

# Numerical Methods for Flow and Transport in Porous Media

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## **Abstract**

In this short course we will start by deriving the basic conservation laws for mass, momentum and energy. We will extend the results to mixtures in general and then to multiphase flow in porous media. We will describe the black-oil models and the Buckley-Leverett problem. Second, we will review the basic numerical methods for solving the differential equations that model a fluid in a porous medium. Finally, we will give some typical problems of flow and transport and show how they can be solved numerically.

# Contents

<b>1</b>	<b>Equations of Motion.</b>	<b>2</b>
1.1	Conservation Laws . . . . .	2
1.2	Mixtures . . . . .	6
1.3	Multiphase Flows in Porous Media . . . . .	10
1.4	Multiphase-multispecies Flows . . . . .	12
<b>2</b>	<b>Numerical Methods.</b>	<b>15</b>
2.1	Basic Methods for Parabolic Equations . . . . .	15
2.2	Numerical Methods for Elliptic Equations . . . . .	25
<b>3</b>	<b>Numerical Methods for some Problems in Porous Media.</b>	<b>29</b>
3.1	1-D Steady Flow . . . . .	29
3.2	Slightly Compressible Fluid . . . . .	31
3.3	Non-steady Aquifer . . . . .	33
3.4	Mixed Finite Element Example . . . . .	34
3.5	Transport of a Solute . . . . .	37
3.6	Modified Method of Characteristics for Transport . . . . .	38
3.7	Multiphase Flow . . . . .	41

# Chapter 1

## Equations of Motion.

### 1.1 Conservation Laws

We will start by deriving the equations of motion for a simple fluid consisting of only one phase and one component. Assume the continuum hypothesis. Let  $\tilde{x} = (x, y, z)$  be a point in space.

Let  $\tilde{v}(\tilde{x}, t)$  be the velocity of a particle of fluid moving through  $\tilde{x}$  at time  $t$ .

Let  $\rho(\tilde{x}, t)$  be the mass density, so that the mass of a fluid region  $W$  is

$$m(W, t) = \int_W \rho(\tilde{x}, t) dV$$

The equations of motion are based on the following conservation principles:

1. Mass is neither created nor destroyed.
2. The rate of change of momentum equals the applied force.
3. Energy is conserved.

#### 1. Conservation of Mass

Let  $W$  be a fixed region, the rate of change of mass in this region is

$$\frac{d}{dt} m(W, t) = \int_W \frac{\partial \rho}{\partial t}(\tilde{x}, t) dV.$$

This rate of increase (decrease) of mass in  $W$  equals the rate of mass getting into (exiting) the volume:

$$\frac{d}{dt} \int_W \rho dV = \oint_{\partial W} \rho \tilde{v} \cdot \tilde{n} dA,$$

where  $\partial W$  is the surface of  $W$  and  $\tilde{n}$  is the outward unit normal vector. The divergence theorem states that:

$$\oint_{\partial W} \tilde{f} \cdot \tilde{n} dA = \int_W \operatorname{div} \tilde{f} dV.$$

Applying it, we then have

$$\int_W \left[ \frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \tilde{v}) \right] dV = 0.$$

This is the conservation law in integral form. Since this is valid for all  $W$  we have the differential conservation form:

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \tilde{v}) = 0.$$

2. Conservation of momentum:

Let the velocity be

$$\tilde{v}(\tilde{x}, t) = \frac{d\tilde{x}(t)}{dt}$$

and the acceleration be

$$\tilde{a}(t) = \frac{d^2\tilde{x}(t)}{dt^2}.$$

Then using the chain rule we have

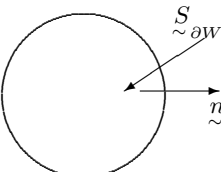
$$\begin{aligned} \tilde{a}(t) &= \frac{\partial \tilde{v}}{\partial x} \dot{x} + \frac{\partial \tilde{v}}{\partial y} \dot{y} + \frac{\partial \tilde{v}}{\partial z} \dot{z} + \frac{\partial \tilde{v}}{\partial t} \\ &= \partial_t \tilde{v} + \tilde{v} \cdot \nabla \tilde{v}. \end{aligned}$$

Let  $\frac{D}{Dt} = \partial_t + \tilde{v} \cdot \nabla$  be the material derivative, that is, the derivative following a fluid particle.

First let's work with an ideal fluid: the only force is the pressure, there are no tangential stresses.

The force across the surface per unit area is  $p(\tilde{x}, t)\tilde{n}$ , where  $p(\tilde{x}, t)$  is the pressure and  $\tilde{n}$  is the outward unit normal.

Then the total force exerted on the fluid through the boundary is

$$\tilde{S}_{\partial W} = - \oint_{\partial W} p \tilde{n} dA.$$


The diagram shows a circle representing a fluid element. A horizontal arrow labeled  $\tilde{n}$  points to the right from the center of the circle, representing the outward unit normal. Another arrow labeled  $\tilde{S}_{\partial W}$  points from the right edge of the circle towards the center, representing the force exerted on the fluid through the boundary.

For any fixed vector  $\tilde{e}$ :

$$\tilde{e} \cdot \tilde{S}_{\partial W} = - \oint_{\partial W} p \tilde{e} \cdot \tilde{n} dA = - \int_W \operatorname{div}(p\tilde{e}) dV = - \int_W (\operatorname{grad} p) \cdot \tilde{e} dV.$$

The second equality is obtained using the divergence theorem and the third one by using the vector identity  $\text{div}(\phi \underline{a}) = \phi \text{div} \underline{a} + \underline{a} \cdot \text{grad} \phi$  with  $\underline{a}$  fixed. Therefore we have that the surface force due to the pressure is

$$\underline{S}_{\partial W} = - \int_W \text{grad} p dV.$$

If  $\underline{b}(\underline{x}, t)$  is the body force per unit mass, usually only the force of gravity, then the total body force is

$$\underline{B} = \int_W \rho \underline{b} dV.$$

Therefore, for any piece of material, the force per unit volume is  $-\text{grad} p + \rho \underline{b}$ . By Newton's second law, (which states that, for constant density, the force is equal to the mass times the acceleration), we have the balance of momentum law

$$\rho \frac{D \underline{v}}{Dt} = -\text{grad} p + \rho \underline{b}.$$

### 3. Conservation of Energy

First we will deal only with mechanical energy, that is, kinetic energy. Over a volume  $W_t$ , that always has the same molecules, it is defined as

$$E_k = \frac{1}{2} \int_{W_t} \rho \|\underline{v}\|^2 dV$$

Its rate of change with time is

$$\begin{aligned} \frac{d}{dt} E_k &= \frac{d}{dt} \left[ \frac{1}{2} \int_{W_t} \rho \|\underline{v}\|^2 dV \right] \\ &= \frac{1}{2} \int_{W_t} \rho \frac{D \|\underline{v}\|^2}{Dt} dV \\ &= \int_{W_t} \rho \left( \underline{v} \cdot \left( \frac{\partial \underline{v}}{\partial t} + (\underline{v} \cdot \nabla) \underline{v} \right) \right) dV. \end{aligned}$$

The last equality is since  $\frac{1}{2} \frac{D \|\underline{v}\|^2}{Dt} = \underline{v} \cdot \frac{\partial \underline{v}}{\partial t} + (\underline{v} \cdot \nabla) \underline{v}$  as can be proven working component-wise.

#### Incompressible Flow

The rate of change of the kinetic energy equals the rate at which the pressure and body forces do work:

$$\frac{d}{dt} E_k = - \int_{\partial W_t} p \underline{v} \cdot \underline{n} dA + \int_{W_t} \rho \underline{v} \cdot \underline{b} dV,$$

and using the divergence theorem we get:

$$\int_{W_t} \rho \left[ \tilde{v} \cdot \left( \frac{\partial \tilde{v}}{\partial t} + \tilde{v} \cdot \nabla \tilde{v} \right) \right] dV = - \int_{W_t} \operatorname{div}(\rho \tilde{v}) - (\rho \tilde{v} \cdot b) dV.$$

Since the fluid is incompressible the law of mass conservation,  $\frac{D\rho}{Dt} + \rho \operatorname{div} \tilde{v} = 0$ , implies that  $\operatorname{div} \tilde{v} = 0$ .

Therefore the last integral is

$$- \int_{W_t} \left( \tilde{v} \cdot \nabla p - \rho \tilde{v} \cdot \tilde{b} \right) dV.$$

And, since the volume is arbitrary:

$$\rho \left[ \tilde{v} \cdot \left( \frac{\partial \tilde{v}}{\partial t} + \tilde{v} \cdot \nabla \tilde{v} \right) \right] = -\tilde{v} \cdot \nabla p + \rho \tilde{v} \cdot \tilde{b}$$

or  $\rho \frac{D\tilde{v}}{Dt} = -\nabla p + \rho \tilde{b}$  which is the conservation of momentum law.

### Navier-Stokes Equations

Now we will include the viscous forces, so the force acting on a surface  $S$  per unit area is  $-p(\tilde{x}, t)\tilde{n} + \tilde{\sigma}(x, t) \cdot \tilde{n}$ , where  $\tilde{\sigma}$  is the shear stress tensor, which is of rank 2.

We need more assumptions to be able to close the system. We assume that the fluid is newtonian, for which the shear tensor is given by

$$\tilde{\sigma} = 2\mu \left[ D - \frac{1}{3} \operatorname{div} \tilde{v} I \right] + \zeta (\operatorname{div} \tilde{v}) I,$$

where  $\mu$  is the first coefficient of viscosity,

$\zeta = \lambda + \frac{2}{3}\mu$  is the second coefficient of viscosity and

$D$  is the deformation tensor, given by  $D = \frac{1}{2} \left[ \operatorname{grad} \tilde{v} + (\operatorname{grad} \tilde{v})^T \right]$ .

Component-wise the deformation tensor is  $D_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ .

And  $I$  is the identity matrix.

Using the divergence theorem as before, the moment balance law gives the Navier-Stokes equations:

$$\rho \frac{D\tilde{v}}{Dt} = -\nabla p + (\lambda + \mu) \nabla (\operatorname{div} \tilde{v}) + \mu \Delta \tilde{v},$$

$$\text{where } \Delta \tilde{v} = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \tilde{v}.$$

## 1.2 Mixtures

Many real life problems involve fluids that consist of more than one phase (liquid, gas) and more than one component or species (water, methane). So we have to determine how to study solutions, or fluids in permeable media, or mixtures with chemical reactions? To answer these questions we need to obtain the conservation laws for mixtures.

Definition: A mixture is a collection of  $N$  bodies called constituents, forming overlapping continua. At each point in space,  $\tilde{x}$ , we can have material from each constituent.

For example: Salt water has water and sodium,  $N_a^+$ , and chloride,  $Cl^-$ . From a molecular point of view the species are separated but macroscopically they occupy the same space.

Another example is sandstone, which is a porous and permeable rock, filled with water. The segregation of the phases is observable at a microscopic scale much larger than the molecular scale. But macroscopically sandstone and water occupy the same space.

Suppose we have  $N$  constituents,  $\alpha = 1, \dots, N$ . Each one has its own motion:

$$\tilde{x}^\alpha = \tilde{x}^\alpha(\tilde{X}^\alpha, t)$$

$$\tilde{X}^\alpha = \tilde{X}^\alpha(\tilde{x}^\alpha, t),$$

where  $\tilde{X}^\alpha$  is the Lagrangian label of the particle initially at spatial (eulerian) position  $\tilde{x}^\alpha$ .

Also its own velocity:

$$\tilde{V}^\alpha(\tilde{X}^\alpha, t) = \frac{\partial \tilde{x}^\alpha}{\partial t}(\tilde{X}^\alpha, t); \quad \tilde{v}^\alpha(\tilde{x}^\alpha, t) = \tilde{V}^\alpha(\tilde{X}^\alpha(\tilde{x}^\alpha, t), t),$$

and its own density  $\rho^\alpha(\tilde{x}^\alpha, t)$  (mass of  $\alpha$  per unit volume of  $\alpha$ ).

The total mass of  $\alpha$  in a part  $P$  of the mixture is

$$M^\alpha(P) = \int_{\tilde{x}^\alpha(P)} \rho^\alpha dV$$

For multiphase mixtures, we assign to each constituent  $\alpha$  a volume fraction,  $\phi^\alpha(\tilde{x}^\alpha, t)$ , which is the fraction of the volume occupied by  $\alpha$ . So that in any part  $P$  of the mixture the total volume within  $P$  occupied by  $\alpha$  is

$$F^\alpha(P) = \int_{\tilde{x}^\alpha(P)} \phi^\alpha dV,$$

where  $\phi^\alpha = \frac{\text{volume of } \alpha}{\text{volume of mixture}}$ . Therefore,  $0 \leq \phi^\alpha \leq 1$  and  $\sum_{\alpha=1}^N \phi^\alpha = 1$ .

