Pinter Consulting
New Series Nos. 12.

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Motto

- Meg(g)y? Nem meg(g)y?
- Meg(g)y, de néha eröltetni kell az igényes matematikai továbbképzést.

- **Private studies for professional development**
- **béláim, gondolkozzunk, amig lehet**
- Socratic Programme for Q1 2017
- Pólya - Szegö : Aufgaben und Lehrsätze aus der Analysis
- Memoirs of Applied Mathematics
- Continuous improvement with corrections
- Collection of problems with our own solutions
- Il n'est point besoin espérer pour entreprendre ni réussir pour persévérer.

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Introduction

Pinter Consulting of Calgary, Alberta practices Mathematics, promotes clear thinking and offers Consultations, Tutorials and Seminars in Mathematics.

Summary

The Report is concerned with Mathemathical Modelling. We calculate errors of difference schemes, stability by both Fourier and matrix methods, analyze the block tri-diagonal algorithm for the solution of systems of linear equations, and formulate the partial differential equation for 1D waterflood.

Contents

13.0 Assignment 32. 2
13.1 Assignment 33. 7
13.2 Assignment 34. 16
13.3 Assignment 35. 22
13.4 Assignment 36. 27

13.0 Assignment 32.

Summary

- Mathematical Modelling
- *Westbrook, Ames*
- Last revision May 13, 2017

1. Use Taylor series to show that the difference schemes with $h = k$

$$\frac{1}{h^2}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}\right) =$$
$$(\triangle u)_{ij} + \frac{h^2}{12}\left[\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4}\right]_{ij} + \emptyset(h^4), \quad (a)$$

and

$$\frac{1}{2h^2}\left(u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1} - 4u_{i,j}\right) =$$
$$(\triangle u)_{ij} + \frac{h^2}{12}\left[\frac{\partial^4 u}{\partial x^4} + 6\frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^4}\right]_{ij} + \emptyset(h^4). \quad (b)$$

If $f(x, y)$ is m times continuously differentiable on $\mu P + (1-\mu)Q$, $0 \leq \mu \leq 1$ with $P = (x_0, y_0)$ and $Q = (x_0 + h, y_0 + k)$ then

$$f(x_0 + h, y_0 + k) = \sum_{\lambda=0}^{m-1} \frac{1}{\lambda!}\left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^{\lambda} f(x_0, y_0) + R_m^{(h,k)}$$

where

$$R_m^{(h,k)} = \frac{1}{m!}\left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y}\right)^{m} f(x_0 + h, y_0 + k), \ \ 0 < \theta < 1.$$

For Problems (1) and (2) we assume that there exists a domain D in the positive quadrant of the Cartesian coordinate system, $u = u(x, y)$ is defined and is continuously differentiable in D at least six times. Furthermore, we assume that there is a regular mesh with increments h and k, $h = k$ discretizing D. Let (x_0, y_0) be a mesh point sufficiently far from the boundaries of D, $(x_0, y_0)\epsilon D$. Then we identify $u_{i,j}$ with $u(x_0, y_0)$, $u_{i\pm1,j}$ with $u(x_0 \pm h, y_0)$, $u_{i,j\pm1}$ with $u(x_0, y_0 \pm k)$.

Proof of claim (a)

$$u_{i+1,j} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!}\left(h\frac{\partial}{\partial x}\right)^{\lambda} u + R_6^{(h,0)}$$

$$u_{i-1,j} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!}\left(-h\frac{\partial}{\partial x}\right)^{\lambda} u + R_6^{(-h,0)}$$

$$u_{i,j+1} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!}\left(k\frac{\partial}{\partial y}\right)^{\lambda} u + R_6^{(0,k)}$$

$$u_{i,j-1} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!}\left(-h\frac{\partial}{\partial y}\right)^{\lambda} u + R_6^{(0,-k)}$$

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} = 4u + h^2 u_{xx} + k^2 u_{yy} + \frac{h^4}{12} u_{xxxx} + \frac{k^4}{12} u_{yyyy}$$
$$+\frac{h^6}{6!}\{u(x_0+\theta_1 h, y_0) + u(x_0-\theta_2 h, y_0) + u(x_0, y_0+\theta_3 k) + u(x_0, y_0-\theta_4 k)\}$$

with $h = k$ for some θ_i, $i = 1, 2, 3, 4$; $0 < \theta_i < 1$.

$$\frac{1}{h^2}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u\right) = (u_{xx} + u_{yy}) + \frac{h^2}{12}(u_{xxxx} + u_{yyyy})$$
$$+\frac{h^4}{6!}\{u(x_0+\theta_1 h, y_0) + u(x_0-\theta_2 h, y_0) + u(x_0, y_0+\theta_3 k) + u(x_0, y_0-\theta_4 k)\} =$$
$$(\triangle u)_{ij} + \frac{h^2}{12}\left[\frac{\partial^4}{\partial x^4}u + \frac{\partial^4}{\partial y^4}u\right] + \emptyset(h^4).$$

Proof of claim (b) Consider the following identities for indeterminates a and b

$$(a+b)^k + (-a+b)^k + (a-b)^k + (-a-b)^k =$$

$$\begin{cases} 0 & \text{if } k = 1, 3, 5 \\ 4 & \text{if } k = 0 \\ 4(a^2+b^2) & \text{if } k = 2 \\ 4a^2 + 24a^2b^2 + 4b^2 & \text{if } k = 4. \end{cases}$$

$$u_{i+1,j+1} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!} \left(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y} \right)^{\lambda} + R_6^{(h,k)}$$

$$u_{i+1,j-1} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!} \left(h\frac{\partial}{\partial x} - k\frac{\partial}{\partial y} \right)^{\lambda} + R_6^{(h,-k)}$$

$$u_{i-1,j+1} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!} \left(-h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y} \right)^{\lambda} + R_6^{(-h,+k)}$$

$$u_{i-1,j-1} = \sum_{\lambda=0}^{5} \frac{1}{\lambda!} \left(-h\frac{\partial}{\partial x} - k\frac{\partial}{\partial y} \right)^{\lambda} + R_6^{(-h,-k)}$$

$$u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1} =$$
$$\sum_{\lambda=0}^{5} \frac{1}{\lambda!} \left[(h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y})^{\lambda} + (h\frac{\partial}{\partial x} - k\frac{\partial}{\partial y})^{\lambda} + (-h\frac{\partial}{\partial x} + k\frac{\partial}{\partial y})^{\lambda} + (-h\frac{\partial}{\partial x} - k\frac{\partial}{\partial y})^{\lambda} \right] u$$
$$+ R_6^{(h,k)} + R_6^{(h,-k)} + R_6^{(-h,+k)} + R_6^{(-h,-k)}.$$

Upon applying the identities above with $a = h\frac{\partial}{\partial x}$ and $b = k\frac{\partial}{\partial y}$ we obtain

$$u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1} =$$
$$\left[4u + 2h^2(u_{xx} + u_{yy}) + h^4(\frac{1}{6}u_{xxxx} + u_{xxyy} + \frac{1}{6}u_{yyyy}) \right]$$
$$+ R_6^{(h,k)} + R_6^{(h,-k)} + R_6^{(-h,+k)} + R_6^{(-h,-k)}.$$

Collecting the zeroth order derivatives on the left hand side yields

$$u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1} - 4u =$$
$$2h^2(u_{xx} + u_{yy}) + h^4(\frac{1}{6}u_{xxxx} + u_{xxyy} + \frac{1}{6}u_{yyyy})$$
$$+ \frac{h^4}{6!}\{u(x_0 + \theta_1 h, y_0) + u(x_0 - \theta_2 h, y_0) + u(x_0, y_0 + \theta_3 k) + u(x_0, y_0 - \theta_4 k)\}.$$

Therefore

$$\frac{1}{2h^2} \left(u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1} - 4u_{i,j} \right) =$$
$$(\triangle u)_{ij} + \frac{h^2}{12} \left[\frac{\partial^4 u}{\partial x^4} + 6\frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^4} \right]_{ij} + \emptyset(h^4)$$

as claimed.

