A finite volume method designed for error analysis

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ABSTRACT. *We present a finite volume scheme that allows to reformulate the leading terms of the discretization error in the model equations in terms of local errors in the numerical solution. To ensure that the leading error terms be dominant,* all *variables that are approximated numerically need to be sufficiently smooth functions. This is realized by using the error to steer numerical dissipation mechanisms. The application considered is the shallow-water flow with a hydraulic jump through an irregular channel. It is shown that, contrary to what may have been expected, smoothing may actually improve the accuracy of a numerical simulation. Valuable information about the effect of numerical modeling errors is obtained as well.*

KEYWORDS: *finite volume scheme, error analysis, smoothing, steep gradients*

1. Introduction

As computational models are used more and more routinely in applications of increasing complexity, there is a growing concern about the validity and reliability of model results [HAS 92, MEH 98]. Model assumptions, numerical approximations, and errors in the physical input data all influence the result of a numerical simulation. Due to the complexity of natural systems, it is generally impossible to quantify these effects in applications of practical interest [ORE 94].

It would be very useful if, for any application, it was possible to separate errors that are due to the conceptual model (model equations, geometry, initial and boundary conditions, physical parameters) from those caused by the numerical implementation [FRE 02]. This would provide valuable information on the modeling aspects that determine the quality of a simulation. For example, it would immediately be clear whether physical or numerical parameters should be modified to improve the results.

When flow and transport problems are solved numerically, it is generally very difficult to quantify the effect of discretization errors on the accuracy of a numerical simulation. For this reason, error estimates and error indicators rather than error approximations are used, for example in adaptive grid methods [BOR 01]. Although error estimates exist for increasingly complex equations, they are not yet available for all mathematical models encountered in practical applications [EYM 00]. Moreover, they tend to overestimate the genuine numerical solution error [GES 96]. They also do not provide insight in to what extent the numerical approximation affects the modeled physics.

We have therefore considered an approach that in essence is the method proposed over 50 years ago by Von Neumann and Richtmyer: "utilize the well-known effect on shocks of dissipative mechanisms, such as viscosity" [VON 50]. The idea is to sort of replace local discretization errors by local smoothing errors. If realized by means of an artificial exaggeration of physical dissipation mechanisms, the latter can be interpreted physically by direct comparison with the physical terms and the physical dissipation included in the model. This information can be used advantageously in the assessment of the quality of results and the development of a computational model.

2. Two-step numerical modeling

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 (cf. Figure 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.

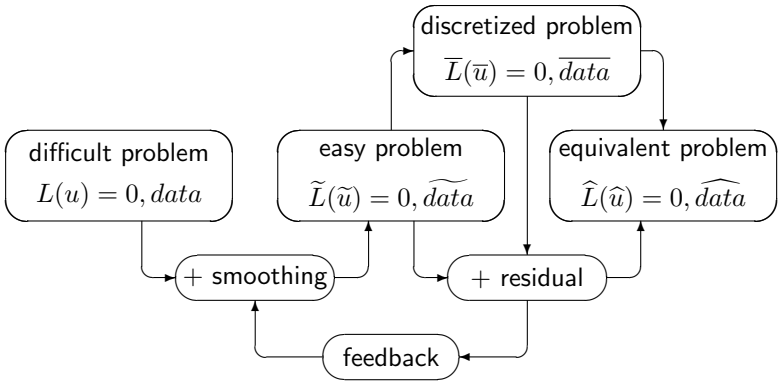

Figure 1. *Outline of the two-step numerical modeling technique*

A tilde ($\widetilde{\ }$) indicates the variables and differential operators of the easy problem. Their discretizations are indicated by a bar ($\overline{\ }$). 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 [BOR 01].

