Journal of Mathematics and System Science 2 (2012) 334-340

A Derivative Recovery Spectral Volume Model for the Analysis of Constituents Transport in One-Dimensional Flows

Luigi Cimorelli[1], Carmine Covelli[1], Luca Cozzolino[2], Renata Della Morte[2] and Domenico Pianese[1]

1. Faculty of Engineering, University of Naples Federico II, Napoli 80125, Italy

2. Faculty of Engineering, University of Naples Parthenope, Napoli 80142, Italy

Received: April 23, 2012 / Accepted: May 16, 2012 / Published: May 25, 2012.

Abstract: The treatment of advective fluxes in high-order finite volume models is well established, but this is not the case for diffusive fluxes, due to the conflict between the discontinuous representation of the solution and the continuous structure of analytic solutions. In this paper, a derivative reconstruction approach is proposed in the context of spectral volume methods, for the approximation of diffusive fluxes, aiming at the reconciliation of this conflict. Two different reconstructions are used for advective and diffusive fluxes: the advective reconstruction makes use of the information contained in a spectral cell, and allows the formation of discontinuities at the spectral cells boundaries; the diffusive reconstruction makes use of the information contained in contiguous spectral cells, imposing the continuity of the reconstruction at the spectral cells boundaries. The method is demonstrated by a number of numerical experiments, including the solution of shallow-water equations, complemented with the advective-diffusive transport equation of a conservative substance, showing the promising abilities of the numerical scheme proposed.

Key words: Spectral volume method, derivative recovery method, advection-diffusion problems, C-property, well-balanced.

1. Introduction

The increasing interest of public audience and researchers towards environmental problems has prompted the study and the design of numerical models able to simulate the transport and the fate of constituents and pollutants in surface water bodies. For instance, numerous finite volume models for the solution of the shallow-water equations, coupled with the passive transport of a constituent, at most second-order accurate in time and space, are available in literature, based on different approaches. The treatment of advective fluxes in high-order finite volume models (spectral volume, ENO, WENO among the others) is well established, and the discontinuous representation of the solution can naturally accommodate for the discontinuities of the true solution. Conversely, high-order treatment of diffusive fluxes can be difficult in finite volume models, in that the discontinuous representation of the solution conflicts with the analytic solution, which is always continuous. Recently, a number of approaches have been proposed and adopted for the calculation of diffusive fluxes in the context of Spectral Volume methods, namely the LSV (local spectral volume) approach and the penalty SV (spectral volume) by Sun and Wang [1], the penalty SV approach by Kannan and Wang [2]. These methods exhibit one or more of the following problems: lack of symmetry, lack of compactness and sub-optimal order of convergence. Especially the first two problems stressed above can decrease the convergence speed of algorithms in the case of implicit time-marching methods. Starting from

Corresponding author: Domenico Pianese, professor, research fields: hydraulics, hydrology, water resources planning and management, river engineering. E-mail: pianese@unina.it.

these considerations, in this paper a numerical model for the solution of the one-dimensional shallow-water equations:

$$\begin{aligned} &\frac{\partial h}{\partial t}+\frac{\partial hU}{\partial x}=0 \\ &\frac{\partial hU}{\partial t}+\frac{\partial}{\partial x}\left(\frac{g}{2}h^2+hU^2\right)=-gh\frac{dz_b}{dx} \end{aligned} \tag{1}$$

is presented, coupled with the equation for the passive transport of dissolved substances, which takes into account also the diffusion of constituents:

$$\frac{\partial hC}{\partial t}+\frac{\partial}{\partial x}hUC=\frac{\partial}{\partial x}\left(Dh\frac{\partial C}{\partial x}\right) \tag{2}$$

In the Eqs. (1) and (2) the following definitions hold: x = space independent variable, t = time independent variable, $z_b\ (x)$ = bed elevation, $h(x,t)$ = water depth, $U(x,t)$ = vertically averaged flow velocity, $C(x,t)$ = vertically averaged constituent concentration, g = gravity acceleration constant, $D(x,t)$ = dispersion coefficient. We observe that the system of Eq. (1) is hyperbolic, while the coupling of Eqs. (1) and (2) leads to an advection-dominated parabolic system of equations.

