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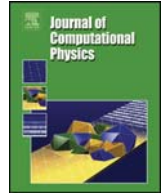
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Short note

On high order finite-difference metric discretizations satisfying GCL on moving and deforming grids [☆]Björn Sjögren ^{a,1}, H.C. Yee ^b, Marcel Vinokur ^b^a Lawrence Livermore National Laboratory, Livermore, CA 94551, United States^b NASA Ames Research Center, Moffett Field, CA 94035, United States

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ABSTRACT

In this note we generalize our previous treatment of the discretizations of geometric conservation laws on steady grids (Vinokur and Yee, 2000) to general time dependent grids. The commutative property of mixed difference operators is generalized to apply to time metrics and Jacobians. Our treatment uses half the number of terms as those used in a recent paper by Abe et al. (2012). We also derive the proper temporal discretizations of both Runge–Kutta and linear multistep methods to satisfy the commutativity property for higher than first order.

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1. Introduction

The purpose of this short communication is to present a straightforward extension of the work of Vinokur and Yee [9] for 3D curvilinear moving grids in the high order finite-difference frame work to include deforming grids that satisfy the GCL (Geometric Conservation Law). The main ingredient that was used in Vinokur and Yee is based on the commutative property of mixed difference operators for metric evaluations. This property can be applied to mixed difference operators including time metric evaluations for deforming grids. The natural and obvious candidates to satisfy the commutative property are linear time and spatial difference operators. For separable difference schemes using the method of lines (MOL) approach, all first-order linear operators and high order linear multiple step methods (LMMs) temporal discretizations satisfy the GCL. Examples of spatial operators are all orders of central difference operators or any order of linear difference operators. For in-separable Lax–Wendroff-type difference schemes (second-order or higher) some analysis is needed to make sure the desired accuracy is maintained.

Recently, Abe et al. [1] made use of the commutative property presented in Vinokur and Yee to construct a conservative metric evaluation that satisfies the GCL identity. The first purpose of this note is to illustrate that the Abe et al. [1] formulation can be simplified to just half of the terms needed to satisfy the GCL identity. In addition, Abe et al. made use of the linear difference operators that automatically satisfy the commutative property for first order time discretization. For general multistage Runge–Kutta (RK) methods that are higher than first order, the majority are not explicitly linear. Special construction of higher than first-order RK methods is needed to insure the commutative property and maintain the desired order of accuracy. Abe et al. used a standard second-order RK method in their examples. However, they did

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not prove that RK methods satisfy the commutative property. In addition it is uncertain whether or not this RK method maintains second-order accuracy on their time metric evaluation. The second purpose of this note is to show that some of the typical explicit and implicit LMMs popularized by Beam and Warming [2] do satisfy the commutative property. A construction of multistage RK methods with the commutative property is included. The following expands the discussion further.

We consider a finite difference approximation of partial differential equations, where a curvilinear grid discretizes the computational domain. The grid is generated by a coordinate mapping from a reference cube $(\xi, \eta, \zeta) \in [0, 1]^3$ with time τ to the physical domain $(x, y, z) \in \Omega$ with time t , and is given by an invertible mapping

$$x = x(\xi, \eta, \zeta, \tau) \quad (1)$$

$$y = y(\xi, \eta, \zeta, \tau) \quad (2)$$

$$z = z(\xi, \eta, \zeta, \tau) \quad (3)$$

$$t = \tau. \quad (4)$$

The mapping transforms the conservation law

$$u_t + f(u)_x + g(u)_y + h(u)_z = 0$$

on Ω into

$$\begin{aligned} (Ju)_\tau + (J\xi_x f + J\xi_y g + J\xi_z h + J\xi_t u)_\xi \\ + (J\eta_x f + J\eta_y g + J\eta_z h + J\eta_t u)_\eta + (J\zeta_x f + J\zeta_y g + J\zeta_z h + J\zeta_t u)_\zeta = 0 \end{aligned} \quad (5)$$

on the domain $[0, 1]^3$. Partial derivatives are denoted by subscript notation. For example, ξ_x denotes the partial derivative $\partial\xi/\partial x$. The Jacobian of the mapping, J , is the determinant of the matrix of partial derivatives $\partial(x, y, z)/\partial(\xi, \eta, \zeta)$. The derivation of the conservative form (5) makes use of the so called geometric conservation laws

$$(J\xi_x)_\xi + (J\eta_x)_\eta + (J\zeta_x)_\zeta = 0 \quad (6)$$

$$(J\xi_y)_\xi + (J\eta_y)_\eta + (J\zeta_y)_\zeta = 0 \quad (7)$$

$$(J\xi_z)_\xi + (J\eta_z)_\eta + (J\zeta_z)_\zeta = 0 \quad (8)$$

$$J_\tau + (J\xi_t)_\xi + (J\eta_t)_\eta + (J\zeta_t)_\zeta = 0. \quad (9)$$

Here, the term ‘geometric conservation law’ is somewhat misleading, since (6)–(9) are really identities that are satisfied by any of the given differentiable functions (1)–(3). It is straightforward to see that (6)–(9) guarantee that any constant u is a solution of (5). We will show how to discretize (5) in such a way that (6)–(9) are satisfied exactly by the discretization. When (6)–(9) are satisfied exactly, regions of constant u , such as a free stream state, will be preserved exactly. In general, a finite difference discretization only guarantees that a free stream state is constant up to the order of truncation error of the discretization. There are many examples where an approximation that has the exact free stream preserving property is advantageous.