3. 1D shallow-water model

The application that we consider is the simulation of flow through an open channel of uniform width, described by the equations for mass and momentum conservation:

$$\frac{\partial H}{\partial t} + \frac{\partial q}{\partial x} = 0 \,, \qquad [1]$$

$$\frac{\partial q}{\partial t} + \frac{\partial q^2/H}{\partial x} + gH\frac{\partial \zeta}{\partial x} = \frac{\partial}{\partial x}\left(\nu_{\text{art}} H \frac{\partial q/H}{\partial x}\right) \,, \qquad [2]$$

with $H(x,t)$ the total water depth, $q(x,t)$ the depth-integrated flow velocity, $\zeta(x,t)$ the water elevation, and g the constant gravitational acceleration. The difference between H and ζ is the specified still water depth $h(x)$: $H = \zeta + h$. Depth-average flow velocity $u(x,t)$ is equal to q/H. Bottom friction has been left out of [2], but viscosity is included. Although the latter can be used to model physical effects, it is used here solely to create an easy problem by taking artificial viscosity coefficient $\nu_{\text{art}} > 0$. Note that this requires the data,

in particular h, to be smooth as well. For convenience, the tilde has been omitted in [1] and [2], which can be combined to the energy equation:

$$\begin{aligned} &\frac{\partial}{\partial t}\left(H\left(\frac{1}{2}u^2+g\zeta-\frac{1}{2}gH\right)\right)+\frac{\partial}{\partial x}\left(uH\left(\frac{1}{2}u^2+g\zeta\right)\right) \\ &\quad=-\nu_{\rm art}H\left(\frac{\partial u}{\partial x}\right)^2+\frac{\partial}{\partial x}\left(u\nu_{\rm art}H\frac{\partial u}{\partial x}\right)\ . \end{aligned} \qquad [3]$$

If $\nu_{\rm art}$ and h are smooth, then this equation is also valid in shock regions. By adding artificial viscosity, discontinuous hydraulic jumps are replaced by steep but smooth gradients. These jumps are still modeled accurately if the amount of smoothing is small enough, because the conservative form of [1] and [2] ensures that across the smoothed hydraulic jump the correct jump conditions are applied [VON 50].

The discretization of the model equations in space is straightforward. First, piecewise linear approximations of all primary variables (H, q, h, $\nu_{\rm art}$, x) are defined in a computational space with uniform grid, using values defined at grid points. This defines also the discrete approximation of secondary variables (ζ, u). There is now one set of locations where fluxes, including the viscous flux, can be approximated with second-order accuracy: the cell centers. This prescribes automatically the discretization method to be applied: integrate the equations over the finite volumes formed by the cell centers with an accuracy of fourth order or better to avoid second-order integration errors. For this reason, the viscous flux is written prior to the discretization as:

$$\frac{\partial}{\partial x}\left(\nu_{\rm art}H\frac{\partial q/H}{\partial x}\right)=\frac{\partial}{\partial x}\left(\nu_{\rm art}\frac{\partial q}{\partial x}\right)-\frac{\partial}{\partial x}\left(\nu_{\rm art}\frac{q}{H}\frac{\partial H}{\partial x}\right)\ . \qquad [4]$$

To our knowledge, this is the only way to construct a discretization fully compatible with the underlying discretization of the variables. It has the unique property that *all* lowest-order terms in the residual can be written in terms of errors in the solution and other variables. For example, the equation equivalent with [2] discretized on a uniform grid is:

$$\begin{aligned} &\frac{\partial}{\partial t}\left[\widehat{q}+\gamma_0 D_x(\widehat{q})\right]+\frac{\partial}{\partial x}\left[\frac{(\widehat{q}+\gamma_1 D_x(\widehat{q}))^2}{\widehat{H}+\gamma_1 D_x(\widehat{H})}\right] \\ &\quad+g\left(\widehat{H}+\gamma_0 D_x(\widehat{H})\right)\frac{\partial}{\partial x}\left[\widehat{\zeta}+\gamma_1 D_x(\widehat{\zeta})\right]+\frac{g}{24}\frac{\partial\widehat{H}}{\partial x}D_x(\widehat{\zeta}) \\ =\ &\frac{\partial}{\partial x}\left[\left(\widehat{\nu}_{\rm art}+\gamma_1 D_x(\widehat{\nu}_{\rm art})\right)\frac{\partial}{\partial x}\left(\widehat{q}+\gamma_2 D_x(\widehat{q})\right)\right] \\ &\quad-\frac{\partial}{\partial x}\left[\frac{\left(\widehat{\nu}_{\rm art}+\gamma_1 D_x(\widehat{\nu}_{\rm art})\right)\left(\widehat{q}+\gamma_1 D_x(\widehat{q})\right)}{\widehat{H}+\gamma_1 D_x(\widehat{H})}\frac{\partial}{\partial x}\left(\widehat{H}+\gamma_2 D_x(\widehat{H})\right)\right] \\ &\quad+O(\Delta x^4)\ , \end{aligned} \qquad [5]$$

with $\gamma_0 = (\frac{2}{3} - \gamma)/8$, $\gamma_1 = (1 - \gamma)/8$, $\gamma_2 = (\frac{1}{3} - \gamma)/8$, γ a parameter ($\geq 0, \leq 1$) that depends on how the smooth approximations ($\widehat{q}$, etc.) of the piecewise linear functions ($\overline{q}$, etc.) are defined [BOR 01], and $D_x = \Delta x^2 \partial^2/\partial x^2$. The error analysis to obtain this result can be found in [BOR 01] where the equation equivalent with a discretization on a moving, non-uniform grid is derived.

The comparison of [5] with [2] and [4] shows that the discretized system solves equations of the same form as the easy model equations, but with variables perturbed by discretization errors. The errors are of the same form and size as the leading interpolation error of the piecewise linear approximation used for the variables [BOR 01]. This result demonstrates the compatibility between the discretization of the flow equations and the applied discrete function approximations.

The fourth-order errors in [5] can be neglected if all variables are sufficiently smooth. This is obtained by taking ν_{art} equal to the sum of the scaled discretization error in the kinetic part and in the potential part of the energy head $\frac{1}{2}u^2/g + \zeta$ [BOR 01]. However, since H and ζ should both be smooth functions, $h = H - \zeta$ must be smooth as well. Obviously, the smoothing of the geometry must depend on the discretization errors in the numerical solution, but this has not been fully developed and implemented yet. Instead, we have used the function smoothing procedure of [BOR 98], which turns out to be sufficient to demonstrate the importance of geometry smoothing.

4. Results

To illustrate the performance of the presented shallow-water model, we consider a steady-state sub-/supercritical flow with hydraulic jump over a bar. In order to make discretization errors due to a non-smooth geometry large enough to be noticeable, a steep upstream slope has been used. Apart from this, the test case is equal to the one considered in [BOR 01].

Figure 2 shows the numerical result if no geometry smoothing is applied, using a fairly coarse grid of 50 finite volumes. It is compared with the exact solution, obtained by solving [1] and [2] for $\nu_{\text{art}} = 0$. It can be observed that, despite the smoothing due to the artificial viscosity, the hydraulic jump is modeled very well. Although it is spread over about 5 grid cells, its position, indicated by $\text{Fr} = 1$ (with $\text{Fr} = u/\sqrt{gH}$ the Froude number), is predicted within a fraction of the grid size. Also the energy loss across the jump is predicted accurately. The undershoot of the energy head at the position of the jump is the result of the viscous energy redistribution modeled by the second term in the right-hand side of [3] [BOR 01].