We need some definitions.

Definition.- Overall mass density:

$$\rho = \begin{cases} \sum_{\alpha=1}^N \rho^\alpha & \text{multispecies mixtures} \\ \sum_{\alpha=1}^N \phi^\alpha \rho^\alpha & \text{multiphase mixtures} \end{cases}$$

Definition.- Mass fraction:

$$w^\alpha = \begin{cases} \frac{\rho^\alpha}{\rho} & \text{multispecies mixtures} \\ \phi^\alpha \frac{\rho^\alpha}{\rho} & \text{multiphase mixtures} \end{cases}$$

Note that

$$\sum_{\alpha=1}^N w^\alpha = 1.$$

Definition.- Baricentric velocity (mass weighted mean of velocities):

$$\tilde{v} = \begin{cases} \frac{1}{\rho} \sum_{\alpha=1}^N \rho^\alpha \tilde{v}^\alpha & \text{multispecies} \\ \frac{1}{\rho} \sum_{\alpha=1}^N \phi^\alpha \rho^\alpha \tilde{v}^\alpha & \text{multiphase} \end{cases}$$

The diffusion velocity of a constituent  $\alpha$  with respect to the mean mixture flow velocity is

$$\tilde{v}^\alpha = v^\alpha - \tilde{v}.$$

Note that for multispecies mixtures

$$\begin{aligned} \sum_{\alpha} w^\alpha \tilde{v}^\alpha &= \frac{1}{\rho} \sum_{\alpha} \rho^\alpha (v^\alpha - \tilde{v}) = \frac{1}{\rho} \left[ \sum_{\alpha} \rho^\alpha \tilde{v}^\alpha - \tilde{v} \sum_{\alpha} \rho^\alpha \right] \\ &= \tilde{v} - \frac{1}{\rho} \tilde{v} \rho = \tilde{v} - \tilde{v} = 0. \end{aligned}$$

And similarity for multiphase mixtures. For mixtures the general global balance laws are:

Multispecies

$$\sum_{\alpha=1}^N \left( \frac{d}{dt} \int_{V_\alpha} \rho^\alpha \psi^\alpha dV - \oint_{\partial V_\alpha} \tilde{\mathcal{T}}^\alpha \cdot \tilde{n} dA - \int_{V_\alpha} \rho^\alpha g^\alpha dV \right) = 0.$$

Multiphase

$$\sum_{\alpha=1}^N \left( \frac{d}{dt} \int_{\nu_\alpha} \phi^\alpha \rho^\alpha \psi^\alpha dV - \oint_{\partial\nu_\alpha} \tilde{\tau}^\alpha \cdot \tilde{n} dA - \int_{\nu_\alpha} \phi^\alpha \rho^\alpha g^\alpha dV \right) = 0.$$

Local or differential mixture balance laws are obtained in a similar way to the one constituent case.

Multispecies:

$$\sum_{\alpha=1}^N \left[ \frac{D^\alpha}{Dt} (\rho^\alpha \psi^\alpha) + \rho^\alpha \psi^\alpha \operatorname{div} \tilde{v}^\alpha - \operatorname{div} \tilde{\tau}^\alpha - \rho^\alpha g^\alpha \right] = 0.$$

Multiphase:

$$\sum_{\alpha=1}^N \left[ \frac{D^\alpha}{Dt} (\phi^\alpha \rho^\alpha \psi^\alpha) + \phi^\alpha \rho^\alpha \psi^\alpha \operatorname{div} \tilde{v}^\alpha - \operatorname{div} \tilde{\tau}^\alpha - \phi^\alpha \rho^\alpha g^\alpha \right] = 0.$$

Here

$$\frac{D^\alpha}{Dt} = \begin{cases} \frac{\partial}{\partial t} & \text{for functions of Lagrange coordinates } (\tilde{X}^\alpha, t) \\ \frac{\partial}{\partial t} + \tilde{v}^\alpha \cdot \nabla & \text{for functions of spatial coordinates } (\tilde{x}^\alpha, t). \end{cases}$$

To write the conservation law for each constituent we need to take into account the interactions among constituents. Let  $e^\alpha$  be a measurement of the exchange of  $\psi$  into constituent  $\alpha$  from other constituents.

Therefore we have:

Multispecies

$$\frac{D^\alpha}{Dt} (\rho^\alpha \psi^\alpha) + \rho^\alpha \psi^\alpha \operatorname{div} \tilde{v}^\alpha - \operatorname{div} \tilde{\tau}^\alpha - \rho^\alpha g^\alpha = e^\alpha, \quad \alpha = 1, \dots, N.$$

Multiphase

$$\frac{D^\alpha}{Dt} (\phi^\alpha \rho^\alpha \psi^\alpha) + \phi^\alpha \rho^\alpha \psi^\alpha \operatorname{div} \tilde{v}^\alpha - \operatorname{div} \tilde{\tau}^\alpha - \phi^\alpha \rho^\alpha g^\alpha = e^\alpha, \quad \alpha = 1, \dots, N.$$

From the laws for the whole mixture we can see that

$$\sum_{\alpha=1}^N e^\alpha = 0.$$

As a first example, consider the transport of a dissolved contaminant by a fluid.

The constituents are:  $S$ =solute(contaminant)       $F$ =fluid.

So we have a multispecies mixture with no chemical reactions.

Looking at the mass balance:  $\psi^\alpha = 1$        $\tau^\alpha = 0$ ,       $g^\alpha = 0$ ,       $e^\alpha = 0$ .

( $e^\alpha$  is the production of constituent  $\alpha$  by chemical reaction but in this case there is none).

$$\frac{D^\alpha \rho^\alpha}{Dt} + \rho^\alpha \operatorname{div} \tilde{v}^\alpha = \frac{\partial \rho^\alpha}{\partial t} + \operatorname{div}(\rho^\alpha \tilde{v}^\alpha) = 0 \quad \alpha = S, F$$

$$\frac{\partial \rho^\alpha}{\partial t} + \operatorname{div}(\rho^\alpha \tilde{v}^\alpha) + \operatorname{div} \tilde{j}^\alpha = 0,$$

where:  $\tilde{j}^\alpha = \rho^\alpha \tilde{v}^\alpha$  is the diffusive flux.

Consider the solute, we need a constitutive law for  $\tilde{j}^S$ . Use Fick's Law:

$$\tilde{j}^S = -K^S \nabla \rho^S \quad \text{with } K^S > 0, \text{ the diffusion coefficient.}$$

$$\text{This implies } \frac{\partial \rho^S}{\partial t} + \operatorname{div}(\rho^S \tilde{v}^S) - \operatorname{div}(K^S \nabla \rho^S) = 0 \quad \text{Advection-diffusion transport equation.}$$

Example: Fluid Flow in porous rock. Even for one fluid this is multiphase. We have two constituents:  $F$  fluid,  $R$ , rock. Assume that the flow is chemically inert (no mass exchanges) and that the rock is immobile ( $\tilde{v}^R = 0$ ). Lets look at the conservation of momentum law:

$$\begin{aligned} \psi^\alpha &= \tilde{v}^\alpha, & \text{velocity} \\ \tilde{\tau}^\alpha &= \mathbf{t}^\alpha, & \text{stress tensor} \\ \tilde{g}^\alpha &= \tilde{b}^\alpha, & \text{body forces} \\ e^\alpha &= \tilde{m}^\alpha, & \text{rate of momentum exchange.} \end{aligned}$$

The differential conservation law is then:

$$\begin{aligned} \frac{D^\alpha}{Dt} (\phi^\alpha \rho^\alpha \tilde{v}^\alpha) + \phi^\alpha \rho^\alpha \tilde{v}^\alpha \operatorname{div} \tilde{v}^\alpha - \operatorname{div} \mathbf{t}^\alpha - \phi^\alpha \rho^\alpha \tilde{b}^\alpha &= \tilde{m}^\alpha \\ \rho^\alpha \phi^\alpha \frac{D^\alpha \tilde{v}^\alpha}{Dt} + v^\alpha \underbrace{\left[ \frac{D}{Dt} (\phi^\alpha \rho^\alpha) + \phi^\alpha \rho^\alpha \operatorname{div} \tilde{v}^\alpha \right]}_{\text{mass balance}} - \operatorname{div} \mathbf{t}^\alpha - \phi^\alpha \rho^\alpha \tilde{b}^\alpha &= \tilde{m}^\alpha \end{aligned}$$

Suppose the fluid is inviscid:

$$t^F = -pI.$$

and that the only body force is gravity:

$$\phi^F \tilde{b}^F = g \nabla z, \quad z \text{ is the depth below a reference level.}$$

Suppose the momentum transfer is given by Stokes drag which says that  $\tilde{m}^F$  is proportional to the fluid velocity:

$$\tilde{m}^F = \frac{\phi^F}{\Lambda} (-\tilde{v}^F) = -\frac{\phi^F}{\Lambda} \tilde{v}^F, \quad \text{where } \Lambda \text{ is the fluid mobility.}$$

The conservation law is now:

$$\phi^F \rho^F \frac{D^F \tilde{v}^F}{Dt} + \nabla p^F - \rho^F g \nabla z = -\frac{\phi^F}{\Lambda} \tilde{v}^F.$$

A common assumption is that the fluid inertia is negligible compared with the pressure, gravity and momentum exchanges:

$$\frac{D^F \tilde{v}^F}{Dt} = 0.$$

So the conservation law simplifies to:

$$\tilde{v}^F = \frac{\Lambda}{\phi^F} (\nabla p^F - \rho^F g \nabla z).$$

The fluid mobility,  $\Lambda$ , depends on both the fluid and the rock:

$$\Lambda = \frac{k}{\mu^F},$$

where  $\mu^F$  is the fluid dynamic viscosity and  $k$  is the permeability of the rock. So finally, we obtain the well known Darcy's law:

$$\tilde{v}^F = -\frac{k}{\mu^F \phi^F} (\nabla p^F - \rho^F g \nabla z).$$

To a macroscopic observer  $\tilde{v}^F$  is the mean fluid velocity through the pores of the rock. An observer at the pore scale would need to use the Navier-Stokes equations on the irregular geometry given by the pores. Darcy derived the law that has his name from experimental observations.

For many sedimentary porous media, the flow is anisotropic. To take this into account let  $k$  be a tensor

$$\tilde{v}^k = -\frac{\mathbf{k}}{\phi \mu^F} \cdot (\nabla p^F - \rho^F g \nabla z)$$

Although  $k$  is supposed to depend only on the rock it is different for gases than for liquids. For liquids there is friction between the liquid and the rock, there is a no-slip boundary condition between the two. For gases the friction is negligible.

### 1.3 Multiphase Flows in Porous Media

Lets look at the simplest of what is commonly called multiphase flow. That is, a flow with two fluid phases. So we have three phases: rock  $R$ , aqueous fluid  $W$ , and nonaqueous fluid  $N$ . Assume Darcy's Law holds for both  $W$  and  $N$ :

$$\begin{aligned} \tilde{v}^W &= -\frac{\Lambda^W}{\phi^W} (\nabla p_W - \rho^W g \nabla z) \\ \tilde{v}^N &= -\frac{\Lambda^N}{\phi^N} (\nabla p_N - \rho^N g \nabla z). \end{aligned}$$

A lot of work has been done into simplifying the problem. One possibility is to work with different variables. Let  $\phi = 1 - \phi^R = \phi^W + \phi^N$  be the porosity of the rock. Define the saturations as

$$S_W = \frac{\phi^W}{\phi}, \quad S_N = \frac{\phi^N}{\phi}, \quad \text{fraction of pore spore occupied by the respective fluids.}$$

So we have

$$S_W + S_N = 1.$$

Decompose the fluid mobilities,  $\Lambda^W$  and  $\Lambda^N$ , into

$$\Lambda^W = \frac{k_W}{\mu^W}, \quad \Lambda^N = \frac{k_N}{\mu_N}.$$

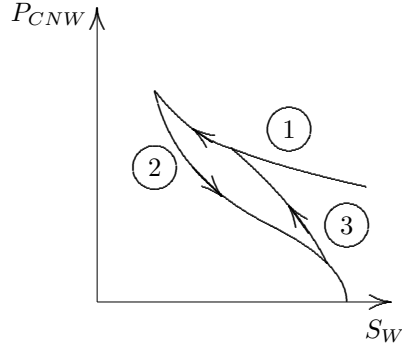
$k_W$  and  $k_N$  are no longer rock properties alone, since one fluid blocks the flow of the other. Suppose that the effective permeability depends on the fluid saturation of the phase increasing with its saturation. This is because the more we have of fluid  $\alpha$  the less the other fluid interferes with its flow.

$$\begin{aligned} k_W &= k k_{rW}(S_W), \\ k_N &= k k_{rN}(S_W), \quad S_N = 1 - S_W. \end{aligned}$$

For two fluids with a fixed interfacial tension, the interfacial geometry varies with saturation so we can expect  $p_N - p_W$  to be a function of the saturation  $S_W$  :

$$p_N - p_W = p_{CNW}(S_W).$$

The capillary pressure may be a multivalued function due to hysteresis.



