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Rapport N°2:

1. Implementation of Implicit and explicit Fluctuation Splitting Schemes in WW3

1.1. Introduction

As an alternative to well know family of Finite Volume Schemes or Finite Element Schemes the Family of Residual Distribution Schemes (RD; also known as "Fluctuation Splitting Schemes") have been considered for implementation in the WW3 model. The RD-schemes are a new family of numerical schemes which borrow ideas from the Finite Element (FE) and the Finite Volume (FV) framework. As a result, compact schemes and accurate solutions can be achieved on the framework of the philosophy of fluctuation splitting. Abgrall (2006) gives a recent review on the history and future trends of fluctuation splitting schemes. The Residual Distribution technique was first introduced by Roe (1982) and further improved and modified by many other scientists (e.g. Abgrall, Deconinck, Roe and others).

As a starting point, the RD-philosophy will be explained for the linear advection equation following the thesis of Tomaich (1995). The linear advection equations for the WAE or for any scalar quantity in a divergence free flow reads:

$$\frac{\partial N}{\partial t} + \boldsymbol{c}_X \nabla_X N = 0 \tag{1.1}$$

This form of the advection equation is valid for deep water waves that are not interacting with the bottom or the ambient currents. The derivation of the RD-schemes for the general case of the WAE (eq.(1.2)) is shown hereinafter.

$$\frac{\partial N}{\partial t} + \nabla_X \left(\boldsymbol{c}_X N \right) = 0 \tag{1.2}$$

Eq. 1.2 can be integrated by isolating the time derivative and integrating eq. 1.2 over the whole domain Ω.

$$\int_\Omega \frac{\partial N}{\partial t} dA = -\int_\Omega \mathrm{c}_g \nabla N dA \quad . \tag{1.3}$$

where the domain Ω is divided into a triangular mesh with a conformal triangulation (see Figure 1).

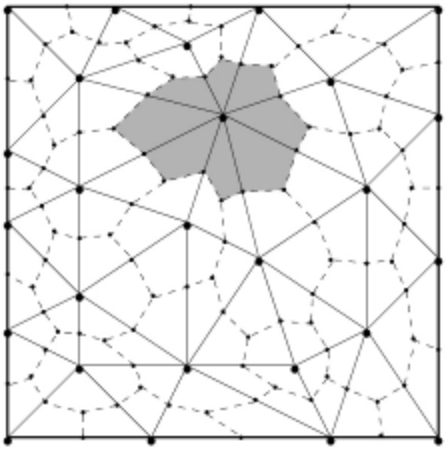

Figure 1: Sample grid with median dual areas, adapted from Tomaich (1995)

A cell is defined with its vertices i that are numbered counter clock wise and have unique coordinates i(xi,yi). The discrete solutions are stored at the vertices of the triangulation. Eq. 1.3 can be rewritten as the sum of the integrals over each triangular cell N.

$$\int_{\Omega} \frac{\partial N}{\partial t} dA = \sum_{i=1}^{N} \int_{T} \frac{\partial N}{\partial t} dA \tag{1.4}$$

The integral on the right hand side of eq. (1.4) can be reformulated with the aid of eq. (1.3) as

$$\int_{T} \frac{\partial N}{\partial t} dA = -\int_{T} \boldsymbol{c}_X \nabla N dA = \Phi_T \tag{1.5}$$

Here “the integral of the time derivative over the cell is equal the fluctuation of that cell” (cf. Tomaich, 1995). The “total fluctuation” of a cell or “the residual of a cell” is named Φ_T .

For evaluation of these integrals over a triangular cell a distribution function within a cell for the unknown quantity must be assumed. In the fluctuation-splitting framework, usually a linear variation of the dependent variable within the triangular cell is assumed resulting in a linear basis function in every triangular element. The approximate solution of the unknowns can be expressed as

$$\tilde{N}_{(t,x,y)} = \sum_{i=1}^{3} w_{(x,y)} \cdot N_{(t)i} \tag{1.6}$$

where wi are the linear basis functions (see Figure) defined at each vertex. The RD-schemes borrows at this stage the idea from the Finite Element Method, see e.g. Donea (1985), eq. (1.6) is similar to his eq. 7.

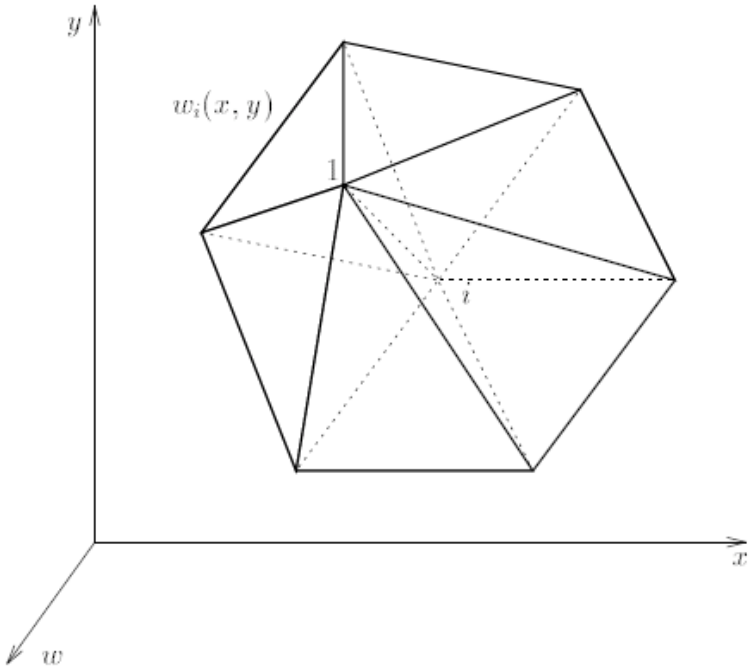

Figure 2: Two dimensional linear basis functions for triangular elements (adopted from Tomaich, 1995).

The total cell fluctuation (eq. **Fehler! Verweisquelle konnte nicht gefunden werden.**) can now be written in a discrete form introducing the spatial derivative of wave action, which is given for a linear basis function wi within the element as:

$$\nabla N = -\frac{1}{2S_T}\sum_{i=1}^{3} N_i \boldsymbol{n_i} \tag{1.7}$$

Substituting eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** in the right hand side of eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** one can rewrite the total fluctuation as follows:

$$\begin{aligned}\Phi_T &= -\int_T \boldsymbol{c}_X \nabla N dA \\ &= \sum_{i=1}^{3} \frac{1}{2}\lambda \cdot N_i \cdot \boldsymbol{n_i} = \sum_{i=1}^{3} N_i \left(\frac{1}{2}\lambda \cdot \boldsymbol{n_i}\right) = \sum_{i=1}^{3} k_i N_i\end{aligned} \tag{1.8}$$