The energy loss over the steep upstream slope is plain wrong. A comparison between the hydrostatic pressure term (the third term in the left-hand side of [2]) and the artificial viscosity term, both shown in Figure 2, provides the

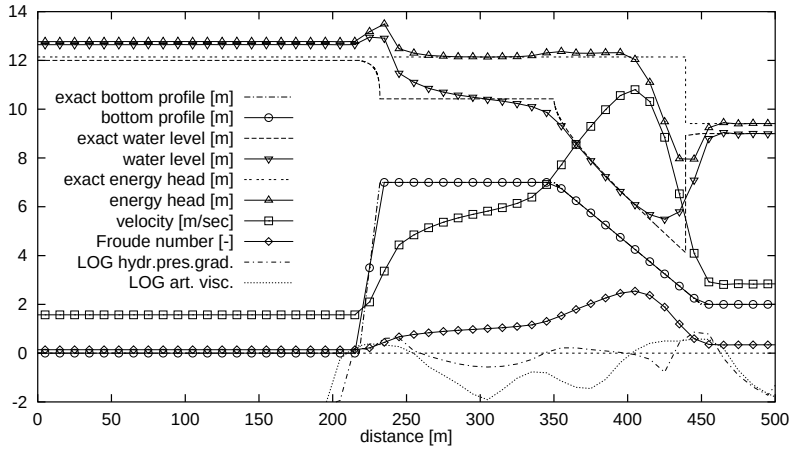

Figure 2. *Flow over a bar using 50 finite volumes*

explanation. As expected, these terms are equally important in the jump area where artificial viscosity is required to balance the physical modeling terms, to prevent them from becoming too large to be discretized accurately. They are, however, also of the same size at the upstream slope, where the non-smooth geometry introduces large errors that the model attempts to compensate by introducing a large amount of artificial viscosity.

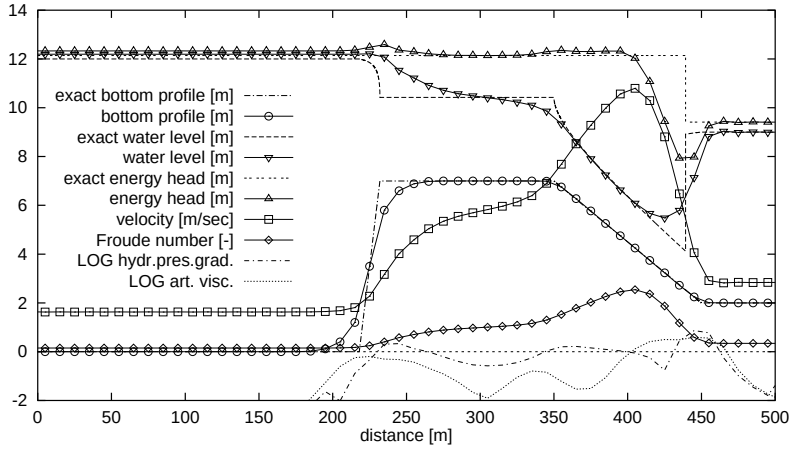

Figure 3. *Flow over a bar using 50 finite volumes and geometry smoothing*

This compensation is not required if the geometry is properly smoothed. Figure 3 shows that this leads to significantly better results, despite the fact that the geometry is modeled 'less accurately'. The advantage of strongly reduced discretization errors clearly outweighs the disadvantage of larger smooth-

ing errors. Notice that the level of artificial viscosity may still be considered to be fairly large near the upstream slope. We expect to obtain better results once we have implemented the correct geometry smoothing procedure.

