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MUSCL schemes for the shallow water sensitivity equations with passive scalar transport

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ABSTRACT

A higher-order numerical technique is presented for the direct sensitivity analysis of the shallow water equations with passive scalar transport. The continuous sensitivity equations are modified to account for the possible presence of shocks in the solution, that result in Dirac source terms for the sensitivity across flow discontinuities. Higher-order accuracy is achieved via a MUSCL reconstruction technique with slope limiting, which makes the numerical solution Total Variation Diminishing (TVD). The Harten–Lax–Van Leer (HLL) approximate Riemann solver is modified so as to account for the influence of source terms in both the flow and sensitivity solutions. Several options are tested for the wave speed estimates and the order of the MUSCL time stepping, such as the MUSCL-Hancock, MUSCL-EVR and MUSCL-HLLG techniques. Convergence analyses on continuous and discontinuous flow problems with analytical solutions indicate that first-order time stepping is approximately twice as fast as second-order time stepping and that it yields more accurate sensitivity solutions.

1. Introduction

Sensitivity equations for flow problems and optimization have gained attention over the past years. The applications of sensitivity analysis include local and global sensitivity, uncertainty analysis of model response, as well as reliability analysis [4,11,13,26,34], inverse modeling [8], optimization, design and control [16,25,35]. Several approaches to sensitivity modeling are available. The direct (or forward) sensitivity approach is mainly used when the sensitivity of several variables to a few parameters is to be investigated, while the adjoint (or backward) sensitivity approach is advised when the purpose is to investigate the influence of numerous parameters on a limited set of variables [4]. Calculation methods include continuous and discrete approaches. In the continuous approach, the set of sensitivity equations are obtained by differentiating the governing flow equations with respect to the parameters of interest. The sensitivity equations are then solved numerically (see e.g. [9,15,18–21,23,24,29,35,36]). In the discrete approach, the governing flow equations are first solved numerically, then differentiated with respect to the parameter of interest to provide a discrete sensitivity solution. Examples of such methods are complex differentiation [30], code differentiation [14], and finite difference evaluation of the sensitivity [27], also called empirical sensitivity calculation.

In the field of free surface flow modeling, the sensitivity approach has been applied in the form of adjoint approaches [13,36,35] and direct approaches [9,15,20,23], mostly in the form of continuos methods. Most existing applications to date are valid for continuous flow solutions only, because discontinuous flow solutions make the derivatives locally meaningless. As shown in [2,25], Dirac source terms appear across discontinuities. Such terms are not accounted for in classical sensitivity calculation techniques and the sensitivity solution may become unstable when computed numerically. In [2], the sensitivity equations are reformulated in the framework of the theory of distributions and the Rankin–Hugoniot (jump) relationships are presented for the sensitivity. Such relationships are much more complex than the jump relationships for the flow variables and their discretization poses a number of issues, as shown in this paper.

So far, the numerical techniques presented for the shallow water sensitivity equations in the presence of discontinuous solutions are based on first-order finite volume approaches [9,23,20,21,10] and have been applied to flows over smooth topographies. The purpose of the present paper is (i) to propose a number of MUSCL-based, finite volume methods for direct sensitivity computation for the shallow water equations, (ii) to assess the computational efficiency and accuracy of the various approaches, (iii) to present an improvement over the method initially proposed

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in [10] for source term discretization, and (iv) to assess the influence of classical wave speed estimates used in the Riemann solver on the accuracy of the solution.

The paper is organized as follows. In Section 2, the governing flow and sensitivity equations are presented, as well as an overview of the finite volume discretization. Section 3 focuses on the Riemann solver used to compute the fluxes and source terms for both the hydrodynamic and sensitivity variables. Section 4 presents the MUSCL-based schemes used. In Section 5, the various numerical approaches are applied to various test cases and convergence analyses are carried out. Section 6 is devoted to concluding remarks.