ST is the area of the triangle and n_i the edge normal vector defined according to Figure. The vectors n_i are scaled with the edge length to opposite to its vertices. is the linearized advection vector of the cell. In this special case it was assumed that it is constant in spatial space (no currents, deep water) so it follows that:

$$\lambda = \frac{1}{3}\sum_{i=1}^{3} \boldsymbol{c}_{X,i} = \boldsymbol{c}_{X,i} \text{ for } \boldsymbol{c}_{X,i} \neq \boldsymbol{c}_{X,i(X)} \tag{1.9}$$

Introducing the scalars ki

$$k_i = \frac{1}{2}\lambda \boldsymbol{n_i} \tag{1.10}$$

one can see that the sum of all vectors ni is zero so that following identity is valid:

$$\sum_{i=1}^{3} \boldsymbol{n_i} = 0 \quad . \tag{1.11}$$

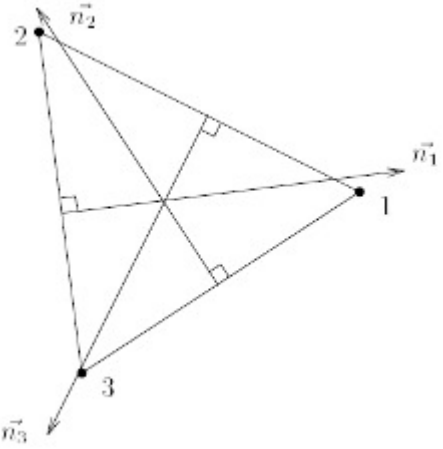

Figure 3: Definition of the edge normal vectors (adapted from Tomaich, 1995).

From eq. (1.11) immediately follows that

$$\sum_{i=1}^{3} k_i = 0 \tag{1.12}$$

These relationships are important for the further derivation of the RD-schemes. The total fluctuation of a triangular cell for the linear conservation law can now be rewritten using the above-defined relationships as follows:

$$\Phi_T = \sum_{i=1}^{3} k_i N_i = \sum_{i=1}^{3} \alpha_i \Phi_T = \sum_{i=1}^{3} \Phi_{i,T} \quad , \tag{1.13}$$

α_i are the redistribution coefficients that must be in their sum unity in order to guarantee conservation,

$$\sum_{i=1}^{3} \alpha_i = 1 \tag{1.14}$$

Si is the median dual cell area (see Fig. 11), which can be evaluated as the sum of one third of the cell areas Ai connected to the certain vertex.

$$S_i = \sum_{i=1}^{N_{con.}} \frac{1}{3} \cdot A_i \tag{1.15}$$

The approximation of eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** is then obtained through the following finite volume type time updating procedure.

$$N_i^{n+1} = N_i^n + \frac{\Delta t}{S_i} \sum_{T, i \in D_i} \Phi_{i,T} \quad . \tag{1.16}$$

In order to update the solution, the contribution of all fluctuations $\Phi_{i,T}$, that are members of the set of triangles Di (element patch) connected to node I, are cumulated. The cumulated cell fluctuations are weighted by the area of the median dual cell, which results in an updating scheme, which is very similar to cell-vertex FV-schemes (e.g. Qian et al. 2007). One advantage of the above described updating procedure is that for FV-schemes the nodal update is calculated as the sum of the edge fluxes defining the median dual cell, which are twice more than cells needed for the update in the FS scheme. This is a computational advantage of the RD-schemes in comparison to the cell-vertex FV-schemes. The sum of all nodal fluctuations, contributing to the nodal update, vanishes when eq. (1.16) reaches its steady state solution:

$$\sum_{T,i\in T_i} \Phi_{i,T} = 0 \tag{1.17}$$

After the total fluctuation of a certain cell has been calculated, it must be distributed over the vertices of the cell. The main problem in designing the schemes lies in the definition of the redistribution coefficients αi, which characterizes the final advection scheme. Certain design principles are defined in order to develop proper redistribution schemes. These criteria are

Conservation or property (C) requires that the solution at the new time level n+ 1 conserves the depended variable. This is guaranteed as long as the distribution coefficients αi in eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** are in their sum unity.

Positivity of the scheme, or the so called property (P). For a linear scheme, the solution at the new time level can be written as sum of the product between the coefficients ck, resulting from the discretization of a certain scheme. The values of the updated solution are positive if the coefficients $\tilde{c}_k$ are positive (eq. **Fehler! Verweisquelle konnte nicht gefunden werden.**)

$$u_i^{n+1} = \sum_{k=1}^{N} \tilde{c}_k \cdot u_k^n \tag{1.18}$$

For explicit schemes this condition is normally strictly connected to a CFL stability criterion, which must be maintained in order to get stable and monotone solutions. For the explicit schemes, in the RD-framework this criterion is:

$$\Delta t_i = \max_{T,i\in D_i} \left(\frac{k_i^+}{A_i} \right) \tag{1.19}$$

Linear Preservation (LP); Condition LP prescribes that the numerical scheme maintains 2nd order accuracy at steady state in smooth regions of the solution while retaining monotonicity when fulfilling the CFL-like condition.

Linear schemes[1] cannot be both P and LP at the same time according to “Godunov's order barrier theorem”, which states that linear monotone schemes cannot be of second order without producing oscillative solutions. It is possible to construct second order linear preserving schemes, but this makes a nonlinear redistribution of the fluctuations necessary. In the framework of explicit time integration schemes, this can be done with the application of so called “Flux limiters” or with the aid of blending of linear monotone and nonlinear non-monotone schemes (e.g. Roe, Leonard and many others). In the framework of Finite Volume schemes, this is called “Total Variation Diminishing” criterion. The second order fluxes of the non-monotone schemes are limited near the strong gradients, where these schemes would otherwise produce non-positive values, and monotone first order schemes are used to obtain the solution. The art of designing such limiters is to apply them only in situations where the second order schemes lead to non-monotone results maintaining second order accuracy as often as possible. In the RD-framework, similar technique can be applied as done in e.g. by Hubbard & Roe(2002). One advantage of explicit integration schemes is that they are faster than implicit schemes because no linear equation system has to be solved. Another advantage is that nonlinear schemes can be designed in order to fulfil all the above-mentioned design criteria. The results are non-oscillatory monotone higher order space/time schemes with a high accuracy.

However, in certain applications, where a high spatial resolution is needed, the limiting factor for the explicit schemes becomes the stability criterion of eq. **Fehler! Verweisquelle konnte nicht gefunden werden.**. The numerical scheme can become unfeasible with respect to the needed computational time.

Implicit schemes have with respect to this a clear advantage, they can be designed in such a way that their stability and monotonicity does not depend on the CFL criterion. The price to pay is the solution of a linear equation system that evolved in the solution procedure. The computational time for the implicit scheme is roughly two times greater than for

1 Linear schemes, in the sense, that the solution at the new time level is a linear combination of the old values of the solution.

the implicit schemes for the case of the explicit and implicit N-scheme (see next subsection). In order to obtain an unconditionally monotone implicit scheme that is also LP will lead, because of the Godunov theorem, to a nonlinear scheme (see e.g. Abgrall & Mezine, 2002 and Richuotto et al., 2005). The resulting equation system becomes in this case naturally also nonlinear and iterative methods have to be used for the solution. For the WAE this is a crux since the advection part must be solved for each spectral component that average around 800 -1200 quantities with different advection velocities makes an application of a nonlinear equation solver to a computationally very expensive task. In this thesis, the author did not consider nonlinear implicit schemes because of the necessary iterative solution procedure and the associated computational costs. As long as the implicit schemes are linear and monotonicity should be retained the schemes cannot be second order in space and time and though LP. Higher order linear schemes will always be limited by a CFL as condition for which monotonicity is retained.