### Mass Balance

The differential mass balance is given by:

$$\frac{\partial}{\partial t} (\phi^\alpha \rho^\alpha) + \text{div} (\phi^\alpha \rho^\alpha \tilde{v}^\alpha) = r^\alpha$$

If we assume there is no interphase mass transfer,  $r^\alpha = 0$ .

Eliminating the mass fractions in favor of the saturations,  $\phi^\alpha = \phi S_\alpha$  we have

$$\frac{\partial}{\partial t} (\phi S_\alpha \rho^\alpha) + \text{div} (\phi S_\alpha \rho^\alpha \tilde{v}^\alpha) = 0.$$

Substitute  $\tilde{v}^\alpha$  from Darcy's law (which is the conservation of momentum) into the conservation of  $W$  and  $N$ :

$$\begin{aligned}\frac{\partial}{\partial t} (\phi S_W \rho^W) - \operatorname{div} \left[ \rho^W \frac{k k_{rW}}{\mu_W} (\nabla p_W - \rho^W g \nabla z) \right] &= 0 \\ \frac{\partial}{\partial t} (\phi (1 - S_W) \rho^N) - \operatorname{div} \left[ \rho^N \frac{k k_{rN}}{\mu_N} (\nabla p_W + \nabla p_{CNW} - \rho^N g \nabla z) \right] &= 0.\end{aligned}$$

Here,  $p_W$  and  $S_W$  are considered the primary unknowns. Empirical measurements are necessary to establish the relationships

$$\begin{aligned}k_{r\alpha} &= k_{r\alpha}(S_W) \quad \alpha = W, N \\ p_{CNW} &= p_{CNW}(S_W) \\ \rho^W &= \rho^W(p_W) \\ \rho^N &= \rho^N(p_N) = \rho^N(p_W, p_{CNW}(S_W))\end{aligned}$$

We also need initial conditions  $p_W(\underline{x}, 0)$ ,  $S_W(\underline{x}, 0)$ . These are known from measurements and interpolated to get the desired functions.

The final thing that we need are boundary conditions. Specify  $p_W$  at the boundaries of the flow region. Also, specify the normal flux of aqueous fluid across the boundaries. That is, give

$$\tilde{v}^W \cdot \tilde{n} = -\frac{\Lambda^W}{\phi^W} (\nabla p_W - \rho^W g \nabla z) \cdot \tilde{n}$$

Many times, such as in oil reservoirs, there is no flux at the boundary:  $\tilde{v}^W \cdot \tilde{n} = 0$ .

## 1.4 Multiphase-multispecies Flows

Many mixtures of interest, such as oil reservoirs, consist of several phases and several species. They consist of several phases including rock, oil, water and gas. They also consist of many molecular species such as methane, propane, water and salt.

Let the species be  $i = 1, \dots, N+1$  and consider three fluid phases, aqueous( $W$ ), oil( $O$ ) and gas( $G$ ) and one rock phase( $R$ ). One of the species is the rock material, for example, sandstone. In contamination problems, the phase may be rock, water and DNAPL (dense nonaqueous phase liquids) or maybe even bacteria. We will concentrate on modelling an oil reservoir.

In this mixture each pair  $(i, \alpha)$  with  $i$  chosen from the species indices and  $\alpha$  from the phases is a constituent. Example: methane in gas is one constituent and methane in oil is another.

$\rho_i^\alpha$ , intrinsic mass density of species  $i$  in phase  $\alpha$  (mass of  $i$ /unit volume of  $\alpha$ )

$\phi_\alpha$ , volume fraction of phase  $\alpha$

$S_\alpha$ , saturation of phase  $\alpha = \phi_\alpha/\phi$ ,  $\phi = 1 - \phi_R$ , porosity

$\rho^\alpha = \sum_{i=1}^N \rho_i^\alpha$ , intrinsic mass density of phase  $\alpha$

$W_i^\alpha = \frac{\rho_i^\alpha}{\rho^\alpha}$ , mass fraction of species  $i$  in phase  $\alpha$  [mass  $i$ /mass  $\alpha$ ]

$\rho = \phi \sum_{\alpha \neq R} S_\alpha \rho^\alpha$ , bulk density of fluids [mass of fluids/volume]

$W_i = \left(\frac{\phi}{\rho}\right) \sum_{\alpha \neq R} S_\alpha \rho^\alpha W_i^\alpha$ , total mass fraction of species  $i$  in the fluids [mass of  $i$ /mass of fluids]

The baricentric velocity of phase  $\alpha$  is

$$\underset{\sim}{v}^\alpha = \frac{1}{\rho^\alpha} \sum_{i=1}^n \rho_i^\alpha \underset{\sim}{v}_i^\alpha.$$

The diffusion velocity of species  $i$  in phase  $\alpha$  is

$$\underset{\sim}{u}_i^\alpha = \underset{\sim}{v}_i^\alpha - \underset{\sim}{v}^\alpha.$$

Constraints

$$\sum_{i=1}^N W_i = \sum_{i=1}^N W_i^\alpha = 1, \quad \text{for every } \alpha$$

$$\sum_{\alpha} \phi_\alpha = \sum_{\alpha \neq R} S_\alpha = 1$$

$$\sum_{i=1}^N \rho_i^\alpha \underset{\sim}{u}_i^\alpha = 0.$$

The mass balance law for constituent  $(i, \alpha)$  is:

$$\frac{\partial}{\partial t} (\phi_\alpha \rho_i^\alpha) + \text{div} \left( \phi_\alpha \rho_i^\alpha \underset{\sim}{v}_i^\alpha \right) = r_i^\alpha. \quad (*)$$

exchange terms

Rewrite (\*) as

$$\frac{\partial}{\partial t} \left( \underbrace{\phi S_\alpha}_{\phi_\alpha} \underbrace{\rho^\alpha W_i^\alpha}_{\rho_i^\alpha} \right) + \text{div} \left( \phi S_\alpha \rho^\alpha W_i^\alpha \underbrace{\underset{\sim}{v}}_{\text{velocity of phase}} \right) + \text{div} \underset{\sim}{j}_i^\alpha = r_i^\alpha, \quad (**)$$

where  $\underset{\sim}{j}_i^\alpha = \phi S_\alpha \rho^\alpha W_i^\alpha \underset{\sim}{u}_i^\alpha$  is the diffusive flux.

Assume no intraphase chemical reactions and  $\sum_{\alpha \neq R} r_i^\alpha = 0$  for each species.

Sum (\*\*) over all fluid phases to get the total balance law for each species.

$$\begin{aligned} \frac{\partial}{\partial t}(\rho W_i) + \operatorname{div} \left[ \phi \left( S_W \rho^W W_i^W \tilde{v}^W + S_O \rho^O W_i^O \tilde{v}^O + S_G \rho^G W_i^G \tilde{v}^G \right) \right] \\ + \operatorname{div} \left( \tilde{j}_i^W + \tilde{j}_i^O + \tilde{j}_i^G \right) = 0 \quad i = 1, \dots, W. \end{aligned}$$

Assume Darcy's law for each phase

$$\tilde{v}^\alpha = -\frac{k k_{r\alpha}}{\mu^\alpha \phi S_\alpha} (\nabla p^\alpha - \rho^\alpha g \nabla z) \quad \alpha = W, O, G.$$

Assume the hydrodynamic dispersion is small

$$\begin{aligned} \tilde{j}_i^W + \tilde{j}_i^O + \tilde{j}_i^G \simeq 0 \\ \frac{\partial}{\partial t} \left[ \phi \left( S_W \rho^W W_i^W + S_O \rho^O W_i^O + S_G \rho^G W_i^G \right) \right] \\ - \operatorname{div} \left[ \frac{k k_{rW} \rho^W W_i^W}{\mu^W} (\nabla p_W - \rho_g^W \nabla z) + \frac{k k_{rO} \rho^O W_i^O}{\mu^O} (\nabla p_O - \rho^O g \nabla z) \right. \\ \left. - \frac{k k_{rG} \rho^G W_i^G}{\mu^G} (\nabla p_G - \rho^G g \nabla z) \right] = 0 \quad i = 1, \dots, N. \end{aligned}$$

To close the system, we need some supplementary constraints. Some are the equations of state:

$$\begin{aligned} \rho^\alpha &= \rho^\alpha(W_1^\alpha, \dots, W_N^\alpha, p_\alpha) & \alpha &= W, O, G \\ W_i^\alpha &= W_i^\alpha(W_1, \dots, W_N, p_\alpha) & \alpha &= W, O, G \\ S_\alpha &= S_\alpha(W_1, \dots, W_N, p_\alpha) & \alpha &= W, O, G, \end{aligned}$$

which may be given explicitly, implicitly or in tabular form.

The other constraints are the constitutive relations:

$$\begin{aligned} p_O - p_W &= p_{COW} = p_{COW}(S_O, S_G) \\ p_G - p_O &= p_{CGO}(S_0, S_G) \\ k_{r\alpha} &= k_{r\alpha}(S_0, S_G) \quad \alpha = W, O, G. \end{aligned}$$

The previous material is based partially on [2], [6], [3] and [4].

# Chapter 2

## Numerical Methods.

### 2.1 Basic Methods for Parabolic Equations

We will review some numerical methods for parabolic differential equations. We will look at

- Finite Difference Methods
- Weighted Residual Methods
- Finite Volume Methods
- Characteristic Methods
- Nonstandard Methods
- Other Methods

#### Finite Difference Methods

They are the easiest to think about:

Replace derivatives by finite differences

- $\left(\frac{du}{dx}\right)_i \approx \frac{u_{i+1}-u_i}{\Delta x}$  *forward difference*
- $\left(\frac{du}{dx}\right)_i \approx \frac{u_i-u_{i-1}}{\Delta x}$  *backward difference*
- $\left(\frac{du}{dx}\right)_i \approx \frac{u_{i+1}-u_{i-1}}{2\Delta x}$  *central difference*
- $\left(\frac{d^2u}{dx^2}\right)_i = \frac{d}{dx} \left(\frac{du}{dx}\right)_i \approx \frac{1}{\Delta x} \left[ \left(\frac{du}{dx}\right)_{i+1} - \left(\frac{du}{dx}\right)_i \right] = \frac{1}{\Delta x} \left( \frac{u_{i+1}-u_i}{\Delta x} - \frac{u_i-u_{i-1}}{\Delta x} \right) = \frac{u_{i+1}-2u_i+u_{i-1}}{\Delta x^2}$

We will start with an ordinary differential equation example:

Second order equation

$$\frac{d^2u}{dx^2} + 2 = 0$$

with Dirichlet boundary conditions:

$$u = 0 \quad \text{at } x = 0$$

$$u = 0 \quad \text{at } x = 1.$$

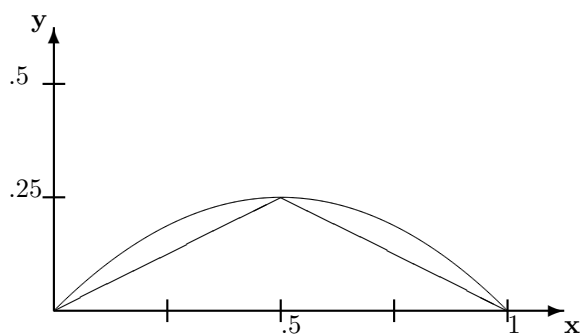
Replacing the second derivative by finite differences we obtain:

$$\frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + 2 = 0,$$

which is a system of equations in  $u_i$ .

If  $\Delta x = 1/2$ , then we have three points. With  $u_0 = 0$  and  $u_2 = 0$  from the boundary conditions, we have  $u_1 = 1/4$  which is the exact value at  $x = 1/2$ .

The finite difference solution is



### Method of Weighted Residuals

We seek an approximate solution  $\hat{u}$  of the form

$$\hat{u}(x) = \sum_{i=0}^N u_i \varphi_i(x)$$

$\uparrow \quad \uparrow$   
 Unknown    Known  
 Coefficients    Basic functions

The basis functions (Legendre, trigonometric, piecewise Lagrange) are usually chosen to satisfy the b.c. but not the equation.

