

Mathematical Physics of Water Systems

Exam

code: 195400900, year: 2010/11

date: 15 April 2011, time: 13:45-17:15, location: OH-114

Introduction

This exam consists of 14 numbered items, worth a total of 26 points. You are allowed to write your answers in either English or Dutch. After the exam, this paper must be handed in along with your answers. Time: 3.5 hours. Good luck!

Equilibrium solutions to a diffusion problem (8p)

In a one-dimensional space domain of length L , let us consider the PDE

$$\frac{\partial u}{\partial t} = \delta \frac{\partial^2 u}{\partial x^2}, \quad (0 < x < L, \quad t > 0), \quad (1)$$

with coefficient $\delta > 0$. The unknown $u(x, t)$ is a function of the spatial coordinate x and time t . We impose an arbitrary initial profile $u(x, 0) = u_0(x)$ and Dirichlet BCs: $u(0, t) = U_{\text{left}}$ and $u(L, t) = U_{\text{right}}$ with $0 < U_{\text{left}} < U_{\text{right}}$.

- (1p) **1.** Show whether the PDE (1) is hyperbolic, parabolic or elliptic.
- (2p) **2.** Derive and plot the equilibrium profile to this problem. Describe the diffusive flux of this equilibrium.

To solve this problem numerically, let us define $x_j = j \Delta x$ and $t_k = k \Delta t$ with space step Δx and time step Δt . Furthermore, $u_{j,k}$ denotes the numerical solution at $(x, t) = (x_j, t_k)$. The well-known FTCS-scheme reads

$$u_{j,k+1} = \mathcal{D}u_{j-1,k} + (1 - 2\mathcal{D})u_{j,k} + \mathcal{D}u_{j+1,k}, \quad (2)$$

with diffusion number $\mathcal{D} = \delta \frac{\Delta t}{(\Delta x)^2}$. Based on equation (2), one may state:

- A. “The numerical value at $x = x_j$ decreases in time as long as it is larger than the average of its neighbouring values.”
- B. “The numerical value at $x = x_j$ increases in time as long as it is smaller than the average of its neighbouring values.”
- (2p) **3.** Show that statements A and B are true (for points *not* on the boundary). What do these statements imply for the *numerical* equilibrium solution?
- (3p) **4.** Using a Von Neumann stability analysis, derive the stability properties of the FTCS-scheme in equation (2).

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Advection and decay in one-dimensional flow

Formulation (6p)

We consider a section of length L in an elongated test channel, where a biogeomorphologist investigates the behaviour of a certain type of biota subject to a steady current. This type of biota experiences two phenomena: advection by the current and decay due to biochemical processes.

The biomass density per unit length is given by $f(x, t)$ (in milligrams per meter: mg m^{-1}), defined as a function of the spatial coordinate x in m ($0 < x < L$) and time t in s ($t > 0$). The quantity $f(x, t)$ satisfies the following differential equation:

$$\frac{\partial f}{\partial t} + \gamma \frac{\partial f}{\partial x} = -\beta f^3, \quad (3)$$

with coefficients β and γ . Introducing a coefficient $f_0 > 0$, the initial and boundary conditions are given by

$$f(x, 0) = f_0 \sin(\pi x/L), \quad \text{for } 0 < x < L, \quad (4)$$

$$f(0, t) = 0, \quad \text{for } t > 0. \quad (5)$$

(1p) **5.** Derive the dimension of β .

(2p) **6.** Classify equation (3) in the following respects: ODE/PDE, linear/nonlinear and (if applicable!) homogeneous/nonhomogeneous. Do this for three cases by copying and completing the table below.

case	param. values	ODE/PDE	linear/nonlin.	hom./nonhom.
I.	$\gamma = 0, \beta > 0$	...	...	...
II.	$\gamma > 0, \beta = 0$	...	...	...
III.	$\gamma > 0, \beta > 0$	...	...	...

(2p) **7.** Plot the initial profile according to equation (4) and calculate the total biomass F initially present in the section of the test channel.

(1p) **8.** Sketch the domain of the differential problem in the (x, t) -plane. In your sketch, clearly indicate the initial and boundary conditions.