2. Explicit Residual Distribution schemes

2.1 The CRD N-scheme

The basis of all RD-schemes is the N-Scheme, which has its name because of its narrow numerical stencil as it uses only the nearest neighbour nodes to compute the nodal update of the solution. In order to describe the N-Scheme for the general nonlinear conservation law, first the scheme for a linear conservation law given by eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** will be derived. The standard N-scheme can be designed introducing an upwinding for the distribution of the total fluctuation over the nodes of the elements. In order to do so it must be distinguished between two and one-sided inflow triangles (e.g. Tomaich, 1995). The amount of inflow sides and the upwind nodes are defined through the signs of the k-values. For the simple case of one inflow side, the whole fluctuation Φ_T is sent to the upwind node. For the more complicated case of two inflow sides, the total fluctuation is split between the nodes. The method of this splitting defines the final character of the scheme. The total fluctuation can be rewritten using eq. (1.11), for the case of two inflow edges as shown in Figure , as

$$\Phi_T = k_2 \cdot (N_2 - N_1) + k_3 \cdot (N_3 - N_1) \,. \tag{1.20}$$

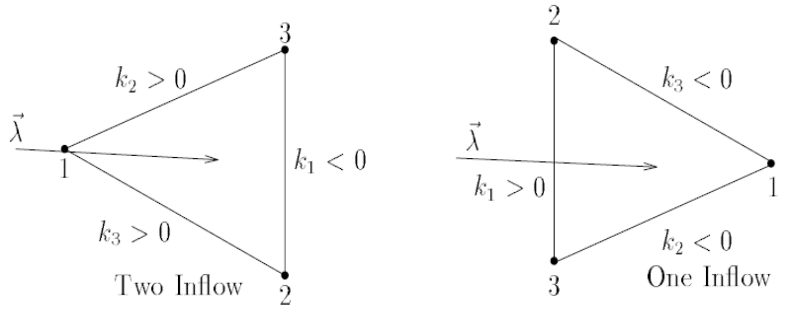

Figure 4: Two and one side inflow within a triangle according to Tomaich (1995)

From eq. (1.20) the splitting is obvious and the redistribution of the fluctuations for the N-scheme reads

$$\begin{aligned} \Phi_{1,T} &= 0 \\ \Phi_{2,T} &= k_2 \cdot (N_2 - N_1) \\ \Phi_{3,T} &= k_3 \cdot (N_3 - N_1) \end{aligned} \tag{1.21}$$

Following e.g. Abgrall (2006) the N-scheme can be written in a more compact form introducing positive and the negative k's

$$k_i^+ = \max(k_i, 0)$$
$$k_i^- = \min(k_i, 0) \tag{1.22}$$

so that

$$k_i = k_i^+ + k_i^- \tag{1.23}$$

and the upwind residual becomes

$$\tilde{N} = \tilde{n} \cdot \left(\sum_{i=1}^{3} k_i^- N_i \right) \tag{1.24}$$

With

$$\tilde{n} = \left(\sum_{i=1}^{3} k_i^- \right)^{-1} \tag{1.25}$$

The resulting splitting for the total fluctuation may now be written as

$$\Phi_{i,T} = k_i^+ (N_i - \tilde{N}) \tag{1.26}$$

It can be easily seen that, when cumulating all nodal fluctuations according to eq. (1.27), the total fluctuation of the cell is obtained which renders the scheme a conservative one.

$$\Phi_T = \sum_{i=1}^{3} \Phi_{i,T} \tag{1.27}$$

The above set of equations define the standard N-scheme for linear conservations laws according to eq. **Fehler! Verweisquelle konnte nicht gefunden werden.**. The resulting scheme is valid only for the WAE in the case of the deep-water waves without ambient currents when the group velocities are divergence free in geographic space. The flux form, which is valid in the general case, is defined as

$$\frac{\partial N}{\partial t} + \nabla_X \left(\boldsymbol{c}_X N \right) = 0 \tag{1.28}$$

and can be rewritten using the product rule giving eq.(1.29)

$$\frac{\partial N}{\partial t} + \nabla_X \left(\boldsymbol{c}_X N \right) = \frac{\partial N}{\partial t} + \boldsymbol{c}_X \nabla_X N + N \nabla_X \boldsymbol{c}_X \tag{1.29}$$

Since the last term of the right hand side of eq. (1.29) does not vanish[2] in the general case, there is no obvious linearization for eq. (1.28) and therefore the conservative form must be solved given through eq. (1.28).

2 The solution of the linearized equations in shallow water would result e.g. in an absence of the shoaling effect.

In order to construct a conservative scheme in terms of the RD-framework, Csik et al (2002) introduced the CRD-scheme (Conservative contour Integral based Residual Distribution scheme) where the total cell fluctuation is evaluated over the cell contour integrating an arbitrary flux function F with a higher order integration method for the evolving Gauss integral eq. (1.30).

$$\Phi_T = -\oint_{\partial T} \nabla \mathbb{F} \cdot \vec{n} dS \tag{1.30}$$

For the WAE, the flux function is defined as

$$\mathbb{F} = \boldsymbol{c}_X \cdot \mathrm{N} \tag{1.31}$$

For the case of the conservative form of the WAE, which is valid for general nonlinear conservation laws, the nodal residual must be calculated according to Csik et al. (2002). The authors suggested replacing eq. (1.24) with the following formula in order to conserve an arbitrary flux function F.

$$\tilde{N} = \tilde{n} \cdot \left(\sum_{i=1}^{3} k_i^+ N_i - \Phi_T \right) \tag{1.32}$$

Eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** can easily be derived when rewriting eq. (1.8) for the case of the two inflow edges and calculating the contribution of the upwind node, but with the difference that the total fluctuation Φ_T is an unknown quantity. This leads directly to eq. (1.33), which is equivalent to eq. (1.32).

$$N_1 = \frac{1}{k_1} \left(k_2 \cdot N_2 + k_3 \cdot N_3 - \Phi_T \right) \tag{1.33}$$

If the upwind contribution is calculated this way it can be seen, when cumulating all contributions from the nodes of each element according to eq.**Fehler! Verweisquelle konnte nicht gefunden werden.**, that the total fluctuation is conserved when using eq. (1.32). Since the upwind contribution is now evaluated of terms of the total fluctuation Φ_T, integrating eq. (1.30) numerically, the conservation of arbitrary flux functions F is enforced. The linearized state, defined through the average velocity in the element, is used only for the identification of the upwind direction. This procedure can be seen as a correction of the linear advection scheme for the additional nonlinear flux.

