An explicit and conservative remapping strategy for semi-Lagrangian advection

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Abstract

A conservative semi-Lagrangian advection scheme has recently been proposed by Cotter et al. (2007). It is based on a remapped particle-mesh implementation using bicubic B-spline as basis functions. It has been shown that the method is of comparable accuracy as standard bicubic semi-Lagrangian advection schemes. A potential drawback of the, so called, remapped particle-mesh semi-Lagrangian (RPM SL) advection scheme is that it requires the solution of tridiagonal linear systems of equations. In this note, we demonstrate that the solution of linear equations can be avoided without sacrificing the conservation and accuracy properties of the original RPM SL method.

Keywords: semi-Lagrangian advection schemes, conservation of mass, particle-mesh methods, remapping, cubic B-splines, quasi-interpolants

1 Introduction

The standard semi-Lagrangian algorithm (see, e.g., Staniforth & Coté (1991)) calculates departure points, i.e., the positions of Lagrangian particles which will be advected onto the grid during the time step. The momentum and density equations are then solved along the trajectory of the particles. This calculation requires interpolation to obtain velocity and density values at the departure point. It has been found that cubic Lagrangian and cubic spline interpolation are both accurate and computationally tractable (see, e.g., Staniforth & Coté (1991)).

Ideally, as well as being efficient and accurate, a density advection scheme should exactly preserve mass in order to be useful for, e.g., climate prediction or atmospheric chemistry calculations. A conservative semi-Lagrangian scheme based on forward-trajectories has been proposed by Cotter et al. (2007) and compared to existing conservative semi-Lagrangian schemes. The scheme is based on the Hamiltonian particle-mesh method, as introduced by Frank et al. (2002), combined with a conservative remapping strategy, which leads, in general, to the solution of tridiagonal linear systems of equations.

In this paper, we further develop the remapped particle-mesh semi-Lagrangian (RPM SL) advection scheme by showing how the inversion of linear systems of equations can be avoided without having to sacrifice accuracy and conservation properties. Numerical results from the slotted-cylinder problem (Nair et al., 1999*b*; Zerroukat et al., 2002) and the idealized vortex problem of Doswell (1984) are presented to demonstrate the similar behavior of the newly proposed variant of the RPM SL method to the one presented in Cotter et al. (2007).

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2 The remapped particle-mesh semi-Lagrangian (RPM SL) advection scheme

In this section, we summarize the remapped particle-mesh semi-Lagrangian advection (RPM SL) scheme. See Cotter et al. (2007) for more details. For simplicity, we restrict the discussion to two-dimensional flows. We begin with the continuity equation

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

where ρ is the density and $\mathbf{u} = (u, v)^T \in \mathbb{R}^2$ is the fluid velocity as a function of space $\mathbf{x} = (x, y)^T \in \mathbb{R}^2$ and time $t \geq 0$. We denote the initial density by $\rho^0(\mathbf{x}) = \rho(\mathbf{x}, 0)$.

The RPM SL scheme is based on the following discrete Lagrangian approximation scheme. We introduce a finite set of Lagrangian particles $\mathbf{X}_\beta(t) = (X_\beta(t), Y_\beta(t))^T \in \mathbb{R}^2$, $\beta = 1, \ldots, N$, and a fixed Eulerian grid $\mathbf{x}_{k,l} = (x_k, y_l)^T = (k \cdot \Delta x, l \cdot \Delta y)^T$, $k, l = 0, \ldots, M$. Each Eulerian grid point $\mathbf{x}_{k,l}$ carries a basis function $\psi_{k,l}(\mathbf{x}) \geq 0$, which satisfy the normalization condition $\int \psi_{k,l}(\mathbf{x}) \, \mathrm{d}A(\mathbf{x}) = 1$ and the partition of unity (PoU) property

$$\sum_{k,l} \psi_{k,l}(\mathbf{x}) \, A_{k,l} = 1, \qquad A_{k,l} := \Delta x \Delta y, \tag{2}$$

for all $\mathbf{x} \in \mathbb{R}^2$. We approximate the Eulerian grid density $\rho_{k,l}(t) \approx \rho(\mathbf{x}_{k,l}, t)$ by

$$\rho_{k,l}(t) = \sum_\beta m_\beta^0 \, \psi_{k,l}(\mathbf{X}_\beta(t)), \tag{3}$$

where m_β^0 is the "mass" of particle β. The time evolution of the particle positions $\mathbf{X}_\beta(t)$ under given velocities $\mathbf{u}_\beta$ is defined by

$$\frac{d}{dt} \mathbf{X}_\beta = \mathbf{u}_\beta. \tag{4}$$

We assume that

$$\mathbf{X}_\beta(0) := \mathbf{x}_{i,j}, \qquad \beta = 1 + i + j \cdot (M+1) \tag{5}$$

at initial time.

