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Inflow-implicit/outflow-explicit finite volume methods for solving advection equations



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ABSTRACT

We introduce a new class of methods for solving non-stationary advection equations. The new methods are based on finite volume space discretizations and a semi-implicit discretization in time. Its basic idea is that outflow from a cell is treated explicitly while inflow is treated implicitly. This is natural, since we know what is outflowing from a cell at the old time step but we leave the method to resolve a system of equations determined by the inflows to a cell to obtain the solution values at the new time step. The matrix of the system in our inflow-implicit/outflow-explicit (IIOE) method is determined by the inflow fluxes which results in an M-matrix yielding favorable stability properties for the scheme. Since the explicit (outflow) part is not always dominated by the implicit (inflow) part and thus some oscillations can occur, we build a stabilization based on the upstream weighted averages with coefficients determined by the flux-corrected transport approach [2,19] yielding high resolution versions, S¹IIOE and S²IIOE, of the basic scheme. We prove that our new method is exact for any choice of a discrete time step on uniform rectangular grids in the case of constant velocity transport of quadratic functions in any dimension. We also show its formal second order accuracy in space and time for 1D advection problems with variable velocity. Although designed for non-divergence free velocity fields, we show that the basic IIOE scheme is locally mass conservative in case of divergence free velocity. Finally, we show L²-stability for divergence free velocity in 1D on periodic domains independent of the choice of the time step, and L^{∞} -stability for the stabilized high resolution variant of the scheme. Numerical comparisons with the purely explicit schemes like the fully explicit up-wind and the Lax-Wendroff schemes were discussed in [13] and [14] where the basic IIOE was originally introduced. There it has been shown that the new scheme has good properties with respect to a balance of precision and CPU time related to a possible choice of larger time steps in our scheme. In this contribution we compare the new scheme and its stabilized variants with widely used fully implicit up-wind method. In this comparison our new schemes show better behavior with respect to stability and precision of computations for time steps several times exceeding the CFL stability condition. Our new stabilized methods are L^{∞} stable, second order accurate for any smooth solution and with accuracy of order 2/3 for solutions with moving discontinuities. This is opposite to implicit up-wind schemes which have accuracy order 1/2 only. All these properties hold for any choice of time step thus making our new method attractive for practical applications.

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1. Introduction

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In this article we present the inflow-implicit/outflow-explicit (IIOE) method, and its stabilized (S¹IIOE, S²IIOE) high-resolution variants, for solving general time dependent variable velocity advection equations of the form

$$u_t + \mathbf{v} \cdot \nabla u = 0 \tag{1}$$

where $u \in \mathbb{R}^d \times [0, T]$ is the unknown function and **v** is a vector field which may vary in space, e.g. $\mathbf{v} = \mathbf{v}(x, u, \nabla u)$. Variable velocity vector fields arise in many applications, e.g. in transport equations with non-divergence free velocities or nonlinear conservation laws [11], in the Eulerian level set methods for evolving fronts [18], in a tangentially stabilized Lagrangean methods for evolving interfaces [1,16] or in other applications like an image segmentation by active contours in a form of generalized subjective surface method [3,4,9,15,17,20]. In such case of image segmentation, the spatially varying vector field $\mathbf{v}(x)$ depends on the gradient of the image intensity function. For motion of level sets in normal direction with speed F(x) we have $\mathbf{v} = F(x) \frac{\nabla u}{|\nabla u|}$ [12,18]. In this case the basic IIOE method coincides with the semi-implicit forward-backward diffusion approach recently presented by the authors in [12]. In the context of level set equations the originality of the approach in [12] consists in rewriting the level set equation for motion in normal direction in terms of an equation containing the forward and backward diffusion. Then naturally, the forward diffusion dominated parts of the model are treated implicitly, while the backward diffusion dominated parts are treated explicitly. The resulting scheme is a semi-implicit second order numerical scheme that allows large time steps. Hence, our new IIOE method presented in [13,14] and in this paper can be seen as a generalization of the approach from [12] to arbitrary variable velocity advection equations.

The basic idea of our new IIOE method is that outflow from a cell is treated explicitly while inflow is treated implicitly. Such an approach is natural, since we know what is flowing out from a cell at an old time step n - 1 but we leave the method to resolve a system of equations determined by the inflows to obtain a new value in the cell at time step n. Since the matrix of the system is determined by the inflow fluxes, it is an M-matrix and thus it has favorable solvability and stability properties. It is worth to note that a similar idea to construct the M-matrix in the implicit part has also been introduced by Kuzmin and his co-authors by using a purely algebraic approach in the context of solving advection equations by the Galerkin finite element method combined usually with the Crank–Nicolson time stepping, see [10] for the latest state-of-the-art and related references.

Since the explicit (outflow) part is not always dominated by the implicit (inflow) part, some oscillations can occur in the basic IIOE scheme. One way is to leave them propagate and perform some postprocessing of the numerical solution, or another way is to incorporate a stabilization mechanism into the scheme itself. As it was shown in [12], a special local averaging was sufficient to stabilize the forward-backward diffusion approach in order to get stable second order solution in case of smooth level set interface motion in normal direction, but in general, such local averaging does not guarantee fulfilling sharply the discrete minimum-maximum principle. In this paper we build a new stabilization of the basic IIOE scheme based on the so-called flux-corrected transport approach [2,19] yielding L^{∞} stable high resolution variant of the scheme.

We also present theoretical results for our new scheme, namely, its exactness for any choice of time step on uniform rectangular grids in the case of constant velocity transport of quadratic functions in any dimension and its formal second order accuracy in space and time for 1D advection problems with variable velocity. Although designed for non-divergence free velocity fields, we show that the basic IIOE scheme is locally mass conservative in case of divergence free velocity. Finally, we show L^2 -stability for divergence free velocity in 1D on periodic domains independent of the choice of the time step, and L^{∞} -stability for the stabilized high resolution variant of the scheme.

Numerical comparisons with the fully explicit schemes like the fully explicit up-wind and the (limited) Lax–Wendroff method were discussed in [13] and [14]. There, the positive properties of the new scheme have been shown with respect to a balance of precision and CPU time. Thus, in this paper we concentrate mainly on a comparison of the new IIOE scheme and its stabilized variants with the well-known and widely used fully implicit up-wind method for solving advection equations. We show superior behavior of our new schemes with respect to stability and precision of computations for time steps largely exceeding CFL stability condition. Our new schemes are L^{∞} stable, second order accurate for smooth solutions and with accuracy of order 2/3 for solutions with moving discontinuities, opposite to the implicit up-wind schemes which have accuracy order only 1/2 in the discontinuous case. Moreover, all these properties hold for any choice of time step and thus make our new methods attractive from the point of view of practical applications where no concern on CFL restrictions is preferable.

The rest of the article is organized as follows. In Section 2 we introduce the general formulation of the basic and stabilized IIOE schemes on unstructured grids in several space dimensions. In Section 3, for clarity and also due to the reasons of our theoretical study, we write a 1D version of the IIOE scheme and also its higher dimensional form in the case of advective motion of level sets in normal direction in order to clearly see its relation to the forward–backward diffusion approach from [12]. In Section 4 we present theoretical results for our new schemes and in Section 5 we present several representative 1D and higher dimensional numerical experiments demonstrating interesting properties of the method.

2. The inflow-implicit/outflow-explicit scheme

Let us consider Eq. (1) in a bounded polygonal domain $\Omega \subset \mathbb{R}^d$, d = 2, 3, and time interval [0, T]. Let Q_h denote a primal polygonal partition of Ω . Let p be a finite volume (cell) of a corresponding dual Voronoi tessellation \mathcal{T}_h with measure m_p and let e_{pq} be an edge between p and q, $q \in N(p)$, where N(p) is a set of neighboring finite volumes (i.e. $\bar{p} \cap \bar{q}$ has nonzero (d-1)-dimensional measure). Let us note that the Voronoi property is introduced just due to a formulation of the scheme for advective motion of level sets in normal direction, presented in Section 3.2, where approximation of the solution gradient is necessary. Let c_{pq} be the length of e_{pq} and n_{pq} be the unit outer normal vector to e_{pq} with respect to p. We shall consider \mathcal{T}_h to be an admissible mesh in the sense of [5], i.e., there exists a representative point x_p in the interior of every finite volume p such that the joining line between x_p and x_q , $q \in N(p)$, is orthogonal to e_{pq} . We denote by x_{pq} the intersection of this line segment with the edge e_{pq} . The length of this line segment is denoted by d_{pq} , i.e. $d_{pq} := |x_q - x_p|$. As we have constructed \mathcal{T}_h based on the primal mesh \mathcal{Q}_h , we assume that the points x_p coincide with the vertices of \mathcal{Q}_h . Let us denote by u_p a (constant) value of the solution in a finite volume p computed by the scheme. For the solution representation inside the finite volume p we either use this value u_p or a reconstructed (but again constant) value denoted by \overline{u}_{pq} .

In order to motivate our new scheme, let us rewrite (1) in the formally equivalent form with conserving and nonconserving parts [7,8]

$$u_t + \nabla \cdot (\mathbf{v}u) - u\nabla \cdot \mathbf{v} = 0. \tag{2}$$

Integrating (2) over a finite volume *p* then yields

$$\int_{p} u_t \, dx + \int_{p} \nabla \cdot (\mathbf{v}u) \, dx - \int_{p} u \nabla \cdot \mathbf{v} \, dx = 0.$$

Using a constant representation of the solution on the cell p denoted by \bar{u}_p and applying the divergence theorem we get

$$\int_{p} u_t \, dx + \sum_{q \in N(p)} \int_{e_{pq}} u \mathbf{v} \cdot n_{pq} \, ds - \overline{u}_p \sum_{q \in N(p)} \int_{e_{pq}} \mathbf{v} \cdot n_{pq} \, ds = 0.$$

Denoting by \bar{u}_{pq} another representative constant value of the solution on the interface e_{pq} , we further get

$$\int_{p} u_t \, dx + \sum_{q \in N(p)} \overline{u}_{pq} \int_{e_{pq}} \mathbf{v} \cdot n_{pq} \, ds - \overline{u}_p \sum_{q \in N(p)} \int_{e_{pq}} \mathbf{v} \cdot n_{pq} \, ds = 0$$

If we denote the integrated fluxes in the inward normal direction to the finite volume p by

$$\bar{\nu}_{pq} = -\int\limits_{e_{pq}} \mathbf{v} \cdot n_{pq} \, ds,\tag{3}$$

we finally arrive at the balance law

$$\int_{D} u_t \, dx + \sum_{q \in N(p)} \bar{v}_{pq} (\bar{u}_p - \bar{u}_{pq}) = 0. \tag{4}$$

The major new idea of our scheme is to split the resulting fluxes into the corresponding inflow and outflow parts to the cell *p*. This is done by defining

$$a_{pq}^{in} = \max(\bar{\nu}_{pq}, 0), \qquad a_{pq}^{out} = \min(\bar{\nu}_{pq}, 0).$$
 (5)

We then approximate u_t by the time difference $\frac{u_p^n - u_p^{n-1}}{\tau}$, where τ is a uniform time step size, and take the inflow parts implicitly and the outflow parts explicitly in (4). This yields the following system of equations for the finite volume solution u_p^n , $p \in T_h$ at the *n*-th discrete time step

$$u_{p}^{n} + \frac{\tau}{m_{p}} \sum_{q \in N(p)} a_{pq}^{in} (\bar{u}_{p}^{n} - \bar{u}_{pq}^{n}) = u_{p}^{n-1} - \frac{\tau}{m_{p}} \sum_{q \in N(p)} a_{pq}^{out} (\bar{u}_{p}^{n-1} - \bar{u}_{pq}^{n-1})$$
(6)

for all $p \in T_h$.