Case I: decay only (3p)

Now let us proceed by considering the differential problem (3)-(5) for $\gamma = 0$ and $\beta > 0$. This means that advection is absent, and that only biochemical decay is present.

(3p) **9.** Solve $f(x_0, t)$ at the fixed position $x_0 = \frac{1}{2}L$. Next, describe the solution at other positions x .

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Case II: advection only (4p)

Alternatively, let us consider the differential problem (3)-(5) for $\gamma > 0$ and $\beta = 0$. This means that biochemical decay is absent, and that only advection is present. The solution is then given by

$$f(x, t) = \begin{cases} f_0 \sin(\pi[x - \gamma t]/L) & \text{if } x > \gamma t, \\ 0 & \text{if } x \leq \gamma t. \end{cases} \quad (6)$$

- (2p) **10.** By substitution, show that the solution to the differential problem (3)-(5) (with $\beta = 0$) is indeed given by equation (6).
- (1p) **11.** Regarding the solution, explain the role of the lines in the (x, t) -plane, characterized by constant values of $x - \gamma t$.
- (1p) **12.** What has happened to the solution at $t = L/\gamma$? Explain this in terms of the initial and boundary conditions.

Case III: both advection and decay (5p)

Finally, we consider the most general case in which both advection and decay are present, i.e. $\beta > 0$ and $\gamma > 0$.

- (2p) **13.** Describe the solution qualitatively in this case. What kind of behaviour takes place along the lines characterized by constant values of $x - \gamma t$?

For $\beta > 0$ and $\gamma > 0$, the above differential problem (3)-(5) can also be solved numerically, e.g. using the method of finite differences. To this end, let us define $x_j = j \Delta x$ and $t_k = k \Delta t$ with space step Δx and time step Δt . Furthermore, $f_{j,k}$ denotes the numerical solution at $x = x_j$ and $t = t_k$.

We will now derive a so-called *semi-implicit upwind scheme*, which combines the following discretizations:

- *Backward-Euler* for the time derivative
- *Upwind* for the space derivative
- A ‘mixed’ representation of the term on the right-hand side of equation (3): write f^3 as a suitable product of the solutions at the old time level (f^2) and new time level (f). Note that this is a consistent discretization!

- (3p) **14.** Derive the semi-implicit numerical scheme for the differential problem, i.e. express $f_{j,k+1}$ in terms of $f_{j-1,k+1}$ and $f_{j,k}$:

$$f_{j,k+1} = \dots$$

end of exam ◁

Answers

Item 1 (1p)

Whether the diffusion equation (1) is parabolic, hyperbolic or elliptic, follows from calculating the discriminant $\text{Discr} = B^2 - 4AC$ [1/5] in which $B = 0$, $A = \pm\delta$ and $C = 0$ [1/5] (or, equivalently, A and C defined the other way around), which leads to $\text{Discr} = 0$ [1/5]. This finally shows that the diffusion equation is *parabolic* [2/5].

Item 2 (2p)

The correct answer consists of the following three steps.

- Equilibrium profiles $u_{\text{eq}}(x)$ satisfy $\frac{\partial u_{\text{eq}}}{\partial t} = 0$, i.e. $\frac{\partial^2 u_{\text{eq}}}{\partial x^2} = 0$ [1/3]. Integrating the latter expression twice with respect to x implies a linear equilibrium profile $u_{\text{eq}}(x) = Ax + B$ for some constants A and B [1/3]. Imposing the boundary conditions resolves these constants, which finally gives [1/3]:

$$u_{\text{eq}}(x) = U_{\text{left}} + \frac{U_{\text{right}} - U_{\text{left}}}{L}x. \quad (7)$$

- The plot should show a linear curve with a positive slope and correctly display the axes labels as well as the meaning of the parameters U_{left} , U_{right} and L [1/2].
- There is a spatially uniform diffusive flux $F_{\text{diff}} = -\delta \frac{\partial u_{\text{eq}}}{\partial x} = -\delta \frac{U_{\text{right}} - U_{\text{left}}}{L}$ directed to the left, i.e. pointing in the negative x -direction [1/2].