The total cell fluctuation can be calculated with aid of the Simpson integration. The Gauss integral over the triangle edges (eq. (1.30)) must be evaluated with a higher order integration scheme (e.g. Simpson Rule) because if first order schemes, such as the “Trapezoidal Rule”, are used, the resulting scheme will not accurately conserve the fluctuations of the cell and may generate greater negative values in the vicinity of large gradients in the solution. The flux at the middle of each edge can be defined as the product of the average edge normal velocities and wave action densities at the nodes of each edge.

$$\Phi_T = -\oint_{\partial T} \nabla \mathbb{F} \cdot \mathrm{n} ds = \sum_{j=1}^{3} \int_{l_j} \mathbb{F} \cdot \mathrm{n}_j ds_j \tag{1.34}$$

The Simpson rule for one edge reads:

$$\int_{l_i} \mathbb{F} \cdot \mathrm{n} ds = \frac{l_j}{6} \left(F_\perp(a) + 4F_\perp\left(\frac{a+b}{2} \right) + F_\perp(b) \right) \tag{1.35}$$

$F_\perp$ are the edge normal fluxes at the beginning and the endpoint of the edge and are defined as:

$$F_{\perp}(a) = c^{\perp}_{a,j} \cdot N_a$$
$$F_{\perp}(b) = c^{\perp}_{b,j} \cdot N_b \tag{1.36}$$

a and b are representing the beginning and the endpoint of the edge and the index j runs over the edges of the triangle. N_a and N_b are the wave actions and $c^{\perp}_{a,j}$ and $c^{\perp}_{b,j}$ are the advection velocities normal to the edge j at point a and b respectively. The average wave-action-flux at the middle of the edge j is defined as with the average values of the wave action and the normal advection velocity at each node of edge j.

$$F_{\perp}\left(\frac{a+b}{2}\right) = \frac{c^{\perp}_{a,j} + c^{\perp}_{b,j}}{2} \cdot \frac{N_a + N_b}{2} \tag{1.37}$$

This can be rewritten as

$$4F_{\perp}\left(\frac{a+b}{2}\right) = N_a\left(c^{\perp}_{a,j} + c^{\perp}_{b,j}\right) + N_b\left(c^{\perp}_{a,j} + c^{\perp}_{b,j}\right) \tag{1.38}$$

Using eq. (1.35) and eq. (1.36) one can rewrite eq. (1.34) as:

$$\int_{l_j} \mathbb{F} \cdot \vec{n} ds = \frac{l_j}{6}\left(N_a\left(2c^{\perp}_{a,j} + c^{\perp}_{b,j}\right) + N_b\left(2c^{\perp}_{a,j} + c^{\perp}_{b,j}\right)\right) \tag{1.39}$$

For all edges of a certain element this can be written in a discrete form introducing node numbers i, i+1 and i+2 for a, b and c as

$$\begin{aligned}\oint_{\partial T} \nabla\mathbb{F} \cdot \vec{n} ds = {} & N_i\left(\frac{l_1}{6}\left(2c^{\perp}_{i,1} + c^{\perp}_{i+1,1}\right) + \frac{l_3}{6}\left(2c^{\perp}_{i+2,3} + c^{\perp}_{i,3}\right)\right) + \\ & N_{i+1}\left(\frac{l_2}{6}\left(2c^{\perp}_{i+1,2} + c^{\perp}_{i+2,2}\right) + \frac{l_1}{6}\left(2c^{\perp}_{i,1} + c^{\perp}_{i+1,1}\right)\right) + \\ & N_{i+2}\left(\frac{l_3}{6}\left(2c^{\perp}_{i+2,3} + c^{\perp}_{i,3}\right) + \frac{l_2}{6}\left(2c^{\perp}_{i+1,2} + c^{\perp}_{i+2,2}\right)\right)\end{aligned} \tag{1.40}$$

With some algebra eq.(1.39) can be expressed as

$$\Phi_T = \oint_{\partial T} \nabla\mathbb{F} \cdot \vec{n} ds = \sum_{i=1}^{3} N_i \delta_i \tag{1.40}$$

With

$$\begin{aligned}\delta_1 &= \frac{l_1}{6}\left(2c^{\perp}_{i,1} + c^{\perp}_{i+1,1}\right) + \frac{l_3}{6}\left(2c^{\perp}_{i+2,3} + c^{\perp}_{i,3}\right) \\ \delta_2 &= \frac{l_2}{6}\left(2c^{\perp}_{i+1,2} + c^{\perp}_{i+2,2}\right) + \frac{l_1}{6}\left(2c^{\perp}_{i,1} + c^{\perp}_{i+1,1}\right) \\ \delta_3 &= \frac{l_3}{6}\left(2c^{\perp}_{i+2,3} + c^{\perp}_{i,3}\right) + \frac{l_2}{6}\left(2c^{\perp}_{i+1,2} + c^{\perp}_{i+2,2}\right)\end{aligned} \tag{1.41}$$

The coefficient δi depends on the velocities at the edges and the geometry of the triangle. Using eq. (1.40) and eq. (1.30) eq. (1.34) can be rewritten as

$$\begin{aligned}\tilde{N} &= \tilde{n}\cdot\left(\sum_{i=1}^{3} k_i^+ N_i - \Phi_T\right)\\ &= \tilde{n}\cdot\left(\sum_{i=1}^{3} k_i^+ N_i - \sum_{i=1}^{3}\delta_i N_i\right)\\ &= \tilde{n}\cdot\left(\sum_{i=1}^{3} N_i\left(k_i^+ - \delta_i\right)\right)\end{aligned} \tag{1.42}$$

In this way, the upwind fluctuation can be expressed only with the nodal values that are functions of the geometry and the wave kinematics. This is important for the derivation of the implicit FS schemes. The CRD-N scheme has very similar characteristics as the standard N-Scheme. It is as explicit as the first order space/time scheme that is monotone under the CFL condition given in eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** and conservative. However, the presented variant of the N-scheme is quasi-positive, since for the CRD-approaches positivity cannot be proven due to the numerical integration of the flux function along the edges (Csik et al. 2002). However, the resulting scheme is monotone and the negative values are negligible and do not alter the conservation of the scheme when set to zero. The above set of discrete equations describes the CRD-N scheme as it is implemented in the WWM II.

2.2 The CRD-LDA (Low Diffusion Approximation) scheme

The LDA (Low Diffusion Approximation) scheme is of first order in time, second order in cross flow direction and first order in longitudal flow direction. The scheme is LP, but since it is linear, it is not positive and therefore non-monotone due to the Godunov theorem. However, the LDA-scheme is used in combination with lower order schemes (e.g. N-scheme) to design nonlinear schemes which fulfil all the above-mentioned design criteria such as the PSI (Positive Streamline Invariant) scheme or the FCT scheme using residual distribution. The nodal fluctuation of the standard LDA scheme reads for a certain element (e.g. Abgrall, 2006):

$$\Phi_{i,T} = -\tilde{n}k_i^+\Phi_T \tag{1.43}$$

It is easy to see that the above given scheme is conservative since the sum of the redistribution coefficients is unity when cumulated over all nodes of the element:

$$\sum_{i=1}^{3} -\tilde{n}k_i^+ = \sum_{i=1}^{3}\alpha_i = 1 \tag{1.44}$$

In order to formulate a contour integration based LDA scheme, the total fluctuation in eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** must be replaced by eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** in order to solve the conservative form of the WAE. The LDA scheme is a higher order linear scheme and therefore not positive and non-monotone. The resulting scheme achieves first order accuracy in time and second order in cross flow direction and first order in longitudal flow direction.