2. Use (a) and (b) of Problem 1. to obtain a 9 point difference stencil which has an error of $\emptyset(h^4)$ when u is a solution of $\triangle u = 0$. First note that $\triangle u = 0$ implies $u_{xx} = -u_{yy}$. Then $u_{xxxx} = -u_{yyxx}$ and $u_{xxyy} = -u_{yyyy}$, hence

$$u_{xxxx} = -u_{yyxx} = -u_{xxyy} = u_{yyyy}.$$

By $1(a)$ and (b)

$$\frac{2}{h^2}(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}) =$$
$$2(\triangle u)_{ij} + \frac{h^2}{12}\left[2u_{xxxx} + 2u_{yyyyy}\right] + \emptyset(h^4)$$

$$\frac{1}{2h^2}(u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1} - 4u_{i,j}) =$$
$$(\triangle u)_{ij} + \frac{h^2}{12}\left[u_{xxxx} + 6u_{xxyy} + u_{yyyyy}\right] + \emptyset(h^4)$$

By summing the last two lines

$$\frac{1}{h^2}[2(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}) +$$
$$\frac{1}{2}(u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1}) - 10u_{i,j}] =$$
$$3(\triangle u)_{ij} + \frac{h^2}{12}\left[3u_{xxxx} + 6u_{xxyy} + 3_{yyyy}\right] + \emptyset(h^4).$$

By hypothesis, $(\triangle u)_{ij} = 0$; and by $u_{xxxx} = -u_{xxyy} = u_{yyyy}$ the second term on the right hand side is zero as well. Therefore the scheme

$$\frac{1}{3h^2}[2(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1})$$
$$+\frac{1}{2}(u_{i+1,j+1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i-1,j-1})$$
$$-10u_{i,j}]$$

has an error of $\emptyset(h^4)$ when $\triangle u = 0$.

3. For the Problem

$$\begin{aligned} u_t &= u_{xx};\ 0 < x < 1, t > 0 \\ u(0,t) &= u(1,t) = 0 \\ u(x,0) &= \begin{cases} 2x & 0 < x \leq 1 \\ 2(1-x) & \frac{1}{2} \leq x \leq 1. \end{cases} \end{aligned}$$

use the (explicit) finite difference scheme

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

let $h = 0.1$ write $r = \dfrac{k}{h^2}$ and choose time step k so that $r = \dfrac{1}{10}, \dfrac{1}{6}, \dfrac{1}{2}, \dfrac{3}{4}$, respectively and tabulate numerical solution $u(x, 0.1)$ at

$$x = 0.00,\ 0.10,\ 0.20,\ 0.30,\ 0.40,\ 0.50,\ 0.60$$

x	$r = \frac{1}{10}$	$r = \frac{1}{6}$	$r = \frac{1}{2}$	$r^* = \frac{3}{4}$	*true*
0.00	0.0000	0.0000	0.0000	0.0000	0.0000
0.10	0.0944	0.0941	0.0949	38.10	0.0934
0.20	0.1796	0.1790	0.1717	−73.22	0.1776
0.30	0.2472	0.2464	0.2484	103.14	0.2444
0.40	0.2907	0.2897	0.2778	−122.47	0.2873
0.50	0.3056	0.3046	0.3071	130.08	0.3021
0.60	0.2907	0.2897	0.2778	−122.47	0.2873

$(*)$ the finite difference scheme is unstable for $r > \dfrac{1}{2}$.

13.1 Assignment 33.

Summary

- Mathematical Modelling
- *Westbrook*
- Last revision May 13, 2017

Problem 1.

Discuss the Fourier stability of the DuFort-Frankel scheme:

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

Write

$$u(i,j) = F(i)G(j)$$

$$F(j) = \exp(\alpha jk), \quad G(i) = \exp(\sqrt{(-1)}\beta ih)$$

$$F(j_1 + j_2) = F(j_1)F(j_2), \; G(i_1 + i_2) = G(i_1)G(i_2)$$

$$u_{i,j+1} = F(j+1)G(i) = F(j)F(1)G(i)$$

$$u_{i,j-1} = F(j-1)G(i) = F(j)F(-1)G(i)$$

$$u_{i-1,j} = F(j)G(i-1) = F(j)G(i)G(-1)$$

Next, we examine the propagation of error, or the growth factor for a single term in the finite Fourier series of errors at $t = 0$.

The DuFort-Frankel scheme takes the form

$$F(j)G(i)[F(1) - F(-1)] \;\; = \;\; \frac{2k}{h^2}F(j)G(i)[G(1) - F(1) - F(-1) + G(-1)].$$

$$F(1) - F(-1) = 2r[G(1) - F(1) - F(-1) + G(-1)]; \; r = \frac{k}{h^2}$$

$$(1+2r)F(1) - (1-2r)F(-1) = 2r[G(1) + G(-1)]$$

$$[G(1)+G(-1)] = \exp(\sqrt{(-1)}\beta ih) + \exp(\sqrt{-(-1)}\beta ih) = 2\cos(\beta h)$$

$$(1+2r)\exp(\alpha k) - (1-2r)\exp(-\alpha k) - 2r[2\cos(\beta h)] = 0$$

$$x = \exp(\alpha k);\ q = \cos(\beta h)$$

$$(1+2r)x^2 - 4rqx - (1-2r) = 0$$

$$x_{1,2} = \frac{4rq \pm \sqrt{16r^2q^2 + 4(1+2r)(1-2r)}}{2(1+2r)}$$

$$d = 16r^2q^2 + (1+2r)(1-2r) = \begin{cases} > 0 \\ = 0 \\ < 0 \end{cases}$$

Case 1, $d > 0$, two real roots

$$f(x) = (1+2r)x^2 - 4rqx - (1-2r)$$

$$a = (1+2r),\ b = -4rq,\ c = -(1-2r)$$

$$f(x) = ax^2 + bx + c$$

$$f(x) = f(\xi) + f'(\xi)(x-\xi) + \frac{1}{2}f"(\xi)(x-\xi)^2$$

(Taylor polynomial for $f(x)$, expanded about $x = 1$.)

$$f(x) = (a\xi^2 + b\xi + c) + (2a\xi + b)(x-\xi) + a(x-\xi)^2$$

$$\xi = 1$$

$$f(x) = (1+2r-4rq-(1-2r)) + (2(1+2r)-4rq)(x-1) + (1+2r)(x-1)^2$$

$$f(x) = 4r(1-q) + (2+4r(1-q))(x-1) + (1+2r)(x-1)^2,\ x > 1$$

$$4r(1-q) \geq 0,\ (2+4r(1-q)) > 0,\ (1+2r).0,\ x-1 > 0$$

Therefore $f(x) > 0$ when $x > 1$. Next let $g(x) = f(-x)$ and let $x > 1$.

$$g(x) = (1+2r)x^2 + 4rqx - (1-2r)$$

$$g'(x) = 2(1+2r)x + 4rq$$

$$g"(x) = 2(1+2r)$$

$$g(x) = 4r(1+q) + [2+4r(1+q)](x-1) + (1+2r)(x-1)^2$$

(Taylor polynomial for $g(x)$, expanded about $x = 1$.)

$$4r(1-q) \geq 0,\ (2+4r(1-q)) > 0,\ (1+2r).0,\ x-1 > 0$$

Therefore $g(x) > 0$ when $x > 1$, so $f(-x) > 0$ as well. This shows that $f(x)$ is all positive outside $[-1, 1]$, hence it does not have real roots whose absolute values exceed one. Since $f(x)$ is known to have two real roots, they are in $[-1, 1]$, thus $|x_1| \leq 1$; $|x_2| \leq 1$.

