# Highlights

## Analysis of finite-volume transport schemes on cubed-sphere grids and an accurate scheme for divergent winds

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- The transport scheme employed in the dynamical core of United States' Global Forecast System is revisited.
- Numerical simulations show that this scheme has reduced accuracy for divergent winds.
- An alternative scheme is proposed, which is much more accurate for divergent winds than the revisited scheme.
- The proposed scheme adds only a slight increase in computational cost.

## Analysis of finite-volume transport schemes on cubed-sphere grids and an accurate scheme for divergent winds

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#### Abstract

The cubed-sphere finite-volume dynamical core (FV3), developed by GFDL-NOAA-USA, serves as the dynamical core for many models worldwide. In 2019, it was officially designated as the dynamical core for the new Global Forecast System of the National Weather Service in the USA, replacing the spectral model. The finite-volume approach employed by FV3 to solve horizontal dynamics involves the application of transport finite-volume fluxes for different variables. Hence, the transport scheme plays a key role in the model. Therefore, this work proposes to revisit the details of the transport scheme of FV3 with the aim of adding enhancements. We proposed modifications to the FV3 transport scheme, which notably enhanced accuracy, particularly in the presence of divergent winds, as evidenced by numerical experiments. In contrast to the FV3 scheme's first-order accuracy in the presence of divergent winds, the proposed scheme achieves second-order accuracy. For divergencefree winds, both schemes are second-order, with our scheme being slightly more accurate. Additionally, the proposed scheme exhibits slight computational overhead but is easily implemented in the current code. In summary, the proposed scheme offers significant improvements in accuracy, particularly

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in the presence of divergent winds, which are present in various atmospheric phenomena, while maintaining computational efficiency.

*Keywords:* Cubed-sphere, finite-volume, transport, advection, numerical weather prediction, divergent winds.

## 1 1. Introduction

The Finite Volume Cubed-Sphere Dynamical Core (FV3), developed by 2 the National Oceanic and Atmospheric Administration's Geophysical Fluid 3 Dynamics Laboratory (NOAA-GFDL), has been embraced as the dynamical 4 core for several atmospheric models (cf. eg. [1, 2, 3, 4, 5, 6]). In 2019, FV3 5 attained significant recognition when it was adopted as the new dynamical 6 core for the Global Forecast System operated by the U.S. National Weather Service (NWS), replacing the spectral transform dynamical core. Addition-8 ally, FV3 is used in the Hurricane Analysis and Forecast System (HAFS) 9 from the NWS for tropical cyclone forecasts [7]. 10

Currently, FV3 solves the non-hydrostatic and compressible Euler equations, as described in the technical report [8], using the vertical Lagrangian coordinate approach outlined in [9]. This method treats the vertical terms implicitly, and the horizontal winds are updated using the shallow-water equations (SWEs) on the designated Lagrangian surfaces. Consequently, the SWEs solver assumes a pivotal role within the FV3 non-hydrostatic solver.

On the other hand, within FV3, the solution of the SWEs is derived using 17 the finite-volume method proposed by [10] extended to the cubed-sphere grid. 18 This approach takes into account the SWEs in their vector invariant form, 19 combining both the C and D-grid staggering in Arakawa notation introduced 20 in [11]. The idea of combining C and D-grids is a unique feature of the scheme 21 proposed by [10] and has also been explored in [12]. Another major feature 22 of this scheme is that the computation of fluid pressure, absolute vorticity, 23 and kinetic energy fluxes is carried out using only transport finite-volume 24 fluxes. Additionally, on the Lagrangian surfaces, the transport scheme is 25 also used for the advection of virtual potential temperature [8, Section 6.1]. 26 Thus, the transport scheme assumes a critical role in shaping the horizontal 27 dynamics of FV3, beyond its traditional function in the dynamical core, as 28 usually observed in tracer transport [13]. 29

The transport scheme employed in FV3, proposed by [14], extends the method introduced by [15] and also by [16] at the same time, moving from latitude-longitude grids to cubed-sphere grids, aiming for better performance
on massive parallel supercomputers, which is difficult to achieve on latitudelongitude grids due to the pole problem [13, 17]. Cubed-sphere grids were
originally proposed by [18] and revisited by [19, 20]. This type of grid is
an instance of grids based on Platonic solids [17], which consider a Platonic
solid circumscribed on the sphere, project its faces onto the sphere's surface,
and apply subdivision on the projected faces to generate the grid cells.

The approach of [15, 14] involves constructing a two-dimensional (2D) 39 scheme by combining the solution of one-dimensional (1D) conservative trans-40 port equations using a direction-splitting strategy on each cube face. The 41 1D equations are solved using the finite-volume approach of the Piecewise 42 Parabolic Method (PPM) [21, 22]. A notable feature of the scheme proposed 43 by [15] is its elimination of the splitting error under conditions where the 44 initial transported scalar field density is constant and the wind is divergence-45 free. This property is attained through modifications to the inner advection 46 operators employed within the scheme. 47

Therefore, given the relevance of the FV3 dynamical core, the goal of this 48 study is to reassess and suggest enhancements for the current FV3 transport 49 scheme originally developed by [14], given its pivotal role in the horizontal 50 dynamics of FV3. It is demonstrated in this work that the scheme proposed 51 by [14] assumes constant metric terms during the application of the PPM to 52 each 1D flux integration domain and employs a first-order departure point 53 calculation for the 1D fluxes. We propose a new scheme that incorporates a 54 second-order departure point calculation for the 1D fluxes and eliminates the 55 assumption of constant metric terms. While the proposed scheme does not 56 retain the property of splitting error elimination for divergence-free winds and 57 constant scalar fields, it ensures second-order errors in such scenarios. The 58 proposed scheme performs slightly better for divergence-free wind simulations 59 of the advection equation on the sphere. Notably, the proposed scheme 60 achieves second-order accuracy for divergent winds, while the FV3 scheme is 61 only first-order accurate in this scenario. 62

This work considers the duo-grid version of FV3 developed by [23], which has been shown to significantly reduce grid imprinting. This improvement is achieved by replacing edge extrapolations from [14] with a scheme that extends gridlines continuously, aligning them with neighboring panels and enabling more accurate stencil computations through 1D Lagrange interpolation. The new scheme is easy to implement in the duo-grid version of the FV3 code and adds only a small extra computational cost within this framework. The extra cost is mainly due to the second-order departure point computation, which requires 1D linear interpolations at each cell edge in both directions of each cubed-sphere panel. However, the duo-grid interpolation creates a computational overhead for parallel computing [24]. Nevertheless, once the computational performance of the duo-grid version of FV3 is optimized, the new scheme presents an attractive alternative for a more accurate transport scheme.

This work is outlined as follows: Section 2 presents the cubed-sphere grids, revisiting both the equiangular and equi-edge grids, and also discusses the treatment of ghost cells, providing all the notations needed for this work. In Section 3, the FV3 transport scheme of [14] is revisited on the cubed-sphere and an alternative scheme is proposed. In Section 4, numerical simulations comparing the proposed scheme with the current FV3 transport scheme are reported. Final thoughts are presented in Section 5.

#### <sup>84</sup> 2. Cubed-sphere grids

The goal of this section is to briefly review the concept of cubed-sphere 85 grids, particularly those available in FV3. To start with, the mapping be-86 tween the cube and the sphere introduced by [18], also known as the equidis-87 tant mapping, is presented in Section 2.1. After that, it is shown that by using 88 a change of coordinates, the equidistant mapping can be utilized to create 89 other mappings from the cube to the sphere. Namely, Section 2.2 introduces 90 the equiangular mapping introduced by [20], and Section 2.3 introduces the 91 equi-edge mapping introduced by [24]. Section 2.4 demonstrates how these 92 mappings are utilized to generate cubed-sphere grids and introduces all the 93 notations and tools necessary for the subsequent parts of this work. Finally, 94 on the cubed-sphere, it is needed to define ghost cells, which are cells added 95 outside each cubed-sphere face that allow for stencil computation near to the 96 edges of the spherical cube. Therefore, in Section 2.5, it is demonstrated how 97 the needed ghost cells are generated. 98

### 99 2.1. Equidistant mapping

<sup>100</sup> Considering a cube circumscribed on a sphere, [18] introduces a mapping <sup>101</sup> between the cube faces and the sphere, generating a spherical cube. This <sup>102</sup> mapping is also called equidistant mapping and generates the equidistant <sup>103</sup> grid. Given R > 0, the sphere of radius R centered at the origin of  $\mathbb{R}^3$  is 104 denoted as:

$$\mathbb{S}_{R}^{2} = \{ P = (p_{x}, p_{y}, p_{z}) \in \mathbb{R}^{3} : p_{x}^{2} + p_{y}^{2} + p_{z}^{2} = R^{2} \}.$$
 (1)

For the purposes of this work, the Earth radius  $R = 6.371 \times 10^6$  meters is considered. The equidistant mapping considers a cube centered at the origin with a side length of  $\frac{2R}{\sqrt{3}}$  and radially projects the cube faces onto the sphere (Figure 1a).

The equidistant mapping is a family of maps  $\Gamma_p : [-1,1] \times [-1,1] \to \mathbb{S}^2_R$ , where  $p = 1, \ldots, 6$ , defined as follows:

$$\Gamma_1(X,Y) = \frac{R}{\sqrt{1+X^2+Y^2}}(1,X,Y),$$
(2)

$$\Gamma_2(X,Y) = \frac{R}{\sqrt{1+X^2+Y^2}}(-X,1,Y),$$
(3)

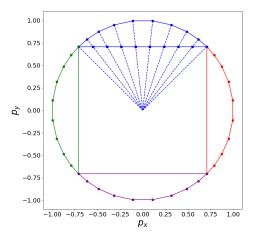
$$\Gamma_3(X,Y) = \frac{R}{\sqrt{1+X^2+Y^2}}(-X,-Y,1),$$
(4)

$$\Gamma_{3+k}(X,Y) = -\Gamma_k(Y,X), \quad k = 1, 2, 3.$$
 (5)

These mappings are defined individually for each of the 6 cube faces, 111 also called panels, denoted by p, and they allow for the coverage of the 112 sphere. The idea behind this mapping is illustrated in Figure 1a, where the 113 coordinates (X, Y) are thought to live on the cube faces. Figure 1a shows 114 how the grid points are equally spaced on the cube and then projected onto 115 the sphere, hence the name equidistant. Note that there are other ways to 116 arrange the coordinates over the panels. Each one defines a connectivity pat-117 tern between the panels, as discussed by [24, Section 2.1]. The connectivity 118 pattern presented here is known as the staircase arrangement (see Figure 2 119 in [24]), which is used in FV3 and provides some advantages for exchanging 120 information between panels. 121

The derivative of  $\Gamma_p$  is a  $3 \times 2$  matrix denoted by  $d\Gamma_p$ . Explicit formulas are provided in Appendix A. With the aid of the derivative, a basis of tangent vectors  $\{\partial_X \Gamma_p, \partial_Y \Gamma_p\}$  may be defined at each point on the sphere, where  $\partial_X \Gamma_p$ is given by the first column of  $d\Gamma_p$  and  $\partial_Y \Gamma_p$  is given by the second column of  $d\Gamma_p$ . Along side, the metric tensor is defined as  $G_{\Gamma} := (d\Gamma_p)^T \cdot d\Gamma_p$ . It is easy to see that the metric tensor does not depend on the panel p. The Jacobian of the metric tensor  $G_{\Gamma}$  is then defined as  $\sqrt{\mathfrak{g}_{\Gamma}} := \sqrt{|\det G_{\Gamma}|}$ .