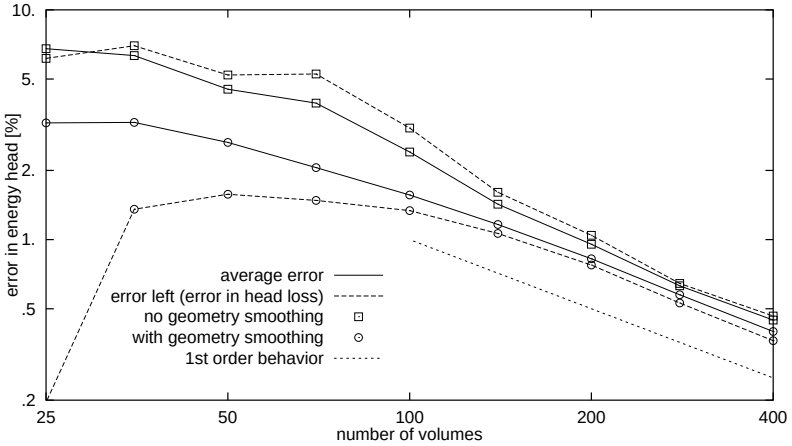

Figure 4. *Error in energy head as a function of the grid size*

Figure 4 shows the difference between the computed and the exact energy head as a function of the number of grid points. It can be observed that with geometry smoothing the errors are not only smaller, but are also a smooth function of the number of grid points, i.e., they depend primarily on the grid size. If the geometry is not smoothed, the error is also sensitive to the position of the grid points with respect to the edges of the bar, which changes constantly as the number of volumes is varied. This confirms the conclusion of [BOR 01] that geometry smoothing is essential for error-minimizing grid adaptation, which requires the error to be a smooth function of the grid size only. See also [BOR 98]. The difference between the errors with and without geometry smoothing vanishes as the number of grid points increases, since then the first-order error due to the smoothed hydraulic jump becomes dominant.

An interesting advantage of smoothness is that the nonlinear algebraic system of discretized equations can be solved very efficiently [BOR 01]. Starting from a uniform water level and zero discharge, the solution process converged in only 30 (25 volumes) to 78 (400 volumes) iterations to a convergence error of less than 10^{-11} in the water level and less than 10^{-13} in the flow velocity.

5. Concluding remarks

We presented a numerical solution technique that uses error-based artificial smoothing to keep discretization errors small. In many applications, neither the effect of conceptual modeling errors and data errors, nor the effect of nu-

merical errors can be quantified. With the proposed method, where artificial smoothing is the dominant numerical error, it is at least possible to interpret numerical errors physically and compare them with physical modeling terms. This information can be very useful in the development and use of computational models for complex applications.

The results that were presented indicate that artificial smoothing does not necessarily lead to larger solution errors, since discretization errors become smaller. Moreover, smoothness allows to apply central discretization schemes that are generally more accurate and easier to implement than upwind methods. The development of suitable smoothing mechanisms may be rather complicated, but we do have indications that discretizations and dissipation techniques simpler than those presented here may work nearly as well.

References

[BOR 98] Borsboom M., "Development of an Error-Minimizing Adaptive Grid Method", *Appl. Num. Math.*, vol. 26, 1998, pp. 13–21.

[BOR 01] Borsboom M., "Development of a 1-D Error-Minimizing Moving Adaptive Grid Method", in: *Adaptive Method of Lines*, A. Vande Wouwer, Ph. Saucez, and W.E. Schiesser (eds.), CRC Press, 2001, pp. 139–180.

[EYM 00] Eymard R., Gallouët T., Herbin R., "The Finite Volume Method", in: *Handbook of Numerical Analysis VII*, P.G. Ciarlet, J.L. Lions (eds.), North Holland, 2000, pp. 715–1022.

[FRE 02] Freitas C.J., "The Issue of Numerical Uncertainty", *Appl. Math. Modelling*, vol. 26, 2002, pp. 237–248.

[GES 96] Gessner T., Kröner D., Schupp B., Wierse M., "Finite Volume Methods for Conservation Laws and Convection-Dominated Diffusion Equations", in: *Finite Volumes for Complex Applications*, F. Benkhaldoun, R. Vilsmeier (eds.), Hermes, 1996, pp. 61–76.

[HAS 92] Hassanizadeh S.M., Carrera, J., "Editorial", *Adv. Water Res.*, vol. 15, 1992, pp. 1–3.

[MEH 98] Mehta U.B., "Credible Computational Fluid Dynamics Simulations", *AIAA Journal*, vol. 36, 1998, pp. 665–667.

[ORE 94] Oreskes N., Shrader-Frechette K., Belitz, K., "Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences", *Science*, vol. 263, 1994, pp. 641–646.

[VON 50] Von Neumann J., Richtmyer R.D., "A Method for the Numerical Calculation of Hydrodynamic Shocks", *J. Applied Physics*, vol. 21, 1950, pp. 232–237.