Case 2, $d = 0$ double root, real

$$x_{1,2} = \frac{4rq}{2(1+2r)} = \frac{2rq}{(1+2r)}$$

$$|x_{1,2}| = \left|\frac{2rq}{(1+2r)}\right| < \left|\frac{2r}{(1+2r)}\right| < 1.$$

Case 3, $d < 0$ two complex conjugate roots

$$x_1 = \bar{x}_2 \Rightarrow |x_1| = |x_2|.$$

$$|x_1| = \frac{4rq}{2(1+2r)} + \imath\frac{\sqrt{16r^2q^2 + 4(1+2r)(1-2r)}}{2(1+2r)}$$

$$|x_1|^2 = \frac{16r^2q^2}{4(1+2r)^2} + \frac{-16r^2q^2 - 4(1+2r)(1-2r)}{4(1+2r)^2}$$

$$\frac{-4(1+2r)(1-2r)}{4(1+2r)(1-2r)} = \frac{2r-1}{2r+1} < 1.$$

The calculation shows that the growth factor $|\exp(\alpha k)|$, for a single term in the finite Fourier series of errors at $t = 0$ is not greater than one. The term is not amplified out of bounds. Therefore, by superposition, the errors at $t = 0$ remain bounded, and the DuFort-Frankel scheme is unconditionally stable.

Problem 2.

For $\theta \geq 0$ examine the three level scheme

$$(1+\theta)\frac{U_{i,j+1}-U_{i,j}}{k} - \theta\left(\frac{U_{i,j}-U_{i,j-1}}{k}\right) = \frac{U_{i+1,j+1}-2U_{i,j+1}+U_{i-1,j+1}}{h^2}$$

for stability using the matrix method. Write V_j for the vector of mesh values along the j line and

$$AV_{j+1} = BV_j + CV_{j-1}$$

for the general three-level recurrence relation. (cf. Extension of matrix stability analysis, Ames)

Claim 1.

Let A, B, C, I be $n \times n$ matrices and

$$P = \begin{bmatrix} A^{-1}B & A^{-1}C \\ I & 0 \end{bmatrix}$$

Then the characteristic roots are

$$|P - \mu I| = |\mu^2 A - \mu B - C| = 0.$$

Proof Claim 1.

Schur complementation:

$$[P - \mu I] = \begin{bmatrix} A^{-1}B - \mu I & A^{-1}C \\ I & -\mu I \end{bmatrix} =$$

$$\begin{bmatrix} I & A^{-1}C(-\mu I)^{-1} \\ 0 & I \end{bmatrix} \times \begin{bmatrix} A^{-1}B - \mu I - A^{-1}C(-\mu I)^{-1}I & 0 \\ 0 & -\mu I \end{bmatrix} \times \begin{bmatrix} I & 0 \\ -(\mu I)^{-1}I & I \end{bmatrix}$$

$$\mu \neq 0.$$

By the elementary product rule of determinants

$$|P - \mu I| = |A^{-1}B - \mu I - A^{-1}C(-\mu I)^{-1}I||-\mu I|$$

Since $|-\mu I| \neq 0$

$$|P - \mu I| = |A^{-1}B - \mu I - A^{-1}C(-\mu I)^{-1}I| = 0.$$

$$A^{-1}B - \mu I - A^{-1}C(-\mu I)^{-1}I = A^{-1}(B - \mu A + C\mu^{-1})$$

$$|A| \neq 0$$

Therefore

$$|P - \mu I| = 0 \iff |\mu^2 A - \mu B - C| = 0,$$

and the eigenvalues of P can be calculated from the second equation.

Claim 2.

For the specific case under consideration

$$A = rT - 2rI - (1+\theta)I, \quad B = -(1+2\theta)I, \quad C = \theta I$$

where

$$I = \text{identity matrix}, \quad r = \frac{k}{r^2};$$

$$T = [t_{i,j}]; \quad t_{i,j} = \begin{cases} 1 & \text{for } |i-j| = 1 \\ 0 & \text{for } |i-j| \neq 1 \end{cases}$$

Proof Claim 2.

The equation

$$-(1+2\theta)U_{i,j} + \theta U_{i,j-1} = r\left(U_{i+1,j+1} - 2U_{i,j+1} + U_{i-1,j+1}\right) - (1+\theta)U_{i,j+1}$$

turns into

$$(1+2\theta)IV_j + \theta IV_{j-1} = rTV_{j+1} - 2rIV_{j+1} - (1+\theta)IV_{j+1}$$

$$(1+2\theta)IV_j + \theta IV_{j-1} = r\left(T - 2rI - (1+\theta)I\right)V_{j+1}.$$

with matrix notation. Therefore

$$A = rT - 2rI - (1+\theta)I$$

$$B = -(1+2\theta)I$$

$$C = \theta I.$$

Claim 3.

$$T = \begin{bmatrix} 0 & 1 & 0 & \dots & \dots & 0 \\ 1 & 0 & 1 & 0 & \dots & 0 \\ 0 & 1 & 0 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & 1 & 0 & 1 \\ 0 & 0 & \dots & \dots & 1 & 0 \end{bmatrix}_{N\times N}$$

symmetric band matrix with eigenvalues

$$\lambda = 2\cos(\phi_k); \quad (N+1)\phi_k = \pi k.$$

Eigenvalues of P.

The roots of the characteristic equation $|P - \mu I|$ are identical with the roots of $|\mu^2 A - \mu B - C|$. By **Claim 2.**

$$\mu^2 A - \mu B - C = \mu^2(rT - 2rI - (1+\theta)I) + \mu(1+2\theta)I - \theta I$$

$$= \mu^2 rT - 2r\mu^2 I - (1+\theta)\mu^2 I + \mu I + 2\theta\mu I - \theta I$$

$$= \mu^2 rT - (2r\mu^2 + (1+\theta)\mu^2 - (1+2\theta)\mu + \theta)I$$

$$T - \frac{2r\mu^2 + (1+\theta)\mu^2 - (1+2\theta)\mu + \theta)}{\mu^2 r} I = T - \lambda I$$

$$\lambda = \frac{2r\mu^2 + (1+\theta)\mu^2 - (1+2\theta)\mu + \theta)}{\mu^2 r}$$

$$|\mu^2 A - \mu B - C| = 0 \;\leftrightarrow\; |T - \lambda I| = 0 \;\leftrightarrow\; \lambda \,\epsilon\, \sigma(T)$$

where $\sigma(T)$ is the spectrum of matrix T, the set of all distinct eigenvalues. Recall the another expression for λ in **Claim 3.** :

$$\mu^2 r 2\cos(\phi_k) = 2r\mu^2 + (1+\theta)\mu^2 - (1+2\theta)\mu + \theta$$

$$\theta > 0, \quad r > 0, \quad \phi_k = \frac{\pi k}{N+1}, \quad k = 1 \dots N$$

$$\mu^2(2r + (1+\theta) - 2r\cos(\phi_k)) - \mu(1+2\theta) + \theta = 0$$

This is a quadratic equation in μ.

$$\mu_{1,2}^{(k)} = \frac{(1+2\theta) \pm \sqrt{(1+2\theta)^2 - 4\theta(2r(1-\phi_k)+(1+\theta)}}{2\left[2r(1-\cos\phi_k)+(1+\theta)\right]}$$

$$= \frac{1+2\theta \pm \sqrt{1-4\theta\cdot 2(1-\phi_k)r}}{2\left[2r(1-\cos\phi_k)+(1+\theta)\right]}.$$

Stability of finite difference scheme

The finite difference scheme is stable if $\max|\mu_l| \leq 1$, $\mu_l \,\epsilon\, \sigma(P)$. Write

$$d = 1 - 4\theta \cdot 2(1-\phi_k)r$$

and note

$$1 - \phi_k \geq 0.$$

Case 1, $d < 0$

$$|\mu_{1,2}^{(k)}|^2 = \frac{(1+2\theta)^2 + 4\theta\cdot 2r(1-\cos(\theta_k)) - 1}{2^2[(2r(1-\cos(\phi_k))+1)+\theta]^2}$$

$$= \frac{1+4\theta+4\theta^2+4\theta\cdot 2r(1-\cos(\theta_k)-1}{4[(2r(1-\cos(\phi_k))+1)+\theta]^2}$$

$$= \frac{\theta^2 + 2r(1-\cos(\phi_k)\theta}{\theta^2 + 2\cdot(2r(1-\cos(\phi_k))+1)\theta + (2r(1-\cos(\phi_k))+1)^2} < \ 1,$$

since $(2r(1-\cos(\phi_k))+1) > 0$, $\theta > 0$ and the numerator is less than the denominator.