Let us assume that it is given a function  $\beta : [-a, a] \to [-1, 1]$ , for some positive a > 0, supposed to be bijective and  $C^1$  with inverse  $C^1$  as well. That



(a) Cube and sphere equidistant mapping for  $p_z = 0$ .

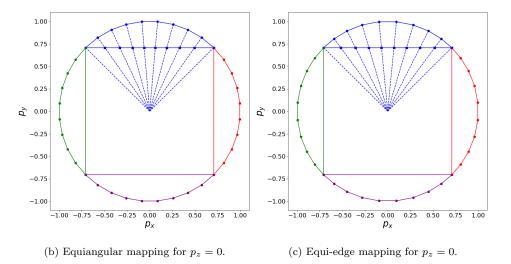


Figure 1: Illustration of the cube-to-sphere projection using the equidistant (a), equiangular (b) and the equi-edge (c) mappings. This figure uses a cross section obtained with  $p_z = 0$ .

<sup>131</sup> is,  $\beta$  is a change of coordinates. Then, new cube-to-sphere mappings may be <sup>132</sup> constructed. Indeed, we may define  $\Psi_p : [-a, a] \times [-a, a] \to \mathbb{S}^2_R$ , given by

$$\Psi_p(x,y) := \Gamma_p(\beta(x),\beta(y)). \tag{6}$$

<sup>133</sup> Using the derivatives of  $\Psi_p(x, y)$ , a basis of tangent vectors  $\{\partial_x \Psi_p, \partial_y \Psi_p\}$ <sup>134</sup> induced by this mapping is defined. The metric tensor of  $\Psi_p$ , denoted by <sup>135</sup>  $G_{\Psi}$ , is defined as  $G_{\Gamma}$ , namely  $G_{\Psi} = (d\Psi_p)^T d\Psi_p$ . Finally, the metric term for <sup>136</sup>  $\Psi$  is defined as  $\sqrt{\mathfrak{g}_{\Psi}} := \sqrt{|\det G_{\Psi}|}$ , which may also be expressed as

$$\sqrt{\mathfrak{g}_{\Psi}}(x,y) = \|\partial_x \Psi_p\| \|\partial_y \Psi_p\| \sin \alpha(x,y,p),\tag{7}$$

where  $\|\cdot\|$  is the Euclidian norm of  $\mathbb{R}^3$ ,  $\alpha$  is the angle between  $\partial_x \Psi_p$  and  $\partial_y \Psi_p$  that satisfies

$$\cos\alpha(x, y, p) = \langle \boldsymbol{e}_x(x, y, p), \boldsymbol{e}_y(x, y, p) \rangle, \qquad (8)$$

<sup>139</sup> where  $\langle \cdot, \cdot \rangle$  denotes the standard inner product of  $\mathbb{R}^3$  and  $\{e_x, e_y\}$  is the <sup>140</sup> normalization of the tangent vector basis  $\{\partial_x \Psi_p, \partial_y \Psi_p\}$ .

Given a tangent vector field  $\boldsymbol{u}$  on the sphere, also known as wind, we may represent it using the basis obtained by cubed-sphere coordinates:

$$\boldsymbol{u}(x,y,p) = \boldsymbol{u}(x,y,p)\partial_x \Psi_p(x,y) + \boldsymbol{v}(x,y,p)\partial_y \Psi_p(x,y).$$
(9)

This representation (u, v) is known as the contravariant representation, and they are the components of the wind on the tangent basis defined by the cubed-sphere mapping. A detailed discussion on how the cubed-sphere wind representation is related to the zonal and meridional representation is presented in Appendix B. In practice, FV3 schemes [14, 8] use the normalized contravariant wind (u, v) given by:

$$\boldsymbol{u}(x,y,p) = \boldsymbol{\mathsf{u}}(x,y,p)\boldsymbol{e}_x(x,y,p) + \boldsymbol{\mathsf{v}}(x,y,p)\boldsymbol{e}_y(x,y,p), \tag{10}$$

where  $e_x$  and  $e_y$  are the normalized cubed-sphere tangent vectors, which may be computed easily in terms of the grid points [24, Appendix C2]. It is easy to see that:

$$u(x, y, p) = \frac{\mathsf{u}(x, y, p)}{\|\partial_x \Psi_p(x, y)\|}, \quad v(x, y, p) = \frac{\mathsf{v}(x, y, p)}{\|\partial_y \Psi_p(x, y)\|}.$$
 (11)

Finally, we recall that the horizontal divergence operator for a wind u on the sphere is defined in terms of the cubed-sphere metric terms as follows:

$$[\nabla \cdot \boldsymbol{u}](x, y, p) := \frac{1}{\sqrt{\mathfrak{g}_{\Psi}(x, y)}} \bigg( \partial_x(\sqrt{\mathfrak{g}_{\Psi}}u)(x, y, p) + \partial_y(\sqrt{\mathfrak{g}_{\Psi}}v)(x, y, p) \bigg), \quad (12)$$

for  $x, y \in [-a, a]$ , p is the panel and u and v are the contravariant wind components. The divergence operator shall be used in the transport model in Section 3.

#### 157 2.2. Equiangular mapping

Another cubed-sphere mapping is the equiangular mapping, introduced by [20], which leads to a more uniform grid on the sphere. This mapping is obtained by considering  $\beta(x) = \tan x$  and  $a = \frac{\pi}{4}$ . In this case,  $\beta(x)$  represents the angular coordinates, and the cubed-sphere is obtained by partitioning the angle between grid points equally, as illustrated in Figure 1b, hence the name equiangular.

#### 164 2.3. Equi-edge mapping

Another cubed-sphere mapping is the equi-edge mapping, initially intro-165 duced by [24], which utilizes  $\beta(x) = \sqrt{2} \tan x$  and  $a = \arcsin\left(\frac{1}{\sqrt{3}}\right)$ . It is 166 worth noting that while this mapping technique had been used previously 167 in FV3, it was not formally documented until the work [24]. The idea be-168 hind the equi-edge mapping lies in partitioning the edges of the spherical 169 cube equally and then generating the other cells, resulting in an equidistant-170 along-edges grid, that we will here call "equi-edge", according to previous 171 use of this terminology [24]. Also, this mapping leads to more uniform grid 172 cells after applying the grid stretching option of FV3 [25, 24]. This mapping 173 is illustrated in Figure 1c. 174

#### 175 2.4. Cubed-sphere grid generation

Let us fix two positive integers N and  $\nu$ , where N represents the number of 176 cells in both the x and y directions, and  $\nu$  represents the number of ghost cell 177 layers. The equiangular or equi-edge mappings, denoted by  $\Psi_p$ , introduced 178 previously, are considered to generate the cubed-sphere grid. The notation 179  $\Psi_p$  is used for both equiangular and equi-edge mappings, as what will be 180 discussed does not depend particularly on the mapping. For simplicity, the 181 metric term  $\sqrt{\mathfrak{g}}_{\Psi}$  is denoted by  $\sqrt{\mathfrak{g}}$ . To generate the cubed-sphere grid, the 182 domain  $[-a, a] \times [-a, a]$  is discretized using uniformly spaced points. 183

$$x_{i+\frac{1}{2}} = -a + i\Delta x, \quad y_{j+\frac{1}{2}} = -a + j\Delta y,$$
 (13)

where  $\Delta x = \Delta y = \frac{2a}{N}$ ,  $i, j = -\nu + 1, \dots, N + 1 + \nu$ . The center coordinates are defined as:

$$x_{i} = \frac{x_{i+\frac{1}{2}} + x_{i-\frac{1}{2}}}{2}, \quad y_{j} = \frac{y_{j+\frac{1}{2}} + y_{j-\frac{1}{2}}}{2}, \tag{14}$$

for  $i, j = -\nu + 1, ..., N + \nu$ . Notice that the mappings  $\Psi_p$  defined before can be computed outside the range [-a, a], and the cubed-sphere mapping can be applied to all these ghost cell points. Firstly, we shall focus the attention on the interior cells; the generation of ghost cells shall be addressed in Section 2.5.

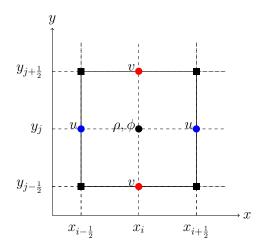


Figure 2: Illustration of the discrete grid indexes for a cell. The corner points are depicted using black squares, while the centroids are represented using black circles. The left-right and up-down midpoints of the edges, are illustrated in blue and red circles, respectively. Additionally, this figure shows the positions of the contravariant wind components u and v in a C-grid discretization for the transport model, along with the fluid density  $\rho$  and tracer concentration  $\phi$  at the centers.

There are four types of grid points on the cubed-sphere that are needed to be computed: the center, corners, right-left edge midpoints, and up-down edge midpoints. These points are illustrated in Figure 2. The corner points are computed as:

$$\Psi_{i+\frac{1}{2},j+\frac{1}{2},p} := \Psi_p(x_{i+\frac{1}{2}}, y_{j+\frac{1}{2}}), \tag{15}$$

i, j = 0, ..., N. To ease the notation hereafter, the dependence on p is omitted because it does not interfere with what is going to be discussed in this section. Figure 3 shows the obtained grid lines in for N = 10.

The center, corners, right-left edge midpoints, and up-down edge midpoints could be computed similarly using Equation (15). However, in FV3, these points are replaced by averages of the corner points. Thus, the center

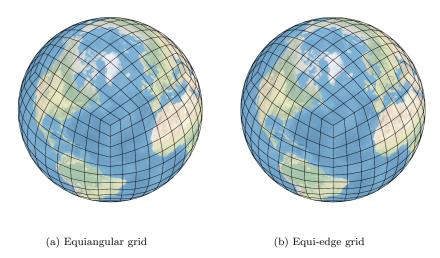


Figure 3: (a) Illustration of the resulting gridlines for the cubed-sphere equiangular and equi-edge mapping for N = 10.

