Propagation of Diffusing Pollutant by a Hybrid Eulerian-Lagrangian Method

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We present a hybrid numerical method for computing the propagation of a diffusing passive pollutant in shallow water. The flow is modeled by the Saint-Venant system of shallow water equations and the pollutant propagation is described by a convection-diffusion equation.

In this paper, we extend the hybrid finite-volume-particle (FVP) method, which was originally introduced in [CK04, CKP06] for the model of inviscid pollutant propagation, to the case of a diffusing pollutant. The idea behind the FVP method is to use different schemes for the flow and pollution computations: the shallow water equations are numerically integrated using a finite-volume scheme, while the transport equation for the propagation of passive pollutant is solved by a deterministic particle method. When the pollutant diffuses, the second step of the FVP method has to be modified. We propose a new hybrid Eulerian-Lagrangian method, in which the convection term is treated by the method of characteristics (which is, in the context of scalar transport equations is very similar to the deterministic particle method), while the diffusion is resolved using the fast explicit operator splitting method recently developed in [CKP].

1 Introduction

Prediction of a pollution propagation is an important problem in many industrial and environmental projects. Different mathematical models are used to describe this phenomenon and to obtain an accurate location and concentration of pollutant.

In this paper, we consider the transport of a passive pollutant by a flow modeled by the Saint-Venant system of shallow water equations [Sai1871]. In the one-dimensional (1-D) case, the system reads:

$$\begin{cases} h_t + (hu)_x = S, \\ (hu)_t + \left(hu^2 + \dfrac{gh^2}{2}\right)_x = -ghB_x. \end{cases} \tag{1}$$

Here, h and u are the depth and the velocity of the water, g is the gravity constant, and S is a source term. The function B represents the bottom topography.

The propagation of the pollutant is modeled by the convection-diffusion equation:

$$(hT)_t + (uhT)_x = T_S S + \nu h T_{xx}, \tag{2}$$

where T is the pollutant concentration, the coefficient T_S represents a concentration of the pollutant at the source, and ν is the viscosity coefficient.

For simplicity, we will assume that the pollution source has already been turned off, that is, we will only consider the $S \equiv 0$ case (numerical treatment of the source term was discussed in detail in [CK04, CKP06]). Under this assumption, equations (2) and (1) are coupled only through the velocity u. This suggests the following strategy for developing numerical methods for the system (1)–(2): first, solve the Saint-Venant system (1), and then substitute the obtained velocity field u into equation (2), which can be whereupon viewed as a linear convection-diffusion equation with possibly discontinuous coefficients. Since equations (2) and (1) can be solved separately, they can be solved by two different methods: one method should be designed for the hyperbolic system of balance laws (1), while the other method should be capable to accurately solve the convection-diffusion equation (2). This simple hybrid strategy was realized in [CK04, CKP06], where the FVP method was introduced: the Saint-Venant system (1) was solved by a shock-capturing finite-volume method (the central-upwind scheme from [KL02, KNP01, KT00]), while the inviscid transport equation, (2) with $\nu = 0$, was accurately solved by the deterministic particle method (see, e.g., [Rav85] for a comprehensive description of particle methods for transport equations).

The main advantage of the FVP hybrid strategy is its flexibility. There is a wide variety of reliable finite-volume methods for the Saint-Venant system (see, e.g., [ABBKP04, AB03, GHS03, JW05, KL02, KP, NPPN06, XS06] for just a few examples of recently proposed methods). One may select one's favorite method for the first part of the hybrid algorithm. When the system (1) is solved for h and hu, a global approximation of u at each time level can be computed by dividing a piecewise polynomial approximation of hu by a piecewise polynomial approximation of h. This gives one a velocity coefficient in equation (2), which can be thus treated as a linear equation. Since particle methods are specifically designed as a non-diffusive numerical methods for transport equations, they allow to very accurately resolve contact discontinuities that typically appear in the pollutant concentration field, as it was demonstrated in [CK04, CKP06].

In this work, we extend the FVP method to the case of diffusing pollutant ($\nu \neq 0$). The first part of our hybrid algorithm (an Eulerian finite-volume method) is not affected by the presence of diffusion in equation (2), therefore, only its second part is to be modified. There are several ways to implement particle methods for convection-diffusion equations (see, e.g., [CHO73, CK00, DM91, DM90, LM99, RUS90]). These methods can be, in principle, applied to equation (2), but will require either smearing the particle approximation, which may introduce an extensive amount of numerical diffusion (especially in the convection-dominated case), or computing the numerical derivatives on a nonuniform mesh, formed by the particle locations, which may be inaccurate (especially in the two-dimensional (2-D) case).