Item 3 (2p)

Statements A and B follows from rewriting the numerical scheme (2) into the following expression [2/3]:

$$u_{j,k+1} = u_{j,k} - 2\mathcal{D}[u_{j,k} - u_{\text{avg}}], \quad u_{\text{avg}} = \frac{u_{j-1,k} + u_{j+1,k}}{2}. \quad (8)$$

Written this way, it is immediately seen that the numerical value *decreases* in time ($u_{j,k+1} < u_{j,k}$) if it is *larger* than the average of its neighbouring values ($u_{j,k} > u_{\text{avg}}$) [1/3]. Conversely, the numerical value *increases* in time ($u_{j,k+1} > u_{j,k}$) if it is *smaller* than the average of its neighbouring values ($u_{j,k} < u_{\text{avg}}$) [1/3]. This proves statements A and B.

Finally, statements A and B imply that a *numerical* equilibrium solution is characterized by the fact that every numerical value is exactly the average of its neighbouring values: $u_{j,k} = u_{\text{avg}} = \frac{u_{j-1,k} + u_{j+1,k}}{2}$, for all $0 < j < J_{\text{max}}$ [2/3].

Item 4 (3p)

The Von Neumann analysis of the FTCS-scheme (2) involves the following six steps.

- Adopt the numerical trial solution $u_{j,k} = \hat{U}R^k \exp(ij\varphi)$ for complex parameter R , phase angle φ ($0 < \varphi \leq \pi$) and some constant $\hat{U}$ [1/2].

- Substitution of this trial solution gives: $R = 1 - 2\mathcal{D} + \mathcal{D}[\exp(i\varphi) + \exp(-i\varphi)]$ [1/2].
- Using the definition of the cosine, this expression can be rewritten to find $R = 1 - 2\mathcal{D}(1 - \cos \varphi)$ [1/2].
- Since R is real-valued, the requirement that $|R| < 1$ is equivalent to the condition $-1 < R < 1$ [1/2].
- Accounting for all φ under consideration, this implies $\mathcal{D} < \frac{1}{2}$ [1/2].
- Conclusion: the FTCS-scheme conditionally stable, i.e. subject to the condition $\mathcal{D} < \frac{1}{2}$ [1/2].

Item 5 (1p)

Using the requirement that every term in a differential equation must carry the same dimension, the dimension of β is found to be identical to that of f^{-2} per second, i.e. $\text{m}^2 \text{mg}^{-2} \text{s}^{-1}$ or, equivalently, $\frac{\text{m}^2}{\text{mg}^2 \text{s}}$ [1].

Item 6 (2p)

The correct table is the following ([2/9] for each correct entry):

case	param. values	ODE/PDE	linear/nonlin.	hom./nonhom.
I.	$\gamma = 0, \beta > 0$	ODE	nonlinear	not applicable
II.	$\gamma > 0, \beta = 0$	PDE	linear	homogeneous
III.	$\gamma > 0, \beta > 0$	PDE	nonlinear	not applicable

Item 7 (2p)

The plot of the initial profile should show (the first half of a) sine-curve, with an amplitude f_0 on a domain $0 < x < L$ [1]. The total amount of biomass initially present in the domain is obtained by integrating the initial profile over the domain, which leads to the following expression [1]:

$$F = \int_0^L f(x, 0) dx = \int_0^L f_0 \sin\left(\frac{\pi x}{L}\right) dx = \frac{-Lf_0}{\pi} \left[\cos\left(\frac{\pi x}{L}\right) \right]_0^L = \frac{2Lf_0}{\pi}. \quad (9)$$

Item 8 (1p)

The plot should show the space-time domain in the (x, t) -plane, bounded to the left by $x = 0$ (with boundary condition), bounded to the right by $x = L$ without boundary condition, and bounded below by $t = 0$ (with initial condition) [1].