<sup>201</sup> points are computed by averaging the values of 4 corner points:

$$\Psi_{ij} := R \frac{\Psi_{i+\frac{1}{2},j+\frac{1}{2}} + \Psi_{i+\frac{1}{2},j-\frac{1}{2}} + \Psi_{i-\frac{1}{2},j+\frac{1}{2}} + \Psi_{i-\frac{1}{2},j-\frac{1}{2}}}{\|\Psi_{i+\frac{1}{2},j+\frac{1}{2}} + \Psi_{i+\frac{1}{2},j-\frac{1}{2}} + \Psi_{i-\frac{1}{2},j+\frac{1}{2}} + \Psi_{i-\frac{1}{2},j-\frac{1}{2}}\|}.$$
 (16)

Similarly, the right-left edge points  $\Psi_{i+\frac{1}{2},j}$  are obtained by averaging the values of 2 corner points and the up-down edge points  $\Psi_{i,j+\frac{1}{2}}$  are also given by the average of 2 corner points. It is easy to see that generating the grid points using these averages has an  $\mathcal{O}(\Delta x^2)$  difference compared to generating these points using a cubed-sphere mapping  $\Psi_p$ .

The following geodesic distances in x and y directions, respectively, are introduced:

$$\hat{l}_{ij}^{\hat{x}} = d(\Psi_{i+\frac{1}{2},j}, \Psi_{i-\frac{1}{2},j}), \quad \hat{l}_{ij}^{\hat{y}} = d(\Psi_{i,j+\frac{1}{2}}, \Psi_{i,j-\frac{1}{2}}), \tag{17}$$

where  $d(P,Q) = R \arccos(\langle P,Q \rangle)$ , for  $P,Q \in \mathbb{S}^2_R$ . These distances may be represented in terms of the tangent vector norms as:

$$\widehat{l_{ij}^x} = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \|\partial_x \Psi_p\|(x, y_j) \, dx, \quad \widehat{l_{ij}^y} = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \|\partial_y \Psi_p\|(x_i, y) \, dy. \tag{18}$$

<sup>211</sup> Hence, their midpoint approximations are defined as:

$$l_{ij}^{x} = \|\partial_x \Psi_p(x_i, y_j)\| \Delta x, \quad l_{ij}^{y} = \|\partial_y \Psi_p(x_i, y_j)\| \Delta y.$$
(19)

We point out that  $l_{ij}^x$  and  $l_{ij}^y$  are replaced in FV3 code by the geodesic distances that they approximate whenever they appear, which are second-order accurate by the midpoint rule. A control volume of the cubed-sphere is denoted by  $\Omega_{ijp}$ , defined as  $\Omega_{ijp} = \Psi_p(\Omega_{ij})$ . The area of  $\Omega_{ijp}$  is denoted by  $|\Omega_{ij}|$ , since the area does not depend on the panel due to the grid symmetry. The control volume area may be expressed as:

$$|\Omega_{ij}| = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \sqrt{\mathfrak{g}}(x,y) \, dx \, dy = |\hat{\Omega}_{ij}| + \mathcal{O}(\Delta x^2), \tag{20}$$

218 where

$$|\hat{\Omega}_{ij}| = \sqrt{\mathfrak{g}}_{ij} \Delta x \Delta y, \qquad (21)$$

<sup>219</sup>  $\sqrt{\mathfrak{g}}_{ij} = \sqrt{\mathfrak{g}}(x_i, y_j)$  and the last equality in Equation (20) follows from the <sup>220</sup> midpoint rule for integration. Similar to the grid lengths, the approximated areas  $|\hat{\Omega}_{ij}|$  are replaced by the exact area  $|\Omega_{ij}|$  in the FV3 code.

Table 1: Mean length, minimum length, and maximum length for different values of N considering the equiangular grid.

N	Mean Length (km)	Min Length (km)	Max Length (km)	$\frac{Max}{Min}$
48	220	202	240	1.1890
96	109	99	118	1.1892
192	54	49	59	1.1892
384	27	24	29	1.1892
768	13	12	14	1.1892

221

Tables 1 and 2 display the lengths of the equiangular and equi-edge grids 222 for  $N = 48 \times 2^k$ , where  $k = 0, \ldots, 4$ . These values of N are considered in this 223 work. It can be observed that in terms of length of the cells, the equi-edge 224 grid is less uniform than the equiangular grid. Despite this, the equi-edge 225 grid is the operational grid in some applications of FV3 [8, 24], such as, for 226 instance, the Next Generation Global Prediction System (NGGPS) [26]. As 227 mentioned in Section 2.3, the equi-edge grid has greater uniformity near the 228 original cube edges, which are the critical regions of the cube-sphere in terms 229 of grid imprinting [24]. Grid imprinting, which refers to the appearance of 230

N	Mean Length (km)	Min Length (km)	Max Length (km)	$\frac{Max}{Min}$
48	218	175	266	1.5192
96	108	86	131	1.5195
192	54	43	65	1.5196
384	26	21	32	1.5197
768	13	10	16	1.5197

Table 2: As Table 1 but considering the equi-edge grid.

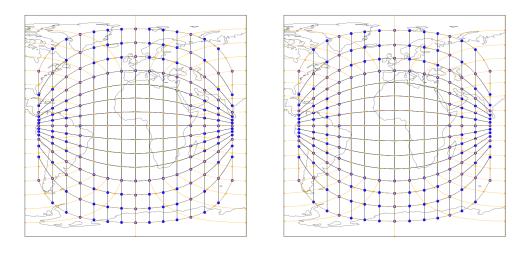
grid features on the solution (cf. eg., [27, 28, 23]), is a common problem that appears when using Platonic solid based spherical grids, and is highly undesirable due to its lack of physical meaning.

#### 234 2.5. Ghost cells

Currently, FV3 uses the cells of the adjacent panels as ghost cells, em-235 ploying an approach named kinked grid by [23]. This was the approach used 236 by [14], alongside with extrapolations to compute stencils at or close to a 237 cube edge. In this work, we shall use the extended grid lines of the cubed-238 sphere mapping to generate the ghost cells, in an approach named duo-grid 239 recently introduced by [24], as it uses the kinked grid values to fill the ex-240 tended grid values. This approach was recently exploited in FV3 by [23] and 241 helps to reduce grid imprinting, and it shall be considered in this work (see 242 data availability statement). This approach, however, has some scalability 243 issues for parallel computing that we discuss in Section 3.7. 244

The corner ghost cell points are generated by applying Equation (15) for *i* and *j* out of the range 0 to N+1. The other grid points are again computed by averaging the corner points, as in the interior grid points. Figure 4a show how the corner ghost points of the equiangular grid are aligned on common geodesics of the adjacent panels. This property has been known since the work of [20].

The extended grid alignment property is very useful because it allows us 251 to use 1D Lagrange interpolation to estimate the function values at the ghost 252 cells using function values from neighboring panels, and it has been widely 253 used in the literature [29, 30, 31, 32, 33, 24]. A complete description of this 254 process has been provided by [34]. However, the analogous property does not 255 hold for the equi-edge grid. To address this problem, [24] proposes modifying 256 the ghost values of the x and y coordinates by mirroring certain points. This 257 generates the new ghost points, aligning them on the same geodesic as those 258



(a) Extended equiangular grid. (b) Mirrored equi-edge grid.

Figure 4: Grid lines of panel 1, including ghost cells, for the extended equiangular grid (a) and the mirrored equi-edge grid (b). Corner ghost points are denoted by blue circles, and the corner interior points are denoted by orange points.

from the neighboring panel, as illustrated in Figure 4b. More formally, for  $g = 1, 2, ..., \nu$ , the mirrored values are given by:

$$\hat{x}_{-g+\frac{1}{2}} = \arctan\left(\frac{1}{a}\tan\left(-\frac{\pi}{2} - \arctan\left(a\tan x_{g+\frac{1}{2}}\right)\right)\right),\tag{22}$$

and  $\hat{x}_{N+g+\frac{1}{2}} = -\hat{x}_{-g+\frac{1}{2}}$  to replace  $x_{-g+\frac{1}{2}}, x_{N+g+\frac{1}{2}}$ , respectively. Similar formulas are used for the *y* component. To conclude this section, we note that this work will consider the duo-grid interpolation performed using cubic Lagrange interpolation in the numerical experiments presented in Section 4.

#### <sup>265</sup> 3. The conservative transport equation on the cubed-sphere

The goal of this section is to present and solve numerically the conservative transport equation on the cubed-sphere. We are going to consider the equi-edge or equiangular cubed-sphere mappings  $\Psi_p$  and their respective local coordinates (x, y). Once again, the metric term is denoted by  $\sqrt{\mathfrak{g}}_{\Psi}$  by  $\sqrt{\mathfrak{g}}$ for simplicity. Following [35], the transport model without sources or sinks <sup>271</sup> is considered:

$$[\partial_t \rho + \nabla \cdot (\rho \boldsymbol{u})](x, y, p, t) = 0, \qquad (23)$$

$$[\partial_t(\rho\phi) + \nabla \cdot (\rho\phi \boldsymbol{u})](x, y, p, t) = 0, \qquad (24)$$

for  $x, y \in [-a, a], t \in [0, T]$ , where T is the final time, **u** is the wind, u and 272 v are the contravariant wind components (Equation 9),  $\rho$  is the fluid density 273 and  $\phi$  is the tracer concentration. Additionally, for the transport model, it is 274 assumed that the initial conditions are given as  $\rho(x, y, p, 0) = \rho_0(x, y, p)$  and 275  $\phi(x, y, p, 0) = \phi_0(x, y, p)$ , given  $\rho_0$  and  $\phi_0$ . Equation (23) is the continuity 276 equation and Equation (24) is the conservative advection equation. In this 277 framework,  $\rho\phi$  represents the tracer density, and the total masses of  $\rho$  and 278  $\rho\phi$  are preserved. Therefore, these quantities are referred to as conserved 279 quantities. Higher-order moments of  $\rho$  and  $\rho\phi$  are also preserved; however, 280 this work focuses solely on the first moment, namely the mass, which is what 281 we mean by conserved in this context and what we aim to reproduce with 282 the numerical schemes investigated in this paper. 283

In the transport model, one can easily see that the tracer variable  $\phi$  is advected. That is,  $\phi$  satisfies the non-conservative advection equation:

$$[\partial_t \phi + \langle \boldsymbol{u}, \nabla \phi \rangle](x, y, p, t) = 0.$$
<sup>(25)</sup>

Equations (23) and (24) have the same form. Hence, it follows from the definition of the divergence operator in terms of the cubed-sphere mapping (Equation (12)) that the equation that needs to be solved may be uniquely expressed as:

$$[\partial_t(\sqrt{\mathfrak{g}}q) + \partial_x(u\sqrt{\mathfrak{g}}q) + \partial_y(v\sqrt{\mathfrak{g}}q)](x, y, p, t) = 0,$$
(26)

where  $q = \rho$  or  $q = \rho \phi$ . Additionally, it is assumed that q(x, y, p, 0) =290  $q_0(x, y, p)$  for some given  $q_0$ . Equation (26) is referred to as the conservative 291 transport equation. The goal now is to solve Equation (26), which will allow 292 for the solution of the transport model on the sphere. In the shallow-water 293 model, Equation (26) is satisfied for the fluid depth and the absolute vorticity. 294 For simplicity, the dependence on the panel p is omitted as the discussion 295 here does not depend on p. Initially, the time is discretized by introducing 296 the time step  $\Delta t = \frac{T}{N_T}$ , for some integer  $N_T > 0$ , and the discrete time 297 instants are given by  $t^n = n\Delta t$ , for  $n = 0, \ldots, N_T$ . We are particularly 298 interested in proposing a scheme that approximates the values of  $q(x_i, y_j, t^n)$ 299

for i, j = 1, ..., N and  $n = 1, ..., N_T$ , where the numerical approximation is denoted by  $q_{ij}^n$ . It is assumed, of course, that  $q_{ij}^0 = q(x_i, y_j, 0)$ .

