Two step FVE method

A numerical modeling technique designed for error insight

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Symbol	Unit	Description
Δt	s	Time increment
Δx	m	Space increment, $\Delta x_{i+\frac{1}{2}} = x_{i+1} - x_i$
ε	$\mathrm{m\,s^{-2}}$	Multiplier of the correction term for the essential boundary condition, ζ-boundary
ε	$\mathrm{s^{-1}}$	Multiplier of the correction term for the essential boundary condition, q-boundary
ν	$\mathrm{m^2\,s^{-1}}$	Kinematic viscosity
Ω	-	Finite volume
Ψ	$\mathrm{m^2\,s^{-1}}$	Artificial smoothing coefficient
θ	-	θ-method. If $\theta = 1$ then it is a fully implicit method and if $\theta = 0$ then it is a fully explicit method.
$\boldsymbol{E}$	-	Error vector function, defined in computational space
ξ	-	Relative coordinate
ζ	m	Water level w.r.t. reference plane, positive upward
c_Ψ	$(.)^{-1}$	Artificial smoothing variable
g	$\mathrm{m\,s^{-2}}$	Gravitational constant
h	m	Total water depth
i	-	node counter
q	$\mathrm{m^2\,s^{-1}}$	The water flux in x-direction, $q = hu$
r	$\mathrm{m^2\,s^{-1}}$	The water flux in y-direction, $r = hv$
t	s	Time coordinate
t_{reg}	s	The regularization time for the given time-series
u	$\mathrm{m\,s^{-1}}$	Velocity in x-direction
v	$\mathrm{m\,s^{-1}}$	Velocity in y-direction
x	m	x-coordinate
z_b	m	Bed level w.r.t. reference plane, positive upward

List of To Do's

1 Introduction

Nature can be described by mathematical models, these models approximate the behaviour of nature. The main question is: "How well will these mathematical models describe nature?". This document is based on Borsboom (1998), where the mathematical model is called the "*difficult problem*".

To show that the mathematical model does not match with nature by using a numerical method, it is needed that the numerical error of the numerical method can be quantified. The numerical errors should be very small compared to the errors made in the mathematical model. In that case the results of the numerical model is a reliable approximation of the mathematical model. A mismatch in results of the numerical method w.r.t. the nature is then fully determined by the mismatch of the mathematical model.

In this report a derivation is reported of a numerical model that automatically is adjusted to assure that the numerical result is close enough to the solution of the mathematical model. To obtain such a numerical model the mathematical model should be adjusted to a state which is suitable to determine what and how large the mismatch is. The mathematical model is adjusted in that way that the second derivatives of all data is smooth. After smoothing of the data the mathematical model is called "*easy problem*". This step in the procedure is called "*regularization*" and is the first step of the two step FVE method (Finite Volume Element method).

The regularization step has to ensure that the lowest-order terms of the residual of the discretization step are dominant, so that we can limit ourselves to the analysis of the leading terms of the error expansion. The regularization is assumed to be such that the easy problem can be discretized accurately on the available grid, and that the leading terms of the series expansions are dominant.

To obtain this goal the numerical scheme should be central in space, no dissipation is added to the model by the numerical method, just dispersion. All examples in this document will be performed with a fully implicit time-integrator using a iteration mechanism based on the Newton-linearization. The Newton-iteration process benefits of the regularized data. This is the second step of the two step FVE method (Finite Volume Element method).

When all the mentioned items are fulfilled then the numerical scheme is:

1 accurate (2nd order, due to the requirement that there is no numerical dissipation),
2 reliable (numerical errors are reduced to be much less then the modelling deviations),
3 robust (no numerical restrictions on time step other then physical restrictions),
4 flexible (separation of numerical and physical part, lot of numerical methods can be used without hampering the physical part),
5 efficient (Newton method is a second order method),
6 fast (fully implicit).

The feasibility of this method is shown by performing this method on the 1D shallow water equations. Towards these shallow water equations we will look first to the hyperbolic part of these equations. The boundary conditions are separated in a strictly outgoing and a strictly ingoing signal. When selecting a special combination of these signals a weakly-reflective or absorbing boundary condition can be prescribed, including a prescribed ingoing signal.

In chapter 2: Two-step numerical modeling, error minimizing, the error-minimizing integration method is presented. The error-minimizing integration method is based on the assumption that a function can be made smooth so that the numerical discretization and the regularized function are so close that the numerical error is negligible for that function.

In chapter 3: 1-D Space discretization, the one dimensional space discretization. Which consist of a finite volume method and central discretizations and piecewise linear functions between the nodes. Also an estimation of the regularization coefficient for a given function based on the second order of accuracy of the discretization is presented. So the user is able to justify the quality of the numerical solution and in that way to judge where to adjust the regularization or adapt the grid in certain regions.

In chapter 4: Time integration scheme, the fully implicit time integration is based on Newton iteration presented. Due to the regularization of the data the Newton iteration converges extremely well, that is second order in also the more complex areas.

In chapter 5: Towards the shallow water equations, the fully implicit time integration is presented for one dimensional shallow water equations. We start with the implementation of the 1D advection/transport equation, then with the implementation of the wave equation without convection. This 1D wave equation consist of two independent advection/transport equation for a right and left going signal. At the boundary these two equations are coupled and will therefor generate reflections in the numerical model. We start with 1D advection/transport equation because this equation has the same nature as the right going signal of the wave equation.

In chapter 6: Numerical experiments, several numerical experiments will be shown. Starting with some examples with just a source/sink-term, so only a time integration and without transport and diffusion (Air pollution and Brusselator). Followed by numerical experiments of the advection-diffusion equation (with and without diffusion), the 1D-wave equation and 2D-wave equation.

In section 6.3.1: Outflow boundary layer, the fully implicit time integration is presented for the advection-diffusion equation. Showing a flow from left to right with a Dirichlet boundary condition at the outflow side of the domain. The Dirichlet value at the outflow boundary is so chosen that there will appear an outflow boundary layer.

In section 6.3.2: Interface problem, the fully implicit time integration is presented for the advection-diffusion equation. Showing a flow from left to right with a interface in the diffusion coefficient for the transported constituent.

2 Two-step numerical modeling, error minimizing

For the realization of our objective, an error analysis is required to gain insight in the relative importance of discretization errors. This has to be in the form of power series expansions to be genuinely generally applicable. Smoothness is required to ensure fast converging series and dominant lowest-order terms that can be used as a basis for reliable local error approximations. Artificial smoothing is added to satisfy this requirement, if necessary. To enable the physical interpretation of numerical errors afterwards, smoothing can only involve the artificial enhancement of physical dissipation. Taylor-series expansions can be used to determine the leading terms of the residual. The residual, however, is not a suitable error measure since it indicates the local discretization error in the equations, not in the solution. In order to be useful, the residual needs to be reformulated in terms of local solution errors. We did not find any existing scheme that allows for such a transformation, and so we developed a discretization method that does. The result turns out to be a method of finite volume type. The discretization consists of integrating the model equations over control volumes, using uniquely defined discrete approximations of all variables. The proposed numerical modeling technique solves the conceptual model problem in two steps (Figure 2.1: in the first step the difficult problem to be solved is changed into an easy problem by adding artificial smoothing; in the second step the easy problem is discretized.

Showing the two-step method in general

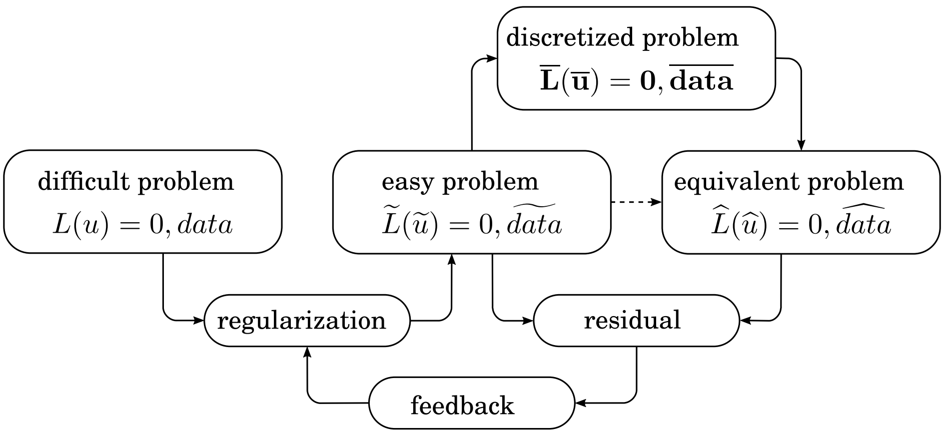


Figure 2.1: *Graphical presentation of the error-minimizing two step method*

Notation agreements:

u	Non-regularized/non-smoothed function, to be determined numerically.
$\widetilde{u}$	Regularized/smoothed function, denoted by the wavy line.
$\overline{u}$	Piecewise linear function, denoted by the bar.
$\widehat{u}$	Numerical solution on the nodes.

A tilde ($\widetilde{u}$) indicates the variables and differential operators of the easy problem. Their discretizations are indicated by a bar, $\overline{u}$. Next, we define the smooth and infinitely differentiable function $\widehat{u}$ that is a very close approximation of numerical solution $\overline{u}$. By means of an error analysis we determine the differential problem that $\widehat{u}$ is a solution of. Note that the data pertaining to the computational model are also included in the procedure. Independent variables describing, e.g., the geometry and initial and boundary conditions also need to be discretized and hence need to be sufficiently smooth, to ensure that all higher-order error terms are sufficiently small and can be neglected. Sufficient smoothness is obtained automatically by using smoothing coefficients that are a function of the discretization errors. See also Borsboom (2001).

3 1-D Space discretization

We are looking for a second order central space discretization together with the finite volume approach. So the higher order terms in the Taylor series expansion are negligible. For this numerical discretization method no dissipation is added, only there is some dispersion for the shorter waves, i.e. dependent on the third derivative in the Taylor expansion. To fulfill this requirement the data should be smooth according to the truncation error of the numerical discretization. If not, the data should be made smooth with a procedure in which you can see on which location the smoothing is severe. The process of smoothing is called regularization. If the truncation error (high values of second derivatives) is severe on locations that the user do not expect and do not accept then the user can adjust the discretization in that part of the domain. There are two options to adjust the data:

1 increase the smoothing coefficient or

2 choose a smaller grid size.

3.1 Finite volume approach

We will discuss the finite volume approach for the one dimensional case of the function $u(x,t)$, for the grid shown in Figure 3.1

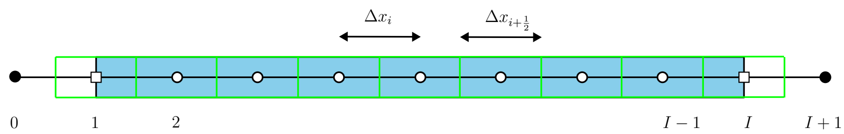


Figure 3.1: *Water body (blue area), finite volumes (green boxes), computational points (open dots), virtual computational points (black dots), boundary points (open squares) are at $i = 1$ (west boundary) and $i = I$ (east boundary).*

The control volume is defined on the interval $x_{i-\frac{1}{2}}$ to $x_{i+\frac{1}{2}}$, see Figure 3.1. The grid in Figure 3.1 is equidistant but that is not necessarily, the method which is described in this document also holds for a non-equidistant grid.

3.1.1 Quadrature rule, source term

The finite volume approach for the function $u(x,t)$ reads:

$$\int_{\Omega} u \, d\Omega = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u \, dx \tag{3.1}$$

Using piecewise linear functions between the non-equidistant nodes the quadrature rule reads:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u \, dx = \int_{x_{i-\frac{1}{2}}}^{x_i} u \, dx + \int_{x_i}^{x_{i+\frac{1}{2}}} u \, dx \approx \tag{3.2}$$

$$\approx \frac{\Delta x_{i-\frac{1}{2}}}{2} \frac{u_{i-1} + 3u_i}{4} + \frac{\Delta x_{i+\frac{1}{2}}}{2} \frac{3u_i + u_{i+1}}{4} \tag{3.3}$$

where the control volume is split into two adjacent sub-control volumes $[x_{i-\frac{1}{2}}, x_i]$ and $[x_i, x_{i+\frac{1}{2}}]$. A graphical interpretation is given in Figure 3.2.

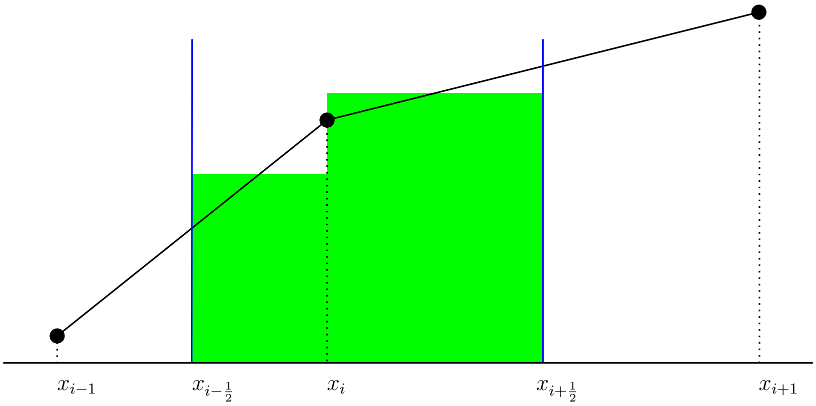


Figure 3.2: *Integration at x_i over the control volume from $x_{i-\frac{1}{2}}$ to $x_{i+\frac{1}{2}}$.*

Higher order quadrature rules may be chosen, but they are not discussed in this report.

3.1.2 Quadrature rule, flux term

3.1.3 Boundary conditions

At the west and east boundary boundary conditions need to be supplied. If it is a prescribed boundary condition (ingoing signal) it is called an **essential**-boundary condition, if the boundary condition is determined by the outgoing signal it is called a **natural**-boundary condition (Logan, 1987; Kan et al., 2008). In case of a wave equation we have a right and left going signal. When no reflection at an open boundary is required then at the west boundary a signal need to prescribed without disturbing the left going signal. And at the east boundary the other way around.

Further more we have the prescribed boundary signal at the boundary node of the grid. This assumption is made because the users are acquainted with the fact that open boundaries are given at nodes. But for the outgoing signal this is not necessarily, for the outgoing signal we stick to the finite volume approach.

When we consider a one dimensional right going signal (see section 5.2.1) the boundary at the west side is located at x_1 and the outflow condition is located at $x_{I+\frac{1}{2}}$. The prescribed function reads:

$$c(0,t) = f(t) \tag{3.4}$$

Because we use a 3-point stencil for the interior, we aim for a 3-point stencil for the essential boundary condition. One possible quadratic interpolation is a parabolic fit through the grid points, giving an under specification of the solution at the boundary regardless of its position.

$$\begin{aligned} c_{GP}(\xi) &= c_0\,(1-\xi) + c_1\,\xi + \frac{1}{2}(c_0 - 2\,c_1 + c_2)\,(\xi - 1)\,\xi = \\ &= (1-\xi)\left(1 - \frac{1}{2}\xi\right) c_0 + \xi\,(2-\xi)\,c_1 + \frac{1}{2}\xi\,(\xi-1)\,c_2 \end{aligned} \tag{3.5}$$

where $\xi \in [0,1]$ is the weight function between c_0 and c_1.

Another possible quadratic fit is the one through Cell-Centered values:

$$c_{CC}(\xi) = c_0\,(1-\xi) + c_1\,\xi + \frac{1}{2}(c_0 - 2c_1 + c_2)\left(\xi - \frac{1}{2}\right)^2 \tag{3.6}$$

$$= \left(1 - \xi + \frac{1}{2}\left(\xi - \frac{1}{2}\right)^2\right) c_0 + \left(\xi - \left(\xi - \frac{1}{2}\right)^2\right) c_1 + \left(\frac{1}{2}\left(\xi - \frac{1}{2}\right)^2\right) c_2 \tag{3.7}$$

The parabolic fit that gives neither underspecification nor overspecification of imposed values at boundaries is a combination of Equation (45) and (49). It is easy to show that that combination consists of $1/3$ times Equation (3.5) plus $2/3$ times Equation (3.7):

$$c_{opt}(\xi) = \left(\frac{13}{12} - \frac{3}{2}\xi - \frac{1}{2}\xi^2\right) c_0 + \left(-\frac{1}{6} + 2\xi - \xi^2\right) c_1 + \left(\frac{1}{12} - \frac{1}{2}\xi + \frac{1}{2}\xi^2\right) c_2 \tag{3.8}$$

Which lead to the following interpolations for $\xi = \frac{1}{2}$ and $\xi = 1$:

$$c_{opt}\left(\frac{1}{2}\right) = \frac{11}{24}c_0 + \frac{14}{24}c_1 - \frac{1}{24}c_2 \tag{3.9}$$

$$c_{opt}\left(1\right) = \frac{1}{12}c_0 + \frac{10}{12}c_1 + \frac{1}{12}c_2 \tag{3.10}$$

Where Equation (3.9) will be used for the natural boundary condition and Equation (3.10) will be used for the essential boundary condition.

Verification of its correctness by means of integration over the outermost finite volume:

$$\int_{\xi_{\frac{1}{2}}}^{\xi_{\frac{3}{2}}} c_{opt}(\xi)\, d\xi = \frac{1}{8}c_0 + \frac{3}{4}c_1 + \frac{1}{8}c_2 \tag{3.11}$$

In the right-hand side we see the weights of the mass matrix of the piecewise linear FVE method, i.e. averaged over the left outermost finite volume the quadratic function c_{opt} equals the piecewise linear function used in the FVE scheme.

3.2 Regularization of artificial viscosity Ψ

To get an error-minimizing method we need to regularize all data, as mentioned in chapter 2. Regularization of the artificial viscosity Ψ is performed as described in Borsboom (2001, eq. 14).

$$\int_{\Omega} \Psi\, d\omega - \alpha_\psi \int_{\Omega} \Delta\xi^2 \frac{\partial^2 \Psi}{\partial \xi^2}\, d\omega = \int_{\Omega} \beta_\psi Err_{\beta_\psi}\, d\omega \tag{3.12}$$

When discretized it yields (Borsboom, 2001, eq. 18):

$$\left(\frac{1}{8} - \alpha_\psi\right)\Psi_{i-1} + \left(\frac{3}{4} + 2\alpha_\psi\right)\Psi_i + \left(\frac{1}{8} - \alpha_\psi\right)\Psi_{i+1} = \frac{\beta_\psi}{\Delta\xi}\int_{\xi_{i-\frac{1}{2}}}^{\xi_{i+\frac{1}{2}}} Err_{\beta_\psi}\, d\xi \tag{3.13}$$

The right hand side of Equation (3.13) can be approximated by:

$$\frac{\beta_\psi}{\Delta\xi}\int_{\xi_{i-\frac{1}{2}}}^{\xi_{i+\frac{1}{2}}} Err_{\beta_\psi}\, d\xi = \frac{\beta_\psi}{\Delta\xi}\int_{\xi_{i-\frac{1}{2}}}^{\xi_i} Err_{\beta_\psi}\, d\xi + \frac{\beta_\psi}{\Delta\xi}\int_{\xi_i}^{\xi_{i+\frac{1}{2}}} Err_{\beta_\psi}\, d\xi \approx \tag{3.14}$$

$$\approx \frac{\beta_\psi}{\Delta\xi}\frac{1}{2\Delta\xi}(Err_{\beta_\psi})_{i-\frac{1}{4}} + \frac{\beta_\psi}{\Delta\xi}\frac{1}{2\Delta\xi}(Err_{\beta_\psi})_{i+\frac{1}{4}} \tag{3.15}$$

For Err_{β_ψ} the following expression is used (comparable to Borsboom (2001, eq. 42), a derivation of this expression is given in Appendix C):

$$Err_{\beta_\psi} = \Delta\xi\, \overline{x}_\xi \left(\frac{1}{16}\sqrt{\frac{g}{\overline{h}}}\left|D_\xi(\overline{\zeta})\right| + \frac{1}{16}\sqrt{2}\left|\frac{D_\xi(\overline{q})}{\overline{h}} - \frac{\overline{q}D_\xi(\overline{h})}{\overline{h}^2}\right|\right) \tag{3.16}$$

For the Weir experiment (section 6.4.2) the following parameters are used, $\alpha_\psi = c_\Psi$ and $\beta_\psi = 32c_\Psi$ *which are educational guesses!*.

Using (with $\overline{u} \in \{\overline{h}, \overline{q}\}$):

$$\overline{u}_{i-\frac{1}{4}} = \frac{1}{4}(u_{i-1} + 3u_i), \qquad \overline{u}_{i+\frac{1}{4}} = \frac{1}{4}(u_{i+1} + 3u_i) \tag{3.17}$$

and

$$(\overline{x}_\xi)_{i-\frac{1}{4}} = x_i - x_{i-1}, \qquad (\overline{x}_\xi)_{i+\frac{1}{4}} = x_{i+1} - x_i \tag{3.18}$$

and for equidistant meshes we use (Borsboom, 2001, eq. 35) :

$$D_\xi(\overline{u}) = \Delta\xi^2 \frac{\partial^2}{\partial \xi^2} \approx u_{i-1} - 2u_i + u_{i+1}. \tag{3.19}$$

3.3 Regularization of given function

To get an error-minimizing method we need to regularize all data, as mentioned in chapter 2. Regularization of a given function is performed as described in Borsboom (1998) and Borsboom (2003). The given function to regularize reads:

$$u_{giv}(x). \tag{3.20}$$

Some notation agreements are:

u	Non-regularized/non-smoothed function, to be determined numerically.
$\widetilde{u}$	Regularized/smoothed function, denoted by the wavy line.
$\overline{u}$	Piecewise linear function, denoted by the bar.
u_i	Value of the numerical value at point x_i, denoted by the subscript.

The regularized function $\widetilde{u}$ satisfy the next equation (Borsboom, 1998, eq. 6):

$$\widetilde{u} - \frac{\partial}{\partial x}\Psi\frac{\partial \widetilde{u}}{\partial x} = u_{giv}, \qquad \Psi = c_\Psi \Delta x^2 E, \tag{3.21}$$

where

u_{giv}	Given function, ex. bathymetry, viscosity, ..., $[\cdot]$.
$\widetilde{u}$	Regularized/smoothed function of u_{giv}, $[\cdot]$.
Ψ	(Artificial) smoothing coefficient, $[\mathrm{m}^2]$
Δx	Space discretization, $\Delta x_{i+\frac{1}{2}} = x_{i+1} - x_i$, $[\mathrm{m}]$
c_Ψ	Smoothing factor (set by user), $[1/\cdot]$
E	Error function, $[\cdot]$ (see section 3.3.1)

First the discretization of Equation (3.21) is discussed and second the determination of the artificial smoothing coefficient Ψ.

The finite volume approach of Equation (3.21) reads:

$$\int_{\Omega} \widetilde{u}\, d\Omega - \int_{\Omega} \frac{\partial}{\partial x} \Psi \frac{\partial \widetilde{u}}{\partial x}\, d\Omega = \int_{\Omega} u_{giv}\, d\Omega \tag{3.22}$$

Integration of the first term

Integration of the first term yields:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \widetilde{u}\, dx \approx \frac{1}{2}\Delta x_{i-\frac{1}{2}} \left(\frac{1}{4}u_{i-1} + \frac{3}{4}u_i\right) + \frac{1}{2}\Delta x_{i+\frac{1}{2}} \left(\frac{3}{4}u_i + \frac{1}{4}u_{i+1}\right) \tag{3.23}$$

Integration of the second term

Integration of the second term, with $\Psi_{i+\frac{1}{2}} = \frac{1}{2}(\Psi_i + \Psi_{i+1})$:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x} \Psi \frac{\partial \widetilde{u}}{\partial x} dx = \Psi \frac{\partial \widetilde{u}}{\partial x}\bigg|_{i+\frac{1}{2}} - \Psi \frac{\partial \widetilde{u}}{\partial x}\bigg|_{i-\frac{1}{2}} \approx \tag{3.24}$$

$$\approx \Psi_{i+\frac{1}{2}} \frac{u_{i+1} - u_i}{\Delta x_{i+\frac{1}{2}}} - \Psi_{i-\frac{1}{2}} \frac{u_i - u_{i-1}}{\Delta x_{i-\frac{1}{2}}} = \tag{3.25}$$

$$= \frac{\Psi_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}} u_{i-1} - \left(\frac{\Psi_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}} + \frac{\Psi_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}}\right) u_i + \frac{\Psi_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}} u_{i+1} \tag{3.26}$$

Integration of the right hand side

For the integration of the right hand side we could use a smaller integration step size, to incorporate the sub-grid scale effects. If the function u_{giv} is for example an analytic function this integral can be computed exact or data is given by a lot of measurement points per finite volume, see for example Figure 3.3. When integrating over a finite volume the sub-grid scale effects will be taken into account

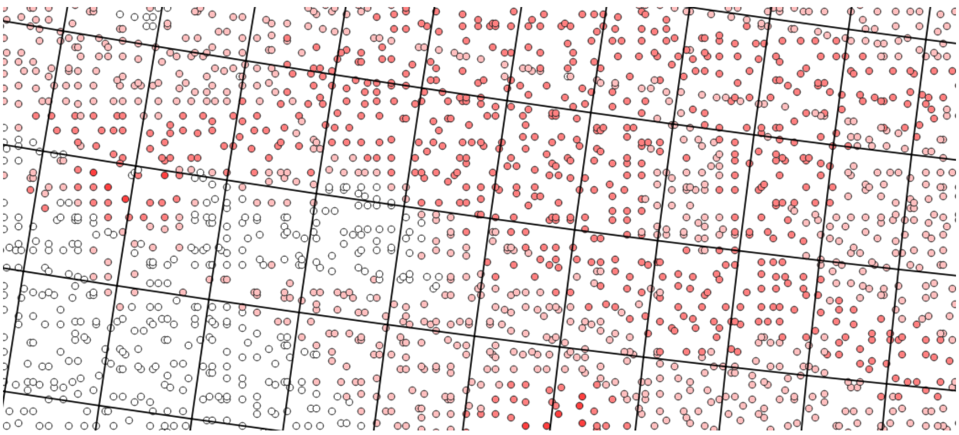


Figure 3.3: *Two dimensional example of a lot of data points per grid cell. The data points are used to compute the integral at the righthand side of Equation (3.28).*

Discretization of Equation (3.22)

So the discretization of Equation (3.22) with $\alpha = \frac{1}{8}$, read (i.e. Borsboom (1998, eq. 7) and Borsboom (2003, eq. 6)):

$$\left(\frac{\Delta x_{i-\frac{1}{2}}}{8} - \frac{\Psi_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}}\right) u_{i-1} + \left(\frac{3\Delta x_{i-\frac{1}{2}}}{8} + \frac{\Psi_{i-\frac{1}{2}}}{\Delta x_{i-\frac{1}{2}}} + \frac{3\Delta x_{i+\frac{1}{2}}}{8} + \frac{\Psi_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}}\right) u_i + \tag{3.27}$$

$$+ \left(\frac{\Delta x_{i+\frac{1}{2}}}{8} - \frac{\Psi_{i+\frac{1}{2}}}{\Delta x_{i+\frac{1}{2}}}\right) u_{i+1} = \int_{x_{i-1/2}}^{x_{i+\frac{1}{2}}} u_{giv}\, dx \tag{3.28}$$

The boundary conditions to close the three diagonal system are $u_0 = u_{giv}(x_0)$ and $u_{I+1} = u_{giv}(x_{I+1})$.