To overcome these difficulties, we propose the following Lagrangian strategy for solving (2). First, we rewrite equation (2) in an equivalent nonconservative form:

$$T_t + uT_x = \nu T_{xx}, \tag{3}$$

We then use the Strang operator splitting [Str68] and solve the convection equation:

$$T_t + uT_x = 0, \tag{4}$$

and the diffusion equation:

$$T_t = \nu T_{xx}, \tag{5}$$

separately. As it has been shown in [CK04], the particle method applied to (2) with $\nu = 0$ is basically equivalent to the method of characteristics applied to equation (4). The linear heat equation (5) is very simple and can be solved exactly by convolving the initial condition with the heat kernel, as it has been done in [CKP]. Since we need to obtain point values of T after each parabolic step of the operator splitting method, a certain quadrature rule should be applied to the integral form of the solution, and this may be rather computationally expensive, especially in the 2-D case. However, in the convection-dominated case (that is, when $\nu << 1$), splitting increments $\Delta t_{\rm spl}$ can be made very large (since the splitting error is proportional to $\nu^3(\Delta t_{\rm spl})^2$) and we can obtain a very accurate approximate solution by applying only a small number of operator splitting steps.

2 Description of the Method

In this section, we provide a description of our 1-D hybrid Eulerian-Lagrangian method for the system (1),(3). Similarly, to the FVP method, the new hybrid method consists of two parts. We first solve the Saint-Venant system (1) by the semi-discrete second-order well-balanced positivity preserving central-upwind scheme, recently proposed in [KP], with time evolution carried out by the third-order strong stability preserving (SSP) Runge-Kutta solver [GST01]. We would like to emphasize that this part of our hybrid Eulerian-Lagrangian algorithm can be replaced with one's favorite finite-volume method.

We now focus on the second part of out hybrid algorithm: the Lagrangian version of the fast explicit operator splitting method for the convection-diffusion equation (3). In the following, we will assume that an approximate velocity $u(x,\cdot)$ is available at every time level. We split the convection-diffusion equation (3) into the convection equation (4) and the diffusion one (5). We denote the solution operators, associated with these equations by $S_{\mathcal{C}}$ and $S_{\mathcal{D}}$, respectively. Then, according to [Str68], the solution of the convection-diffusion equation (3) satisfies:

$$T(t+\Delta t_{\rm spl}) = S_{\mathcal{C}}(\Delta t_{\rm spl}/2)S_{\mathcal{D}}(\Delta t_{\rm spl})S_{\mathcal{C}}(\Delta t_{\rm spl}/2) + E(\Delta t_{\rm spl}), \tag{6}$$

where $\Delta t_{\rm spl}$ is a splitting time increment, and the one time-step splitting error, $E(\Delta t_{\rm spl})$, is proportional to $\nu^3(\Delta t_{\rm spl})^3$ (an accumulative splitting error is then proportional to $\nu^3(\Delta t_{\rm spl})^2$). Notice that a success of the fast explicit operator splitting method hinges on smallness of the viscosity coefficient ν, since then the splitting error is small even for sufficiently large values of $\Delta t_{\rm spl}$ and one can obtain a very accurate solution with only few splitting steps (see [CKP] for details).

In practice, the exact solution operators $S_{\mathcal{C}}$ and $S_{\mathcal{D}}$ are to be replaced with approximate ones. We use the (Lagrangian) method of characteristics to solve equation (4). To this end, we assume that a set of characteristic points, $\{x_i(t)\}$, and the corresponding pollution concentration values, $\{T(x_i(t),t)\}$, are available at a certain time level t. We then perform the first convection substep of (6) by evolving the characteristics points according to the following system of ODEs:

$$\frac{dx_i(t)}{dt} = u(x_i(t),t),$$

which is numerically solved by the same SSP Runge-Kutta method used for time evolution of the shallow water solution. At the end of this substep, the solution will be realized as a set of point values $\{T_i^* := T(x_i^*, t+\Delta t_{\rm spl}/2) \equiv T(x_i(t),t)\}$, where $x_i^* := x_i(t+\Delta t_{\rm spl}/2)$. The diffusion substep is then carried out by evolving this intermediate solution exactly according to:

$$S_{\mathcal{D}}(\Delta t_{\rm spl})T(x,\cdot) = T(x,\cdot) + \int\limits_{-\infty}^{\infty} G(x-\xi, \nu\Delta t_{\rm spl})(T(\xi,\cdot) - T(x,\cdot))\,d\xi, \tag{7}$$

where $G(x,t) := (4\pi t)^{-1/2}\exp(-x^2/4t)$ is the heat kernel. Since after the first convection substep only a discrete set of values $\{T_i^*\}$ is available, we apply the trapezoidal rule to formula (7) and end up with the new set of point values of T at the same locations $\{x_i^*\}$:

$$T_i^{**} = T_i^* + \sum_j G(x_i^* - x_j^*, \nu\Delta t_{\rm spl})(T_j^* - T_i^*). \tag{8}$$