The numerical model presented in this paper, which is high-order accurate far from discontinuities of the flow field, extends to the case of transport of passive constituents the approaches already proposed by some of the authors [3, 4], based on the spectral volume method, and makes use of the HLLC (harten–lax–van leer contact wave) approximate Riemann solver to evaluate the advective fluxes at the interfaces between the spectral cells. In order to ensure the C-property, the source terms are upwinded at the interfaces, after a so-called “hydrostatic reconstruction”. The diffusive fluxes are calculated using a novel approach, called DRSV (derivative recovery spectral volume), which is linked to the derivative recovery method [5, 6] and to the direct discontinuous galerkin method [7], recently introduced for the diffusive fluxes calculation in RKDG (Runge-Kutta discontinuous galerkin methods). The DRSV exhibits good properties, namely high-order accuracy, local symmetry and compactness of the numerical stencil. A number of preliminary numerical experiments are reported, showing the promising capabilities of the method.

The paper is organized as follows: in Section 2, the numerical method is discussed; in Section 3, the numerical method is verified by means of numerical experiments; in Section 4, the results are discussed.

2. The Numerical Method

In this section, at first, the spectral volume method [8] for hyperbolic systems of differential equations is briefly reviewed; then, the derivative recovery spectral volume is introduced for the solution of parabolic problems. Finally, it is shown how these approaches are applied for the solution of the one-dimensional shallow-water equations, complemented with the passive transport of a constituent.

2.1 The Spectral Volume Method for Hyperbolic Equations

A system of hyperbolic equations can be considered as :

$$\frac{\partial \mathbf{u}}{\partial t}+\frac{\partial \mathbf{f}(\mathbf{u})}{\partial x}=\mathbf{s}(x,\mathbf{u}), \quad x\in[0\,;L] \quad t>0 \tag{3}$$

where $\mathbf{u}$ is the vector of conserved variables, $\mathbf{f}(\mathbf{u})$ is the vector of physical fluxes and $\mathbf{s}(x,\mathbf{u})$ is the vector of source terms. In order to apply the spectral volume method, the computational domain is partitioned in NS non-overlapping cells named “spectral volumes” or “spectral cells”, indexed by i. Then, the generic spectral cell is defined by $S_i = [x_{i-1/2},\ x_{i+1/2}]$. Each spectral cell is in turn partitioned in k non-overlapping finite volumes: the generic finite volume $V_{i,j}$ contained in the spectral volume S_i is defined by $V_{i,j} = [x_{i,j-1/2}, x_{i,j+1/2}]$, and its length is $\Delta x_{i,j} = x_{i,j+1/2} - x_{i,j-1/2}$. It can be observed that the following obvious congruency conditions holds: $x_{i,1/2} = x_{i-1/2}$ and $x_{i,k+1/2} = x_{i+1/2}$. If Eq. (3) is integrated in each finite volume $V_{i,j}$, the following systems of ordinary differential equations is obtained:

$$\frac{d\,\mathbf{u}_{i,j}}{dt} = -\frac{1}{\Delta x_{i,j}}\left[\mathbf{F}_{i,j+\frac{1}{2}} - \mathbf{F}_{i,j-\frac{1}{2}}\right] + \mathbf{s}_{i,j} \tag{4}$$