The most natural choice for reconstructions \bar{u}_p^m and \bar{u}_{pq}^m , m = n, n - 1 is given by

$$\bar{u}_{p}^{m} = u_{p}^{m}, \qquad \bar{u}_{pq}^{m} = \frac{1}{2} \left(u_{p}^{m} + u_{q}^{m} \right)$$
(7)

and leads to the basic IIOE scheme

$$u_p^n + \frac{\tau}{2m_p} \sum_{q \in N(p)} a_{pq}^{in} (u_p^n - u_q^n) = u_p^{n-1} - \frac{\tau}{2m_p} \sum_{q \in N(p)} a_{pq}^{out} (u_p^{n-1} - u_q^{n-1})$$
(8)

which for a uniform squared grids in two space dimensions with a finite volume side width h reduces to the following simple system

$$u_{p}^{n} + \frac{\tau}{2h^{2}} \sum_{q \in N(p)} a_{pq}^{in} (u_{p}^{n} - u_{q}^{n}) = u_{p}^{n-1} - \frac{\tau}{2h^{2}} \sum_{q \in N(p)} a_{pq}^{out} (u_{p}^{n-1} - u_{q}^{n-1}).$$
(9)

Before proceeding further let us remark that, Eq. (4) has the form of a discretization of a diffusion equation, where \bar{v}_{pq} would represent the so-called transmissive coefficients (integrated diffusion fluxes divided by distances between cell centers). In a standard forward diffusion all these coefficients are strictly positive which leads to a weighted averaging of the solution and the implicit schemes are natural in this case. On the other hand the negative coefficients would correspond to a backward diffusion in which case information propagates outside the cell and explicit schemes are thus natural. In our case the sign of the coefficients is given by the inflow or outflow character of the cell boundary and the inflow-implicit/outflow-explicit approach is thus natural. This forward-backward diffusion relationship with the inflow-outflow fluxes is inspired by [12] where the forward-backward diffusion formulation was used for solving advective motion of level sets in normal direction. Let us also note that a term h^{d-1} is included in the definition of the numerical fluxes \bar{v}_{pq} and a term h^d in definition of m_p . Thus, taking this into account we see that a τ/h term is in front of the sums in (9) which is standard in advection discretization schemes. It is also well-known that in any second order scheme for solving advection equations one can identify the "forward diffusion" part (like the first order up-winding) and the "backward diffusion" part (additional sharpening terms coming (sometimes surprisingly) from the second order Taylor's expansions), a classical example is e.g. the Lax–Wendroff scheme [11]. In our method this splitting arises naturally and, as we will see theoretically in Section 4, it gives the second order accuracy. Since the "backward diffusion" part of the scheme is clearly given, its stabilization can be built straightforwardly if it is necessary to suppress some (not unboundedly growing) oscillations.

The basic scheme (8) allows to use any time step size τ and obtain a solution of the linear system given by the left hand implicit side. This follows from the M-matrix property of the system and we call it the *solvability property* of the scheme. However, the right hand explicit side may cause oscillations especially in case of singularities or large gradients in a solution. These oscillations do not grow unboundedly in time, but if one prefers to remove them we present here a strategy how to make our method *unconditionally stable* in the L^{∞} sense and keep its *second order accuracy* for smooth solutions. The stabilization approach is based on an adaptive upstream weighted choice for the averages \bar{u}_{pq}^m , m = n, n - 1at the cell interfaces. Instead of taking $\bar{u}_{pq}^m = \frac{1}{2}(u_p^m + u_q^m)$ as suggested for the basic scheme, we relax (7) to the choice

$$\bar{u}_p^m = u_p^m, \qquad \bar{u}_{pq}^m = \left(1 - \theta_{pq}^m\right)u_p^m + \theta_{pq}^m u_q^m \tag{10}$$

for some weighting parameter $\theta_{pq}^m \in [0, 1]$ that we will choose locally in such a way that the resulting scheme becomes unconditionally stable in L[∞]. With this relaxation we recover the basic scheme for $\theta_{pq}^n = \theta_{pq}^{n-1} = 1/2$, while $\theta_{pq}^m = 1$ corresponds to full up-wind for inflows (and full down-wind for outflows) and $\theta_{pq}^m = 0$ to full down-wind for inflows (and full up-wind for outflows). Since in our scheme the inflows appear in the implicit part, i.e. with index m = n, and outflows appear in the explicit part, i.e. for m = n - 1, we will use notation $\theta_{pq}^{in,n}$ for inflow relaxation parameters and $\theta_{pq}^{out,n-1}$ for outflow relaxation parameters. Plugging reconstructions (10) in both inflow-implicit and outflow-explicit parts of (6) we get

$$u_{p}^{n} + \frac{\tau}{m_{p}} \sum_{q \in N(p)} a_{pq}^{in} \left(u_{p}^{n} - \left(\left(1 - \theta_{pq}^{in,n} \right) u_{p}^{n} + \theta_{pq}^{in,n} u_{q}^{n} \right) \right) \\ = u_{p}^{n-1} - \frac{\tau}{m_{p}} \sum_{q \in N(p)} a_{pq}^{out} \left(u_{p}^{n-1} - \left(\left(1 - \theta_{pq}^{out,n-1} \right) u_{p}^{n-1} + \theta_{pq}^{out,n-1} u_{q}^{n-1} \right) \right)$$
(11)

from where we obtain the general form of a stabilized IIOE scheme

$$u_{p}^{n} + \frac{\tau}{m_{p}} \sum_{q \in N(p)} \theta_{pq}^{in,n} a_{pq}^{in} (u_{p}^{n} - u_{q}^{n}) = u_{p}^{n-1} - \frac{\tau}{m_{p}} \sum_{q \in N(p)} \theta_{pq}^{out,n-1} a_{pq}^{out} (u_{p}^{n-1} - u_{q}^{n-1})$$
(12)

where $\theta_{pq}^{out,n-1}$, $\theta_{pq}^{in,n}$ will be chosen using ideas of the so-called flux-corrected transport (FCT) methodology [2,19]. The stabilized IIOE scheme can be understood as a high-resolution variant of the basic IIOE scheme which may locally decrease the outflow contributions, and, when not considering the outflows at all, it corresponds to a fully implicit up-wind method, where only inflows are considered. The local choice of the relaxation parameters will be done in such a way, that the stabilized IIOE scheme reduces to the basic IIOE in case of well resolved smooth solutions (and thus it is second order in smooth case), whereas it switches locally towards a fully implicit discretization at grid points where the minimum-maximum principle would be violated. We show by numerical computations that unlike the classical first order implicit up-wind method

which has for linearly advected solutions with discontinuities convergence order 1/2, the new method has in such cases convergence order 2/3 for any choice of time step.

As noticed above, the choice of θ -stabilization coefficients follows the FCT approach. In our semi-implicit method, the only part which may cause the violation of the global minimum–maximum principle is the right hand explicit side of (12). Thus, we require that the relaxation parameters $\theta_{pq}^{out,n-1}$ are chosen in such a way that the following two conditions are fulfilled locally in every finite volume p

$$u_p^{n-1} - \frac{\tau}{m_p} \sum_{q \in N(p)} \theta_{pq}^{out, n-1} a_{pq}^{out} \left(u_p^{n-1} - u_q^{n-1} \right) \le u_p^{max, n-1},\tag{13}$$

$$u_p^{n-1} - \frac{\tau}{m_p} \sum_{q \in N(p)} \theta_{pq}^{out, n-1} a_{pq}^{out} \left(u_p^{n-1} - u_q^{n-1} \right) \ge u_p^{min, n-1}.$$
(14)

Here, $u_p^{max,n-1}$ and $u_p^{min,n-1}$ denote a maximum, respectively minimum in a local neighborhood of p at time step n-1. A particular choice of the parameters $\theta_{pq}^{out,n-1}$ is determined as follows. Let us denote by n^{out} the number of nonzero outflows from the finite volume p, i.e.

$$n^{out} = -\sum_{q \in N(p)} \operatorname{sign}(a_{pq}^{out}).$$

For all $q \in N(p)$ where $a_{pq}^{out} < 0$ and $(u_p^{n-1} - u_q^{n-1}) \neq 0$ we require that the following two conditions are satisfied

$$\frac{1}{n^{out}}u_p^{n-1} - \frac{\tau}{m_p}\theta_{pq}^{out,n-1}a_{pq}^{out}\left(u_p^{n-1} - u_q^{n-1}\right) \le \frac{1}{n^{out}}u_p^{max,n-1},\tag{15}$$

$$\frac{1}{n^{out}}u_p^{n-1} - \frac{\tau}{m_p}\theta_{pq}^{out,n-1}a_{pq}^{out}\left(u_p^{n-1} - u_q^{n-1}\right) \ge \frac{1}{n^{out}}u_p^{min,n-1}.$$
(16)

It is clear that by summation of the conditions (15) over all $q \in N(p)$ we get (13) and similarly by summation of (16) we get (14). The conditions (15), (16) are not necessarily optimal ones, but they are sufficient to get (13) and (14). Since on the right hand side of (13), (14) there are local minima and maxima which are inside the range of the global minimum and maximum at the time step n - 1, due to the M-matrix property of the system on the left hand side of (12), we have that the overall solution in the new time step fulfills the global minimum–maximum principle. From (15) and (16) we get two conditions for $\theta_{pq}^{out,n-1}$

$$\theta_{pq}^{out,n-1} \le \frac{\frac{1}{n^{out}} (u_p^{max,n-1} - u_p^{n-1})}{-\frac{\tau}{m_n} a_{pq}^{out} (u_p^{n-1} - u_q^{n-1})}, \quad \text{if } \left(u_p^{n-1} - u_q^{n-1} \right) > 0, \tag{17}$$

$$\theta_{pq}^{out,n-1} \le \frac{\frac{1}{n^{out}} (u_p^{min,n-1} - u_p^{n-1})}{-\frac{\tau}{m_p} a_{pq}^{out} (u_p^{n-1} - u_q^{n-1})}, \quad \text{if } \left(u_p^{n-1} - u_q^{n-1} \right) < 0$$
(18)

from which we define

$$\theta_{pq}^{out,n-1} = \operatorname{Min}\left(\frac{1}{2}, \frac{m_p(u_p^{max,n-1} - u_p^{n-1})}{\tau n^{out} a_{pq}^{out}(u_q^{n-1} - u_p^{n-1})}\right) \quad \text{if } a_{pq}^{out}(u_q^{n-1} - u_p^{n-1}) > 0 \tag{19}$$

$$\theta_{pq}^{out,n-1} = \operatorname{Min}\left(\frac{1}{2}, \frac{m_p(u_p^{min,n-1} - u_p^{n-1})}{\tau n^{out} a_{pq}^{out}(u_q^{n-1} - u_p^{n-1})}\right) \quad \text{if } a_{pq}^{out}\left(u_q^{n-1} - u_p^{n-1}\right) < 0.$$

$$(20)$$

If $a_{pq}^{out} = 0$ or $u_p^{n-1} - u_q^{n-1} = 0$, $\theta_{pq}^{out,n-1}$ could be theoretically arbitrary, but we set

$$\theta_{pq}^{out,n-1} = \frac{1}{2}, \quad \text{if } a_{pq}^{out} \left(u_q^{n-1} - u_p^{n-1} \right) = 0.$$
(21)

Finally, it remains to define the relaxation parameters $\theta_{pq}^{in,n}$ for the implicit inflow parts. If $\theta_{pq}^{in,n}$ is considered for an inflow face to volume p, it is natural that $\theta_{qp}^{out,n-1}$ is associated with an outflow face of the neighboring cell q. Thus, a natural choice that makes the reconstruction \overline{u}_{pq}^n at the interface e_{pq} unique, is

$$\theta_{pq}^{in,n} = 1 - \theta_{qp}^{out,n-1} \tag{22}$$

where $\theta_{qp}^{out,n-1}$ is defined through (19)–(21). The scheme (12) with the choice of relaxation parameters given by (19)–(22) represent our first stabilized **S**¹**IIOE** scheme. Let us note that our definitions of relaxation parameters ensure that for outflow

faces we always have $\theta_{pq}^{out,n-1} \in [0, 1/2]$ and for inflow faces $\theta_{pq}^{in,n} \in [1/2, 1]$. Thus, the relaxation may only shift the reconstruction at cell interfaces towards an upstream average. The conditions (19)–(21) guarantee L^{∞} stability, while condition (22) keeps the scheme consistent and ensures uniqueness of the cell interface reconstructions.