Second-order spatial discretizations that satisfy the identities (6)–(8) were developed by [7] in non-symmetric form. Vinokur and Yee showed in [9] how a coordinate invariant, or symmetric, form for high order spatial difference operators can be devised. The spatial discretizations used in the work by Visbal and Gaitonde [10] and by Ou and Jameson [5] are not symmetric and they do not make use of the commutative property in their metric construction. Recently, Abe et al. [1] developed a discretization that satisfies (9). Making use of the Vinokur and Yee symmetric formulation for moving grids in the high order finite-difference framework, it will be shown that we can straightforwardly extend the idea of Vinokur and Yee to include deforming grid time metrics that satisfy the GCL identity (9). From our formulation we will show how the construction by Abe et al. can be considerably simplified with just half of their indicated terms. In addition, we will extend the results to LLMs and multi-stage Runge–Kutta time discretizations.

Remark. If we are only given the time dependent mapping on the boundary, the spatial grid generation mapping in the interior can be used to obtain the mappings (1)–(4). For example, to compute x_τ , one would have to use the chain rule and derive a formula that is the differential of the grid generation mapping times the time derivative of the boundary coordinates. This could be rather complicated to implement, but the principle is straightforward.

2. Geometric conservation laws

We introduce the notation

$$\mathbf{S}^{(\xi)} = J \begin{pmatrix} \xi_x \\ \xi_y \\ \xi_z \end{pmatrix}, \quad \mathbf{S}^{(\eta)} = J \begin{pmatrix} \eta_x \\ \eta_y \\ \eta_z \end{pmatrix}, \quad \mathbf{S}^{(\zeta)} = J \begin{pmatrix} \zeta_x \\ \zeta_y \\ \zeta_z \end{pmatrix}. \tag{10}$$

In this notation, (6)–(8) become

$$(\mathbf{S}^{(\xi)})_{\xi} + (\mathbf{S}^{(\eta)})_{\eta} + (\mathbf{S}^{(\zeta)})_{\zeta} = \mathbf{0}. \tag{11}$$

The vector $\mathbf{S}^{(\xi)}$ can be evaluated in terms of the derivatives of the coordinate mapping because of the relations

$$\mathbf{S}^{(\xi)} = \mathbf{r}_{\eta} \times \mathbf{r}_{\zeta}, \quad \mathbf{S}^{(\eta)} = \mathbf{r}_{\zeta} \times \mathbf{r}_{\xi}, \quad \mathbf{S}^{(\zeta)} = \mathbf{r}_{\xi} \times \mathbf{r}_{\eta}. \tag{12}$$

Here, \mathbf{r} denotes the vector of spatial coordinates,

$$\mathbf{r}(\xi, \eta, \zeta, \tau) = \begin{pmatrix} x(\xi, \eta, \zeta, \tau) \\ y(\xi, \eta, \zeta, \tau) \\ z(\xi, \eta, \zeta, \tau) \end{pmatrix} \tag{13}$$

and the partial derivatives of the coordinate vector are denoted

$$\mathbf{r}_{\xi} = (x_{\xi} \ y_{\xi} \ z_{\xi})^T, \quad \mathbf{r}_{\eta} = (x_{\eta} \ y_{\eta} \ z_{\eta})^T, \tag{14}$$

$$\mathbf{r}_{\zeta} = (x_{\zeta} \ y_{\zeta} \ z_{\zeta})^T, \quad \mathbf{r}_{\tau} = (x_{\tau} \ y_{\tau} \ z_{\tau})^T. \tag{15}$$

For a derivation of (12), see [8]. The coordinate invariant form by Vinokur and Yee is obtained by rewriting (12) as the mathematically equivalent

$$\mathbf{S}^{(\xi)} = \frac{1}{2} [(\mathbf{r} \times \mathbf{r}_{\zeta})_{\eta} - (\mathbf{r} \times \mathbf{r}_{\eta})_{\zeta}] \tag{16}$$

$$\mathbf{S}^{(\eta)} = \frac{1}{2} [(\mathbf{r} \times \mathbf{r}_{\xi})_{\zeta} - (\mathbf{r} \times \mathbf{r}_{\zeta})_{\xi}] \tag{17}$$

$$\mathbf{S}^{(\zeta)} = \frac{1}{2} [(\mathbf{r} \times \mathbf{r}_{\eta})_{\xi} - (\mathbf{r} \times \mathbf{r}_{\xi})_{\eta}] \tag{18}$$

before approximating. Let the derivatives with respect to $(\xi \ \eta \ \zeta)$ in (16)–(18) be approximated by difference operators $D^{(\xi)}$, $D^{(\eta)}$, and $D^{(\zeta)}$ respectively. The approximations of (16)–(18) are

$$\mathbf{S}_h^{(\xi)} = \frac{1}{2} [D^{(\eta)}(\mathbf{r} \times D^{(\zeta)}\mathbf{r}) - D^{(\zeta)}(\mathbf{r} \times D^{(\eta)}\mathbf{r})] \tag{19}$$

$$\mathbf{S}_h^{(\eta)} = \frac{1}{2} [D^{(\zeta)}(\mathbf{r} \times D^{(\xi)}\mathbf{r}) - D^{(\xi)}(\mathbf{r} \times D^{(\zeta)}\mathbf{r})] \tag{20}$$

$$\mathbf{S}_h^{(\zeta)} = \frac{1}{2} [D^{(\xi)}(\mathbf{r} \times D^{(\eta)}\mathbf{r}) - D^{(\eta)}(\mathbf{r} \times D^{(\xi)}\mathbf{r})]. \tag{21}$$