When we substitute the approximation of the true solution into an equation  $Lu = f$ , we get a residual,  $R$ :

$$R(\hat{u}) = L\hat{u} - f$$

The residuals are made zero in an average sense: Pick  $N$  weighting functions  $w_j$ ,  $j = 1, 2, \dots, N$ .

Define the weighted average as:

$$\langle w, u \rangle = \int_{\Omega} w u dx$$

and make

$$\langle w_j, R(\hat{u}) \rangle = 0 \quad j = 1, 2, \dots, N,$$

which is a system of  $N$  linear equations.

### Weighted Residual Methods

- Subdomain: divide the domain  $\Omega$  into subdomains  $\Omega_j$  not necessarily disjoint and choose

$$w_j = \begin{cases} 1 & (x, y) \in \Omega_j \\ 0 & \text{otherwise} \end{cases}$$

- Collocation: pick  $N$  points  $(x_j, y_j)$  in  $\Omega$  and choose  $w_j(x, y) = \delta((x, y) - (x_j, y_j))$

$$\langle w_j, R\hat{u} \rangle = \int_{\Omega} \delta((x, y) - (x_j, y_j)) R(\hat{u}) dx dy = R(\hat{u}(x_j, y_j)) = 0$$

So equation is satisfied exactly at  $(x_j, y_j)$ .

- Least squares

$$w_j = \frac{\partial R}{\partial u_j}$$

$$\int_{\Omega} R \frac{\partial R}{\partial u_0} dx = \frac{1}{2} \int_{\Omega} \frac{\partial R^2}{\partial u_j} dx = 0$$

- Bubnov-Galerkin

$$w_j = \varphi_j$$

### Finite Elements

The method of finite elements requires that the basis functions,  $\varphi_j(x)$  be finite elements, that is, they be zero except for a small portion of the domain.

Lets start with a one-dimensional example:

$$\frac{du}{dx} + bu = h \quad 0 < x < 1$$

$$u(0) = 1$$

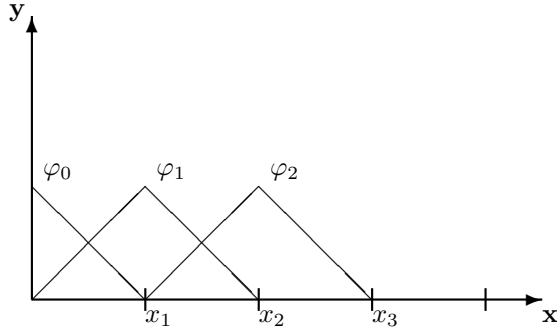
Define grid:  $x_0, x_1, \dots, x_N$  Let

$$\{\varphi_j(x)\}_{j=0}^N$$

be piecewise Lagrange polynomials on  $x_0, x_1, \dots, x_N$

$$\varphi_j(x) = \begin{cases} \frac{x - x_{j-1}}{x_j - x_{j-1}} & x_{j-1} \leq x \leq x_j \\ \frac{x_{j+1} - x}{x_{j+1} - x_j} & x_j < x \leq x_{j+1} \\ 0 & \text{otherwise} \end{cases}$$

The piecewise linear basis functions are:



$u_0$  is known from the b.c.:

$$u(0) = \hat{u}(0) = u_0 = 1$$

$$\Rightarrow \hat{u}(x) = \varphi_0(x) = \sum_{j=1}^N u_j \varphi_j(x)$$

The residual is then:  $R(\hat{u}) = \varphi'_0 + \sum_{j=1}^N u_j \varphi'_j + k \left( \varphi_0 + \sum_{j=1}^N u_j \varphi_j \right) - h$ . In this method the weight functions are the same as the basis functions so pick  $w_j = \varphi_j \quad j = 1, \dots, N$ .

$$\int_0^1 R(\hat{u}) \varphi_j dx = 0 \quad j = 1, \dots, N$$

The above integrals involve only basis functions. They can usually be calculated exactly, as in this case, or using Gaussian quadrature formulas. We obtain a system of sparse linear equations, which can be solved using a Gaussian elimination method designed for tridiagonal matrices known as the Thomas algorithm.

### Collocation

The collocation method is similar differing only in the choice of weight functions:

- Choose grid
- Choose collocation points (where solution is exact)
- Define basis functions,  $\varphi_j$
- Satisfy Dirichlet boundary conditions
- Write approximating function

$$\hat{u}(x) = \varphi_0(x) + \sum_{j=1}^2 u_j \varphi_j(x)$$

- Substitute approximate solution into equation and find residual function
- Define weight functions,  $w_i(x) = \delta(x - \bar{x}_i)$

- Multiply residual by weight functions and integrate
- Integrals are immediate because of the  $\delta$  functions
- Solve sparse linear system

### Finite Volume Methods

Consider

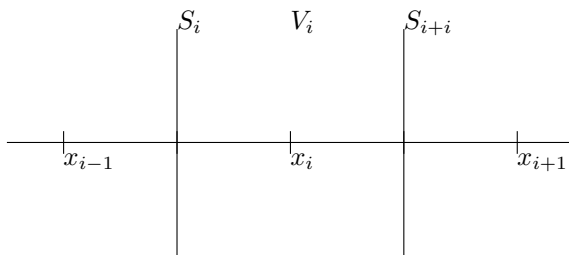
$$\frac{d^2 u}{dx^2} - 2 = 0, \quad 0 < x < 1$$

. Divide the domain into finite volumes and integrate the equation

$$\int_{x_{i-1}}^{x_{i+1}} \left( \frac{d^2 u}{dx^2} - 2 \right) dx = 0$$

. Integrating

$$\frac{du}{dx} \Big|_{x_{i-1}}^{x_{i+1}} - \int_{x_{i-1}}^{x_{i+1}} 2 dx = 0$$



Finite volume methods can be based on finite differences or on finite elements. Using finite differences:

$$\frac{u_{i+1} - u_i}{\Delta x} - \frac{u_i - u_{i-1}}{\Delta x} = 2\Delta x.$$

Using finite elements the method is:

- Choose basis functions
- Write approximate solution as linear combination
- Substitute into integrated expression
- Get same results as for finite differences.

### Parabolic equations

Parabolic equations are of the form

$$u_t = f(u_{xx}, u_x, u, x, t)$$

An example is

$$\begin{aligned}u_t &= u_{xx} & 0 < x < 1, \quad 0 < t \\u(x, 0) &= f(x) \\u(0, t) &= g_0(t), u(1, t) = g_1(t)\end{aligned}$$

The simplest method is the method of lines which consists of

- Discretize the x part of the equation using finite differences or finite elements
- Get a system of ordinary differential equations in time
- Solve using Euler, Runge-Kutta, etc. Usually the method is Euler or backward Euler or an average of both.

The numerical method that we choose needs to have some properties:

- Consistency: The discretized equations approach the exact equation as the grid is refined.
- Convergence: The approximate solution approaches the exact solution as the grid is refined.
- Stability: Errors don't grow.

The proof of consistency is easy, but have we really want is that we have convergence. The easiest way of proving convergence is to use the Lax equivalence theorem:

If the scheme inconsistent, then stability  $\Leftrightarrow$  convergence.

### Model equation

The heat equation is

$$u_t = Du_{xx}, \quad 0 < x < x_{\max}, \quad 0 < t \quad u(x, 0) = u_I, \quad 0 < x < x_{\max}$$

$$\left. \begin{aligned}u(0, t) &= u_2 \\u(x_{\max}, t) &= u_k\end{aligned} \right\} t > 0$$

If we use an explicit scheme

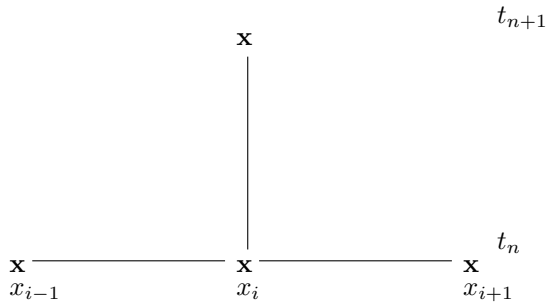
$$u_j^{n+1} - u_j^n = \frac{\Delta t}{\Delta x^2} (u_{j-1}^n - 2u_j^n + u_{j+1}^n).$$

t is stable if

$$\lambda = \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2},$$

which gives a restriction to very small time steps.

Explicit molecule:



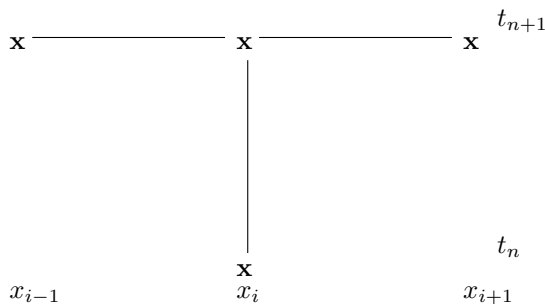
Fully Implicit:

$$u_j^{n+1} - u_j^n = \lambda (u_{j-1}^{n+1} - 2u_j^{n+1} + u_{j+1}^{n+1})$$

$$(1 + 2\lambda)u_j^{n+1} - \lambda (u_{j+1}^{n+1} + u_{j-1}^{n+1}) = u_j^n$$

This scheme is unconditionally stable, but we need to solve a system of algebraic equations. It also introduces artificial viscosity.

The implicit molecule is



Crank-Nicolson's method is an average of the explicit and implicit methods:

$$u_j^{n+1} - u_j^n = \left[ \theta (u_{j+1}^{n+1} - 2u_j^{n+1} + u_{j-1}^{n+1}) + (1 - \theta) (u_{j+1}^n - 2u_j^n + u_{j-1}^n) \right] \lambda$$

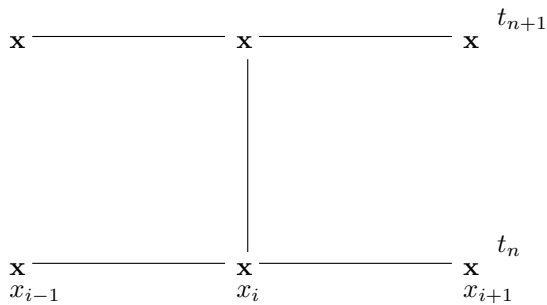
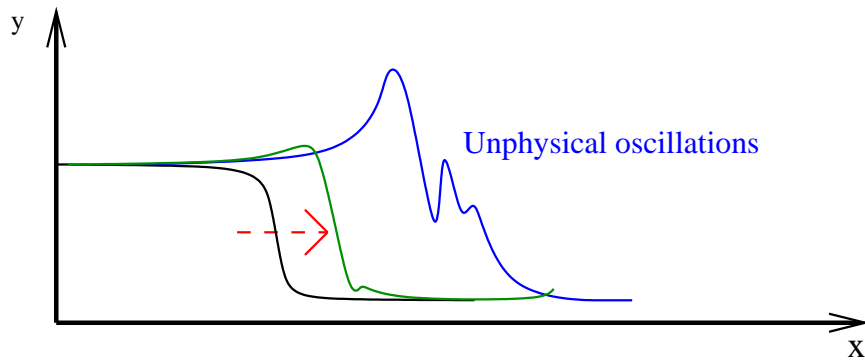
$\theta = 0$  explicit

$\theta = 1$  full implicit

$\theta = \frac{1}{2}$  Crank Nicolson

Crank-Nicolson's scheme is unconditionally stable, has better accuracy than the fully implicit method but still requires solution of algebraic systems

The Crank-Nicolson's molecule is



### Convection-diffusion equations

A model equation is

$$\frac{\partial u}{\partial t} = \frac{1}{Pe} \frac{\partial^2 u}{\partial x^2} - \frac{\partial u}{\partial x},$$

where  $Pe = \text{Peclet number} = \frac{v x_{\max}}{\Delta}$ . Applying Crank-Nicolson to the equation we get

$$\begin{aligned} \frac{\partial u}{\partial t} &\simeq \frac{u_i^{n+1} - u_i^n}{\Delta t} \\ \frac{\partial u}{\partial x} &\simeq \frac{1}{2} \frac{u_{i+1}^{n+1} - u_{i-1}^{n+1}}{2\Delta x} + \frac{1}{2} \frac{u_{i+1}^n - u_{i-1}^n}{2\Delta x} \\ \frac{\partial^2 u}{\partial x^2} &\simeq \frac{1}{2} \frac{(u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1})}{\Delta x^2} \\ &\quad + \frac{1}{2} \frac{(u_{i+1}^n - 2u_i^n + u_{i-1}^n)}{\Delta x^2}. \end{aligned}$$

The truncation error is  $\theta(\Delta t^2 + \Delta x^2)$

If  $\Delta x > \frac{2}{Pe}$  we have spurious oscillations that produce instabilities.