Performing numerical experiments, we have found and built also a second approach to stabilization that results in our S^2 IIOE scheme which is given by a two-step procedure in every discrete time step:

1st step: first use the basic IIOE scheme, i.e. solve (12) with
$$\theta_{pq}^{in,n} = \theta_{pq}^{out,n-1} = 1/2$$
.
2nd step: if $u_p^n > u_p^{max,n-1}$ or $u_p^n < u_p^{min,n-1}$ we redefine $\theta_{pq}^{out,n-1}$ and $\theta_{qp}^{in,n}$ according to (19)–(22). (23)

The usage of the S²IIOE scheme is motivated by the fact that conditions (13), (14) may be too strong. Although they are not fulfilled sharply, the implicit part can keep the numerical solution in the minimum–maximum range. Thus, we mark the points where the minimum–maximum principle is violated when applying the basic IIOE scheme and only in those points we redefine the relaxation parameters. On the first view, this approach seems slower concerning CPU than S¹IIOE, because we have to solve the linear system twice. But, on the other hand, the redefinition of relaxation parameters, which takes its own CPU time, occurs only in few points while in S¹IIOE it is done in every grid point. Our computational experience is that S²IIOE scheme is only slightly (like 10–20%) slower than S¹IIOE scheme while, especially in case of smooth solutions, it increases precision significantly.

Further useful modification of both stabilized schemes is that we can consider $u_p^{max,n-1}$ and $u_p^{min,n-1}$ in (13), (14) and subsequent formulas taking into account a local quadratic reconstruction of the numerical solution at time step n - 1. This can be useful, because the maximum (minimum) does not necessarily transfer to a grid point in a consecutive time step. The quadratic reconstruction allows the reconstructed numerical solution to be slightly higher (lower) than just values at grid points and thus keeps overall maximum (minimum) with higher order accuracy. In particular, it makes our stabilized S²IIOE method exact for an advection of a quadratic function by a constant velocity for any choice of time step, similarly to such property of the basic IIOE scheme, because the θ coefficients are not redefined when using quadratic reconstruction.

We summarize our new inflow-implicit/outflow-explicit methods in the following general definition.

Definition 2.1 (*IIOE schemes*). Let initial data $u_0 \in C^0(\Omega)$ and Dirichlet boundary data $u_D \in C^0(\partial \Omega \times [0, T])$ be given. Furthermore, let R_p and R_{pq} denote suitable local reconstructions of the solution on the cell p and the interface e_{pq} , respectively and g_{pq} denote a suitable numerical flux that approximates $-\int_{e_{pq}} \mathbf{v} \cdot n_{pq} \, ds$. These operators may differ depending on the inflow or outflow character of the cell interface (such dependence will be denoted by superscripts *in* and *out*).

Then the general inflow-implicit/ outflow-explicit method (IIOE) is defined as follows:

Initial data: For n = 0 define the piecewise constant approximation u_h^0 through

$$u_{h}^{0}|_{p}(x) := u_{p}^{0} := \pi_{p}(u_{0}), \quad \forall x \in p, \ p \in \mathcal{T}_{h},$$
(24)

where $\pi_p : C^0(p) \to \mathbb{P}_0(p)$ is a suitable local projection to a constant.

Time step $(\mathbf{n} - \mathbf{1}) \rightarrow \mathbf{n}$: For n > 0 we define u_h^n through u_p^n , $p \in \mathcal{T}_h$ as follows

a) Definition of boundary values at time t^n : For all $x_p \in \partial \Omega$ we set

$$u_p^n := u_D(x_p, t^n). \tag{25}$$

b) Definition of the interior values at time t^n :

i) Inflow/outflow splitting of the fluxes. For all interfaces e_{pq} we define

$$a_{pq}^{in,n} = \max(g_{pq}^{in}(\mathbf{v}, u_h^n), 0), \qquad a_{pq}^{out,n-1} = \min(g_{pq}^{out}(\mathbf{v}, u_h^{n-1}), 0).$$
(26)

ii) For all $x_p \in \Omega \setminus \partial \Omega$ we define u_p^n as the solution of the following linear system

$$u_{p}^{n} + \frac{\tau}{m_{p}} \sum_{q \in N(p)} a_{pq}^{in,n} \left(R_{p}^{in}(u_{h}^{n}) - R_{pq}^{in}(u_{h}^{n}) \right)$$

= $u_{p}^{n-1} + \frac{\tau}{m_{p}} \sum_{q \in N(p)x} a_{pq}^{out,n-1} \left(R_{p}^{out}(u_{h}^{n-1}) - R_{pq}^{out}(u_{h}^{n-1}) \right).$ (27)

Note that (26) and (27) may result in a non-linear system of equations for u_h^n , if the velocity field depends on the solution.

c) Definition of u_h^n :

We define the piecewise constant approximation u_h^n as

$$u_h^n|_p(x) := u_p^n, \quad \forall x \in p, \, p \in \mathcal{T}_h$$

A specific IIOE scheme is obtained by specifying the reconstruction operators R_p^{in} , R_{pq}^{out} , R_{pq}^{out} , R_{pq}^{out} and the numerical flux function g_{pq}^{in} , g_{pq}^{out} . The most natural choice of reconstruction operators are given in (7) and (3) and lead to our basic **IIOE scheme**. More sophisticated choices are given by (10) with stabilization parameters chosen from (19)–(22), or from (23) and lead to the **S¹IIOE**, and **S²IIOE** schemes, respectively. These schemes are used in all computations presented in Section 5. Further particular choices of reconstructions are possible, e.g. a local averaging, as presented in the context of motion of level sets in normal direction in [12].

3. Special cases of the IIOE scheme

For clearer exposition and to prepare for the theoretically analysis in Section 4, we now detail the method in two particular cases, for one dimensional transport with variable velocity, and for motion of level sets in normal direction.

3.1. IIOE scheme for 1D variable velocity case

Let us derive the scheme for the one-dimensional equation

$$u_t + v u_x = 0, \tag{28}$$

where v = v(x). Again (28) is written in the form

$$u_t + (vu)_x - uv_x = 0, (29)$$

and integrated in p_i , the cell with the spatial index i, length h, center point x_i , left border $x_{i-\frac{1}{2}}$ and right border $x_{i+\frac{1}{2}}$. Let us denote $v_i = v(x_i)$, $v_{i-\frac{1}{2}} = v(x_{i-\frac{1}{2}})$, $v_{i+\frac{1}{2}} = v(x_{i+\frac{1}{2}})$, u_i^n the value of the numerical solution at time step n and \overline{u}_i^n , $\overline{u}_{i-\frac{1}{2}}^n$ the reconstructed values. Using the Newton–Leibniz formula we get

$$\int_{p_i} u_t \, dx + v_{i+\frac{1}{2}} \overline{u}_{i+\frac{1}{2}} - v_{i-\frac{1}{2}} \overline{u}_{i-\frac{1}{2}} - \overline{u}_i (v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}) = 0,$$

which can be rewritten as

$$\int_{p_i} u_t \, dx + v_{i-\frac{1}{2}} (\bar{u}_i - \bar{u}_{i-\frac{1}{2}}) + (-v_{i+\frac{1}{2}}) (\bar{u}_i - \bar{u}_{i+\frac{1}{2}}) = 0$$

If $v_{i-\frac{1}{2}} > 0$ it represents inflow from the left to the cell and if $(-v_{i+\frac{1}{2}}) > 0$ it represents inflow from the right to the cell. If the signs are opposite it represents outflows. Thus, we define

$$\begin{aligned} a_{i-\frac{1}{2}}^{in} &= \max(v_{i-\frac{1}{2}}, 0), \qquad a_{i-\frac{1}{2}}^{out} &= \min(v_{i-\frac{1}{2}}, 0), \\ a_{i+\frac{1}{2}}^{in} &= \max(-v_{i+\frac{1}{2}}, 0), \qquad a_{i+\frac{1}{2}}^{out} &= \min(-v_{i+\frac{1}{2}}, 0). \end{aligned}$$

If we use a finite difference approximation of the time derivative, take inflow implicitly and outflow explicitly and use the simple reconstructions $\bar{u}_i^n = u_i^n$, $\bar{u}_{i-\frac{1}{2}}^n = \frac{1}{2}(u_i^n + u_{i-1}^n)$ in both time steps, we end up with the basic **one-dimensional IIOE scheme**:

$$u_{i}^{n} + \frac{\tau}{2h} a_{i-\frac{1}{2}}^{in} \left(u_{i}^{n} - u_{i-1}^{n} \right) + \frac{\tau}{2h} a_{i+\frac{1}{2}}^{in} \left(u_{i}^{n} - u_{i+1}^{n} \right) = u_{i}^{n-1} - \frac{\tau}{2h} \left(a_{i-\frac{1}{2}}^{out} \left(u_{i}^{n-1} - u_{i-1}^{n-1} \right) + a_{i+\frac{1}{2}}^{out} \left(u_{i}^{n-1} - u_{i+1}^{n-1} \right) \right).$$

$$(30)$$

The scheme (30) requires to solve a tridiagonal system in every time step which is very fast using the standard tridiagonal solver (also called the Thomas algorithm). The stabilized one-dimensional **S¹IIOE** and **S²IIOE** schemes are obtained by (12) with the formulas (19)–(22) and (19)–(23), respectively.