Assuming that the values  $q_{ij}^n$  for i, j = 1, ..., N are given, we are going to use the dimension-splitting approach as discussed in [15] to obtain  $q_{ij}^{n+1}$ . Beforehand, the ghost cell interpolation method described in Section 2.5 is used on the grid function  $q^n$ , so the values  $q_{ij}^n$  for  $i, j = -\nu + 1, ..., N + \nu$ are obtained.

The scheme proposed by [15] is based on replacing the two-dimensional conservative transport equation (Equation (26)) by combining the solutions of the conservative transport equation when considering only the x direction and then separately when considering only the y direction. More precisely,  $N + 2\nu$  one-dimensional conservative transport equations in the x-direction are considered:

$$[\partial_t(\sqrt{\mathfrak{g}}q^x) + \partial_x(u\sqrt{\mathfrak{g}}q^x)](x, y_j, t) = 0, \qquad (27)$$

for  $j = -\nu + 1, \dots, N + \nu$ , and  $N + 2\nu$  one-dimensional conservative transport equations in the *y*-direction

$$[\partial_t(\sqrt{\mathfrak{g}}q^y) + \partial_y(v\sqrt{\mathfrak{g}}q^y)](x_i, y, t) = 0, \qquad (28)$$

for  $i = -\nu + 1, \ldots, N + \nu$ , using  $q_{ij}^n$  as initial data. Therefore, the solution to the 1D conservative transport equation needs to be specified. A finite-volume approach is going to be used to solve Equations (27) and (28), as described in the next subsection.

The goal now is to describe the details of the numerical method proposed 319 by [14], known as the FV3 scheme, currently used in FV3. In each part of 320 the FV3 method that will described, we will propose modifications aimed 321 at improvements. Additionally, the scheme proposed in this work is named 322 LT2. The justification for its name will be provided in the next sections, as 323 it utilizes an average of two Lie-Trotter splittings [36], along with a second-324 order Runge-Kutta method for the departure point equation that we shall 325 obtain soon. 326

## 327 3.1. The one-dimensional finite-volume discretization

This subsection is dedicated to describing the 1D finite-volume scheme for solving the conservative transport equation separately in the x and ydirections. The description here will only consider the conservative transport equation in the x direction (Equation 27), but everything here generalizes straightforwardly to the conservative transport equation in the y direction. For each  $j = -\nu + 1, \dots, N + \nu$  fixed, the following linear conservative transport equation in the conservative form is considered:

$$\begin{cases} [\partial_t(\sqrt{\mathfrak{g}}q) + \partial_x(u\sqrt{\mathfrak{g}}q)](x,t) = 0, \quad \forall (x,t) \in [-a,a] \times [0,T], \\ q(x,0) = q_0(x), \quad \forall x \in [-a,a]. \end{cases}$$
(29)

where the notation  $\sqrt{\mathfrak{g}}(x) = \sqrt{\mathfrak{g}}(x, y_j)$  and  $u(x, t) = u(x, y_j, t)$  are being used, along with the notations  $\sqrt{\mathfrak{g}}_i = \sqrt{\mathfrak{g}}(x_i, y_j)$  and  $u_{i+\frac{1}{2}}^n = u(x_{i+\frac{1}{2}}, y_j, t^n)$ . Furthermore, the dependence on j is omitted to ease notation. The average values in the x direction for the *i*-th cell are defined as:

$$\overline{(\sqrt{\mathfrak{g}}q)}_i(t) = \frac{1}{\Delta x} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} (\sqrt{\mathfrak{g}}q)(x,t) \, dx. \tag{30}$$

Following the finite-volume approach as in [37], Equation (29) is integrated in space on  $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$  followed by an integration in time on  $[t^n, t^{n+1}]$ , leading to the integral version of the conservative transport equation:

$$\overline{(\sqrt{\mathfrak{g}}q)}_{i}(t^{n+1}) = \overline{(\sqrt{\mathfrak{g}}q)}_{i}(t^{n}) - \frac{\Delta t}{\Delta x}\frac{\delta_{x}}{\Delta t}\left(\int_{t^{n}}^{t^{n+1}} (u\sqrt{\mathfrak{g}}q)(x_{i},t)\,dt\right),\tag{31}$$

 $\forall i = 1, \ldots, N, \forall n = 0, \ldots, N_T - 1 \text{ and } \delta_x \varphi(x_i) = \varphi(x_{i+\frac{1}{2}}) - \varphi(x_{i-\frac{1}{2}}), \text{ for any}$ 342 function  $\varphi$ . It is important to note that no approximations have been made 343 in Equation (31). Equation (31) needs to approximate the time-averaged 344 flux at the cell edges  $x_{i\pm\frac{1}{2}}$  to derive a finite-volume scheme. This flux, in 345 principle, requires knowledge of q over the entire interval  $[t^n, t^{n+1}]$ . To over-346 come this, the temporal integral is expressed as a spatial integral at time  $t^n$ . 347 This approach avoids the need for information about q throughout the entire 348 interval  $[t^n, t^{n+1}]$ . Furthermore, this spatial integral domain is closely related 349 to the definition of the departure point. 350

To introduce the definition of departure point, for each  $s \in [t^n, t^{n+1}]$ , the following Cauchy problem backward in time is introduced:

$$\begin{cases} \partial_t x_{i+\frac{1}{2}}^d(t,s) = u\left(x_{i+\frac{1}{2}}^d(t,s),t\right), & t \in [t^n,s] \\ x_{i+\frac{1}{2}}^d(s,s) = x_{i+\frac{1}{2}}. \end{cases}$$
(32)

The point  $x_{i+\frac{1}{2}}^d(t^n, s)$  is called departure point at time  $t^n$  of the point  $x_{i+\frac{1}{2}}$ at time s. In Theorem 1 from Appendix C, it is shown that:

$$\int_{t^n}^{t^{n+1}} (u\sqrt{\mathfrak{g}}q)(x_{i+\frac{1}{2}},s) \, ds = \int_{x_{i+\frac{1}{2}}^d(t^n,t^{n+1})}^{x_{i+\frac{1}{2}}} (\sqrt{\mathfrak{g}}q)(x,t^n) \, dx. \tag{33}$$

Therefore, replacing Equation (33) in Equation (31), it is clear that at each 355 time step, the values of  $\overline{(\sqrt{\mathfrak{g}}q)}_i(t^{n+1})$  are computed based on  $\overline{(\sqrt{\mathfrak{g}}q)}_i(t^n)$  and 356 the integrals of  $(\sqrt{\mathfrak{g}}q)(x,t^n)$  over specific intervals that are defined by the 357 departure points. To perform these computations, the departure points from 358 the edges of all control volumes are needed to calculate the required integrals. 359 This idea serves as the motivation for defining finite-volume Semi-Lagrangian 360 schemes, also known as flux-form Semi-Lagrangian schemes, as explored by 361 [15]. The idea of deriving a scheme by obtaining formulas for integrals with 362 domains that depend on departure points has also been explored in one 363 dimension, albeit somewhat differently, in [38, 39]. These schemes involve 364 estimating the departure points and reconstructing the function  $\sqrt{\mathfrak{g}}q$  at time 365  $t^n$  using their average values  $(\sqrt{\mathfrak{g}}q)_i(t^n)$ , which enables the computation of 366 the necessary integrals. Therefore, this serves as motivation to look for a 367 scheme of the form: 368

$$\overline{(\sqrt{\mathfrak{g}}q)}_{i}^{n+1} = \overline{(\sqrt{\mathfrak{g}}q)}_{i}^{n} - \frac{\Delta t}{\Delta x} \bigg( F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} \bigg), \tag{34}$$

369 for i = 1, ..., N, where

$$F_{i+\frac{1}{2}} = \frac{1}{\Delta t} \int_{\tilde{x}_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}} (\widetilde{\sqrt{\mathfrak{g}q}})(x, t^n) \, dx, \tag{35}$$

is the numerical flux, where  $(\sqrt{\mathfrak{g}q})$  is a subgrid reconstruction function of  $\sqrt{\mathfrak{g}q}$ 370 using the average values  $\overline{(\sqrt{\mathfrak{g}}q)}_i^n$  and  $\tilde{x}_{i+\frac{1}{2}}^n$ , which is the estimated departure 371 point obtained by solving numerically Equation (32). Since the Courant-372 Friedrichs-Lewy (CFL) condition is assumed in this work, this integral shall 373 be constrained to a single cell, namely  $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$  or  $[x_{i+\frac{1}{2}}, x_{i+\frac{3}{2}}]$ , as will be 374 discussed in detail in Section 3.3. This scheme allows for the use of large time 375 steps, as discussed in [15, 40], but it is not considered in this work, since the 376 FV3 discretization assumes the CFL condition. 377

In practice, the scheme from Equation (34) is replaced by using the midpoint rule for integration, that is  $\overline{(\sqrt{\mathfrak{g}}q)}_i^n \approx q_i^n \sqrt{\mathfrak{g}}_i$ , and therefore the scheme becomes a method to update cell center values, namely:

$$q_i^{n+1} = q_i^n - \frac{\Delta t \Delta y}{|\hat{\Omega}_{ij}|} \left( F_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} \right), \tag{36}$$

where we used Equation (21).

382 3.2. One-dimensional departure point computation

Integrating Equation (32) over the interval [t, s], yields:

$$x_{i+\frac{1}{2}}^{d}(t,s) = x_{i+\frac{1}{2}} - \int_{t}^{s} u\left(x_{i+\frac{1}{2}}^{d}(\theta,s),\theta\right) d\theta.$$
(37)

Therefore, the estimated departure point, denoted by  $\tilde{x}_{i+\frac{1}{2}}^n$ , takes the form:

$$\tilde{x}_{i+\frac{1}{2}}^{n} = x_{i+\frac{1}{2}} - \tilde{u}_{i+\frac{1}{2}}^{M} \Delta t, \qquad (38)$$

where M stands for the employed method. When the FV3 method is used, M = FV3; when the proposed scheme is used, M = LT2. This notation shall be used for the remainder of this work.