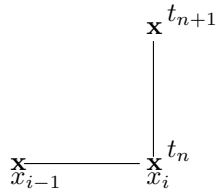
The convection-diffusion equation is also written as

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} - \frac{\partial}{\partial x} (D \partial c \partial x) = 0,$$

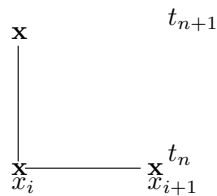
where  $v$  is the velocity of the fluid, and  $D$  is the diffusion coefficient. For most problems in porous media, the convection term dominates. For example in modeling transport of a solute in a fluid. Then the behavior

is close to that of hyperbolic equations. Which means that the numerical scheme needs to move information in the same direction as the differential equation. Upwind schemes are designed to do it:

If  $v > 0$ , forward differences:



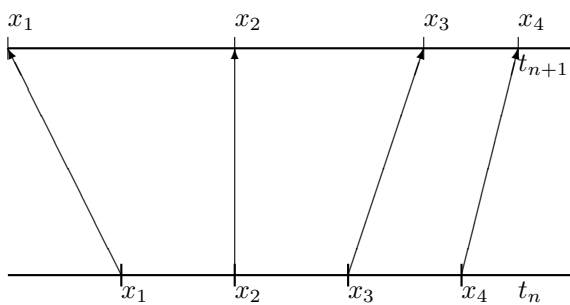
and if  $v < 0$  then use backward differences:



For finite elements the same effect is obtained with the Petrov-Galerkin method, which uses weight functions that are larger in the direction of propagation.

### Characteristic Methods

The method of characteristics is used to integrate the hyperbolic (transport) part. The main problem is that the mesh gets deformed.



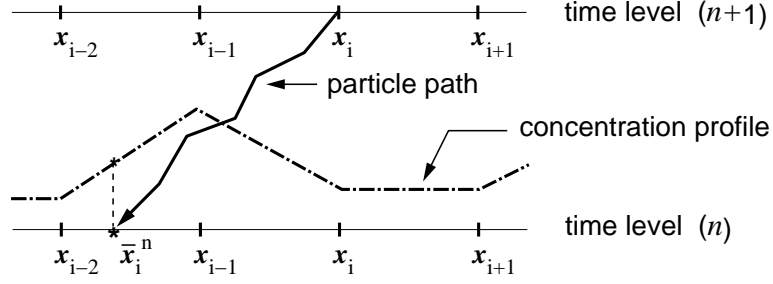
One way to deal with this is to use the modified method of characteristics (MMOC), which uses a regular mesh and integrates back along the characteristics. The characteristic does not get back at a grid point, but since we know the solution at that time level we can interpolate to find the value at this “back track point”. This is a lagrangian method.

If we consider the transport equation

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} - \frac{\partial}{\partial x} \left( D \frac{\partial c}{\partial x} \right) = R(c)$$

The modified method of characteristics is

$$\frac{Dc}{Dt} = \frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} \simeq \frac{C^{n+1}(x) - C^n(x - v^n \Delta t)}{\Delta t}$$



- Finite-Difference Approximation (*FD*):

$$\frac{C_i^{n+1} - C^n(x_i - v^n \Delta t)}{\Delta t} - \delta_{\bar{x}}(D\delta_x C^{n+1})_i = R(C_i^{n+1})$$

### Other Methods

- Mixed finite elements. Write second order equation as system of first order equations
- Eulerian-Lagrangian Methods: approximate part of the equation using Lagrangian coordinates (following physical particles) and part using Eulerian coordinates
- ELLAM (Eulerian-Lagrangian localized adjoint method)
- Particle in cell: Follow the motion of particles
- Nonstandard methods: Integrate transport-reaction part exactly using characteristics

## 2.2 Numerical Methods for Elliptic Equations

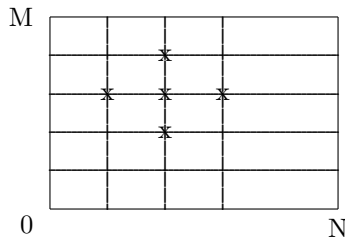
In two dimensions Poisson's equation is

$$\begin{aligned} u_{xx} + u_{yy} &= -f(x, y) && \text{in } (0, 1) \times (0, 1) \\ u &= u_{\partial}(x, y) && \text{on the boundary} \end{aligned}$$

Finite difference approximation

$$\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{\Delta y^2} = -f_{ij} \quad \begin{array}{l} i = 1, \dots, N-1 \\ j = 1, \dots, M-1 \end{array}$$

$$\begin{aligned} x_i &= i\Delta x & \Delta x &= \frac{1}{N} \\ y_j &= j\Delta y & \Delta y &= \frac{1}{M} \end{aligned}$$



$(N-1)(M-1)$  interior points with unknowns.

Solving for  $u_{ij}$

$$\begin{aligned} u_{ij} &= \frac{1}{2\Delta x^2 + 2\Delta y^2} [(u_{i+1,j} + u_{i-1,j}) \Delta y^2 + (u_{i,j+1} + u_{i,j-1}) \Delta x^2 \\ &\quad + f_{ij} \Delta x^2 \Delta y^2] \\ &= \delta_1 (u_{i+1,j} + u_{i-1,j}) + \delta_2 (u_{i,j+1} + u_{i,j-1}) + \delta f_{ij}, \end{aligned}$$

$$\text{where } \delta_1 = \frac{\Delta y^2}{2\Delta x^2 + 2\Delta y^2}, \quad \delta_2 = \frac{\Delta x^2}{2\Delta x^2 + 2\Delta y^2}, \quad \delta = \frac{\Delta x^2 \Delta y^2}{2\Delta x^2 + 2\Delta y^2}.$$

### Iterative Methods

Jacobi

$$u_{ij}^{(n+1)} = \delta_1 (u_{i+1,j}^{(n)} + u_{i-1,j}^{(n)}) + \delta_2 (u_{i,j+1}^{(n)} + u_{i,j-1}^{(n)}) + \delta f_{ij}$$

Gauss-Seidel Use updated variables as soon as they are available:

$$u_{ij}^{(n+1)} = \delta_1 (u_{i+1,j}^{(n)} + u_{i-1,j}^{(n+1)}) + \delta_2 (u_{i,j+1}^{(n)} + u_{i,j-1}^{(n+1)}) + \delta f_{ij}$$

## SOR

$$\begin{aligned}\bar{u}_{ij}^{(n+1)} &= \delta_1 \left( u_{i+1,j}^{(n)} + u_{i-1,j}^{(n+1)} \right) + \delta_2 \left( u_{i,j+1}^{(n)} + u_{i,j-1}^{(n+1)} \right) + \delta f_{ij} \\ u_{ij}^{(n+1)} &= u_{i,j}^{(n)} + w \left( \bar{u}_{i,j}^{(n+1)} - u_{i,j}^{(n)} \right)\end{aligned}$$

with  $0 < w < 2$  for convergence ( $w = 1$  Gauss Seidel).

Line iterative methods: improve all points in a line at the same time.

Line Jacobi

$$u_{ij}^{(n+1)} - \delta_1 \left( u_{i+1,j}^{(n+1)} + u_{i-1,j}^{(n+1)} \right) = \delta_2 \left( u_{i,j+1}^{(n)} + u_{i,j-1}^{(n)} \right) + \delta f_{ij}$$

In each iteration we have to solve a tridiagonal system (direct method).

Line Gauss-Seidel (by columns)

$$u_{ij}^{(n+1)} - \delta_1 \left( u_{i+1,j}^{(n+1)} + u_{i-1,j}^{(n+1)} \right) = \delta_2 \left( u_{i,j+1}^{(n)} + u_{i,j-1}^{(n+1)} \right) + \delta f_{ij}$$

Line SOR (by columns)

$$\begin{aligned}\bar{u}_{ij}^{(n+1)} - \delta_1 \left( \bar{u}_{i+1,j}^{(n+1)} + \bar{u}_{i-1,j}^{(n+1)} \right) &= \delta_2 \left( u_{i,j+1}^{(n)} + u_{i,j-1}^{(n+1)} \right) + \delta f_{ij} \\ u_{ij}^{(n+1)} &= u_{i,j}^{(n)} + w \left( \bar{u}_{i,j}^{(n+1)} - u_{i,j}^{(n)} \right)\end{aligned}$$

## **Alternating Direction Methods**

Consist of a row line iteration, then a column line iteration and so on.

For example, ADLSOR is:

$$\begin{aligned}u_{ij}^{(n+\frac{1}{2})} - \delta_1 \left( \bar{u}_{i+1,j}^{(n+\frac{1}{2})} + \bar{u}_{i-1,j}^{(n+\frac{1}{2})} \right) &= \delta_2 \left( u_{i,j+1}^{(n)} + u_{i,j-1}^{(n+\frac{1}{2})} \right) + \delta f_{ij} \\ u_{ij}^{(n+\frac{1}{2})} &= u_{i,j}^{(n)} + w \left( \bar{u}_{i,j}^{(n+\frac{1}{2})} - u_{i,j}^{(n)} \right) \\ \bar{u}_{i,j}^{(n+1)} - \delta_2 \left( \bar{u}_{i,j+1}^{(n+1)} + \bar{u}_{i,j-1}^{(n+1)} \right) &= \delta_1 \left( u_{i+1,j}^{(n+\frac{1}{2})} + u_{i-1,j}^{(n+1)} \right) + \delta f_{ij} \\ u_{i,j}^{(n+1)} &= u_{i,j}^{(n+\frac{1}{2})} + w \left( \bar{u}_{i,j}^{(n+1)} - u_{i,j}^{(n+\frac{1}{2})} \right)\end{aligned}$$

One advantage is that the influence of b.c. spreads faster into the whole domain. This implies better convergence.

Conjugate Gradient Methods

- Symmetric matrices: Conjugate gradient and preconditioned conjugate gradient
- Nonsymmetric matrices: Orthomin, GMRES, . . . .

**Finite Elements** In 1-D we have for piecewise linear basis functions, that are given by piecewise Lagrange polynomials. They can also be written in terms of functions defined in  $[-1, 1]$ :

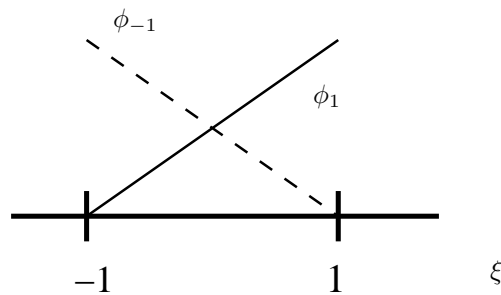


Figure 2.1: Linear basis functions in terms of  $\xi$

$$\begin{aligned} \varphi_{-1}(\xi) &= \frac{1}{2}(1 - \xi) & \varphi_1(\xi) &= \frac{1}{2}(1 + \xi) \\ \text{or } \varphi_{\xi_i} &= \frac{1}{2}(1 + \xi\xi_i) & \text{where } \xi_i &= -1, 1 \end{aligned}$$

In two dimensions the easiest is to form the product of two one-dimensional bases, one in each direction

$$\varphi = \frac{1}{4}(1 + \xi\xi_i)(1 + \eta\eta_i)$$

Triangular elements

The linear basis functions are of the form

$\phi(x, y) = ax + by + c$  making it one at one node and zero at the others we get

$$\varphi_i(x, y) = \frac{x(y_j - y_k) + y(x_k - x_j) + (x_j y_k - x_k y_j)}{\det(P)}$$

where  $(i, j, k)$  is a cyclic permutation of  $(1, 2, 3)$

and  $P$  is  $\begin{pmatrix} x_i & y_i & 1 \\ x_j & y_j & 1 \\ x_k & y_k & 1 \end{pmatrix}$

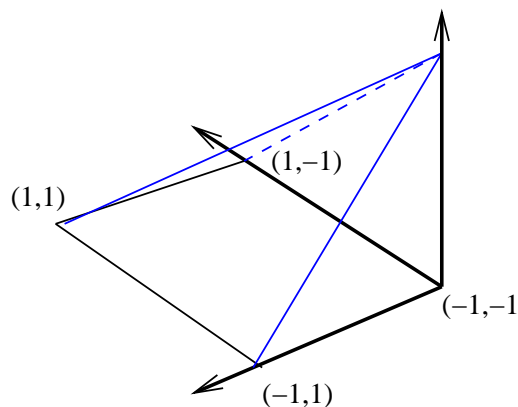


Figure 2.2: Example of a 2-D linear basis function

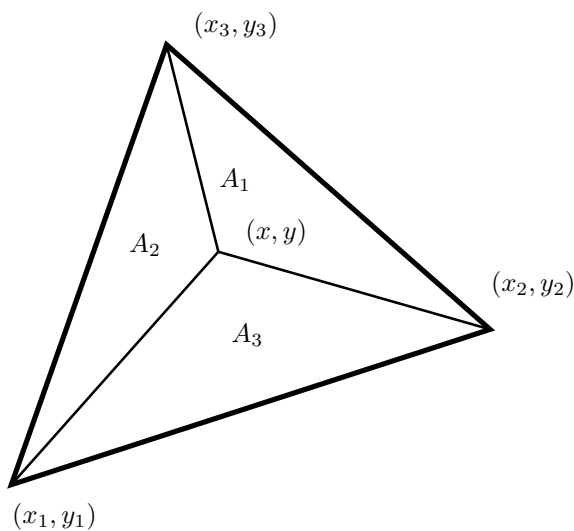


Figure 2.3: A triangular element

Let  $P_i$  be the matrix obtained from  $P$  when  $(x_i, y_i)$  is replaced by  $(x, y)$  then  $\varphi_i = \frac{\det(P_i)}{\det(P)}$

or in terms of the areas of the triangles (since  $A = \frac{1}{2} \det(P)$ )

$$\varphi_i(x, y) = \frac{A_i}{A}$$

All three  $\varphi_i$  are not independent since

$$A_1 + A_2 + A_3 = A$$

and  $\varphi_3 = 1 - \varphi_1 - \varphi_2$

## Chapter 3

# Numerical Methods for some Problems in Porous Media.

### 3.1 1-D Steady Flow

We consider the steady flow of water through a porous medium consisting of three zones with different hydraulic properties. Water is injected at a unit rate into the left side of the medium and at the right end the head is maintained at a constant value of 5.