3.2. IIOE scheme for motion of level sets in normal direction

In the case of motion of level sets in normal direction we consider Eq. (1) with velocity depending on the gradient of solution, i.e. $\mathbf{v} = F \frac{\nabla u}{|\nabla u|}$. Let us consider Cartesian grids in two space dimensions with finite volume side width *h* and define

$$\overline{v}_{pq} = Fh \; \frac{(\overline{u}_p^{n-1} - \overline{u}_{pq}^{n-1})}{(h/2)|\nabla u_{pq}^{n-1}|} = \frac{2F(\overline{u}_p^{n-1} - \overline{u}_{pq}^{n-1})}{|\nabla u_{pq}^{n-1}|} \tag{31}$$

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where $|\nabla u_{pq}^{n-1}|$ is computed by the diamond-cell strategy as detailed in [12]. Plugging expression (31) for integrated inward fluxes into the basic IIOE scheme (9) and comparing it with the scheme (2.5) in [12] we see that they form exactly the same system. One can also see the correspondence of the forward diffusion coefficients in [12] and inflow coefficients in the IIOE scheme (9), respectively the backward diffusion coefficients in [12] and outflow coefficients in the IIOE scheme (9). The FBD and FBD2 schemes from [12] are obtained using their reconstruction stencils (Definitions 2.3 and 3.1), and the role of the forward diffusion contribution D_p^f respectively the backward diffusion contribution D_p^b in general Definition 2.1 of [12] is played by the total inflow D_p^{in} respectively the total outflow D_p^{out} defined by

$$D_{p}^{in} = \sum_{q \in N(p)} a_{pq}^{in}, \qquad D_{p}^{out} = \sum_{q \in N(p)} a_{pq}^{out}.$$
(32)

Numerical experiments for such an IIOE scheme are presented in [12] and also the results of the new stabilized versions of the basic scheme presented in this paper in Section 5.3 are similar to those.

4. Analysis of the scheme

The aim of this section is to give some theoretical backup for the IIOE schemes. In particular we address local mass conservation, exactness for transport of quadratic polynomials with constant velocity with arbitrary time steps, formal order of consistency, $L^{\infty}(L^2)$ stability, as well as $L^{\infty}(L^{\infty})$ stability. As we first look at local mass conservation, let us first recall that such property is automatically satisfied for the general class of finite volume schemes in conservation form, defined as follows.

Definition 4.1 (*Finite volume scheme in conservation form*). Let $\Theta \in [0, 1]$. A finite volume scheme is in conservation form if it can be written in the form

$$u_p^n - u_p^{n-1} = -\frac{\tau}{m_p} \left(\Theta \sum_{q \in N(p)} g_{pq}^n + (1 - \Theta) \sum_{q \in N(p)} g_{pq}^{n-1} \right)$$

where the fluxes need to be conservative in the sense that $g_{pq} = -g_{qp}$. In 1D on uniform partitions this reduces to

$$u_i^n - u_i^{n-1} = -\frac{\tau}{h} \left(\Theta \left(g_{i+1/2}^n - g_{i-1/2}^n \right) + (1 - \Theta) \left(g_{i+1/2}^{n-1} - g_{i-1/2}^{n-1} \right) \right)$$

Lemma 4.2 (Local conservation property). For divergence free velocity field, the basic IIOE is locally mass conservative and can be written in conservation form with numerical fluxes at inflow boundaries (with respect to cell *p*) $g_{pq} := g_{pq}^{in} := \frac{1}{2}(g_{pq}^{in,n} + g_{pq}^{in,n-1})$ with $g_{pq}^{in,n} := -a_{pq}^{in}u_q^n$, $g_{pq}^{in,n-1} := -a_{pq}^{in}u_p^{n-1}$ and at outflow boundaries $g_{pq} := g_{pq}^{out} := \frac{1}{2}(g_{pq}^{out,n} + g_{pq}^{out,n-1})$ and $g_{pq}^{out,n} := -a_{pq}^{out}u_q^n$, $g_{pq}^{out,n-1} := -a_{pq}^{out}u_q^{n-1}$. The conservation property holds, as we have with these definitions

$$g_{pq}^{in} = -g_{qp}^{out}$$
, or respectively $g_{pq}^{out} = -g_{qp}^{in}$

In the simple 1D case with constant positive velocity, the basic IIOE scheme thus reads

$$u_{i}^{n} - u_{i}^{n-1} = -\frac{\tau}{h} \left(\underbrace{\frac{\nu}{2} (u_{i}^{n} + u_{i+1}^{n-1})}_{=:g_{i+1/2}} - \underbrace{\frac{\nu}{2} (u_{i-1}^{n} + u_{i}^{n-1})}_{=:g_{i-1/2}} \right).$$

It is locally conservative with $\Theta := \frac{1}{2}$ and the following definition of the fluxes

$$g_{i+1/2}^n := v u_i^n, \qquad g_{i+1/2}^{n-1} := v u_{i+1}^{n-1}, \qquad g_{i-1/2}^n := v u_{i-1}^n, \qquad g_{i-1/2}^{n-1} := v u_i^{n-1}.$$

Proof. The divergence free velocity field implies in our discrete setting that we have for a cell *p*

$$\sum_{q\in N(p)}a_{pq}^{in}+\sum_{q\in N(p)}a_{pq}^{out}=0.$$

This implies a rewriting of the IIOE scheme as follows

$$u_{p}^{n} = u_{p}^{n-1} - \frac{\tau}{2m_{p}} \sum_{q \in N(p)} a_{pq}^{in} (u_{p}^{n} - u_{q}^{n}) - \frac{\tau}{2m_{p}} \sum_{q \in N(p)} a_{pq}^{out} (u_{p}^{n-1} - u_{q}^{n-1})$$
$$= u_{p}^{n-1} - \frac{\tau}{2m_{p}} \sum_{q \in N(p)} a_{pq}^{in} u_{p}^{n} + \frac{\tau}{2m_{p}} \sum_{q \in N(p)} a_{pq}^{in} u_{q}^{n}$$

$$\begin{aligned} &-\frac{\tau}{2m_{p}}\sum_{q\in N(p)}a_{pq}^{out}u_{p}^{n-1}+\frac{\tau}{2m_{p}}\sum_{q\in N(p)}a_{pq}^{out}u_{q}^{n-1}\\ &=u_{p}^{n-1}+\frac{\tau}{2m_{p}}\sum_{q\in N(p)}a_{pq}^{out}u_{p}^{n}+\frac{\tau}{2m_{p}}\sum_{q\in N(p)}a_{pq}^{in}u_{q}^{n}\\ &+\frac{\tau}{2m_{p}}\sum_{q\in N(p)}a_{pq}^{in}u_{p}^{n-1}+\frac{\tau}{2m_{p}}\sum_{q\in N(p)}a_{pq}^{out}u_{q}^{n-1}\\ &=u_{p}^{n-1}+\frac{\tau}{m_{p}}\sum_{q\in N(p)}a_{pq}^{in}\frac{1}{2}(u_{q}^{n}+u_{p}^{n-1})+\frac{\tau}{m_{p}}\sum_{q\in N(p)}a_{pq}^{out}\frac{1}{2}(u_{p}^{n}+u_{q}^{n-1})\\ &=-g_{pq}^{in} \end{aligned}$$

Let us consider that e_{pq} is an inflow boundary with respect to p, and hence an outflow boundary for q. With $a_{pq}^{in} = -a_{qp}^{out}$, we then obtain

$$g_{pq} + g_{qp} = g_{pq}^{in} + g_{qp}^{out} = -a_{pq}^{in} \frac{1}{2} (u_q^n + u_p^{n-1}) - \underbrace{a_{qp}^{out}}_{=-a_{pq}^{in}} \frac{1}{2} (u_q^n + u_p^{n-1}) = 0.$$

If e_{pq} is an outflow boundary with respect to p and inflow with respect to q, we analogously get

$$g_{pq} + g_{qp} = g_{pq}^{out} + g_{qp}^{in} = -a_{pq}^{out} \frac{1}{2} (u_p^n + u_q^{n-1}) - \underbrace{a_{qp}^{in}}_{=-a_{pq}^{out}} \frac{1}{2} (u_p^n + u_q^{n-1}) = 0.$$

This proves the lemma. \Box

Note, that the property of local mass conservation gets lost for the stabilized versions of the scheme. However, by numerical experiments we see that the global mass error for smooth solutions vanishes with the same order h^2 as the solution error in case of S¹IIOE scheme and with the much higher order h^4 for the S²IIOE scheme, cf. Table 2. The area error is negligible, for dense grids below machine precision, in case of moving discontinuities by linear advection, cf. Table 3.

Theorem 4.3 (Exactness for quadratic polynomials). Let us consider Eq. (1) with constant velocity vector **v** and IIOE scheme (8) on uniform rectangular grids with grid sizes h_i . Let the initial condition be given as a second order polynomial. Then the IIOE scheme (8) gives the exact solution for any choice of time step τ .

Proof. For simplicity let us first consider the 1D case. A general second order polynomial initial condition is of the form $u_0(x) = ax^2 + bx + c$ and exact solution at time τ is given by $u(x, \tau) = u^0(x - v\tau)$. With positive v the scheme (30) takes the form

$$u_i^n + \frac{\tau v}{2h} (u_i^n - u_{i-1}^n) = u_i^{n-1} - \frac{\tau (-v)}{2h} (u_i^{n-1} - u_{i+1}^{n-1})$$
(33)

If we plug into the scheme (33) the exact values in grid points x_i , x_{i-1} , x_{i+1} at time steps $t^{n-1} = 0$ and $t^n = \tau$, namely

$$u_i^{n-1} = ax_i^2 + bx_i + c, \qquad u_{i+1}^{n-1} = a(x_i + h)^2 + b(x_i + h) + c,$$

$$u_i^n = a(x_i - v\tau)^2 + b(x_i - v\tau) + c, \qquad u_{i-1}^n = a(x_i - h - v\tau)^2 + b(x_i - h - v\tau) + c,$$
(34)

we end-up with true identity. In fact, it can be easily checked, e.g. by a symbolic computing system like Mathematica, that both sides are equal to $ax_i^2 + bx_i - av\tau x_i - \frac{1}{2}bv\tau - \frac{1}{2}ahv\tau + c$ and thus their difference is 0. In case of negative velocity v the scheme (30) takes the form

$$u_i^n + \frac{\tau(-\nu)}{2h} \left(u_i^n - u_{i+1}^n \right) = u_i^{n-1} - \frac{\tau \nu}{2h} \left(u_i^{n-1} - u_{i-1}^{n-1} \right)$$
(35)

and again plugging the exact values (34) into (35) gives true identity, both sides are equal to $ax_i^2 + bx_i - av\tau x_i - \frac{1}{2}bv\tau + \frac{1}{2}ahv\tau + c$.

In the 3D case a general quadratic polynomial has the form $a_0 + a_1x + a_2y + a_3z + a_4xy + a_5xz + a_6yz + a_7x^2 + a_8y^2 + a_9z^2$ and the same procedure can be performed in a symbolic computer algebra system. Such calculations surely generalize to arbitrary space dimensions. \Box

Theorem 4.4 (Formal second order consistency). Let us consider Eq. (1) in 1D with variable smooth velocity and the IIOE scheme (30) on a uniform grid. Then the scheme is formally second order and the consistency error is of order $\mathcal{O}(h^2) + \mathcal{O}(\tau h) + \mathcal{O}(\tau^2)$.

Proof. As the scheme depends on inflow/outflow properties of the cell boundaries, we have to distinguish four cases: a) $v_{i-1/2}$, $v_{i+1/2} \ge 0$, b) $v_{i-1/2}$, $v_{i+1/2} \le 0$, c) $v_{i-1/2} < 0$, $v_{i+1/2} > 0$, and d) $v_{i-1/2} > 0$, $v_{i+1/2} < 0$. In both cases, a) and b), we have one inflow and one outflow cell boundary, while in case c) we have only outflows and in d) only inflows.