One possible way to estimate the departure point, which is used in FV3, is:

$$\tilde{u}_{i+\frac{1}{2}}^{FV3} = u_{i+\frac{1}{2}}^{n+\frac{1}{2}},\tag{39}$$

<sup>390</sup> which leads to a first-order accurate scheme in time.

To achieve second-order accuracy in time, a second-order Runge-Kutta (RK2) method may be employed to integrate Equation (32). Following [41], this scheme results in:

$$\tilde{u}_{i+\frac{1}{2}}^{LT2} = \begin{cases} \left(1 - \alpha_{i+\frac{1}{2}}^{n}\right)u_{i+\frac{1}{2}}^{n+\frac{1}{2}} + \alpha_{i+\frac{1}{2}}^{n}u_{i-\frac{1}{2}}^{n+\frac{1}{2}} & \text{if } u_{i+\frac{1}{2}}^{n} \ge 0, \\ -\alpha_{i+\frac{1}{2}}^{n}u_{i+\frac{3}{2}}^{n+\frac{1}{2}} + \left(1 + \alpha_{i+\frac{1}{2}}^{n}\right)u_{i+\frac{1}{2}}^{n+\frac{1}{2}} & \text{if } u_{i+\frac{1}{2}}^{n} < 0, \end{cases}$$
(40)

where

$$\alpha_{i+\frac{1}{2}}^n = \frac{u_{i+\frac{1}{2}}^n \Delta t}{2\Delta x}$$

Notice that, in order for the linear interpolation of Equation (40) to make 394 sense, it is necessary to ensure that  $|\alpha_{i+\frac{1}{2}}^n| \in [0,1]$ . This requirement is 395 particularly fulfilled when the Courant number is less than one, as discussed 396 in Section 3.3. The LT2 scheme requires the wind at two time levels, while 397 FV3 uses only one time level. Since this work performs simulations with 398 prescribed winds, it is assumed that the wind is known at time levels n and 390  $n+\frac{1}{2}$ . However, in the FV3 shallow-water solver, the C-grid step first takes 400 the D-grid wind and convert it to a C-grid wind at time level n, and then 401 the C-grid wind at the time level  $n + \frac{1}{2}$  is computed. Therefore, considering 402 the horizontal solver, the LT2 scheme will use information that is already 403 available by the shallow-water solver. 404

#### 405 3.3. The time-averaged and upwind Courant number

In order to compute the integral in Equation (35), it will be useful to introduce the time-averaged Courant number at the edges. This integral in FV3 is expressed in terms of this number. For the LT2 scheme, the Courant number at the edges is defined naturally as

$$\tilde{c}_{i+\frac{1}{2}}^{LT2} = \tilde{u}_{i+\frac{1}{2}}^{LT2} \frac{\Delta t}{\Delta x} = \tilde{u}_{i+\frac{1}{2}}^{LT2} \frac{\Delta t}{l_{i+\frac{1}{2}}^x},\tag{41}$$

where  $\tilde{u}_{i+\frac{1}{2}}^{LT2}$  is just a normalization of  $\tilde{u}_{i+\frac{1}{2}}^{LT2}$  (Equation (11)). FV3, on the other hand, uses the upwind Courant number approach from [42], namely:

$$c_{i+\frac{1}{2}}^{FV3} = \tilde{\mathbf{u}}_{i+\frac{1}{2}}^{FV3} \frac{\Delta t}{l_{i+\frac{1}{2}}^{x,*}},\tag{42}$$

412 where

$$l_{i+\frac{1}{2}}^{x,*} = \begin{cases} l_i^x, & \text{if } \tilde{\mathbf{u}}_{i+\frac{1}{2}}^{FV3} \ge 0, \\ l_{i+1}^x, & \text{if } \tilde{\mathbf{u}}_{i+\frac{1}{2}}^{FV3} < 0. \end{cases}$$
(43)

<sup>413</sup> Then Equation (38) may is expressed in terms of the Courant number as:

$$\tilde{x}_{i+\frac{1}{2}}^{n} = x_{i+\frac{1}{2}} - \tilde{c}_{i+\frac{1}{2}}^{M} \Delta x, \qquad (44)$$

where M = FV3 or M = LT2. It is easy to see that assuming the absolute value of the Courant number is less than one, then  $\tilde{x}_{i+\frac{1}{2}}^n \in [x_{i+\frac{1}{2}}, x_{i+\frac{3}{2}}]$  if  $\tilde{c}_{i+\frac{1}{2}}^M$ is positive, and  $\tilde{x}_{i+\frac{1}{2}}^n \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$  otherwise. Then, as mentioned earlier before, the integral of Equation (35) is constrained to a single control-volume under the CFL condition. Also, the upwind approach of the numerical flux becomes clear at this point.

#### 420 3.4. PPM reconstruction

<sup>421</sup> Now that the computation of the departure points has been addressed,
<sup>422</sup> the next step is to describe the subgrid reconstruction process, which allows
<sup>423</sup> the evaluation of the flux in Equation (35).

In FV3, it is assumed that the metric  $\sqrt{\mathfrak{g}}$  appearing in Equation (35) is constant over the integration domain, specifically equal to  $\sqrt{\mathfrak{g}}_{i+\frac{1}{2}}$ , hence only q needs to be reconstructed instead of  $\sqrt{\mathfrak{g}}q$ . This implies the following approximation in Equation (45):

$$\int_{x_{i+\frac{1}{2}}^{d}(t^{n},t^{n+1})}^{x_{i+\frac{1}{2}}} (\sqrt{\mathfrak{g}}q)(x,t^{n}) \, dx = \sqrt{\mathfrak{g}}_{i+\frac{1}{2}} \int_{x_{i+\frac{1}{2}}^{d}(t^{n},t^{n+1})}^{x_{i+\frac{1}{2}}} q(x,t^{n}) \, dx + \mathcal{O}(\Delta x).$$
(45)

The scheme proposed in this work, on the other hand, considers the reconstruction of  $\sqrt{\mathfrak{g}}q$ , avoiding the approximation in Equation (45). The reconstruction employed here for both the FV3 and LT2 schemes uses the PPM scheme from [21, 22]. We introduce the grid function  $q^M$  expressed as:

$$q^{M} = \begin{cases} q^{n}, & \text{if } M = \text{FV3}, \\ \sqrt{\mathfrak{g}}q^{n}, & \text{if } M = \text{LT2}. \end{cases}$$
(46)

Following [8], the PPM reconstruction on the *i*-th cell for a grid function  $q^M$ may be expressed as:

$$\widetilde{q^{M}}(x) = \widetilde{q_{i}^{M}}(x) = a_1 + a_2 \left(\frac{x - x_{i-\frac{1}{2}}}{\Delta x}\right) + a_3 \left(\frac{x - x_{i-\frac{1}{2}}}{\Delta x}\right)^2, \quad (47)$$

434 for  $x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ , where

$$a_1 = q_{L,i}^M, \quad a_2 = -(4b_{L,i}^M + 2b_{R,i}^M), \quad a_3 = 3(b_{L,i}^M + b_{R,i}^M),$$
 (48)

435 where the following perturbation values of  $q_i^M$  named by [8] are introduced

$$b_{L,i}^M = q_{L,i}^M - q_i^M, \quad b_{R,i}^M = q_{R,i}^M - q_i^M,$$
(49)

and  $q_i^M$  are the average or centroid values at the *i*-th cell. It is easy to see that integrating Equation (47) on  $x \in [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$  gives  $q_i^M \Delta x$ , therefore the PPM reconstructions preserves the mass on each cell. It is also easy to see that:

$$\lim_{x \to x^+_{i-\frac{1}{2}}} q^M(x) = q^M_{L,i}, \quad \lim_{x \to x^-_{i+\frac{1}{2}}} q^M(x) = q^M_{R,i}.$$
(50)

Therefore, the values  $q_{L,i}^M$  and  $q_{R,i}^M$  should approximate  $q_{i-\frac{1}{2}}^M$  and  $q_{i+\frac{1}{2}}^M$ , respectively. Furthermore, we consider:

$$q_{R,i}^{M} = \begin{cases} q_{R,i}, & \text{if } M = \text{FV3}, \\ \sqrt{\mathfrak{g}}_{i+\frac{1}{2}}q_{R,i}, & \text{if } M = \text{LT2}, \end{cases}$$
(51)

and similarly to  $q_{L,i}^M$ , where  $q_{L,i}$  and  $q_{R,i}$  should approximate  $q_{i-\frac{1}{2}}^n$  and  $q_{i+\frac{1}{2}}^n$ , respectively. One possible way of doing this approximation is by employing a reconstruction method based on primitive functions [37, Chapter 17]. For instance, [21] uses

$$q_{R,i} = \frac{7}{12} \left( q_{i+1}^n + q_i^n \right) - \frac{1}{12} \left( q_{i+2}^n + q_{i-1}^n \right), \tag{52}$$

and  $q_{L,i} = q_{R,i-1}$  for the unlimited PPM reconstruction. This formula is fourth-order accurate if the exact average values are used and second-order accurate if the centroid values are used. This scheme is referred to as UNLIM. This work also considers the monotonic scheme outlined in [9, Appendix B], where the values of  $q_{L,i}$  and  $q_{R,i}$  are determined by equations B3 and B4 in the same appendix. This scheme is referred to as MONO. Finally, both UNLIM and MONO schemes require  $\nu = 3$  layers of ghost cells.