The flow is given by Darcy's law:

$$v = -\frac{k\rho g}{\mu} \left( \frac{1}{\rho g} \frac{\partial p}{\partial x} + \frac{\partial z}{\partial x} \right).$$

Define the hydraulic head as  $h = p/(\rho g) + z$  and the hydraulic conductivity coefficient as  $K = \rho g k/\mu$ , then Darcy's law is

$$v = -K \frac{\partial h}{\partial x}.$$

We discretize the medium using three elements, and four nodes: at the left end, two at the boundaries between elements and one at the right end.

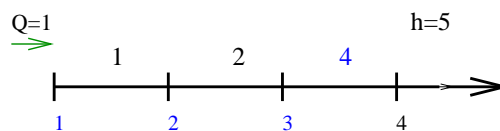


Figure 3.1: Three element composite porous medium

Consider an element  $e$  with local nodes 1 and 2. The flow is positive if it is entering the element. We will use linear basis functions. Darcy's equation at each node is

$$Q_1 = KA \frac{h_1 - h_2}{L}$$

and

$$Q_2 = KA \frac{h_2 - h_1}{L},$$

where  $K$  is the hydraulic conductivity,  $A$  the cross-sectional area and  $L$  the length of the element.

Writing the system in matrix form

$$\begin{bmatrix} \frac{KA}{L} & -\frac{KA}{L} \\ -\frac{KA}{L} & \frac{KA}{L} \end{bmatrix}^e \begin{Bmatrix} h_1 \\ h_2 \end{Bmatrix}^e = \begin{Bmatrix} Q_1 \\ Q_2 \end{Bmatrix}^e,$$

or

$$[C]^e h^e = Q^e.$$

Here the  $e$  denotes we are working at the element level.

To assemble the global set of equations, we write the above equations for each node: For element 1

$$\begin{bmatrix} c_{11}^{(1)} & c_{12}^{(1)} & 0 & 0 \\ c_{21}^{(1)} & c_{22}^{(1)} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{Bmatrix} = \begin{Bmatrix} Q_1^1 \\ Q_2^1 \\ 0 \\ 0 \end{Bmatrix}.$$

For element 2

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & c_{11}^{(2)} & c_{12}^{(2)} & 0 \\ 0 & c_{21}^{(2)} & c_{22}^{(2)} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{Bmatrix} = \begin{Bmatrix} 0 \\ Q_1^2 \\ Q_2^2 \\ 0 \end{Bmatrix}.$$

For element 3

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & c_{11}^{(3)} & c_{12}^{(3)} \\ 0 & 0 & c_{21}^{(3)} & c_{22}^{(3)} \end{bmatrix} \begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ Q_1^3 \\ Q_2^3 \end{Bmatrix}.$$

Adding the three matrices we get

$$[C]h = Q,$$

where

$$h = \begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{Bmatrix},$$

$$Q = \begin{Bmatrix} Q_1^{(1)} \\ Q_2^{(1)} + Q_1^{(2)} \\ Q_2^{(2)} + Q_1^{(3)} \\ Q_2^{(3)} \end{Bmatrix},$$

and

$$[C] = \begin{bmatrix} c_{11}^{(1)} & c_{12}^{(1)} & 0 & 0 \\ c_{21}^{(1)} & c_{22}^{(1)} + c_{11}^{(2)} & c_{12}^{(2)} & 0 \\ 0 & c_{21}^{(2)} & c_{22}^{(2)} + c_{11}^{(3)} & c_{12}^{(3)} \\ 0 & 0 & c_{21}^{(3)} & c_{22}^{(3)} \end{bmatrix}.$$

Note that  $c_{ij} = c_{ji}$ . Enforcing the continuity of flow at the internal nodes 2 and 3:  $Q_2^{(1)} = Q_1^{(2)}$  and  $Q_2^{(2)} = Q_1^{(3)}$ , so the right hand side vector becomes

$$Q = \begin{Bmatrix} Q_1^{(1)} \\ 0 \\ 0 \\ Q_2^{(3)} \end{Bmatrix}.$$

Using the boundary conditions we have  $Q_1^{(1)} = Q_1 = 1$ . The other boundary condition  $h_4 = 5$  has to be incorporated carefully to keep the symmetry of the system:

$$\begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 \\ c_{21} & c_{22} & c_{23} & 0 \\ c_{31} & c_{32} & c_{33} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \begin{Bmatrix} h_1 \\ h_2 \\ h_3 \\ h_4 \end{Bmatrix} = \begin{Bmatrix} 1 - 5c_{14} \\ -5c_{24} \\ -5c_{34} \\ 5 \end{Bmatrix}.$$

Finally we need to solve the linear system.

### 3.2 Slightly Compressible Fluid

The continuity equation is now

$$\frac{\partial v}{\partial x} = -(\alpha + \phi\beta) \frac{\partial p}{\partial t}.$$

Since

$$\frac{\partial h}{\partial t} = \frac{1}{\rho g} \frac{\partial p}{\partial t}$$

the equation of continuity can be written as

$$-(\alpha + \phi\beta) \frac{\partial p}{\partial t} = -\rho g(\alpha + \phi\beta) \frac{\partial h}{\partial t} = S_s \frac{\partial h}{\partial t},$$

where  $S_s = \rho g(\alpha + \phi\beta)$  is called the specific storage. Combining this equation and the continuity equation with Darcy's law we obtain

$$\frac{\partial}{\partial x} \left( K \frac{\partial h}{\partial x} \right) = S_s \frac{\partial h}{\partial t}.$$

Consider the above equation on  $0 \leq x \leq X$ , with the initial and boundary conditions  $h(x, 0) = h_0$ ,  $h(0, t) = 0$  and  $h(X, t) = 0$ . Using the Galerkin finite element approach, approximate  $h$  by

$$h(x, t) = \sum_{J=0}^n \Phi_J(x) h_J(t).$$

Substituting this approximation, multiplying by the weight function  $\Phi_I(x)$ , integrating over  $x$  and integrating by parts the term with the second  $x$  derivative we get:

$$\sum_J \left( \int_0^X \frac{\partial \Psi_I}{\partial x} \frac{d\Psi_J}{dx} h_J dx + \int_0^X S_s \Psi_I \Psi_J \frac{dh_J}{dt} dx \right) = 0.$$

Or

$$\sum_J \left( C_{IJ} h_J + M_{IJ} \frac{dh_J}{dt} \right) = 0, \quad \text{for } I = 2, 3, \dots, n-1.$$

Here

$$C_{IJ} = \int_0^X K \frac{d\Psi_I}{dx} \frac{\Psi_J}{dx} dx$$

and

$$M_{IJ} = \int_0^X S_s \Psi_I \Psi_J dx.$$

The time derivative can be approximated by finite differences or finite elements. Lets do finite differences.

Use a super index  $k + \theta$  to denote the time level, with  $0 \leq \theta \leq 1$ :

$$\sum \left( C_{IJ} h_J^{k+\theta} + M_{IJ} \left( \frac{dh_J}{dt} \right)^{k+\theta} \right) = 0.$$

The time derivative is approximated as

$$\left( \frac{dh_J}{dt} \right)^{k+\theta} = (h_J^{k+1} - h_J^k) / \delta t$$

and the values of the head at  $k + \theta$  by

$$h_J^{k+\theta} = (1 - \theta) h_J^k + \theta h_J^{k+1}.$$

Our system is now

$$\sum \left( C_{IJ} [\theta h_J^{k+1} + (1 - \theta) h_J^k] + \frac{M_{IJ}}{\delta t} (h_J^{k+1} - h_J^k) \right) = 0.$$

For  $\theta = 0$  we obtain the following explicit scheme

$$\sum \left[ \frac{M_{IJ}}{\delta t} h_J^{k+1} = \sum \left( \frac{M_{IJ}}{\delta t} - C_{IJ} \right) h_J^k. \right.$$

For  $\theta = 1$  the scheme is fully implicit. After moving all the terms at the new time level  $k + 1$  to the left and all the terms at the  $k$  level to the right we have

$$\sum \left[ C_{IJ} + \frac{M_{IJ}}{\delta t} \right] h_J^{k+1} = \sum \frac{M_{IJ}}{\delta t} h_J^k.$$

And finally for  $\theta = 1/2$  we have the Crank-Nicolson scheme

$$\sum \left[ \frac{C_{IJ}}{2} + \frac{M_{IJ}}{\delta t} \right] h_J^{k+1} = \sum \left[ \frac{M_{IJ}}{\delta t} - \frac{C_{IJ}}{2} \right] h_J^k.$$

The explicit scheme is the easiest to solve but is only conditionally stable. Both the implicit and Crank-Nicolson are unconditionally stable.

The two previous examples are from [3].

### 3.3 Non-steady Aquifer

Consider an aquifer with uniform thickness  $b$  and assume that it is uniform in the vertical direction. Assume that there is recharge from precipitation or extraction by wells given by a function  $R$ , the volume of water added or subtracted per unit time per unit area. Take a small rectangular region of size  $\Delta x$  by  $\Delta y$  by  $b$ . The continuity equation is now

$$\nabla \cdot \mathbf{v} = R/b.$$

Substituting Darcy's law  $\mathbf{v} = -K\nabla h$  we get

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = -\frac{R(x, y)}{T}.$$

where  $T$  is the transmissivity defined as  $T = Kb$ . The finite difference form of this Poisson equation is

$$\frac{h_{i-1,j} - 2h_{i,j} + h_{i+1,j}}{(\Delta x)^2} + \frac{h_{i,j-1} - 2h_{i,j} + h_{i,j+1}}{(\Delta y)^2} = \frac{R}{T}.$$

It can be solved using Gauss-Seidel iteration.

For problems with pumping of water through wells we need to introduce the storage coefficient  $S$  which represents the volume of water released from storage per unit area per unit decline of head

$$S = \frac{-\Delta V_w}{\Delta x \Delta y \Delta h},$$

where  $\Delta V_w$  is the volume of water released from storage within the element of volume with area  $\Delta x \Delta y$  and thickness  $b$ . Adding this term to the continuity equation we get

$$\nabla \cdot \mathbf{v} = \frac{R}{b} - \frac{S}{b} \frac{\partial h}{\partial t}.$$

Substituting Darcy's law we get

$$\frac{\partial^2 h}{\partial x^2} + \frac{\partial^2 h}{\partial y^2} = \frac{S}{T} \frac{\partial h}{\partial t} - \frac{R(x, y, t)}{T}.$$

If we use a forward difference time approximation

$$\frac{\partial h}{\partial t} \approx \frac{h_{ij}^{n+1} - h_{ij}^n}{\Delta t}$$

and the usual approximation for the second space derivatives we get

$$\frac{h_{i-1,j}^n - 2h_{i,j}^n + h_{i+1,j}^n}{(\Delta x)^2} + \frac{h_{i,j-1}^n - 2h_{i,j}^n + h_{i,j+1}^n}{(\Delta y)^2} = \frac{S}{T} \frac{h_{ij}^{n+1} - h_{ij}^n}{\Delta t} - \frac{R_{ij}^n}{T}.$$

Letting  $\Delta x = \Delta y = a$  and solving for  $h_{ij}^{n+1}$

$$h_{ij}^{n+1} = \left(1 - \frac{4T\Delta t}{Sa^2}\right) h_{ij}^n + \left(\frac{4T\Delta t}{Sa^2}\right) \left(\frac{h_{i-1,j}^n + h_{i+1,j}^n + h_{i,j-1}^n + h_{i,j+1}^n}{4} + \frac{R_{ij}^n \Delta t}{S}\right).$$

This example is done in [5].