3.3.1 Determination of artificial smoothing coefficient Ψ

The artificial smoothing coefficient Ψ ($= c_\psi \Delta x^2 E$, Equation (3.21)) is dependent on error E, the smoothing coefficent c_E and the second derivative of the given function u_{giv} (Borsboom, 1998, eq. 8). The error E will be computed in computational space, meaning that a disturbance is spreaded over an equal number of cells before and after the location of the disturbance:

$$\left(\frac{\Delta\xi}{8} - \frac{c_E}{\Delta\xi}\right) E_{i-1} + \left(\frac{6\Delta\xi}{8} + \frac{2c_E}{\Delta\xi}\right) E_i + \left(\frac{\Delta\xi}{8} - \frac{c_E}{\Delta\xi}\right) E_{i+1} = \int_{\xi_{i-\frac{1}{2}}}^{\xi_{i+\frac{1}{2}}} |D_i|\, d\xi \tag{3.29}$$

with $\Delta\xi = 1$ it reads:

$$\left(\frac{1}{8} - c_E\right) E_{i-1} + \left(\frac{6}{8} + 2c_E\right) E_i + \left(\frac{1}{8} - c_E\right) E_{i+1} = |D_i| \tag{3.30}$$

Choose $\mathbf{c_E}$ equal to $\mathbf{c}_\psi$ and take into account that D_i is constant over a control volume

$$D_i = \Delta\xi^2 \frac{\partial^2 u_{giv}}{\partial \xi^2} \qquad \text{(Borsboom, 1998, eq. 2)} \tag{3.31}$$

$$\approx u_{giv_{i-1}} - 2u_{giv_{i-1}} + u_{giv_{i+1}} \tag{3.32}$$

Now system the system of Equation (3.29) can be solved and where $\boldsymbol{\Psi}$ is set to:

$$\boldsymbol{\Psi} = c_\Psi \Delta x^2 \boldsymbol{E} \tag{3.33}$$

For an estimation of c_Ψ see section A.2, in this document we use $c_\Psi = 4$.

The boundary conditions to close the three diagonal system are:

$$2E_0 - E_1 = |D_1| \quad \text{and} \tag{3.34}$$

$$-E_I + 2E_{I+1} = |D_I|\,. \tag{3.35}$$

3.3.2 Step function (Heaviside function)

For a full description of this example see Borsboom (2003, eq. 5). The function is initially defined as:

$$u_{given}(x) = \begin{cases} 0, & \text{if} \quad 0\ [m] \leq x \leq 1000\ [m], \\ 1, & \text{if} \quad 1000\ [m] < x \leq 2000\ [m], \end{cases} \tag{3.36}$$

For illustration, the step is chosen to be exactly on a grid point (in the middle of a control volume at $1000\ [m]$) and at the finite volume boundary, i.e. a half Δx shifted to the right.

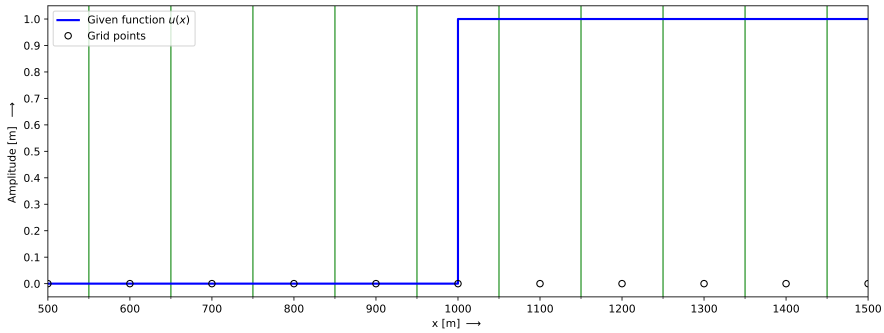
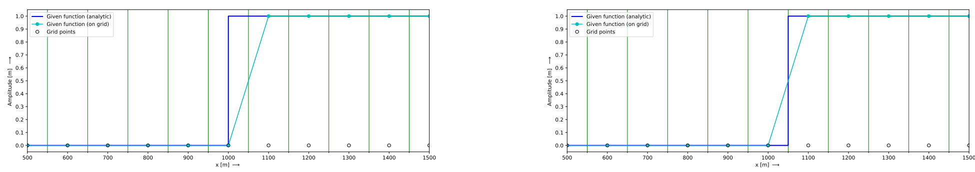


Figure 3.4: *Step function to be estimated. The thin green vertical lines indicate the borders of the finite volumes.*

A straight forward piecewise approximation is shown in Figure 3.5. Both figures does show the same discretization function (cyan colored) but the step is at a different location.

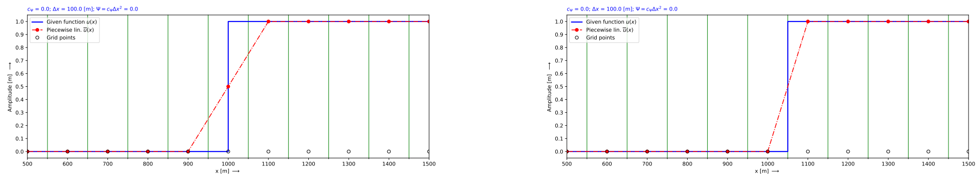


(a) *Step at grid node,* $x = 1000\ [m]$

(b) *Step at boundary of a finite volume,* $x = 1050\ [m]$

Figure 3.5: *As seen from this figures the function defined on the grid nodes does not see the exact location of the step. Both function through the grid nodes have the same profile, but the step is at another location.*

A piecewise approximation with a regularization coefficient of zero ($c_\Psi = 0$) is shown in Figure 3.6.



(a) *Step at grid node, $x = 500$ $[m]$*

(b) *Step at boundary finite volume, $x = 550$ $[m]$*

Figure 3.6: *Step function approximated by a piecewise linear function (red line with dots at the nodes), $c_\Psi = 0$, $\Delta x = 100$ $[m]$ and $\Psi = 0$. The thin green vertical lines indicate the borders of the finite volumes.*

As seen from Figure 3.6 the step is more taken into account as is presented in Figure 3.5. Which looks quite well, but what are the values of the second derivative of the solution. For $\Delta x = 100\,[\mathrm{m}]$ the absolute value of the second derivative is $0.5/(100)^2$ (Figure 3.6a) and $1.0/(100)^2$ (Figure 3.6b).

There are two options to estimate this step function by a piecewise linear smooth function with the same numerical accuracy:

1 Regularization with using a large grid size, the numerical solution is less close to the step function (see Figure 3.7)

2 Regularization with using a small grid size, the numerical solution is closer to the step function (see Figure 3.8),

Both options has the same value for $c_\Psi = 4$. Meaning that the step is represented by the same number of grid cells. How to estimate c_Ψ can be read in Appendix A. It is up to the user which regularization is can be used for the numerical simulation. A better representation of the step function need a smaller grid size.

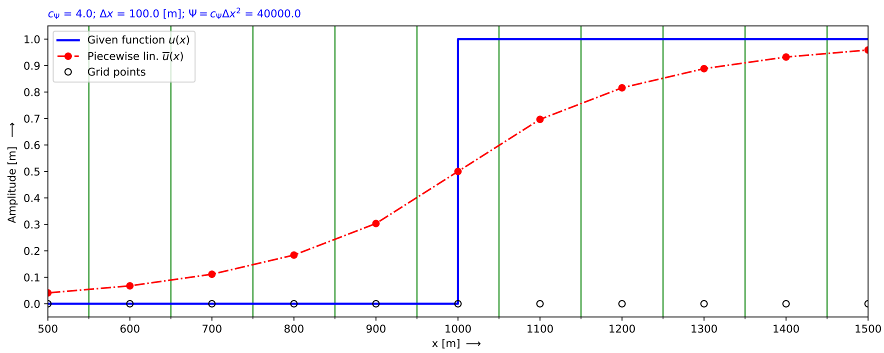


Figure 3.7: *Step function approximated by a piecewise linear function (red line with dots at the nodes), $c_\Psi = 4$, $\Delta x = 100$ $[m]$ and $\Psi = 40000$. The thin green vertical lines indicate the borders of the finite volumes.*

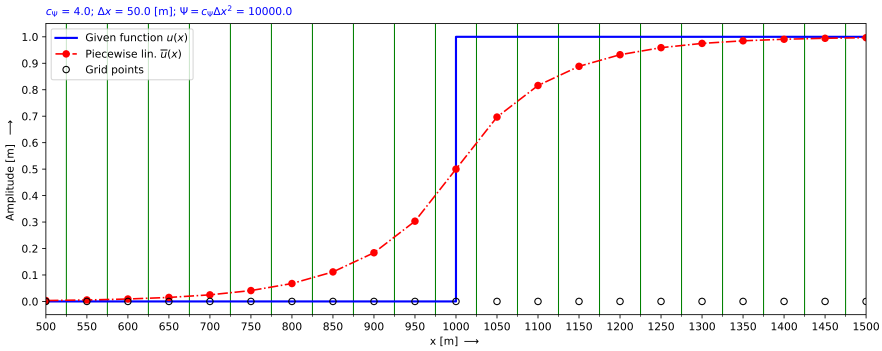


Figure 3.8: *Step function approximated by a piecewise linear function (red line with dots at the nodes),* $c_\Psi = 4$, $\Delta x = 50$ $[m]$ *and* $\Psi = 10000$. *he thin green vertical lines indicate the borders of the finite volumes.*

3.3.3 Small and a large gradient in the data set

To show the influence of regularization a more general data set is chosen, Borsboom (1998) (given function, here adjusted). A given function with a small (smooth) and large (steep) gradients in the data set is chosen. The function is defined by:

$$u_{given}(x) = \begin{cases} 10\left(\frac{1}{2} - \frac{1}{2}\tanh\left(20x/1000 - 6\right)\right), & \text{if} \quad 0\ [m] \leq x \leq 650\ [m], \\ 10, & \text{if} \quad 650\ [m] < x \geq 1000\ [m], \end{cases} \tag{3.37}$$

and shown in Figure 3.9:

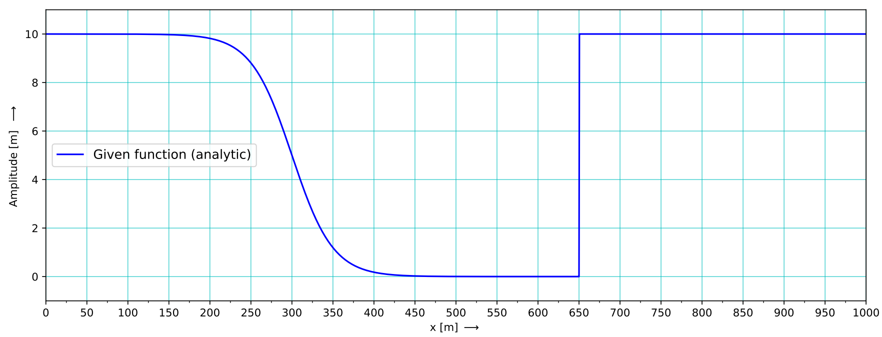
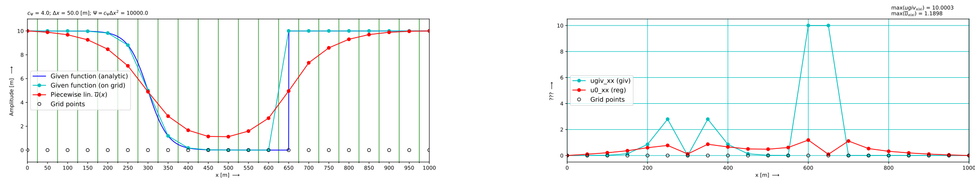


Figure 3.9: *Large and small gradients in given function.*

First guess of regularization:



***(a)** Grid size $\Delta x = 50\ [m]$*

***(b)** Second derivatives, normalized grid size $\Delta\xi = 1$.*

***Figure 3.10:** Initial guess ($c_\Psi = 4, \Delta x = 50\ [m]$)*

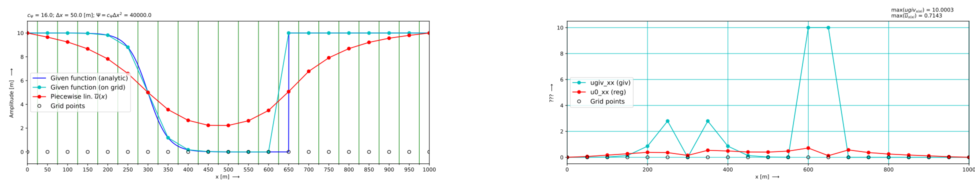
There are two options to adjust the data:

1 increase the regularization coefficient or

2 choose a smaller grid size.

Regularization coefficient increased

Increasing the regularization coefficient c_Ψ:



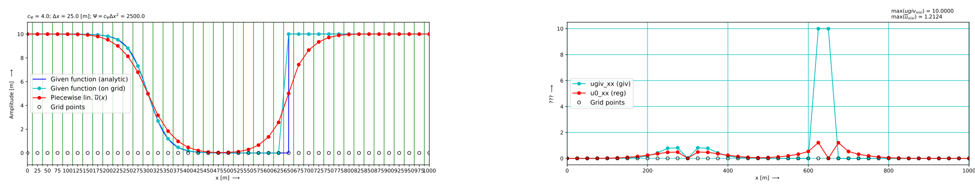
***(a)** Grid size $\Delta x = 50\ [m]$*

***(b)** Second derivatives, normalized grid size $\Delta\xi = 1$.*

***Figure 3.11:** Regularization coefficient increased to 16 ($c_\Psi = 16, \Delta x = 50\ [m]$)*

Grid size decreased

Decrease the grid size Δx:



***(a)** Step at grid node, $c_\Psi = 4, \Delta x = 25\ [m]$*

***(b)** Second derivatives.*

***Figure 3.12:** Grid size decreased to $25\ [m]$ ($c_\Psi = 4, \Delta x = 25\ [m]$)*

3.4 Compatible initialization

To assure that the given initial condition(s) are compatible with the numerical scheme, the given function need to fulfill the follow equation:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \overline{u}_{initial}\, dx = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_{given}\, dx \tag{3.38}$$

where $\overline{u}$ is the piecewise function and u_{given} the given initial condition. In case the function u_{given} is an integrable analytic function the integral can be exact computed. In discrete form the equation for each control volume reads:

$$\frac{\Delta x_{i-\frac{1}{2}}}{2}\,\frac{u_{i-1}+3u_i}{4} + \frac{\Delta x_{i+\frac{1}{2}}}{2}\,\frac{3u_i+u_{i+1}}{4} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} u_{given}\, dx \tag{3.39}$$

Extra equations are needed for the boundary conditions, the following boundary treatment is used at $x = 2$ (see section 3.1.3):

$$\frac{1}{12}u_0 + \frac{10}{12}u_1 + \frac{1}{12}u_2 = u_{given}(2) \tag{3.40}$$

and similar at the other boundary ($x = 10$). An illustration off the result of Equation (3.38) is given in Figure 3.13.

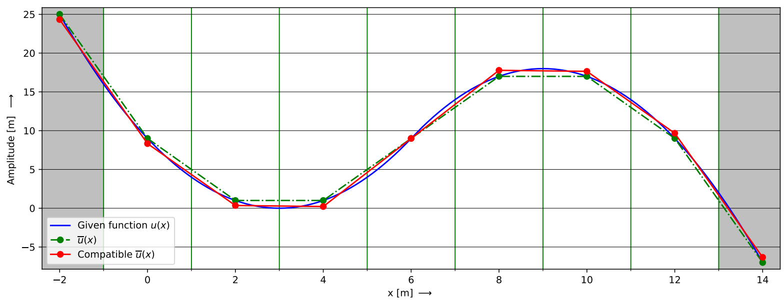


Figure 3.13: *Illustration of compatible quadratic function. Given function in blue. Compatible function in red. In green lines through nodes lying on the given function. Control volumes in between the green vertical lines. And the gray areas are virtual and are not belonging to the water body (see Figure 3.1). The integral over the control volume of the the given function is better represented by the red-function then by the green-function.*

Some numerical items used to generate Figure 3.13 are $x \in [0, 12]$, $\Delta x = 2$ and the given function reads:

$$u_{given}(x) = \begin{cases} (x-3)^2 & x < 6 \\ -(x-3)^2 + 18 & x \geq 6 \end{cases} \tag{3.41}$$

4 Time integration scheme

To derive a time integration we start from the PDE:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{f}(\boldsymbol{u}) = 0 \tag{4.1}$$

For conservation types it can be written as:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \nabla \cdot \boldsymbol{f}(\boldsymbol{u}) = \mathrm{S} \tag{4.2}$$

and when the finite volume approach is applied, we get

$$\int_\Omega \frac{\partial \boldsymbol{u}}{\partial t}\, d\Omega + \int_\Omega \nabla \cdot \boldsymbol{f}(\boldsymbol{u})\, d\Omega = \int_\Omega \mathrm{S}\, d\Omega, \tag{4.3}$$

and after Green's theorem

$$\int_\Omega \frac{\partial \boldsymbol{u}}{\partial t}\, d\Omega + \int_\Gamma \boldsymbol{f}(\boldsymbol{u}) \cdot \boldsymbol{n}\, d\Gamma = \int_\Omega \mathrm{S}\, d\Omega, \tag{4.4}$$

4.1 Fully implicit time integration by adding an iteration process

The system of Equations (4.1) can be written as, including the θ method:

$$\Delta t_{inv} \mathrm{M} \left(\boldsymbol{u}^{n+1} - \boldsymbol{u}^{n} \right) + \boldsymbol{f}\left(\boldsymbol{u}^{n+\theta} \right) = 0 \tag{4.5}$$

with $\Delta t_{inv} = 1/\Delta t$, M a mass-matrix and $0 \leq \theta \leq 1$. The mass-matrix used in this document for three adjacent grid nodes reads:

$$\mathrm{M} = \begin{pmatrix} \frac{1}{8} & \frac{6}{8} & \frac{1}{8} \end{pmatrix} \tag{4.6}$$

representing a piecewise linear approximation of the function between the grid nodes.

To reach a fully implicit time integration an iteration process p is added (Borsboom, 2019, eqs. 15/16):

$$\Delta t_{inv} \mathrm{M} \left(\boldsymbol{u}^{n+1,p+1} - \boldsymbol{u}^{n} \right) + \boldsymbol{f}\left(\boldsymbol{u}^{n+\theta,p+1} \right) = 0 \tag{4.7}$$

iterating from $p \to p+1$ until convergence.

The **first** term is split to get a so called "Delta" formulation, taking into account the previous iteration:

$$\Delta t_{inv} \mathrm{M} \left(\boldsymbol{u}^{n+1,p+1} - \boldsymbol{u}^{n+1,p} + \boldsymbol{u}^{n+1,p} - \boldsymbol{u}^{n} \right) + \cdots = 0 \tag{4.8}$$

$$\Delta t_{inv} \mathrm{M} \Delta \boldsymbol{u}^{n+1,p+1} + \cdots = -\Delta t_{inv} \mathrm{M} \left(\boldsymbol{u}^{n+1,p} - \boldsymbol{u}^{n} \right) \tag{4.9}$$

with $\Delta\boldsymbol{u}^{n+1,p+1} = \boldsymbol{u}^{n+1,p+1} - \boldsymbol{u}^{n+1,p}$. The right hand side is fully explicit (i.e. known at the previous iteration level p). And if the iteration process is converged, the term at the left hand side is zero (i.e. $\Delta\boldsymbol{u}^{n+1,p+1} = 0$) so the right handside represent the time derivative.

The **second** term of Equation (4.5)

$$\ldots + \boldsymbol{f}\left(\boldsymbol{u}^{n+\theta,p+1}\right) = 0 \tag{4.10}$$

will be linearized around the iteration step p (Newton linearization) and yields

$$\boldsymbol{f}(\boldsymbol{u}^{n+\theta,p+1}) = \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p}) + \frac{\partial \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p})}{\partial \boldsymbol{u}^{n+1,p}}(\boldsymbol{u}^{n+\theta,p+1} - \boldsymbol{u}^{n+\theta,p}) \tag{4.11}$$

$$= \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p}) + \frac{\partial \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p})}{\partial \boldsymbol{u}^{n+1,p}}\Delta\boldsymbol{u}^{n+\theta,p+1} \tag{4.12}$$

with

$$\Delta\boldsymbol{u}^{n+\theta,p+1} = \boldsymbol{u}^{n+\theta,p+1} - \boldsymbol{u}^{n+\theta,p} \tag{4.13}$$

$$= \theta\boldsymbol{u}^{n+1,p+1} + (1-\theta)\boldsymbol{u}^{n} - \theta\boldsymbol{u}^{n+1,p} - (1-\theta)\boldsymbol{u}^{n} \tag{4.14}$$

$$= \theta\boldsymbol{u}^{n+1,p+1} - \theta\boldsymbol{u}^{n+1,p} \tag{4.15}$$

$$= \theta\Delta\boldsymbol{u}^{n+1,p+1} \tag{4.16}$$

After subtitution of Equation (4.16) into Equation (4.12) we get:

$$\boldsymbol{f}(\boldsymbol{u}^{n+\theta,p+1}) = \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p}) + \theta\frac{\partial \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p})}{\partial \boldsymbol{u}^{n+1,p}}\Delta\boldsymbol{u}^{n+1,p+1} \tag{4.17}$$

The Jacobian

$$\mathbf{J}^{n+1,p} = \frac{\partial \boldsymbol{f}(\boldsymbol{u}^{n+\theta,p})}{\partial \boldsymbol{u}^{n+1,p}} = \frac{\partial \boldsymbol{f}(\theta\boldsymbol{u}^{\boldsymbol{n+1,p}} + (1-\theta)\boldsymbol{u}^{n})}{\partial \boldsymbol{u}^{n+1,p}} \tag{4.18}$$

is the approximate linearization of $\boldsymbol{f}$ as a function of $\theta\boldsymbol{u}^{n+1} + (1-\theta)\boldsymbol{u}^{n}$ with respect to $\boldsymbol{u}^{n+1,p}$. The Jacobians needed for the shallow water equations are described in section 4.2.

The total time integration method read:

$$\boxed{\begin{aligned}&\left(\Delta t_{inv}\mathbf{M} + \theta\mathbf{J}^{n+1,p}\right)\Delta\mathbf{u}^{n+1,p+1} = \\ &\quad = -\left(\Delta t_{inv}\mathbf{M}\left(\boldsymbol{u}^{n+1,p} - \boldsymbol{u}^{n}\right) + \boldsymbol{f}\left(\theta\boldsymbol{u}^{n+1,p} + (1-\theta)\boldsymbol{u}^{n}\right)\right)\end{aligned}} \tag{4.19}$$

with $\boldsymbol{u}^{n+1,p+1} = \boldsymbol{u}^{n+1,p} + \Delta\boldsymbol{u}^{n+1,p+1}$ and right hand side is explicit w.r.t. the iterator p. In case the Newton iteration process converges, i.e.:

$$\lim_{p\to\infty}\left(\Delta\boldsymbol{u}^{n+1,p+1}\right) = \lim_{p\to\infty}\left(\boldsymbol{u}^{n+1,p+1} - \boldsymbol{u}^{n+1,p}\right) = 0. \tag{4.20}$$

then the left hand side of Equation (4.19) is equal to zero and thus it solves the original system of equations:

$$0 = \Delta t_{inv} \mathrm{M} \left(\boldsymbol{u}^{n+1,p} - \boldsymbol{u}^{n} \right) + \boldsymbol{f} \left(\theta \boldsymbol{u}^{n+1,p} + (1-\theta) \boldsymbol{u}^{n} \right). \tag{4.21}$$

Because in the previous part we consider only the first derivative (Jacobian) and assumed that the second derivative is nearly zero, which is not always through. Therefor we will extend the iteration process, see section 4.1.1. See also: Borsboom (1998) and Pulliam (2014)

4.1.1 Pseudo time stepping

In section 4.1 we assumed that only the Jacobian is relevant and the second derivative is negligible. But in some case it is not the cases we have to assure that the following inequality is true:

$$\left| \frac{1}{2} \frac{\partial^2 \boldsymbol{f}(\theta \boldsymbol{u}^{n+1,p} + (1-\theta)\boldsymbol{u}^{n})}{(\partial \boldsymbol{u}^{n+1,p})^2} \Delta \boldsymbol{u}^{n+1,p+1} \right| < O \left(\left| \frac{\partial \boldsymbol{f}(\theta \boldsymbol{u}^{n+1,p} + (1-\theta)\boldsymbol{u}^{n})}{\partial \boldsymbol{u}^{n+1,p}} \right| \right) \tag{4.22}$$

Therefor the time integration is extended with a (so called) pseudo timestep method, which read:

$$\boxed{\begin{aligned} &\left(\mathrm{M}_{pseu} \boldsymbol{T}_{pseu}^{n+1,p} + \Delta t_{inv} \mathrm{M} + \theta \mathbf{J}^{n+1,p} \right) \Delta \mathbf{u}^{n+1,p+1} = \\ &\quad = - \left(\Delta t_{inv} \mathrm{M} \left(\boldsymbol{u}^{n+1,p} - \boldsymbol{u}^{n} \right) + \boldsymbol{f} \left(\theta \boldsymbol{u}^{n+1,p} + (1-\theta) \boldsymbol{u}^{n} \right) \right) \end{aligned}} \tag{4.23}$$

where $\boldsymbol{T}_{pseu}^{n+1,p}$ is a vector containing the inverse of the pseudo timestep, which may vary for all grid nodes, and M_{pseu} a mass-matrix operating on the pseudo timestep vector. See for a more detailed description and how to choose the term $\mathrm{M}_{pseu} \boldsymbol{T}_{pseu}^{n+1,p}$ Borsboom (2019) and Buijs (2024).

4.2 Jacobians

As seen in section 4.1 Jacobians need to be computed. These Jacobians does not contain only derivatives to the major variables but also to place derivatives, which need special attention (section 4.2.3). For example for the two dimensional convection flux ($\boldsymbol{q}\boldsymbol{q}^T$) and presure term $gh\nabla\zeta$, where $\boldsymbol{q} = (q, r)^T$ and ζ the water level.

As example we take the integral form of the two dimensional non-linear wave equation. This equation reads:

$$\int_{\Omega} \frac{\partial \boldsymbol{u}}{\partial t} \, d\Omega + \int_{\Omega} \nabla \cdot \boldsymbol{F} \, d\Omega = 0 \Leftrightarrow \int_{\Omega} \frac{\partial \boldsymbol{u}}{\partial t} \, d\Omega + \oint_{\Gamma} \boldsymbol{F} \cdot \boldsymbol{n} \, d\Gamma = 0 \tag{4.24}$$

with vector $\boldsymbol{u} = (h, q, r)^T$ the Jacobian read. With

h	The total water depth, $[\mathrm{m}]$
q	The water flux in x-direction, $[\mathrm{m}^2\,\mathrm{s}^{-1}]$
r	The water flux in y-direction, $[\mathrm{m}^2\,\mathrm{s}^{-1}]$

The Jacobian of the function $F(h, q, r)$ as used in the two dimensional shallow water equations reads:

$$\mathbf{J} = \begin{pmatrix} J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{pmatrix} = \begin{pmatrix} \frac{\partial F_1}{\partial h} & \frac{\partial F_1}{\partial q} & \frac{\partial F_1}{\partial r} \\ \frac{\partial F_2}{\partial h} & \frac{\partial F_2}{\partial q} & \frac{\partial F_2}{\partial r} \\ \frac{\partial F_3}{\partial h} & \frac{\partial F_3}{\partial q} & \frac{\partial F_3}{\partial r} \end{pmatrix} \tag{4.25}$$

4.2.1 Non-linear term, product

If the Jacobian contains non-linear terms, each variable of $\boldsymbol{u}$ is linearized before using it in the non-linear term. As an example a product of two quantities is taken, say q and r (like the convection term in two dimensional shallow water equations) and $\Delta q^{n+1,p+1} = \Delta q$ and $\Delta r^{n+1,p+1} = \Delta r$:

$$(qr)\big|^{n+\theta,p+1} = \left(q^{n+\theta,p} + \theta\Delta q\right)\left(r^{n+\theta,p} + \theta\Delta r\right) \approx \tag{4.26}$$

$$\approx q^{n+\theta,p} r^{n+\theta,p} + \theta q^{n+\theta,p}\Delta r + \theta r^{n+\theta,p}\Delta q \tag{4.27}$$

omitting the quadratic term $O((\Delta q)^2, \Delta q\Delta r, (\Delta r)^2)$.