where $i = 1, 2, \dots, NS$; $j = 1, 2, \dots, k$; and $t > 0$. In the Eq. (4), $\mathbf{u}_{i,j}$ is the cell averaged value of the vector of conserved variables in $V_{i,j}$, $\mathbf{F}_{i,j+1/2}$ is the vector of numerical fluxes through the interface $x_{i,j+1/2}$ between $V_{i,j}$ and $V_{i,j+1}$, $\mathbf{s}_{i,j}$ is the vector of numerical source terms in $V_{i,j}$. In order to evaluate the terms at the right-hand side of Eq. (4), the conserved variables are reconstructed in each spectral cell S_i by means of a piecewise polynomial conservative reconstruction $\mathbf{u}_i(x)$ of order $p = k - 1$, which ensures that:

$$\mathbf{u}_{i,j} = \frac{1}{\Delta x_{i,j}} \int_{x_{i,j-1/2}}^{x_{i,j+1/2}} \mathbf{u}_i(x)dx\ ;\ j = 1,2...k \tag{5}$$

The reconstructed variables are used to evaluate high-order approximations of source terms in finite volumes, and fluxes at the interfaces: after evaluation of the right-hand side of Eq. (4), a system of ordinary differential equations is obtained, and a high-order Runge-Kutta scheme is used to make the solution marching in time. It can be observed that the conserved variables and fluxes can be discontinuous passing through the interface between two finite volumes, after variables reconstruction. In this case, the numerical fluxes are calculated by solving the local Riemann problem.

2.2 Derivative Recovery Spectral Volume for Diffusive Fluxes Calculation

When applying the Finite Volume Method on uniform grids, in order to approximate the solution of the diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}\ ,\ x \in [0\,;L] \quad t > 0 \tag{6}$$

the following second-order accurate scheme is often used:

$$\frac{du_i}{dt} = \frac{u_{i+1} - 2u_i + u_{i+1}}{\Delta x^2} \tag{7}$$

where u_i is the averaged value of $u(x)$ in the finite volume V_i, and Δx is the length of the finite volumes. The finite volume scheme Eq. (7) is analogous to the finite difference scheme for the diffusion [9], where u_i should be intended as the approximation of $u(x)$ at the location x_i, and for this reason it is sometimes called "finite difference approach". Of course, the Eq. (7) can be derived in the context of the finite volume method. In fact, having defined the flux $F = -\partial u/\partial x$, the application of the finite volume method to the Eq. (6) allows writing, for each finite volume, the equation:

$$\frac{du_i}{dt} = -\frac{1}{\Delta x}\left[F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\right] \tag{8}$$

where $F_{i+1/2}$ is a consistent approximation of the flux $F(x_{i+1/2})$ between the finite volumes V_i and V_{i+1} [10]. In order to evaluate $F_{i+1/2}$, it can be observed [5] that a conservative reconstruction of the solution $u(x)$ on the stencil $V_{i,i+1}=V_i \cup V_{i+1}$ is:

$$u_{i,i+1}(x) = \left(x - x_{i+1/2}\right)\frac{u_{i+1} - u_i}{\Delta x} + \frac{u_{i+1} + u_i}{2} \tag{9}$$

which very naturally supplies:

$$\frac{\partial u}{\partial x}\left(x_{i+1/2}\right) \approx \frac{\partial u_{i,i+1}}{\partial x}\left(x_{i+1/2}\right) = \frac{u_{i+1} - u_i}{\Delta x} \tag{10}$$

So, a good approximation of $F(x_{i+1/2}) = -\partial u/\partial x$ is $F_{i+1/2} = -(u_{i+1} - u_i)/\Delta x$, and the scheme Eq. (7) is obtained.

The concept can be generalized to the case of the spectral volume method. In order to evaluate the diffusive flux $F_{i,k+1/2}$ between the spectral volumes S_i and S_{i+1}, let's consider the stencil $S_{i,i+1}=S_i \cup S_{i+1}$, which consists of $2k$ finite volumes: in this stencil, the solution can be reconstructed by means of a polynomial $u_{i,i+1}(x)$ of order $p = 2k - 1$, and this polynomial can be used in turn to supply a high-order approximation of $F(x)= -\partial u/\partial x$ at the interface between the two spectral volumes. The diffusive fluxes are needed also for internal interfaces: the arithmetic average $0.5[u_{i-1,i}(x) + u_{i,i+1}(x)]$ of the reconstructions $u_{i-1,i}(x)$ and $u_{i,i+1}(x)$ supplies a $2k$ accurate approximation of the solution $u(x)$ in the spectral volume S_i, which can be used for the evaluation of $\partial u/\partial x$ at internal faces. It is clear that, on irregular grids, the expected nominal order of accuracy is $p = 2k - 1$.