### 3.4 Mixed Finite Element Example

Assume a rigid porous medium saturated with a viscous, incompressible fluid, If the medium is also assumed to be homogeneous and isotropic and the fluid and solid are in thermal equilibrium, the equations of the fluid are

$$\frac{\partial u_i}{\partial x_i} = 0 \quad (3.1)$$

$$\frac{\rho}{\phi} \frac{\partial u_j}{\partial t} + \left( \frac{\rho \hat{c}}{\sqrt{\kappa}} \|\mathbf{u}\| + \frac{\mu}{\kappa} \right) u_i = \frac{\partial}{\partial x_j} \left[ -P \delta_{ij} + \mu_e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \rho f_i. \quad (3.2)$$

Here  $\rho$  is the density,  $\kappa$  is the permeability,  $\phi$  is the porosity,  $\hat{c}$  is the inertia coefficient and  $\|\mathbf{u}\|$  is the magnitude of the velocity.  $\mu$  is the viscosity coefficient,  $P$  is the pressure,  $\mathbf{f}$  is the body force, and the subindex  $e$  refers to effective viscosity. We sum over repeated indices.

The above system is a generalization of the Darcy's equations for isothermal flow in a saturated medium. It is called the *Forchheimer-Brinkman* model.

The boundary conditions are the same as for viscous flow: *Dirichlet boundary conditions*:

$$u_i = f_i^u(s, t) \quad \text{on } \Gamma_u$$

or *Neumann boundary conditions*:

$$\tau_i = \sigma_{ij}(s, t) n_j(s) = f_i^\tau(s, t) \quad \text{on } \Gamma_\tau,$$

where  $s$  is the coordinate along the boundary,  $t$  is time,  $n_i$  the outward unit normal and  $\Gamma$  the boundary.

The weak form of the above equations is obtained by multiplying by weight functions  $(Q, \mathbf{w})$  and integrating over the domain  $\Omega$ .

Using the shorthand  $f_1 = 0$  and  $\mathbf{f}_2 = \mathbf{f}_3$  for equations 3.1 and 3.2 we get

$$\int_{\Omega} Q f_1 d\mathbf{x} = 0$$

and

$$\int_{\Omega} \mathbf{w} \cdot \mathbf{f}_2 d\mathbf{x} = \int_{\Omega} \mathbf{w} \cdot \mathbf{f}_3 d\mathbf{x}.$$

Integrating by parts the term inside the square brackets in the second equation we get

$$0 = \int_{\Omega} Q \left( \frac{\partial u_i}{\partial x_i} \right) d\mathbf{x}$$

$$0 = \int_{\Omega} \left[ w_i \frac{\rho}{\phi} \frac{\partial u_j}{\partial t} + w_i \left( \frac{\rho \hat{c}}{\sqrt{\kappa}} \|\mathbf{u}\| + \frac{\mu}{\kappa} \right) u_i + \frac{\partial w_i}{\partial x_j} \left( -P \delta_{ij} + \mu_e \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) - \rho w_i f_i \right] d\mathbf{x} - \oint_{\Gamma} w_i \tau_i ds.$$

As in any Galerkin finite element approximation we write  $\mathbf{u}$  and  $P$  in terms of basis functions and use the same basis functions for the weight functions

$$u_i(\mathbf{x}, t) = \sum_{m=1}^M \psi_m(\mathbf{x}) u_i^m(t) = \mathbf{\Psi}^T \mathbf{u}_i$$

$$P(\mathbf{x}, t) = \sum_{l=1}^L \phi_l(\mathbf{x}) P_l(t) = \Phi^T \mathbf{P}$$

$Q = \Phi$  and  $\mathbf{w} = \Psi$ .

Substituting into the equations for conservation of mass and momentum we get

$$\begin{aligned} & - \left[ \int_{\Omega} \Phi \frac{\partial \Psi^T}{\partial x_i} d\mathbf{x} \right] \mathbf{u}_i = 0 \\ & \left[ \int_{\Omega} \frac{\rho}{\phi} \Psi \Psi^T d\mathbf{x} \right] \dot{\mathbf{u}}_i + \left[ \int_{\Omega} \frac{\rho \hat{c}}{\sqrt{\kappa}} \Psi (\Psi^T \|\mathbf{u}\|) \Psi^T d\mathbf{x} \right] \mathbf{u}_i + \left[ \int_{\Omega} \frac{\mu}{\kappa} \Psi \Psi^T d\mathbf{x} \right] \dot{\mathbf{u}}_i \\ & + \left[ \int_{\Omega} \text{mega} \mu_e \frac{\partial \Psi}{\partial x_j} \frac{\partial \Psi^T}{\partial x_j} d\mathbf{x} \right] \mathbf{u}_i + \left[ \int_{\Omega} \mu_e \frac{\partial \Psi^T}{\partial x_j} \frac{\partial \Psi^T}{\partial x_i} d\mathbf{x} \right] \mathbf{u}_i - \left[ \int_{\Omega} \frac{\partial \Psi}{\partial x_i} \Phi^T d\mathbf{x} \right] \mathbf{P} \\ & = \left[ \int_{\Omega} \rho f_i \Psi d\mathbf{x} \right] + \left\{ \int_{\Gamma} \tau_i \Psi ds \right\} \end{aligned}$$

The above equations can be written in matrix form as

$$-\tilde{\mathbf{Q}}^T \mathbf{u} = \mathbf{0}$$

and

$$\tilde{\mathbf{M}} \dot{\mathbf{u}} + \tilde{\mathbf{C}}(\mathbf{u}) \mathbf{u} + \tilde{\mathbf{A}} \mathbf{u} + \tilde{\mathbf{K}} \mathbf{u} - \tilde{\mathbf{Q}} \mathbf{P} = \tilde{\mathbf{F}}$$

where  $\mathbf{u} = (\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3)^T$  and

$$\begin{aligned} \tilde{\mathbf{M}} &= \int_{\Omega} \frac{\rho}{\phi} \Psi \Psi^T d\mathbf{x} \\ \tilde{\mathbf{C}}(\mathbf{u}) &= \int_{\Omega} \frac{\rho \hat{c}}{\sqrt{\kappa}} \Psi (\Psi^T \|\mathbf{u}\|) \Psi^T d\mathbf{x} \\ \tilde{\mathbf{A}} &= \int_{\Omega} \frac{\mu_e}{\kappa} \Psi \Psi^T d\mathbf{x} \\ \tilde{\mathbf{K}}_{ij} &= \int_{\Omega} \mu_e \frac{\partial \Psi^T}{\partial x_j} \frac{\partial \Psi^T}{\partial x_i} d\mathbf{x} \\ \tilde{\mathbf{Q}}_i &= \int_{\Omega} \frac{\partial \Psi}{\partial x_i} \Phi^T d\mathbf{x} \\ \tilde{\mathbf{F}}_i &= \int_{\Omega} \rho f_i \Psi d\mathbf{x} + \int_{\Gamma} \tau_i \Psi ds. \end{aligned}$$

Writing it as a single matrix equation

$$\begin{bmatrix} \tilde{\mathbf{M}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{P}} \end{Bmatrix} + \begin{bmatrix} \tilde{\mathbf{C}}(\mathbf{u}) + \tilde{\mathbf{A}} + \tilde{\mathbf{K}} & -\tilde{\mathbf{Q}} \\ -\tilde{\mathbf{Q}}^T & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{u} \\ \mathbf{P} \end{Bmatrix} = \begin{Bmatrix} \tilde{\mathbf{F}} \\ \mathbf{0} \end{Bmatrix}.$$

For Darcy's case,  $\hat{c} = 0$  and  $\mu_e = 0$ , the system simplifies to

$$\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \dot{\mathbf{u}} \\ \dot{\mathbf{P}} \end{Bmatrix} + \begin{bmatrix} \tilde{\mathbf{A}} & -\tilde{\mathbf{Q}} \\ -\tilde{\mathbf{Q}}^T & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{u} \\ \mathbf{P} \end{Bmatrix} = \begin{Bmatrix} \tilde{\mathbf{F}} \\ \mathbf{0} \end{Bmatrix}.$$

It can be shown that for the discrete system not to be overconstrained the basis functions for the pressure must be at least one order lower than the basis functions for the velocity. Furthermore, the pressure does not need to be continuous across elements. The Ladyzhenskaya-Babuska-Brezzi (LBB) condition needs to be satisfied, so there are additional restrictions on which basis functions work with the given elements.

For 2-D problems a common element is a rectangle with nine nodes, one in each corner, one in the middle of each side and one in the center. The velocity is represented using biquadratic Lagrange functions. The

pressure can be given as a bilinear which is continuous across elements and defined at the corners of the rectangle. Or it could be given as bilinear but discontinuous.

This section was inspired by [4].

### 3.5 Transport of a Solute

The transport of a nonreactive, nonradioactive solute in the absence of adsorption is given by

$$\frac{\partial}{\partial t} \phi c + \frac{\partial}{\partial x_i} v_i c = \frac{\partial}{\partial x_i} \left( \phi D_{ij} \frac{\partial c}{\partial x_j} \right),$$

where summation over repeated indices is assumed.  $c$  is the concentration of the solute per unit volume,  $D_{ij}$  is the dispersion coefficient and  $\phi$  the porosity. To obtain the velocity we need solve the pressure equation

$$H \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} [M_{ij} (\frac{\partial p}{\partial x_j} + \rho g_j)] = 0$$

where  $H = -\rho(\alpha + \phi\beta)$  and  $M_{ij} = \rho k_{ik}/\mu$  and substitute the pressure into Darcy's law

$$v_i = -\frac{k_{ij}}{\mu} (\frac{\partial p}{\partial x_j} + \rho g_j).$$

To simplify notation lets introduce the central difference  $\delta u_r = u_{r+1/2} - u_{r-1/2}$  and the backward difference  $\nabla_t u_r = u_r - u_{r-1}$  and use a subindex to denote the variable with respect to we take the difference.

$$\frac{1}{\Delta x_i} \delta_{x_i} \left( \phi \rho D_{ij} \frac{\delta_{x_j} c}{\Delta x_j} \right) + \frac{\rho k_{ij}}{\mu} \left( \frac{\delta_{x_i} p}{\Delta x_j} + \rho g_j \right) \frac{\delta_{x_i} c}{\Delta x_i} = \frac{\rho}{\Delta t} \nabla_t (\phi c)$$

$$\frac{H}{\Delta t} \nabla_t p + \frac{1}{\Delta x_i} \delta_{x_i} \left[ M_{ij} \left( \frac{1}{\Delta x_j} \delta_{x_j} p + \rho g_j \right) \right] = 0.$$

We have a system of  $2N$  nonlinear equations in  $2N$  unknowns,  $p$  and  $c$ , where  $N$  is the number of nodal points. These equations are weakly nonlinear and are usually solved sequentially. That is, first solve for the pressure, and find the velocity, and then solve for the concentration. Explicit finite difference schemes are commonly used, in spite of having to restrict the time step to avoid nonphysical oscillations. But implicit methods that don't have this restriction, introduce artificial diffusion. They also require to calculate second cross derivatives which increase the number of off-diagonal elements in the system matrix.

The material in this section is based on [3].

## 3.6 Modified Method of Characteristics for Transport

### Problem Description 1.- Fluid flow equation

In this section we consider transient groundwater flow in a 2-D aquifer. There is a dissolved solute that is transported by the flow and also diffuses.

The pressure equation is

$$S \frac{\partial p}{\partial t} - \nabla \cdot (K \nabla p) = f,$$

where  $S(\mathbf{x}, t)$  is the specific storage,  $p(\mathbf{x}, t)$  is the pressure or hydraulic head,  $K(\mathbf{x}, t)$  is the saturated hydraulic conductivity and  $f(\mathbf{x}, t)$  represents the sources or sinks.