2. Governing equations and finite volume discretization

2.1. The shallow water equations

The one-dimensional shallow water equations with passive scalar transport can be written in conservation form as

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S} \tag{1}$$

where t and x are respectively the time and space coordinates, and the conserved hydrodynamic variable $\mathbf{U}$, the flux $\mathbf{F}$ and the source term $\mathbf{S}$ are defined as

$$\mathbf{U} = \begin{bmatrix} h \\ q \\ m \end{bmatrix} = \begin{bmatrix} h \\ hu \\ hv \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} q \\ \frac{q^2}{h} + \frac{g}{2}h^2 \\ qv \end{bmatrix}, \quad \mathbf{S} = \begin{bmatrix} 0 \\ (S_0 - S_f)gh \\ 0 \end{bmatrix} \tag{2}$$

where g is the gravitational acceleration, h is the water depth, m is the amount of the variable v per unit length, q is the unit discharge, S_0 and S_f are respectively the bottom and friction slope, u is the flow velocity and v is the advected variable. For example, if the variable v is a solute concentration, m is the solute mass per unit length and width of channel. S_0 and S_f are defined as

$$S_0 = -\frac{\partial z_b}{\partial x} \tag{3a}$$

$$S_f = n_M^2 u|u|h^{-4/3} \tag{3b}$$

where n_M is Manning's friction coefficient. Eq. (1) can also be written in non-conservation form as

$$\frac{\partial \mathbf{U}}{\partial t} + \mathbf{A}\frac{\partial \mathbf{U}}{\partial x} = \mathbf{S} - \left(\frac{\partial \mathbf{F}}{\partial x}\right)_{\mathbf{U}=\mathrm{Const}} \tag{4}$$

where $\mathbf{A}$ is the Jacobian matrix of $\mathbf{F}$ with respect to $\mathbf{U}$:

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 \\ c^2 - u^2 & 2u & 0 \\ -uv & v & u \end{bmatrix} \tag{5}$$

with $c = (gh)^{1/2}$ the speed of the waves in still water. The eigenvalues of $\mathbf{A}$ are

$$\lambda^{(1)} = u - c \tag{6a}$$

$$\lambda^{(2)} = u \tag{6b}$$

$$\lambda^{(3)} = u + c \tag{6c}$$

and the matrix of eigenvectors of $\mathbf{A}$ is

$$\mathbf{K} = \begin{bmatrix} 1 & 0 & 1 \\ \lambda^{(1)} & 0 & \lambda^{(3)} \\ v & 1 & v \end{bmatrix} \tag{7}$$

The purpose is to solve Eq. (1) over a domain $[0, L]$ of space for times $t > 0$. The problem is well-posed, that is, the existence and uniqueness of the solution of Eq. (1) is guaranteed, provided that the initial condition $\mathbf{U}(x, t)$ is known for all $x \in [0, L]$ at time $t = 0$, and that as many boundary conditions are prescribed as there are characteristics $\frac{dx}{dt} = \lambda^{(p)}$ $(p = 1, 2, 3)$ entering the domain [6]. Such initial and boundary conditions are written in the form

$$\mathbf{U}(x, 0) = \mathbf{U}_0(x) \quad \forall x \in [0, L] \tag{8a}$$

$$\mathbf{f}(\mathbf{U}(0, t)) = \mathbf{f}_{b,0}(t) \quad \forall t > 0 \tag{8b}$$

$$\mathbf{f}(\mathbf{U}(L, t)) = \mathbf{f}_{b,L}(t) \quad \forall t > 0 \tag{8c}$$

where $\mathbf{U}_0(x)$, $\mathbf{f}_{b,0}(t)$ and $\mathbf{f}_{b,L}(t)$ are known functions for the initial and boundary conditions.