It can be observed that the DRSV method is compact, in that the diffusive fluxes through the external and internal interfaces of the spectral volume S_i depend solely on the variables conserved in the finite volumes of the cells S_{i-1}, S_i and S_{i+1}. In order to make an example, it can be observed that, in the case of $k = 2$ and uniform grid with spectral volumes of length Δx, the following scheme is obtained:

$$\frac{d}{dt}\begin{pmatrix} u_{i,1} \\ u_{i,2} \end{pmatrix} = \frac{1}{6\Delta x^2}\left\{\begin{pmatrix} -1 & 27 \\ -1 & 3 \end{pmatrix}\begin{pmatrix} u_{i-1,1} \\ u_{i-1,2} \end{pmatrix} + \begin{pmatrix} -50 & 22 \\ 22 & -50 \end{pmatrix}\begin{pmatrix} u_{i,1} \\ u_{i,2} \end{pmatrix} + \begin{pmatrix} 3 & -1 \\ 27 & -1 \end{pmatrix}\begin{pmatrix} u_{i+1,1} \\ u_{i+1,2} \end{pmatrix}\right\} \tag{11}$$

2.3 Spectral Volume Shallow-Water Equations Model with Constituents Transport

The spectral volume method can be applied for the solution of Eqs. (1) and (2). First, the conserved variables h, hU, hC and $z_b + h$ are reconstructed in each spectral volume; then, the HLLC approximate Riemann solver is used to evaluate the advective fluxes at the interfaces between the spectral cells (see Section 2.1). The TVBM (total variation bounded in the means) limiter [11] is used to limit the reconstructions near shocks, ensuring the algorithm stability. In order to force the equilibrium in steady-state calculations the source terms must balance the advective fluxes (C-property): aiming at this, the source terms are firstly subdivided into in-cell contribution and interface contributions; then, the interface contributions are upwinded [12] following the so-called “hydrostatic reconstruction”. For the integration of the in-cell source term contribution, the Romberg formulas are applied. Diffusive fluxes are calculated by recovering the derivatives of h and hC, and applying the DRSV approach (see Section 2.2).

After the evaluation of fluxes and source terms, a system of ordinary differential equations is obtained, whose solution is approximated by means of the third-order TVD (total variation diminishing) Runge-Kutta scheme.

3. Numerical Experiments

In this section, a number of numerical experiments are presented, in order to test the numerical scheme.

3.1 Diffusion of a Sinusoidal Wave

In the first numerical experiment, an accuracy test is accomplished considering the approximate solution of the following equation:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}, \; x \in [0\,;\,2\pi]; \quad t > 0 \tag{12}$$

with sinusoidal initial conditions:

$$u_0(x) = u\,(x,0) = \sin(x), \; x \in [0\,;\,2\pi] \tag{13}$$

and periodic boundaries conditions. The problem admits the exact solution:

$$u\,(x,t) = e^{-Dt}\sin(x) \tag{14}$$

The value D = 1 m^2/s was chosen. In order to generate a non-uniform grid for this numerical test, the following technique was adopted: the computational domain, $L = 2\pi$ long, was firstly subdivided in NS uniform spectral volumes, each $\Delta x = 2\pi/NS$ long; then, the interface between two spectral volumes was randomly moved by the distance $0.1\Delta x$ to the left or to the right. The fluxes between the finite volumes were calculated using the DRSV approach, while the time-marching method used was the third-order TVD Runge-Kutta method. The numerical solution was carried out up to t = 1 s, with time step Δt small enough to consider the time error negligible. The test was repeated for $k = 1$, 2 and 3 finite volumes per cell, and for increasing NS. The L_∞ and L_1 norms of the error, calculated with reference to the finite volume-averaged values of u, are presented in Table 1. From inspection of Table 1, it is apparent that the convergence order of the DRSV method is greater than the nominal value $2k - 1$, and very close to $2k$. It is noticed that, for $k = 3$ and $NS = 40$, the spatial error is proportional to 10^{-10}, and the time error dominates.