We use the subscript h to denote a quantity that has been discretized on a grid. If the operators along the different coordinate directions commute, e.g., $D^{(\xi)}D^{(\eta)} = D^{(\eta)}D^{(\xi)}$, then the finite difference approximation satisfies the discretized (11),

$$D^{(\xi)}\mathbf{S}_h^{(\xi)} + D^{(\eta)}\mathbf{S}_h^{(\eta)} + D^{(\zeta)}\mathbf{S}_h^{(\zeta)} = \mathbf{0} \tag{22}$$

exactly. To see this, we insert (19)–(21) into (22) and obtain the following expression for the left hand side of (22),

$$\begin{aligned} & D^{(\xi)} \left[\frac{1}{2} (D^{(\eta)}(\mathbf{r} \times D^{(\zeta)}\mathbf{r}) - D^{(\zeta)}(\mathbf{r} \times D^{(\eta)}\mathbf{r})) \right] \\ & + D^{(\eta)} \left[\frac{1}{2} (D^{(\zeta)}(\mathbf{r} \times D^{(\xi)}\mathbf{r}) - D^{(\xi)}(\mathbf{r} \times D^{(\zeta)}\mathbf{r})) \right] \\ & + D^{(\zeta)} \left[\frac{1}{2} (D^{(\xi)}(\mathbf{r} \times D^{(\eta)}\mathbf{r}) - D^{(\eta)}(\mathbf{r} \times D^{(\xi)}\mathbf{r})) \right]. \end{aligned} \tag{23}$$

Reordering the terms, we find that (23) is equivalent with the sum of three pairs of differences,

$$\begin{aligned} & \frac{1}{2} [D^{(\xi)} D^{(\eta)} (\mathbf{r} \times D^{(\zeta)} \mathbf{r}) - D^{(\eta)} D^{(\xi)} (\mathbf{r} \times D^{(\zeta)} \mathbf{r}) \\ & + D^{(\eta)} D^{(\zeta)} (\mathbf{r} \times D^{(\xi)} \mathbf{r}) - D^{(\zeta)} D^{(\eta)} (\mathbf{r} \times D^{(\xi)} \mathbf{r}) \\ & + D^{(\zeta)} D^{(\xi)} (\mathbf{r} \times D^{(\eta)} \mathbf{r}) - D^{(\xi)} D^{(\zeta)} (\mathbf{r} \times D^{(\eta)} \mathbf{r})]. \end{aligned} \tag{24}$$

The expression (24) is zero because the first two terms cancel when $D^{(\xi)}$ commutes with $D^{(\eta)}$. Similarly, terms three and four cancel because $D^{(\eta)}$ and $D^{(\zeta)}$ commutes. The last pair, terms five and six, cancel in the same way. The commutative property holds for standard centered difference operators; see e.g., [9] for a proof. Note that the result (22) is obtained because the same difference operator $D^{(\eta)}$ as used in (19) and (21), is also used in (22). Similarly, the operators $D^{(\zeta)}$ and $D^{(\xi)}$ that are used in (19) and (20) are also used in (22). Note that there is no requirement that the difference operators used along the different coordinate directions be the same one dimensional operators.

It can be seen from the pairwise cancellations that occur in (24), that the ‘innermost’ difference operators do not contribute to the cancellation. These operators could therefore be replaced by other operators $\tilde{D}^{(\xi)}$, $\tilde{D}^{(\eta)}$, and $\tilde{D}^{(\zeta)}$, so that the metric discretization (19)–(21) instead becomes

$$\mathbf{S}_h^{(\xi)} = \frac{1}{2} (D^{(\eta)} (\mathbf{r} \times \tilde{D}^{(\zeta)} \mathbf{r}) - D^{(\zeta)} (\mathbf{r} \times \tilde{D}^{(\eta)} \mathbf{r})) \tag{25}$$

$$\mathbf{S}_h^{(\eta)} = \frac{1}{2} (D^{(\zeta)} (\mathbf{r} \times \tilde{D}^{(\xi)} \mathbf{r}) - D^{(\xi)} (\mathbf{r} \times \tilde{D}^{(\zeta)} \mathbf{r})) \tag{26}$$

$$\mathbf{S}_h^{(\zeta)} = \frac{1}{2} (D^{(\xi)} (\mathbf{r} \times \tilde{D}^{(\eta)} \mathbf{r}) - D^{(\eta)} (\mathbf{r} \times \tilde{D}^{(\xi)} \mathbf{r})). \tag{27}$$

The identity (22) would still hold. This possibility is discussed by Deng et al. in [4], who conclude that the accuracy is better when $\tilde{D}^{(\xi)} = D^{(\xi)}$, $\tilde{D}^{(\eta)} = D^{(\eta)}$, and $\tilde{D}^{(\zeta)} = D^{(\zeta)}$.

We remark here that for spatial discretizations it is a standard procedure to use the same difference metric operator for all spatial directions, even if different spatial discretizations in each of the inviscid flux derivative spatial directions might be employed. Here, we only consider separable finite difference schemes of the MOL type. Temporal finite difference operator construction is different from the spatial discretizations. Often, different orders and different types of finite difference temporal discretizations are employed from the spatial difference operators. These MOL discretizations are employed in our high order metric constructions as well.