As before this equation is derived by combining the mass balance law

$$S \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{v} = f$$

with Darcy's law for the groundwater velocity

$$K^{-1} \mathbf{v} + \nabla p = 0.$$

### Numerical Solution of the Flow Equation

$$S \frac{\partial p}{\partial t} - \nabla \cdot (K \nabla p) = f \quad \text{vs.} \quad \begin{cases} S \frac{\partial p}{\partial t} + \nabla \cdot \mathbf{v} = f \\ K^{-1} \mathbf{v} + \nabla p = 0 \end{cases}$$

- Mixed Finite-Element Method

- variational formulation:

$$\int_{\Omega} K^{-1} \mathbf{v}_h \mathbf{w} - \int_{\Omega} p_h \nabla \cdot \mathbf{w} = 0, \quad \forall \mathbf{w} \in W_h = W_h^x \times W_h^y$$

$$\int_{\Omega} q S \frac{\partial p_h}{\partial t} + \int_{\Omega} q \nabla \cdot \mathbf{v}_h = \int_{\Omega} q f, \quad \forall q \in Q_h$$

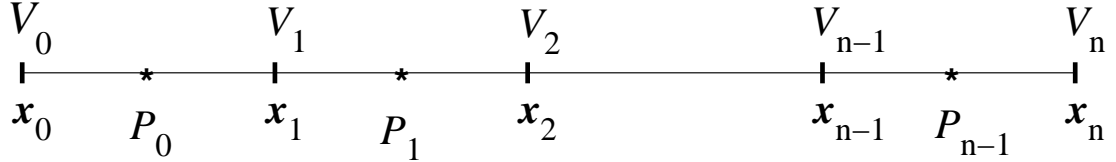
- lowest-order *Raviart-Thomas* spaces –  $Q_h, W_h$

- forward-difference and matrix splitting

Or writing it as a matrix system:

$$\begin{bmatrix} D & N \\ N^T & \Delta t^{-1} M \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix}^{n+1, m+1} = \begin{bmatrix} D - A & N \\ N^T & \Delta t^{-1} M \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix}^{n+1, m} + \begin{bmatrix} 0 \\ G \end{bmatrix}^n.$$

- Multigrid based solver at each iteration level
- Pressure and velocity nodal values:



The error estimates:

the approximate pressures and velocities obey equal-order  $L^2$  global error estimates that are  $\mathcal{O}(\Delta \mathbf{x})$ .

### Problem Description 2.- Solute transport equation

The convection-dispersion-reaction equation for single species transport in a 2-D aquifer is

$$\frac{\partial \phi c}{\partial t} + \nabla \cdot (\mathbf{v}c) - \nabla \cdot (\mathbf{D} \cdot \nabla c) = r(c),$$

where  $c(\mathbf{x}, t)$  is the solute concentration,  $\mathbf{v}(\mathbf{x}, t)$  is fluid (barycentric) velocity,  $r(c)$  are the reaction and source terms and  $\mathbf{D}(\mathbf{v})$  is the hydrodynamic dispersion tensor:

$$\mathbf{D}(\mathbf{v}) = d_m \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{d_L}{|\mathbf{v}|} \begin{bmatrix} v_x^2 & v_x v_y \\ v_y v_x & v_y^2 \end{bmatrix} + \frac{d_T}{|\mathbf{v}|} \begin{bmatrix} v_y^2 & -v_y v_x \\ -v_x v_y & v_x^2 \end{bmatrix},$$

where  $d_m$  is the molecular diffusion coefficient, and  $d_L$  and  $d_T$  are the longitudinal and transverse dispersivities.

The derivation of the transport equation is based on combining the mass balance law

$$\frac{\partial \phi c}{\partial t} + \nabla \cdot (\mathbf{v}c) + \nabla \cdot \mathbf{j} = r(c)$$

with Fick's law for the diffusive flux

$$\mathbf{j} = -\mathbf{D} \cdot \nabla c.$$

It is important to remember the changing nature of the solute transport equation

- hyperbolic (convection-dominated) – preserves sharp fronts
- parabolic (diffusion-dominated) – smoothes sharp fronts

### Numerical Solution of the Transport Equation

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c - \nabla \cdot (\mathbf{D} \cdot \nabla c) = r(c).$$

A very reliable method to solve the above equation is the *MMOC-Galerkin Method*. Its two parts are

1. Modified method of characteristics:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{Dc}{Dt}(\mathbf{x}, t_{n+1}) \simeq \frac{c(\mathbf{x}, t_{n+1}) - c(\bar{\mathbf{x}}^n, t_n)}{\Delta t},$$

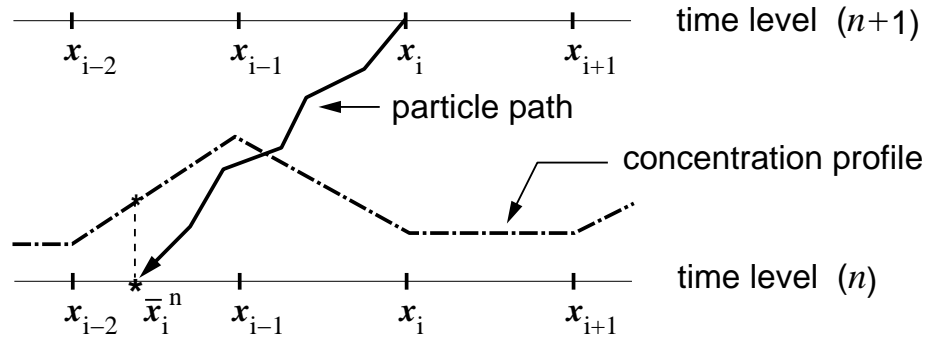
where the *backtrack* point is  $\bar{\mathbf{x}}^n = \mathbf{x} - \mathbf{v} \Delta t$

2. Galerkin finite-element method:

$$\frac{1}{\Delta t} \int_{\Omega} (c_h^{n+1} - \bar{c}_h^n) \varphi + \int_{\Omega} D \nabla c_h^{n+1} \cdot \nabla \varphi = \int_{\Omega} r(c_h^{n+1}) \varphi.$$

Gauss quadrature method is used to calculate  $\bar{c}_h^n(\mathbf{x}) = c_h^n(\bar{\mathbf{x}}^n)$ . Also Picard's iteration is needed to accommodate  $r(c_h^{n+1})$

Following particle paths:



### An alternative numerical solution of the transport equation

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c - \nabla \cdot (\mathbf{D} \cdot \nabla c) = r(c)$$

It is called the *MMOC* – Streamline Diffusion Method

- Modified method of characteristics:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{Dc}{Dt}(\mathbf{x}, t_{n+1}) \simeq \frac{c(\mathbf{x}, t_{n+1}) - c(\mathbf{x} - \mathbf{v}^{n+1} \Delta t, t_n)}{\Delta t}$$

- Streamline diffusion method:  $\varphi \rightarrow \varphi + \gamma \mathbf{v} \cdot \nabla \varphi$

$$\begin{aligned} \frac{1}{\Delta t} \int_{\Omega} (c_h^{n+1} - c_h^*) \varphi + \gamma \int_{\Omega} (\mathbf{v} \cdot \nabla c_h^{n+1})(\mathbf{v} \cdot \nabla \varphi) \\ + \int_{\Omega} \mathbf{D} \cdot \nabla c_h^{n+1} \cdot \nabla \varphi = \int_{\Omega} r(c_h^{n+1}) \varphi. \end{aligned}$$

The new integral term mimics the *longitudinal* entries of the hydrodynamic dispersion tensor  $\mathbf{D}(\mathbf{v})$

$$\gamma \begin{bmatrix} v_x^2 & v_x v_y \\ v_y v_x & v_y^2 \end{bmatrix}.$$

The error estimates for the combined *MMOC-SD* method are  $L^2$  error bounds:  $\mathcal{O}(\Delta x + \Delta t)$ .

### 3.7 Multiphase Flow

Here we consider an oil reservoir with two phases: water and oil. Darcy's law is

$$v_{if} = -\frac{k_{ij}k_{rf}}{\mu_f} \left( \frac{\partial p_f}{\partial x_j} + \rho_f g \frac{\partial z}{\partial x_j} \right), \quad f = w, o.$$

To account for volume changes due to the different pressures at the reservoir and at the surface it is convenient to introduce a formation volume factor,  $B_f = V_f/V_{fs}$ . Thus we obtain the following continuity equations

$$-\frac{\partial}{\partial x_i} \left( \frac{v_{if}}{B_f} \right) = \frac{\partial}{\partial t} \left( \frac{\phi S_f}{B_f} \right),$$

where  $S_f$  is the saturation of phase  $f$ , defined as  $\phi_f/\phi$ , with  $\phi_f$  the volume fraction occupied by fluid  $f$  and  $\phi$  is the porosity. Substituting the Darcy's velocities into this equation we get

$$\frac{\partial}{\partial x_i} \left[ \frac{k_{ij}\lambda_f}{B_f} \left( \frac{\partial p_f}{\partial x_j} + \rho_f g \frac{\partial z}{\partial x_j} \right) \right] = \frac{\partial}{\partial t} \left( \frac{\phi S_f}{B_f} \right),$$

where  $\lambda_f$  is the mobility factor defined as  $\lambda_f = k_{rf}/\mu_f$ .

Averaging over the vertical thickness  $b$

$$\frac{\partial}{\partial x_i} \left[ b \frac{k_{ij}\lambda_f}{B_f} \left( \frac{\partial p_f}{\partial x_j} + \rho_f g \frac{\partial z}{\partial x_j} \right) \right] = b \frac{\partial}{\partial t} \left( \frac{\phi S_f}{B_f} \right).$$

Assuming  $k_{12} = k_{21} = 0$  the finite difference form can be written

$$\frac{1}{(\Delta x_i)^2} \delta_{x_i} \left[ \frac{bk_{ii}\lambda_f}{B_f} (\delta_{x_i} p_f + \rho_f g \delta_{x_i} z) \right] = \frac{1}{\Delta t} \nabla_t \left( \phi \frac{S_f}{B_f} \right). \quad (3.3)$$

All the terms in the left hand side are evaluated at time  $s+1$ , which gives a coupled nonlinear system of equations.

The Implicit pressure-Explicit Saturation method (IMPES) proposes to be a more efficient method. The idea is to eliminate the saturation terms and obtain an equation that contains only the pressure as the dependent variable. This equation is solved using an implicit finite difference approximation. Then the saturation can be solved explicitly from the original equations.

Assume that the capillary pressure  $p_{cow} = p_o - p_w$  does not change over a time step. Therefore  $\nabla_t p_w = \nabla_t p_o$  and letting  $p \equiv p_o$  gives

$$\delta_{x_i} [a_{wi}(\delta_{x_i} p - \delta_{x_i} p_{cow} + \rho_w g \delta_{x_i} z)] = \frac{d_{w1}}{\Delta t} \nabla_t p + \frac{d_{w2}}{\Delta t} \nabla_t S_w$$

and

$$\delta_{x_i} [a_{oi}(\delta_{x_i} p + \rho_o g \delta_{x_i} z)] = \frac{d_{o1}}{\Delta t} \nabla_t p + \frac{d_{o2}}{\Delta t} \nabla_t S_o,$$

where

$$a_{fi} = \frac{bk_{ii}\lambda_f}{(\Delta x_i)^2 B_f} \quad i = 1, 2,$$

$$d_{f1} = \frac{1}{\Delta t} \left[ (S_f \phi)_s \frac{(1/B_f)}{dp_f} + \frac{S_{fs}}{B_{fs+1}} \frac{d\phi}{dp} \right],$$

and

$$d_{f2} = (\phi/B_f)_{s+1}.$$

Here  $s$  refers to the time level. Remembering that  $S_w + S_o = 1$ , we reduce the above two equations to an equation in the pressure by multiplying the first one by  $d_{o2}$ , the second one by  $d_{w2}$  and adding

$$d_{o2}\delta_{x_i}[a_{wi}(\delta_{x_i}p - \delta_{x_i}p_{cow} + \rho_w g \delta_{x_i}z)] + d_{w2}\delta_{x_i}[a_{oi}(\delta_{x_i}p + \rho_o g \delta_{x_i}z)] = \left( \frac{d_{o2}d_{w1}}{\Delta t} + \frac{d_{o1}d_{w2}}{\Delta t} \right) \nabla_t p.$$

Using the capillary pressure at time  $s$ , we can rewrite this equation in a similar form to that for a one-phase flow:

$$\delta_{x_i}[a_{wi}(\delta_{x_i}p + \rho_w g \delta_{x_i}z)] + \frac{d_{w2}}{d_{o2}}\delta_{x_i}[a_{oi}(\delta_{x_i}p + \rho_o g \delta_{x_i}z)] = \left( \frac{d_{w1}}{\Delta t} + \frac{d_{o1}d_{w2}}{d_{o2}\Delta t} \right) \nabla_t p + \delta_{x_i}(a_{wi}\delta_{x_i}p_{cow,s}).$$

This is an implicit nonlinear difference equation for  $p_{s+1}$ . Equations (3.3),  $f = o, w$  can now be solved explicitly for the saturations.

Similar procedures can be used for the case of three phases: water, oil and gas. For more information see [2], [6] and [3].

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