Jacobian

When the Jacobian notation is used for the function $F(q, r) = qr$

$$\mathbf{J} = \begin{pmatrix} J_{11} & J_{12} \end{pmatrix} = \begin{pmatrix} \frac{\partial F}{\partial q} & \frac{\partial F}{\partial r} \end{pmatrix} = \begin{pmatrix} \frac{\partial qr}{\partial q} & \frac{\partial qr}{\partial r} \end{pmatrix} = \begin{pmatrix} r & q \end{pmatrix} \tag{4.28}$$

it leads to following approximation

$$(qr)\big|^{n+\theta,p+1} \approx q^{n+\theta,p} r^{n+\theta,p} + \theta J_{11}^{n+\theta,p}\Delta q + \theta J_{12}^{n+\theta,p}\Delta r = \tag{4.29}$$

$$= q^{n+\theta,p} r^{n+\theta,p} + \theta r^{n+\theta,p}\Delta q + q^{n+\theta,p}\Delta r \tag{4.30}$$

4.2.2 Non-linear term, quotient

If the Jacobian contains non-linear terms, each variable of $\boldsymbol{u}$ is linearized before using it in the non-linear term. in this example a quotient of two quantities is taken, say q and h (representing the velocity in the two dimensional shallow water equations) and $\Delta q^{n+1,p+1} = \Delta q$ and $\Delta h^{n+1,p+1} = \Delta h$:

$$\left(\frac{q}{h}\right)\Bigg|^{n+\theta,p+1} = \frac{q^{n+\theta,p} + \theta\Delta q}{h^{n+\theta,p} + \theta\Delta h} \approx \tag{4.31}$$

$$\approx \frac{q^{n+\theta,p} + \theta\Delta q}{h^{n+\theta,p}} \left(1 - \frac{\theta}{h^{n+\theta,p}}\Delta h + O\left((\Delta h)^2\right)\right) \approx \tag{4.32}$$

$$\approx \left(\frac{q^{n+\theta,p}}{h^{n+\theta,p}} + \frac{\theta}{h^{n+\theta,p}}\Delta q\right)\left(1 - \frac{\theta}{h^{n+\theta,p}}\Delta h + O\left((\Delta h)^2\right)\right) \approx \tag{4.33}$$

$$\approx \frac{q^{n+\theta,p}}{h^{n+\theta,p}} - \theta\frac{q^{n+\theta,p}}{(h^{n+\theta,p})^2}\Delta h + \theta\frac{1}{h^{n+\theta,p}}\Delta q \tag{4.34}$$

omitting the quadratic term $O((\Delta q)^2, \Delta q\Delta h, (\Delta h)^2)$.

Jacobian

When the Jacobian notation is used for the function $F(h, q) = q/h$

$$\mathbf{J} = \begin{pmatrix} J_{11} & J_{12} \end{pmatrix} = \begin{pmatrix} \frac{\partial F}{\partial h} & \frac{\partial F}{\partial q} \end{pmatrix} = \begin{pmatrix} \frac{\partial q/h}{\partial h} & \frac{\partial q/h}{\partial q} \end{pmatrix} = \begin{pmatrix} -\frac{q}{h^2} & \frac{1}{h} \end{pmatrix} \tag{4.35}$$

it leads to following approximation

$$(qr)|^{n+\theta,p+1} \approx \frac{q^{n+\theta,p}}{r^{n+\theta,p}} + \theta J_{11}^{n+\theta,p}\Delta h + \theta J_{12}^{n+\theta,p}\Delta q = \tag{4.36}$$

$$= q^{n+\theta,p}r^{n+\theta,p} - \theta\frac{q^{n+\theta,p}}{(h^{n+\theta,p})^2}\Delta h + \theta\frac{1}{h^{n+\theta,p}}\Delta q \tag{4.37}$$

4.2.3 Terms with an operator

The Jacobian of an operator is also applied to the argument of the operator. As an example the pressure term of the shallow water equations is taken, where $\Delta h^{n+1,p+1} = \Delta h$ and $\Delta\zeta^{n+1,p+1} = \Delta\zeta$:

$$gh\frac{\partial\zeta}{\partial x}\Bigg|^{n+\theta,p+1} \approx g\left(h^{n+\theta,p} + \theta\Delta h\right)\frac{\partial}{\partial x}\left(\zeta^{n+\theta,p} + \theta\Delta\zeta\right) \approx \tag{4.38}$$

$$\approx gh^{n+\theta,p}\frac{\partial\zeta^{n+\theta,p}}{\partial x} + \theta gh^{n+\theta,p}\frac{\partial\Delta\zeta}{\partial x} + \theta g\frac{\partial\zeta^{n+\theta,p}}{\partial x}\Delta h \tag{4.39}$$

omitting the quadratic term $O(\Delta h\, \partial\Delta\zeta/\partial x)$. The term $\partial\Delta\zeta/\partial x$ is not always small and therefor a psuedo time step method is introduced, see section 4.1.1.

In discrete form it reads on location $x_{i+\frac{1}{2}}$:

$$gh\frac{\partial\zeta}{\partial x}\bigg|_{i+\frac{1}{2}}^{n+\theta,p+1} \approx gh_{i+\frac{1}{2}}^{n+\theta,p}\frac{\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p}}{\Delta x_i} + \theta gh_{n+\frac{1}{2}}^{n+\theta,p}\frac{\Delta\zeta_{i+1}-\Delta\zeta_i}{\Delta x_i} + \tag{4.40}$$

$$+\,\theta g\frac{\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p}}{\Delta x_i}\Delta h_{i+\frac{1}{2}} \tag{4.41}$$

Remember that the gradient over a grid cell Δx_i is constant, due to the piece-wise linear approximation between two nodes.

Jacobian

When the Jacobian notation is used for the function $F(q,h) = gh\,\partial\zeta/\partial x$

$$\mathbf{J} = \begin{pmatrix} J_{11} & J_{12}\end{pmatrix} = \begin{pmatrix} \frac{\partial F}{\partial h} & \frac{\partial F}{\partial \zeta}\end{pmatrix} = \begin{pmatrix} \frac{\partial(gh\,\partial\zeta/\partial x)}{\partial h} & \frac{\partial(gh\,\partial\zeta/\partial x)}{\partial\zeta}\end{pmatrix} = \begin{pmatrix} g\,\frac{\partial\zeta}{\partial x} & gh\,\frac{\partial}{\partial x}\end{pmatrix} \tag{4.42}$$

it leads to following approximation

$$gh\frac{\partial\zeta}{\partial x}\bigg|_{i+\frac{1}{2}}^{n+\theta,p+1} \approx gh^{n+\theta,p}\frac{\partial\zeta^{n+\theta,p}}{\partial x} + \theta J_{11}\Delta h + \theta J_{12}\frac{\partial}{\partial x}(\Delta\zeta) \approx \tag{4.43}$$

$$\approx gh^{n+\theta,p}\frac{\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p}}{\Delta x_i} + \theta g\frac{\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p}}{\Delta x_i}\Delta h_{i+\frac{1}{2}} + \tag{4.44}$$

$$+\,\theta gh_{n+\frac{1}{2}}^{n+\theta,p}\frac{\Delta\zeta_{i+1}-\Delta\zeta_i}{\Delta x_i} \tag{4.45}$$

5 Towards the shallow water equations

Consider the non-linear wave equation when the pressure gradient is explicitly expressed as the gradient of the water level (ζ):

$$\underbrace{\frac{\partial h}{\partial t}}_{\textit{Time derivative}} + \underbrace{\frac{\partial q}{\partial x}}_{\textit{Mass flux}} = 0, \tag{5.1a}$$

$$\underbrace{\frac{\partial q}{\partial t}}_{\textit{Time derivative}} + \underbrace{\frac{\partial q^2/h}{\partial x}}_{\textit{Convection}} + \underbrace{gh\frac{\partial \zeta}{\partial x}}_{\textit{Pressure gradient}} + \\ + \underbrace{c_f \frac{q\,|q|}{h^2}}_{\textit{Bed shear stress}} - \underbrace{\frac{\partial}{\partial x}\left(\nu h \frac{\partial q/h}{\partial x}\right)}_{\textit{Viscosity}} = 0, \tag{5.1b}$$

$$\zeta = h + z_b \tag{5.1c}$$

with

h	Total water depth ($h = \zeta - z_b$), $[\mathrm{m}]$.
z_b	Bed level w.r.t. reference plane, positive upward, $[\mathrm{m}]$.
q	Flow ($q = hu$), $[\mathrm{m^2\,s^{-1}}]$.
ζ	Water level w.r.t. reference plane ($\zeta = h + z_b$), positive upward, $[\mathrm{m}]$.
u	Velocity ($u = q/h$), $[\mathrm{m\,s^{-1}}]$.
g	Acceleration due to gravity, $[\mathrm{m\,s^{-2}}]$.
ν	Kinematic viscosity, $[\mathrm{m^2\,s^{-1}}]$.

If u is needed for other processes (like morphology and/or post processing) it can be computed according the next equation:

$$u = \frac{q}{h}. \tag{5.2}$$

In the finite volume approach these equations read:

$$\int_\Omega \frac{\partial h}{\partial t}\,d\omega + \int_\Omega \frac{\partial q}{\partial x}\,d\omega = 0, \tag{5.3a}$$

$$\int_\Omega \frac{\partial q}{\partial t}\,d\omega + \int_\Omega \frac{\partial q^2/h}{\partial x}\,d\omega + \int_\Omega gh\frac{\partial \zeta}{\partial x}\,d\omega + \\ + \int_\Omega c_f \frac{q\,|q|}{h^2}\,d\omega - \int_\Omega \frac{\partial}{\partial x}\left(\nu h \frac{\partial q/h}{\partial x}\right)\,d\omega = 0, \tag{5.3b}$$

$$\int_\Omega \zeta\,d\omega = \int_\Omega h\,d\omega + \int_\Omega z_b\,d\omega \tag{5.3c}$$

In this document we will end up with an implementation description of the 1D shallow water equation. We start a zero-dimensional implementation of a source term, representing the source and sink of external influences, like a power plant. Here we will show the results of a Brusselator (Ault and Holmgreen, 2003) and of a air pollution model (Hundsdorfer and Verwer, 2003, ex. 1.1 pg. 7). Then we continue with the one dimensional advection/transport equation than a one dimensional wave equation without convection, then with convection and at last with a bottom friction term. in this sequence we are missing the viscosity term, that term will be investigated by the advection-diffusion equation.

Because we will handle the shallow water equations in the variables h and q and not in ζ and u the equations does have always a non-linear behaviour, only for very small amplitude the behaviour is like a linear system. For linear wave equations the behaviour is always linear, even for large amplitudes, which is not the case for the equations we consider.

5.1 0-D Source/sink term

In this section a zero-dimensional model is implementation of the source term, representing the source and sink of external influences, like a power plant. The main (simple) equation will look like:

$$\frac{\partial \boldsymbol{u}}{\partial t} = \boldsymbol{f}(\boldsymbol{u}, t) \tag{5.4}$$

Here we will show the mathematical and implementation of an air pollution model, section 5.1.1 (Hundsdorfer and Verwer, 2003, ex. 1.1 pg. 7) and a Brusselator, section 5.1.2 (Ault and Holmgreen, 2003). Some results are shown in section 6.1.

5.1.1 Air pollution

Analytic description

We illustrate the mass action law by the following three reactions between oxygen O_2, atomic oxygen O, nitrogen oxide NO, and nitrogen dioxide NO_2 (Hundsdorfer and Verwer, 2003, eq. 1.1, page 7):

$$NO_2 + h\nu \xrightarrow{k_1} NO + O, \tag{5.5}$$

$$O + O_2 \xrightarrow{k_2} O_3, \tag{5.6}$$

$$NO + O_3 \xrightarrow{k_3} O_2 + NO_2. \tag{5.7}$$

These reactions are basic to any tropospheric air pollution model. The firstreaction is photochemical and says that NO and O are formed from $N02$ by photo-dissociation caused by solar radiation, indicated by $h\nu$. This depends on the time of the day and therefore $k_l = k_l(t)$. We consider the concentrations u_1 = [O], u_2 = [NO], u_3 = [NO2], u_4 = [O3]. The oxygen concentration [O_2] is treated as constant, and we assume there is a constant source term σ_2 simulating emission of nitrogen oxide. The rate functions and stoichiometric matrix are

$$g(t,u) = \begin{pmatrix} k_1(t)u_3 \\ k_2u_1 \\ k_3u_2u_4 \end{pmatrix}, \qquad S = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix} \tag{5.8}$$

The corresponding ODE system reads:

$$\frac{\partial u_1}{\partial t} = k_1u_3 - k_2u_1 \tag{5.9}$$
$$\frac{\partial u_2}{\partial t} = k_1u_3 - k_3u_2u_4 + \sigma_2 \tag{5.10}$$
$$\frac{\partial u_3}{\partial t} = k_3u_2u_4 - k_1u_3 \tag{5.11}$$
$$\frac{\partial u_4}{\partial t} = k_2u_1 - k_3u_2u_4 \tag{5.12}$$

We see that

$$\frac{\partial u_1}{\partial t} + \frac{\partial u_3}{\partial t} + \frac{\partial u_4}{\partial t} = 0, \tag{5.13}$$

and

$$\frac{\partial u_2}{\partial t} + \frac{\partial u_3}{\partial t} = \sigma_2 t \tag{5.14}$$

hence [O] + [NO2] + [O3] is a conserved quantity while [NO] + [NO2] growths with $\sigma_2 t$. By considering the null-space of S^T it is seen that these are the two mass laws for this chemical model.

With $\boldsymbol{u}(0) = (0.0, 2.0 \times 10^{-1}, 2.0 \times 10^{-3}, 2.0 \times 10^{-1})^T$ and $\sigma_2 = 10^{-7}$, and the coefficients k are defined as (this given conditions are different from the conditions as defined in Hundsdorfer and Verwer (2003, pg. 8):

$$k_1 = \begin{cases} 10^{-5} \exp\left(7\ g(t)\right) \\ 10^{-40}, & \text{during night} \end{cases} \tag{5.15}$$
$$k_2 = 2.0 \times 10^{-2} \tag{5.16}$$
$$k_3 = 1.0 \times 10^{-3} \tag{5.17}$$

with

$$g(t) = \left(\sin\left(\frac{\pi}{16}(t_h - 4)\right)\right)^{0.2}, \qquad t_h = \frac{t}{3600}; \tag{5.18}$$

where t_h is the time in hours. How these equations are discretized is given in Equation (5.1.1).

Numerical discretization

The discretization in Δ-formulation reads:

$$\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} = -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + k_1(u_3^{n+\theta,p+1}) - k_2(u_1^{n+\theta,p+1}) \tag{5.19}$$

$$\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} = -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_1(u_3^{n+\theta,p+1}) - k_3(u_2^{n+\theta,p+1})(u_4^{n+\theta,p+1}) + \sigma_2 \tag{5.20}$$

$$\frac{1}{\Delta t}\Delta u_3^{n+1,p+1} = -\frac{1}{\Delta t}(u_3^{n+1,p} - u_3^n) + k_3(u_2^{n+\theta,p+1})(u_4^{n+\theta,p+1}) - k_1(u_3^{n+\theta,p+1}) \tag{5.21}$$

$$\frac{1}{\Delta t}\Delta u_4^{n+1,p+1} = -\frac{1}{\Delta t}(u_4^{n+1,p} - u_4^n) + k_2(u_1^{n+\theta,p+1}) - k_3(u_2^{n+\theta,p+1})(u_4^{n+\theta,p+1}) \tag{5.22}$$

with linearization of $\boldsymbol{u}^{n+\theta,p+1}$ yields:

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} &= -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + \\ &+ k_1(u_3^{n+\theta,p} + \theta\Delta u_3^{n+1,p+1}) - k_2(u_1^{n+\theta,p} + \theta\Delta u_1^{n+1,p+1})\end{aligned} \tag{5.23}$$

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} &= -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_1(u_3^{n+\theta,p} + \theta\Delta u_3^{n+1,p+1}) + \\ &- k_3(u_2^{n+\theta,p} + \theta\Delta u_2^{n+1,p+1})(u_4^{n+\theta,p} + \theta\Delta u_4^{n+1,p+1}) + \sigma_2\end{aligned} \tag{5.24}$$

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_3^{n+1,p+1} &= -\frac{1}{\Delta t}(u_3^{n+1,p} - u_3^n) + k_3(u_2^{n+\theta,p} + \theta\Delta u_2^{n+1,p+1})(u_4^{n+\theta,p} + \\ &+ \theta\Delta u_4^{n+1,p+1}) - k_1(u_3^{n+\theta,p} + \theta\Delta u_3^{n+1,p+1})\end{aligned} \tag{5.25}$$

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_4^{n+1,p+1} &= -\frac{1}{\Delta t}(u_4^{n+1,p} - u_4^n) + k_2(u_1^{n+\theta,p} + \theta\Delta u_1^{n+1,p+1}) + \\ &- k_3(u_2^{n+\theta,p} + \theta\Delta u_2^{n+1,p+1})(u_4^{n+\theta,p} + \theta\Delta u_4^{n+1,p+1})\end{aligned} \tag{5.26}$$

and rearrange the system of equations to $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$, yields

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} - k_1\theta\Delta u_3^{n+1,p+1} + k_2\theta\Delta u_1^{n+1,p+1} &= \\ = -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + k_1 u_3^{n+\theta,p} - k_2 u_1^{n+\theta,p}\end{aligned} \tag{5.27}$$

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} - k_1\theta\Delta u_3^{n+1,p+1} + k_3\theta u_4^{n+1,p}\Delta u_2^{n+1,p+1} + k_3\theta u_2^{n+1,p}\Delta u_4^{n+1,p+1} &= \\ = -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_1 u_3^{n+\theta,p} - k_3 u_2^{n+\theta,p} u_4^{n+\theta,p} + \sigma_2\end{aligned} \tag{5.28}$$

$$\begin{aligned}\frac{1}{\Delta t}\Delta u_3^{n+1,p+1} - k_3 u_2^{n+\theta,p}\theta\Delta u_4^{n+1,p+1} - k_3 u_4^{n+\theta,p}\theta\Delta u_2^{n+1,p+1} + k_1\theta\Delta u_3^{n+1,p+1} &= \\ = -\frac{1}{\Delta t}(u_3^{n+1,p} - u_3^n) + k_3 u_2^{n+\theta,p} u_4^{n+\theta,p} - k_1 u_3^{n+\theta,p}\end{aligned} \tag{5.29}$$

$$
\begin{aligned}
\frac{1}{\Delta t}\Delta u_4^{n+1,p+1} - k_2\theta\Delta u_1^{n+1,p+1} + k_3 u_2^{n+\theta,p}\theta\Delta u_4^{n+1,p+1} + k_3 u_4^{n+\theta,p}\theta\Delta u_2^{n+1,p+1} = \\
= -\frac{1}{\Delta t}(u_4^{n+1,p} - u_4^n) + k_2 u_1^{n+\theta,p} - k_3 u_2^{n+\theta,p} u_4^{n+\theta,p} \qquad (5.30)
\end{aligned}
$$

5.1.2 Brusselator

Analytic description

The ODE system for the Brusselator reads Ault and Holmgreen (2003, eq. 14, 15):

$$
\frac{\partial u_1}{\partial t} = 1 - (k_2 + 1)u_1 + k_1 u_1^2 u_2, \qquad (5.31)
$$

$$
\frac{\partial u_2}{\partial t} = k_2 u_1 - k_1 u_1^2 u_2 \qquad (5.32)
$$

with $k_1 = 1$ and $k_2 = 2.5$ and initial values $u_1(0) = 0$ and $u_2(0) = 0$.

Numerical discretization

The ODE system for the brusselator reads (Ault and Holmgreen, 2003, eq. 14, 15):

$$
\frac{\partial u_1}{\partial t} = 1 - (k_2 + 1)u_1 + k_1 u_1^2 u_2, \qquad (5.33)
$$

$$
\frac{\partial u_2}{\partial t} = k_2 u_1 - k_1 u_1^2 u_2 \qquad (5.34)
$$

The discretization in Δ-formulation reads:

$$
\begin{aligned}
\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} &= -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + 1 - (k_2 + 1)u_1^{n+\theta,p+1} + \\
&\quad + k_1 \left(u_1^{n+\theta,p+1}\right)^2 u_2^{n+\theta,p+1} \qquad (5.35)\\
\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} &= -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_2(u_1^{n+\theta,p+1}) + \\
&\quad - k_1 \left(u_1^{n+\theta,p+1}\right)^2 u_2^{n+\theta,p+1} \qquad (5.36)
\end{aligned}
$$

with linearization of $\boldsymbol{u}^{n+\theta,p+1}$ yields:

$$
\begin{aligned}
\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} &= -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + 1 - (k_2 + 1)\left(u_1^{n+\theta,p} + \theta\Delta u_1^{n+1,p+1}\right) + \\
&\quad + k_1 \left(u_1^{n+\theta,p} + \Delta u_1^{n+1,p+1}\right)^2 \left(u_2^{n+\theta,p} + \Delta u_1^{n+1,p+1}\right) \qquad (5.37)\\
\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} &= -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_2(u_1^{n+\theta,p} + \theta\Delta u_1^{n+1,p+1}) + \\
&\quad - k_1 \left(u_1^{n+\theta,p} + \Delta u_1^{n+1,p+1}\right)^2 \left(u_2^{n+\theta,p} + \Delta u_1^{n+1,p+1}\right) \qquad (5.38)
\end{aligned}
$$

and rearrange the system of equations to $\mathbf{A}\boldsymbol{x} = \boldsymbol{b}$ and omitting the second order terms, yields

$$\frac{1}{\Delta t}\Delta u_1^{n+1,p+1} - \theta\left((k_2+1) + 2k_1 u_1^{n+\theta,p} u_2^{n+\theta,p}\right)\Delta u_1^{n+1,p+1} - \theta k_1 \left(u_1^{n+1,p+1}\right)^2 \Delta u_2^{n+1,p+1} =$$
$$= -\frac{1}{\Delta t}(u_1^{n+1,p} - u_1^n) + 1 - (k_2+1)u_1^{n+\theta,p} + k_1\left(u_1^{n+\theta,p}\right)^2 u_2^{n+\theta,p} \qquad (5.39)$$
$$\frac{1}{\Delta t}\Delta u_2^{n+1,p+1} + \theta\left(k_2 + 2k_1 u_1^{n+\theta,p} u_2^{n+\theta,p}\right)\Delta u_1^{n+1,p+1} + \theta k_1 \left(u_1^{n+1,p+1}\right)^2 \Delta u_2^{n+1,p+1} =$$
$$= -\frac{1}{\Delta t}(u_2^{n+1,p} - u_2^n) + k_2 u_1^{n+\theta,p} - k_1\left(u_1^{n+\theta,p}\right)^2 u_2^{n+\theta,p} \qquad (5.40)$$

This system can be implemented and solved, some results are presented in section 5.1.2.

5.2 1-D Advection-diffusion equation

In this section we will discuss the discretization of an advection-diffusion equation when the constituent does not need to be positive and when the constiuent must be positive.

5.2.1 Not strictly positive constituent

The considered advection-diffusion equation reads:

$$\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} - \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial c}{\partial x}\right) = 0, \qquad u > 0. \qquad (5.41)$$

A constituent c is transported from the left to the right with the constant velocity $u\,[\mathrm{m\,s^{-1}}]$. Which is discretised on the grid

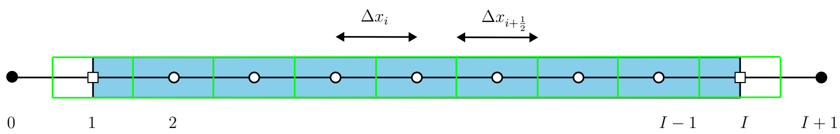


Figure 5.1: *Water body (blue area), finite volumes (green boxes), computational points (open dots), virtual computational points (black dots), boundary points are at x_1 (inflow/west boundary) and $x_{I+\frac{1}{2}}$ (outflow/east boundary).*

The finite volume approach for control volume $\Delta x_{i+\frac{1}{2}}$ of Equation (5.41) reads:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial c}{\partial t}\,dx + \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial uc}{\partial x}\,dx - \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial c}{\partial x}\right)dx = 0 \qquad (5.42)$$

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial c}{\partial t}\,dx + (uc)|_{i+\frac{1}{2}} - (uc)|_{i-\frac{1}{2}} - \left(\varepsilon\left.\frac{\partial c}{\partial x}\right|_{i+\frac{1}{2}} - \varepsilon\left.\frac{\partial c}{\partial x}\right|_{i-\frac{1}{2}}\right) = 0 \qquad (5.43)$$

Discretization interior

The discretization in Δ-formulation in the interior of domain Ω and for equidistant grid and the mass-matrix as given in Equation (4.6) reads

$$
\begin{aligned}
&\Delta x \Delta t_{inv} \left(\frac{1}{8} \Delta c_{i-1}^{n+1,p+1} + \frac{6}{8} \Delta c_{i}^{n+1,p+1} + \frac{1}{8} \Delta c_{i+1}^{n+1,p+1} \right) + \\
&+ \left\{ \Delta x \Delta t_{inv} \left(\frac{1}{8} \left(c_{i-1}^{n+1,p} - c_{i-1}^{n} \right) + \frac{6}{8} \left(c_{i}^{n+1,p} - c_{i}^{n} \right) + \frac{1}{8} \left(c_{i+1}^{n+1,p} - c_{i+1}^{n} \right) \right) \right\} + \\
&\quad + u \left(\frac{1}{2} (c_{i}^{n+\theta,p+1} + c_{i+1}^{n+\theta,p+1}) - \frac{1}{2} (c_{i-1}^{n+\theta,p+1} + c_{i}^{n+\theta,p+1}) \right) + \\
&\quad - \left(\varepsilon_{i+\frac{1}{2}} \frac{c_{i+1}^{n+\theta,p+1} - c_{i}^{n+\theta,p+1}}{\Delta x} - \varepsilon_{i-\frac{1}{2}} \frac{c_{i}^{n+\theta,p+1} - c_{i-1}^{n+\theta,p+1}}{\Delta x} \right) = 0
\end{aligned}
\tag{5.44}
$$

After linearization of $c^{n+\theta,p+1}$ the discretization reads:

$$
\begin{aligned}
&\Delta x \Delta t_{inv} \left(\frac{1}{8} \Delta c_{i-1}^{n+1,p+1} + \frac{6}{8} \Delta c_{i}^{n+1,p+1} + \frac{1}{8} \Delta c_{i+1}^{n+1,p+1} \right) \\
&\quad \frac{1}{2} \theta u \left(\Delta c_{i}^{n+1,p+1} + \Delta c_{i+1}^{n+1,p+1} - \left(\Delta c_{i-1}^{n+1,p+1} + \Delta c_{i}^{n+1,p+1} \right) \right) + \\
&\quad - \theta \frac{\varepsilon_{i+\frac{1}{2}}}{\Delta x} \Delta c_{i+1}^{n+1,p+1} + \theta \left(\frac{\varepsilon_{i+\frac{1}{2}}}{\Delta x} + \frac{\varepsilon_{i-\frac{1}{2}}}{\Delta x} \right) \Delta c_{i}^{n+1,p+1} - \theta \frac{\varepsilon_{i-\frac{1}{2}}}{\Delta x} \Delta c_{i-1}^{n+1,p+1} = \\
&\quad = - \left\{ \Delta x \Delta t_{inv} \left(\frac{1}{8} \left(c_{i-1}^{n+1,p} - c_{i-1}^{n} \right) + \frac{6}{8} \left(c_{i}^{n+1,p} - c_{i}^{n} \right) + \frac{1}{8} \left(c_{i+1}^{n+1,p} - c_{i+1}^{n} \right) \right) + \right. \\
&\qquad + \frac{1}{2} u \left((c_{i}^{n+\theta,p} + c_{i+1}^{n+\theta,p}) - (c_{i-1}^{n+\theta,p} + c_{i}^{n+\theta,p}) \right) + \\
&\qquad \left. - \left(\varepsilon_{i+\frac{1}{2}} \frac{c_{i+1}^{n+\theta,p} - c_{i}^{n+\theta,p}}{\Delta x} - \varepsilon_{i-\frac{1}{2}} \frac{c_{i}^{n+\theta,p} - c_{i-1}^{n+\theta,p}}{\Delta x} \right) \right\}
\end{aligned}
\tag{5.45}
$$

Discretization at boundaries

An **essential** boundary condition at the inflow boundary is needed, left side of the domain. And, at the right side an outflow boundary 'condition' is required for numerical reasons (called a **natural** boundary condition), i.e. a discretization of the model equation at the outflow boundary. The natural boundary conditions is fully determined by the outgoing signal and therefor we use the equation of the outgoing signal, i.e. Equation (5.59). For the 1-D advection-diffusion equation when omitting the viscosity term it reads:

$$
\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} = 0, \qquad u > 0. \tag{5.46}
$$