Next, we show a natural generalization of the above to obtain a time metric discretization that satisfies (9) exactly. It holds that,

$$J = \mathbf{r}_\xi \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta),$$

and

$$J_{\xi t} = -\mathbf{r}_\tau \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta) \tag{28}$$

$$J_{\eta t} = -\mathbf{r}_\tau \cdot (\mathbf{r}_\zeta \times \mathbf{r}_\xi) \tag{29}$$

$$J_{\zeta t} = -\mathbf{r}_\tau \cdot (\mathbf{r}_\xi \times \mathbf{r}_\eta). \tag{30}$$

The terms in the identity (9) can be rewritten in a way similar to (16)–(18) by noting that

$$J = \mathbf{r}_\xi \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta) = \frac{1}{3} ((\mathbf{r} \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta))_\xi + (\mathbf{r} \cdot (\mathbf{r}_\zeta \times \mathbf{r}_\xi))_\eta + (\mathbf{r} \cdot (\mathbf{r}_\xi \times \mathbf{r}_\eta))_\zeta). \tag{31}$$

Applying (31) to each of (28)–(30) with obvious modifications gives

$$J_{\xi t} = -\frac{1}{3} ((\mathbf{r} \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta))_\tau + (\mathbf{r} \cdot (\mathbf{r}_\zeta \times \mathbf{r}_\tau))_\eta + (\mathbf{r} \cdot (\mathbf{r}_\tau \times \mathbf{r}_\eta))_\xi) \tag{32}$$

$$J_{\eta t} = -\frac{1}{3} ((\mathbf{r} \cdot (\mathbf{r}_\zeta \times \mathbf{r}_\xi))_\tau + (\mathbf{r} \cdot (\mathbf{r}_\xi \times \mathbf{r}_\tau))_\zeta + (\mathbf{r} \cdot (\mathbf{r}_\tau \times \mathbf{r}_\zeta))_\xi) \tag{33}$$

$$J_{\zeta t} = -\frac{1}{3} ((\mathbf{r} \cdot (\mathbf{r}_\xi \times \mathbf{r}_\eta))_\tau + (\mathbf{r} \cdot (\mathbf{r}_\eta \times \mathbf{r}_\tau))_\xi + (\mathbf{r} \cdot (\mathbf{r}_\tau \times \mathbf{r}_\xi))_\eta). \tag{34}$$

Let the discretization of J , $J_{\xi t}$, $J_{\eta t}$, and $J_{\zeta t}$ be done by replacing all derivatives with respect to $(\xi \ \eta \ \zeta \ \tau)$ in (31) and (32)–(34) by commuting finite difference operators, $D^{(\xi)}$, $D^{(\eta)}$, $D^{(\zeta)}$, and $D^{(\tau)}$; e.g., (32) would be discretized by

$$\begin{aligned} (J_{\xi t})_h &= -\frac{1}{3} (D^{(\tau)} (\mathbf{r} \cdot (D^{(\eta)} \mathbf{r} \times D^{(\zeta)} \mathbf{r})) \\ & + D^{(\eta)} (\mathbf{r} \cdot (D^{(\zeta)} \mathbf{r} \times D^{(\tau)} \mathbf{r})) + D^{(\zeta)} (\mathbf{r} \cdot (D^{(\tau)} \mathbf{r} \times D^{(\eta)} \mathbf{r}))). \end{aligned} \tag{35}$$

It is then straightforward to verify that this discretization satisfies the following discrete version of (9),

$$D^{(\tau)} J_h + D^{(\xi)} (J \xi_t)_h + D^{(\eta)} (J \eta_t)_h + D^{(\zeta)} (J \zeta_t)_h = 0. \tag{36}$$

A more careful study shows that the cancellation of terms that leads to (36) occurs in two groups. It is therefore possible to make the more general discretization of the metric coefficient

$$(J \xi_t)_h = -\frac{1}{3} (D^{(\tau)} (\mathbf{r} \cdot (D^{(\eta)} \mathbf{r} \times D^{(\zeta)} \mathbf{r})) + D^{(\eta)} (\tilde{\mathbf{r}} \cdot (D^{(\zeta)} \tilde{\mathbf{r}} \times \tilde{D}^{(\tau)} \mathbf{r})) + D^{(\zeta)} (\tilde{\mathbf{r}} \cdot (\tilde{D}^{(\tau)} \mathbf{r} \times D^{(\eta)} \tilde{\mathbf{r}}))) \tag{37}$$

and similarly for $(J \eta_t)_h$ and $(J \zeta_t)_h$. Here, $\tilde{\mathbf{r}}$, denotes the grid evaluated at a time that is different from the time at which \mathbf{r} is evaluated, and $\tilde{D}^{(\tau)}$ is an approximation of the time derivative that is different from $D^{(\tau)}$. The identity (36) will still hold, as long as all terms of the discretization of the Jacobian, J_h , are evaluated at \mathbf{r} . The more general form (37) will be useful when generalizing Runge–Kutta methods to moving grids, as described in the next section.

The metric discretization given in [1] also satisfies (36). However, in [1], Eq. (31) is further decomposed by applying (16)–(18) to the cross products. This leads to the Jacobian being rewritten as

$$\begin{aligned} J &= \mathbf{r}_\xi \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta) = \frac{1}{3} [(\mathbf{r} \cdot (\mathbf{r}_\eta \times \mathbf{r}_\zeta))_\xi + (\mathbf{r} \cdot (\mathbf{r}_\zeta \times \mathbf{r}_\xi))_\eta + (\mathbf{r} \cdot (\mathbf{r}_\xi \times \mathbf{r}_\eta))_\zeta] \\ &= \frac{1}{3} \left[\left(\mathbf{r} \cdot \left(\frac{1}{2} ((\mathbf{r} \times \mathbf{r}_\zeta)_\eta - (\mathbf{r} \times \mathbf{r}_\eta)_\zeta) \right) \right)_\xi + \left(\mathbf{r} \cdot \left(\frac{1}{2} ((\mathbf{r} \times \mathbf{r}_\xi)_\zeta - (\mathbf{r} \times \mathbf{r}_\zeta)_\xi) \right) \right)_\eta \right. \\ &\quad \left. + \left(\mathbf{r} \cdot \left(\frac{1}{2} ((\mathbf{r} \times \mathbf{r}_\eta)_\xi - (\mathbf{r} \times \mathbf{r}_\xi)_\eta) \right) \right)_\zeta \right] \end{aligned} \tag{38}$$

before discretizing. For the time metrics, their formulas (32)–(34) are also rewritten in a similar way. Hence, this discretization requires double the number of terms.