Case 2, $d = 0$

$$\mu_{1,2}^{(k)} = \frac{1+2\theta}{2[2r(1-\cos(\phi_k))+1+\theta]}$$

$$0 < \mu_{1,2}^{(k)} < 1.$$

Case 3, $d > 0$

$$0 < 1 - 4\theta\cdot 2r\cdot(1-\phi_k) \leq 1 \implies \sqrt{d} \ \leq \ 1$$

$$0 \leq 2\theta \leq 1 + 2\theta \pm \sqrt{d} \leq 2 + 2\theta$$

Hence

$$\frac{2\theta}{2[2r(1-\cos(\phi_k)) + 1 + \theta]} \leq \frac{1 + 2\theta \pm \sqrt{d}}{2[2r(1-\cos(\phi_k)) + 1 + \theta]}$$

$$\frac{1 + 2\theta \pm \sqrt{d}}{2[2r(1-\cos(\phi_k)) + 1 + \theta]} \leq \frac{2 + 2\theta}{2[2r(1-\cos(\phi_k)) + 1 + \theta]}$$

and

$$0 \leq \mu_{1,2}^{(k)} \leq 1.$$

Therefore the finite difference scheme is unconditionally stable for $\theta \geq 0$.

Truncation error

Assuming sufficient differentiability

$$u(x_0 + h, y_0) = \sum_{\lambda=0}^{m-1} \frac{1}{\lambda!} \left(h \frac{\partial}{\partial x} \right)^{\lambda} u(x_0, y_0) + R_m^{(h,0)}$$

$$u(x_0 - h, y_0) = \sum_{\lambda=0}^{m-1} \frac{1}{\lambda!} \left(-h \frac{\partial}{\partial x} \right)^{\lambda} u(x_0, y_0) + R_m^{(-h,0)}$$

$$u(x_0 + h, y_0) + u(x_0 - h, y_0) - 2u(x_0, y_0) =$$

$$= \sum_{\lambda=2}^{m-1} \frac{1}{\lambda!} \left(h \frac{\partial}{\partial x} \right)^{\lambda} u(x_0, y_0) + R; \quad R = R_m^{(h,0)} + R_m^{(-h,0)}.$$

$$\frac{u(x_0 + h, y_0) - 2u(x_0, y_0) + u(x_0 - h, y_0)}{h^2} =$$

$$= \sum_{\lambda=2}^{m-1} \frac{h^{\lambda-2}}{\lambda!} \left(\frac{\partial}{\partial x} \right)^{\lambda} u(x_0, y_0) + \frac{R}{h^2} =$$

$$= \frac{\partial^2}{\partial x^2} u(x_0, y_0) + 2 \sum_{\lambda=4}^{m-1} \frac{h^{\lambda-2}}{\lambda!} \left(\frac{\partial}{\partial x} \right)^{\lambda} u(x_0, y_0) + \frac{h^{m-2}}{m!} M =$$

where M is a constant determined by $R_m^{(h,0)}$ and $R^{(-h,0)}$ and terms with λ odd cancel each other

$$= \frac{\partial^2}{\partial x^2}u(x_0, y_0) + h^2\frac{2}{4!}\frac{\partial^2}{\partial x^2}u(x_0, y_0) + \sum_{\lambda=6}^{m-1}\frac{h^{\lambda-2}}{\lambda!}\left(\frac{\partial}{\partial x}\right)^\lambda u(x_0, y_0) + \frac{h^{m-2}}{m!}M =$$

$$\frac{\partial^2}{\partial x^2}u(x_0, y_0) + \emptyset(h^2).$$

Similarly,

$$u(x_0, y_0 + k) = \sum_{\lambda=0}^{n-1}\frac{1}{\lambda!}\left(k\frac{\partial}{\partial y}\right)^\lambda u(x_0, y_0) + R_n^{(0,k)}$$

$$u(x_0, y_0 - k) = \sum_{\lambda=0}^{n-1}\frac{1}{\lambda!}\left(-k\frac{\partial}{\partial y}\right)^\lambda u(x_0, y_0) + R_n^{(0,k)}$$

$$\frac{u(x_0, y_0 + k) - u(x_0, y_0)}{k} =$$

$$= \frac{\partial}{\partial y}u(x_0, y_0) + \sum_{\lambda=2}^{n-1}\frac{k^{\lambda-1}}{\lambda!}\left(\frac{\partial}{\partial y}\right)^\lambda u(x_0, y_0) + \frac{R_n^{(0,k)}}{k}$$

$$= \frac{\partial}{\partial y}u(x_0, y_0) + \frac{k}{2}\frac{\partial^2}{\partial x^2}u(x_0, y_0) + \sum_{\lambda=3}^{n-1}\frac{k^{\lambda-1}}{\lambda!}\left(\frac{\partial}{\partial y}\right)^\lambda u(x_0, y_0) + k^{n-1}M_1$$

$$= \frac{\partial}{\partial y}u(x_0, y_0) + \emptyset(k).$$

Now repeat it with $-k$

$$\frac{u(x_0, y_0 - k) - u(x_0, y_0)}{k} =$$

$$= \frac{\partial}{\partial y}u(x_0, y_0) + \sum_{\lambda=2}^{n-1}\frac{-k^{\lambda-1}}{\lambda!}\left(\frac{\partial}{\partial y}\right)^\lambda u(x_0, y_0) + \frac{R_n^{(0,-k)}}{k}$$

$$= \frac{\partial}{\partial y}u(x_0, y_0) - \frac{k}{2}\frac{\partial^2}{\partial x^2}u(x_0, y_0) + \sum_{\lambda=3}^{n-1}\frac{-k^{\lambda-1}}{\lambda!}\left(\frac{\partial}{\partial y}\right)^\lambda u(x_0, y_0) + k^{n-1}M_2$$

$$= \frac{\partial}{\partial y}u(x_0, y_0) + \emptyset(k),$$

$M_1 = \text{const}$ $M_2 = \text{const}$

Truncation error for the finite difference scheme is $\emptyset(h^2) + \emptyset(k)$.

13.2 Assignment 34.

Summary

- Mathematical Modelling
- *Ciarlet, Ames*
- Last revision May 13, 2017

Problem 1.

Consider the linear system whose matrix is block tridiagonal

$$\begin{bmatrix} B_1 & C_1 & & & \\ A_2 & B_2 & C_2 & & \\ & A_3 & B_3 & C_3 & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & A_N & B_N \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ \\ V_N \end{bmatrix} = \begin{bmatrix} D_1 \\ D_2 \\ \vdots \\ \\ D_N \end{bmatrix}. \tag{13.1}$$

With the provision of certain hypothesis, which should be stated explicitly, show that the solution of this linear system may be obtained by constructing successively the three sequences $\{Z\}, \{W\}, \{V\}$, the first of matrices, the other two of vectors,

$$Z_1 = B_1^{-1}C_1,\ Z_k = (B_k - A_k Z_{k-1})^{-1}C_k,\ k = 2, 3, \ldots N,$$

$$W_1 = B_1^{-1}D_1,\ W_k = (B_k - A_k Z_{k-1})^{-1}(D_k - A_k W_{k-1}),\ k = 2, 3, \ldots N,$$

$$V_N = W_N,\ V_k = W_k - Z_k V_{k+1}, k = N-1, N-2, \ldots, 1$$

Proof:

$A_2, \ldots A_N$, $B_1, B_2, \ldots B_N$; and $C_1, C_2, \ldots C_{N-1}$ are blocks of size $n \times n$ whereas $V_1, V_2, \ldots V_N$, and $D_1, D_2, \ldots D_N$ are vectors of size n. Note that $A's, B's, C's, D's$ are input.