The **essential** boundary condition at the inflow boundary reads:

$$
c(0,t) = c_0(t), \quad t > 0 \qquad \text{(essential boundary)} \tag{5.47}
$$

The essential boundary condition is supplied at x_1 with the following discretization (Equation (3.10))

$$\frac{1}{12}\Delta c_0^{n+1,p+1} + \frac{10}{12}\Delta c_1^{n+1,p+1} + \frac{1}{12}\Delta c_2^{n+1,p+1} =$$
$$= c_0(t) - \left(\frac{1}{12}c_0^{n+1,p} + \frac{10}{12}c_1^{n+1,p} + \frac{1}{12}c_2^{n+1,p}\right) \tag{5.48}$$

TODO 5.1:** The implementation is not stable, check implementation!* ***TODO

The **natural** is chosen in that way that as less as possible left going spurious numerical waves are generated at the outflow boundary, i.e. nearly no reflection. The natural boundary condition is supplied at x_I with the discretization constants as determined by Equation (3.9) and boundary condition Equation (5.46) which yields:

$$\left(\frac{1+\alpha_{bnd}}{\Delta t} + \theta\frac{u}{\Delta x}\right)\Delta c_{I+1}^{n+1,p+1} + \left(\frac{1-2\alpha_{bnd}}{\Delta t} - \theta\frac{u}{\Delta x}\right)\Delta c_I^{n+1,p+1} + \frac{\alpha_{bnd}}{\Delta t}\Delta c_{I-1}^{n+1,p+1} = \tag{5.49}$$

$$= -\left\{\frac{1+\alpha_{bnd}}{\Delta t}\left(c_{I+1}^{n+1,p} - c_{I+1}^n\right) + \frac{1-2\alpha_{bnd}}{\Delta t}\left(c_I^{n+1,p} - c_I^n\right) + \frac{\alpha_{bnd}}{\Delta t}\left(c_{I-1}^{n+1,p} - c_{I-1}^n\right) + \right. \tag{5.50}$$

$$\left. + \frac{u}{\Delta x}\left(c_{I+1}^{n+\theta,p} - c_I^{n+\theta,p}\right)\right\} \tag{5.51}$$

where $\alpha_{bnd} = 2\alpha - \frac{1}{2}$ ($\alpha_{bnd} = -\frac{1}{4}$ when $\alpha = \frac{1}{8}$)

5.2.2 Strictly positive constituent

When c needs a strickly positive value (like a concentration) then due to numerical discretization the value c could become negative, even if the initial and boundary values are positive. In certain applications a positive value is required and even small negative are not allowed. To ensure the positivity of the constituent c we will write the equation with variable ϕ, where ϕ is defined as:

$$c = \exp(\ln(c)) = \exp(\phi), \quad \text{with} \quad \phi = \ln(c) \tag{5.52}$$

The considered advection-diffusion equation than reads:

$$\int_\Omega \frac{\partial e^\phi}{\partial t}\,d\omega + \int_\Omega \frac{\partial\left(ue^\phi\right)}{\partial x}\,d\omega - \int_\Omega \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial e^\phi}{\partial x}\right)\,d\omega = 0, \tag{5.53}$$

Discretization interior

Not yet documented

Discretization at boundaries

Not yet documented

5.3 1-D wave equation

The hyperbolic part of the one dimensional shallow water equations (assuming that the viscosity term vanish) are diagonalized to separate the left and right going wave. We start from the follwoing equations, with convection for flat bottom ($\frac{1}{2}g\,\partial h^2/\partial x = gh\,\partial h/\partial x$ and $\partial z_b/\partial x = 0$), reads

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0 \qquad \textit{continuity eq.} \tag{5.54}$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{h}\right) + gh\frac{\partial h}{\partial x} = 0 \qquad \textit{momentum eq.} \tag{5.55}$$

These one dimensional shallow water equations can be written in matrix and vector notation as:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \mathbf{A}\frac{\partial \boldsymbol{u}}{\partial x} = 0 \tag{5.56}$$

To find the characteristic equations this set of equations should be written in a set of equation representing left and right going waves. The diagonalisation is performed as follows:

$$\frac{\partial \boldsymbol{u}}{\partial t} + \mathbf{P}\,\underbrace{\mathbf{P}^{-1}\mathbf{A}\mathbf{P}}_{\boldsymbol{\Lambda}}\,\mathbf{P}^{-1}\frac{\partial \boldsymbol{u}}{\partial x} = 0 \tag{5.57}$$

multiply this with $\mathbf{P}^{-1}$

$$\mathbf{P}^{-1}\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{\Lambda}\mathbf{P}^{-1}\frac{\partial \boldsymbol{u}}{\partial x} = 0 \tag{5.58}$$

with $\boldsymbol{\Lambda}$ a diagonal matrix and thus the left and right going signals are independent. For the one dimensional shallow water equations the two independent equations read:

$$\begin{array}{c} \text{right going} \\ \text{left going} \end{array} \quad \begin{pmatrix} \sqrt{gh} + \frac{q}{h} & -1 \\ \sqrt{gh} - \frac{q}{h} & 1 \end{pmatrix} \begin{pmatrix} \textit{continuity eq.} \\ \textit{momentum eq.} \end{pmatrix} = 0 \tag{5.59}$$

See for a derivation Appendix B.

We have split the hyperbolic wave equation into a right and left going wave. Now we are able to apply the **natural** boundary conditions as described in section 5.2.1 for each of the waves. The **essential** boundary condition is chosen to be an absorbing boundary, so no reflections at the boundaries will appear.

For the space discretizations of an arbitrary function u, the following space interpolations are used:

$$u_{i+\frac{1}{2}} = \frac{1}{2}\left(u_{i+1} + u_i\right) \qquad \textit{interface of control volume} \tag{5.60}$$

$$u_{i+\frac{1}{4}} = \frac{1}{4}\left(3u_i + u_{i+1}\right) \qquad \textit{quadrature point of sub-control volume} \tag{5.61}$$

$$u_{i-\frac{1}{4}} = \frac{1}{4}\left(3u_i + u_{i-1}\right) \qquad \textit{quadrature point of sub-control volume} \tag{5.62}$$

These formulas are visualized in Figure 3.2.

5.3.1 Discretizations continuity equation

The discretization of the continuity equation will be presented term by term of Equation (5.54).

5.3.1.1 Time derivative

The discretization of the time derivative term of the continuity equation reads:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial h}{\partial t}\, dx \tag{5.63}$$

which will be approximated by

$$\begin{aligned}
&\frac{1}{2}\Delta x_{i-\frac{1}{2}}\left(\frac{1}{4}\frac{\partial h_{i-1}}{\partial t} + \frac{3}{4}\frac{\partial h_i}{\partial t}\right) + \frac{1}{2}\Delta x_{i+\frac{1}{2}}\left(\frac{3}{4}\frac{\partial h_i}{\partial t} + \frac{1}{4}\frac{\partial h_{i+1}}{\partial t}\right) \approx \\
&\approx \frac{\Delta x_{i-\frac{1}{2}}}{\Delta t}\left(\frac{1}{8}\left(\Delta h_{i-1}^{n+1,p+1} + h_{i-1}^{n+1,p} - h_{i-1}^{n}\right) + \frac{3}{8}\left(\Delta h_{i}^{n+1,p+1} + h_{i}^{n+1,p} - h_{i}^{n}\right)\right) + \\
&+ \frac{\Delta x_{i+\frac{1}{2}}}{\Delta t}\left(\frac{3}{8}\left(\Delta h_{i}^{n+1,p+1} + h_{i+1}^{n+1,p} - h_{i}^{n}\right) + \frac{1}{8}\left(\Delta h_{i+1}^{n+1,p+1} + h_{i+1}^{n+1,p} - h_{i+1}^{n}\right)\right)
\end{aligned} \tag{5.64}$$

after rearranging the equation into an implicit left hand side and an explicit right hand side it reads:

$$\begin{aligned}
&\frac{\Delta x_{i-\frac{1}{2}}}{\Delta t}\left(\frac{1}{8}\Delta h_{i-1}^{n+1,p+1} + \frac{3}{8}\Delta h_{i}^{n+1,p+1}\right) + \frac{\Delta x_{i+\frac{1}{2}}}{\Delta t}\left(\frac{3}{8}\Delta h_{i}^{n+1,p+1} + \frac{1}{8}\Delta h_{i+1}^{n+1,p+1}\right) = \\
&= -\left\{\frac{\Delta x_{i-\frac{1}{2}}}{\Delta t}\left(\frac{1}{8}\left(h_{i-1}^{n+1,p} - h_{i-1}^{n}\right) + \frac{3}{8}\left(h_{i}^{n+1,p} - h_{i}^{n}\right)\right) + \right. \\
&\left. + \frac{\Delta x_{i+\frac{1}{2}}}{\Delta t}\left(\frac{3}{8}\left(h_{i+1}^{n+1,p} - h_{i}^{n}\right) + \frac{1}{8}\left(h_{i+1}^{n+1,p} - h_{i+1}^{n}\right)\right)\right\}
\end{aligned} \tag{5.65}$$

5.3.1.2 Mass flux

The discretization of the mass flux term of the continuity equation reads:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial q}{\partial x}\, dx \tag{5.66}$$

which will be approximated by the θ-method and using Green's theorem:

$$q_{i+\frac{1}{2}}^{n+\theta,p+1} - q_{i-\frac{1}{2}}^{n+\theta,p+1}. \tag{5.67}$$

The linearization of the flux q around iteration level p reads then:

$$q_{i+\frac{1}{2}}^{n+\theta,p} + \theta\Delta q_{i+\frac{1}{2}}^{n+1,p+1} - q_{i-\frac{1}{2}}^{n+\theta,p} - \theta\Delta q_{i-\frac{1}{2}}^{n+1,p+1} \tag{5.68}$$

after rearranging the equation into an implicit left hand side and an explicit right hand side it reads:

$$\frac{1}{2}\theta\Delta q_i^{n+1,p+1} - \frac{1}{2}\theta\Delta q_{i-1}^{n+1,p+1} + \left\{\frac{1}{2}q_{i+1}^{n+\theta,p} - \frac{1}{2}q_{i-1}^{n+\theta,p}\right\} \tag{5.69}$$

5.3.2 Discretizations momentum equation

The discretization of the momentum equation will be presented term by term of Equation (5.55).

5.3.2.1 Time derivative

The discretization of the time derivative term of the momentum equation reads and is similar as for the continuity equation:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial q}{\partial t}\, dx \tag{5.70}$$

which will be approximated by

$$\begin{aligned} &\frac{1}{2}\Delta x_{i-\frac{1}{2}}\left(\frac{1}{4}\frac{\partial q_{i-1}}{\partial t} + \frac{3}{4}\frac{\partial q_i}{\partial t}\right) + \frac{1}{2}\Delta x_{i+\frac{1}{2}}\left(\frac{3}{4}\frac{\partial q_i}{\partial t} + \frac{1}{4}\frac{\partial q_{i+1}}{\partial t}\right) \approx \\ &\approx \frac{\Delta x_{i-\frac{1}{2}}}{\Delta t}\left(\frac{1}{8}\left(\Delta q_{i-1}^{n+1,p+1} + q_{i-1}^{n+1,p} - q_{i-1}^{n}\right) + \frac{3}{8}\left(\Delta q_i^{n+1,p+1} + q_i^{n+1,p} - h_i^n\right)\right) + \\ &+ \frac{\Delta x_{i+\frac{1}{2}}}{\Delta t}\left(\frac{3}{8}\left(\Delta q_i^{n+1,p+1} + q_{i+1}^{n+1,p} - q_i^n\right) + \frac{1}{8}\left(\Delta q_{i+1}^{n+1,p+1} + q_{i+1}^{n+1,p} - q_{i+1}^n\right)\right) \end{aligned} \tag{5.71}$$

after rearranging the equation into an implicit left hand side and an explicit right hand side it reads:

$$\frac{\Delta x_{i-\frac{1}{2}}}{\Delta t}\left(\frac{1}{8}\Delta q_{i-1}^{n+1,p+1}+\frac{3}{8}\Delta q_{i}^{n+1,p+1}\right)+\frac{\Delta x_{i+\frac{1}{2}}}{\Delta t}\left(\frac{3}{8}\Delta q_{i}^{n+1,p+1}+\frac{1}{8}\Delta q_{i+1}^{n+1,p+1}\right)+$$
$$+\left\{\frac{\Delta x_{i-\frac{1}{2}}}{\Delta t}\left(\frac{1}{8}\left(q_{i-1}^{n+1,p}-q_{i-1}^{n}\right)+\frac{3}{8}\left(q_{i}^{n+1,p}-q_{i}^{n}\right)\right)+\right.$$
$$\left.+\frac{\Delta x_{i+\frac{1}{2}}}{\Delta t}\left(\frac{3}{8}\left(q_{i+1}^{n+1,p}-q_{i}^{n}\right)+\frac{1}{8}\left(q_{i+1}^{n+1,p}-q_{i+1}^{n}\right)\right)\right\} \tag{5.72}$$

5.3.2.2 Pressure term

The pressure term is dependent on the gradient of the water level ζ and reads:

$$\int_{i-\frac{1}{2}}^{i+\frac{1}{2}} gh\frac{\partial\zeta}{\partial x}\,dx. \tag{5.73}$$

The acceleration due to gravity is assumed to be constant ($g = constant$). We first linearize the equation and then discretize in space. The linearization of the pressure term around iteration level p reads:

$$gh\left.\frac{\partial\zeta}{\partial x}\right|^{n+\theta,p+1} \approx \tag{5.74}$$

$$\approx gh^{n+\theta,p}\frac{\partial\zeta^{n+\theta,p}}{\partial x}+\theta g\frac{\partial\zeta^{n+\theta,p}}{\partial x}\Delta h^{n+1,p+1}+\theta gh^{n+\theta,p}\frac{\partial}{\partial x}\Delta\zeta^{n+1,p+1} \tag{5.75}$$

Computing the integral over the finite volume:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} gh\frac{\partial\zeta}{\partial x}\,dx=\int_{x_{i-\frac{1}{2}}}^{x_i} gh\frac{\partial\zeta}{\partial x}\,dx+\int_{x_i}^{x_{i+\frac{1}{2}}} gh\frac{\partial\zeta}{\partial x}\,dx \tag{5.76}$$

with piecewise linear h en piecewise linear ζ, thus piecewise constant $\partial\zeta/\partial x$. The first term of Equation (5.75) becomes:

$$\int_{x_{i-\frac{1}{2}}}^{x_i} gh^{n+\theta,p}\frac{\partial\zeta^{n+\theta,p}}{\partial x}\,dx+\int_{x_i}^{x_{i+\frac{1}{2}}} gh^{n+\theta,p}\frac{\partial\zeta^{n+\theta,p}}{\partial x}\,dx \approx$$
$$\approx\frac{\Delta x_{i-\frac{1}{2}}}{2}gh_{i-\frac{1}{4}}^{n+\theta,p}\frac{\zeta_i^{n+\theta,p}-\zeta_{i-1}^{n+\theta,p}}{\Delta x_{i-\frac{1}{2}}}+\frac{\Delta x_{i+\frac{1}{2}}}{2}gh_{i+\frac{1}{4}}^{n+\theta,p}\frac{\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p}}{\Delta x_{i+\frac{1}{2}}} \tag{5.77}$$
$$=\frac{1}{2}gh_{i-\frac{1}{4}}^{n+\theta,p}\left(\zeta_i^{n+\theta,p}-\zeta_{i-1}^{n+\theta,p}\right)+\frac{1}{2}gh_{i+\frac{1}{4}}^{n+\theta,p}\left(\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p}\right) \tag{5.78}$$

The second term of Equation (5.75)

$$\int_{x_{i-\frac{1}{2}}}^{x_i}\theta g\frac{\partial\zeta^{n+\theta,p}}{\partial x}\Delta h_{i-\frac{1}{4}}^{n+1,p+1}\,dx+\int_{x_i}^{x_{i+\frac{1}{2}}}\theta g\frac{\partial\zeta^{n+\theta,p}}{\partial x}\Delta h_{i+\frac{1}{4}}^{n+1,p+1}\,dx \approx \tag{5.79}$$
$$\approx\frac{1}{2}\theta g(\zeta_i^{n+\theta,p}-\zeta_{i-1}^{n+\theta,p})\Delta h_{i-\frac{1}{4}}^{n+1,p+1}+\frac{1}{2}\theta g(\zeta_{i+1}^{n+\theta,p}-\zeta_{i}^{n+\theta,p})\Delta h_{i+\frac{1}{4}}^{n+1,p+1} \tag{5.80}$$

The third term of Equation (5.75)

$$\int_{x_{i-\frac{1}{2}}}^{x_i} \theta g h_{i-\frac{1}{4}}^{n+\theta,p} \frac{\partial}{\partial x} \Delta\zeta^{n+1,p+1}\, dx + \int_{x_{i+\frac{1}{2}}}^{x_i} \theta g h_{i+\frac{1}{4}}^{n+\theta,p} \frac{\partial}{\partial x} \Delta\zeta^{n+1,p+1}\, dx = \tag{5.81}$$

$$= \frac{1}{2}\theta g h_{i-\frac{1}{4}}^{n+\theta,p} \left(\Delta\zeta_i^{n+1,p+1} - \Delta\zeta_{i-1}^{n+1,p+1}\right) + \frac{1}{2}\theta g h_{i+\frac{1}{4}}^{n+\theta,p} \left(\Delta\zeta_{i+1}^{n+1,p+1} - \Delta\zeta_i^{n+1,p+1}\right) \tag{5.82}$$

In a formulation of the shallow-water equations, where the water level is expressed as $\zeta = h + z_b$. The equations can be simplified, because

$$\Delta\zeta = \Delta(h + z_b) = \Delta h + \Delta z_b. \tag{5.83}$$

and if $\Delta z_b = 0$, i.e. time independent, the contributions to the $\Delta\zeta$-equations need to be incorporated in the Δh-equations. Adjusting the matrix coefficients and right-hand side change accordingly.

5.3.2.3 Convection

The convection term read:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial q^2/h}{\partial x}\, dx = \left.\frac{q^2}{h}\right|_{i+\frac{1}{2}}^{n+\theta,p+1} - \left.\frac{q^2}{h}\right|_{i-\frac{1}{2}}^{n+\theta,p+1} \tag{5.84}$$

The linearization of the convection term around iteration level p reads:

$$\left.\frac{q^2}{h}\right|^{n+\theta,p+1} \approx \frac{(q^{n+\theta,p})^2}{h^{n+\theta,p}} + 2\frac{q^{n+\theta,p}}{h^{n+\theta,p}}\theta\Delta q^{n+1,p+1} - \frac{(q^{n+\theta,p})^2}{(h^{n+\theta,p})^2}\theta\Delta h^{n+1,p+1} \tag{5.85}$$

(where $\Delta q^{n+\theta,p+1} = \theta\Delta q^{n+1,p+1}$ and $\Delta h^{n+\theta,p+1} = \theta\Delta h^{n+1,p+1}$, see Equation (4.16)).

5.3.2.4 Bed shear stress

The bed shear stress term reads:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} c_f \frac{q\,|q|}{h^2}\, dx = \int_{x_{i-\frac{1}{2}}}^{x_i} c_f \frac{q\,|q|}{h^2}\, dx + \int_{x_i}^{x_{i+\frac{1}{2}}} c_f \frac{q\,|q|}{h^2}\, dx \approx \tag{5.86}$$

$$\approx \frac{\Delta x_{i-\frac{1}{2}}}{2}\left(c_{f\,i-\frac{1}{4}} \frac{q_{i-\frac{1}{4}}\left|q_{i-\frac{1}{4}}\right|}{(h_{i-\frac{1}{4}})^2}\right) + \frac{\Delta x_{i+\frac{1}{2}}}{2}\left(c_{f\,i+\frac{1}{4}} \frac{q_{i+\frac{1}{4}}\left|q_{i+\frac{1}{4}}\right|}{(h_{i+\frac{1}{4}})^2}\right) \tag{5.87}$$

To avoid the discontinue derivative of the abs-function, this function is replaced by the following C^2-continue function:

$$|q| = F_{abs}(q) \approx \left(q^4 + \varepsilon^4\right)^{1/4}, \qquad \varepsilon = 0.01 \tag{5.88}$$

We first linearize the equation and then discretize/integrate in space. The linearization of the bed shear stress term around iteration level p reads expressed at $x_{i-\frac{1}{4}}$:

$$c_{f\,i-\frac{1}{4}} F_{abs}(q_{i-\frac{1}{4}}) \frac{q_{i-\frac{1}{4}}}{(h_{i-\frac{1}{4}})^2}\Bigg|^{n+\theta,p+1} \approx \tag{5.89}$$

$$\approx c_{f\,i-\frac{1}{4}} F_{abs}(q^{n+\theta,p}_{i-\frac{1}{4}}) \frac{q^{n+\theta,p}_{i-\frac{1}{4}}}{(h^{n+\theta,p}_{i-\frac{1}{4}})^2} +$$
$$+ c_{f\,i-\frac{1}{4}} \frac{\partial}{\partial q}\left\{F_{abs}(q^{n+\theta,p}_{i-\frac{1}{4}})\right\} \frac{q^{n+\theta,p}_{i-\frac{1}{4}}}{(h^{n+\theta,p}_{i-\frac{1}{4}})^2}\theta\Delta q^{n+1,p+1}_{i-\frac{1}{4}} +$$
$$+ c_{f\,i-\frac{1}{4}} F_{abs}(q^{n+\theta,p}_{i-\frac{1}{4}}) \frac{1}{(h^{n+\theta,p}_{i-\frac{1}{4}})^2}\theta\Delta q^{n+1,p+1}_{i-\frac{1}{4}} +$$
$$- c_{f\,i-\frac{1}{4}} F_{abs}(q^{n+\theta,p}_{i-\frac{1}{4}}) \frac{2q^{n+\theta,p}_{i-\frac{1}{4}}}{(h^{n+\theta,p}_{i-\frac{1}{4}})^3}\theta\Delta h^{n+1,p+1}_{i-\frac{1}{4}} \tag{5.90}$$

and

$$\frac{\partial}{\partial q}\left\{F_{abs}(q^{n+\theta,p}_{i-\frac{1}{4}})\right\} = (q^{n+\theta,p}_{i-\frac{1}{4}})^3\left(((q^{n+\theta,p}_{i-\frac{1}{4}})^4 + \varepsilon^4\right)^{-3/4} \tag{5.91}$$

The integral was split into two parts, both parts are integrated separately. For the left part ($x_{i-\frac{1}{4}}$) we use:

$$c_{f\,i-\frac{1}{4}} = \frac{1}{4}\left(c_{f\,i-1} + 3c_{f\,i}\right), \tag{5.92}$$
$$h^{n+\theta,p}_{i-\frac{1}{4}} = \frac{1}{4}\left(h^{n+\theta,p}_{i-1} + 3h^{n+\theta,p}_{i}\right), \tag{5.93}$$
$$q^{n+\theta,p}_{i-\frac{1}{4}} = \frac{1}{4}\left(q^{n+\theta,p}_{i-1} + 3q^{n+\theta,p}_{i}\right), \tag{5.94}$$

and for the right part ($x_{i+\frac{1}{4}}$) we use

$$c_{f\,i+\frac{1}{4}} = \frac{1}{4}\left(3c_{f\,i} + c_{f\,i+1}\right), \tag{5.95}$$
$$h^{n+\theta,p}_{i+\frac{1}{4}} = \frac{1}{4}\left(3h^{n+\theta,p}_{i} + h^{n+\theta,p}_{i+1}\right), \tag{5.96}$$
$$q^{n+\theta,p}_{i+\frac{1}{4}} = \frac{1}{4}\left(3q^{n+\theta,p}_{i} + q^{n+\theta,p}_{i+1}\right). \tag{5.97}$$

5.3.2.5 Viscosity

The viscosity term read:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(\nu h \frac{\partial(q/h)}{\partial x}\right)\,dx \;= \nu\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right)\Bigg|_{i+\frac{1}{2}} - \nu\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right)\Bigg|_{i-\frac{1}{2}} \tag{5.98}$$

The linearization of the viscosity term ($\nu = constant$) around iteration level p reads (see section D.1 for a derivation):

$$\nu\left(\frac{\partial q^{n+\theta,p+1}_{i+\frac{1}{2}}}{\partial x} - \frac{q^{n+\theta,p+1}_{i+\frac{1}{2}}}{h^{n+\theta,p+1}_{i+\frac{1}{2}}}\frac{\partial h^{n+\theta,p+1}_{i+\frac{1}{2}}}{\partial x}\right) \approx \tag{5.99}$$

$$\begin{aligned}
&\approx \nu\frac{\partial q^{n+\theta,p}_{i+\frac{1}{2}}}{\partial x} - \nu\frac{q^{n+\theta,p}_{i+\frac{1}{2}}}{h^{n+\theta,p}_{i+\frac{1}{2}}}\frac{\partial h^{n+\theta,p}_{i+\frac{1}{2}}}{\partial x} + \\
&+ \theta\underbrace{\nu}_{\mathcal{A}}\frac{\partial \Delta q^{n+1p+1}_{i+\frac{1}{2}}}{\partial x} - \theta\underbrace{\nu\frac{1}{h^{n+\theta,p}}\frac{\partial h^{n+\theta,p}_{i+\frac{1}{2}}}{\partial x}}_{\mathcal{B}}\Delta q^{n+1p+1}_{i+\frac{1}{2}} + \\
&+ \theta\underbrace{\nu\frac{q^{n+\theta,p}_{i+\frac{1}{2}}}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2}\frac{\partial h^{n+\theta,p}_{i+\frac{1}{2}}}{\partial x}}_{\mathcal{C}}\Delta h^{n+1p+1}_{i+\frac{1}{2}} - \theta\underbrace{\nu\frac{q^{n+\theta,p}_{i+\frac{1}{2}}}{h^{n+\theta,p}_{i+\frac{1}{2}}}}_{\mathcal{D}}\frac{\partial \Delta h^{n+1,p+1}_{i+\frac{1}{2}}}{\partial x}
\end{aligned} \tag{5.100}$$

where $\theta\mathcal{A}$, $\theta\mathcal{B}$, $\theta\mathcal{C}$ and $\theta\mathcal{D}$ are coefficients in the matrix of the Δ-formulation. For the part at $x_{i-\frac{1}{2}}$ a similar expression is feasible.

5.3.3 Discretizations at boundary

For the 1D linear wave equations (Equation (5.1)) at each boundary one boundary condition need to be prescribed, that is the ingoing wave, called **essential** boundary condition (Dirichlet or Neumann condition). And one boundary condition to handle the outgoing wave, called **natural** boundary condition.

The boundary conditions are presented for the left/west boundary. First the **natural** boundary is discussed and after that the **essential** boundary condition. A similar derivation can be given for right/east boundary.

The **essential** boundary condition is to be assumed somewhere in the first control volume, ($x_{i_{bc}}$ with $i_{bc} \in [i-\frac{1}{2}, i+\frac{1}{2}]$). For simplicity the boundary condition is chosen to be on node $i = 1$ (location x_1).