To close the approximation scheme, we need to state a procedure for computing the particle masses

$$m_\beta^0 = m_{i,j}^0, \qquad \beta = 1 + i + j \cdot (M+1) \tag{6}$$

in (3). The RPM SL method is based on the interpolation condition

$$\rho_{k,l}^0 = \sum_{i,j} m_{i,j}^0 \, \psi_{k,l}(\mathbf{x}_{i,j}) \tag{7}$$

for given initial densities $\rho_{k,l}^0 = \rho^0(\mathbf{x}_{k,l})$, which leads, in general, to a linear system of equations in the particle masses $m_{i,j}^0$. See Cotter et al. (2007) for a detailed discussion in the context of bicubic B-spline basis functions.

We finally note that (2) ensures conservation of mass since

$$\sum_{k,l} \rho_{k,l}(t) \, A_{k,l} = \sum_{k,l} \sum_\beta m_\beta^0 \, \psi_{k,l}(\mathbf{X}_\beta(t)) \, A_{k,l} = \sum_\beta m_\beta^0. \tag{8}$$

3 An explicit RPM SL advection scheme

The proposed explicit variant of the RPM SL advection scheme is based on a blended approximation using bilinear and bicubic B-splines as basis functions. These basis functions are more precisely given by

$$\psi^{\mathrm{H}}_{k,l}(\mathbf{x}) := \frac{1}{\Delta x \Delta y}\,\psi_{\mathrm{cs}}\left(\frac{x-x_k}{\Delta x}\right)\cdot\psi_{\mathrm{cs}}\left(\frac{y-y_l}{\Delta y}\right), \tag{9}$$

where $\psi_{\mathrm{cs}}(r)$ is the cubic B-spline

$$\psi_{\mathrm{cs}}(r) = \begin{cases} \frac{2}{3} - |r|^2 + \frac{1}{2}|r|^3, & |r| \le 1, \\ \frac{1}{6}(2-|r|)^3, & 1 < |r| \le 2, \\ 0, & |r| > 2. \end{cases}, \tag{10}$$

and

$$\psi^{\mathrm{L}}_{k,l}(\mathbf{x}) := \frac{1}{\Delta x \Delta y}\,\psi_{\mathrm{ls}}\left(\frac{x-x_k}{\Delta x}\right)\cdot\psi_{\mathrm{ls}}\left(\frac{y-y_l}{\Delta y}\right), \tag{11}$$

where $\psi_{\mathrm{ls}}(r)$ is the linear B-spline

$$\psi_{\mathrm{ls}}(r) = \begin{cases} 1-|r|, & |r| \le 1, \\ 0, & |r| > 1, \end{cases}, \tag{12}$$

respectively.

In case of linear splines, i.e., $\psi_{k,l} = \psi^{\mathrm{L}}_{k,l}$ in (3), the interpolation problem (7) is simply solved by

$$m^0_{i,j} := \rho^0_{i,j}\,A_{i,j}. \tag{13}$$

The resulting low-order advection scheme possesses the desirable property that $\rho^0_{k,l} \ge 0$ for all k,l implies that $\rho_{k,l}(t) \ge 0$ for all k,l and all $t \ge 0$. Local conservation of mass, in the sense of finite-volume methods, and monotonicity are also achieved.

In case of cubic splines, i.e., $\psi_{k,l} = \psi^{\mathrm{H}}_{k,l}$ in (3), we propose to use a quasi-interpolant (Powell, 1981). Quasi-interpolation leads to the explicit formula

$$m^0_{i,j} := \frac{1}{6}\left(8\widehat{m}_{i,j} - \widehat{m}_{i,j+1} - \widehat{m}_{i,j-1}\right), \qquad \widehat{m}_{i,j} := \frac{1}{6}\left(8\rho^0_{i,j} - \rho^0_{i+1,j} - \rho^0_{i-1,j}\right)A_{i,j}. \tag{14}$$

The quasi-interpolant has the same approximation order as the interpolant implicitly defined by (7) (Powell, 1981). However, even though the difference

$$\Delta\rho^0_{k,l} := \rho^0_{k,l} - \sum_{i,j} m^0_{i,j}\,\psi^{\mathrm{H}}_{k,l}(\mathbf{x}_{i,j}) \tag{15}$$

will be small for smooth $\rho^0(\mathbf{x})$, it implies a diffusive behavior of the resulting RPM SL scheme under zero advection, i.e., $\mathbf{u}_\beta = \mathbf{0}$ in (4).

