and better accuracy in areas of rapid changes in pressures and saturations, such as in the neighborhood of production and injection wells. For the simple one-dimensional system, a variable grid system would be:



the Taylor expansions become (dropping the time index):

$$P_{i+1} = P_i + \frac{(\Delta x_i + \Delta x_{i+1})/2}{1!}P_i' + \frac{\left[(\Delta x_i + \Delta x_{i+1})/2\right]^2}{2!}P_i'' + \frac{\left[(\Delta x_i + \Delta x_{i+1})/2\right]^3}{3!}P_i''' \ldots..$$

$$P_{i-1} = P_i + \frac{-(\Delta x_i + \Delta x_{i-1})/2}{1!}P_i' + \frac{\left[-(\Delta x_i + \Delta x_{i-1})/2\right]^2}{2!}P_i'' + \frac{\left[-(\Delta x_i + \Delta x_{i-1})/2\right]^3}{3!}P_i''' \ldots..$$

to yield

$$P_i'' = 4\,\frac{2\left(\dfrac{\Delta x_i + \Delta x_{i-1}}{2\Delta x_i + \Delta x_{i+1} + \Delta x_{i-1}}\right)P_{i+1} - 2P_i + 2\left(\dfrac{\Delta x_i + \Delta x_{i+1}}{2\Delta x_i + \Delta x_{i+1} + \Delta x_{i-1}}\right)P_{i-1}}{(\Delta x_i + \Delta x_{i+1})(\Delta x_i + \Delta x_{i-1})} + O(\Delta x).$$

An important difference is now that the error term is of only first order, due to the different block sizes. However, normally the flow terms in our simulation equations will be of the type $\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]$, where $f(x)$ includes permeability, mobility and flow area. Therefore, we will instead derive a central approximation for the first derivative, and apply it twice to this flow term.

$$\left[f(x)\frac{\partial P}{\partial x}\right]_{i+1/2} = \left[f(x)\frac{\partial P}{\partial x}\right]_i + \frac{\Delta x_i/2}{1!}\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_i + \frac{(\Delta x_i/2)^2}{1!}\frac{\partial^2}{\partial x^2}\left[f(x)\frac{\partial P}{\partial x}\right]_i + ...$$

and

$$\left[f(x)\frac{\partial P}{\partial x}\right]_{i-1/2} = \left[f(x)\frac{\partial P}{\partial x}\right]_i + \frac{-\Delta x_i/2}{1!}\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_i + \frac{(-\Delta x_i/2)^2}{1!}\frac{\partial^2}{\partial x^2}\left[f(x)\frac{\partial P}{\partial x}\right]_i + ...$$

which yields

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_i = \frac{\left[f(x)\frac{\partial P}{\partial x}\right]_{i+1/2} - \left[f(x)\frac{\partial P}{\partial x}\right]_{i-1/2}}{\Delta x_i} + O(\Delta x^2).$$

Similarly, we may obtain the following expressions:

$$\left(\frac{\partial P}{\partial x}\right)_{i+1/2} = \frac{P_{i+1} - P_i}{(\Delta x_i + \Delta x_{i+1})/2} + O(\Delta x)$$

and

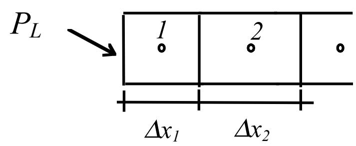
$$\left(\frac{\partial P}{\partial x}\right)_{i-1/2} = \frac{P_i - P_{i-1}}{(\Delta x_i + \Delta x_{i-1})/2} + O(\Delta x).$$

As we can see, due to the different block sizes, the error terms for the last two approximations are again of first order only. By inserting these expressions into the previous equation, we get the following approximation for the flow term:

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_i = \frac{2f(x)_{i+1/2}\frac{(P_{i+1} - P_i)}{(\Delta x_{i+1} + \Delta x_i)} - 2f(x)_{i-1/2}\frac{(P_i - P_{i-1})}{(\Delta x_i + \Delta x_{i-1})}}{\Delta x_i} + O(\Delta x).$$

Boundary conditions

We have seen earlier that we have two types of boundary conditions, *Dirichlet*, or pressure condition, and *Neumann*, or rate condition. If we first consider a pressure condition at the left side of our slab, as follows:



then we will have to modify our approximation of the first derivative at the left face, $i = 1/2$, to become a forward difference instead of a central difference:

$$\left(\frac{\partial P}{\partial x}\right)_{1/2} = \frac{P_1 - P_L}{(\Delta x_1)/2} + O(\Delta x),$$

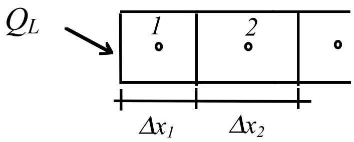
and the flow term approximation thus becomes:

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_1 = \frac{2f(x)_{11/2}\dfrac{(P_2 - P_1)}{(\Delta x_2 + \Delta x_1)} - 2f(x)_{1/2}\dfrac{(P_1 - P_L)}{(\Delta x_1)}}{\Delta x_1} + O(\Delta x) .$$

With a pressure P_R specified at the right hand face, we get a similar approximation for block N:

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_N = \frac{2f(x)_{N+1/2}\dfrac{(P_R - P_N)}{(\Delta x_N)} - 2f(x)_{N-1/2}\dfrac{(P_N - P_{N-1})}{(\Delta x_N + \Delta x_{N-1})}}{\Delta x_N} + O(\Delta x) .$$

For a flow rate specified at the left side (injection/production),



we make use of Darcy's equation:

$$Q_L = -\frac{kA}{\mu B}\left(\frac{\partial P}{\partial x}\right)_{1/2}$$

or

$$\left(\frac{\partial P}{\partial x}\right)_{1/2} = -Q_L\frac{\mu B}{kA} .$$

Then, by substituting into the approximation, we get:

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_1 = \frac{2f(x)_{11/2}\dfrac{(P_2 - P_1)}{(\Delta x_2 + \Delta x_1)} + Q_L\dfrac{\mu B}{kA}}{\Delta x_1} + O(\Delta x) .$$

With a rate Q_R specified at the right hand face, we get a similar approximation for block N:

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_N = \frac{-Q_R\dfrac{\mu B}{kA} - 2f(x)_{N-1/2}\dfrac{(P_N - P_{N-1})}{(\Delta x_N + \Delta x_{N-1})}}{\Delta x_N} + O(\Delta x) .$$

For the case of a no-flow boundary between blocks Q_R and Q_R, the flow terms for the two blocks become:

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_i = \frac{2f(x)_{i+1/2}\dfrac{(P_{i+1} - P_i)}{(\Delta x_{i+1} + \Delta x_i)} - 2f(x)_{i-1/2}\dfrac{(P_i - P_{i-1})}{(\Delta x_i + \Delta x_{i-1})}}{\Delta x_i} + O(\Delta x)$$

$$\frac{\partial}{\partial x}\left[f(x)\frac{\partial P}{\partial x}\right]_i = \frac{2f(x)_{i+1/2}\dfrac{(P_{i+1} - P_i)}{(\Delta x_{i+1} + \Delta x_i)} - 2f(x)_{i-1/2}\dfrac{(P_i - P_{i-1})}{(\Delta x_i + \Delta x_{i-1})}}{\Delta x_i} + O(\Delta x)$$

Time discretization

We showed earlier that by expansion backward in time:

$$P(x,t) = P(x,t+\Delta t) + \frac{-\Delta t}{1!}P'(x,t+\Delta t) + \frac{(-\Delta t)^2}{2!}P''(x,t+\Delta t) + \frac{(-\Delta t)^3}{3!}P'''(x,t+\Delta t) + \ldots .$$

the following backward difference approximation with first order error term is obtained:

$$(\frac{\partial P}{\partial t})_i^{t+\Delta t} = \frac{P_i^{t+\Delta t} - P_i^t}{\Delta t} + O(\Delta t) .$$

An expansion forward in time:

$$P(x, t+\Delta t) = P(x, t) + \frac{\Delta t}{1!} P'(x, t) + \frac{(\Delta t)^2}{2!} P''(x, t) + \frac{(\Delta t)^3}{3!} P'''(x, t) + \ldots .$$

yields a forward approximation, again with first order error term:

$$(\frac{\partial P}{\partial t})_i^{t+\Delta t} = \frac{P_i^{t+\Delta t} - P_i^t}{\Delta t} + O(\Delta t) .$$

Finally, expanding in both directions:

$$P(x, t+\Delta t) = P(x, t) + \frac{\Delta t}{1!} P'(x, t) + \frac{(\Delta t)^2}{2!} P''(x, t) + \frac{(\Delta t)^3}{3!} P'''(x, t) + \ldots .$$

$$P(x, t+\Delta t) = P(x, t) + \frac{\Delta t}{1!} P'(x, t) + \frac{(\Delta t)^2}{2!} P''(x, t) + \frac{(\Delta t)^3}{3!} P'''(x, t) + \ldots .$$

we get a central approximation, with a second order error term:

$$(\frac{\partial P}{\partial t})_i^{t+\Delta t} = \frac{P_i^{t+\Delta t} - P_i^t}{\Delta t} + O(\Delta t)$$

The time approximation used as great influence on the solutions of the equations. Using the simple case of the flow equation and constant grid size as example, we may write the difference form of the equation for the three cases above.

<u>Explicit formulation</u>

Here, we use the forward approximation of the time derivative at time level t . Hence, the left hand side is also at time level Q_t, and we can solve for pressures explicitly:

$$\frac{P_{i+1}^t - 2P_i^t + P_{i-1}^t}{\Delta x^2} \approx (\frac{\phi\mu c_t}{k}) \frac{P_i^{t+\Delta t} - P_i^t}{\Delta t}, \ for \, i = 1, \ldots, N$$

As discussed previously, this formulation has limited stability, and is therefore seldom used.

<u>Implicit formulation</u>

Here, we use the backward approximation of the time derivative at time level Q_R , and thus left hand side is also at time level Q_R :

$$\frac{P_{i+1}^{t+\Delta t} - 2P_i^{t+\Delta t} + P_{i-1}^{t+\Delta t}}{\Delta x^2} = (\frac{\phi\mu c}{k}) \frac{P_i^{t+\Delta t} - P_i^t}{\Delta t}$$

Now we have a set of N equations with N unknowns, which must be solved simultaneously, for instance using the Gaussian elimination method. The formulation is unconditionally stable.

Crank-Nicholson formulation

Finally, by using the central approximation of the time derivative at time level Q_R , and thus left hand side is also at time level Q_R :

$$\frac{1}{2}\left[\frac{P_{i+1}^{t} - 2P_{i}^{t} + P_{i-1}^{t}}{\Delta x^2} + \frac{P_{i+1}^{t+\Delta t} - 2P_{i}^{t+\Delta t} + P_{i-1}^{t+\Delta t}}{\Delta x^2}\right] = \left(\frac{\phi\mu c}{k}\right)\frac{P_{i}^{t+\Delta t} - P_{i}^{t}}{\Delta t}$$

The resulting set of linear equations may be solved simultaneously just as in the implicit case. The formulation is unconditionally stable, but may exhibit oscillatory behavior, and is seldom used.