3. Time integration

For moving deformable grids it is important to distinguish between the two cases: (a) The grid mapping is a known, given, function of time, and (b) The grid depends on the computed solution, and therefore needs to be solved for in time together with the solution of the PDE. Here our discussion focuses on (a). We are not sure if any of the theory could be used for (b) as well.

The forward time difference

$$D^{(\tau)} u^n = (u^{n+1} - u^n) / \Delta t \tag{39}$$

is a linear difference operator, and hence it can be used in time to define a discretization that satisfies (36), as outlined in the previous section. Here, superscript n denotes time level. We assume that time has been discretized with a uniform time step Δt , so that the time levels are $t_n = n \Delta t$, $n = 0, 1, \dots$. Similarly, time discretizations that can be written of the form

$$Dy_n = f(y^*, t_*)$$

for some y^* , t_* , when applied to the ODE $y_t = f(y, t)$, allow straightforward inclusion of the moving grid terms. The operator D is any linear finite difference operator approximating the time derivative. Examples of methods of this form are the backward Euler, leap-frog, and backward differentiation (BDF) methods. Furthermore, it is possible to include the moving grid terms in general LMMs to obtain the exact conservation (36) in the sense that the local truncation error is exactly zero for constant u . For higher order methods it is important to verify that the order of accuracy is not degraded by adding the moving grid terms.

For higher order of accuracy, Runge–Kutta (RK) methods are standard choices. RK methods are not explicitly linear difference operators, but by making use of (36) it is possible to choose the metric at the different RK stages to perfectly preserve a free stream state on a moving and deforming grid. For simplicity we assume that $f(u) = g(u) = h(u) = 0$, so that (5) becomes

$$(Ju)_\tau + (J \xi_t u)_\xi + (J \eta_t u)_\eta + (J \zeta_t u)_\zeta = 0. \tag{40}$$

Let

$$s_h(\mathbf{r}(\tau_1), \mathbf{r}(\tau_2), \mathbf{r}(\tau_3), u) = D^{(\xi)} ((J \xi_t)_h u) + D^{(\eta)} ((J \eta_t)_h u) + D^{(\zeta)} ((J \zeta_t)_h u),$$

where the time differences of the metric are approximated by differences between $\mathbf{r}(\tau_2)$ and $\mathbf{r}(\tau_1)$, and where grid terms not differentiated in time are evaluated at τ_3 . For example,

$$\begin{aligned}
(J\xi_t)_h &= -\frac{1}{3\Delta t}(\mathbf{r}(\tau_2) \cdot (D^{(\eta)}\mathbf{r}(\tau_2) \times D^{(\zeta)}\mathbf{r}(\tau_2)) \\
&\quad - \mathbf{r}(\tau_1) \cdot (D^{(\eta)}\mathbf{r}(\tau_1) \times D^{(\zeta)}\mathbf{r}(\tau_1)) \\
&\quad + D^{(\eta)}(\mathbf{r}(\tau_3) \cdot (D^{(\zeta)}\mathbf{r}(\tau_3) \times (\mathbf{r}(\tau_2) - \mathbf{r}(\tau_1)))) \\
&\quad + D^{(\zeta)}(\mathbf{r}(\tau_3) \cdot ((\mathbf{r}(\tau_2) - \mathbf{r}(\tau_1)) \times D^{(\eta)}\mathbf{r}(\tau_3))). \tag{41}
\end{aligned}$$

The notation is here simplified by writing $\mathbf{r}(\tau)$ for $\mathbf{r}(\xi, \eta, \zeta, \tau)$. The discretization (41) is of the form (37), with $\tilde{\mathbf{r}} = \mathbf{r}(\tau_3)$ and $\tilde{D}^{(\tau)}\mathbf{r} = D^{(\tau)}\mathbf{r} = (\mathbf{r}(\tau_2) - \mathbf{r}(\tau_1))/\Delta t$. Note that the grid $\mathbf{r}(\tau)$ can be evaluated at any τ , because it is assumed to be a given function. When u is a constant, it follows from (36) that

$$\Delta t s_h(\mathbf{r}(\tau_1), \mathbf{r}(\tau_2), \mathbf{r}(\tau_3), u) = (-J_h(\tau_2) + J_h(\tau_1))u, \tag{42}$$

where the Jacobian can be evaluated at any τ , since it is a function of the grid. The spatial derivatives in (41) are evaluated at τ_3 .

The two-stage RK method in conservative form

$$J_h(\tau_{n+1})u^{(1)} = J_h(\tau_n)u^n - \Delta t s_h(\mathbf{r}(\tau_n), \mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_n), u^n) \tag{43}$$

$$(2J_h(\tau_{n+1}) - J_h(\tau_n))u^{(2)} = J_h(\tau_{n+1})u^{(1)} - \Delta t s_h(\mathbf{r}(\tau_n), \mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_{n+1}), u^{(1)}) \tag{44}$$

$$J_h(\tau_{n+1})u^{n+1} = \frac{1}{2}(J_h(\tau_n)u^n + (2J_h(\tau_{n+1}) - J_h(\tau_n))u^{(2)}) \tag{45}$$

approximates (40) to second order accuracy and preserves constants perfectly. When the metric is stationary, (43)–(45) is the standard second order TVD RK method [6].