This disadvantage of the explicit mass definition (14) can be eliminated by the following blended scheme:

$$\rho_{k,l}(t) = \sum_{i,j} m^0_{i,j}\,\psi^{\mathrm{H}}_{k,l}(\mathbf{X}_{i,j}(t)) + \sum_{i,j} \Delta m^0_{i,j}\,\psi^{\mathrm{L}}_{k,l}(\mathbf{X}_{i,j}(t)), \tag{16}$$

where $m^0_{i,j}$ is defined by (14) and $\Delta m^0_{i,j} := \Delta\rho^0_{i,j}\,A_{i,j}$ with $\Delta\rho^0_{i,j}$ given by (15).

The blended method (16) possesses the same approximation order as the bicubic RPM SL method considered in Cotter et al. (2007) and satisfies the interpolation condition $\rho_{k,l}(0) = \rho^0_{k,l}$. Contrary to the bicubic scheme of Cotter et al. (2007), the RPM SL advection scheme, defined by (16), is entirely explicit. Following the discussion of Cotter et al. (2007) it is straightforward to extend the blended RPM SL scheme to a spherical longitude-latitude grid. We will present numerical results in section 5.

4 Algorithmic summary

The explicit RPM SL advection scheme can be summarized as follows. Given a gridded density approximation $\{\rho^n_{k,l}\}_{k,l}$ at time-level t_n and a gridded velocity field $\{\mathbf{u}^{n+1/2}_{i,j}\}_{i,j}$ at time-level $t_{n+1/2} = t_n + \Delta t/2$, we find a gridded density approximation $\{\rho^{n+1}_{k,l}\}_{k,l}$ at time-level $t_{n+1} = t_n + \Delta t$ through the following steps:

(i) Compute particle masses

$$m^n_{i,j} := \frac{1}{6}\left(8\widehat{m}_{i,j} - \widehat{m}_{i,j+1} - \widehat{m}_{i,j-1}\right), \qquad \widehat{m}_{i,j} := \frac{1}{6}\left(8\rho^n_{i,j} - \rho^n_{i+1,j} - \rho^n_{i-1,j}\right) A_{i,j}. \tag{17}$$

(ii) Compute correction terms

$$\Delta m^n_{k,l} := \left[\rho^n_{k,l} - \sum_{i,j} m^n_{i,j}\,\psi^{\mathrm{H}}_{k,l}(\mathbf{x}_{i,j})\right] A_{k,l}. \tag{18}$$

(iii) Compute arrival points

$$\mathbf{X}^{\mathrm{a}}_{i,j} := \mathbf{x}_{i,j} + \Delta t\,\mathbf{u}^{n+1/2}_{i,j}. \tag{19}$$

(iv) Compute new density approximations

$$\rho^{n+1}_{k,l} := \sum_{i,j} m^n_{i,j}\,\psi^{\mathrm{H}}_{k,l}(\mathbf{X}^{\mathrm{a}}_{i,j}) + \sum_{i,j} \Delta m^n_{i,j}\,\psi^{\mathrm{L}}_{k,l}(\mathbf{X}^{\mathrm{a}}_{i,j}). \tag{20}$$

5 Numerical results

To assess the accuracy of the newly proposed RPM SL advection scheme in planar and spherical geometry, we consider two common test problems; the slotted-cylinder problem (Zerroukat et al., 2002; Nair et al., 1999*b*) and the idealized vortex problem of Doswell (1984). To eliminate errors due to the approximate nature of (19), arrival points are calculated from analytic solutions for both test problems.

5.1 Planar advection: Slotted-cylinder problem

The slotted-cylinder problem consists of a solid-body rotation of a slotted cylinder in a flow field that rotates with constant angular velocity about a fixed point. We implement the slotted-cylinder problem as, for example, described in Zerroukat et al. (2002); Nair et al. (1999*b*).