Let us first look at the cases a) and b). We write our transport equation as $\partial_t u + f(v, \partial_x u) = 0$ with $f(v, \partial_x u) := v(x)\partial_x u$. We will use notations $u^n := u(t^n)$, $f^n := f(v, \partial_x u^n)$. The Taylor expansion in time yields

$$u^{n} = u^{n-1} + \tau \,\partial_{t} u^{n-1} + \frac{\tau^{2}}{2} \,\partial_{t}^{2} u^{n-1} + \mathcal{O}(\tau^{3}), \qquad u^{n-1} = u^{n} - \tau \,\partial_{t} u^{n} + \frac{\tau^{2}}{2} \,\partial_{t}^{2} u^{n} + \mathcal{O}(\tau^{3}).$$

Subtracting these two equations we derive relation

$$u^{n} - u^{n-1} = \frac{\tau}{2} \left(\partial_{t} u^{n} + \partial_{t} u^{n-1} \right) + \frac{\tau^{2}}{4} \left(\partial_{t}^{2} u^{n-1} - \partial_{t}^{2} u^{n} \right) + \mathcal{O}(\tau^{3}).$$
(36)

We can see that the second term on the right hand side is also $O(\tau^3)$ and using the equation $\partial_t u + f(v, \partial_x u) = 0$, we get for the first term of the right hand side

$$I = \frac{\tau}{2} \left(\partial_t u^n + \partial_t u^{n-1} \right) = -\frac{\tau}{2} \left(f^n + f^{n-1} \right)$$
(37)

Using the notation $f_i := f(x_i) = v(x_i)\partial_x u(x_i)$, by the Taylor expansion in space we have for case a)

$$f_{i-1/2}^{n} = f_{i}^{n} - \frac{h}{2} \partial_{x} f_{i}^{n} + \mathcal{O}(h^{2}), \qquad f_{i+1/2}^{n-1} = f_{i}^{n-1} + \frac{h}{2} \partial_{x} f_{i}^{n-1} + \mathcal{O}(h^{2})$$
(38)

or for case b)

$$f_{i-1/2}^{n-1} = f_i^{n-1} - \frac{h}{2} \partial_x f_i^{n-1} + \mathcal{O}(h^2), \qquad f_{i+1/2}^n = f_i^n + \frac{h}{2} \partial_x f_i^n + \mathcal{O}(h^2)$$
(39)

We continue for case a). Using (37)–(38) we derive

$$I_{i} = -\frac{\tau}{2} (f_{i}^{n} + f_{i}^{n-1}) = -\frac{\tau}{2} \bigg(f_{i-1/2}^{n} + f_{i+1/2}^{n-1} + \frac{h}{2} (\partial_{x} f_{i}^{n} - \partial_{x} f_{i}^{n-1}) + \mathcal{O}(h^{2}) \bigg).$$

The term $\frac{h}{2}(\partial_x f_i^n - \partial_x f_i^{n-1})$ in the brackets on the right hand side is of order $\mathcal{O}(\tau h)$ and we shall analyze the term $f_{i-1/2}^n + f_{i+1/2}^{n-1}$. We know that

$$\partial_{x}u_{i-1/2}^{n} = \frac{1}{h}(u_{i}^{n} - u_{i-1}^{n}) + \mathcal{O}(h^{2}), \qquad \partial_{x}u_{i+1/2}^{n-1} = \frac{1}{h}(u_{i+1}^{n-1} - u_{i}^{n-1}) + \mathcal{O}(h^{2})$$

and resubstituting for $f_{i-1/2}^n = v_{i-1/2} \partial_x u_{i-1/2}^n$ and $f_{i+1/2}^{n-1} = v_{i+1/2} \partial_x u_{i+1/2}^{n-1}$ we get

$$I_{i} = -\frac{\tau}{2} \left(\nu_{i-1/2} \frac{1}{h} \left(u_{i}^{n} - u_{i-1}^{n} \right) + \nu_{i+1/2} \frac{1}{h} \left(u_{i+1}^{n-1} - u_{i}^{n-1} \right) \right) + \mathcal{O}(\tau^{2}h) + \mathcal{O}(\tau h^{2}).$$

$$\tag{40}$$

From (36) and (40) we finally get

$$u_i^n - u_i^{n-1} = -\frac{\tau}{2} \left(\frac{\nu_{i-1/2}}{h} (u_i^n - u_{i-1}^n) + \frac{\nu_{i+1/2}}{h} (u_{i+1}^{n-1} - u_i^{n-1}) \right) + \mathcal{O}(\tau^2 h) + \mathcal{O}(\tau h^2) + \mathcal{O}(\tau^3)$$

where we recognize the scheme (30) for case a), cf. also (33), and dividing by τ we get the consistency error of the IIOE scheme stated in the theorem. The result for case b) follows analogously to a), using (39) instead of (38).

The cases c) and d) have to be treated differently, as in c) only explicit fluxes and in d) only implicit fluxes are used in the scheme. Let us start with case c). We start from Taylor expansion in time with only explicit evaluations of time derivatives.

$$u^{n} - u^{n-1} = \tau \partial_{t} u^{n-1} + \frac{\tau^{2}}{2} \partial_{t}^{2} u^{n-1} + \mathcal{O}(\tau^{3}).$$
(41)

With the expansion of the explicit fluxes

$$f_{i-1/2}^{n-1} = f_i^{n-1} - \frac{h}{2} \partial_x f_i^{n-1} + \mathcal{O}(h^2), \qquad f_{i+1/2}^{n-1} = f_i^{n-1} + \frac{h}{2} \partial_x f_i^{n-1} + \mathcal{O}(h^2)$$
(42)

we now obtain using $\partial_t u + f(v, \partial_x u) = 0$,

$$\tau \partial_t u_i^{n-1} = -\tau f_i^{n-1} = -\frac{\tau}{2} \left(f_{i-1/2}^{n-1} + f_{i+1/2}^{n-1} + \mathcal{O}(h^2) \right)$$
(43)

Next, we will show that the term $\frac{\tau^2}{2}\partial_t^2 u^{n-1}$ of (41) is actually $\mathcal{O}(\tau^2 h)$ due to the smallness of the velocity in this case. Using $\partial_t u + f(v, \partial_x u) = 0$, we get

$$\partial_t^2 u_i^{n-1} = \partial_t f_i^{n-1} = v_i \partial_t \partial_x u_i^{n-1}.$$
(44)

As the velocity field is smooth and changes sign within the cell $(x_{i-1/2}, x_{i+1/2})$, there exists some $x^* \in (x_{i-1/2}, x_{i+1/2})$ with $v(x^*) = 0$. Hence, by Taylor expansion we get

$$v_i = v(x_i) = \underbrace{v(x^{\star})}_{=0} + (x_i - x^{\star}) \partial_x v(x^{\star}) + \mathcal{O}(h^2).$$

Thus, we have $v_i = \mathcal{O}(h)$ and we obtain

$$\frac{\tau^2}{2}\partial_t^2 u_i^{n-1} = \frac{\tau^2}{2} v_i \partial_t \partial_x u_i^{n-1} = \mathcal{O}(\tau^2 h).$$
(45)

Together with (41) and (43) we thus obtain the result, i.e.

$$u^{n} - u^{n-1} = -\frac{\tau}{2} \left(f_{i-1/2}^{n-1} + f_{i+1/2}^{n-1} \right) + \mathcal{O}(\tau h^{2}) + \mathcal{O}(\tau^{2}h) + \mathcal{O}(\tau^{3}).$$

Case d) is obtained analogously to c) by using Taylor expansion in time with only implicit evaluations of time derivatives and replacing the explicit fluxes by corresponding implicit ones.

Theorem 4.5 ($L^{\infty}(L^2)$ stability). Let us consider the advection equation in 1D with constant velocity $v \ge 0$ (or $v \le 0$) and the IIOE scheme on a uniform grid with periodic boundary conditions. Then the scheme is L^2 stable and the following a priori estimate holds

$$\sum_{i \in I} \int_{p_i} (u_i^N)^2 + \sum_{i \in I} \int_{p_i} \frac{|v|\tau}{4h} (u_i^N - u_{i-1}^N)^2 = \sum_{i \in I} \int_{p_i} (u_i^0)^2 + \sum_{i \in I} \int_{p_i} \frac{|v|\tau}{4h} (u_{i+1}^0 - u_i^0)^2.$$

Proof. Without loss of generality, let us assume constant velocity $v \ge 0$. The basic IIOE scheme then reads

$$\frac{u_i^n - u_i^{n-1}}{\tau} + \frac{1}{2}\nu\left(\frac{u_i^n - u_{i-1}^n}{h} + \frac{u_{i+1}^{n-1} - u_i^{n-1}}{h}\right) = 0,$$

where $i \in I$, n = 1, ..., N, I is the number of finite volumes and N is the number of time steps. Testing with $\frac{1}{2}(u_i^n + u_i^{n-1})$ yields after integration over cell p_i and time interval (t^n, t^{n+1}) and summation

$$\sum_{n=1}^{N} \sum_{i \in I} \int_{t^n}^{t^{n+1}} \int_{p_i}^{f} (T_t + T_s) = 0,$$
(46)

where the time and space terms are given as

$$T_t := \frac{1}{2\tau} (u_i^n - u_i^{n-1}) (u_i^n + u_i^{n-1}) = \frac{1}{2\tau} ((u_i^n)^2 - (u_i^{n-1})^2),$$
(47)

$$T_s := \frac{\nu}{4h} \left(\left(u_i^n - u_{i-1}^n \right) + \left(u_{i+1}^{n-1} - u_i^{n-1} \right) \right) \left(u_i^n + u_i^{n-1} \right).$$
(48)

By simple algebraic manipulation, we further get for T_s

$$T_{s} = \frac{v}{8h} ((u_{i}^{n} - u_{i-1}^{n}) + (u_{i+1}^{n-1} - u_{i}^{n-1}))((u_{i}^{n} - u_{i-1}^{n}) - (u_{i+1}^{n-1} - u_{i}^{n-1})) + \frac{v}{8h} ((u_{i}^{n} + u_{i+1}^{n-1}) - (u_{i-1}^{n} + u_{i}^{n-1}))((u_{i}^{n} + u_{i+1}^{n-1}) + (u_{i-1}^{n} + u_{i}^{n-1})) = \frac{v}{8h} (\underbrace{(u_{i}^{n} - u_{i-1}^{n})^{2}}_{=:(\Delta_{i-1}^{n-1})^{2}} - \underbrace{(u_{i+1}^{n-1} - u_{i}^{n-1})^{2}}_{=:(\Delta_{i}^{n-1})^{2}} + \underbrace{(u_{i}^{n} + u_{i+1}^{n-1})^{2}}_{=:(S_{i}^{n+1/2})^{2}} - \underbrace{(u_{i-1}^{n} + u_{i}^{n-1})^{2}}_{=:(S_{i-1}^{n+1/2})^{2}}.$$

In this form of the space term, it can be seen that the term $(\Delta_i^{n-1})^2$ is a space-time shift of $(\Delta_{i-1}^n)^2$, and $(S_i^{n+1/2})^2$ is a space shift of $(S_{i-1}^{n+1/2})^2$. We thus obtain from (46) with periodicity and using the shift correlation in the T_t and T_s -terms

$$0 = \sum_{i \in I} \int_{p_i} \frac{1}{2} \left(\left(u_i^N \right)^2 - \left(u_i^0 \right)^2 \right) + \sum_{i \in I} \int_{p_i} \frac{v\tau}{8h} \left(\left(\Delta_{i-1}^N \right)^2 - \left(\Delta_i^0 \right)^2 \right).$$
(49)

Hence, we obtain with the definition of the Δ -terms

$$\sum_{i \in I} \int_{p_i} (u_i^N)^2 + \sum_{i \in I} \int_{p_i} \frac{v\tau}{4h} (u_i^N - u_{i-1}^N)^2 = \sum_{i \in I} \int_{p_i} (u_i^0)^2 + \sum_{i \in I} \int_{p_i} \frac{v\tau}{4h} (u_{i+1}^0 - u_i^0)^2.$$

As the proof of the stability estimate only relies on space and time shifts, it transfers immediately also to the case of uniform rectangular grids in multiple space dimensions. \Box

Theorem 4.6 $(L^{\infty}(L^{\infty})$ stability of the stabilized IIOE scheme). Let us consider the advection equation (1) with given variable velocity. Then, the stabilized S¹IIOE is unconditionally stable in the $L^{\infty}(L^{\infty})$ sense and the following minimum–maximum property holds

$$\min_{q\in\mathcal{T}_h} u_q^0 \le u_p^n \le \max_{q\in\mathcal{T}_h} u_q^0, \quad \forall q\in\mathcal{T}_h, \ n=0,\dots,N.$$
(50)

Proof. The theorem follows from the construction of the stabilized scheme as discussed in Section 2 above.