5.3.3.1 Natural boundary condition

The **natural** boundary condition for the left/west boundary, describing the undisturbed outgoing wave, reads (Equation (5.59)):

$$-\left(\sqrt{gh}+\frac{q}{h}\right)\underbrace{\left(\frac{\partial h}{\partial t}+\frac{\partial q}{\partial x}+\dots\right)}_{\text{continuity eq.}}+\underbrace{\left(\frac{\partial q}{\partial t}+gh\frac{\partial \zeta}{\partial x}+\dots\right)}_{\text{momentum eq.}}=0 \tag{5.101}$$

For the **natural** boundary the values at the boundary ($x_{i+\frac{1}{2}}$ with $i=0$) of h and q are computed as follows:

$$\begin{aligned} h_{i+\frac{1}{2}} &= \frac{1}{2}\left(h_i+h_{i+1}\right)+\frac{\alpha_{bnd}}{2}\left(h_i-2h_{i+1}+h_{i+2}\right)\\ &= \frac{1}{2}\left(1+\alpha_{bnd}\right)h_i+\frac{1}{2}\left(1-2\alpha_{bnd}\right)h_{i+1}+\frac{1}{2}\alpha_{bnd}h_{i+2} \end{aligned} \tag{5.102}$$

$$\begin{aligned} q_{i+\frac{1}{2}} &= \frac{1}{2}\left(q_i+q_{i+1}\right)+\frac{\alpha_{bnd}}{2}\left(q_i-2q_{i+1}+q_{i+2}\right)\\ &= \frac{1}{2}\left(1+\alpha_{bnd}\right)q_i+\frac{1}{2}\left(1-2\alpha_{bnd}\right)q_{i+1}+\frac{1}{2}\alpha_{bnd}q_{i+2} \end{aligned} \tag{5.103}$$

Time derivative, continuity equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i=0$) the time discretization of the continuity equation for the **natural** boundary condition, describing the outgoing wave, reads:

$$\frac{\partial h}{\partial t}\approx\frac{1}{\Delta t}\left(h^{n+1}_{i+\frac{1}{2}}-h^{n}_{i+\frac{1}{2}}\right) \tag{5.104}$$

A diffusion like term is added to the boundary equation to damp the reflection of spurious waves. A coefficient α_{bnd} is placed before that extra term, the optimal value of this coefficient is taken from the analysis in *Reference not yet known* (n.d.).

$$\begin{aligned} &\frac{1}{\Delta t}\left(\frac{1}{2}\left(h_i^{n+1,p+1}+h_{i+1}^{n+1,p+1}\right)+\frac{\alpha_{bnd}}{2}\left(h_i^{n+1,p+1}-2h_{i+1}^{n+1,p+1}+h_{i+2}^{n+1,p+1}\right)+\right.\\ &\qquad\left.-\left(\frac{1}{2}\left(h_i^n+h_{i+1}^n\right)+\frac{\alpha_{bnd}}{2}\left(h_i^n-2h_{i+1}^n+h_{i+2}^n\right)\right)\right) \end{aligned} \tag{5.105}$$

After rearranging the equation into an implicit and an explicit part it reads:

$$\begin{aligned} &\frac{1}{\Delta t}\left(\frac{1}{2}\left(\Delta h_i^{n+1,p+1}+\Delta h_{i+1}^{n+1,p+1}\right)+\right.\\ &\qquad\left.+\frac{\alpha_{bnd}}{2}\left(\Delta h_i^{n+1,p+1}-2\Delta h_{i+1}^{n+1,p+1}+\Delta h_{i+2}^{n+1,p+1}\right)\right)+\\ &\qquad+\frac{1}{\Delta t}\left\{\frac{1}{2}\left(h_i^{n+1,p}+h_{i+1}^{n+1,p}\right)+\frac{\alpha_{bnd}}{2}\left(h_i^{n+1,p}-2h_{i+1}^{n+1,p}+h_{i+2}^{n+1,p}\right)+\right.\\ &\qquad\left.-\left(\frac{1}{2}\left(h_i^n+h_{i+1}^n\right)+\frac{\alpha_{bnd}}{2}\left(h_i^n-2h_{i+1}^n+h_{i+2}^n\right)\right)\right\} \end{aligned} \tag{5.106}$$

Mass flux, continuity equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i = 0$) the discretization of the mass flux for the **natural** boundary condition, describing the outgoing wave, reads:

$$\frac{\partial q}{\partial x} \approx \frac{1}{\Delta x}\left(q_{i+1}^{n+\theta,p+1} - q_i^{n+\theta,p+1}\right) \tag{5.107}$$

which will be approximated by

$$\frac{1}{\Delta x}\left(\left(q_{i+1}^{n+\theta,p} + \theta\Delta q_{i+1}^{n+1,p+1}\right) - \left(q_i^{n+\theta,p+1} + \theta\Delta q_i^{n+1,p+1}\right)\right) \tag{5.108}$$

$$\Leftrightarrow \tag{5.109}$$

$$\frac{\theta}{\Delta x}\left(\Delta q_{i+1}^{n+1,p+1} - \Delta q_i^{n+1,p+1}\right) + \frac{1}{\Delta x}\left\{q_{i+1}^{n+\theta,p} - q_i^{n+\theta,p+1}\right\} \tag{5.110}$$

Time derivative, momentum equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i = 0$) the time discretization of the momentum equation for the **natural** boundary condition, describing the outgoing wave, reads:

$$\frac{\partial q}{\partial t} \approx \frac{1}{\Delta t}\left(q_{i+\frac{1}{2}}^{n+1} - q_{i+\frac{1}{2}}^{n}\right) \tag{5.111}$$

A diffusion like term is added to the boundary equation to damp the reflection of spurious waves. A coefficient α_{bnd} is placed before that extra term, the optimal value of this coefficient is taken from the analysis in *Reference not yet known* (n.d.).

$$\begin{aligned}\frac{1}{\Delta t}\Bigg(&\frac{1}{2}\left(q_i^{n+1,p+1} + q_{i+1}^{n+1,p+1}\right) + \frac{\alpha_{bnd}}{2}\left(q_i^{n+1,p+1} - 2q_{i+1}^{n+1,p+1} + q_{i+2}^{n+1,p+1}\right) + \\ &- \left(\frac{1}{2}\left(q_i^n + q_{i+1}^n\right) + \frac{\alpha_{bnd}}{2}\left(q_i^n - 2q_{i+1}^n + q_{i+2}^n\right)\right)\Bigg)\end{aligned} \tag{5.112}$$

After rearranging the equation into an implicit and an explicit part it reads:

$$\begin{aligned}\frac{1}{\Delta t}\Bigg(&\frac{1}{2}\left(\Delta q_i^{n+1,p+1} + \Delta q_{i+1}^{n+1,p+1}\right) + \\ &+ \frac{\alpha_{bnd}}{2}\left(\Delta q_i^{n+1,p+1} - 2\Delta q_{i+1}^{n+1,p+1} + \Delta q_{i+2}^{n+1,p+1}\right)\Bigg) + \\ &+ \frac{1}{\Delta t}\left\{\frac{1}{2}\left(q_i^{n+1,p} + q_{i+1}^{n+1,p}\right) + \frac{\alpha_{bnd}}{2}\left(q_i^{n+1,p} - 2q_{i+1}^{n+1,p} + q_{i+2}^{n+1,p}\right) + \right. \\ &\left. - \frac{1}{2}\left(q_i^n + q_{i+1}^n\right) - \frac{\alpha_{bnd}}{2}\left(q_i^n - 2q_{i+1}^n + q_{i+2}^n\right)\right\}\end{aligned} \tag{5.113}$$

Pressure term, momentum equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i = 0$) the discretization of the pressure term for the **natural** boundary condition, describing the outgoing wave, reads:

$$gh\frac{\partial \zeta}{\partial x} \approx gh_{i+\frac{1}{2}}^{n+\theta,p+1}\frac{\partial}{\partial x}\left(\zeta_{i+\frac{1}{2}}^{n+\theta,p+1}\right) \tag{5.114}$$

In a formulation of the shallow-water equations, where the equation for the free-surface level ζ reduces to $\zeta = h + z_b$ (excluding drying and flooding), the equations can be simplified, because $\Delta\zeta = \Delta h$ (when z_b is not time dependent). In this case, the contributions to the $\Delta\zeta$-equations need to be incorporated in the Δh-equations. The pressure term will then be approximated by

$$\begin{aligned}
&\frac{1}{\Delta x} g h^{n+\theta,p}_{i+\frac{1}{2}} \left(\zeta^{n+\theta,p}_{i+1} - \zeta^{n+\theta,p}_{i}\right) + \\
&\quad + \frac{1}{\Delta x} g \left(\zeta^{n+\theta,p}_{i+1} - \zeta^{n+\theta,p}_{i}\right) \theta \Delta h^{n+1,p+1}_{i+\frac{1}{2}} + \\
&\quad + \frac{1}{\Delta x} g h^{n+\theta,p}_{i+\frac{1}{2}} \theta \left(\Delta\zeta^{n+1,p+1}_{i+1} - \Delta\zeta^{n+1,p+1}_{i}\right)
\end{aligned} \tag{5.115}$$

After rearranging the equation into an implicit and an explicit part it reads:

$$\begin{aligned}
&\frac{1}{\Delta x} g \left(\zeta^{n+\theta,p}_{i+1} - \zeta^{n+\theta,p}_{i}\right) \theta \Delta h^{n+1,p+1}_{i+\frac{1}{2}} + \frac{1}{\Delta x} g h^{n+\theta,p}_{i+\frac{1}{2}} \theta \left(\Delta\zeta^{n+1,p+1}_{i+1} - \Delta\zeta^{n+1,p+1}_{i}\right) + \\
&\quad + \left\{ \frac{1}{\Delta x} g h^{n+\theta,p}_{i+\frac{1}{2}} \left(\zeta^{n+\theta,p}_{i+1} - \zeta^{n+\theta,p}_{i}\right) \right\}
\end{aligned} \tag{5.116}$$

Convection term, momentum equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i = 0$) the discretization of the convection term for the **natural** boundary condition, describing the outgoing wave, reads:

$$\begin{aligned}
\frac{\partial q^2/h}{\partial x} &= \frac{2q}{h}\frac{\partial q}{\partial x} - \frac{q^2}{h^2}\frac{\partial h}{\partial x} \approx \\
&\approx \frac{2q^{n+\theta,p+1}_{i+\frac{1}{2}}}{h^{n+\theta,p+1}_{i+\frac{1}{2}}} \frac{\partial q^{n+\theta,p+1}_{i+\frac{1}{2}}}{\partial x} - \frac{(q^{n+\theta,p+1}_{i+\frac{1}{2}})^2}{(h^{n+\theta,p+1}_{i+\frac{1}{2}})^2} \frac{\partial h^{n+\theta,p+1}_{i+\frac{1}{2}}}{\partial x}
\end{aligned} \tag{5.117}$$

which will be approximated by

$$\begin{aligned}
&\left.\frac{2q}{h}\frac{\partial q}{\partial x}\right|_{i+\frac{1}{2}} - \left.\frac{q^2}{h^2}\frac{\partial h}{\partial x}\right|_{i+\frac{1}{2}} \approx \\
&\quad \approx \underbrace{\frac{2q^{n+\theta,p}_{i+\frac{1}{2}}}{h^{n+\theta,p}_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(q^{n+\theta,p}_{i+\frac{1}{2}}\right) - \frac{(q^{n+\theta,p}_{i+\frac{1}{2}})^2}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2} \frac{\partial}{\partial x}\left(h^{n+\theta,p}_{i+\frac{1}{2}}\right)}_{\textit{to right handside}} + \\
&\quad + \theta \underbrace{\left(-\frac{2q^{n+\theta,p}_{i+\frac{1}{2}}}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2} \frac{\partial}{\partial x}\left(q^{n+\theta,p}_{i+\frac{1}{2}}\right) + \frac{2(q^{n+\theta,p}_{i+\frac{1}{2}})^2}{(h^{n+\theta,p}_{i+\frac{1}{2}})^3} \frac{\partial}{\partial x}\left(h^{n+\theta,p}_{i+\frac{1}{2}}\right) \right)}_{\mathcal{A}} \Delta h^{n+1,p+1}_{i+\frac{1}{2}} + \\
&\quad + \theta \underbrace{\left(\frac{2}{h^{n+\theta,p}_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(q^{n+\theta,p}_{i+\frac{1}{2}}\right) - \frac{2q^{n+\theta,p}_{i+\frac{1}{2}}}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2} \frac{\partial}{\partial x}\left(h^{n+\theta,p}_{i+\frac{1}{2}}\right) \right)}_{\mathcal{B}} \Delta q^{n+1,p+1}_{i+\frac{1}{2}} +
\end{aligned} \tag{5.118}$$

$$+\theta\underbrace{\left(-\frac{(q^{n+\theta,p}_{i+\frac{1}{2}})^2}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2}\right)}_{\mathcal{C}}\frac{\partial}{\partial x}\left(\Delta h^{n+1,p+1}_{i+\frac{1}{2}}\right)+\theta\underbrace{\frac{2q^{n+\theta,p}_{i+\frac{1}{2}}}{h^{n+\theta,p}_{i+\frac{1}{2}}}}_{\mathcal{D}}\frac{\partial}{\partial x}\left(\Delta q^{n+1,p+1}_{i+\frac{1}{2}}\right) \tag{5.119}$$

where $\theta\mathcal{A}$, $\theta\mathcal{B}$, $\theta\mathcal{C}$ and $\theta\mathcal{D}$ are coefficients in the matrix of the Δ-formulation.

Bed shear stress term, momentum equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i=0$) the discretization of the bed shear stress term for the **natural** boundary condition, describing the outgoing wave, reads:

$$c_f\frac{q\,|q|}{h^2}\approx c_{f\,i+\frac{1}{2}}\frac{q^{n+\theta,p+1}_{i+\frac{1}{2}}\left|q^{n+\theta,p+1}_{i+\frac{1}{2}}\right|}{(h^{n+\theta,p+1}_{i+\frac{1}{2}})^2} \tag{5.120}$$

To avoid the discontinue derivative of the abs-function, this function is replaced by a C^2-continue function (Equation (5.88))

$$|q|\approx F_{abs}(q)=\left(q^4+\varepsilon^4\right)^{1/4},\qquad \varepsilon=0.01 \tag{5.121}$$

which will be approximated by

$$\begin{aligned}&c_{f\,i+\frac{1}{2}}\frac{q^{n+\theta,p}_{i+\frac{1}{2}}F_{abs}(q^{n+\theta,p}_{i+\frac{1}{2}})}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2}+\\
&\quad+c_{f\,i+\frac{1}{2}}\frac{F_{abs}(q^{n+\theta,p}_{i+\frac{1}{2}})}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2}\theta\Delta q^{n+1,p+1}_{i+\frac{1}{2}}+\\
&\quad+c_{f\,i+\frac{1}{2}}\frac{q^{n+\theta,p}_{i+\frac{1}{2}}}{(h^{n+\theta,p}_{i+\frac{1}{2}})^2}\frac{\partial}{\partial q}\left(F_{abs}(q^{n+\theta,p}_{i+\frac{1}{2}})\right)\theta\Delta q^{n+1,p+1}_{i+\frac{1}{2}}+\\
&\quad-c_{f\,i+\frac{1}{2}}\frac{2q^{n+\theta,p}_{i+\frac{1}{2}}F_{abs}(q^{n+\theta,p}_{i+\frac{1}{2}})}{(h^{n+\theta,p}_{i+\frac{1}{2}})^3}\theta\Delta h^{n+1,p+1}_{i+\frac{1}{2}}\end{aligned} \tag{5.122}$$

with

$$\frac{\partial}{\partial q}\left(F_{abs}(q^{n+\theta,p}_{i+\frac{1}{2}})\right)=(q^{n+\theta,p}_{i+\frac{1}{2}})^3\left((q^{n+\theta,p}_{i+\frac{1}{2}})^4+\varepsilon^4\right)^{-3/4} \tag{5.123}$$

Viscosity term, momentum equation

At the left/west boundary ($x_{i+\frac{1}{2}}$ with $i=0$) the discretization of the viscosity term for the **natural** boundary condition, describing the outgoing wave, reads:

Remark:

- Strictly spoken there is no separation between left and right going waves when there is a viscosity term.

$$\frac{\partial}{\partial x}\left(\nu h \frac{\partial (q/h)}{\partial x}\right) = \tag{5.124}$$

$$= \frac{\partial \nu}{\partial x}\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right) + \nu \frac{\partial h}{\partial x}\left(\frac{1}{h}\frac{\partial q}{\partial x} - \frac{q}{h^2}\frac{\partial h}{\partial x}\right) +$$

$$-\nu \frac{1}{h}\frac{\partial q}{\partial x}\frac{\partial h}{\partial x} + \nu \frac{\partial^2 q}{\partial x^2} - \nu \frac{1}{h}\frac{\partial h}{\partial x}\frac{\partial q}{\partial x} - \nu \frac{2q}{h^2}\frac{\partial h}{\partial x}\frac{\partial h}{\partial x} + \nu \frac{q}{h}\frac{\partial^2 h}{\partial x^2} \tag{5.125}$$

which will be approximated by the following discretizations:

$$\frac{\partial \nu}{\partial x} \approx \frac{\nu_{i+1} - \nu_i}{\Delta x} \tag{5.126}$$

$$\frac{\partial q}{\partial x} \approx \frac{q_{i+1}^{n+\theta,p+1} - q_i^{n+\theta,p+1}}{\Delta x} \tag{5.127}$$

$$\frac{\partial h}{\partial x} \approx \frac{h_{i+1}^{n+\theta,p+1} - h_i^{n+\theta,p+1}}{\Delta x} \tag{5.128}$$

$$\frac{\partial^2 q}{\partial x^2} \approx \frac{q_{i-1}^{n+\theta,p+1} - 2q_i^{n+\theta,p+1} + q_{i+1}^{n+\theta,p+1}}{\Delta x} \tag{5.129}$$

$$\frac{\partial^2 h}{\partial x^2} \approx \frac{h_{i-1}^{n+\theta,p+1} - 2h_i^{n+\theta,p+1} + h_{i+1}^{n+\theta,p+1}}{\Delta x} \tag{5.130}$$

TODO 5.2: *Natural boundary: viscosity term* ***TODO***

5.3.3.2 Essential boundary condition

The **essential** boundary condition is to be assumed somewhere in the first control volume, ($x_{i_{bc}}$ with $i_{bc} \in [i-\frac{1}{2}, i+\frac{1}{2}]$). For simplicity the boundary condition is chosen to be on node $i = 1$ (location x_1).

The **essential** boundary condition for the left/west boundary at x_1 reads, describing the ingoing wave (indicated with h^+, q^+) with as less as possible disturbing the outgoing wave (Equation (5.59)):

$$\left(\sqrt{gh} - \frac{q}{h}\right)\frac{\partial h^+}{\partial t} + \frac{\partial q^+}{\partial t} = F(t) \tag{5.131}$$

$$\left(\sqrt{gh} + \frac{q}{h}\right)\frac{\partial h^+}{\partial t} - \frac{\partial q^+}{\partial t} = 0 \tag{5.132}$$

Equation (5.132) means that the ingoing wave does not disturb the outgoing wave.

The essential boundary condition for the right/east boundary at $x_{I+\frac{1}{2}}$ reads, describing the ingoing wave (indicated with h^-, q^-) with as less as possible disturbing the outgoing wave (Equation (5.59)):

$$\left(\sqrt{gh} + \frac{q}{h}\right)\frac{\partial h^-}{\partial t} - \frac{\partial q^-}{\partial t} = G(t) \tag{5.133}$$

$$\left(\sqrt{gh} - \frac{q}{h}\right)\frac{\partial h^-}{\partial t} + \frac{\partial q^-}{\partial t} = 0 \tag{5.134}$$

Equation (5.134) means that the ingoing wave does not disturb the outgoing wave.

Given water level at left/west boundary

Adding the equations ((5.131) + (5.132)) yields

$$2\sqrt{gh}\frac{\partial h}{\partial t} = F(t) \tag{5.135}$$

So the essential boundary condition for incoming signal (if $\partial z_b/\partial t = 0$) reads

$$\boxed{\left(\sqrt{gh} - \frac{q}{h}\right)\frac{\partial h^+}{\partial t} + \frac{\partial q^+}{\partial t} = 2\sqrt{gh}\frac{\partial \zeta_{given}}{\partial t} + \varepsilon(\zeta_{given} - \zeta)} \tag{5.136}$$

a correction term is added, to prevent drifting away of the solution (an integration constant is missing). The variable ε has dimension $[\mathrm{m\,s^{-2}}]$.

The discretization of boundary Equation (5.136) at $x = i + \frac{1}{2}$ reads

$$\begin{aligned}&\left(\sqrt{gh^{n+\theta,p+1}} - \frac{q^{n+\theta,p+1}}{h^{n+\theta,p+1}}\right)\frac{\partial h^+}{\partial t} + \frac{\partial q^+}{\partial t} = \\ &= 2\sqrt{gh^{n+\theta,p+1}}\frac{\partial \zeta_{given}}{\partial t} + \varepsilon\left((\zeta_{given} - z_b) - h^{n+1,p}\right)\end{aligned} \tag{5.137}$$

Given water flux at left/west boundary

Subtracting the equations ((5.131) − (5.132)), yields:

$$-2\frac{q}{h}\frac{\partial h}{\partial t} + 2\frac{\partial q}{\partial t} = F(h, q, t) \tag{5.138}$$

and using Equation (5.132) (ingoing information does not disturb outgoing information)

$$\left(\sqrt{gh} + \frac{q}{h}\right)\frac{\partial h}{\partial t} - \frac{\partial q}{\partial t} = 0 \tag{5.139}$$

$$\frac{\partial h}{\partial t} = \frac{1}{\sqrt{gh} + \frac{q}{h}}\frac{\partial q}{\partial t} \tag{5.140}$$

So the essential boundary condition for incoming signal reads

$$\left(\sqrt{gh} - \frac{q}{h}\right)\frac{\partial h^+}{\partial t} + \frac{\partial q^+}{\partial t} = -2\frac{q}{h}\frac{\partial h}{\partial t} + 2\frac{\partial q}{\partial t} \tag{5.141}$$

substituting Equation (5.134) into the right hand side, yields

$$\boxed{\left(\sqrt{gh} - \frac{q}{h}\right)\frac{\partial h^+}{\partial t} + \frac{\partial q^+}{\partial t} = 2\left(\frac{\sqrt{gh}}{\sqrt{gh} + \frac{q}{h}}\right)\frac{\partial q_{given}}{\partial t} + \varepsilon(q_{given} - q)} \tag{5.142}$$

a correction term is added, to prevent drifting away of the solution (an integration constant is missing). The variable ε has dimension $[\mathrm{s}^{-1}]$. The discretization of boundary Equation (5.142) at $x = i + \frac{1}{2}$ reads

$$
\begin{aligned}
&\left(\sqrt{gh^{n+\theta,p+1}} - \frac{q^{n+\theta,p+1}}{h^{n+\theta,p+1}}\right)\frac{\partial h}{\partial t} + \frac{\partial q}{\partial t} = \\
&= 2\left(\frac{\sqrt{gh^{n+\theta,p+1}}}{\sqrt{gh^{n+\theta,p+1}} + \frac{q^{n+\theta,p+1}}{h^{n+\theta,p+1}}}\right)\frac{\partial q_{given}}{\partial t} + \varepsilon\left(q_{given} - q^{n+1,p}\right)
\end{aligned}
\tag{5.143}
$$

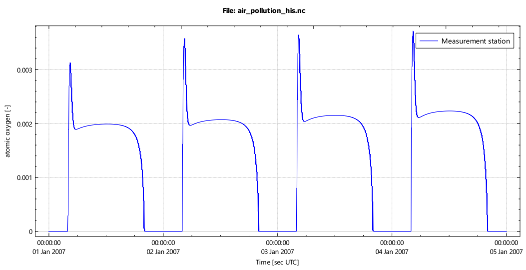
6 Numerical experiments

6.1 0-D, sources and sinks

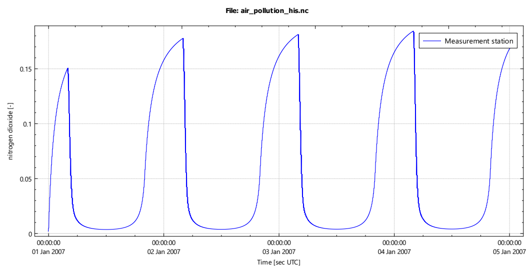
In this section the numerical results are given for the 0-dimensional air pollution example as described in section 5.1.1 and for the Brusselator, as described in section 5.1.2.

6.1.1 Air pollution

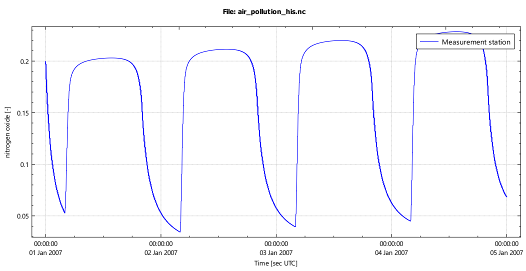
Some numerical results of the air pollution example (section 5.1.1) is:



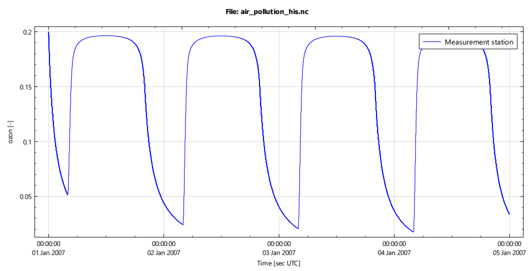
(a) *Concentration of Atomic Oxygen.*



(b) *Concentration of Nitrogen Dioxide.*



(c) *Concentration of Nitrogen Oxide.*



(d) *Concentration of Ozon.*

Figure 6.1: *Result plots of the different constituents, compute with the fully implicit time integration method with a time step of* 0.5 [s].

Different time integrators

Numerical stability for different values of Δt are studied for Euler-explicit, Runga-Kutta-4 and the fully implicit Δ-formulation.

Table 6.1: Stability for different time integrators

	Time step [s]	Euler explicit	Runge-Kutta 4	Fully Implicit Δ-formulation
1	0.5	-	✓	✓
2	60	✓	✓	✓
3	120	Unstable	✓	✓
4	180	-	Unstable	✓
5	240	-	-	✓
6	300	-	-	✓
7	900	-	-	✓
8	1800	-	-	✓
9	3600	-	-	✓

6.1.2 Brusselator

Some numerical results of the brusselator example (section 5.1.2) is:

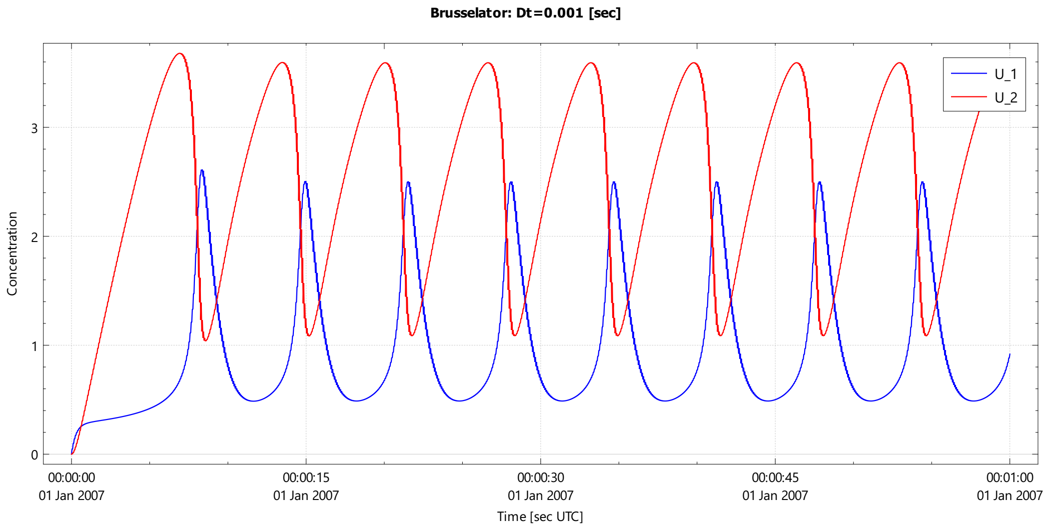
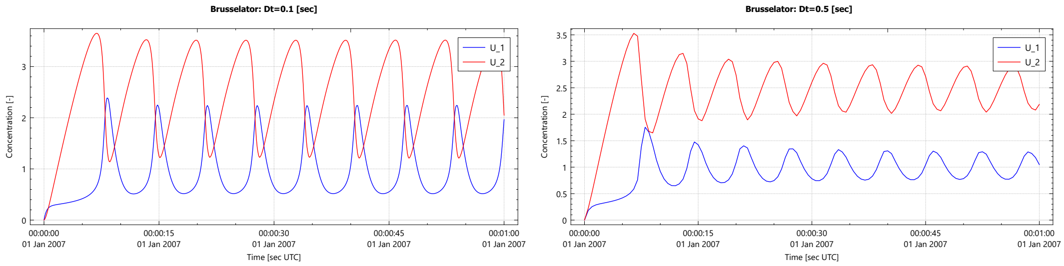


Figure 6.2: *Fully Implicit:* $\Delta t = 0.001$ [s], $k_1 = 1$, $k_2 = 2.5$.

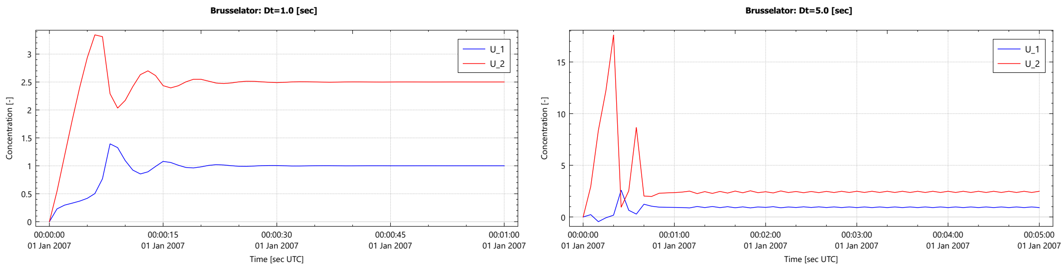
The solution presented in Figure 6.2 is assumed to be the reference (analytic) solution of Equation (5.32).