The first block row is

$$B_1V_1 + C_1V_2 = D_1$$

Assuming that B^{-1} exists we have

$$V_1 + B_1^{-1} C_1 V_2 = B_1^{-1} D_1$$

Write

$$Z_1 = B_1^{-1} C_1,\ W_1 = B_1^{-1} D_1,\ T_1^{-1} = B_1^{-1}.$$

Both matrix Z_1 and vector W_1 are computable, $\{T\}$ is an auxiliary set of matrices. Thus we are led to

$$V_1 + Z_1 V_2 = W_1$$

and

$$V_1 = W_1 - Z_1 V_2.$$

Next, we substitute this expression into second block row:

$$A_2 V_1 + B_2 V_2 + C_2 V_3 = D_2$$

$$A_2(W_1 - Z_1 V_2) + B_2 V_2 + C_2 V_3 = D_2$$

$$(B_2 - A_2 Z_1) V_2 + C_2 V_3 = D_2 - A_2 W_1$$

Again, assuming the existence of the inverse of the auxiliary matrix T_2

$$T_2^{-1} = (B_2 - A_2 Z_1)^{-1}$$

$$V_2 + (B_2 - A_2 Z_1)^{-1} C_2 V_3 = (B_2 - A_2 Z_1)^{-1} (D_2 - A_2 W_1)$$

Write

$$Z_2 = (B_2 - A_2 Z_1)^{-1} C_2 = T_2^{-1} C_2$$

$$W_2 = (B_2 - A_2 Z_1)^{-1} (D_2 - A_2 W_1) = T_2^{-1} (D_2 - A_2 W_1)$$

Then

$$V_2 + Z_2 C_3 = W_2$$

and finally

$$V_2 = W_2 - Z_2 V_3.$$

We can proceed to the next line

$$A_3V_2 + B_3V_3 + C_3V_4 = D_3$$

to obtain

$$V_3 = W_3 - Z_3V_4.$$

We repeat this procedure up to $N-1$. At each step

$$Z_k = (B_k - A_kZ_k)^{-1}C_k$$

$$W_k = (B_{N-}D_k - A_kW_{k-1})$$

$$V_k = W_{k-1} - Z_kV_{k+1}.$$

$$T_k^{-1} = (B_k - A_kZ_{k-1})^{-1}$$

where T_k is assumed to have an inverse. When we get to the last row

$$A_NV_{N-1} + B_NV_N = D_N$$

we can eliminate V_{N-1}

$$A_N(W_{N-1} - Z_{N-1}V_N) + B_NV_N = D_N$$

$$(B_N - A_NZ_{N-1})V_N = D_N - A_NW_{N-1}$$

$$V_N = (B_N - A_NZ_{N-1})^{-1}(D_N - A_NW_{N-1})$$

$$V_N = W_N$$

Thus V_N is resolved because W_N is computable at the $N-th$ step. Finally, backsubstitution into

$$V_k = W_{k-1} - Z_kV_{k+1}.$$

yields $V_{N-1}, V_{N-2}, \ldots V_2, V_1$, recursivelly. Therefore the solution to (1) can be calculated by constructing the following three sequences

$$Z_1 = B_1^{-1}C_1,\ Z_k = (B_k - A_kZ_{k-1})^{-1}C_k,\ k = 2, 3, \ldots N,$$

$$W_1 = B_1^{-1}D_1,\ W_k = (B_k - A_kZ_{k-1})^{-1}(D_k - A_kW_{k-1}),\ k = 2, 3, \ldots N,$$

$$V_N = W_N,\ V_k = W_k - Z_kV_{k+1}, k = N-1, N-2, \ldots, 1$$

provided that the fourth sequence exists:

$$T_1 = B_1^{-1},\ T_k = (B_k - A_kZ_{k-1})^{-1},\ k = 2, 3, \ldots N,$$

This is the equivalent of the standard algorithm for tridiagonal matrices. (cf. Thomas algorithm)

Demonstration:

Consider the following minimal 4×4 system:

$$\begin{bmatrix} b_1 & c_1 & & \\ a_2 & b_2 & c_2 & \\ & a_3 & b_3 & c_3 \\ & & b_4 & c_4 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ d_4 \end{bmatrix}$$

First row:

$$b_1 v_1 + c_1 v_2 = d_1$$

$$v_1 = b_1^{-1}(d_1 - c_1 v_2),\ b_1 \neq 0$$

$$z_1 = b_1^{-1} c_1,\ w_1 = b_1^{-1} d_1,\ t_1^{-1} = b_1^{-1}.$$

$$v_1 + z_1 v_2 = w_1$$

$$v_1 = w_1 - z_1 v_2.$$

Second row:

$$a_2 v_1 + b_2 v_2 + c_2 v_3 = d_2$$

$$a_2(w_1 - z_1 v_2) + b_2 v_2 + c_2 v_3 = d_2$$

$$(b_2 - b_2 z_1) v_2 + c_2 v_3 = d_2 - a_2 w_1$$

$$t_2^{-1} = (b_2 - a_2 z_1)^{-1},\ (b_2 - a_2 z_1) \neq 0$$

$$v_2 + (b_2 - a_2 z_1)^{-1} c_2 v_3 = (b_2 - a_2 z_1)^{-1}(d_2 - a_2 w_1)$$

$$z_2 = (b_2 - a_2 z_1)^{-1} c_2 = t_2^{-1} c_2$$

$$w_2 = (b_2 - a_2 z_1)^{-1}(d_2 - a_2 w_1) = t_2^{-1}(d_2 - a_2 w_1)$$

$$v_2 + z_2 c_3 = w_2$$

$$v_2 = w_2 - z_2 v_3.$$

Third row:

$$a_3v_2 + b_3v_3 + c_3v_4 = d_3$$

$$\vdots$$

$$v_3 = w_3 - z_3v_4.$$

Fourth row:

$$a_4v_3 + B_4V_3 = d_4$$

$$a_4(w_3 - z_3v_4) + b_4v_4 = d_4$$

$$(b_4 - a_4z_3)v_4 = d_4 - a_4w_3$$

$$v_4 = (b_4 - a_4z_3)^{-1}(d_4 - a_4w_3)$$

$$v_4 = w_4\surd$$

Recursion:

$$v_k = w_{k-1} - z_kv_{k+1}.$$

thus v_3, v_2, v_1 are computable if t_1, t_2, t_3, t_4 are not zero.

Problem 2.

Let A, B, I be $n \times n$ matrices. (I is the identity matrix.) Suppose $I - AB$ is invertible. Then

$$(I - BA)^{-1} = I + B(I - AB)^{-1}A.$$

Proof:

$$(I - BA)B = B - BAB = B(I - AB)$$

$$(I - BA)B(I - AB)^{-1}A = (B - BAB)(I - AB)^{-1}A =$$

$$B(I - AB)(I - AB)^{-1}A = BA$$

$$(I - BA) + (I - BA)B(I - AB)^{-1}A = (I - BA) + BA$$

$$(I - BA)(I + B(I - AB)^{-1}A) = I$$

$$(I - BA)(I + B(I - AB)^{-1}A) = I$$

$$(I - BA)^{-1} = I + B(I - AB)^{-1}A.$$

q.e.d.