To complete one splitting step, we perform another convection substep and obtain the new set of characteristic points, $\{x_i(t+\Delta t_{\rm spl})\}$, with the same set of solution values there: $\{T(x_i(t+\Delta t_{\rm spl}), t+\Delta t_{\rm spl}) \equiv T_i^{**}\}$.

Remark The 2-D extension of our hybrid Eulerian-Lagrangian method is rather straightforward. We would only like to comment here on the 2-D extension of the trapezoidal quadrature (8), which has been performed by arranging a nonuniform set of characteristics points $\{(x_i^*, y_i^*)\}$ into the Delaunay triangulation by implementing the algorithm based on the open source mesh generation package GeomPack, available at `www.geompack.org` (see also `www.csit.fsu.edu/~burkardt/f_src/geompack/geompack.html`). This determines the continuous piecewise linear approximation of the integrand in the 2-D analog of (7), which, in turn, can be integrated exactly: the integral over each triangle is equal to the area of the triangle multiplied by the average of the integrand values at the triangle vertices.

3 Numerical Examples

In this section, we illustrate the performance of the proposed hybrid Eulerian-Lagrangian method on two numerical examples. We compare the obtained results with those obtained by a "purely" Eulerian finite-volume method (we have used the second-order central upwind scheme with the MinMod1.5 limiter [KL02, KNP01, KP]) applied to the Saint-Venant system (1) and the convection-diffusion equation (2) separately, as it has been suggested in [CKP06] as the way to improve the resolution of contact waves in T captured by the central-upwind scheme. In all our numerical experiments, the gravitation constant was taken $g = 1$ and viscosity coefficient $\nu = 10^{-5}$.

One-Dimensional Example. We start with the 1-D example taken from [CKP06]. In this example, we assume that the initial water level and the initial discharge are constant: $h(x,0) + B(x) \equiv 1$, $h(x,0)u(x,0) = 0.1$, the bottom topography is given by:

$$B(x) = \begin{cases} 0.25(\cos(10\pi(x-0.5)) + 1, & \text{if } \ 0.4 \le x \le 0.6, \\ 0, & \text{otherwise,} \end{cases}$$

and the initially polluted area is $[0.4, 0.5]$:

$$T(x,0) = \begin{cases} 1, & \text{if } \ 0.4 \le x \le 0.5, \\ 0, & \text{otherwise.} \end{cases}$$

The pollution spot propagates to the right, and we numerically track its evolution. The pollutant concentration at times $t = 0$, 2, and 4, computed by the hybrid Eulerian-Lagrangian and the finite-volume methods, is shown in Figure 1 (left), where both Δx for the central-upwind scheme and the distance between the initially uniformly distributed characteristics points is taken $1/200$. One can clearly see the superiority of the results obtained by our hybrid method. In Figure 1 (right), we refine the mesh employed by the finite-volume method. The solutions are shown at time $t = 4$. One can observe that the resolution achieved by the hybrid Eulerian-Lagrangian method with $\Delta x = 1/200$ is comparable with the one by the finite-volume method with $\Delta x = 1/1600$. The difference becomes even more prominent in the 2-D case, considered in the next numerical example.