The exact solution after six rotations and its numerical approximation using the RPM SL method with either (i) linear splines, (ii) implicit cubic splines (as defined in (Cotter et al., 2007)), or (iii) explicit cubic splines (as defined in section 4) are displayed in figure 1. It can be concluded that bilinear splines are not suitable for this problem. This is in contrast to both bicubic implementations of the RPM SL scheme, which display a rather similar solution accuracy (as expected from the theory of quasi-interpolants (Powell, 1981)). Upon closer inspection, it can be noted that the blended method (panel (d)) leads to a slightly smoother approximation.

5.2 Spherical advection: Smooth deformational flow

To assess the accuracy of the newly proposed RPM SL advection scheme in spherical geometry, we consider the idealized vortex problem of Doswell (1984). The flow field is deformational and an analytic solution is available (see Nair et al. (1999*a*); Nair & Machenhauer (2002) for details).

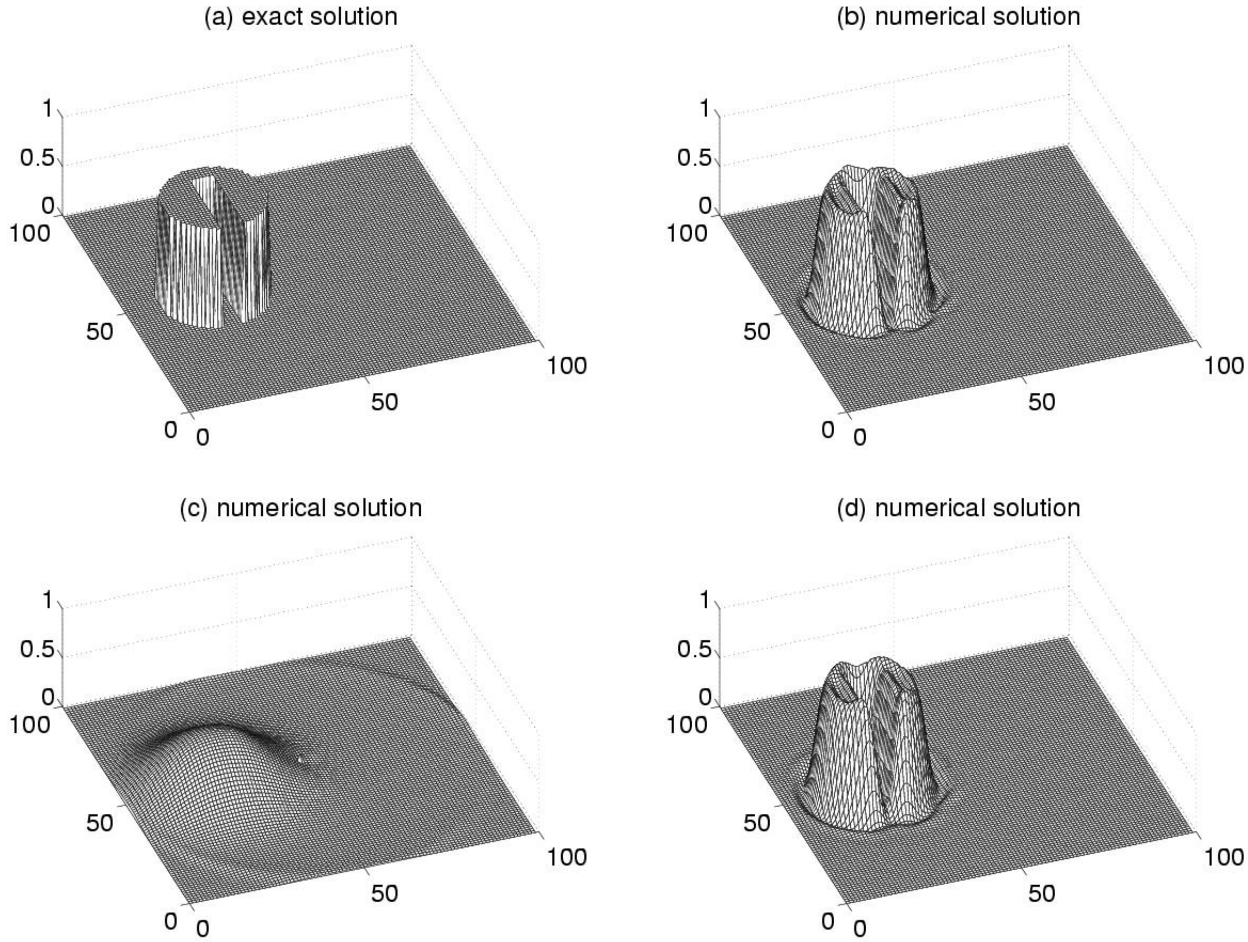

Figure 1: Results from a slotted cylinder problem in planar geometry. The exact solution after six rotations can be found in panels (a). Numerical results are displayed in panels (b)-(d). Panel (b) shows the result using the bicubic RPM SL method of Cotter et al. (2007), while panel (c) displays results using the RPM SL scheme with bilinear splines. Results using the newly proposed explicit RPM SL scheme are shown in panel (d).

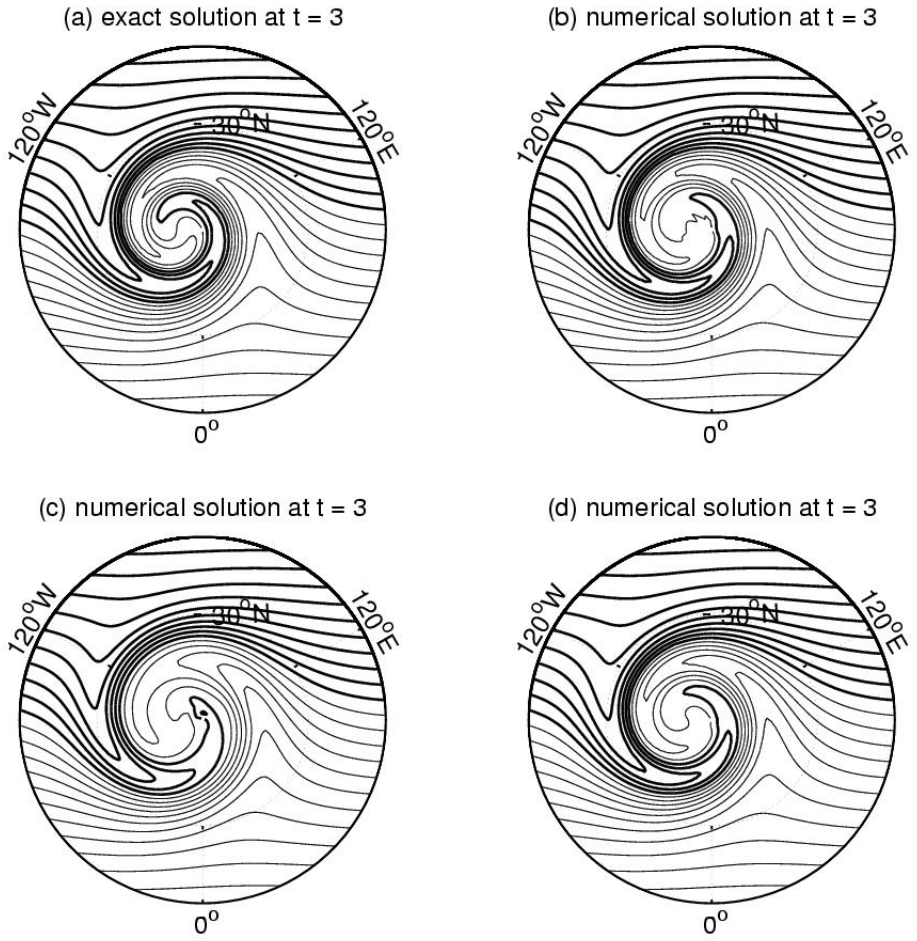

Figure 2: Results from a polar vortex simulation over the sphere. The exact solution at time $t = 3$ can be found in panels (a). Numerical results are displayed in panels (b)-(d). Panel (b) shows the result using the bicubic RPM SL method of Cotter et al. (2007), while panel (c) displays results using the RPM SL scheme with bilinear splines. Results from the newly proposed explicit RPM SL scheme are shown in panel (d). Contours plotted between 0.5 and 1.5 with contour interval 0.05.