3.2 Advection-Diffusion of a Sinusoidal Wave

In this numerical experiment, the following equation is considered:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = D\frac{\partial^2 u}{\partial x^2}, \; x \in [0\,;\,2\pi]; \quad t > 0 \tag{15}$$

with sinusoidal initial conditions given by Eq. (13), with the choices D = 1 m^2/s and c = 1 m/s and periodic

Table 1 Diffusion of a sinusoidal wave on a irregular grid by means of the DRSV method: error norms.

k		NS = 5	NS = 10		NS = 20		NS = 40	
		Error	Error	Order	Error	Order	Error	Order
1	L_∞	4.89E-02	2.48E-02	0.98	5.68E-03	2.13	1.31E-03	2.11
	L_1	1.80E-01	5.91E-02	1.60	1.31E-02	2.17	3.29E-03	1.99
2	L_∞	3.04E-03	2.18E-04	3.80	1.51E-05	3.85	9.11E-07	4.05
	L_1	8.90E-03	5.88E-04	3.92	3.91E-05	3.91	2.41E-06	4.02
3	L_∞	4.06E-05	7.16E-07	5.82	1.20E-08	5.89	-	-
	L_1	7.87E-05	1.62E-06	5.60	2.50E-08	6.01	-	-

boundaries conditions. The problem admits the exact solution:

$$u\left(x,t\right)=e^{-Dt}\sin\left(x-ct\right) \tag{16}$$

The computational domain, $L = 2\pi$ long, was subdivided in *NS* uniform spectral volumes, and the solution was computed up to $t = 1$ s. The diffusive fluxes between the finite volumes were calculated using the DRSV approach, while the simple upwind formula:

$$F_c=\frac{1}{2}u^{+}_{i,j+1}\left(c-\left|c\right|\right)+\frac{1}{2}u^{-}_{i,j+1}\left(c+\left|c\right|\right) \tag{17}$$

was used for the advective flux through the interface $x_{i,j+1/2}$ between the finite volume $V_{i,j}$ and the finite volume $V_{i,j+1}$. The test was repeated for $k = 1$, 2 and 3 finite volumes per cell, and for increasing *NS*. The L_∞ and L_1 norms of the error, calculated with reference to the finite volume-averaged values of u, are presented in Table 2.

It has to be observed that the advective fluxes were calculated with order of accuracy k, while the diffusive fluxes were calculated with order of accuracy greater than $2k - 1$: the global order of accuracy was equal or greater than k, as confirmed by inspection of Table 2.

3.3 Solution of the Shallow-Water Equations with Passive Transport of a Constituent

In this test, inspired to that presented by Xing and Shu [13], the solution of the Eqs. (1) and (2) is considered. In a channel, 1 m long, the initial conditions and the bed elevation were defined by:

$$\begin{cases} h\left(x,0\right)=5+e^{\cos\left(2\pi x\right)} \\ hU\left(x,0\right)=\sin\left(\cos\left(2\pi x\right)\right) \\ hC\left(x,0\right)=1+e^{\sin\left(4\pi x\right)} \\ z_b\left(x\right)=\sin^2\left(\pi x\right) \end{cases} \quad x\in\left[0;1\right] \tag{18}$$

The initial conditions Eq. (18) were complemented by periodic boundary conditions.