2.3 The CRD-PSI-scheme

As given in the introduction of this chapter, a scheme, which is conservative, positive, and linear preserving, must be, due to Godunov's Theorem, a nonlinear scheme. The PSI-scheme fulfils these demands and it was constructed with the aid of a blending parameter, which reduces the contribution of the higher order scheme when non-positive or non-

monotone solutions are expected (e.g. Abgrall, 2001). The nodal fluctuation of the PSI scheme can be defined with the blending parameter according to Abgrall (2002) as:

$$\Phi_{i,T,PSI} = l \cdot \Phi_{i,T,N} + (1-l) \cdot \Phi_{i,T,LDA} \tag{1.45}$$

with

$$l = \max\left(\phi(r_1), \phi(r_2), \phi(r_3)\right) \tag{1.46}$$

and

$$r_i = \frac{\Phi_{i,T,N}}{\Phi_{i,T,LDA}}$$
$$\varphi(x) = \begin{cases} \dfrac{x}{x-1} & \text{if } x < 1, \\ 0 & \text{else,} \end{cases} \tag{1.47}$$

The resulting scheme is nonlinear and it was shown by several authors that the scheme satisfies the above defined design criteria. Using the CRD-N scheme and the CRD-LDA scheme, the resulting CRD-PSI holds for any conservation law as the one given through eq. (1.28). The scheme is first order in time and it is at its best second order in cross flow direction and first order in longitudal flow direction. The scheme is positive for a linear conservation law. The PSI scheme was used hereinafter to construct a truly second order space-time scheme, which retains the above-defined design criteria on the foundation of the CRD approach of Csik et al., 2002.

2.4 The CRD-FCT scheme

Hubbard & Roe (2000) combined two fluctuation splitting schemes, namely the PSI[3] scheme presented above and the non-monotone higher order non-upwind Lax-Wendroff RD-scheme in order to design a monotone and positive scheme. In this thesis, the author used the concept of Csik et al. (2002) to formulate a contour integration based version of the Residual Distribution (CRD) Flux Corrected Transport scheme (CRD-FCT). The Lax-Wendroff scheme in the RD context reads:

$$\Phi_{i,T} = \left(\frac{1}{3} + \frac{\Delta t}{2A_i} k_i\right) \Phi_T \tag{1.48}$$

This was achieved with a generalized FCT approach in the context of the RD-framework. The scheme is written in a form, which isolates the cell contribution and limits the contribution of the non-monotone scheme in an optimal way near discontinuities. This is done in an optimized way in order to retain the higher order solution as often as possible. The FCT approach in the FS context can be described in four basic steps.

First, the higher (HEC) and lower order contributions (LEC) from the Lax-Wendroff and PSI scheme are computed and the difference of the node wise contribution of each schemes is estimated and defined as the so called AEC (Anti diffusive Element Contribution):

$$AEC_i = \Phi_{i,T}^{LAX} - \Phi_{i,T}^{PSI} \tag{1.49}$$

In the 2nd step the low order solution is calculated using eq. (1.26) which gives then

3 In fact, already better then a first order scheme.

$$N_i^{PSI,n+1} = N_i^n + \frac{\Delta t}{S_i} \sum_{T, i \in T_i} \Phi_{i,T}^{PSI} \tag{1.50}$$

In the third, most important step, the AEC must be corrected in such a way that the solution at the new time level is monotone. This is achieved with correction factors βi leading to:

$$AEC_{i,corr} = \beta_i \cdot AEC_i \tag{1.51}$$

The final update is obtained by advancing in time and adding the corrected AEC to the solution of the lower order scheme according to:

$$N_i^{n+1} = N_i^{PSI,n+1} + \frac{\Delta t}{S_i} \sum_{T, i \in T_i} AEC_{corr,i} \tag{1.52}$$

The main problem in such an approach is to formulate the correction factors βi which must also guarantee conservation in the case of the RD-approach. The procedure for the calculation of the correction factors is described in detail in Hubbard & Roe (2000) and will not be repeated for the sake of brevity. The author has also considered in this thesis another non-monotone scheme, which is the 2nd order upwind control volume (UCV) scheme of Paillere (1995) that reads:

$$\Phi_{i,T} = \left(\frac{1}{3} + \frac{3}{3} \frac{k_i}{\sum_{i=1}^{3} k_i^+} \right) \Phi_T \tag{1.53}$$

The scheme was also incorporated in the FCT approach, but the results have been not as good as for the scheme suggested by Hubbard & Roe. As the FCT scheme in this thesis was constructed on the foundation of the above described CRD schemes, the total fluctuation in eq. **Fehler! Verweisquelle konnte nicht gefunden werden.** was calculated numerically integrating the flux function over the element edges. The resulting scheme should be conservative for arbitrary flux functions. In fact the author did not find any situation where the opposite occurs.

3. Implicit fluctuation splitting schemes

3.1 The CRD-N1 and the CRD-N2 scheme

As an alternative to the TG approach, implicit fluctuation splitting schemes, which have been originally introduced by Mezine & Abgrall (2002) and Richuotto et al. (2005), have been considered here. The schemes have been derived in a very similar way as for the explicit schemes though redistributing the fluctuation over a prism for which the vertical dimension is the time. In that way, Mezine & Abgrall formulate the idea of fluctuation splitting for a so called “space-time” element (see Figure). They constructed first and second accurate space-time schemes. In order to avoid the Godunov theorem, the fully second order monotone space-time schemes must be nonlinear and therefore a nonlinear equation system must be solved which was considered by the author to be too expensive to be used in the WWM since in this case a linear equation system must be solved iteratively (e.g. with the Newton method). However, such schemes could be considered in future after a parallelization of the code. The finally implemented schemes are ranging from first to second order accurate approximation of the time derivative and are first order in accurate in space.