2.2. Derivation of the sensitivity equations for continuous solutions

In the conservation and non-conservation forms (1) and (4), the flux $\mathbf{F}$ and the source term $\mathbf{S}$ are functions of a number of parameters such as the gravitaional acceleration g, the bottom slope S_0 and the friction coefficient n_M. Besides, the solution $\mathbf{U}$ at a given (x, t) is a function of the initial and boundary conditions, that may also be considered as parameters of the problem. Therefore, in Eq. (1), $\mathbf{F} = \mathbf{F}(\mathbf{U}, \varphi)$ and $\mathbf{S} = \mathbf{S}(\mathbf{U}, \varphi)$. A sensitivity analysis consists in studying the variations in $\mathbf{U}$ triggered by a variation in the parameter φ. The sensitivity can be seen as the partial derivative of $\mathbf{U}$ with respect to the perturbation amplitude φ_0. It is presented in [4] as a Gateaux differential, that is, a directional derivative.

The shallow water sensitivity equations are derived by assuming an infinitesimal perturbation $\mathrm{d}\varphi$ in the parameter φ:

$$\mathrm{d}\varphi(x, t) = \varphi_0\ \varepsilon(x, t) \tag{9}$$

where φ_0 is the amplitude (assumed infinitesimal) of the perturbation and $\varepsilon(x, t)$ is the so-called support function of the perturbation. $\varepsilon = 0$ in the regions of the solution domain where φ is not to be perturbed, and takes non-zero values at points where φ is assumed to be subjected to a perturbation. Perturbing the parameter φ by $\mathrm{d}\varphi$ induces a perturbation $\mathrm{d}\mathbf{U}$ in $\mathbf{U}$ over the solution domain. The sensitivity $\mathbf{s}$ of $\mathbf{U}$ with respect to φ is defined as the limit ratio

$$\mathbf{s} \equiv \lim_{\varphi_0 \to 0} \frac{\mathrm{d}\mathbf{U}}{\varphi_0} \tag{10}$$

The governing equations for the sensitivity $\mathbf{s}$ are obtained by writing that the perturbed solution $\mathbf{U} + \mathrm{d}\mathbf{U}$ also verifies Eq. (1):

$$\frac{\partial(\mathbf{U} + \mathrm{d}\mathbf{U})}{\partial t} + \frac{\partial(\mathbf{F} + \mathrm{d}\mathbf{F})}{\partial x} = \mathbf{S} + \mathrm{d}\mathbf{S} \tag{11}$$

Under the assumption of an infinitesimal perturbation, one has

$$\mathrm{d}\mathbf{F} = \mathbf{A}\ \mathrm{d}\mathbf{U} + \frac{\partial \mathbf{F}}{\partial \varphi}\mathrm{d}\varphi = \left(\mathbf{A}\mathbf{s} + \frac{\partial \mathbf{F}}{\partial \varphi}\varepsilon\right)\varphi_0 \tag{12a}$$

$$\mathrm{d}\mathbf{S} = \frac{\partial \mathbf{S}}{\partial \mathbf{U}}\ \mathrm{d}\mathbf{U} + \frac{\partial \mathbf{S}}{\partial \varphi}\mathrm{d}\varphi = \left(\frac{\partial \mathbf{S}}{\partial \mathbf{U}}\mathbf{s} + \frac{\partial \mathbf{S}}{\partial \varphi}\varepsilon\right)\varphi_0 \tag{12b}$$

Substituting Eqs. (12a) and (12b) into Eq. (11), subtracting Eq. (1) and dividing by φ_0 leads to

$$\frac{\partial \mathbf{s}}{\partial t} + \frac{\partial \mathbf{G}}{\partial x} = \mathbf{Q} \tag{13}$$

where the sensitivity flux $\mathbf{G}$ and the sensitivity source term $\mathbf{Q}$ are defined as

$$\mathbf{G} = \mathbf{A}\mathbf{s} \tag{14a}$$

$$\mathbf{Q} = \frac{\partial \mathbf{S}}{\partial \mathbf{U}}\mathbf{s} + \frac{\partial \mathbf{S}}{\partial \varphi}\varepsilon - \frac{\partial}{\partial x}\left(\frac{\partial \mathbf{F}}{\partial \varphi}\varepsilon\right) \tag{14b}$$

In this paper, the parameters under consideration for the sensitivity analysis are initial conditions, as well as the geometric parameter involved in the source term $\mathbf{S}$, that is, the bottom elevation z_b. The gravitational acceleration is not considered for analysis