Item 9 (1p)

At $x = L/2$ and assuming $\gamma = 0$, we must solve the following nonlinear ODE-problem:

$$\frac{df}{dt} = -\beta f^3, \quad f(0) = f_0. \quad (10)$$

The solution is found using separation of variables (for ODEs). The first step is the actual separation [1/2]:

$$\int \frac{df}{f^3} = - \int \beta dt. \quad (11)$$

This leads to the following result where we introduce a (single) integration constant C : [1/2]

$$\frac{-1}{2f^2} = -\beta t + C, \quad (12)$$

Imposing the IC immediately implies $C = \frac{-1}{2f_0^2}$ [1/2]. This implies [1/2]

$$\frac{1}{f^2} = 2\beta t + \frac{1}{f_0^2}, \quad (13)$$

Rewriting this finally gives the required solution [1/2]:

$$f(t) = (2\beta t + f_0^{-2})^{-1/2} = \frac{1}{\sqrt{2\beta t + \frac{1}{f_0^2}}}. \quad (14)$$

At other points x_{other} in the domain, we find similar behaviour but with a smaller initial value. In the above result, one should replace f_0 with $f_0 \sin(\pi x_{\text{other}}/L)$ [1/2].

Item 10 (2p)

The correct answer involves three steps:

- Substitution in the PDE should give an identity. For $x \leq \gamma t$, it is seen that $\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x} = 0$ so the PDE is indeed satisfied [1/2]. For $x > \gamma t$, it follows that $\frac{\partial f}{\partial t} = -\gamma f_0 \sin(\gamma[x - \gamma t])$ and $\gamma \frac{\partial f}{\partial x} = \gamma f_0 \sin(\gamma[x - \gamma t])$. Adding these contributions gives $\frac{\partial f}{\partial t} + \gamma \frac{\partial f}{\partial x} = 0$ so the PDE is indeed satisfied [1/2].
- Initial condition should be satisfied, which is immediately seen from substitution of $t = 0$ in the first expression of equation (6) [1/2].
- Boundary condition at $x = 0$ should be satisfied, which is immediately seen from substitution of $x = 0$ in the second expression of equation (6) [1/2].

Item 11 (1p)

These are the so-called *characteristics*, along which the solution to the simple wave equation is constant in the (x, t) -plane [1].

Item 12 (1p)

At $t = L/\gamma$, the separating characteristic through $(x, t) = (0, 0)$ leaves the domain. From this moment onward, the solution is zero everywhere in the domain. It is then controlled fully by the BC at $x = 0$, where the solution is zero. Alternatively formulated, at $t = L/\gamma$, the initial profile has entirely migrated out of the domain [1].

Item 13 (2p)

When both advection and decay are present, the solution resembles that of equation (6). This means that the characteristics are still present [1]. However, instead of showing constant values along a characteristic, the solution now decays according to the answer to item 9 [1].

Item 14 (3p)

The solution involves the following five steps:

- Discretization of time-derivative using Backward Euler [1/2]:

$$\left. \frac{\partial f}{\partial t} \right|_{(x_j, t_{k+1})} \approx \frac{f_{j,k+1} - f_{j,k}}{\Delta t}. \quad (15)$$

- Upwind discretization of the space-derivative in the advective term [1/2]:

$$\gamma \left. \frac{\partial f}{\partial x} \right|_{(x_j, t_{k+1})} \approx \gamma \frac{f_{j,k+1} - f_{j-1,k+1}}{\Delta x}. \quad (16)$$

- Discretization of the cubic decay term [1/2]:

$$-\beta f^3 \big|_{(x_j, t_{k+1})} \approx -\beta f_{j,k}^2 f_{j,k+1}. \quad (17)$$

- Substitution of these three discretizations into the PDE [1/2]:

$$\frac{f_{j,k+1} - f_{j,k}}{\Delta t} + \gamma \frac{f_{j,k+1} - f_{j-1,k+1}}{\Delta x} = -\beta f_{j,k}^2 f_{j,k+1}. \quad (18)$$

- Rewriting the result into a single expression for $f_{j,k+1}$, introducing the well-known Courant number $\mathcal{C} = \gamma \frac{\Delta t}{\Delta x}$ [1]:

$$f_{j,k+1} = \frac{f_{j,k} + \mathcal{C} f_{j-1,k+1}}{1 + \mathcal{C} + \beta(\Delta t) f_{j,k}^2}. \quad (19)$$