We summarize the mathematical formulation. Let (λ', θ') be a rotated coordinate system with the north pole at $(\pi + 0.025, \pi/2.2)$ with respect to the regular spherical coordinates. We consider rotations of the (λ', θ') coordinate system with an angular velocity ω, i.e.,

$$\frac{d\lambda'}{dt} = \omega, \qquad \frac{d\theta'}{dt} = 0, \tag{21}$$

where

$$\omega(\theta') = \frac{3\sqrt{3}\,\mathrm{sech}^2(3\cos\theta')\tanh(3\cos\theta')}{6\cos\theta'}. \tag{22}$$

An analytic solution to the continuity equation (1) in (λ', θ') coordinates is provided by

$$\rho(\lambda', \theta', t) = 1 - \tanh\left[\frac{3\cos\theta'}{5}\sin(\lambda' - \omega(\theta')\,t)\right]. \tag{23}$$

Simulations are performed using a 128×64 grid and a step size of $\Delta t = 0.05$. The exact solution at time $t = 3$ and its numerical approximation using the RPM SL method with either (i) linear splines, (ii) implicit cubic splines (as defined in (Cotter et al., 2007)), or (iii) explicit cubic splines (as defined in section 4) are displayed in figure 2. It can be concluded that bilinear splines lead to unsatisfactory results compared to both bicubic implementations of the RPM SL scheme, which display a rather similar solution accuracy. Upon closer inspection, it can be noted again that the blended method (panel (d)) leads to a slightly smoother approximation.

6 A semi-Lagrangian method for pure advection problems

The algorithm of section 4 can be adjusted to approximate solutions to the advection problem

$$\frac{D\Phi}{Dt} = \Phi_t + \mathbf{u}\cdot\nabla\Phi = 0. \tag{24}$$

We simply make use of the interpolation property of the blended spline approximation combined with a standard backward trajectory technique (Staniforth & Coté, 1991). More specifically, given a gridded approximation $\{\Phi^n_{k,l}\}_{k,l}$ at time-level t_n and a gridded velocity field $\{\mathbf{u}^{n+1/2}_{i,j}\}_{i,j}$ at time-level $t_{n+1/2}$, we find a gridded density approximation $\{\Phi^{n+1}_{k,l}\}_{k,l}$ at time-level t_{n+1} through the following steps:

(i) Compute weights

$$w^n_{i,j} := \frac{1}{6}\left(8\widehat{w}_{i,j} - \widehat{w}_{i,j+1} - \widehat{w}_{i,j-1}\right), \qquad \widehat{w}_{i,j} := \frac{1}{6}\left(8\Phi^n_{i,j} - \Phi^n_{i+1,j} - \Phi^n_{i-1,j}\right)A_{i,j}. \tag{25}$$

(ii) Compute correction terms

$$\Delta w^n_{k,l} := \left[\Phi^n_{k,l} - \sum_{i,j} w^n_{i,j}\,\psi^{\mathrm{H}}_{i,j}(\mathbf{x}_{k,l})\right]A_{k,l}. \tag{26}$$

(iii) Compute departure points

$$\mathbf{X}^{\mathrm{d}}_{k,l} := \mathbf{x}_{k,l} - \Delta t\,\mathbf{u}^{n+1/2}_{k,l}. \tag{27}$$

(iv) Compute new grid approximations

$$\Phi^{n+1}_{k,l} := \sum_{i,j} w^n_{i,j}\,\psi^{\mathrm{H}}_{i,j}(\mathbf{X}^{\mathrm{d}}_{k,l}) + \sum_{i,j}\Delta w^n_{i,j}\,\psi^{\mathrm{L}}_{i,j}(\mathbf{X}^{\mathrm{d}}_{k,l}). \tag{28}$$

7 Summary and outlook

We have further developed the RPM SL method of Cotter et al. (2007) into a low-complexity, accurate, and conservative advection scheme. As demonstrated in Cotter et al. (2007), the RPM SL method may be included into the time-staggered semi-Lagrangian schemes, as proposed by Staniforth et al. (2006) and Reich (2006) for the shallow-water equations, and can be adapted to spherical geometry.

Using a combination of a low-order, monotonic approximation using bilinear splines and a high-order, non-monotonic approximation based on bicubic B-splines, it seems feasible to implement mass-conserving, monotonic filters based on appropriate modifications to the Zalesak corrector (Zalesak, 1979) along the lines of, e.g., Bermejo & Staniforth (1992) and Nair et al. (1999*b*).

We have also outlined an application of the RPM SL method to the advection problem (24). The dual nature of the RPM SL scheme for the continuity equation (1) of section 4 based on forward trajectories and the scheme of section 6 based on backward trajectories for the advection problem (24) should be explored further.

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