5. Numerical experiments

This section is devoted to numerically analyze and validate the robustness and accuracy of our new IIOE scheme at classical benchmark problems and more involved multi-dimensional applications. We start the evaluation with one dimensional advection with constant speed of a quadratic polynomial, a smooth hump and discontinuous piecewise constant initial data. For each case we compare our new basic and stabilized methods with the classical implicit up-wind scheme. Here we are in particular interested in an evaluation of the methods when large time steps are used that exceed the time step given from the CFL condition. For further one dimensional experiments involving also advection with non-divergence free velocity and for comparison with higher order explicit methods we refer to the exposition in [13,14]. Finally, the last part of this section will be devoted to two dimensional benchmark problems and an evaluation of the scheme for real applications in medical image segmentation.

5.1. 1D advection with constant velocity

As a classical benchmark let us consider one dimensional advection with constant speed given by Eq. (28) with $v(x) \equiv 1$. In all our computations, we restrict to the space interval $\Omega = (-1, 1)$ and time interval I = (0, T) with T = 1. We consider three representative examples in this subsection:

- **a)** advection of the quadratic polynomial $u_0(x) = 1 \frac{1}{2}(x^2 + x)$,
- **b)** advection of a smooth hump defined as $u_0(x) = \max(0, \cos^5(\pi (x + 0.5)))$, and
- **c)** advection of a discontinuous piecewise constant profile given as $u_0(x) = 1$ for $x \in [-0.75, -0.25]$ and $u_0(x) = 0$ otherwise.

The exact solution for all these examples is given by shifting in time the initial profile, i.e. $u(x, t) = u_0(x - vt)$.

Case a) As proven in Section 4, the basic IIOE is exact for advection of a quadratic polynomial. This is of course also seen numerically up to machine accuracy, as depicted in the third column of Table 1. However, exactness is not the case for the stabilized S¹IIOE scheme, which is just second order, but it is again true for the stabilized S²IIOE scheme, cf. fourth and fifth columns of Table 1. The fully implicit up-wind scheme gives the first order accuracy. Clearly, the S²IIOE scheme is superior because it conserves the exactness of the quadratic solution for time steps given by an integer multiplication of *h* and when using local quadratic reconstruction also for time steps less than *h*, cf. Table 1.

Case b) For the more general smooth profile we analyze both, the accuracy and the local mass conservation error (area error) of the respective stabilized IIOE schemes. For smooth solutions we observe that the S²IIOE scheme with quadratic reconstruction behaves similarly as the basic IIOE scheme, while the S¹IIOE scheme with quadratic reconstruction stabilizes a bit more and thus shows slightly worse accuracy in the L^1 error and the area error. A visual comparison of all these methods is shown in Fig. 1. While the S²IIOE scheme shows visually perfect matching with the exact solution, there is a little bit more smearing of the hump for the S¹IIOE scheme. However, both new methods show much better behavior as the very dissipative classical implicit up-wind scheme. The visual comparison is detailed in the convergence study with respect to the solution and with respect to the mass conservation error in Table 2. It can be seen that both stabilized IIOE schemes show second order convergence, both for small ($\tau = h$) and large ($\tau = 8h$) time step sizes. The mass conservation error also converges to zero with second order for the S¹IIOE, while it shows higher then fourth order convergence for the S²IIOE scheme.

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Table 1

Case a) $L^1(I, L^1)$ errors of the IIOE, S¹IIOE, S²IIOE and implicit up-wind schemes for advection of a quadratic polynomial. The relation $\tau = h$ is used in the first 4 rows, $\tau = h/2$ in the next 4 rows, $\tau = 2h$ in the next 4 rows, $\tau = 10h$ in the next 4 rows and the last 5 rows report the errors for fixed n = 160 and refining time step from $\tau = 80h$ to $\tau = 5h$.

n	NTS	IIOE	S ¹ IIOE	S ² IIOE	Implicit up-wind
20	10	$1.8 imes 10^{-16}$	$4.63 imes 10^{-3}$	3.8×10^{-16}	$8.80 imes 10^{-2}$
40	20	$3.5 imes 10^{-16}$	1.18×10^{-3}	$4.9 imes10^{-16}$	$4.28 imes10^{-2}$
80	40	$7.5 imes 10^{-16}$	3.12×10^{-4}	$6.3 imes 10^{-16}$	2.11×10^{-2}
160	80	1.4×10^{-15}	8.35×10^{-5}	7.2×10^{-16}	$1.05 imes 10^{-2}$
20	20	$3.7 imes 10^{-16}$	1.75×10^{-3}	$5.2 imes 10^{-16}$	$6.43 imes10^{-2}$
40	40	$8.0 imes 10^{-16}$	$4.60 imes 10^{-4}$	$5.1 imes 10^{-16}$	$3.17 imes10^{-2}$
80	80	1.1×10^{-15}	1.23×10^{-4}	$7.9 imes10^{-16}$	$1.57 imes 10^{-2}$
160	160	2.4×10^{-15}	3.22×10^{-5}	1.2×10^{-15}	$0.78 imes10^{-2}$
20	5	$2.1 imes 10^{-16}$	1.12×10^{-2}	$1.9 imes 10^{-16}$	$1.38 imes 10^{-1}$
40	10	2.1×10^{-16}	2.77×10^{-3}	$2.1 imes 10^{-16}$	$6.60 imes 10^{-2}$
80	20	$3.9 imes 10^{-16}$	$7.04 imes10^{-4}$	$2.6 imes 10^{-16}$	$3.21 imes 10^{-2}$
160	40	5.7×10^{-16}	$1.80 imes 10^{-4}$	4.1×10^{-16}	$1.58 imes10^{-2}$
20	1	$4.3 imes 10^{-16}$	2.18×10^{-1}	$6.4 imes 10^{-16}$	$6.31 imes 10^{-1}$
40	2	1.0×10^{-15}	$4.91 imes 10^{-2}$	$8.5 imes 10^{-16}$	$2.8 imes 10^{-1}$
80	4	$1.5 imes 10^{-15}$	1.13×10^{-2}	$1.8 imes 10^{-15}$	$1.29 imes 10^{-1}$
160	8	2.5×10^{-15}	2.66×10^{-3}	3.1×10^{-15}	$0.61 imes 10^{-1}$
160	1	$2.6 imes 10^{-15}$	2.11×10^{-1}	1.2×10^{-15}	$5.75 imes 10^{-1}$
160	2	$2.6 imes 10^{-15}$	$4.62 imes 10^{-2}$	$2.7 imes 10^{-15}$	$2.61 imes 10^{-1}$
160	4	$2.6 imes 10^{-15}$	$1.07 imes 10^{-2}$	$3.5 imes 10^{-15}$	$1.23 imes 10^{-1}$
160	8	$2.6 imes 10^{-15}$	2.66×10^{-3}	$3.1 imes 10^{-15}$	$6.12 imes 10^{-2}$
160	16	2.6×10^{-15}	7.31×10^{-4}	4.6×10^{-15}	3.23×10^{-2}





Fig. 1. Case b) Smooth initial data (blue curves), exact solution (green curves), and numerical results at T = 1 (red curves) for the stabilized schemes with quadratic reconstruction S²IIOE (top left), S¹IIOE (top right) in comparison to the result obtained with the implicit up-wind scheme (bottom). For these computations, n = 1280 and the relation $\tau = 8h$ is used, i.e. CFL = 8. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 2

		-1	-1	-2	-2	1
n	NTS	S ¹ IIOE L ¹ -error	S ¹ IIOE area error	S ² IIOE L ¹ -error	S ² IIOE area error	Implicit up-wind L ¹ -error
40	20	$9.53 imes10^{-2}$	$6.69 imes 10^{-2}$	$9.19 imes 10^{-2}$	$1.93 imes 10^{-2}$	1.96×10^{-1}
80	40	$3.51 imes 10^{-2}$	$6.58 imes 10^{-3}$	$2.80 imes10^{-2}$	$2.98 imes 10^{-3}$	1.32×10^{-1}
160	80	9.66×10^{-3}	2.06×10^{-3}	$7.69 imes 10^{-3}$	$2.69 imes 10^{-4}$	8.21×10^{-2}
320	160	2.69×10^{-3}	$6.26 imes10^{-4}$	$1.97 imes 10^{-3}$	$1.94 imes 10^{-5}$	$4.71 imes 10^{-2}$
640	320	$7.00 imes 10^{-4}$	$1.63 imes10^{-4}$	$4.97 imes10^{-4}$	$1.28 imes 10^{-6}$	$2.56 imes 10^{-2}$
1280	640	1.80×10^{-4}	4.16×10^{-5}	$1.24 imes 10^{-4}$	8.14×10^{-8}	1.33×10^{-2}
640	40	$1.03 imes 10^{-2}$	$2.96 imes 10^{-3}$	7.23×10^{-3}	$2.81 imes 10^{-4}$	$9.02 imes 10^{-2}$
1280	80	$2.77 imes 10^{-3}$	$7.75 imes 10^{-4}$	$1.86 imes 10^{-3}$	2.03×10^{-5}	5.23×10^{-2}
2560	160	$7.12 imes 10^{-4}$	$1.94 imes10^{-4}$	$4.67 imes10^{-4}$	$1.32 imes 10^{-6}$	$2.86 imes 10^{-2}$
5120	320	$1.82 imes 10^{-4}$	4.81×10^{-5}	$1.16 imes 10^{-4}$	8.35×10^{-8}	$1.49 imes 10^{-2}$

Case b) Report on the $L^1(I, L^1)$ and area errors of the S¹IIOE, S²IIOE schemes (with quadratic reconstruction) and $L^1(I, L^1)$ errors of the implicit up-wind scheme. The relation $\tau = h$ is used in the first 6 rows and $\tau = 8h$ in the next 4 rows.