To see that constants are left unchanged, assume that u^n is given and constant. Eq. (42) applied to the first stage gives that $u^{(1)} = u^n$. Similarly, we obtain for the second stage $u^{(2)} = u^{(1)}$, and hence $u^{(2)} = u^n$, so that by (45) $u^{n+1} = u^n$. Second order accuracy is shown in Appendix A.

Similarly, we define the third order TVD RK method with moving metric as

$$J_h(\tau_{n+1})u^{(1)} = J_h(\tau_n)u^n - \Delta t s_h(\mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_n), \mathbf{r}(\tau_n), u^n) \tag{46}$$

$$\frac{1}{2}(J_h(\tau_{n+1}) + J_h(\tau_n))u^{(2)} = \frac{3}{4}J_h(\tau_n)u^n + \frac{1}{4}J_h(\tau_{n+1})u^{(1)} \tag{47}$$

$$- \frac{1}{4}\Delta t s_h(\mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_n), \mathbf{r}(\tau_{n+1}), u^{(1)}) \tag{48}$$

$$J_h(\tau_{n+1})u^{n+1} = \frac{1}{3}J_h(\tau_n)u^n + \frac{2}{3} \cdot \frac{1}{2}(J_h(\tau_{n+1}) + J_h(\tau_n))u^{(2)} \tag{49}$$

$$- \frac{2}{3}\Delta t s_h(\mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_n), \mathbf{r}(\tau_{n+1/2}), u^{(2)}). \tag{50}$$

Similar to the second order RK method, it is straightforward to see that this method also leaves constant u^n unchanged.

Note that there are many different ways that the moving metric could be discretized in a RK method. For example, the method

$$J_h(\tau_{n+1})u^{(1)} = J_h(\tau_n)u^n - \Delta t s_h(\mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_n), \mathbf{r}(\tau_n), u^n) \tag{51}$$

$$J_h(\tau_{n+2})u^{(2)} = J_h(\tau_{n+1})u^{(1)} - \Delta t s_h(\mathbf{r}(\tau_{n+2}), \mathbf{r}(\tau_{n+1}), \mathbf{r}(\tau_{n+1}), u^{(1)}) \tag{52}$$

$$(J_h(\tau_{n+2}) + J_h(\tau_n))u^{n+1} = J_h(\tau_n)u^n + J_h(\tau_{n+2})u^{(2)} \tag{53}$$

is another generalization of the standard second order TVD RK method that preserves constants, but (51)–(53) is only first order accurate.

3.1. Linear multistep methods

Consider a general linear k -step method approximating the ODE $y_t = f(y, t)$,

$$\begin{aligned}
\alpha_{k+1}y_{n+1} + \alpha_k y_n + \cdots + \alpha_1 y_{n-k+1} \\
= \beta_{k+1}\Delta t f(y_{n+1}, t_{n+1}) + \cdots + \beta_1 \Delta t f(y_{n-k+1}, t_{n-k+1}). \tag{54}
\end{aligned}$$

The method (54) applied to (40), gives

$$\begin{aligned} & \alpha_{k+1} J_h(\tau_{n+1}) u^{n+1} - \Delta t \beta_{k+1} f_h(u^{n+1}, D_{k+1}^{(\tau)}, \tau_{n+1}) \\ &= - \sum_{m=1}^k \alpha_m J_h(\tau_{n-k+m}) u^{n-k+m} + \Delta t \sum_{m=1}^k \beta_m f_h(u^{n-k+m}, D_m^{(\tau)}, \tau_{n-k+m}) \end{aligned} \tag{55}$$

where

$$f_h(u^{n-k+m}, D_m^{(\tau)}, \tau_{n-k+m})$$

denotes

$$-D^{(\xi)}((J_{\xi t})_h u^{n-k+m}) - D^{(\eta)}((J_{\eta t})_h u^{n-k+m}) - D^{(\zeta)}((J_{\zeta t})_h u^{n-k+m}).$$

Here, the operator $D_m^{(\tau)}$ discretizes the temporal derivatives occurring in the metric terms. The spatial part of the metric is discretized on time level $n - k + m$, e.g.,

$$\begin{aligned} (J_{\xi t})_h &= -\frac{1}{3\Delta t} (D_m^{(\tau)}(\mathbf{r}(\tau_{n-k+m})) \cdot (D^{(\eta)}\mathbf{r}(\tau_{n-k+m}) \times D^{(\zeta)}\mathbf{r}(\tau_{n-k+m}))) \\ &\quad + D^{(\eta)}(\mathbf{r}(\tau_{n-k+m})) \cdot (D^{(\zeta)}\mathbf{r}(\tau_{n-k+m}) \times D_m^{(\tau)}\mathbf{r}(\tau_{n-k+m})) \\ &\quad + D^{(\zeta)}(\mathbf{r}(\tau_{n-k+m})) \cdot (D_m^{(\tau)}\mathbf{r}(\tau_{n-k+m}) \times D^{(\eta)}\mathbf{r}(\tau_{n-k+m})). \end{aligned} \tag{56}$$

Note that in (55) we have collected the ‘new’ time level $n + 1$ in the left hand side, and the ‘old’ levels in the right hand side. When $\beta_{k+1} \neq 0$, (55) is implicit. The metric time derivatives $D_m^{(\tau)}$ include the grid at time level $n + 1$, but this does not make the method implicit, because the grid mapping is assumed to be given and can therefore be directly evaluated at any time level.