Problem 3.

$$(A + uv^T)^{-1} = A^{-1} - \frac{(A^{-1}u)(v^T A^{-1})}{1 + v^T A^{-1} u}$$

Discussion:

This is the *Sherman - Morrison* formula. A is an invertible $n \times n$ matrix, u, v are compatible column vectors. Suppose A is modified by a diadic product and the new matrix is $(A + uv^T)$. The formula provides an inverse for the new matrix. $(A + uv^T)$ is an $n \times n$ matrix, $(A^{-1}u)$ is column vector, the product $(v^T A^{-1})$ is a row vector. $(A^{-1}u)(v^T A^{-1})$ is a diadic product, an $n \times n$ matrix. $(1 + v^T A^{-1} u)$ is a (non-zero) scalar, $(v^T A^{-1} u)$ is a scalar, too. We will use the fact that a product of compatible matrices is associative. In particular

$$(uv^T)(A^{-1}u)(v^T A^{-1}) = u(v^T A^{-1} u)(v^T A^{-1}) = (v^T A^{-1} u) u (v^T A^{-1}).$$

Proof:

$$(A + uv^T)\left(A^{-1} - \frac{(A^{-1}u)(v^T A^{-1})}{1 + v^T A^{-1} u}\right) =$$

$$AA^{-1} + uv^T A^{-1} - \frac{(AA^{-1}u)(v^T A^{-1})}{1 + v^T A^{-1} u} - \frac{u(v^T A^{-1} u)(v^T A^{-1})}{1 + v^T A^{-1} u} =$$

$$I + uv^T A^{-1} - \frac{(uv^T A^{-1})}{1 + v^T A^{-1} u} - \frac{(v^T A^{-1} u)(uv^T A^{-1})}{1 + v^T A^{-1} u} =$$

$$I + uv^T A^{-1} - (uv^T A^{-1})\left(\frac{I}{1 + v^T A^{-1} u} + \frac{(v^T A^{-1} u) I}{1 + v^T A^{-1} u}\right) =$$

$$I + (uv^T A^{-1})\left(I - \frac{I}{1 + v^T A^{-1} u} - \frac{(v^T A^{-1} u) I}{1 + v^T A^{-1} u}\right) =$$

$$I + (uv^T A^{-1})\left(\frac{1 + v^T A^{-1} u}{1 + v^T A^{-1} u} I - \frac{I}{1 + v^T A^{-1} u} - \frac{(v^T A^{-1} u) I}{1 + v^T A^{-1} u}\right) =$$

$$I + (uv^T A^{-1})\left(\frac{1 + v^T A^{-1} u}{1 + v^T A^{-1} u} - \frac{1}{1 + v^T A^{-1} u} - \frac{(v^T A^{-1} u)}{1 + v^T A^{-1} u}\right) I =$$

$$I + (uv^T A^{-1})\left(\frac{0}{1 + v^T A^{-1} u}\right) I = I.$$

13.3 Assignment 35.

Summary

- Mathematical Modelling
- *Notes on three-phase fluid flow - Flucht nach vorne*
- Last revision May 13, 2017

1. Units and dimensions The fundamental physical quantities that underline all other in reservoir simulation are time, distance, mass, absolute temperature and amount of substance. Their dimension in SI units are second (s), meter (m), kilogram (kg), kelvin (K) and mole (mol); respectively.

Further quantities can be derived; for example velocity (ms^{-1}), acceleration (ms^{-2}) and force ($kgms^{-2}$). The acceleration of gravity is considered constant in this work

$$g = 9.806\ 65\ ms^2.$$

The composite unit for force is also called the newton (N). Pressure is defined as force per unit area, and is measured in Nm^2, which for convenience is called pascal (Pa). Moreover,

$$1\ bar = 100\ 000\ Pa$$

is also widely used in engineering. One bar is approximately equal to the standard atmosphere, defined as 101 325 Pa.

Let P be a point in a differential element of volume of continuous fluid. The limit ratio of mass to its volume, as the differential element shrinks about point P, is called the density at P. Density is measured in SI unit kgm^{-3}.

2. Viscosity Next, viscosity or internal friction will be described in simple terms. Imagine, that in a laminar flow there are two parallel plates of continuous fluid at distance h. Let one of the plates move relative to the other at constant velocity v_0.

Then, according to experiments, the force per unit area of the plate is directly proportional to v and inversely proportional to h

$$\frac{F}{S} = \frac{\mu v_0}{h}$$

where S is the area of the plate. The facror is called viscosity or dynamic viscosity. The so-called kinematic viscosity

$$\nu = \frac{\mu}{\rho}$$

is the ratio of viscosity to fluid density ρ. The SI unit for viscosity is $kgms^{-2}sm^{-2} = kgm^{-1}s^{-1}$. We note that the consequence of "no slip" boundary condition of real fluids is that all components of velocityof the fluid vanish on the surface of the body at rest. Also, we remark that viscosity can be defined by examining the shearing deformation in real fluid.

3. Conversion The English engineering units - for example in Sheffield's work - are converted to SI units by the following

$$1\ foot = 0.3048\ m$$

$$1\ cu.ft = 0.02831\ m^3$$

$$1\ barrel = 1.589873E - 01\ m^3$$

The unit "oil barrel (bbl)" is standardized, it is cca. $159\,L = 42\,US\ gallons = 35\ Imperial\ gallons$. The Kelvin scale of absolute temperature is related to common Celsius scale by the equation

$$T(K) = t(C) + 273.15.$$

Conversion from psi to bar is

$$1\ psi * 6.894757E - 02 = 1\ bar$$

The conventional units for density and viscosity are $grcm^{-3}$ and centipoise, respectively

$$1\ centipoise = 0.001\ \frac{Ns}{m^2}$$

4. Porosity, permeability We shall describe the physical properties of rocks found in reservoirs. The reservoir rocks are porous and they transmit fluids.They are also vetted by liquids.

Porosity is the volume of the pore space actually in communication with the pores terminating at the well bore divided by the total volume. So porosity is a fraction between 0 and 1.

Local absolute porosity (k) quantifies the ability of the rock to transmit fluid under specified conditions. It is defined by Darcy's law and has the dimension of (m^2). In practice permeability is given in millidarcys

$$1000\ mD = 1\ Darcy = 1.02\ E - 12\ m^{-2}$$

The apparent permeability to a particular phase, - wter, oil, gas - is termed the effective permeability and denoted by $k_w,\ k_o,\ k_g$. The unit of effective permeability is the same as for local permeability.

The ratio of the effective permeability of a particular phase to the local absolute permeability is designated the "relative permeability". It is a dimensionless fraction

$$k_{rw} = \frac{k_w}{k};\ k_{ro} = \frac{k_o}{k};\ k_{rg} = \frac{k_g}{k}.$$

5. Saturation It is a further experimental fact that in case of more than one fluid or phase flowing in the reservoir the presence of one impedes the flow of the other. The extent to which the flow or flows are effected is determined by the saturation of the phases - s_w for water, s_o for oil, s_g for gas.

The saturation of a fluid is the fraction of the space available to flow occupied by that fluid or phase. Since all three phases are flowing

$$s_w + s_o + s_g = 1.$$

The relative permeability to a given fluid depends primarily upon the saturation of that fluid, although when three fluids flow it is effected to some extent by the saturations of the other two fluids. The permeability to a given fluid becomes zero at low saturations. Under no conditions is the permeability simultaneously zero to all fluids present; if a pressure gradient can be established some fluids will flow. However as oil is being produced, it is displaced by another fluid either gas or water. Thus the oil saturation diminishes and the permeability to oil decreases. Eventually the permeability to oil vanishes and the flow of oil ceases. The oil left uncovered in the reservoir due to low saturation is called residual oil.

6. Capillary effects Reservoir rocks as solids are vetted by liquids and there are capillary effects influencing the flow of fluids.A familiar example of movement of fluid due to capillary pressure is the rise of water in a vertical glass tube of small bore whose lower end is immersed in a vessel of water. Although the capillary passages in sands in pores of reservoir rocks do not resemble the uniform bore of a glass capillary tube it is an experimental fact that three-phase fluid flow is influenced by capillary pressures arising in water-oil and oil-gas subsystems.

Each fluid - water, oil, gas - has its specific pressure $p_w,\ p_w,\ p_w$. The difference between oil and water pressure is a monotone function of water saturation. It is called the capillary pressure of the oil-gas subsystem.