Table 3

Case c) Report on the $L^1(I, L^1)$ and area errors of the S¹IIOE, S²IIOE schemes with quadratic reconstruction and on the $L^1(I, L^1)$ errors of the implicit up-wind scheme. The relation $\tau = h$ is used in the first 6 rows and $\tau = 8h$ in the next 4 rows.

n	NTS	S ¹ IIOE L ¹ -error	S ¹ IIOE area error	S ² IIOE L ¹ -error	S ² IIOE area error	Implicit up-wind L ¹ -error
40	20	$2.03 imes10^{-1}$	$1.06 imes 10^{-3}$	$2.02 imes 10^{-1}$	$6.17 imes10^{-4}$	$3.25 imes 10^{-1}$
80	40	1.31×10^{-1}	5.32×10^{-5}	$1.30 imes 10^{-1}$	5.09×10^{-5}	$2.37 imes 10^{-1}$
160	80	$8.38 imes10^{-2}$	$5.47 imes10^{-7}$	$8.38 imes10^{-2}$	$5.47 imes10^{-7}$	$1.68 imes10^{-1}$
320	160	$5.35 imes 10^{-2}$	$5.69 imes 10^{-10}$	$5.34 imes 10^{-2}$	$5.68 imes 10^{-10}$	$1.19 imes 10^{-1}$
640	320	3.41×10^{-2}	3.34×10^{-15}	3.41×10^{-2}	$3.33 imes 10^{-15}$	8.42×10^{-2}
1280	640	2.16×10^{-2}	4.28×10^{-16}	2.16×10^{-2}	4.24×10^{-16}	$5.95 imes 10^{-2}$
640	40	$9.22 imes 10^{-2}$	$4.22 imes 10^{-7}$	$9.22 imes 10^{-2}$	$4.22 imes 10^{-7}$	$1.79 imes 10^{-1}$
1280	80	$5.74 imes 10^{-2}$	$3.77 imes 10^{-10}$	$5.74 imes 10^{-2}$	$3.77 imes 10^{-10}$	$1.27 imes 10^{-1}$
2560	160	$3.58 imes10^{-2}$	$4.01 imes 10^{-15}$	$3.58 imes10^{-2}$	$4.29 imes 10^{-15}$	$8.95 imes10^{-2}$
5120	320	2.24×10^{-2}	4.96×10^{-15}	2.24×10^{-2}	2.60×10^{-14}	$6.32 imes 10^{-2}$

Case c) Finally, we compare our methods for the discontinuous piecewise constant initial profile. Similarly as in case b), Table 3 shows the detailed convergence behavior of the stabilized S^1 IIOE, and S^2 IIOE schemes with quadratic reconstruction. First of all, it can be observed that in this case both new stabilized schemes show approximately the same convergence behavior. Moreover, also the absolute errors in the solution and with respect to mass conservation are nearly the same. In this non-smooth example, the experimental order of convergence is about 2/3 for both stabilized IIOE schemes, while it is only about 1/2 for the classical implicit up-wind scheme. Concerning the mass conservation error, both new stabilized schemes show exponential convergence to zero in this example.

A visual comparison of our new stabilized schemes (with and without quadratic reconstruction) with the implicit upwind scheme is given in Figs. 2, 3. In both figures we only plot the numerical results for the S²IIOE scheme, as the results for the S¹IIOE are the same as for S²IIOE in this example. The results in Fig. 2 were obtained for n = 1280 and $\tau = 2h$, i.e. CFL = 2, while in Fig. 3 n = 1280 and $\tau = 8h$, i.e. CFL = 8, were used. It can be observed that our new method is clearly superior to the classical implicit scheme in both cases. Although our new stabilized scheme is a little bit more diffusive when larger time steps are used, this effect is much more pronounced by the classical implicit up-wind scheme. A comparison of our new stabilized scheme with and without quadratic reconstruction shows that there is nearly no difference in the behavior of the scheme in this example. Thus, both variants may be used and produce nice results also for large time steps which exceed the CFL restriction.

5.2. 2D advection by a constant velocity vector field and by a rotation

First, let us consider a second order radially symmetric polynomial initial function in the form of paraboloid $u_0(x_1, x_2) = x_1^2 + x_2^2 - 0.25$ and the vector field $\mathbf{v}(x_1, x_2) = (-x_2, x_1)$ which rotates the initial function around the origin. Since it is radially symmetric the exact solution does not change in time. This test problem as well as all further 2D examples in this section are solved in the spatial domain $\Omega = (-1, 1) \times (-1, 1)$ which is split into $n \times n$ finite volumes. The time interval (0, T) is equal (0, 1) for this example and one can see in Table 4 that the exact solution is reproduced numerically up to machine precision by any of the IIOE methods. The system matrix and the right hand side of the IIOE method is constructed in such way that it does not touch this exact solution, which holds true in this case also for the stabilized methods.

in such way that it does not touch this exact solution, which holds true in this case also for the stabilized methods. The second example represents transport of the quadratic polynomial $u_0(x_1, x_2) = 2x_1^2 + x_2^2 - x_1 + x_2 - 0.25$ by the constant vector field $\mathbf{v}(x_1, x_2) = (-1.0, 0.5)$. We can see in Table 5 that, as given by the theory, the numerical solution by the IIOE scheme is exact up to a machine precision, while the two stabilized methods are second order.

In the third example we consider the same paraboloid as in the first example but shifted to (0.5, 0), i.e. $u_0(x_1, x_2) = (x_1 - 0.5)^2 + x_2^2 - 0.25$ and the same rotational vector field. The problem is solved in the larger time interval (0, 3.14). All

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Fig. 2. Case c) Results of the S²IIOE (with quadratic reconstruction) (top left) and S²IIOE (without quadratic reconstruction) (top right) schemes, and the implicit up-wind (bottom) scheme. The initial profile is given in blue, the exact solution in green, and the numerical solution in red. We used n = 1280 and the relation $\tau = 2h$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)



Fig. 3. Case c) Here, the same comparison as in Fig. 2 is plotted for larger choice of the time step size, i.e. we used n = 1280 and the relation $\tau = 8h$.

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Table 4

2D centered paraboloid rotated around the origin: report on the $L^1(I, L^1)$ errors of the IIOE, S¹IIOE, and S²IIOE methods for refined space and time step sizes.

n	τ	NTS	IIOE $L^1(I, L^1)$	S ¹ IIOE $L^1(I, L^1)$	$S^2 IIOE L^1(I, L^1)$
20	0.1	10	$5.938 imes 10^{-16}$	$5.938 imes 10^{-16}$	5.938×10^{-16}
40	0.05	20	$7.388 imes 10^{-16}$	$7.388 imes 10^{-16}$	$7.388 imes 10^{-16}$
80	0.025	40	$1.079 imes 10^{-15}$	$1.079 imes 10^{-15}$	$1.079 imes 10^{-15}$
160	0.0125	80	1.367×10^{-15}	$1.367 imes 10^{-15}$	$1.367 imes 10^{-15}$

Table 5

2D paraboloid transported by a constant vector field: report on the $L^1(I, L^1)$ errors of the IIOE, S¹IIOE, and S²IIOE methods for refined space and time step sizes.

n	τ	NTS	IIOE $L^1(I, L^1)$	S ¹ IIOE $L^1(I, L^1)$	$S^2 IIOE L^1(I, L^1)$
20	0.1	10	$2.624 imes 10^{-15}$	$1.838 imes 10^{-2}$	5.544×10^{-3}
40	0.05	20	$8.170 imes 10^{-15}$	2.959×10^{-3}	$1.084 imes 10^{-3}$
80	0.025	40	$1.421 imes 10^{-14}$	$4.987 imes 10^{-4}$	$2.315 imes10^{-4}$
160	0.0125	80	$2.045 imes 10^{-14}$	$8.291 imes 10^{-5}$	$4.537 imes 10^{-5}$

Table 6

2D rotating paraboloid centered outside the origin: report on the $L^1(I, L^1)$ errors of the IIOE, S¹IIOE, and S²IIOE methods for refined space and time step sizes.

n	τ	NTS	IIOE $L^1(I, L^1)$	S^1 IIOE $L^1(I, L^1)$	$S^2 IIOE L^1(I, L^1)$
20	0.157	20	$2.042 imes 10^{-2}$	$3.184 imes 10^{-2}$	2.340×10^{-2}
40	0.0785	40	$4.564 imes 10^{-3}$	6.422×10^{-3}	5.501×10^{-3}
80	0.03925	80	1.068×10^{-3}	1.379×10^{-3}	1.225×10^{-3}
160	0.019625	160	2.571×10^{-4}	$3.104 imes10^{-4}$	2.897×10^{-4}

Table 7

2D rotating smooth hump centered outside the origin: report on the $L^1(I, L^1)$ errors of the IIOE, S¹IIOE, and S²IIOE methods for refined space and time step sizes.

n	τ	NTS	IIOE $L^1(I, L^1)$	S^1 IIOE $L^1(I, L^1)$	S ² IIOE $L^1(I, L^1)$
20	0.157	20	$4.563 imes 10^{-1}$	$2.680 imes 10^{-1}$	2.888×10^{-1}
40	0.0785	40	$1.628 imes 10^{-1}$	$1.210 imes 10^{-1}$	$1.220 imes 10^{-1}$
80	0.03925	80	$4.426 imes 10^{-2}$	3.927×10^{-2}	3.084×10^{-2}
160	0.019625	160	1.112×10^{-2}	$1.091 imes 10^{-2}$	1.061×10^{-2}
320	0.0098125	320	$2.767 imes 10^{-3}$	$2.824 imes 10^{-3}$	2.772×10^{-3}
640	0.00490625	640	6.8982×10^{-4}	7.067×10^{-4}	6.993×10^{-4}

IIOE methods are second order accurate, as one can see in Table 6. Here, no special attention to a CFL condition was given when choosing τ and h.

In the next two experiments we test the IIOE methods in the case of standard 2D benchmarks, the rotations of a smooth hump and a discontinuous function around the origin, i.e. $\mathbf{v}(x_1, x_2) = (-x_2, x_1)$. The initial smooth function is given by $u_0(x_1, x_2) = \cos^5(\pi \sqrt{(x_1 + 0.5)^2 + x_2^2})$ inside a circle with radius 0.5 centered in (-0.5, 0) and by 0 elsewhere. In the case of a rotating cylinder we have $u_0(x_1, x_2) = 1$ inside a circle with radius 0.45 centered in (-0.5, 0) and 0 elsewhere. We compute the numerical solutions until for half a rotation (T = 3.14) without any special care to the CFL condition. In case of the smooth hump rotation we see second order convergence and very precise conservation of the rotating shape, cf. Table 7 and Fig. 4. In case of the discontinuous solution we see a convergence rate of about 2/3 for the stabilized IIOE schemes and also good conservation of the initial shape after half a rotation, cf. Table 8 and Fig. 5. This is much better than for any other standard implicit scheme with large time steps.

5.3. 2D advection by non-divergence free velocities including advective level set motion in normal direction with topological changes

In the next example we test the IIOE schemes for transport in the non-divergence free velocity field

$$\mathbf{v}(x) = -\frac{x}{|x|}, \quad x = (x_1, x_2).$$
(51)

The exact solution is given by $u(x, t) = u_0(x + \frac{tx}{|x|})$ where $u_0(x)$ is an initial profile. We consider the initial function $u_0(x_1, x_2) = -x_1^2 - x_2^2 + 1$ and solve the problem in the time interval (0, 0.6) on subsequently refined grids. In this case there is a point singularity formed in the origin due to subsequent arrival of initial function values from circular neighborhoods. For this example all IIOE methods are second order accurate and give similar results as one can see in Table 9.



Fig. 4. 2D rotating smooth hump centered outside the origin: the initial condition (left) and the S²IIOE numerical solution after half a rotation (right), n = 320, cf. Table 7.