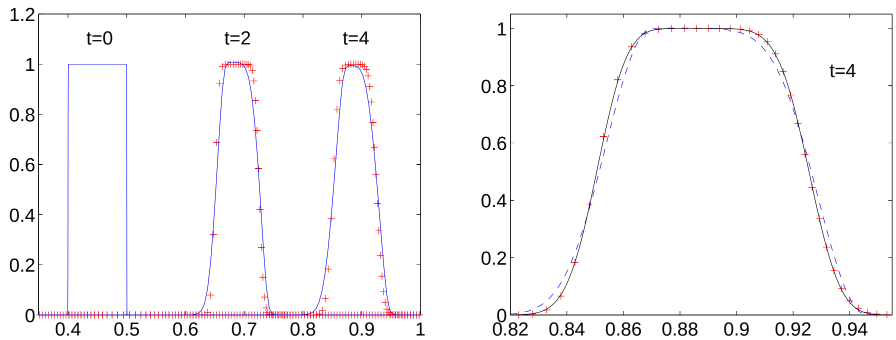

Fig. 1. Propagation of the 1-D pollution spot by the hybrid Eulerian-Lagrangian method ('pluses') and the second-order finite-volume method (solid line) at different times (left figure). In the right figure: comparison of the hybrid solution with the finite-volume ones computed on finer grids with $\Delta x = 1/400$ (dashed line) and $\Delta x = 1/1600$ (solid line).

Two-Dimensional Example. Here, the initial pollutant spot is transfered with the flow over the exponentially shaped bump $B(x, y) = 0.25 \exp(-10x^2 - 5y^2)$. A 2-D version of the system (1),(3) is solved subject to the initial conditions:

$$h(x, y, 0) + B(x, y) = 1, \;\; h(x, y, 0)u(x, y, 0) = 0.2, \;\; h(x, y, 0)v(x, y, 0) = 0.05,$$

where h is, as before, the water depth, and u and v are the x- and y-components of the velocity vector. The initial concentration of the pollutant is:

$$T(x, y, 0) = \begin{cases} 1, & -0.75 \le x \le -0.25, \; -0.25 \le y \le 0.25, \\ 0, & \text{otherwise.} \end{cases}$$

In Figure 2, we show the pollutant concentration T at time $t = 4$, computed by our hybrid Eulerian-Lagrangian method (left) and the second-order central-upwind scheme (right) with $\Delta x = \Delta y = 1/50$ for both the central-upwind scheme and the initial uniform distribution of the characteristic points. One can clearly observe a much better resolution achieved by the hybrid method. As in the 1-D example, we refine the computational grid and apply the second-order central-upwind scheme with $\Delta x = \Delta y = 1/100$ (Figure 3 (left)) and $\Delta x = \Delta y = 1/200$ (Figure 3 (right)). As one can see there, our hybrid method still outperforms the finite-volume one.

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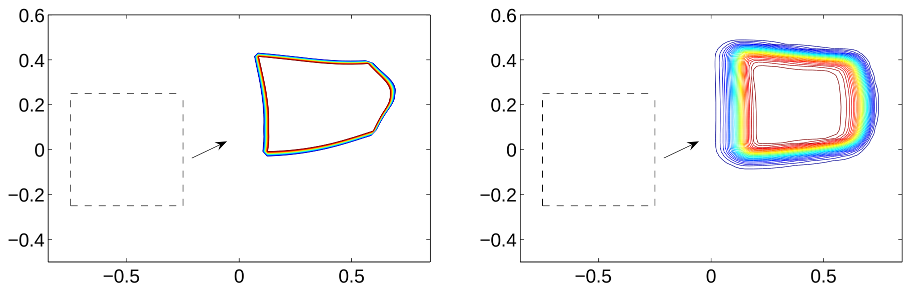

Fig. 2. Propagation of the 2-D pollution spot by the hybrid Eulerian-Lagrangian method (left) and the second-order finite-volume method (right). In both computations $\Delta x = \Delta y = 1/50$. The dashed line represents the boundary of the initially polluted domain.

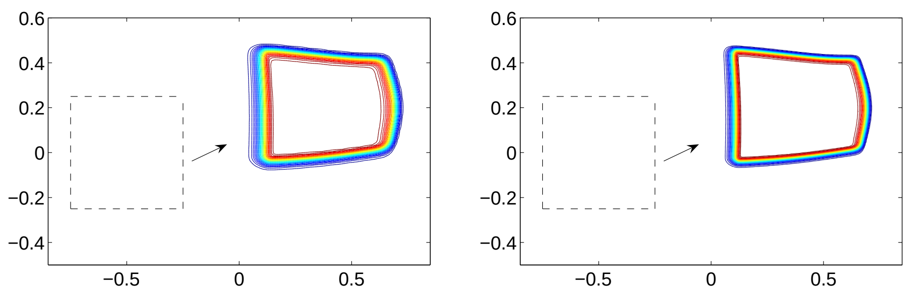

Fig. 3. Propagation of the 2-D pollution spot by the second-order finite-volume method with $\Delta x = \Delta y = 1/100$ (left) and $\Delta x = \Delta y = 1/200$ (right). The dashed line represents the boundary of the initially polluted domain.

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