7. Fluid properties Consider a fixed mass of isotropic fluid isolated from external effects. Such systems are characterized by three measurable coordinates pressure P, volume V, temperature T and are called PVT systems.

The coordinates however are not independent, and the equation of state for equilibrium state can be expressed in a functional form

$$f(P, V, T) = 0$$

or for ideal gas

$$PV = RT$$

where P is pressure, V is molar volume, R is the universal gas constant,

$$R = 8.314\ m^3 Pa\ mol^{-1} K^{-1}$$

A useful, simplified equation of state of real gases is

$$PV = ZRT$$

where Z is a specific constant signifying the ratio of V_{real} per V_{ideal} .

8. Gas in solution In closing we shall illustrate by a textbook example the phase behavior of oil with gas in solution. The expansion and separation of fluids into gasous and liquid phases were observed in a laboratory experiment. The fluid which contains oil and gas in solution is confined in a vertical piston-and-cylinder apparatus in contact with a heat reservoir. The piston is frictionless, cooling is done slowly and all states assumed by the system are equivilibrium states. There are five states recorded.

1)	The initial state	$P_o = 225\ at$, $T = 85\ C$, $V_o = 80.00\ cm^3$
2)	Then pressure is reduced to bubble point pressure	$P_b = 177\ at$ $T = 85\ C$ $V_o = 87.92\ cm^3$
3)	Cooling and further reduction in pressure results in a state with two phases	$P = 27\ at$ $T = 26\ C$ $V_o = 70.05\ cm^3$ $V_g = 191.53\ cm^3$
5)	More cooling	$P = 1\ at$ $T = 15\ C$ $V_o = 63.03\ cm^3$ $V_g = 7790\ cm^3$

The initial state (1) is what we could find in a reservoir and the terminal state (5) is what prevails on the surface. Volumes of free gas and gas in solution vary with pressure and temperature.

13.4 Assignment 36.

Summary

- Mathematical Modelling
- *Douglas*
- Last revision May 13, 2017

Introduction

Let us consider a hypothetical one-dimensional reservoir of porous medium of unit cross-sectional area and of length L extending from $\xi = 0$ to $\xi = L$. Let us suppose that the reservoir contains oil and water and both fluids are incompressible. Assume further that gravitational forces can be neglected.

At one end, say at $\xi = 0$, water is injected into the reservoir. Then from the other end water and oil is produced. This process is known as one-dimensional waterflood or linear waterflood and is performed as a laboratory tube experiment.

In this and subsequent essays we propose to

1. formulate
2. numerically solve
3. illustrate a 1D waterflood with typical reservoir characteristics.

Presently our objective is 1).

Formulation of initial-boundary value problem

$q_w, q_0 -$ water and oil flow rates per unit cross section

$s_w, s_o -$ water and oil saturation

$\phi -$ porosity

$\xi, \tau -$ dimensional space and time

Conservation of mass

$$\frac{\partial q_w}{\partial \xi} = -\phi \frac{\partial s_w}{\partial \tau} \tag{13.2}$$

$$\frac{\partial q_o}{\partial \xi} = -\phi \frac{\partial s_o}{\partial \tau} \tag{13.3}$$

k_w, k_o – effective permeabilitis with respect to water and oil

μ_w, μ_o – viscosity of the phase

p_w, p_o – pressure of the phase

Darcy's law

$$q_w = -\frac{k_w}{\mu_w}\frac{\partial p_w}{\partial \xi} \tag{13.4}$$

$$q_o = -\frac{k_o}{\mu_o}\frac{\partial p_o}{\partial \xi}. \tag{13.5}$$

Note that effective permeabilities are functions of their respective saturations. Capillary pressure

$$p_c = p_o - p_w. \tag{13.6}$$

Saturation, water and oil fill the pore space

$$s = s_o = 1 - s_w. \tag{13.7}$$

Empirical fact, capillary pressure depends on saturation

$$p_c = p_c(s).$$

Flow rate

$$Q(\tau) = q_w(\xi, \tau) + q_o(\xi, \tau). \tag{13.8}$$

Assume constant flow rate Q

$$Q = q_w(\xi, \tau) + q_o(\xi, \tau). \tag{13.9}$$

Next, p_o is replaced by $p_w + p_c$ in 13.5 and substituted with 13.4 into 13.9

$$Q = -\frac{k_w}{\mu_w}\frac{\partial p_w}{\partial \xi} - \frac{k_o}{\mu_o}\frac{\partial (p_w + p_c)}{\partial \xi} = \frac{k_w}{\mu_w}\frac{\partial p_w}{\partial \xi} - \frac{k_o}{\mu_o}\frac{\partial p_w}{\partial \xi} - \frac{k_o}{\mu_o}\frac{\partial p_c}{\partial \xi}.$$

$$\left(\frac{k_w}{\mu_w} + \frac{k_o}{\mu_o}\right)\frac{\partial p_w}{\partial \xi} = -Q - \frac{k_o}{\mu_o}\frac{\partial p_c}{\partial \xi}.$$

$$\frac{\partial p_w}{\partial \xi} = -\frac{Q}{\frac{k_w}{\mu_w} + \frac{k_o}{\mu_o}} - \frac{\frac{k_o}{\mu_o}}{\frac{k_w}{\mu_w} + \frac{k_o}{\mu_o}}\frac{\partial p_c}{\partial \xi}.$$

Since p_c depends only on s we have

$$\frac{\partial p_w}{\partial \xi} = \frac{-Q}{\frac{k_w}{\mu_w} + \frac{k_o}{\mu_o}} - \frac{1}{1 + \frac{k_w \mu_o}{\mu_w k_o}}\frac{\partial p_c}{\partial s}\frac{\partial s}{\partial \xi}. \tag{13.10}$$

Next, substitute 13.10 into 13.4.

$$q_w = -\frac{k_w}{\mu_w}\left(\frac{-Q}{\frac{k_w}{\mu_w} + \frac{k_o}{\mu_o}} - \frac{1}{1 + \frac{k_w \mu_o}{\mu_w k_o}}\frac{\partial p_c}{\partial s}\frac{\partial s}{\partial \xi}\right)$$

$$q_w = \frac{Q}{1 + \frac{\mu_w k_o}{k_w \mu_o}} + \frac{1}{\frac{\mu_w}{k_w} + \frac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\frac{\partial s}{\partial \xi}.$$

Combine this with 13.2 which expresses the conservation of mass

$$\frac{\partial}{\partial \xi}\left(\frac{Q}{1 + \frac{\mu_w k_o}{k_w \mu_o}} + \frac{1}{\frac{\mu_w}{k_w} + \frac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\right) = -\phi\frac{\partial s_w}{\partial \tau}$$

where

$$-\phi\frac{\partial s_w}{\partial \tau} = -\phi\frac{\partial}{\partial \tau}(1 - s) = -\phi\frac{\partial s}{\partial \tau}.$$

Furthermore

$$\frac{\partial}{\partial \xi}\left(\frac{Q}{1+\dfrac{\mu_w k_o}{k_w \mu_o}}\right)+\frac{\partial}{\partial \xi}\left(\frac{1}{\dfrac{\mu_w}{k_w}+\dfrac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\frac{\partial s}{\partial \xi}\right)=\phi\frac{\partial s}{\partial \tau}.$$

$$\frac{\partial}{\partial \xi}\left[\left(\frac{1}{\dfrac{\mu_w}{k_w}+\dfrac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\right)\frac{\partial s}{\partial \xi}\right]+\frac{\partial}{\partial s}\left[\frac{Q}{1+\dfrac{\mu_w k_o}{k_w \mu_o}}\right]\frac{\partial s}{\partial \xi}=\phi\frac{\partial s}{\partial \tau}.$$

This will be made simpler by scaling. New variables x, t are dimensionless.