(a) Fully Implicit: $\Delta t = 0.1$, $k_1 = 1$, $k_2 = 2.5$ *(b) Fully Implicit:* $\Delta t = 0.5$, $k_1 = 1$, $k_2 = 2.5$

Figure 6.3: *Result plots for constant value of* $k_1 = 1$ *and* $k_2 = 2.5$*, computed with a fully implicit (*Δ *formulation) time integration method for different time steps* $\Delta t = 0.1, 0.5$ [s].

Extra attention is needed for the Fully Implicit time integration with larger time step:



(a) Fully Implicit: $\Delta t = 1.0$, $k_1 = 1$, $k_2 = 2.5$ *(b) Fully Implicit:* $\Delta t = 5.0$, $k_1 = 1$, $k_2 = 2.5$

Figure 6.4: *Result plots for constant value of* $k_1 = 1$ *and* $k_2 = 2.5$*, computed with a fully implicit (*Δ *formulation) time integration method for different time steps* $\Delta t = 1.0, 5.0$ [s].

Figure 6.4a converge to the equilibrium state $(u_1, u_2) = (1.0, 2.5)$ and Figure 6.4b looks to converge to the equilibrium state $(u_1, u_2) = (1.0, 2.5)$ but is still wiggling after 5 [min] of simulation time (even after one day — not presented here). How these equations are discretized is given in Equation (5.1.2).

Different time integrators

Numerical stability for different values of Δt are studied for the Runga-Kutta-4 and fully implicit Δ-formulation.

Table 6.2: *Stability of different time integrators for the Brusselator.*

	Time step [s]	**Runge-Kutta 4**	**Fully Implicit** Δ**-formulation**
1	0.1	✓	✓

	Time step [s]	Runge-Kutta 4	Fully Implicit Δ-formulation
2	0.2	✓	✓
3	0.5	✓	✓
4	1.0	Unstable	✓
5	2.0		✓
6	5.0		✓

6.2 1-D Advection equation

The considered advection equation reads:

$$\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} = 0, \tag{6.1}$$

With a velocity of $u = 10\,[\mathrm{m\,s^{-1}}]$, which coincide with the wave celerity of the 1D-wave numerical experiments as described in section 6.4.1.

$$u(x,t) = 10\,[\mathrm{m\,s^{-1}}] \tag{6.2}$$

and with a prescribed boundary condition at the left side of the domain

$$c(0,t) = f_c(t). \tag{6.3}$$

6.2.1 Transport of a constant constituent at the boundary

The prescribed boundary condition for the constituent reads

$$c(0,t) = c_{given} \begin{cases} \frac{1}{2}\left(\cos\left(\pi \frac{t_{reg}-t}{t_{reg}}\right) + 1\right) & \text{if } t < t_{reg}, \\ 1 & \text{if } t \geq t_{reg}, \end{cases} \tag{6.4}$$

where

t_{reg} The regularization time for the given time-series, [s]

Numerical experiment

The numerical experiment is performed with the following parameters:

- Length of the domain, $L_x = 12\,000$ [m]
- Grid size, $\Delta x = 10$ [m]
- Start time, $t_{start} = 0$ [s]
- End time, $t_{stop} = 3600$ [s]
- Timestep, $\Delta t = 5$ [s]
- Regularization time for time-series, $t_{reg} = 600$ [s]
- Prescribed constant velocity, $u_{given}(x,t) = 10\,[\mathrm{m\,s^{-1}}]$

- Prescribed initial value of the constituent, $c(x, 0) = 0$ [−].
- Prescribed constituent on boundary at $x = 0$ is given by Equation (6.4).
- No boundary is prescribed at $x = 12\,000$ [m].

Results of the numerical experiments

A map picture at $t = 3600$ [s] and time-series are given for this experiment. As seen from the map figure there are very small spurious waves traveling from right to left. These spurious waves are fully generated by the numerical scheme at the right boundary, because the continuous advection equation does **not** allow information traveling from right to left.

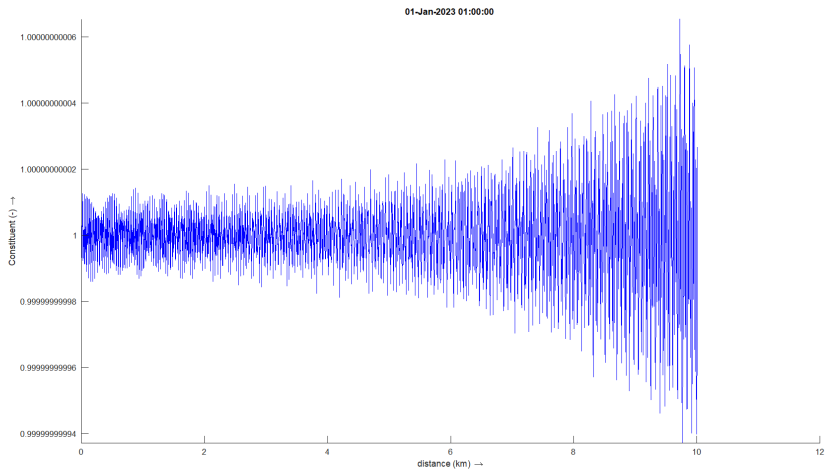


Figure 6.5: *Spurious waves at* $t = 3600$ [s]. *Range from* $1 \pm 8 \times 10^{-9}$

Results for several observation stations along the channel are shown in Figure 6.6

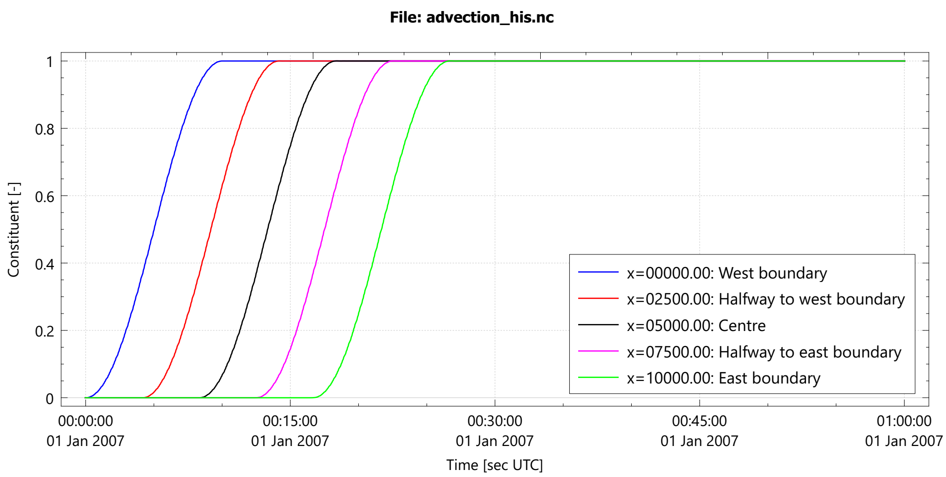


Figure 6.6: *Time-series for several stations in the model, showing the transition behavior between the initial situation and the time-independent solution.*

6.2.2 Transport of a time-dependent constituent at the boundary

The prescribed boundary condition for the constituent reads

$$c(0,t) = c_{given} \begin{cases} \frac{1}{2}\left(\cos\left(\pi\frac{t_{reg}-t}{t_{reg}}\right)+1\right) & \text{if } t < t_{reg}, \\ -\cos\left(\pi\frac{t}{t_{reg}}\right) & \text{if } t \geq t_{reg}, \end{cases} \tag{6.5}$$

where

t_{reg} The regularization time for the given time-series, [s]

Numerical experiment

The numerical experiment is performed with the following parameters:

- Length of the domain, $12\,000$ [m]
- Grid size, $\Delta x = 10$ [m]
- Start time, $t_{start} = 0$ [s]
- End time, $t_{stop} = 3600$ [s]
- Timestep, $\Delta t = 10$ [s]
- Regularization time for time-series, $t_{reg} = 600$ [s]
- Prescribed constant velocity, $u_{given}(x,t) = 10$ [$\mathrm{m\,s^{-1}}$]
- Prescribed initial value of the constituent, $c(x,0) = 0$ [$-$].
- Prescribed constituent on boundary at $x = 0$ is given by Equation (6.4).
- No boundary is prescribed at $x = 12\,000$ [m].

Results of the numerical experiments

Results for several observation stations along the channel are shown in Figure 6.7:

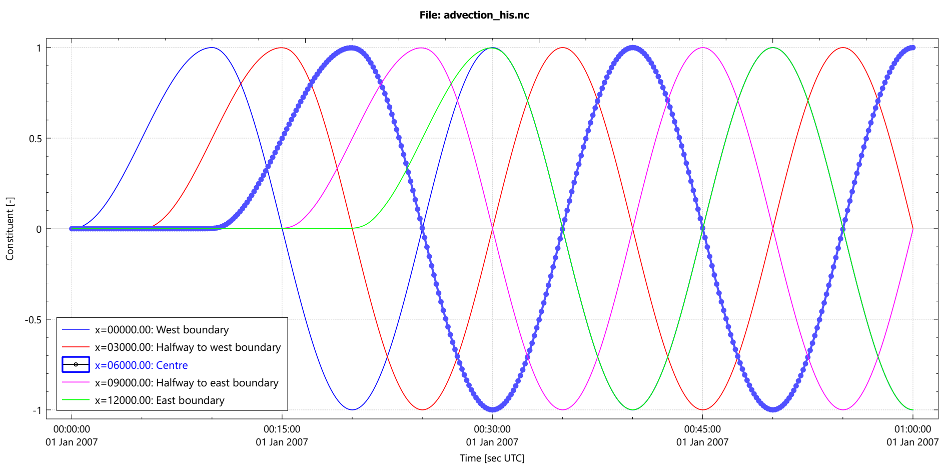


Figure 6.7: *Time-series for several stations in the model, showing the transition behavior between the initial situation and the time-independent solution.*

6.2.3 Transport of a wave package inside the domain

The initial condition are computed as described in section 3.4 and is illustrated in Figure 6.8:

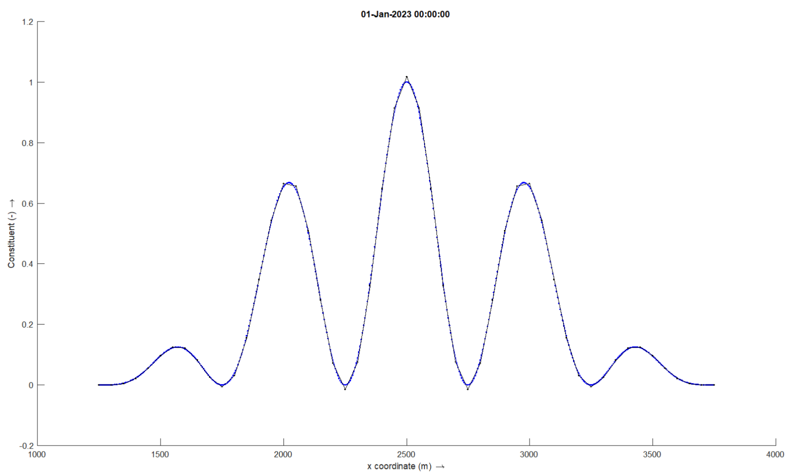


Figure 6.8: *Compatible initial condition of the wave package. Blue: Initial condition when* $\Delta x = 5$ [m]*, Black: Initial condition when* $\Delta x = 50$ [m]

The graphs in Figure 6.8 do not coincide on the grid points because the profiles are computed according section 3.4. The initial condition is defined by:

$$u_{itgiven} = \begin{cases} 0, & 0 < 1250, [\mathrm{m}] \\ (\frac{1}{2} + \frac{1}{2}\cos(5k_{env}(x - x_{cent}))) & \\ \qquad (\frac{1}{2} + \frac{1}{2}\cos(k_{env}(x - x_{cent}))) & 1250 < 3750, [\mathrm{m}] \\ 0, & 3750 < 10000, [\mathrm{m}] \end{cases} \tag{6.6}$$

with

x_{cent}	Location of the centre of the envelope.
L_{env}	Length of the envelope.
k_{env}	$k_{env} = 2\pi/L_{env}$.

Numerical experiment

The numerical experiment is performed with the following parameters:

- Length of the domain $L_x = 10\,000$ [m].
- Length of the envelope 2500 [m], ranging from 1250 [m] to 3750 [m].
- Grid size and time step,
  - $\Delta x = 5$ [m] and $\Delta t = 0.01$ [s]
  - $\Delta x = 10$ [m] and $\Delta t = 0.01$ [s]
  - $\Delta x = 25$ [m] and $\Delta t = 0.01$ [s]

– $\Delta x = 50$ [m] and $\Delta t = 0.01$ [s]

- Start time, $t_{start} = 0$ [s].
- End time, $t_{stop} = 250$ [s].
- Prescribed boundary conditions: $c(0,t) = c(L_x,t) = 0$.
- **No** regularization applied.

Results of the numerical experiments

Results for the four different computations are shown in Figure 6.9

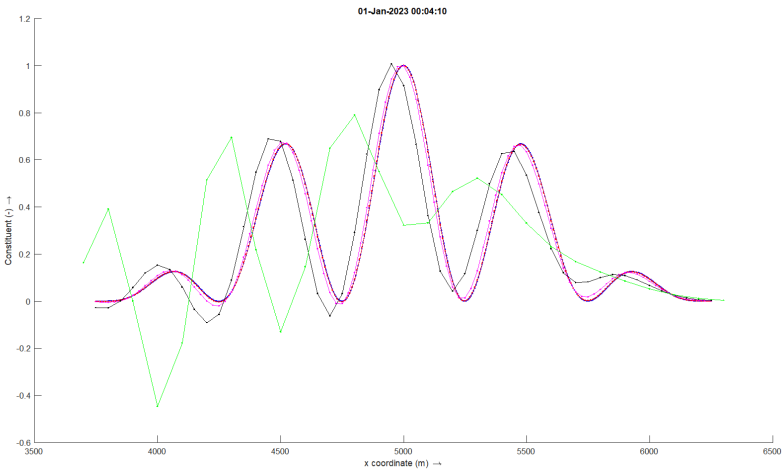


Figure 6.9: *Wave package experiment, results at* $t = 250$ [s] *and* $\Delta t = 0.01$ [s]*: Blue:* $\Delta x = 5$ [m]*, Red:* $\Delta x = 10$ [m]*, Cyan:* $\Delta x = 25$ [m]*, Black:* $\Delta x = 50$ [m]*, Green:* $\Delta x = 100$ [m]*.*

6.2.4 Transport of strictly positive constituent

When c needs a strickly positive value (like a concentration) then due to numerical discretization the value c could become negative, even if the initial and boundary values are positive. In certain applications a positive value is required and even small negative are not allowed. To ensure the positivity of the constituent c we will write the equation with variable ϕ, where ϕ is defined as:

$$c = \exp(\ln(c)) = \exp(\phi), \quad \text{with} \quad \phi = \ln(c) \tag{6.7}$$

The considered advection-diffusion equation than reads:

$$\int_\Omega \frac{\partial e^\phi}{\partial t}\, d\omega + \int_\Omega \frac{\partial \left(u e^\phi\right)}{\partial x}\, d\omega - \int_\Omega \frac{\partial}{\partial x}\left(\varepsilon \frac{\partial e^\phi}{\partial x}\right) d\omega = 0, \tag{6.8}$$

With initial condition for the velocity $u_{given} = 10\ [\mathrm{m\,s^{-1}}]$, which coincide with the wave celerity in the next numerical experiments.

$$u(x,0) = u_{given} \tag{6.9}$$

and with a prescribed boundary condition for the constituent c at the left side of the domain

$$c(0,t) = c_{given} \begin{cases} \frac{1}{2}\cos\left(\pi\left(\frac{t_{reg}-t}{t_{reg}}\right)+1\right) & \text{if } t < t_{reg}, \\ 1 & \text{if } t \geq t_{reg}, \end{cases} \tag{6.10}$$

where

t_{reg} The regularization time for the given time-series, [s]

A value of $c(0,t) = 0$ is estimated by:

$$\phi(0,t) = \ln(c(0,t)) \gtrsim -25 \tag{6.11}$$

Numerical experiment

The numerical experiment is performed with the following parameters:

- Length of the domain, $12\,000$ [m]
- Grid size, $\Delta x = 10$ [m]
- Start time, $t_{start} = 0$ [s]
- End time, $t_{stop} = 3600$ [s]
- Timestep, $\Delta t = 5$ [s]
- Regularization time for time-series, $t_{reg} = 300$ [s]
- Prescribed constant velocity, $u_{given}(x,t) = 10$ [m s^{-1}]
- Prescribed initial value of the constituent, $c(x,0) = 1.4 \times 10^{-11}$, so $\phi = -25$ [$-$].
- Prescribed constant constituent on boundary $c_{given}(0,t) = 1$, so $\phi = \ln(c_{given}(0,t)) = \ln(1) = 0$ [$-$]

Results of the numerical experiments

Not yet documented

6.3 1-D Advection-diffusion equation

In this section we will show the resuls of the advection-diffusion equation with a Dirichlet boundary conditions at both sides of the domain and an interface problem, i.e. a large jump of the diffusion coefficiebt in the middle of the domain.

The considered advection-diffusion equation reads:

$$\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} - \frac{\partial}{\partial x}\left((\varepsilon + \Psi)\frac{\partial c}{\partial x}\right) = 0, \qquad u > 0. \tag{6.12}$$

where

c	Constituent, $[-]$.
u	Advection velocity, $[\mathrm{m\,s^{-1}}]$.
ε	Diffusion coefficient, $[\mathrm{m^2\,s^{-1}}]$.
Ψ	Artificial diffusion, $[\mathrm{m^2\,s^{-1}}]$.

6.3.1 Outflow boundary layer

The Dirichlet value at the outflow boundary is so chosen that there will appear an outflow boundary layer. Due to this outflow boundary the numerical scheme need to have a cell Péclet number ($\mathit{Pe} = u\Delta x/\varepsilon$) smaller then two in the vicinity of that layer. In the Δ-formulation that will be reach by a regularization step, i.e. increase the diffusion in the vicinity of the boundary layer. To force a outflow boundary layer at both boundaries a Dirichlet boundary is prescribed. With the boundary conditions $c(0,t) = a$ and $c(L,t) = b$ the analytic solution read:

$$c(x) = a + (b-a)\frac{e^{\frac{(x-L)}{L}\mathit{Pe}} - e^{-\mathit{Pe}}}{1 - e^{-\mathit{Pe}}}, \tag{6.13}$$

with $\mathit{Pe} = uL/\varepsilon$.

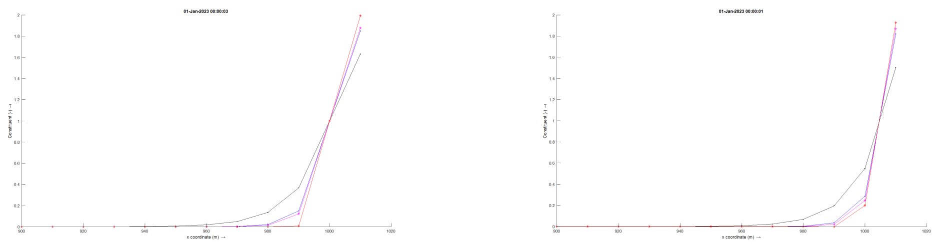
Numerical experiment

The numerical experiment is performed with the following parameters:

- Length of the domain $L_x = 1000$ [m].
- Stationary simulation, $\partial c/\partial t = 0$.
- Prescribed boundary conditions: $c(0,t) = 0$ and $c(L_x,t) = 1$.
- Grid size $\Delta x = 10$ [m],
- Diffusion coefficient $\varepsilon = 10$ $[\mathrm{m^2\,s^{-1}}]$
- Advection velocities, $\mathit{Pe} = u\Delta x/\varepsilon$:
  - $u = 1$ $[\mathrm{m\,s^{-1}}] \rightarrow \mathit{Pe} = 1.0$
  - $u = 1.9$ $[\mathrm{m\,s^{-1}}] \rightarrow \mathit{Pe} = 1.9$
  - $u = 2.1$ $[\mathrm{m\,s^{-1}}] \rightarrow \mathit{Pe} = 2.1$
  - $u = 5.0$ $[\mathrm{m\,s^{-1}}] \rightarrow \mathit{Pe} = 5.0$
- Smoothing factor, $c_\Psi = 4$
- Right hand side to compute artificial viscosity, $\frac{1}{32}c_\Psi u\Delta x\partial^2 c/\partial\xi^2$ (educational guess).

Results of the numerical experiments

Map results are presented for the constituent c and the artificial diffusion Ψ.



(a) *Analytic solution*

(b) *Numerical solution*

Figure 6.10: *Map results for different values of the advection velocity (thus Péclet number). The graphs with an asterix represent results with a cell Péclet number larger then two. Black: Pe* $= 1.0$*; Blue: Pe* $= 1.9$*, Green: Pe* $= 2.1$*; Cyan: Pe* $= 5.0$*.*

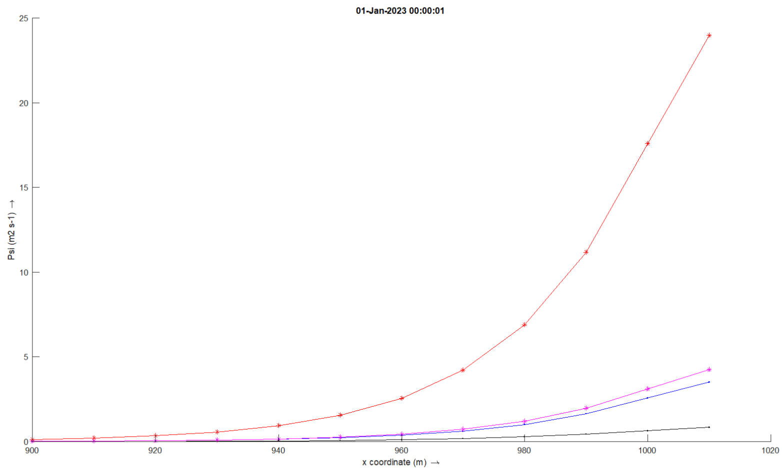


Figure 6.11: *Map results for the used artificial diffusion* Ψ*. Black: Pe* $= 1.0$*; Blue: Pe* $= 1.9$*, Green: Pe* $= 2.1$*; Cyan: Pe* $= 5.0$*.*

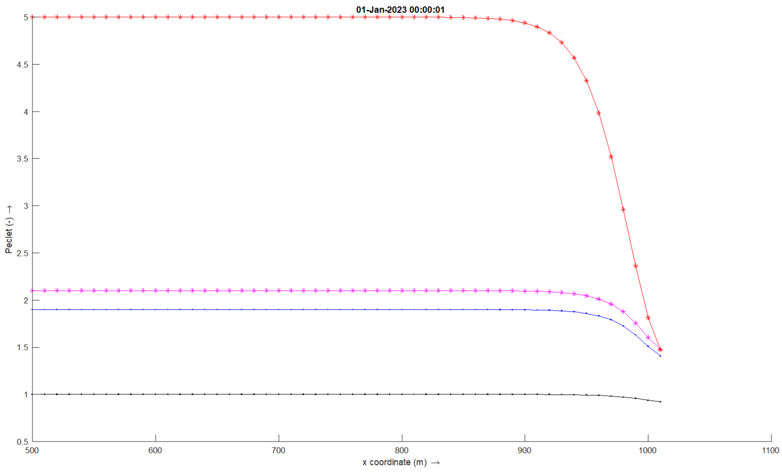


Figure 6.12: *Map results for the used cell Péclet number. Black: Pe* $= 1.0$*; Blue: Pe* $= 1.9$*, Green: Pe* $= 2.1$*; Cyan: Pe* $= 5.0$*.*

6.3.2 Interface problem

A numerical experiments is performed for the stationary advection-diffusion equation with a jump in the diffusion coefficient as described by:

$$\varepsilon(x) = \begin{cases} \breve{\varepsilon}, & \text{if} \quad 0 < x \leq x^*, \\ 1, & \text{if} \quad x^* < x < 1 \end{cases} \tag{6.14}$$

An analytical solution exists in case $u = 0$ and read (Wesseling, 2001, eq. 3.11):

$$c(x) = \begin{cases} \alpha x, & \text{if} \quad 0 < x \leq x^*, \\ \breve{\varepsilon}\alpha x + 1 - \breve{\varepsilon}\alpha, & \text{if} \quad x^* < x < 1 \end{cases} \tag{6.15}$$

$$\alpha = \frac{1}{x^* - \breve{\varepsilon}x^* + \breve{\varepsilon}} \tag{6.16}$$

- If $\varepsilon \frac{\partial c}{\partial x} \equiv 0$ then either $\varepsilon = 0$ or $\frac{\partial c}{\partial x} = 0$. Where $\varepsilon = 0$ is not feasible.

Some numerical experiments are performed with several values of u.

Numerical experiment

The numerical experiment is performed with the following parameters:

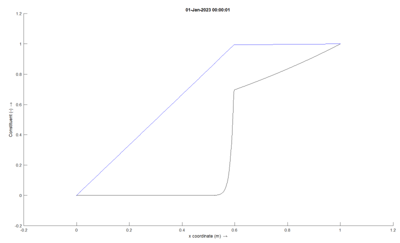
- Length of the domain $L_x = 1$ [m].
- Stationary simulation, $\partial c / \partial t = 0$.
- Prescribed boundary conditions: $c(0, t) = 0$ and $c(L_x, t) = 1$.
- Grid size:
  - $\Delta x = 0.001$ [m] $\rightarrow$ *Pe* $= 0.09$,
  - $\Delta x = 0.01$ [m] $\rightarrow$ *Pe* $= 0.9$,

- $\Delta x = 0.05$ [m] $\rightarrow$ *Pe* $= 4.5$,

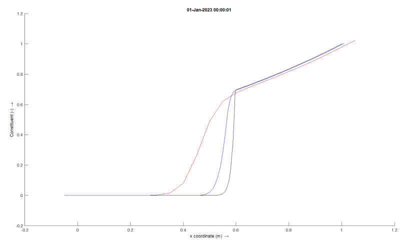
- Diffusion coefficient $\breve{\varepsilon} = 0.01$ [m^2 s^{-1}]
- Advection velocities, *Pe* $= u\Delta x/\varepsilon$:
  - $u = 0$ [m s^{-1}] $\rightarrow$ *Pe* $= 0.0$
  - $u = 0.9$ [m s^{-1}] $\rightarrow$ *Pe* $= 0.09$, *Pe* $= 0.9$ and *Pe* $= 4.5$

Results of numerical experiment

Map results are presented for the constituent c and the artificial diffusion Ψ.



***(a)** High numerical resolution solution $\Delta x = 0.001$ [m]. Blue $u = 0$ [m s^{-1}] and Black $u = 0.9$ [m s^{-1}].*



***(b)** Numerical solution, $u = 0.9$ [m s^{-1}]. Black: $\Delta x = 0.001$ [m] $\rightarrow$ Pe $= 0.09$; Blue: $\Delta x = 0.01$ [m] $\rightarrow$ Pe $= 0.9$ and Red: $\Delta x = 0.05$ [m] $\rightarrow$ Pe $= 4.5$.*

***Figure 6.13:** Map results for different values of the Péclet number.*

6.4 1-D Wave equation

6.4.1 Gaussian hump

The considered 1-D wave equation reads:

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0 \qquad \textit{continuity eq.} \tag{6.17}$$

$$\frac{\partial q}{\partial t} + gh\frac{\partial h}{\partial x} = 0 \qquad \textit{momentum eq.} \tag{6.18}$$

With initial conditions

$$h(x,0) = \zeta(x,0) - z_b(x), \quad [\mathrm{m}] \tag{6.19}$$

$$q(x,0) = 0, \quad [\mathrm{m^2\,s^{-1}}] \tag{6.20}$$

for the the water level a Gaussian hump is prescribed

$$\zeta(x) = 2a_0 \exp\left(\frac{(x-\mu)^2}{2\sigma^2}\right), \quad [\mathrm{m}] \tag{6.21}$$

At the boundaries no ingoing signals are prescribed, so outgoing signals are leaving the domain unhampered, which means no reflections will be present other then numerical reflections.