The temporal operators are assumed to be of the form

$$D_m^{(\tau)} y_{n-k+m} = \frac{1}{\Delta t} \sum_{l=1}^{k+1} \gamma_{l,m} y_{n-k+l}, \quad m = 1, \dots, k + 1$$

for some coefficients $\gamma_{l,m}$. Note that the summation from 1 to $k + 1$ means that $D_m^{(\tau)}$ do not introduce dependencies on other time levels than already present in (54). The subscript m indicates that the temporal difference operators are in general different at different positions in the right hand side of (55). The main result of this section is the following theorem.

Theorem 1. *Let the coefficients in the LMM (54), α_m and β_m , be given such that (54) has p th order of accuracy. Furthermore, assume that $p \leq k$. Then it is always possible to define the operators $D_m^{(\tau)}$ with order of accuracy p , and such that the method (55) exactly preserves a constant u .*

For explicit LMMs the condition $p \leq k$ is necessary for stability according to the Dahlquist stability barrier [3]. If the LMM is implicit, it is possible to have stability for $p \leq k + 1$ (k odd) or $p \leq k + 2$ (k even). It would likely be possible to generalize Theorem 1 to implicit LMMs with $p > k$ by making the operators $D_m^{(\tau)}$ wider.

The following notation is introduced to simplify the description of the proof of the theorem. Let Γ denote the matrix of size $k + 1 \times k + 1$ with elements $\gamma_{l,m}$, let E be the matrix of size $p + 1 \times k + 1$ with elements $E_{i,j} = (j - 1)^{(i-1)}$, and let F be the matrix of size $p + 1 \times k + 1$ with elements $F_{i,j} = (i - 1)(j - 2)^{(i-1)}$, where 0^0 is interpreted as 1. Let \mathbf{a} and \mathbf{b} denote the vectors with elements α_m , and β_m respectively. The proof of Theorem 1 relies on the following observations.

Lemma 1. *The condition for p th order accuracy of (54) is*

$$E\mathbf{a} = F\mathbf{b}. \tag{57}$$

The condition for p th order accuracy of the operators $D_m^{(\tau)}$ is

$$E\Gamma = F. \tag{58}$$

The condition for perfect preservation of constants is

$$\mathbf{a} = \Gamma\mathbf{b}. \tag{59}$$

Proof. We first prove (58). The p th order of accuracy means

$$D_m^{(\tau)} y(\tau_{n-k+m}) = \frac{1}{\Delta t} \sum_{l=1}^{k+1} \gamma_{l,m} y(\tau_{n-k+l}) = y_t(\tau_{n-k+m}) + \mathcal{O}(\Delta t^p).$$

Taylor expansion of both sides around t_{n-k+1} gives the accuracy conditions

$$\sum_{l=1}^{k+1} \gamma_{l,m} = 0, \quad \sum_{l=1}^{k+1} \gamma_{l,m} = 1, \tag{60}$$

$$\sum_{l=1}^{k+1} (l-1)^v \gamma_{l,m} = v(m-1)^{v-1}, \quad v = 2, \dots, p, \quad m = 1, \dots, k+1. \tag{61}$$

It is now straightforward, by the definition of the matrices E and F , that these accuracy conditions can be written as (58). The accuracy condition (57) can be shown similarly by Taylor expansion of (54). The details are left out. Finally (59) is shown. The discrete GCL (36) gives

$$D_m^{(\tau)} J_h(\tau_{n-k+m}) = f_h(u^{n-k+m}, D_m^{(\tau)}, \tau_{n-k+m}).$$

Hence, for constant u (55) becomes

$$\sum_{m=1}^{k+1} \alpha_m J_h(\tau_{n-k+m}) = \Delta t \sum_{m=1}^{k+1} \beta_m D_m^{(\tau)} J_h(\tau_{n-k+m}). \tag{62}$$

Expanding the expressions for $D_m^{(\tau)}$ shows that (62) is satisfied identically if the coefficients satisfy

$$\alpha_l = \sum_{m=1}^{k+1} \beta_m \gamma_{l,m}.$$

This is the matrix vector product (59). \square

Proof of Theorem 1. For given \mathbf{a} and \mathbf{b} satisfying (57), we need to find an operator coefficient matrix Γ satisfying the accuracy condition (58) and the perfect volume conservation (59). Let Γ be a given matrix that satisfies the accuracy condition (58). Such a Γ can always be found, because of the assumption $p \leq k$. Eqs. (57) and (58) give

$$E(\mathbf{a} - \Gamma \mathbf{b}) = \mathbf{0}. \tag{63}$$

If E is a square matrix, i.e., if $p = k$, then the result $\mathbf{a} = \Gamma \mathbf{b}$ follows directly, since E is a full rank matrix. Assume that $p \leq k$. Then, the solution of (63) is

$$\mathbf{a} - \Gamma \mathbf{b} = M \mathbf{k}$$

where columns of the matrix M span the null space of E , and \mathbf{k} is a possibly non-zero vector. The term $M \mathbf{k}$ can be absorbed into Γ since

$$\mathbf{a} - \Gamma \mathbf{b} - M \mathbf{k} = \mathbf{a} - \left(\Gamma - M \frac{\mathbf{k} \mathbf{b}^T}{\mathbf{b}^T \mathbf{b}} \right) \mathbf{b}.$$

We redefine the coefficient matrix

$$\tilde{\Gamma} = \Gamma - M \frac{\mathbf{k} \mathbf{b}^T}{\mathbf{b}^T \mathbf{b}}.$$

The modified coefficient matrix, $\tilde{\Gamma}$, satisfies (59) and also the accuracy condition (58), since $EM = 0$. \square

4. Conclusions

In summary, a systematic formulation of conservative symmetric finite-difference metric discretizations that satisfy the GCL identity exactly in moving deformable grids is presented. A wide class of temporal metric discretizations that satisfy the GCL identity is discussed. In general, higher than first-order RK methods are not explicitly linear difference operators. Construction of multistage RK methods that satisfy the GCL is included.