#### 453 3.5. Numerical flux

Now that the computation of the departure points and the subgrid reconstruction has been addressed, the goal is to integrate the PPM approximation (Equation (47)) in a domain from the departure points (Equation (44)) to the cell edge  $x_{i+\frac{1}{2}}$  to obtain the numerical flux (Equation (35)). The PPM flux is defined by:

$$\mathcal{F}_{i+\frac{1}{2}}^{PPM}(q^{M}; \tilde{c}^{M}) = \frac{1}{\tilde{c}_{i+\frac{1}{2}}^{M} \Delta x} \int_{x_{i+\frac{1}{2}} - \tilde{c}_{i+\frac{1}{2}}^{M} \Delta x}^{x_{i+\frac{1}{2}} - \tilde{c}_{i+\frac{1}{2}}^{M} \Delta x} \widetilde{q^{M}}(x) \, dx \tag{53}$$

$$= \begin{cases} q_{i-1}^{M} + (1 - \tilde{c}_{i+\frac{1}{2}}^{M})(b_{L,i}^{M} - \tilde{c}_{i+\frac{1}{2}}^{M})(b_{L,i}^{M} + b_{R,i}^{M}), & \text{if } \tilde{c}_{i+\frac{1}{2}}^{M} > 0, \\ q_{i}^{M} + (1 + \tilde{c}_{i+\frac{1}{2}}^{M})(b_{L,i+1}^{M} + \tilde{c}_{i+\frac{1}{2}}^{M})(b_{L,i+1}^{M} + b_{R,i+1}^{M}), & \text{if } \tilde{c}_{i+\frac{1}{2}}^{M} \le 0, \end{cases}$$
(54)

for i = 0, ..., N. Recall that the FV3 scheme assumes that the metric term is constant over the integration domain in the numerical flux evaluation (Equation (35)), being equal to  $\sqrt{\mathfrak{g}}_{i+\frac{1}{2}}$ . Therefore, the numerical flux is given by:

$$F_{i+\frac{1}{2}}(q^{M}, \tilde{c}^{M}) = \frac{\Delta x}{\Delta t} \begin{cases} \tilde{c}_{i+\frac{1}{2}}^{FV3} \sqrt{\mathfrak{g}}_{i+\frac{1}{2}} \mathcal{F}_{i+\frac{1}{2}}^{PPM}(q^{n}, \tilde{c}^{FV3}), & \text{if } M = \text{FV3}, \\ \tilde{c}_{i+\frac{1}{2}}^{LT2} \mathcal{F}_{i+\frac{1}{2}}^{PPM}(\sqrt{\mathfrak{g}}q^{n}, \tilde{c}^{LT2}), & \text{if } M = \text{LT2}. \end{cases}$$
(55)

<sup>463</sup> It shall be useful to express Equation (36) as follows,

$$q_i^{n+1} = q_i^n + \mathbf{F}_i^M(q^M, \tilde{c}^M), \tag{56}$$

464 where

$$\mathbf{F}_{i}^{M}(q^{M}, \tilde{c}^{M}) = -\frac{1}{|\hat{\Omega}_{ij}|} \left[ \mathcal{A}_{i+\frac{1}{2}}^{M} \mathcal{F}_{i+\frac{1}{2}}^{PPM}(q^{M}, \tilde{c}^{M}) - \mathcal{A}_{i-\frac{1}{2}}^{M} \mathcal{F}_{i-\frac{1}{2}}^{PPM}(q^{M}, \tilde{c}^{M}) \right], \quad (57)$$

465 and

$$\mathcal{A}_{i+\frac{1}{2}}^{M} = \begin{cases} \Delta x \Delta y \sqrt{\mathfrak{g}}_{i+\frac{1}{2}} \tilde{c}_{i+\frac{1}{2}}^{FV3}, & \text{if } M = \text{FV3}, \\ \Delta x \Delta y \tilde{c}_{i+\frac{1}{2}}^{LT2}, & \text{if } M = \text{LT2}. \end{cases}$$
(58)

Equation (56) is how the 1D solver is implemented in the FV3 code (see data availability statement). Notice that by using Equation (7), it follows that Equation (58) may be rewritten as:

$$\mathcal{A}_{i+\frac{1}{2}}^{FV3} = \binom{l_{i+\frac{1}{2}}^x}{l_{i+\frac{1}{2}}^{x,*}} \Delta t l_{i+\frac{1}{2}}^y \sin \alpha_{i+\frac{1}{2}} \tilde{\mathbf{u}}_{i+\frac{1}{2}}^{FV3}, \tag{59}$$

and recalling the definition of  $l_{i+\frac{1}{2}}^{x,*}$  in Equation (43). In the current FV3 code, the term within parentheses (59) is ignored and assumed to be equal to one. Notice that if the scalar field  $q^n$  is constant equal to Q, the following property holds:

$$\mathbf{F}_{i}^{FV3}(Q,\tilde{c}^{FV3}) = -Q\frac{\Delta t}{\sqrt{\mathfrak{g}}_{i}\Delta x} \left[\sqrt{\mathfrak{g}}_{i+\frac{1}{2}}u_{i+\frac{1}{2}}^{n+\frac{1}{2}} - \sqrt{\mathfrak{g}}_{i-\frac{1}{2}}u_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right].$$
 (60)

This property essentially approximates the term  $\Delta t \partial_x (Q \sqrt{\mathfrak{g}} u) / \sqrt{\mathfrak{g}}$  by a cen-473 tered finite difference. This property shall be very useful to eliminate the 474 splitting error of a constant scalar field for a 2D splitting scheme and justi-475 fies the constant metric term assumption. Furthermore, this property ensures 476 the preservation of a constant scalar field when the wind is divergence free, 477 as highlighted in [15]. This characteristic is known as constancy preserving 478 or consistency in the literature, and ensures that the constant scalar field 479 remains unchanged in this case. For the LT2 scheme, this property does not 480 hold. However, the LT2 scheme ensures second-order accurate preservation 481

<sup>482</sup> of a constant field for divergence-free wind, as it is designed to be second<sup>483</sup> order in general. This will also be demonstrated in the numerical simulations
<sup>484</sup> in Section 4.

Finally, we point out that the 1D FV3 scheme is only first-order accurate 485 since it uses a first-order departure point and assumes a constant metric term 486 over the flux integration domains, while the LT2 scheme is second-order. 487 One could attempt to use RK2 in the departure point calculation in the FV3 488 scheme or refrain from using the constant metric term assumption. In both 489 cases, the property of Equation (60) would be broken, and this property is 490 essential for the elimination of the splitting error in the 2D scheme, as will 491 be explained in the next subsection. 492

#### 493 3.6. The two-dimensional splitting scheme

Now are ready to use the 1D PPM scheme to solve the 2D conserva-494 tive transport equation (Equation (26)). The grid functions  $\mathbf{F}_{ij}^{M}(q^{n}, \tilde{c}_{x}^{M})$ , and  $\mathbf{G}_{ij}^{M}(q^{n}, \tilde{c}_{y}^{M})$ , which represents the version of the PPM numerical update 495 496 (Equation (57)) in the x and y directions, are going to be considered to build 497 the 2D scheme. Additionally,  $\tilde{c}_x^M$  is the time-averaged Courant number as de-498 scribed in Section 3.3 in the x direction using u, and  $\tilde{c}_y^M$  is the time-averaged 499 Courant number in the y direction using v. For the PPM scheme employed in 500 this work (UNLIM and MONO, Section 3.4), the number of ghost cell layers 501 is  $\nu = 3$ . It is worth noting that the 1D scheme employed here could be 502 any one. For instance, in [43], 1D Semi-Lagrangian Discontinuous Galerkin 503 methods and a splitting strategy on the cubed-sphere are exploited. 504

Following [15], the transport equation is solved in the x direction:

$$q_{ij}^{x,n} = q_{ij}^n + \mathbf{F}_{ij}^M(q^n, \tilde{c}_x^M), \tag{61}$$

for i = 1, ..., N,  $j = \nu + 1, ..., N + \nu$ , and then the transport equation in the *y* direction with initial data  $q^{x,n}$  is solved:

$$q_{ij}^{yx,n} = q_{ij}^{x,n} + \mathbf{G}_{ij}^{M}(q^{x,n}, \tilde{c}_{y}^{M}),$$
(62)

for i, j = 1, ..., N. This procedure is also known as Lie-Trotter splitting in general operator splitting methods, and it leads to a first-order scheme at best [36]. Figure 5 illustrates the idea behind this process on a cubed-sphere panel.

Notice that this process may be repeated in the reverse order by solving the conservative transport equation, swapping the x and y directions, to

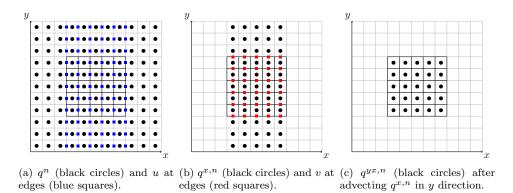


Figure 5: Illustration of the Lie-Trotter splitting on a cubed-sphere panel, where the  $\mathbf{F}^{M}$  operator is applied in the x direction (a) and then in the  $\mathbf{G}^{M}$  operator in the y direction. Interior cells are depicted using black lines, while ghost cells are depicted using gray lines. All the winds shown are the ones used in the FV3 departure point scheme. If the RK2 scheme is used for the departure point calculation, an additional layer of wind ghost values should be added at each boundary in (a) and (b).

obtain another solution  $q_{ij}^{xy,n}$ . Thus the average of the solutions is considered as the final approximation:

$$q^{n+1} = \frac{(q^{xy,n} + q^{yx,n})}{2},\tag{63}$$

<sup>516</sup> or more explicitly:

$$q^{n+1} = q^{n} + \frac{1}{2} \mathbf{F}^{M}(q^{n}, \tilde{c}_{x}^{M}) + \frac{1}{2} \mathbf{F}^{M}\left(q^{n} + \mathbf{G}^{M}(q^{n}, \tilde{c}_{y}^{M}), \tilde{c}_{x}^{M}\right) + \frac{1}{2} \mathbf{G}^{M}(q^{n}, \tilde{c}_{y}^{M}) + \frac{1}{2} \mathbf{G}^{M}\left(q^{n} + \mathbf{F}^{M}(q^{n}, \tilde{c}_{x}^{M}), \tilde{c}_{y}^{M}\right).$$
(64)

<sup>517</sup> This scheme is an average of two Lie-Trotter splitting and was one of the <sup>518</sup> splitting schemes investigated by [44], and it is second-order accurate pro-<sup>519</sup> vided the 1D subproblems are solved with at least second-order accuracy.

As discussed by [15], when the scalar field  $q^n$  is constant and the wind is divergent free, the scheme (64) introduces a splitting error. Aiming to eliminate the splitting error that arises in this situation, [15] proposes to  $_{523}$  consider a modification of the scheme (64) as:

$$q^{n+1} = q^{n} + \frac{1}{2} \mathbf{F}^{M}(q^{n}, \tilde{c}_{x}^{M}) + \frac{1}{2} \mathbf{F}^{M}\left(q^{n} + \mathbf{g}^{M}(q^{n}, \tilde{c}_{y}^{M}), \tilde{c}_{x}^{M}\right) + \frac{1}{2} \mathbf{G}^{M}(q^{n}, \tilde{c}_{y}^{M}) + \frac{1}{2} \mathbf{G}^{M}\left(q^{n} + \mathbf{f}^{M}(q^{n}, \tilde{c}_{x}^{M}), \tilde{c}_{y}^{M}\right),$$
(65)

where, **f** and **g** are called inner advection operators, designed to eliminate the splitting error that arises when the scalar field is constant and the wind is divergence-free. In particular, the inner advection operators of [14, 25] are considered. Their expressions are given by:

$$\mathbf{f}_{ij}^{\text{FV3}}(q^{n}, \tilde{c}_{x}^{\text{FV3}}) = -q_{ij}^{n} + \frac{q_{ij}^{n} + \mathbf{F}_{ij}^{\text{FV3}}(q^{n}, \tilde{c}_{x}^{\text{FV3}})}{1 + \mathbf{F}_{ij}^{\text{FV3}}(\mathbf{1}, \tilde{c}_{x}^{\text{FV3}})},$$
(66)

where, **1** is the constant grid function equal to one. The inner operator  $\mathbf{g}^{\text{FV3}}$ is defined similarly using  $\mathbf{G}^{\text{FV3}}$ . One can easily see that the splitting error is indeed eliminated for the constant scalar field and divergence-free wind when using the FV3 scheme. This happens because the FV3 scheme satisfies Equation (60).

