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A second order residual based predictor–corrector approach for time dependent pollutant transport

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ABSTRACT

We present a second order residual distribution scheme for scalar transport problems in shallow water flows. The scheme, suitable for the unsteady cases, is obtained adapting to the shallow water context the explicit Runge–Kutta schemes for scalar equations [1]. The resulting scheme is decoupled from the hydrodynamics yet the continuity equation has to be considered in order to respect some important numerical properties at discrete level. Beyond the classical characteristics of the residual formulation presented in [1,2], we introduce the possibility to iterate the corrector step in order to improve the accuracy of the scheme. Another novelty is that the scheme is based on a precise monotonicity condition which guarantees the respect of the maximum principle. We thus end up with a scheme which is mass conservative, second order accurate and monotone. These properties are checked in the numerical tests, where the proposed approach is also compared to some finite volume schemes on unstructured grids. The results obtained show the interest in adopting the predictor–corrector scheme for pollutant transport applications, where conservation of the mass, monotonicity and accuracy are the most relevant concerns.

1. Introduction

This paper presents a second order predictor–corrector (PC) scheme for the transport of a passive scalar in shallow water flows. The scheme is conceived to solve practical environmental engineering problems like pollution propagation studies in rivers and estuaries. Therefore, the governing equations are the 2d shallow water equations augmented by a scalar conservation law, necessary to describe the pollutant transport.

Modeling the advection of dissolved substances in the fluid still presents some numerical difficulties related to the particular applications and linked to the particular numerical method. For example, it is important to have high order methods or methods with low numerical diffusion when the goal is to predict pollutant values on long distances. At the same time, it is important that the concentration values obtained are strictly bounded, i.e. local minima and local maxima are not exceeded. This is a fundamental physical property of the pollutant equation, which must be fulfilled by the numerical scheme. Finally, the mass of solute must be perfectly conserved in order to get physical results. This paper deals with these issues: accuracy, preservation of the maximum principle, conservation.

The scheme proposed here, belongs to the family of residual distribution (RD) schemes and it is conceived following the ideas introduced in a series of recent articles about second order schemes in time dependent problems (see [1–3]).

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Indeed, the accuracy in unsteady cases when using unstructured meshes is one of the major concerns in this work. The RD PC scheme is only employed to discretize the pollutant equation, while the rest of the system, i.e. the shallow water equations, are solved through a finite element (FE) method (see [4] for more details about this part). Thus, as the hydrodynamic equations and the pollutant equation are solved in two different steps and by different numerical methods, we define this approach as a decoupled approach (see also [5–9]). In this case, a major challenge is to consistently take into account the continuity equation of the fluid such that mass conservation and monotonicity are strictly enforced for the pollutant. Indeed, even when using a decoupled technique, a conservative scheme for the scalar transport equation cannot be formulated just from the water depths and the velocity fields, but has to consider also the way in which the hydrodynamic equations are solved [9]. The advantage of the decoupled algorithm is that different time discretizations can be used for hydrodynamics and for tracer. This can be useful for processes characterized by different time scaling or when hydrodynamics and tracers do not need the same degree of accuracy and so different time steps can be used.

The RD discretization employed for the conservative pollutant equation is first described for steady problems. This allows to introduce the main elements of our method, namely the N and the PSI schemes and to recall the theory about schemes for steady problems. The construction of the second order scheme envisages as key points the upwind of the derivative in time combined with a time shifted stabilization operator, used on a Runge–Kutta scheme. The final formulation of the predictor–corrector scheme is slightly different from the one proposed in [1]. This is due to two main differences: first, the use of a variational formulation of the problem, which is not current in the RD classical approach; second, the adaptation of the method to the depth-averaged transport equation.

One of the contributions of this work is to improve the accuracy of the classical formulation [1], introducing an iterative scheme on the corrector step, guaranteeing the mass conservation of the advected solute and preserving the maximum principle. The last point is addressed with particular attention. Indeed, it is well known that it is more difficult to preserve the monotonicity when second order methods are used over unstructured meshes (see for example [10] for finite volumes methods). In this work the monotonicity of the predictor–corrector scheme will be ensured by a limitation on the pollutant concentration value obtained by the predictor step, provided a specific time step condition. The monotonicity proof represents a new contribution; this issue was not specifically addressed in the other papers concerning the predictor–corrector schemes, except in [2] where an explicit condition for the positivity of the water depth is given for the limited second order Lax–Friedrichs scheme. In addition, the technique used to get the monotonicity proof can be adapted to other schemes when the theory of positive coefficients scheme cannot be applied.

The article is structured as follows. After the introduction, the section 2 will be dedicated to the governing equations describing the pollutant transport in shallow water flows. Then, in section 3, the residual distribution scheme for the conservative equation for steady problems will be presented. Successively, the predictor–corrector scheme will be described, as well as the monotonicity condition for the pollutant concentration. This section will be followed by a series of test cases, which prove the accuracy of the results, the respect of the maximum principle and the conservation of the solute mass. The paper is ended by a summary of the main contributions, and by an overview of the ongoing and future activities.

2. Governing equations

The conservative scalar transport equation, combined with the continuity equation of the shallow water system, makes up the non-conservative equation for the transport of a passive scalar. The latter can be a solute, a pollutant or any other substance which is advected by the current without influencing the hydrodynamics, which is respectively governed by the shallow water equations (SWEs). The system of equations is thus made up by the shallow water equations augmented by a conservative scalar transport equation for a pollutant:

$$\begin{aligned}
&\frac{\partial h}{\partial t}+\frac{\partial (hu)}{\partial x}+\frac{\partial (hv)}{\partial y}=0\\
&\frac{\partial (hu)}{\partial t}+\frac{\partial (huu)}{\partial x}+\frac{\partial (huv)}{\partial y}=-gh(\eta_x+S_{fx})\\
&\frac{\partial (hv)}{\partial t}+\frac{\partial (huv)}{\partial x}+\frac{\partial (hvv)}{\partial y}=-gh(\eta_y+S_{fy})\\
&\frac{\partial (Ch)}{\partial t}+\frac{\partial (uCh)}{\partial x}+\frac{\partial (vCh)}{\partial y}=0
\end{aligned} \tag{1}$$

where h, u, v, C are the four unknowns of the problems. h is the water depth, $\vec{u}=(u,v)$ is the depth-averaged velocity vector with two components in x and y, C is the concentration of the pollutant. g is the gravity acceleration, η and S_f are respectively the free surface and the friction source term. The system is formed by non-linear partial differential equations and it is strictly hyperbolic for $h > 0$.

The resolution of the entire system is often coupled, which means that the convective fluxes are treated with the same time step and the same kind of discretization for the four equations. Typically, this is the case in the context of finite volume discretizations (see [11–13]). However, solutions where the discretization of the transport equation is different from the hydrodynamics are explored in [9,6,8].