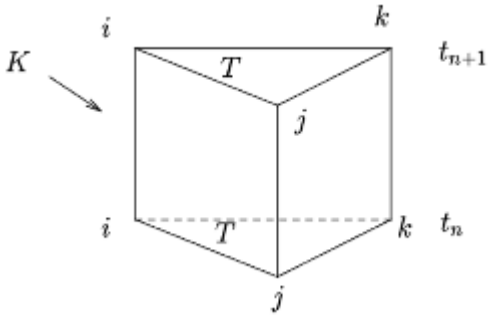

Figure 5: Space time prism for the derivation of the implicit fluctuation splitting schemes. (Adopted from Mezine & Abgrall, 2002)

The 2nd order time accurate N-Scheme reads for the linear problem according to Abgrall & Mezine (2005):

$$\Phi_{i,T} = \frac{A_i}{3}\cdot\left(N_i^{n+1} - N_i^n\right) + \frac{\Delta t}{2}k_i^+\left(N_i^{n+1} - \tilde{N}_i^{n+1}\right) + \frac{\Delta t}{2}k_i^+\left(N_i^n - \tilde{N}_i^n\right) \tag{1.54}$$

In order to have an equivalent formulation for the WAE the CRD framework must be introduced also for the implicit N-Scheme. In the 2nd and 3rd term on the right hand side, the upwind residual must be calculated according to eq. (1.32). Inserting eq. (1.28) in eq. (1.54) gives

$$\begin{aligned}\Phi_{i,T} = {} & \frac{A_i}{3}\cdot\left(N_i^{n+1} - N_i^n\right) \\ & + \frac{\Delta t}{2}k_i^+\left(N_i^{n+1} - \tilde{n}\cdot\left(\sum_{i=1}^{3} N_i^{n+1}\left(k_i^+ - \delta_i^{n+1}\right)\right)\right) \\ & + \frac{\Delta t}{2}k_i^+\left(N_i^n - \tilde{n}\cdot\left(\sum_{i=1}^{3} N_i^n\left(k_i^+ - \delta_i\right)\right)\right)\end{aligned} \tag{1.55}$$

The suggested scheme from Abgrall & Mezine can be identified as a Crank-Nicolson scheme time discretization if one realizes that the above described scheme equals the equation below with θ = 0.5. For θ = 1.0 one obtains a nEuler implicit N-Scheme.

$$\begin{aligned}\Phi_{i,T} = {} & \frac{A_i}{3}\cdot\left(N_i^{n+1} - N_i^n\right) \\ & + \theta\cdot\Delta t k_i^+\left(N_i^{n+1} - \tilde{n}\cdot\left(\sum_{i=1}^{3} N_i^{n+1}\left(k_i^+ - \delta_i^{n+1}\right)\right)\right) \\ & + \left(1-\theta\right)\cdot\Delta t k_i^+\left(N_i^n - \tilde{n}\cdot\left(\sum_{i=1}^{3} N_i^n\left(k_i^+ - \delta_i\right)\right)\right)\end{aligned} \tag{1.56}$$

Eq.(1.56) can be recast into a linear equation system with the aid of eq.(1.17). In order to do so all cell contributions must be cumulated. Writing the old values at the right hand side, the new values on the left hand side of the equation and expanding the summation signs gives back a linear equations system:

$$\boldsymbol{A}\times\boldsymbol{x} = \boldsymbol{b} \tag{1.57}$$

A being the matrix with the coefficients of the unknown at the new time level, the solution vectors x and b represents the values in eq.(1.56) which are known at the actual time level. Hereinafter the scheme with $\theta = 1$ will be called the "N1-scheme" and with $\theta = 0.5$ the "N2-scheme". The N1-scheme is monotone for any integration time step. Due to the CN time, discretization of the N2 scheme the scheme is monotone only for a CFL type condition given by

$$\Delta t_i \leq \frac{2}{3} \max_{T, i \in D_i} \left(\frac{A_i}{k_i^+} \right) \tag{1.58}$$

The above criterion is actually very strict, but numerical experiments showed that the negative values that are evolving, due to the non-monotonic behaviour of the scheme, are small in contrast to other non-monotone schemes as e.g. the Taylor-Galerkin scheme.

4. Parallelization of the implicit and explicit schemes using domain decomposition

A more sustainable way for the parallelization of unstructured meshes is to use the so called "Domain Decomposition" technique. Here a domain is divided into sub-domains where the communication takes place over the so called "ghost nodes" and "ghost elements" for each domain (see fig. 2). The decomposition is done in such a way that the communication halo is minimized by trying to reach equally sized domains for each single thread (for further details consult Schloegel et al., 2002).

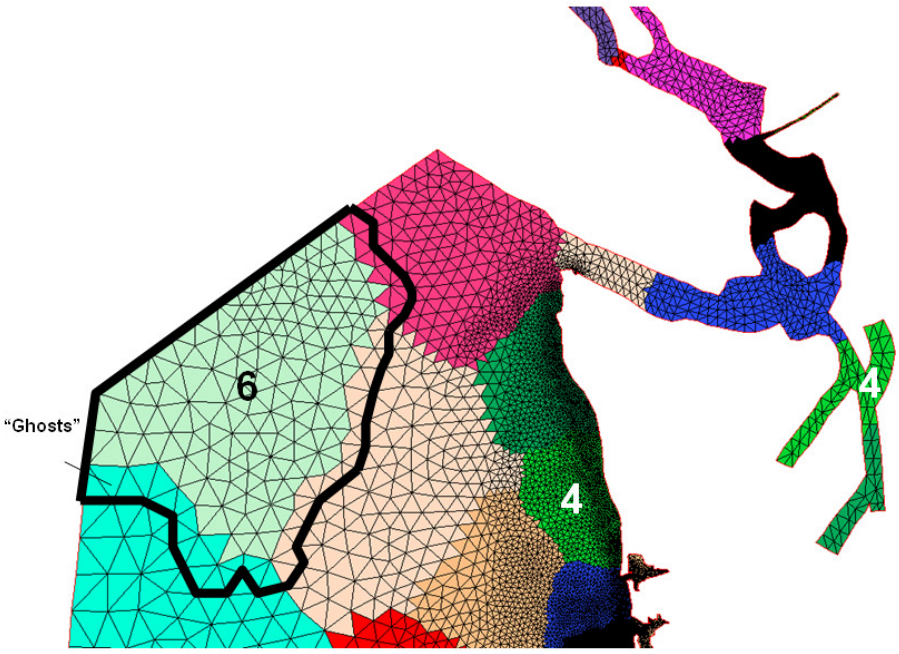

Figure 5: Domain decomposition. Numbers indicate process (CPU rank) numbers, and each color represents a sub-domain. Inside each sub-domain, the nodes/sides/elements are called "residents". Note that the sub-domain of each process may not be contiguous (e.g., "4"). The thick black line indicates the boundary of the augmented domain of rank 6. Those nodes/sides/elements inside the augmented domain but outside the resident domain are called "ghosts". Note that each element is owned by 1 (and 1 only) CPU, but each side or node can be owned by many CPUs (when they are on the border of adjacent sub-domains).

We have implemented the PETSC equation solver within the implicit residual distribution schemes and we have also enhanced the explicit fluctuation splitting schemes for domain decomposition parallelization.

In order to do so we have used the Parallel Decomposition “PDLIB” (Roland & Huxhorn) to establish the needed data structure and interface to ParMetis.

5. Validation of the implicit schemes

The validation of the implicit schemes is by now done on one case, one linear sloping beach where the shoaling can be estimated analytically so we compare the results of the implicit schemes to the analytical solution. In Fig 6. we show the numerical grid and the bathymetry of the analytical test case. Fig. 7 and 8 show the analytical solution and the error ranges using the various numerical schemes available in WW3. The errors of the implicit and explicit schemes are quite comparable. They are well below 1%, just in the last few cells the errors exceed 1% and reach just in the last cells a maximum of 2.5% error to the analytical solution.