Numerical experiment

The numerical experiment is performed with the following parameters:

- Length of the domain, $L_x = 12\,000$ [m], ranging from -6000 [m] to 6000 [m].
- Bed level, $z_b = -10$ [m].
- Grid size, $\Delta x = 10$ [m].
- Start time, $t_{start} = 0$ [s].
- End time, $t_{stop} = 3600$ [s].
- Timestep, $\Delta t = 10$ [s].
- Regularization time for time-series, $t_{reg} = 300$ [s].
- Amplitude of the Gaussian hump at the boundary, $a_0 = 0.01$ [m].
- Centre of the Gaussian hump, $\mu = 3000$ [m].
- Spreading of the Gaussian hump, $\sigma = 700$ [m].

And a second experiment with given boundary values:

- Prescribed discharge boundary at -6000 [m]: $q(0,t) = 0.05$ [m^2 s^{-1}].
- Prescribed water level boundary value at 6000 [m]: $\zeta(0,t) = 0.02$ [m].

Because the boundary values are constant in time the solution is time-independent. Therefore two simulation should be performed:

1 A stationary computation (with $\Delta t = 0$ [s]) and
2 an temporal computation (with $t_{stop} = 10\,800$ [s])

Results of the numerical experiments 1

Not yet documented

Results of the numerical experiments 2

Not yet documented

6.4.2 Weir

The model is taken from Borsboom (2001). The considered 1-D wave equation reads:

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0, \qquad \textit{continuity eq.} \tag{6.22}$$

$$\frac{\partial q}{\partial t} + \frac{\partial (q^2/h)}{\partial x} + gh\frac{\partial h}{\partial x} - \frac{\partial}{\partial x}\left((\nu + \Psi)h\frac{\partial (q/h)}{\partial x}\right) = 0, \qquad \textit{momentum eq.} \tag{6.23}$$

- Length of the domain, 500 [m].
- Artificial viscosity Ψ computated as presented in section 3.2.

Bathymetry [m]:

$$z_b(x) = \begin{cases} -12 & 0 < x \leq 200, \\ -12 + 7(x - 200)/50 & 200 < x \leq 250, \\ -5 & 250 < x \leq 350, \\ -5 - 5(x - 350)/100 & 350 < x \leq 450, \\ -10 & 450 < x \leq 500. \end{cases} \tag{6.24}$$

Initial conditions

$$h(x, 0) = 0, \tag{6.25}$$

$$q(x, 0) = 0 \tag{6.26}$$

Boundary conditions

- Prescribed discharge boundary at 0 [m]: $q(0, t) = 19.8656$ [m^2 s^{-1}].
- Prescribed water level boundary value at 500 [m]: $\zeta(500, t) = -3$ [m].

Numerical experiment

The numerical experiment is performed with the following parameters:

- Grid size and time step,
  - $\Delta x = 10$ [m] and $\Delta t = 2$ [s]
  - $\Delta x = 5$ [m] and $\Delta t = 1$ [s]
  - $\Delta x = 2.5$ [m] and $\Delta t = 0.5$ [s]
  - $\Delta x = 1.25$ [m] and $\Delta t = 0.25$ [s]
- Start time, $t_{start} = 0$ [s].
- End time, $t_{stop} = 7200$ [s].
- Regularization time for time-series, $t_{reg} = 300$ [s].
- Kinematic viscosity, $\nu = 0.01$ [m^2 s^{-1}]
- $\varepsilon_{bc} = 1 \times 10^{-2}$

Results of the numerical experiments

Results for the four different computations are shown in Figure 6.14

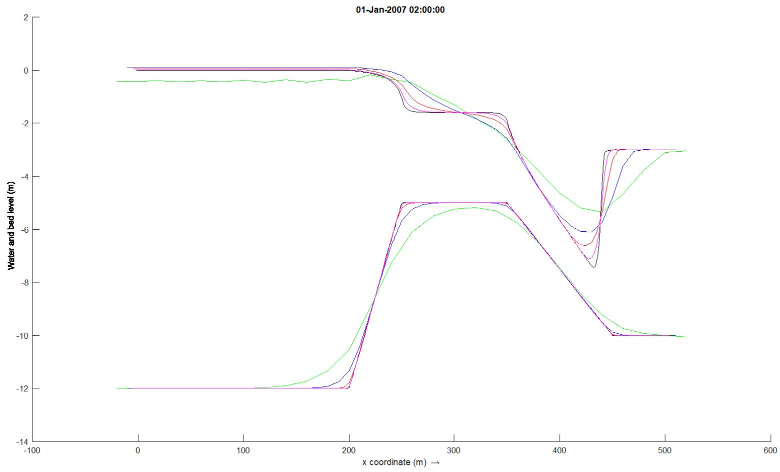
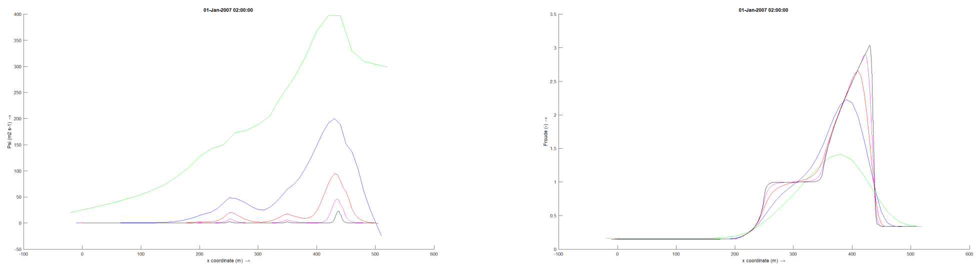


Figure 6.14: *Top graphs present the water level. Lower graphs present the regularized bathymetry. Green:* $\Delta x = 20$ [m], $\Delta t = 4$ [s]*; Blue:* $\Delta x = 10$ [m], $\Delta t = 2$ [s]*; Red:* $\Delta x = 5$ [m], $\Delta t = 1$ [s]*; Cyan:* $\Delta x = 2.5$ [m], $\Delta t = 0.5$ [s]*; Black:* $\Delta x = 1.25$ [m], $\Delta t = 0.25$ [s]



(a) *Artificial viscosity* Ψ.

(b) *Froude number.*

Figure 6.15: *Artificial viscosity* Ψ *and Froude number. Green:* $\Delta x = 20$ [m], $\Delta t = 4$ [s]*; Blue:* $\Delta x = 10$ [m], $\Delta t = 2$ [s]*; Red:* $\Delta x = 5$ [m], $\Delta t = 1$ [s]*; Cyan:* $\Delta x = 2.5$ [m], $\Delta t = 0.5$ [s]*; Black:* $\Delta x = 1.25$ [m], $\Delta t = 0.25$ [s]

7 2-D Shallow water equations

Consider the non-linear wave equation

$$\frac{\partial h}{\partial t} + \nabla \cdot \boldsymbol{q} = 0, \tag{7.1a}$$

$$\frac{\partial \boldsymbol{q}}{\partial t} + \nabla \cdot \left(\boldsymbol{q}\boldsymbol{q}^T/h\right) + \frac{1}{2} g \nabla h^2 = -gh\nabla z_b, \tag{7.1b}$$

or

$$\frac{\partial h}{\partial t} + \nabla \cdot \boldsymbol{q} = 0, \tag{7.2a}$$

$$\frac{\partial \boldsymbol{q}}{\partial t} + \nabla \cdot \left(\boldsymbol{q}\boldsymbol{q}^T/h\right) + gh\nabla\zeta = 0, \tag{7.2b}$$

$$\zeta = h + z_b, \tag{7.2c}$$

with

ζ	Water level w.r.t. reference plane ($\zeta = h + z_b$), [m].
h	Water depth ($h = \zeta - z_b$), [m].
z_b	Bed level w.r.t. reference plane, [m].
$\boldsymbol{q}$	Flow, defined as $\boldsymbol{q} = (q, r)^T = (hu, hv)^T$, [$\mathrm{m^2\,s^{-1}}$].
$\boldsymbol{u}$	Velocity vector, defined as $\boldsymbol{u} = (u, v)^T$, [$\mathrm{m\,s^{-1}}$].
g	Acceleration due to gravity, [$\mathrm{m\,s^{-2}}$].

Finite Volume approach

Integrating the equations over a finite volume Ω yields:

$$\int_\Omega \frac{\partial h}{\partial t}\, d\omega + \int_\Omega \nabla \cdot \boldsymbol{q}\, d\omega = 0, \tag{7.3a}$$

$$\int_\Omega \frac{\partial \boldsymbol{q}}{\partial t}\, d\omega + \int_\Omega \nabla \cdot \left(\boldsymbol{q}\boldsymbol{q}^T/h\right)\, d\omega + \int_\Omega \frac{1}{2} \nabla \left(gh^2\right)\, d\omega = -\int_\Omega gh\nabla z_b\, d\omega, \tag{7.3b}$$

or

$$\int_\Omega \frac{\partial h}{\partial t}\, d\omega + \int_\Omega \nabla \cdot \boldsymbol{q}\, d\omega = 0, \tag{7.4a}$$

$$\int_\Omega \frac{\partial \boldsymbol{q}}{\partial t}\, d\omega + \int_\Omega \nabla \cdot \left(\boldsymbol{q}\boldsymbol{q}^T/h\right)\, d\omega + \int_\Omega gh\nabla\zeta\, d\omega = 0, \tag{7.4b}$$

$$\int_\Omega \zeta\, d\omega = \int_\Omega h\, d\omega + \int_\Omega z_b\, d\omega, \tag{7.4c}$$

7.1 Space discretization, structured

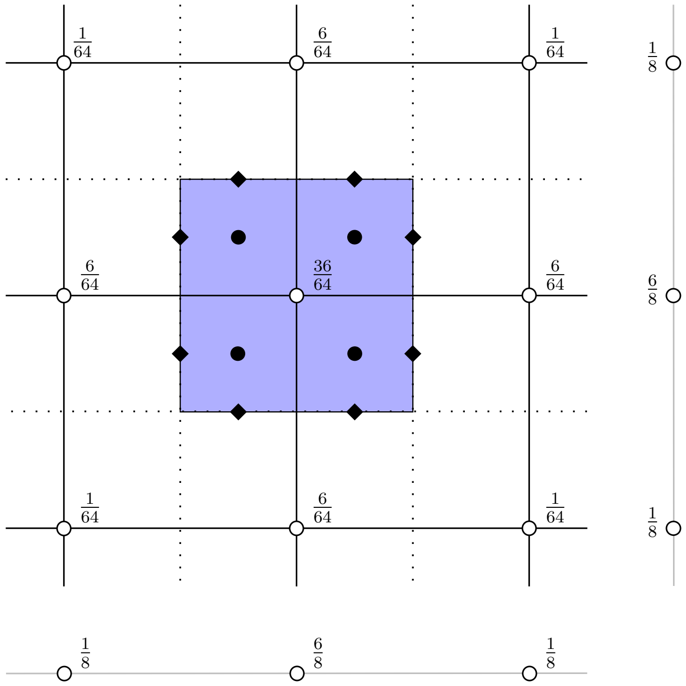


Figure 7.1: *Coefficients for the mass-matrix and the control volume in 2-dimensions in the interior area, on a structured grid. The black dots indicate the location of the quadrature points, and black diamonds the flux points.*

For the space discretizations of an arbitrary function u on the quadrature point of a sub-control volume the following space interpolations are used, $u \in \{h, q, r\}$:

$$u\big|_{i+\frac{1}{4},j+\frac{1}{4}} \approx \frac{1}{16}\left(9u_{i,j} + 3u_{i+1,j} + 3u_{i,j+1} + u_{i+1,j+1}\right) \tag{7.5}$$

$$\left.\frac{\partial u}{\partial x}\right|_{i+\frac{1}{4},j+\frac{1}{4}} \approx \frac{1}{4}\left(3u_{i+1,j} - 3u_{i,j} + u_{i+1,j+1} - u_{i,j+1}\right) \tag{7.6}$$

$$\left.\frac{\partial u}{\partial y}\right|_{i+\frac{1}{4},j+\frac{1}{4}} \approx \frac{1}{4}\left(3u_{i,j+1} - 3u_{i,j} + u_{i+1,j+1} - u_{i+1,j}\right) \tag{7.7}$$

See for the locations Figure 7.1.

7.1.1 Discretizations continuity equation

7.1.2 Discretizations momentum equations

7.1.2.1 Time derivative

Not yet documented

7.1.2.2 Pressure term

In this section we use that the pressure term is dependent on ζ.

$$\int_{\Omega_i} gh\nabla\zeta\, d\omega \tag{7.8}$$

The integral over a control volume will be a sum of integrals over the sub control volumes. On a structured mesh it will be the sum over 4 sub control volumes.

Considering one control volume and only the x-direction (assuming a cartesian grid) it reads:

$$\int_{\Omega_{scv}} gh\nabla\zeta\, d\omega \approx \tag{7.9}$$

$$\approx \frac{1}{4}\Delta x\Delta y\, gh_{qp}^{n+\theta,p+1}\frac{\partial\zeta_{qp}^{n+\theta,p+1}}{\partial x} \tag{7.10}$$

$$\approx \frac{1}{4}\Delta x\Delta y\, g\left(h_{qp}^{n+1,p}+\theta\Delta h^{n+1,p+1}\right)\frac{\partial}{\partial x}\left(\zeta_{qp}^{n+1,p}+\theta\Delta\zeta_q^{n+1,p+1}p\right) \tag{7.11}$$

with qp the location of the quadrature point in the sub-control volume. Assume that the higher order terms are negligible then the discretization for each of the 4 sub-control volumes reads:

$$\frac{1}{4}\Delta x\Delta y\, g\left(h_{qp}^{n+1,p}\frac{\partial\zeta_{qp}^{n+1,p}}{\partial x}+\theta h_{qp}^{n+1,p}\frac{\partial\Delta\zeta_{qp}^{n+1,p+1}}{\partial x}+\theta\frac{\partial\zeta_{qp}^{n+1,p}}{\partial x}\Delta h_{qp}^{n+1,p+1}\right) \tag{7.12}$$

7.1.2.3 Convection

Not yet documented

7.1.2.4 Bed shear stress

Not yet documented

7.1.2.5 Pressure term, dependent on h

In this section we use that the pressure term is dependent on h.

$$\int_{\Omega_i}\frac{1}{2}\nabla\left(gh^2\right)\, d\omega = \int_{\partial\Omega_i}\frac{1}{2}gh^2\hat{\boldsymbol{n}}\, dl \tag{7.13}$$

The linearization of the pressure term in the momentum equation around iteration level p read:

$$\frac{1}{2}g\left(h_{\partial\Omega_i}^{n+\theta,p+1}\right)^2 = \frac{1}{2}g\left(h_{\partial\Omega_i}^{n+\theta,p+1}\right)^2 + gh_{\partial\Omega_i}^{n+\theta,p+1}\left(h^{n+\theta,p+1}-h^{n+\theta,p}\right) = \tag{7.14}$$

$$= \frac{1}{2}g\left(h_{\partial\Omega_i}^{n+\theta,p+1}\right)^2 + \theta gh_{\partial\Omega_j}^{n+\theta,p+1}\Delta h^{n+1,p+1} \tag{7.15}$$

The component in x-direction read:

$$\int_{\partial\Omega_i} \frac{1}{2} g h^2 \hat{\boldsymbol{n}} \cdot \boldsymbol{i_x} \, dl \approx$$
$$\approx \Delta y \left(\frac{1}{2} g \left(h^{n+\theta,p}_{i+\frac{1}{2},j} \right)^2 + \theta g h^{n+\theta,p+1}_{i+\frac{1}{2},j} \Delta h^{n+1,p+1}_{i+\frac{1}{2},j} \right) +$$
$$- \Delta y \left(\frac{1}{2} g \left(h^{n+\theta,p}_{i-\frac{1}{2},j} \right)^2 + \theta g h^{n+\theta,p+1}_{i-\frac{1}{2},j} \Delta h^{n+1,p+1}_{i-\frac{1}{2},j} \right) \tag{7.16}$$

The component in y-direction read:

$$\int_{\partial\Omega_i} \frac{1}{2} g h^2 \hat{\boldsymbol{n}} \cdot \boldsymbol{i_y} \, dl \approx$$
$$\approx \Delta x \left(\frac{1}{2} g \left(h^{n+\theta,p}_{i,j+\frac{1}{2}} \right)^2 + \theta g h^{n+\theta,p+1}_{i,j+\frac{1}{2}} \Delta h^{n+1,p+1}_{i,j+\frac{1}{2}} \right) +$$
$$- \Delta x \left(\frac{1}{2} g \left(h^{n+\theta,p}_{i,j-\frac{1}{2}} \right)^2 + \theta g h^{n+\theta,p+1}_{i,j-\frac{1}{2}} \Delta h^{n+1,p+1}_{i,j-\frac{1}{2}} \right) \tag{7.17}$$

7.1.3 Discretization at boundary

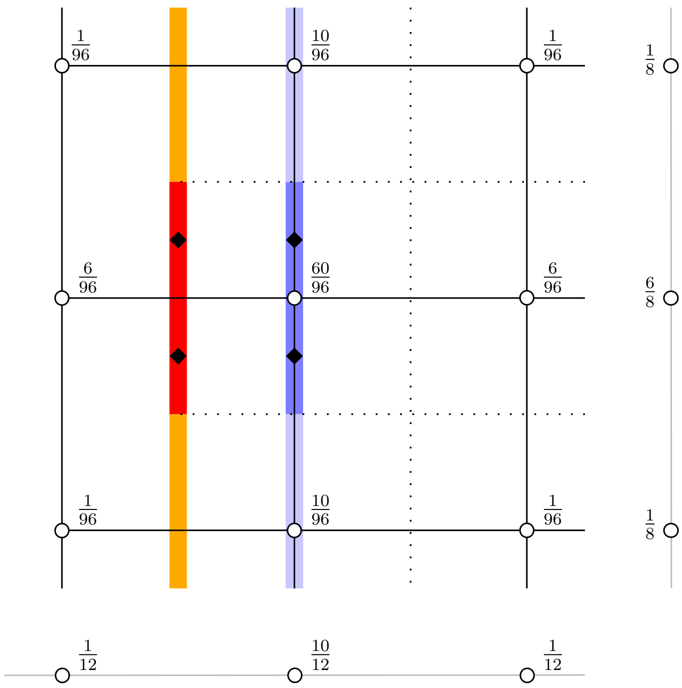


Figure 7.2: *Coefficients of the mass-matrix in 2-dimensions on a structured grid along a straight boundary. The essential boundary condition is located at the cyan-colored line and the natural boundary condition at the orange line.*

For the 2D non-linear wave equations (Equation (7.4)) at each boundary boundary conditions need to be prescribed, the number of boundary conditions depends on the flow direction on the boundary. Considering a hyperbolic system, if the flow is flowing into the domain two boundary conditions need to prescribed and when the flow is flowing out the domain just one boundary need to prescribed. This is according the characteristic theory of 2D hyperbolic systems (Daubert and Graffe, 1967). The ingoing information is called the **essential** boundary condition (Dirichlet or Neumann condition). And a boundary condition to handle the outgoing wave is called the **natural** boundary condition.

7.1.4 Discretization at corner

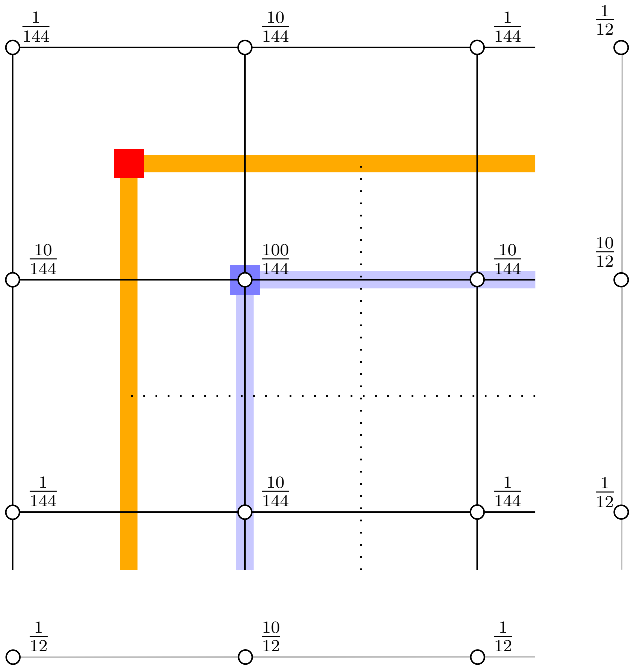


Figure 7.3: *Coefficients for the mass-matrix in 2-dimensions on a structured grid at a corner. No line integrals are performed in the corner.*

7.1.4.1 Weakly reflective boundary conditions

Consider the following weakly reflective boundary conditions:

$$q_{i+\frac{1}{2}} + \sqrt{gh_{i+\frac{1}{2}}} = \sqrt{gh^{\infty}_{i+\frac{1}{2}}}, \quad \text{inflow} \tag{7.18}$$

$$r_{i+\frac{1}{2}} = 0, \quad \text{inflow} \tag{7.19}$$

$$\left.\frac{\partial r}{\partial y}\right|_{i+\frac{1}{2}} = 0, \quad \text{outflow} \tag{7.20}$$

$$q_{i+\frac{1}{2}} - \sqrt{gh_{i+\frac{1}{2}}} = 0, \quad \text{outflow} \tag{7.21}$$

References

Ault, Shaun and Erik Holmgreen (2003). *Dynamics of the Brusselator*. URL: https://mate.unipv.it/~boffi/teaching/download/Brusselator.pdf.

Borsboom, M. (1998). “Development of an error-minimizing adative grid method”. In: *Applied Numerical Mathematics* 26.1, pp. 13–21. ISSN: 0168-9274. DOI: https://doi.org/10.1016/S0168-9274(97)00077-9. URL: https://www.sciencedirect.com/science/article/pii/S0168927497000779.

Borsboom, M. (2001). “Development of a 1-D Error-Minimizing Moving Adaptive Grid Method”. In: ed. by B.Schiesser A. van de Wouwer P. Saucez. CRC Press, to be published. Chap. Adaptive Method of Lines. DOI: https://dx.doi.org/10.1201/9781420035612-8.

Borsboom, M. (2003). *To smooth or not to smooth*. Memo WL | Delft Hydraulics / Deltares. A note on two-step numerical modeling.

Borsboom, M. (2019). *Numerical design of a fast, robust and accurate 1D shallow-water solver for pipe flows with largetime scales – proposal (WORK IN PROGRESS)*.

Borsboom, M. (2024). *Export from MapleSoft: "funcfitsmoothing_Fouriermodeanalysis.pdf"*.

Buijs, J. (2024). *Pseudo-Transient Continuation for the Rapid Convergence of Shallow Water Equation Solvers*. Delft University of Technology, Deltares internship report.

Daubert, A. and O. Graffe (1967). “Quelques aspects des écoulements presque horizontaux à deux dimensions en plan et non permanents, application aux estuaires”. In: *La Houille Blanche - Revue internationale de l’eau* 8, pp. 847–860. DOI: 10.1051/lhb/1967059. URL: https://doi.org/10.1051/lhb/1967059.

Hundsdorfer, W. and J. G. Verwer (2003). *Numerical solution of Time-Dependent Advection-Diffusion-Reaction Equations*. Springer.

Kan, J. van, A. Segal, and F. Vermolen (2008). *Numerical Methods in Scientific Computing*. VSSD. ISBN: 9789071301506. URL: https://books.google.nl/books?id=fCARnQAACAAJ.

Logan, J. David. (1987). *Applied Mathemathics A contemporary approach*. Johan Wiley and Sons, Inc. ISBN: 0-471-85083-7.

Pulliam, T. H. (2014). *Time accuracy and the use of implicit methods*. Tech. rep. NASA Ames Research Center. URL: https://overflow.larc.nasa.gov/wp-content/uploads/sites/54/2014/06/Time_Accurate_Methods_V8.pdf.

Reference not yet known (n.d.).

Wesseling, P. (2001). *Principles of computational fluid dynamics*. Springer.

A Error estimation

In this section a Fourier mode analysis for constant Δx and Ψ of Equation (3.22) is given. For convenience the equation is repeated here:

$$\widetilde{u} - \frac{\partial}{\partial x}\Psi\frac{\partial \widetilde{u}}{\partial x} = u_{giv} \tag{A.1}$$

The Fourier-mode transform of Equation (3.22) reads, when $\Delta x = constant$ and $\Psi = c_\Psi \Delta x^2 = constant$:

$$\widetilde{u}\exp(\mathrm{i}kx)\left(1 + \Psi k^2\right) = \mathcal{F}(u_{giv}) \tag{A.2}$$

multiply Ψ by $\Delta x^2/\Delta x^2 = 1$ yields

$$\widetilde{u}\exp(\mathrm{i}kx)\left(1 + \frac{\Psi}{\Delta x^2}(k\Delta x)^2\right) = \mathcal{F}(u_{giv}) \tag{A.3}$$

which is easier to use in the analysis due to the term $k\Delta x$.

The discretization of Equation (3.28) with constant Δx and Ψ yields:

$$\left(\frac{1}{8} - c_\Psi\right)u_{i-1} + \left(\frac{6}{8} + 2c_\Psi\right)u_i + \left(\frac{1}{8} - c_\Psi\right)u_{i+1} = \tag{A.4}$$

$$= \frac{1}{\Delta x}\int_{x_{i-1/2}}^{x_{i+\frac{1}{2}}} u_{giv}\,dx \tag{A.5}$$

Substitution of the Fourier modes

$$\overline{u}_k = \overline{u}_k\exp(\mathrm{i}k\Delta x) \quad \text{and} \quad u_{giv} = u_{giv,k}\exp(\mathrm{i}k\Delta x) \tag{A.6}$$

in this equation yields:

$$\overline{u}_k\left(\left(\frac{1}{8} - c_\Psi\right)\exp(-\mathrm{i}k\Delta x) + \left(\frac{6}{8} + 2c_\Psi\right) + \left(\frac{1}{8} - c_\Psi\right)\exp(-\mathrm{i}k\Delta x)\right) = \tag{A.7}$$

$$= \frac{u_{giv,k}}{\Delta x}\int_{x_{i-1/2}}^{x_{i+\frac{1}{2}}}\exp(\mathrm{i}k\Delta x)\,dx \tag{A.8}$$

$\Rightarrow$

$$\overline{u}_k\left(\frac{6}{8} + 2c_\Psi + \left(\frac{1}{8} - c_\Psi\right)2\cos(k\Delta x)\right) =$$

$$= u_{giv,k}\frac{-\mathrm{i}(\exp(\frac{\mathrm{i}}{2}k\Delta x) - \exp(\frac{\mathrm{i}}{2}k\Delta x))}{k\Delta x} \tag{A.9}$$

$\Leftrightarrow$

$$\overline{u}_k \left(\frac{6}{8} + 2c_\Psi + \left(\frac{1}{8} - c_\Psi \right) 2\cos(k\Delta x) \right) = u_{giv,k} \frac{2\sin(\frac{1}{2}k\Delta x)}{k\Delta x} \tag{A.10}$$

The ratio between the regularized function $\widetilde{u}$ (Equation (A.3)) and given function reads (see Figure A.1):

$$\widetilde{r} = \left| \frac{\widetilde{u}_k}{u_{giv,k}} \right| = \left| \frac{1}{1 + c_\Psi (k\Delta x)^2} \right| \tag{A.11}$$

and the ratio between the piecewise linear function $\overline{u}$ (Equation (A.10)) and given function reads (see Figure A.1):

$$\overline{r} = \left| \frac{\overline{u}_k}{u_{giv,k}} \right| = \left| \frac{2\sin(\frac{1}{2}k\Delta x)}{k\Delta x \left(\frac{6}{8} + 2c_\Psi + \left(\frac{1}{8} - c_\Psi \right) 2\cos(k\Delta x) \right)} \right| \tag{A.12}$$

$\Leftrightarrow$

$$\overline{r} = \left| \frac{\overline{u}_k}{u_{giv,k}} \right| = \left| \frac{8\sin(\frac{1}{2}k\Delta x)}{k\Delta x \left(3 + \cos(k\Delta x) + 8c_\Psi (1 - \cos(k\Delta x)) \right)} \right| \tag{A.13}$$

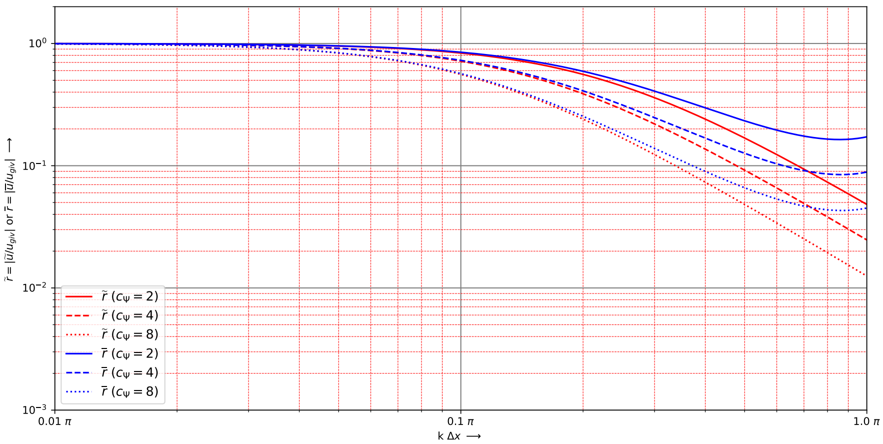


Figure A.1: *Ration between $\widetilde{r} = |\widetilde{u}_k / u_{giv,k}|$, and $\overline{r} = |\overline{u}_k / u_{giv,k}|$. For different values of $c_\Psi = \Psi/\Delta x^2$.*

A.1 Numerical error

Discretization error values are determined when $\Delta x = constant$ and $\Psi = 0$, Equation (3.28) reduces to:

$$\frac{1}{8}u_{i-1} + \frac{6}{8}u_i + \frac{1}{8}u_{i+1} = \frac{1}{\Delta x} \int_{x_{i-1/2}}^{x_{i+\frac{1}{2}}} u_{giv}\, dx \tag{A.14}$$

Numerical error as discretized between grid pints

$$\text{errorFVEgridpoint}(k\Delta x) = \left|1 - \frac{8\sin(\frac{1}{2}k\Delta x)}{k\Delta x(3+\cos(k\Delta x))}\right| \tag{A.15}$$

Numerical error as discretized between cell centres (numerical Fourier-mode through the cell centres)

$$\text{errorFVEcellcentre}(k\Delta x) = \left|1 - \frac{8\sin(\frac{1}{2}k\Delta x)\cos(\frac{1}{2}k\Delta x)}{k\Delta x(3+\cos(k\Delta x))}\right| \tag{A.16}$$

With lowest order estimation of (see Borsboom (2024)):

$$-\frac{1}{24}(k\Delta x)^2 - \frac{7}{960}(k\Delta x)^4 + O(\Delta x^6) \tag{A.17}$$

So if the numerical error needs to be smaller then 1 %, the number of grid cells per wave length ($\lambda = N\Delta x$) is computed as

$$\frac{1}{24}(k\Delta x)^2 < 0.01 \Rightarrow k\Delta x < 0.5 \Rightarrow \tag{A.18}$$

$$\left(\frac{2\pi}{N\Delta x}\right)\Delta x < 0.5 \Rightarrow N > 4\pi \approx 13 \tag{A.19}$$

so per wave detail $\approx$ 7 grid cells.