Table 8
2D rotating cylinder centered outside the origin: report on the $L^1(I, L^1)$ errors of the IIOE, S ¹ IIOE, and S ² IIOE methods for successively refined space and
time step sizes.

n	τ	NTS	IIOE $L^1(I, L^1)$	S ¹ IIOE $L^1(I, L^1)$	S ² IIOE $L^1(I, L^1)$
20	0.157	20	1.532×10^{0}	$8.979 imes 10^{-1}$	9.004×10^{-1}
40	0.0785	40	1.161×10^{0}	$5.758 imes 10^{-1}$	$5.820 imes 10^{-1}$
80	0.03925	80	$8.612 imes 10^{-1}$	3.698×10^{-1}	$3.769 imes 10^{-1}$
160	0.019625	160	$6.357 imes 10^{-1}$	$2.374 imes 10^{-1}$	$2.431 imes 10^{-1}$
320	0.0098125	320	$4.668 imes 10^{-1}$	$1.521 imes 10^{-1}$	$1.560 imes10^{-1}$
640	0.00490625	640	3.413×10^{-1}	$9.720 imes 10^{-2}$	9.998×10^{-2}



Fig. 5. 2D rotating cylinder centered outside the origin: the initial condition (left) and the S²IIOE numerical solution after half a rotation (right), n = 320, cf. Table 8.

In the last example of this section we look at level set motion in normal direction with topological changes. In detail we consider the resolution of the topological changes for the shrinking of an initial quatrefoil (top left in Fig. 6) by a velocity field in normal direction with constant speed equal to 1. Thus, the vector field now depends on the solution and is given by $\mathbf{v} = -\frac{\nabla u}{|\nabla u|}$, cf. also Section 3.2. In the further plots of Fig. 6 we present the evolution of the zero level line representing the quatrefoil evolution (left column) and 2D (middle column) and 3D (right column) plots of the evolution of the level set function *u* computed by the S²IIOE scheme, n = 640, $\tau = 2h$. For further numerical results of IIOE schemes in the level set context we refer to [12] and the discussions therein.

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Fig. 6. 2D level set motion in normal direction: shrinking of the quatrefoil with topological changes. The numerical solution is plotted at the discrete times 0, 0.05, 0.1, 0.15. The zero level line representing the quatrefoil evolution is plotted in the left column, the 2D color coded level set function in the middle and a 3D visualization of the level set function in the right column. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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Table 9

Transport in the non-divergence free velocity field (51) with singular solution in the origin: report on the $L^1(I, L^1)$ errors of the IIOE, S¹IIOE, and S²IIOE methods for successively refined space and time step sizes.

n	τ	NTS	IIOE $L^1(I, L^1)$	S^1 IIOE $L^1(I, L^1)$	$S^2 IIOE L^1(I, L^1)$
20	0.1	6	$6.572 imes 10^{-3}$	6.572×10^{-3}	6.572×10^{-3}
40	0.05	12	$1.480 imes 10^{-3}$	$1.480 imes 10^{-3}$	$1.480 imes 10^{-3}$
80	0.025	24	$3.504 imes 10^{-4}$	$3.504 imes 10^{-4}$	$3.504 imes 10^{-4}$
160	0.0125	48	$8.521 imes 10^{-5}$	$8.521 imes 10^{-5}$	$8.521 imes 10^{-5}$
320	0.00625	96	2.101×10^{-5}	2.101×10^{-5}	$2.101 imes 10^{-5}$



Fig. 7. Prostate segmentation: 2D image (left) and the same image together with a red contour representing segmentation of the prostate by GSUBSURF model (52) using the S²IIOE scheme in the advective part.



Fig. 8. Prostate segmentation: a detail of the nontrivial velocity vector field used in segmentation of the prostate.

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Fig. 9. Prostate segmentation: graphs of subsequently evolving segmentation function, tending from the initial profile (top left) to the final shock-like shape (bottom right) which is used for extracting the segmentation contour plotted in red in Fig. 7 right.

5.4. 2D medical image segmentation

In the last numerical experiment we present an application of the S²IIOE scheme in medical image segmentation. Here, we segment a 2D image with resolution 150×150 pixels, plotted in Fig. 7 left, with the goal to precisely extract the prostate. Prostate segmentation is a very difficult task in medical image analysis due to a poor contrast and a high level of noise intrinsically linked to the image. We use the so-called generalized subjective surface (GSUBSURF) model which represents a robust method for biomedical image segmentation and is a useful generalization of the original approach presented in [17]. The GSUBSURF model has the form of the following PDE [3,15,20]

$$u_t - w_a \nabla g \cdot \nabla u - w_d g \sqrt{\varepsilon^2 + |\nabla u|^2} \nabla \cdot \left(\frac{\nabla u}{\sqrt{\varepsilon^2 + |\nabla u|}}\right) = 0,$$
(52)

where u(t, x) is an evolving segmentation function starting from an initial condition, $u(0, x) = u_0(x)$, usually given by a peak located approximately in the center of the mass of the segmented object. Then, the segmentation function is evolved by the advection (the second term on the left hand side of (52)) regularized by the mean curvature flow (the third term on the left hand side of (52) to a shock-like profile. The central isoline of this profile gives the segmentation result, for the segmentation function evolution see Fig. 9 and for the resulting isoline, which gives very precise localization of the prostate see Fig. 7, right. The important part of the model is given by the advection with the nontrivial velocity vector field $-w_a \nabla g$ where the function $g = \frac{1}{1+Ks^2}$ depends on the norm of the gradient $s = |\nabla I|$ of the image intensity function *I* smoothed by the mean curvature flow filter [6]. This nontrivial velocity field points towards the edges in the image. Its details in the prostate region are plotted in Fig. 8. Opposite to previous implementations of the GSUBSURF model [3,15,20] where the advective part was treated by an explicit scheme - which put a severe restriction to the computational time step - we use here the S²IIOE scheme with a time step size exceeding more than 10 times the standard CFL condition. Similarly to [3,15], for the curvature part we use an unconditionally stable semi-implicit diamond-cell finite volume method. As one can see in the right picture of Fig. 7, we obtain precise results using such overall semi-implicit scheme (both in advection and curvature). Moreover, this scheme always guarantees solvability of the system and stability of the computation and thus represents an important improvement of the GSUBSURF segmentation method. Since we are interested in coming to an "equilibrium" segmentation shape, the choice of larger time step sizes is important from the CPU-time point of view. The model and computational parameters in this example were h = 0.5 (pixel size), $\tau = 5h$, K = 10000, $\varepsilon^2 = 10^{-6}$, $w_a = 5h$, $w_d = 4h$.

6. Conclusions

In this article we discussed inflow-implicit/outflow-explicit (IIOE) finite volume scheme together with its high resolution stabilized variants for solving a variable velocity advection equations. We gave some theoretical and numerical background with respect to solvability, local mass conservation, accuracy and stability for the discussed methods. As demonstrated in several numerical benchmark problems, in particular the S²IIOE scheme with quadratic reconstruction shows experimentally very nice resolution and stability properties. It preserves all solvability and accuracy properties of the basic IIOE scheme for smooth solutions, while at the same time satisfying in all presented numerical experiments L^{∞} -stability, even in settings with discontinuous solutions. Moreover, all presented IIOE schemes keep their accuracy and stability properties for arbitrary large time step sizes which makes this family of methods particular attractive for real applications as demonstrated here for 2D medical image segmentation.

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References

- [1] M. Balažovjech, K. Mikula, A higher order scheme for a tangentially stabilized plane curve shortening flow with a driving force, SIAM J. Sci. Comput. 33 (5) (2011) 2277–2294.
- [2] J.P. Boris, D.L. Book, Flux-corrected transport: I. SHASTA, a fluid transport algorithm that works, J. Comput. Phys. 11 (1973) 38-69.
- [3] P. Bourgine, R. Čunderlík, O. Drblíková, K. Mikula, N. Peyriéras, M. Remešíková, B. Rizzi, A. Sarti, 4D embryogenesis image analysis using PDE methods of image processing, Kybernetika 46 (2) (2010).
- [4] V. Caselles, R. Kimmel, G. Sapiro, Geodesic active contours, Int. J. Comput. Vis. 22 (1997) 61-79.
- [5] R. Eymard, T. Gallouet, R. Herbin, The Finite Volume Methods, in: Ph. Ciarlet, J.L. Lions (Eds.), Handbook for Numerical Analysis, vol. 7, Elsevier, 2000.
- [6] R. Eymard, A. Handlovičová, K. Mikula, Study of a finite volume scheme for the regularised mean curvature flow level set equation, IMA J. Numer. Anal. 31 (2011) 813–846.
- [7] P. Frolkovič, K. Mikula, Flux-based level set method: a finite volume method for evolving interfaces, Appl. Numer. Math. 57 (4) (2007) 436-454.
- [8] P. Frolkovič, K. Mikula, High-resolution flux-based level set method, SIAM J. Sci. Comput. 29 (2) (2007) 579–597.
- [9] S. Kichenassamy, A. Kumar, P. Olver, A. Tannenbaum, A. Yezzi, Conformal curvature flows: from phase transitions to active vision, Arch. Ration. Mech. Anal. 134 (1996) 275–301.
- [10] D. Kuzmin, Linearity-preserving flux correction and convergence acceleration for constrained Galerkin schemes, J. Comput. Appl. Math. (2011), http:// dx.doi.org/10.1016/j.cam.2011.11.019.

- [11] R.J. LeVeque, Finite Volume Methods for Hyperbolic Problems, Cambridge Texts in Applied Mathematics, Cambridge University Press, 2002.
- [12] K. Mikula, M. Ohlberger, A new level set method for motion in normal direction based on a semi-implicit forward-backward diffusion approach, SIAM J. Sci. Comput. 32 (3) (2010) 1527–1544.
- [13] K. Mikula, M. Ohlberger, Inflow-implicit/outflow-explicit scheme for solving advection equations, in: J. Fořt, et al. (Eds.), Finite Volumes in Complex Applications VI, Problems & Perspectives, Prague, June 6–10, 2011, in: Springer Proceedings in Mathematics, vol. 4, Springer-Verlag, 2011, pp. 683–692.
- [14] K. Mikula, M. Ohlberger, A new inflow-implicit/outflow-explicit finite volume method for solving variable velocity advection equations, Preprint 01/10

 N, Angewandte Mathematik und Informatik, Universitaet Münster, June 2010.
- [15] K. Mikula, N. Peyrieras, M. Remešíková, A. Sarti, 3D embryogenesis image segmentation by the generalized subjective surface method using the finite volume technique, in: R. Eymard, J.M. Herard (Eds.), Finite Volumes for Complex Applications V: Problems and Perspectives, ISTE and Wiley, London, 2008, pp. 585–592.
- [16] K. Mikula, D. Ševčovič, M. Balažovjech, A simple, fast and stabilized flowing finite volume method for solving general curve evolution equations, Commun. Comput. Phys. 7 (1) (2010) 195–211.
- [17] A. Sarti, R. Malladi, J.A. Sethian, Subjective surfaces, a method for completing missing boundaries, Proc. Natl. Acad. Sci. USA 12 (2000) 6258–6263.
- [18] J.A. Sethian, Level Set Methods and Fast Marching Methods: Evolving Interfaces in Computational Geometry, Fluid Mechanics, Computer Vision, and Material Science, Cambridge University Press, New York, 1999.
- [19] S.T. Zalesak, Fully multidimensional flux-corrected transport algorithms for fluids, J. Comput. Phys. 31 (1979) 335–362.
- [20] C. Zanella, M. Campana, B. Rizzi, C. Melani, G. Sanguinetti, P. Bourgine, K. Mikula, N. Peyrieras, A. Sarti, Cells segmentation from 3-D confocal images of early zebrafish embryogenesis, IEEE Trans. Image Process. 19 (3) (2010) 770–781.