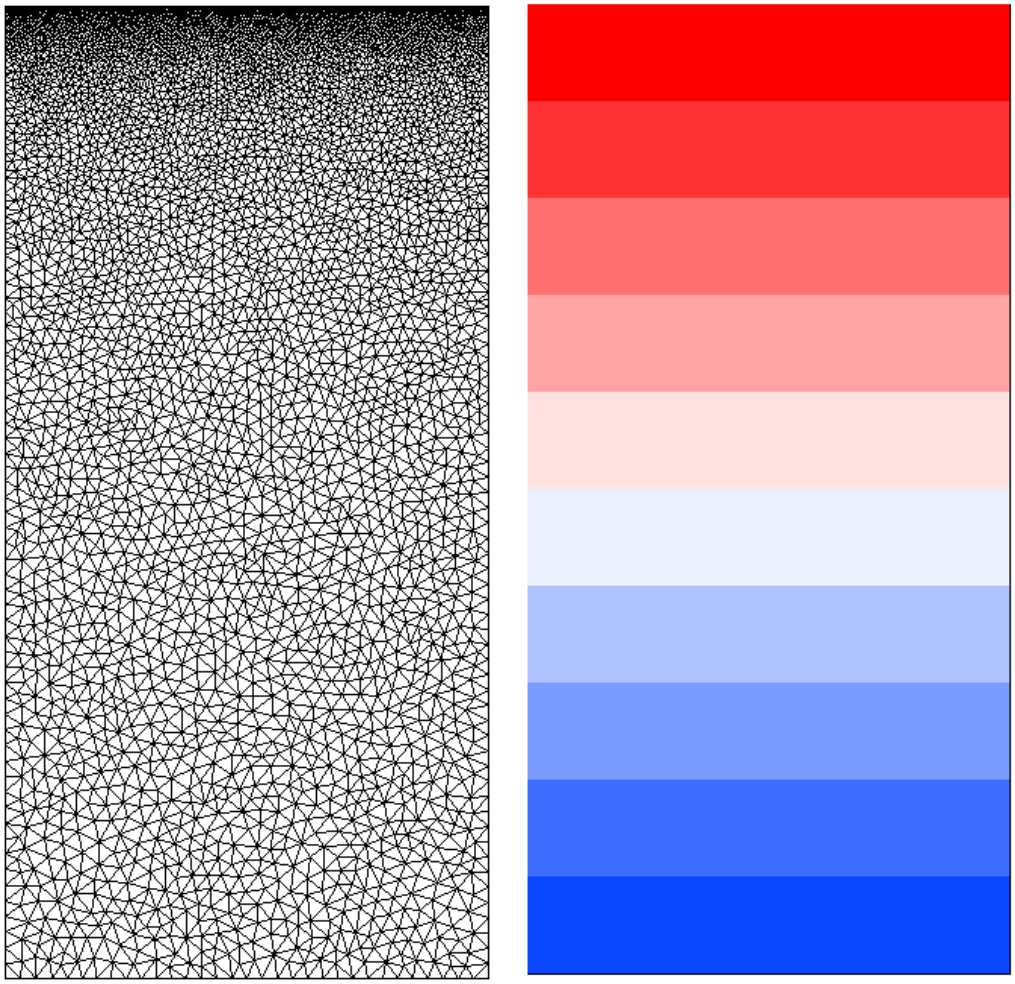

Figure 6: Left: numerical mesh; Right: depth in the computational domain.