The dispersion coefficient depends on the local characteristics of the flow, and could be evaluated [14] by means of the Elder's formula, which is valid for plane turbulent flows. Here, only for demonstrative purposes, the numerical test was accomplished twice, using first a constant dispersion coefficient $D = 0.1$ m^2/s, then a constant dispersion coefficient $D = 0$ m^2/s. For calculations, $NS = 20$ spectral cells and $k = 3$ finite volumes per cell were used. The results are presented in Fig. 1.

Inspection of Fig. 1 shows how the results of the proposed model, with reference to the water surface elevation, compare well with the solutions available in literature [15], also in the case of a modest number of freedom degrees (60 finite volumes). Moreover, in Fig. 1 (panel below), a comparison is made between the concentration distributions obtained using $D = 0$ m^2/s and $D = 0.1$ m^2/s, respectively. The effect of the dispersion coefficient is the smoothing of the concentration distribution, tending to a constant concentration long-term distribution, as expected.

4. Conclusions

In this paper, a spectral volume model for the approximate solution of shallow-water equations has been presented, complemented with the equation of advective-diffusive transport of a passive constituent. The well-balanced model, which is third-order accurate in time and space, makes use of a novel scheme for the diffusive flux calculations, named derivative recovery spectral volume. Preliminary numerical tests seem to

Table 2 Advection-diffusion of a sinusoidal wave on a regular grid by means of the DRSV method: error norms.

k		NS = 5	NS = 10		NS = 20		NS = 40	
		Error	Error	Order	Error	Order	Error	Order
1	L_∞	1.35E-01	8.83E-02	0.614	5.06E-02	0.804	2.70E-02	0.904
	L_1	5.49E-01	5.39E-01	0.614	2.00E-01	0.839	1.08E-01	0.892
2	L_∞	1.49E-02	2.17E-03	2.78	2.92E-04	2.89	3.82E-05	2.93
	L_1	4.17E-02	5.99E-03	2.80	8.15E-04	2.88	1.07E-04	2.93
3	L_∞	1.31E-03	1.56E-04	3.07	2.17E-05	2.84	2.88E-06	2.92
	L_1	4.41E-03	6.22E-04	2.83	8.71E-05	2.84	1.15E-05	2.92

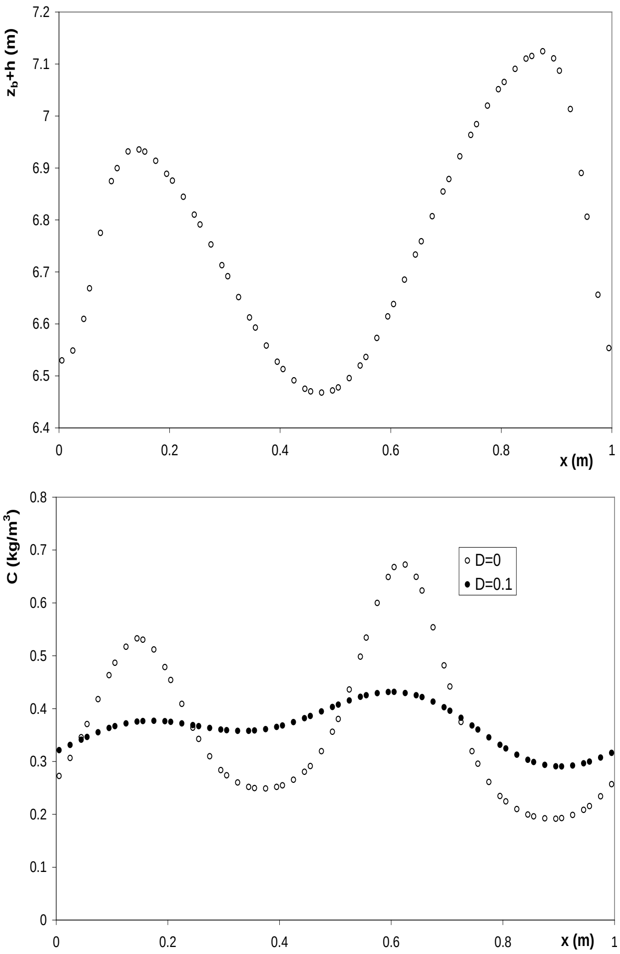

Fig. 1 Periodic wave in a channel. (Above) Water surface height after *t* = 1 s. (Below) Depth-averaged concentration after *t* = 1 s.