Discretization error values are given when $\Psi = c_\Psi \Delta x^2 = 0$ (see Figure A.2):

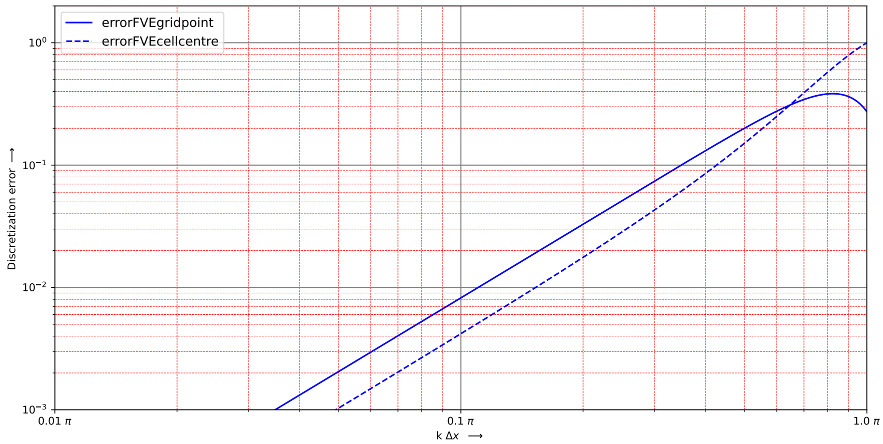


Figure A.2: *Error function for value $\Psi = c_\Psi \Delta x^2 = 0$.*

A.2 Determining the factor c_Ψ

In the limit of $k\Delta x \to \infty$ Equation (A.11) behaves as:

$$\lim_{k\Delta x \to \infty} \frac{1}{1 + c_\Psi (k\Delta x)^2} = \frac{1}{c_\Psi (k\Delta x)^2} \tag{A.20}$$

The cut-off frequency is determined by $1 = 1/(c_\Psi (k\Delta x)^2)$, hence filter parameter $c_\Psi = 1/(k\Delta x)^2$ gives cut-off frequency k, or $k\Delta x = \sqrt{1/c_\Psi}$ is obtained with filter parameter c_Ψ. Given the wave length from the required numerical error (1 %, $N = 13$), the coefficient c_Ψ reads:

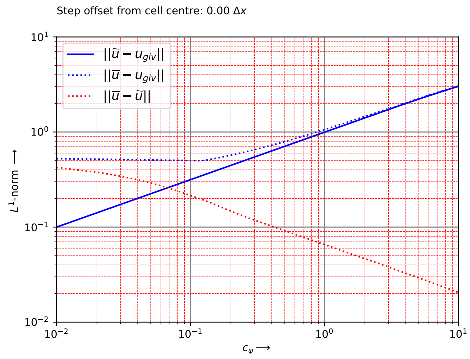
$$c_\Psi = \frac{1}{(k\Delta x)^2} \quad \Rightarrow \quad c_\Psi = \frac{N^2}{(2\pi)^2} \approx 4 \tag{A.21}$$

Table A.1: *Several typical values for numerical accuracy, c_ψ and number of nodes per wavelength (N), the highligthed line is set as default.*

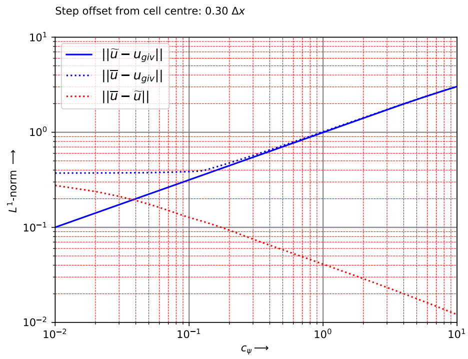
	Accuracy	c_Ψ	N
1	5 %	0.5	4.5
2	2 %	2	8.9
3	1 %	4	12.8
4	0.5 %	10	18.1

A.3 L^1-norm for the functions $\widetilde{u}$, $\overline{u}$ and u_{given}

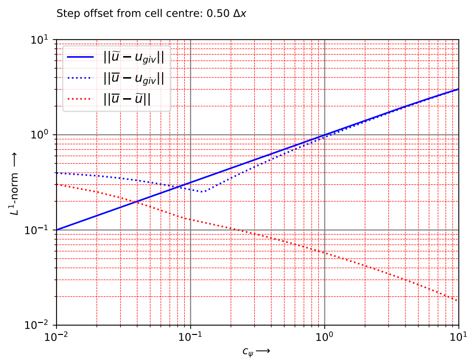
The next figures show the L^1-norm for the functions $||\widetilde{u} - u_{giv}||_1$, $||\overline{u} - u_{giv}||_1$ and $||\overline{u} - \widetilde{u}||_1$



***(a)** Step defined at cell centre.*



***(b)** Step defined with an of set of 0.3 Δx from cell centre.*

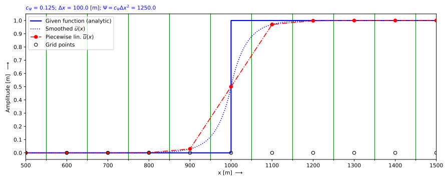


***(c)** Step defined with an of set of 0.5 Δx from cell centre, thus defined at cell face.*

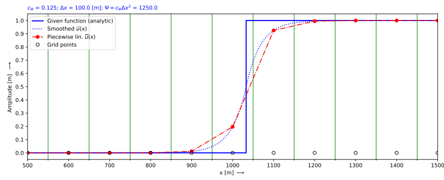
***Figure A.3:** Several plots of L^1-norm for different locations of the step.*

As seen from these figures. When choosing $c_\Psi > 4$ then the L^1-norm of $||\overline{u} - \widetilde{u}||_1$ is for all locations of the step smaller then 2×10^{-2} (red dotted lines in the plots). Also the blue and blue dotted line are close together for $c_\Psi > 4$. That is the region in which we want to have the discetisation because there is the difference between the piecewise linear numerical solution $\overline{u}$ and the regularized solution $\widetilde{u}$ is independent of the location of the step, given by the function u_{giv}.

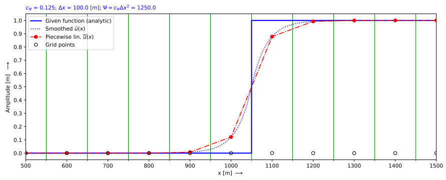
We also see that the dotted blue line is completely above the blue line if the step is located at the cell centre and with an offset of $0.3\Delta x$ (see Figure A.3a and Figure A.3b) and it is partly below the blue line if the offset of the step is located at $0.5\Delta x$ (Figure A.3c). The dotted blue line has also a sharp bend at the location where $c_\Psi = 0.125$. These approximations are presented in the Figure A.4a, Figure A.4b and Figure A.4c. As seen from these plot the piecewise linear approximation shown in Figure A.4c is closer to the Heaviside function as the other two approximations.



(a) *Step defined at cell centre.*



(b) *Step defined with an of set of 0.3 Δx from cell centre.*



(c) *Step defined with an of set of 0.5 Δx from cell centre, thus defined at cell face.*

Figure A.4: *Several plots of the piecewise linear approximation ($\overline{u}$) of the Heaviside function compared to the regularized function ($\widetilde{u}$).*

B Diagonalise 1D wave equation with convection

The one dimensional shallow water equations with convection read

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0 \tag{B.1}$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{h}\right) + gh\frac{\partial \zeta}{\partial x} = 0 \tag{B.2}$$

Using $\zeta = h + z_b$ in the momentum equation the system of equations is written as:

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0 \; \frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{h}\right) + gh\frac{\partial h}{\partial x} \qquad = -gh\frac{\partial z_b}{\partial x} \tag{B.3}$$

The convection term can rewritten in the linear form for the derivatives as:

$$\frac{\partial}{\partial x}\left(\frac{q^2}{h}\right) = \frac{2q}{h}\frac{\partial q}{\partial x} - \frac{q^2}{h^2}\frac{\partial h}{\partial x} \tag{B.4}$$

In matrix notation it reads ($\zeta = h + z_b$ is used):

$$\begin{pmatrix} h \\ q \end{pmatrix}_t + \begin{pmatrix} 0 & 1 \\ gh - \frac{q^2}{h^2} & \frac{2q}{h} \end{pmatrix} \begin{pmatrix} h \\ q \end{pmatrix}_x = -gh\begin{pmatrix} 0 \\ z_b \end{pmatrix}_x 0 \tag{B.5}$$

To make the system of equations diagonal, we have to find the eigen values and the eigen vectors. The eigenvalues of the matrix are (using **Maplesoft**)

$$\lambda_1 = \frac{q}{h} + \sqrt{gh} \qquad \text{and} \qquad \lambda_2 = \frac{q}{h} - \sqrt{gh} \tag{B.6}$$

The eigenvectors are

$$\begin{pmatrix} 1 \\ \frac{q}{h} + \sqrt{gh} \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} 1 \\ \frac{q}{h} - \sqrt{gh} \end{pmatrix} \tag{B.7}$$

The diagonalised SWE with convection read (after multiplying by $2\sqrt{gh}$, using **Maplesoft**)

$$\begin{pmatrix} \sqrt{gh} - \frac{q}{h} & 1 \\ \sqrt{gh} + \frac{q}{h} & -1 \end{pmatrix} \begin{pmatrix} h \\ q \end{pmatrix}_t + \begin{pmatrix} \frac{q}{h} + \sqrt{gh} & 0 \\ 0 & \frac{q}{h} - \sqrt{gh} \end{pmatrix} \begin{pmatrix} \sqrt{gh} - \frac{q}{h} & 1 \\ \sqrt{gh} + \frac{q}{h} & -1 \end{pmatrix} \begin{pmatrix} h \\ q \end{pmatrix}_x =$$

$$= -gh\begin{pmatrix} \sqrt{gh} - \frac{q}{h} & 1 \\ \sqrt{gh} + \frac{q}{h} & -1 \end{pmatrix} \begin{pmatrix} 0 \\ z_b \end{pmatrix}_x \tag{B.8}$$

Written in two separate equations

$$\left(\sqrt{gh}-\frac{q}{h}\right)\frac{\partial h}{\partial t}+\frac{\partial q}{\partial t}+\left(\frac{q}{h}+\sqrt{gh}\right)\left(\left(\sqrt{gh}-\frac{q}{h}\right)\frac{\partial h}{\partial x}+\frac{\partial q}{\partial x}\right)=$$

$$=-gh\frac{\partial z_b}{\partial x}\quad\text{right going}\tag{B.9}$$

$$\left(\sqrt{gh}+\frac{q}{h}\right)\frac{\partial h}{\partial t}-\frac{\partial q}{\partial t}+\left(\frac{q}{h}-\sqrt{gh}\right)\left(\left(\sqrt{gh}+\frac{q}{h}\right)\frac{\partial h}{\partial x}-\frac{\partial q}{\partial x}\right)=$$

$$=gh\frac{\partial z_b}{\partial x}\quad\text{left going}\tag{B.10}$$

First rearrange the equation for the right going wave (keep in mind that also Equation (B.4) is used):

$$\left(\sqrt{gh}-\frac{q}{h}\right)\frac{\partial h}{\partial t}+\frac{\partial q}{\partial t}+\left(gh-\frac{q^2}{h^2}\right)\frac{\partial h}{\partial x}+\left(\frac{q}{h}+\sqrt{gh}\right)\frac{\partial q}{\partial x}=-gh\frac{\partial z_b}{\partial x}\tag{B.11}$$

$$\left(\sqrt{gh}-\frac{q}{h}\right)\left(\frac{\partial h}{\partial t}+\frac{\partial q}{\partial x}\right)+\left(\frac{\partial q}{\partial t}+\frac{\partial}{\partial x}\left(\frac{q^2}{h}\right)+gh\frac{\partial \zeta}{\partial x}\right)=0\tag{B.12}$$

and second, rearrange the equation for the left going wave:

$$\left(\sqrt{gh}+\frac{q}{h}\right)\frac{\partial h}{\partial t}-\frac{\partial q}{\partial t}+\left(\frac{q^2}{h^2}-gh\right)\frac{\partial h}{\partial x}-\left(\frac{q}{h}-\sqrt{gh}\right)\frac{\partial q}{\partial x}=gh\frac{\partial z_b}{\partial x}\tag{B.13}$$

$$\left(\sqrt{gh}+\frac{q}{h}\right)\left(\frac{\partial h}{\partial t}+\frac{\partial q}{\partial x}\right)-\left(\frac{\partial q}{\partial t}+\frac{\partial}{\partial x}\left(\frac{q^2}{h}\right)+gh\frac{\partial \zeta}{\partial x}\right)=0\tag{B.14}$$

Which can be written as a combination of the continuity (B.1) and momentum equation (B.2) (see also Borsboom (2001, eq. 4)),

$$\begin{array}{c}\text{right going}\\ \text{left going}\end{array}\quad\begin{pmatrix}\sqrt{gh}-\frac{q}{h} & 1\\ \sqrt{gh}+\frac{q}{h} & -1\end{pmatrix}\begin{pmatrix}\textit{continuity eq.}\\ \textit{momentum eq.}\end{pmatrix}=0\tag{B.15}$$

or, after multiplying with h

$$\begin{array}{c}\text{right going}\\ \text{left going}\end{array}\quad\begin{pmatrix}h\sqrt{gh}-q & h\\ h\sqrt{gh}+q & -h\end{pmatrix}\begin{pmatrix}\textit{continuity eq.}\\ \textit{momentum eq.}\end{pmatrix}=0\tag{B.16}$$

C Error function needed to regularize the artificial viscosity

Regularization of the artificial viscosity, assumed to be independent of time, is described in section 3.2. The mentioned error-function is derived in this section and is based on Borsboom (2001, eq. 42):

We start from the continuity and momentum equation for non-linear waves (i.e. Equation (5.54) and (5.55) and combine these two equations to one equation representing the energy.

The continuity and momentum equation read:

$$\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0 \qquad \textit{continuity eq.} \tag{C.1}$$

$$\frac{\partial q}{\partial t} + \frac{\partial}{\partial x}\left(\frac{q^2}{h}\right) + gh\frac{\partial h}{\partial x} = 0 \qquad \textit{momentum eq.} \tag{C.2}$$

a suitable combination of these two equations yields the energy equation. The suitable combination is:

$$\left(\frac{1}{2}\frac{q^2}{h^2} + g\zeta\right)(\textit{continuity eq.}) + \frac{q}{h}(\textit{momentum eq.}) = 0 \tag{C.3}$$

and the energy equation reads:

$$\frac{\partial}{\partial t}\left(h\left(\frac{1}{2}\frac{q^2}{h^2} + g\zeta - \frac{1}{2}gh\right)\right) + \frac{\partial}{\partial x}\left(q\left(\frac{1}{2}\frac{q^2}{h^2} + g\zeta\right)\right) = 0 \tag{C.4}$$

For a steady state solution ($\partial/\partial t = 0$ and $q = \textit{Constant}$), when have:

$$\frac{\partial}{\partial x}\left(\frac{1}{2}\frac{q^2}{h^2} + g\zeta\right) = \frac{q}{h^2}\frac{\partial q}{\partial x} - \frac{q^2}{h^3}\frac{\partial h}{\partial x} + g\frac{\partial \zeta}{\partial x} = 0 \tag{C.5}$$

We assume that the artificial viscosity Ψ is proportional to the numerical error of the gradient term.

Based on potential energy

Looking to square root of the potential energy

$$Err\left(\sqrt{g\hat{h}}\right) = \sqrt{g\hat{h}} - \sqrt{g\overline{h}} \approx \tag{C.6}$$

$$\approx \sqrt{g\left(\overline{h} + \frac{1}{8}\Delta x^2 \frac{\partial^2 \overline{h}}{\partial x^2}\right)} - \sqrt{g\overline{h}} = \tag{C.7}$$

$$= \sqrt{g\overline{h}\left(1 + \frac{1}{8\overline{h}}\Delta x^2 \frac{\partial^2 \overline{h}}{\partial x^2}\right)} - \sqrt{g\overline{h}} \approx \tag{C.8}$$

$$\approx \sqrt{g\overline{h}}\left(1 + \frac{1}{16\overline{h}}\Delta x^2 \frac{\partial^2 \overline{h}}{\partial x^2}\right) - \sqrt{g\overline{h}} = \tag{C.9}$$

$$= \frac{1}{16}\Delta x^2 \sqrt{\frac{g}{\overline{h}}}\frac{\partial^2 \overline{h}}{\partial x^2} \tag{C.10}$$

Because $\partial^2 z_b/\partial x^2$ is negligible, due to the regularization of the bedlevel, we get:

$$Err\left(\sqrt{g\hat{h}}\right) = \frac{1}{16}\Delta x^2 \sqrt{\frac{g}{\overline{h}}}\frac{\partial^2 \zeta}{\partial x^2} \tag{C.11}$$

$$\Rightarrow \frac{1}{16}\Delta \xi^2 \sqrt{\frac{g}{\overline{h}}}\frac{\partial^2 \zeta}{\partial \xi^2}, [\mathrm{m\,s^{-1}}]. \tag{C.12}$$

Based on kinetic energy

Looking to square root of the kinetic energy: $\sqrt{u^2/2} = \frac{1}{2}\sqrt{2}\,|u| = \frac{1}{2}\sqrt{2}\,|q/h|$:

$$Err\left(\frac{1}{2}\sqrt{2}\frac{\hat{q}}{\hat{h}}\right) = \frac{1}{2}\sqrt{2}\left(\frac{\hat{q}}{\hat{h}} - \frac{\overline{q}}{\overline{h}}\right) \approx \frac{1}{2}\sqrt{2}\left(\frac{\overline{q} + \frac{1}{8}\Delta x^2 \frac{\partial^2 \overline{q}}{\partial x^2}}{\overline{h} + \frac{1}{8}\Delta x^2 \frac{\partial^2 \overline{h}}{\partial x^2}} - \frac{\overline{q}}{\overline{h}}\right) = \tag{C.13}$$

$$= \frac{1}{2}\sqrt{2}\left(\frac{\overline{q}}{\overline{h}}\frac{1 + \frac{1}{8}\Delta x^2 \frac{1}{\overline{q}}\frac{\partial^2 \overline{q}}{\partial x^2}}{1 + \frac{1}{8}\Delta x^2 \frac{1}{\overline{h}}\frac{\partial^2 \overline{h}}{\partial x^2}} - \frac{\overline{q}}{\overline{h}}\right) \approx \tag{C.14}$$

$$\approx \frac{1}{2}\sqrt{2}\left(\frac{\overline{q}}{\overline{h}}\left(1 + \frac{1}{8}\Delta x^2 \frac{1}{\overline{q}}\frac{\partial^2 \overline{q}}{\partial x^2}\right)\left(1 - \frac{1}{8}\Delta x^2 \frac{1}{\overline{h}}\frac{\partial^2 \overline{h}}{\partial x^2}\right) - \frac{\overline{q}}{\overline{h}}\right) \approx \tag{C.15}$$

$$\approx \frac{1}{2}\sqrt{2}\left(\frac{1}{8}\Delta x^2 \frac{1}{\overline{h}}\frac{\partial^2 \overline{q}}{\partial x^2} - \frac{1}{8}\Delta x^2 \frac{\overline{q}}{\overline{h}^2}\frac{\partial^2 \overline{h}}{\partial x^2}\right) \tag{C.16}$$

$$\Rightarrow \frac{1}{16}\sqrt{2}\Delta \xi^2 \left(\frac{1}{\overline{h}}\frac{\partial^2 \overline{q}}{\partial \xi^2} - \frac{\overline{q}}{\overline{h}^2}\frac{\partial^2 \overline{h}}{\partial \xi^2}\right), [\mathrm{m\,s^{-1}}]. \tag{C.17}$$

The error function for artificial viscosity Err_Ψ reads (comparable with Borsboom (2001, eq. 42)):

$$Err_\Psi = \Delta\xi \overline{x}_\xi \left(\frac{1}{16}\sqrt{\frac{g}{\overline{h}}}\left|D_\xi(\overline{\zeta})\right| + \frac{\sqrt{2}}{16}\left|\frac{1}{\overline{h}}D_\xi(\overline{q}) - \frac{\overline{q}}{\overline{h}^2}D_\xi(\overline{h})\right|\right), \quad [\mathrm{m^2\,s^{-1}}] \tag{C.18}$$

with D_ξ defined as (Borsboom, 2001, eq. 35):

$$D_\xi = \Delta\xi^2 \frac{\partial^2 u}{\partial \xi^2} \approx u_{i-1} - 2u_i + u_{i+1}, \quad u \in \{q, h, \zeta\} \tag{C.19}$$

D Linearization in time

D.1 Viscosity term

The viscosity term read:

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \frac{\partial}{\partial x}\left(\nu h \frac{\partial (q/h)}{\partial x}\right) dx \;= \nu\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right)\bigg|_{x_{i+\frac{1}{2}}} - \nu\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right)\bigg|_{x_{i-\frac{1}{2}}} \tag{D.1}$$

Linearization of the viscosity term at $x_{i+\frac{1}{2}}$ read, where $\Delta h^{n+1,p+1} = \Delta h$ and $\Delta q^{n+1,p+1} = \Delta q$:

$$\nu h \frac{\partial (q/h)}{\partial x}\bigg|^{n+\theta,p+1} = \nu\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right)\bigg|^{n+\theta,p+1} \approx \tag{D.2}$$

$$\approx \nu \frac{\partial}{\partial x}\left(q^{n+\theta,p} + \theta\Delta q\right) - \nu \frac{q^{n+\theta,p} + \theta\Delta q}{h^{n+\theta,p} + \theta\Delta h}\frac{\partial}{\partial x}\left(h^{n+\theta,p} + \theta\Delta h\right) \approx \tag{D.3}$$

with

$$\frac{q^{n+\theta,p} + \theta\Delta q}{h^{n+\theta,p} + \theta\Delta h} \approx \frac{q^{n+\theta,p} + \theta\Delta q}{h^{n+\theta,p}}\left(1 - \frac{\theta\Delta h}{h^{n+\theta,p}} + \left(\frac{\theta\Delta h}{h^{n+\theta,p}}\right)^2 - \left(\frac{\theta\Delta h}{h^{n+\theta,p}}\right)^3 + \dots\right) = \tag{D.4}$$

$$= \frac{q^{n+\theta,p}}{h^{n+\theta,p}} - \frac{q^{n+\theta,p}}{(h^{n+\theta,p})^2}\theta\Delta h + \frac{1}{h^{n+\theta,p}}\theta\Delta q + O\left(\Delta q\Delta h, (\Delta h)^2\right) \tag{D.5}$$

leaving out the terms of $O\left(\Delta q\Delta h, (\Delta h)^2\right)$, yields:

$$\nu h \frac{\partial (q/h)}{\partial x}\bigg|^{n+\theta,p+1} = \nu\left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x}\right)\bigg|^{n+\theta,p+1} \approx \tag{D.6}$$

$$\approx \nu \frac{\partial}{\partial x}\left(q^{n+\theta,p} + \theta\Delta q\right) + \tag{D.7}$$

$$- \nu\left(\frac{q^{n+\theta,p}}{h^{n+\theta,p}} + \frac{1}{h^{n+\theta,p}}\theta\Delta q - \frac{q^{n+\theta,p}}{(h^{n+\theta,p})^2}\theta\Delta h\right)\frac{\partial}{\partial x}\left(h^{n+\theta,p} + \theta\Delta h\right) = \tag{D.8}$$

$$= \nu \frac{\partial q^{n+\theta,p}}{\partial x} + \nu\frac{\partial}{\partial x}\theta\Delta q + \tag{D.9}$$

$$- \nu \frac{q^{n+\theta,p}}{h^{n+\theta,p}}\frac{\partial h^{n+\theta,p}}{\partial x} - \nu\frac{q^{n+\theta,p}}{h^{n+\theta,p}}\frac{\partial}{\partial x}\theta\Delta h - \frac{1}{h^{n+\theta,p}}\frac{\partial h^{n+\theta,p}}{\partial x}\theta\Delta q + \frac{q^{n+\theta,p}}{(h^{n+\theta,p})^2}\frac{\partial h^{n+\theta,p}}{\partial x}\theta\Delta h \tag{D.10}$$

rearranged

$$\nu h \frac{\partial (q/h)}{\partial x}\Bigg|^{n+\theta,p+1} = \nu \left(\frac{\partial q}{\partial x} - \frac{q}{h}\frac{\partial h}{\partial x} \right)\Bigg|^{n+\theta,p+1} \approx \tag{D.11}$$

$$= \nu \frac{\partial q^{n+\theta,p}}{\partial x} - \nu \frac{q^{n+\theta,p}}{h^{n+\theta,p}} \frac{\partial h^{n+\theta,p}}{\partial x} + \tag{D.12}$$

$$+ \nu\theta \frac{\partial \Delta q}{\partial x} - \nu\theta \frac{1}{h^{n+\theta,p}} \frac{\partial h^{n+\theta,p}}{\partial x} \Delta q + \nu\theta \frac{q^{n+\theta,p}}{(h^{n+\theta,p})^2} \frac{\partial h^{n+\theta,p}}{\partial x} \Delta h - \nu\theta \frac{q^{n+\theta,p}}{h^{n+\theta,p}} \frac{\partial \Delta h}{\partial x} \tag{D.13}$$

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