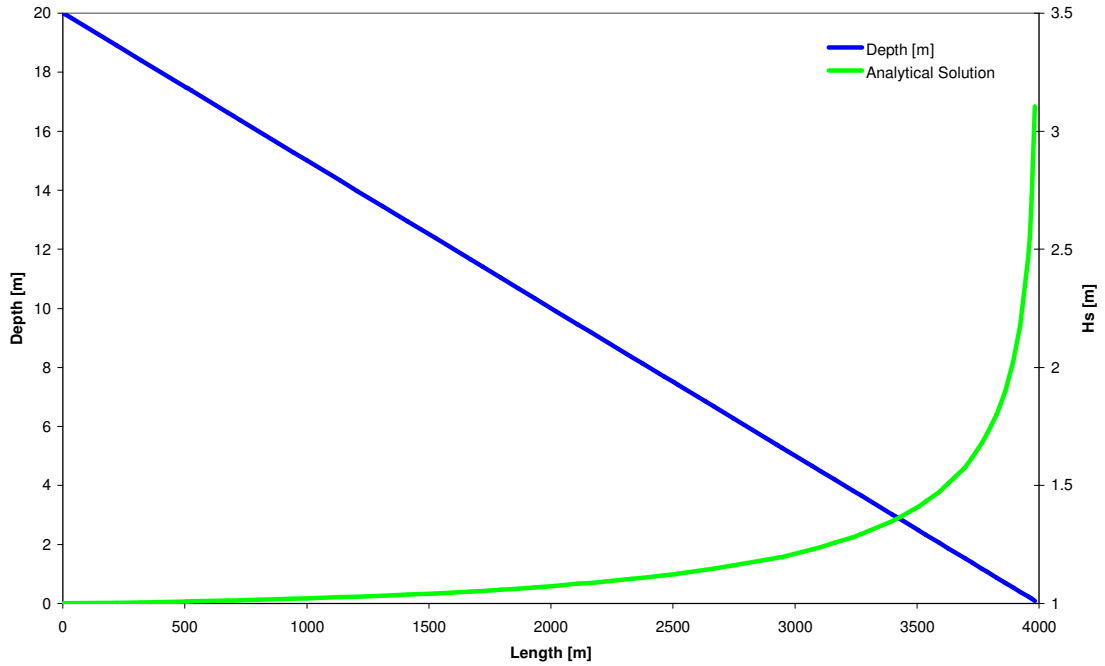

Figure 7: Analytical Solution of the WAE for linear depth profile

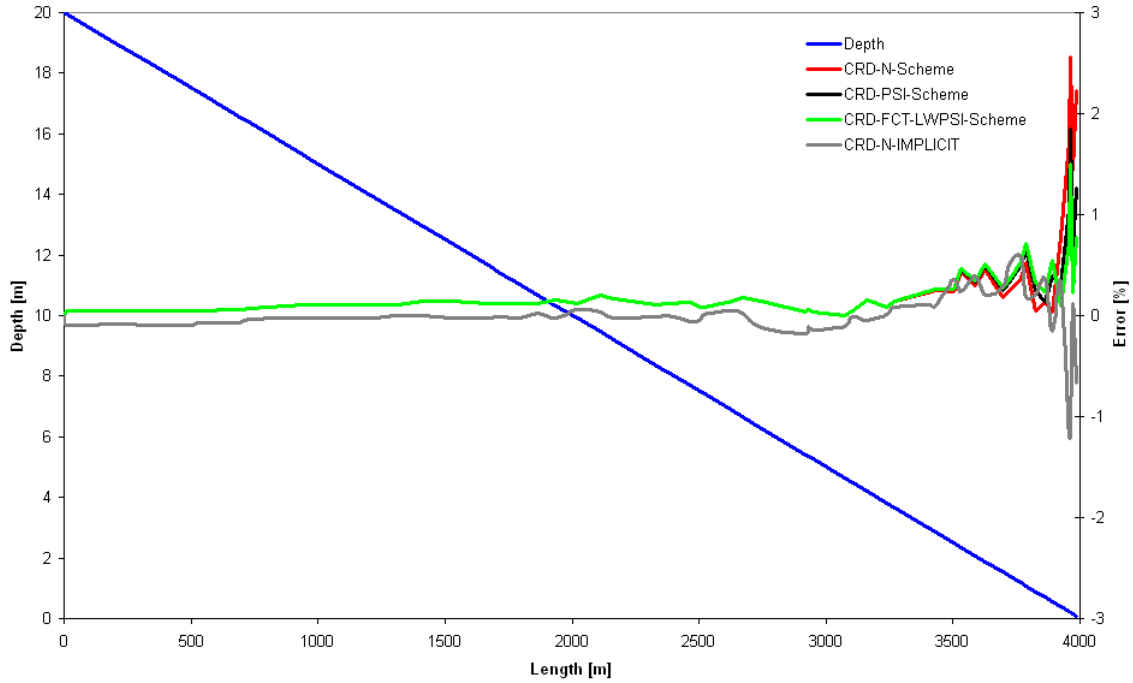

Figure 8: Comparison of the explicit and the implicit schemes to the exact solution.

Another case that is interesting to compare is the harbor of Limon in Costa Rica. The bathymetry and the computational mesh are shown below in Fig. 9. For the boundary conditions 4m swell was set on the eastern boundary from eastern direction and a period of 12s. The low frequency wave is sheltered by the island and the waves refract around the island. In the near-shore region of the island the mesh is resolved up to 1m resolution in geographical space.

Due to the high resolution in the near shore region the explicit schemes need for one integration time step of dt = 30s up to 15s computational time whereas the implicit scheme needs only 2.5, which is more than 5 time faster. Other bathymetry constellation is also possible where even more can be gained by using implicit schemes, e.g. a tidal estuary

with a highly resolved deep channel to get the flow well resolved or very steep bathymetry changes in quite deep water like underwater canyons or continental shelf edges.

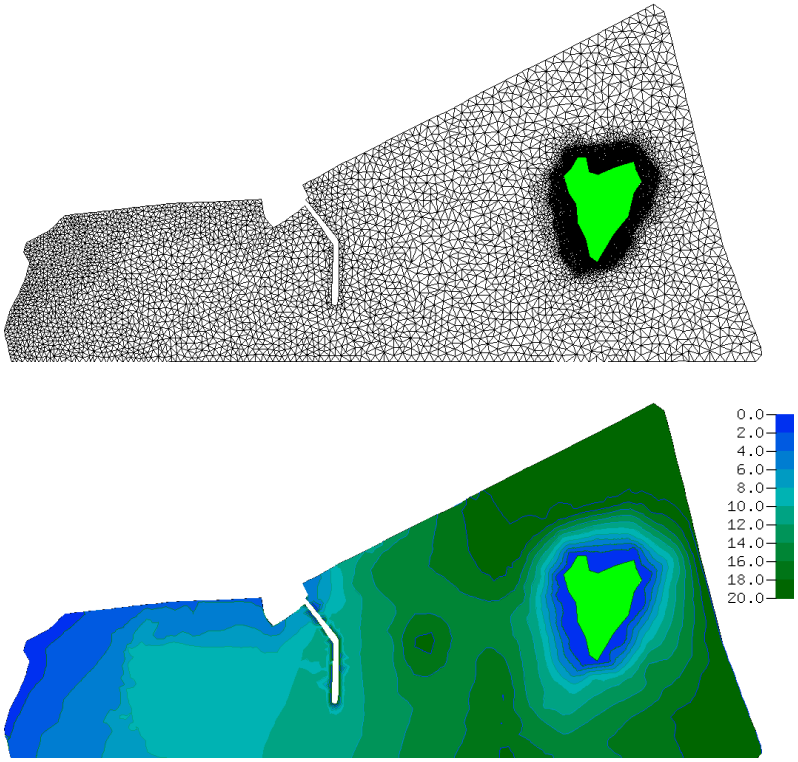

Figure 9: Computational mesh (top) and bathymetry (bottom)

It can be concluded that from the 1st validation runs that the implicit schemes give quite similar results as explicit schemes. The implicit schemes produces very similar error ranges for the analytical shoaling case like explicit schemes. For the real testcase there are hardly any differences visible between both solutions proving the correctness of the implementation.

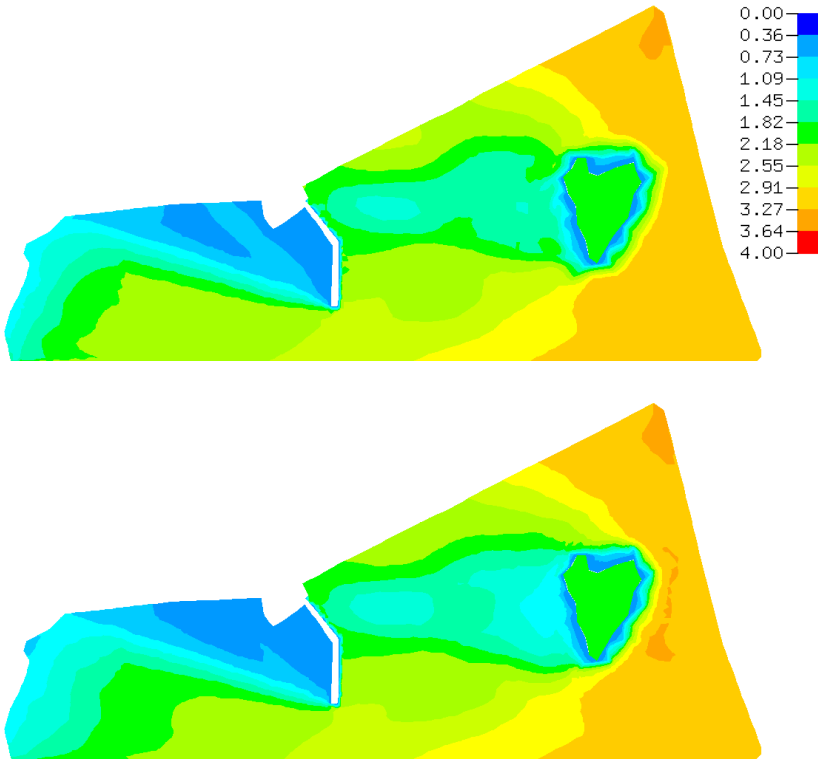

Figure 10: Significant wave height for the implicit (top) and explicit scheme (bottom) , dt = 30s

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