show how the DRSV scheme is a valid alternative to other well known schemes for diffusive fluxes calculation in high-order finite volume schemes. In the next future, the authors plan to find a rigorous demonstration of the accuracy and stability characteristics of the DRSV method, and to implement its application to the case of unstructured grids.

References

[1] Y. Sun, Z.J. Wang, Formulations and analysis of the spectral volume method for the diffusion equation, Communications in Numerical Methods in Engineering 20 (2004) 927-937.

[2] R. Kannan, Z.J. Wang, A study of viscous flux formulations for a p-multigrid spectral volume navier stokes solver, Journal of Scientific Computing 41 (2009) 165-199.

[3] L. Cozzolino, D. Pianese, High-order finite volume modelling of one-dimensional flows, in: R.M.L. Ferreira, E.C.T.L. Alves, J.G.A.B. Leal, A.H. Cardoso (Eds.), Proceedings of River Flow 2006, International Conference on Fluvial Hydraulics, Taylor & Francis Group, London, 2006, pp. 493-502.

[4] L. Cozzolino, R.D Morte, G.D Giudice, A. Palumbo, D. Pianese, A well-balanced spectral volume scheme with the wetting-drying property for the shallow-water equations, Journal of Hydroinformatics 14 (2012) 745-760.

[5] B. van Leer, S. Nomura, Discontinuous Galerkin for diffusion, in: 17th AIAA-CFD Conference, Toronto, Ontario Canada, 2005, pp. 2005-5108.

[6] M. van Raalte, B. van Leer, Bilinear forms for the recovery-based discontinuous Galerkin method for the diffusion, Communications in Computational Physics 5 (2009) 683-693.

[7] H. Liu, J. Yan, The direct discontinuous Galerkin (DDG) methods for diffusion problems, SIAM Journal on Numerical Analysis 47 (2009) 675-698.

[8] Z.J. Wang, Spectral (finite) volume method for conservation laws on unstructured grids: Basic formulation, Journal of Computational Physics 178 (2002) 210-251.

[9] C.A.J. Fletcher, Computational Techniques for Fluid Dynamics 1, Springer-Verlag, Kassel, Germany, 1996.

[10] R. Eymard, T. Gallouët, R. Herbin, Finite Volume Methods, in Handbook for Numerical Analysis, Vol. VII., Ph. Ciarlet and J.L. (Eds.), North Holland, 2000.

[11] B. Cockburn, C.W. Shu, TVB Runge-Kutta local

projection discontinuous Galerkin finite element method for conservation laws II: General framework, Mathematics of Computation 52 (1989) 411-435.

[12] E. Audusse, F. Bouchut, M.O. Bristeau, R. Klein, B. Perthame, A fast and stable well-balanced scheme with the hydrostatic reconstruction for shallow water flows, SIAM Journal on Scientific Computing 25 (2004) 2050-2065.

[13] Y. Xing, C.W. Shu, High order well-balanced finite volume WENO schemes and discontinuous Galerkin methods for a class of hyperbolic systems with source terms, Journal of Computational Physics 214 (2006) 567-598.

[14] H.B. Fisher, E.J. List, R.C. Koh, J. Imbberger, N.H. Brooks, Mixing in Inland and Coastal Waters, Academic Press, Waltham, Massachusetts, 1979.

[15] V. Caleffi, A. Valiani, A. Bernini, Fourth-order balanced source term treatment in central WENO schemes for shallow water equations, Journal of Computational Physics 218 (2006) 228-245.