Numerical experiments are planned to evaluate the performance of the new methods, and to compare the accuracy with previous techniques. We expect the proposed discretization to be more accurate than previous discretizations, which were

based on solving (9) by a numerical scheme. The advantages of the proposed discretizations could be very significant for long time integrations, because the exact volume conservation avoids discretization errors from (9) that accumulate over time.

Another generalization of the proposed method is to consider the GCL satisfying discretizations in the presence of boundary conditions, such as, e.g., finite difference operators that are boundary modified to satisfy a summation by parts identity.

Finally, it will be interesting to generalize the volume conservative discretizations to the case where the grid deformation depends on the computed solution of the PDE. There are many interesting applications where accurate discretization of solution dependent deforming grids are important, for example, in structural mechanics problems with large deformations, and in fluid/structure interaction problems.

Appendix A. Second order of accuracy

To demonstrate the accuracy of (43)–(45), consider the scheme applied to the equation $(Ju)_t + D(a_t u) = 0$, where $J = J(x, t)$ and $a = a(x, t)$ are known functions, and $u = u(x, t)$ is the unknown. D is an unspecified difference operator acting only in the x -direction. The truncation error of (43)–(45), denoted T_E , is obtained by inserting the exact solution, u , into the RK method,

$$\begin{aligned}
 T_E &= J_h^{n+1} u^{n+1} - \frac{1}{2} (J_h^n u^n + J_h^{n+1} u^{(1)} - D((a^{n+1} - a^n) u^{(1)})) \\
 &= J_h^{n+1} u^{n+1} - \frac{1}{2} \left(J_h^n u^n + J_h^n u^n - D((a^{n+1} - a^n) u^n) \right. \\
 &\quad \left. - D\left(\frac{a^{n+1} - a^n}{J_h^{n+1}} (J_h^n u^n - D((a^{n+1} - a^n) u^n))\right) \right) \tag{64}
 \end{aligned}$$

and performing a Taylor expansion in the time variable around t_n . The spatial accuracy is assumed to be order two or higher. The part of the truncation error from the operator D will not be considered below. To simplify the notation, denote $J = J_h^n$, $u = u^n$, and $a = a^n$. The time step is denoted by h . Taylor expansion up to second order gives

$$\begin{aligned}
 T_E &= \left(J + h J_t + \frac{h^2}{2} J_{tt} \right) \left(u + h u_t + \frac{h^2}{2} u_{tt} \right) - J u - \frac{1}{2} \left(D \left(\left(h a_t + \frac{h^2}{2} a_{tt} \right) u \right) \right. \\
 &\quad \left. - D \left(\left(h a_t + \frac{h^2}{2} a_{tt} \right) \left(\frac{1}{J} - h \frac{J_t}{J^2} \right) (J u - D(h a_t u)) \right) \right) + \mathcal{O}(h^3) \\
 &= h (J u)_t + \frac{h}{2} D(a_t u) + \frac{h^2}{2} (J u)_{tt} + \frac{h^2}{4} D(a_{tt} u) + T + \mathcal{O}(h^3) \tag{65}
 \end{aligned}$$

where

$$\begin{aligned}
 T &= \frac{1}{2} D \left(\left(h a_t + \frac{h^2}{2} a_{tt} \right) \left(u - h \frac{1}{J} D(a_t u) - h \frac{J_t}{J} u \right) \right) \\
 &= \frac{1}{2} D \left(h a_t u - h^2 a_t \frac{1}{J} D(a_t u) - h^2 a_t \frac{J_t}{J} u + \frac{h^2}{2} a_{tt} u \right) + \mathcal{O}(h^3). \tag{66}
 \end{aligned}$$

Substitute $D(a_t u) = -(J u)_t$ in the second term to obtain

$$\begin{aligned}
 T &= \frac{1}{2} D \left(h a_t u + h^2 a_t \frac{1}{J} (J u)_t - h^2 a_t \frac{J_t}{J} u + \frac{h^2}{2} a_{tt} u \right) + \mathcal{O}(h^3) \\
 &= \frac{1}{2} D \left(h a_t u + h^2 a_t u_t + \frac{h^2}{2} a_{tt} u \right) + \mathcal{O}(h^3). \tag{67}
 \end{aligned}$$

The final result becomes

$$\begin{aligned}
 T_E &= h (J u)_t + \frac{h}{2} D(a_t u) + \frac{h^2}{2} (J u)_{tt} + \frac{h^2}{4} D(a_{tt} u) + \frac{h}{2} D(a_t u) + \frac{h^2}{2} D(a_t u_t) \\
 &\quad + \frac{h^2}{4} D(a_{tt} u) + \mathcal{O}(h^3). \tag{68}
 \end{aligned}$$

Collecting terms and making use of the equation and its derivative, $(J u)_{tt} + D((a_t u)_t) = 0$, yield the final result

$$T_E = \mathcal{O}(h^3)$$

and, hence, the order of accuracy is two.

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