The LT2 scheme does not satisfy Equation (60). Therefore, this scheme 533 considers simply  $\mathbf{f}^{\text{LT2}} = \mathbf{F}^{\text{LT2}}$  and  $\mathbf{g}^{\text{LT2}} = \mathbf{G}^{\text{LT2}}$ . Despite the elimination 534 of the splitting error for the constant scalar field and divergence free wind 535 will no longer hold, since the 1D LT2 scheme is second-order accurate, the 536 final LT2 scheme is expected to be second-order accurate, since it is given by 537 Equation (64). Although the 1D FV3 scheme is only first-order accurate, the 538 elimination property of the final FV3 scheme guarantees that it behaves as 539 second-order for divergence-free winds, as will be demonstrated in numerical 540 simulations. 541

We would like to point out that both FV3 and LT2 schemes, as they use 542 the PPM as the 1D solver, result in the final 2D schemes employing a C-grid 543 staggering, as named by [11], for the wind positions (Figure 2). The trans-544 ported quantity is located at the cell centers. Furthermore, both schemes 545 are written in flux-form, making them adequate for preserving total mass. 546 However, on the cubed-sphere, as pointed out by [29, 24, 23], the fluxes at 547 the cube edges are computed twice, potentially leading to a mismatch that 548 disrupts total mass conservation. To address this and ensure mass conser-549 vation, this work considers a simple average of the fluxes at the cube edges, 550 following the works mentioned before. 551

As pointed out in Figure 5, both FV3 and LT2 schemes require C-grid 552 contravariant wind components at ghost cells, with the LT2 scheme requiring 553 only an extra ghost cell layer at each boundary. These values may be obtained 554 similarly to the interpolation process described in Section 2.5, but conversions 555 from cube to latitude-longitude coordinates (Appendix B) are needed to 556 avoid the cubed-sphere discontinuity. The inverse transform is performed 557 after the interpolation is done. This process's details are highlighted in [23, 558 Section 2.3]. 559

Regarding the linear numerical stability of both schemes, we recall that 560 linear stability analysis is usually performed in a planar geometric framework. 561 therefore without metric terms and assuming a constant wind, in the so-called 562 frozen coefficients approach [45, p. 59]. In this scenario, it is easy to see that 563 both the FV3 and LT2 schemes are identical, and therefore, they have the 564 same linear stability properties. Specifically, they are stable if the maximum 565 absolute value of the Courant number in both x and y directions is less than 566 one, which follows from the stability analysis of [15] and [46]. 567

To concluded this section, the transport model described by Equations (23) and (24) may be solved using the scheme from Equation (65), applied considering  $q^n = \rho^n$  and  $q^n = (\rho\phi)^n$  simultaneously. In this framework, the tracer concentration is given by  $\phi^n = \frac{(\rho\phi)^n}{\rho^n}$ .

#### <sup>572</sup> 3.7. Computational efficiency and scalability

Both the FV3 and LT2 schemes reduce to the application of the formula 573 presented in Equation (65). This formula requires the computation of the 574 Courant numbers (see Section 3.3), evaluation of the coefficients in Equation 575 (3.3) in the x and y directions, and four PPM flux computations (recall 576 Equation (53)). At each time step, we first need to reconstruct the scalar 577 field at the ghost cell positions (see Figure 5) to apply both schemes. This 578 reconstruction is performed in this work using the duo-grid interpolation 579 described in Section 2.5. 580

The additional step required for the LT2 scheme is to apply the upwind 581 linear interpolation formula from Equation (40) for u, and similarly for v, 582 needed to compute the Courant numbers. The LT2 scheme utilizes winds 583 at time levels n and  $n + \frac{1}{2}$ , while the FV3 scheme employs winds only at 584 time levels  $n + \frac{1}{2}$  (see Equation (39)). Both schemes need to reconstruct the 585 velocity at the ghost cell points. Therefore, the LT2 scheme must reconstruct 586 the wind at the ghost cells for both time levels. However, the shallow-water 587 solver of FV3 developed by [10] employs a combination of C and D-grid 588

<sup>599</sup> approaches, using a half time step on a C-grid followed by a complete time <sup>590</sup> step on the D-grid. On the duo-grid framework, the winds at time level n<sup>591</sup> require duo-grid interpolation, as well as the winds at time level  $n + \frac{1}{2}$ , which <sup>592</sup> are obtained after the half time step on the C-grid. Hence, the LT2 scheme <sup>593</sup> will take advantage of information that has already been computed, with the <sup>594</sup> extra cost mainly arising from the upwind linear formula in Equation (40), <sup>595</sup> having the same number of duo-grid interpolations as the FV3 scheme.

The major drawback of the approach described here is the duo-grid in-596 terpolation. As pointed out by [24, 23], the duo-grid interpolation brings the 597 benefits of reducing grid imprinting but comes at the cost of adding overhead 598 for parallel computations, which affects scalability on high-performance com-599 puting. Additionally, as we discussed in Section 3.6, this approach requires 600 a flux average at the original cube edges, which, as noted by [24], demands 601 more MPI communications. Optimizing the code of [23] and exploring dif-602 ferent ways of fixing the mass at the cube edges is ongoing work. 603

## 604 4. Numerical experiments

In this section, the goal is to present simulations of the numerical solu-605 tion of the transport model, governed by Equations (23) and (24), utilizing 606 the FV3 and LT2 schemes. The duo-grid interpolation described in Section 607 [2.5 to compute the ghost cell values is performed using cubic interpolation. 608 As mentioned earlier, the tracer concentration  $\phi$  is advected in the trans-609 port model. To specify the simulation, including the initial condition for 610 the tracer concentration  $\phi_0$ , the zonal wind component denoted by  $u_{\lambda}$ , and 611 the meridional wind component denoted by  $v_{\theta}$ , need to be defined. The 612 conversion from these wind components to cubed-sphere contravariant wind 613 components (Equation (9)) is detailed in Appendix B. 614

The initial density  $\rho$  is assumed to be equal to one for all tests. For all simulations presented here it is adopted  $R = 6.371 \times 10^6$  meters, equivalent to the Earth's radius. The final integration time is set to  $T = 12 \times 86400$ seconds, equivalent to 12 days.

To compute convergence, cubed-sphere grids with values of  $N_k = 48 \times 2^k$ and time steps  $\Delta t^{(k)} = \frac{\Delta t^{(0)}}{2^k}$  for  $k = 0, \ldots, 4$  are considered, where the value of  $\Delta t^{(0)}$  will be specified for each test case. The *p*-norm,  $p \ge 1$ , for a cubed-sphere grid function  $q_{ijm}$  is defined as:

$$\|q\|_{p} = \begin{cases} \left(\sum_{m=1}^{6} \sum_{i,j=1}^{N} |q_{ijm}|^{p} |\Omega_{ij}|\right)^{\frac{1}{p}} & \text{if } 1 \le p < \infty, \\ \max_{i,j=1,\dots,N,m=1,\dots,6} |q_{ijm}| & \text{if } p = \infty. \end{cases}$$
(67)

<sup>623</sup> The relative error in the *p*-norm are computed as:

$$E_p^{(k)} = \frac{\|q^{\text{REF}} - q\|_p}{\|q^{\text{REF}}\|_p},$$
(68)

for k = 0, ..., 4, where  $q^{\text{REF}}$  is the reference solution. In particular, p = 2(corresponding to the  $L_2$  error) and  $p = \infty$  (corresponding to the  $L_{\infty}$  error) are considered for the tracer concentration, where  $q = \phi$ . The order of convergence is computed as

order = 
$$\ln\left(\frac{E_4}{E_3}\right)\frac{1}{\ln 2}$$
. (69)

628 4.1. Rotated zonal wind experiments

622

In this section, the following rotated zonal wind field based on [47] is considered:

$$\begin{cases} u_{\lambda}(\lambda,\theta,t) = u_0(\cos(\theta)\cos(\alpha) + \sin(\theta)\cos(\lambda)\sin(\alpha)), \\ v_{\theta}(\lambda,\theta,t) = -u_0\sin(\lambda)\sin(\alpha), \end{cases}$$
(70)

where  $\lambda \in [-\pi, \pi]$  represents longitude and  $\theta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$  represents latitude. 631 It is easy to see that the this wind is divergence free. The parameter  $\alpha$  is 632 the rotation angle. Following [14], the rotation angle is set as  $\alpha = \frac{\pi}{4}$  so 633 that the wind is oriented with the cube corners. Finally, the parameter  $u_0$  is 634 defined as  $u_0 = \frac{2\pi R}{T}$ . With this choice, the simulation period is 12 days. The 635 solution should converge to the initial condition after this period, enabling 636 us to compute the final error. Therefore, the temporal evolution of the error 637 may be analyzed. For an expression of the exact solution in this case and a 638 general initial condition, refer to [48, Theorem 5.1, p. 155]. The time step 639 for N = 48 is given by  $\Delta t^{(0)} = 3600$  seconds, leading to a Courant number 640 of approximately 0.95. 641

Initially, the initial condition is given by the following Gaussian hill at a cube corner:

$$\phi_0(P) = \exp(-b_0((p_x - p_x^0)^2 + (p_y - p_y^0)^2 + (p_z - p_z^0)^2)), \tag{71}$$

for  $P \in \mathbb{S}_R^2$ . It is considered  $p_x^0 = p_y^0 = p_z^0 = \frac{1}{\sqrt{3}}$  and  $b_0 = 10$ . Therefore, the Gaussian hill is indeed centered at a cube corner. Hence, in this test, the Gaussian hill is translated over 4 cube corners, enabling the assessment of the schemes' sensitivity to these corners.

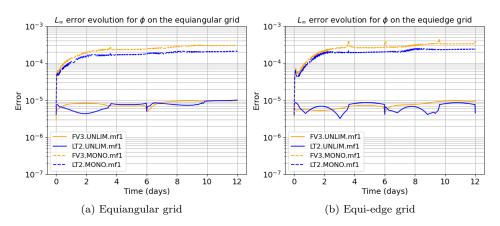


Figure 6: The  $L_{\infty}$  error evolution for the tracer concentration  $\phi$  in the transport model with a Gaussian hill as the initial condition using the rotated zonal wind is illustrated on the equiangular (a) and on the equi-edge (b) grids for 12 days and N = 768. Blue lines indicate the use of the LT2 scheme, while orange lines represent the FV3 scheme. Solid lines represent the results with the unlimited PPM (UNLIM) scheme, whereas dashed lines represent the results with the monotonic (MONO).