$$x=\xi/L \tag{13.11}$$

$$t=Q\tau/L\phi \tag{13.12}$$

Hence

$$\xi = Lx$$

$$d\xi = Ldx$$

$$\tau = L\phi t/Q$$

$$d\tau = \left(\frac{L\phi}{Q}\right)dt.$$

$$\frac{\partial}{L\partial x}\left[\left(\frac{1}{\dfrac{\mu_w}{k_w}+\dfrac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\right)\frac{\partial s}{L\partial x}\right]+\frac{\partial}{\partial s}\left[\frac{Q}{1+\dfrac{\mu_w k_o}{k_w \mu_o}}\right]\frac{\partial s}{L\partial x}=\phi\frac{1}{\dfrac{L\phi}{Q}}\frac{\partial s}{\partial t}.$$

Substitution and simplification give

$$\frac{\partial}{\partial x}\left[\left(\frac{1}{\dfrac{\mu_w}{k_w}+\dfrac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\right)\frac{\partial s}{L\partial x}\right]+\frac{\partial}{\partial s}\left[\frac{Q}{1+\dfrac{\mu_w k_o}{k_w \mu_o}}\right]\frac{\partial s}{L\partial x}=Q\frac{\partial s}{\partial \tau}.$$

$$\frac{\partial}{\partial x}\left[\frac{1}{QL}\left(\frac{1}{\dfrac{\mu_w}{k_w}+\dfrac{\mu_o}{k_o}}\frac{\partial p_c}{\partial s}\right)\frac{\partial s}{\partial x}\right]+\frac{\partial}{\partial s}\left[\frac{1}{1+\dfrac{\mu_w k_o}{k_w \mu_o}}\right]\frac{\partial s}{\partial x}=\frac{\partial s}{\partial \tau}.$$

Typical coefficients and dimensionless groups

In order to further simplify the last equation let us introduce the following notations

$K -$ total permeability

$k_{ro}, krw -$ relative permeabilities

$\gamma(s) -$ dimensionless capillary pressure gradient

$h(s) -$ flow function

$f(s) -$ fractional flow function

$g(s) -$ permeability - capillary pressure function

$$\gamma(s) = \frac{dp_c}{ds}\left[\frac{dp_c}{ds}\right]_{char}^{-1}$$

$$h(s) = \frac{d}{ds}f(s)$$

$$f(s) = \frac{1}{1 + \frac{\mu_w k_o}{k_w \mu_o}}$$

$$g(s) = \frac{K\left[\frac{dp_c}{ds}\right]_{char}}{QL\mu_o}\frac{k_{ro}k_{rw}}{k_{rw} + \frac{\mu_w}{\mu_o}}\gamma(s).$$

The saturation profile at any time depends on the value of the dimensionless groups C_1 and C_2:

$$C_1 = \frac{QL\mu_o}{K\left[\frac{dp_c}{ds}\right]_{char}},$$

$$C_2 = \frac{\mu_w}{\mu_o}.$$

Aided by the foregoing notation, the partial differential equation for 1D waterflood can be written as

$$\frac{\partial}{\partial x} g(s) \frac{\partial}{\partial x} s + h(s) \frac{\partial}{\partial x} s = \frac{\partial s}{\partial t}, \quad 0 \le x \le 1, \quad 0 \le t \le T. \tag{13.13}$$

What are the boundary conditions? Let s_{low} and s_{upp} denote the minimum and maximum of the relative saturation of the non-vetting (i.e. oil) phase. We suppose that the flooding starts at s_{init} and our numerical simulation stops just before the water saturation attains its maximum at the outflow ($\xi = L$) face. It is verified experimentally, that during this interval only oil is produced at the outflow face and only water flows through the inflow ($\xi = 0$) face.

So to set boundary conditions at ($\xi = 0$) , we write

$$q_o(0, t) = 0 \tag{13.14}$$

signifying that oil does not flow through there. Hence

$$0 = q_0 = -\frac{k_0}{\mu_o} \frac{\partial p_o}{\partial \xi} = -\frac{k_0}{\mu_o} \frac{\partial p_o}{L \partial x}$$

and

$$\frac{\partial p_o}{\partial \xi} = \frac{\partial p_o}{L \partial x} = 0.$$

Therefore

$$-\frac{\partial k_w}{\mu_w} \frac{\partial p_w}{L \partial x} = Q$$

at this boundary. Note the capillary pressure gradient

$$\frac{\partial p_c}{\partial x} = \frac{dp_c}{ds} \frac{\partial s}{\partial x}.$$

By construction

$$g(s) = \frac{k_w k_o \frac{dp_c}{ds}}{QL(k_w \mu_o + k_o \mu_w)}.$$

Thus

$$g(s) \frac{\partial s}{\partial x} = \frac{k_w k_o \frac{dp_c}{ds} \frac{\partial s}{\partial x}}{QL(k_w \mu_o + k_o \mu_w)}.$$

and

$$\frac{dp_c}{ds}\frac{\partial s}{\partial x} = \frac{\partial p_c}{\partial x} = \frac{\partial p_o}{\partial x} - \frac{\partial p_w}{\partial x} = \frac{QL\mu_w}{k_w}$$

give

$$g(s)\frac{\partial s}{\partial x} = \frac{k_w k_o \dfrac{QL\mu_w}{k_w}}{QL(k_w\mu_o + k_o\mu_w)}.$$

Whence

$$\frac{\partial s}{\partial x} = \frac{1}{g(s)}\frac{1}{1 + \dfrac{k_w\mu_o}{k_o\mu_w}}.$$

Next, let us define

$$\alpha(s) = \frac{1}{g(s)}\frac{1}{1 + \dfrac{k_{rw}\mu_o}{k_{ro}\mu_w}} \tag{13.15}$$

the boundary condition at the inflow face where water is injected in the reservoir.

To find the boundary conditions at the other end we start with

$$q_w(0,t) = 0 \tag{13.16}$$

and by similar argument as above we arrive at

$$\beta(s) = \frac{1}{g(s)}\frac{-1}{1 + \dfrac{k_{ro}\mu_w}{k_{rw}\mu_o}}, \tag{13.17}$$

where β is the boundary condition at the outflow face describing $\dfrac{\partial s}{\partial x}$ at $(\xi = L)$. Note the different directions of the flows at the ends are reflected in the different signs. Our model does not extend to water breakthrough.

This completes the setting of initial and boundary conditions.

Before we collect our results in a grand formal statement of the problem let us examine the coefficient functions. First, k_{rw} and k_{ro} are functions of their respective saturations; if they are expressed as functions of a sole variable, oil saturation s, (cf. 13.7) , then

$$\frac{dk_{rw}}{ds} < 0$$

$$\frac{dk_{ro}}{ds} > 0$$

over the range $s_{low} < s < s_{upp}$.

The dimensionless capillary pressure gradient function, $\gamma(s)$ ranges over (s_{low}, s_{upp}) and it is strictly positive. It has singularity at the endpoints. These curves describe the physical characteristics of the reservoir.

The dimensionless group C_1 is defined by

$$C_1 = \frac{QL\mu_o}{K\left[\frac{dp_c}{ds}\right]_{char}}.$$

Note that if Q increases so does C_1. Thus - assuming that other parameters are fixed - C_1 can indicate the influx of water in the reservoir. The rate of viscosities of the two phases are expressed by C_2.

Statement of the problem

Find numerical approximation for $s(x,t)$ in

$$\frac{\partial}{\partial x} g(s) \frac{\partial}{\partial x} s + h(s) \frac{\partial}{\partial x} s = \frac{\partial s}{\partial t}, \quad 0 \leq x \leq 1, \quad 0 \leq t \leq T. \tag{13.18}$$

$$\frac{\partial}{\partial x} s_{|x=0} = \alpha; \quad \frac{\partial}{\partial x} s_{|x=1} = \beta \tag{13.19}$$

where

$$s_{init} = 0.125; \; s_{low} = 0.15; \; s_{upp} = 0.9625$$

$$C_1 = 1; \; C_2 = 0.5$$

and

$$\alpha, \; \beta, \; \gamma, \; k_{rw}, \; k_{ro}, \; f, \; g, \; h$$

are defined above.