647

In fact, Figure 6 shows how the error evolves with time over 12 days in the 648  $L_{\infty}$  norm for N = 768 for both equi-edge and equiangular grids. This Figure 649 use orange lines to represent the FV3 scheme and blue lines to represent 650 the LT2 scheme. Dashed lines represent the monotonic while solid lines 651 represent the unlimited PPM. From Figure 6 some small spikes are observed 652 in the  $L_{\infty}$  error on the equi-edge grid (Figure 6b) when using both schemes 653 with MONO, which is less pronounced on the equiangular grid (Figure 6a). 654 On the equi-edge grid (Figure 6b), the spikes are less pronounced for the LT2 655 scheme. 656

Figure 7 illustrates the final error at a cube corner for the equi-edge grid. Similar results are obtained for the equiangular grid, but are omitted here. It is clear that the errors for the FV3 scheme are larger at the corners (Figure 7a) compared to the corner errors of the LT2 scheme (Figure 7b), being almost 1.6 times bigger.

662

Finally, Figures 8 and 9 show the error convergence in  $L_{\infty}$  and  $L_2$  norms.

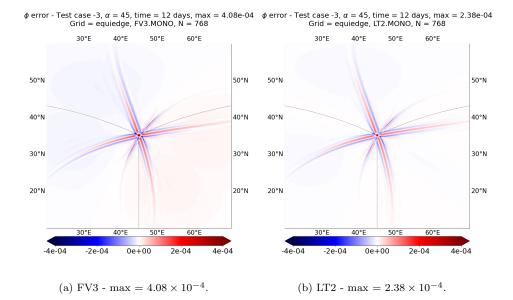


Figure 7: Errors at a cube corner after 12 days of the tracer concentration  $\phi$  in the transport model for the test case using the Gaussian hill and the rotated zonal wind, employing the monotonic scheme (MONO) with FV3 (a) and LT2 schemes (b) on the equi-edge grid with N = 768.

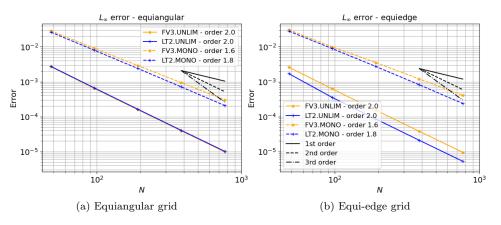


Figure 8:  $L_{\infty}$  error convergence for the tracer concentration  $\phi$  in the transport model using the Gaussian hill as the initial condition and the rotated zonal wind on the equiangular (a) and on the equi-edge (b) grids after 12 days. Blue lines indicate the use of the LT2 scheme, while orange lines represent the FV3 scheme. Solid lines represent the results with the unlimited PPM (UNLIM) scheme, whereas dashed lines represent the results with the monotonic PPM (MONO).

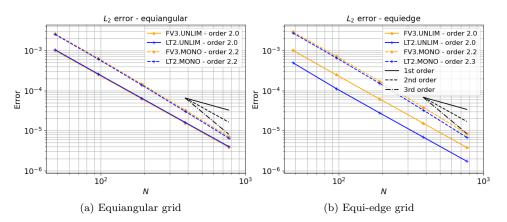


Figure 9: As Figure 8 but using  $L_2$  norm.

It can be observed that all schemes with the unlimited PPM (UNLIM) 663 achieve second-order accuracy as expected. However, for MONO, the or-664 der is reduced, which is also expected. Additionally, it is observed that 665 MONO with LT2 has smaller errors when comparing the blue dashed lines 666 with the orange dashed lines, for both  $L_{\infty}$  and  $L_2$  norms on both equian-667 gular (a) and the equi-edge (b) grid, indicating that LT2 is slightly more 668 accurate. In general, the errors of the equi-edge are slightly smaller than 669 those of equiangular. 670

To assess the difference between the UNLIM and MONO schemes for both FV3 and LT2 schemes, the slotted cylinder from [35] centered a cube corner is considered. To define the slotted cylinder, it is introduced

$$r(\lambda,\theta) = 2R \arcsin\left(\sqrt{\sin^2\left(\frac{\theta-\theta_0}{2}\right) + \cos\theta\cos\theta_0\cos^2\left(\frac{\lambda-\lambda_0}{2}\right)}\right), \quad (72)$$

where r is the geodesic distance from  $(\lambda, \theta)$  to a cube corner fixed point ( $\lambda_0, \theta_0$ ) with  $\lambda_0 = \frac{\pi}{4}, \ \theta_0 = \frac{\pi}{2} - \arccos\left(\frac{1}{\sqrt{3}}\right)$ . The slotted cylinder is defined as:

$$\phi(\lambda,\theta) = \begin{cases} 0.1, & \text{if } r(\lambda,\theta) > r_0, \\ 0.1, & \text{if } r(\lambda,\theta) \le r_0, \\ 1, & \text{otherwise,} \end{cases} \quad |\lambda - \lambda_0| \ge 0.05, \quad \theta \ge \theta_0, \tag{73}$$

677 where  $r_0 = \frac{R}{3}$ .

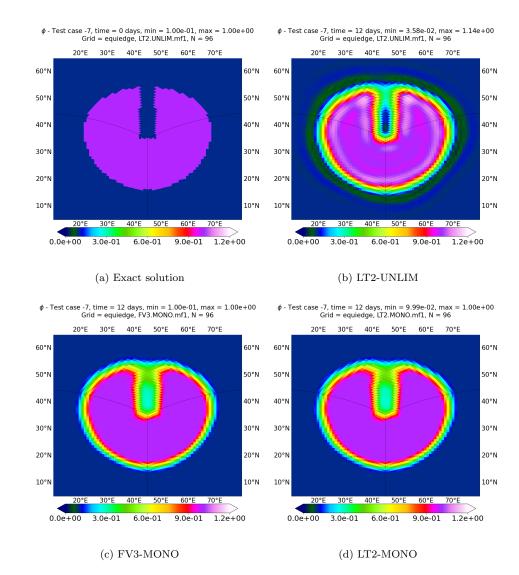


Figure 10: Advection of a cylinder at corner, representing the tracer concentration  $\phi$ , with N = 96 after 12 days for the schemes FV3-MONO (a), LT2-MONO (b), LT2-UNLIM (c) at the equi-edge grid and the exact solution (d).

The slotted cylinder is depicted in Figure 10a. The goal is to test MONO's ability to remove numerical oscillations, which create new extrema, in the case of advecting a cylinder. Similar to the Gaussian hill case, the cylinder is translated through 4 cube corners in this test. Figure 10 presents the results for the MONO scheme with both FV3 (Figure 10c) and LT2 (Figure 10d) schemes on the equi-edge grid with N =96. Result for UNLIM with LT2 are show in Figure 10b. Similar results with the FV3 scheme for UNLIM are obtained and omitted here. The initial cylinder is depicted in Figure 10a. It is observed that the MONO scheme effectively removes the oscillations present in the UNLIM results. Similar results for the equiangular grid are obtained and omitted here.

As we pointed out in Section 3.5, the FV3 scheme satisfies the constancy-689 preserving property, while the LT2 scheme does not. Therefore, in Table 690 3, we present the  $L_{\infty}$  errors after 12 days for the density  $\rho$  in the rotated 691 zonal wind experiment for both equiangular and equi-edge grids, considering 692 the LT2-UNLIM scheme. This allows us to measure the magnitude of the 693 error for the constant scalar, noting that  $\rho$  is initialized with the value 1 at 694 every point. It is clear from Table 3 that the LT2-UNLIM scheme achieves 695 second-order accuracy with the equi-edge grid. Furthermore, in the equian-696 gular grid, we observe that the errors approach third-order accuracy, sur-697 passing expectations. Therefore, although the LT2 scheme does not have the 698 constancy-preserving property, it solves the constant scalar field accurately 699 for this test case.

Table 3: Comparison of  $L_{\infty}$  errors for the density  $\rho$  after 12 fays in the rotated zonal wind test case using LT2-UNLIM. The table presents  $L_{\infty}$  error values for density  $\rho$  after 12 days, with a comparison between equiangular and equi-edge grids. The error ratios are computed as the ratios of successive errors,  $E_{\infty}^{k+1}/E_{\infty}^{k}$ , for  $k = 0, \ldots, 3$ , as detailed in Equation (68).

N	Equiangular		Equi-edge	
1 1 1	$L_{\infty}$ error	Ratio	$L_{\infty}$ error	Ratio
48	$5.06 \times 10^{-5}$	-	$6.02 \times 10^{-4}$	-
96	$6.42 \times 10^{-6}$	8.10	$1.42 \times 10^{-4}$	4.23
192	$8.31 \times 10^{-7}$	7.50	$3.47 \times 10^{-5}$	4.09
384	$1.08 \times 10^{-7}$	7.69	$8.58 \times 10^{-6}$	4.04
768	$1.40 \times 10^{-8}$	7.71	$2.14\times10^{-6}$	4.00

700

### 701 4.2. Flow deformation through a divergence free wind

The divergence free deformational test case from [35] is considered, where the time-dependent winds are given by

$$\begin{cases} u_{\lambda}(\lambda,\theta,t) = u_0 \sin^2(\lambda_p) \sin(2\theta) \cos(\frac{\pi t}{T}) + u_0 \cos\theta, \\ v_{\theta}(\lambda,\theta,t) = u_0 \sin(2\lambda_p) \cos(\theta) \cos(\frac{\pi t}{T}), \end{cases}$$
(74)

where  $\lambda_p = \lambda - \frac{2\pi t}{T}$  and  $u_0 = \frac{2\pi R}{T}$ . As pointed out in [35], a zonal background is added in  $u_{\lambda}$ , namely  $u_0 \cos \theta$ , to avoid error cancellations. The time step for N = 48 is adopted as  $\Delta t^{(0)} = 1600$  seconds, leading to a Courant number of approximately 0.73.

As the initial condition, two Gaussian hills are considered, each one centered on a cube-edge. Specifically,

$$\phi_0(P) = \exp(-b_0[(p_x - p_x^0)^2 + (p_y - p_y^0)^2 + (p_z - p_z^0)^2]) + \exp(-b_0[(p_x - p_x^1)^2 + (p_y - p_y^1)^2 + (p_z - p_z^1)^2]),$$
(75)

for  $P \in \mathbb{S}_R^2$ . Here  $(p_x^0, p_y^0, p_z^0)$  and  $(p_x^1, p_y^1, p_z^1)$  are the  $\mathbb{R}^3$  coordinates of the latitude-longitude points  $(\lambda_1, \theta_1) = (-\frac{\pi}{4}, 0)$  and  $(\lambda_2, \theta_2) = (\frac{\pi}{4}, 0)$ , respectively. The parameter  $b_0$  is set as  $b_0 = 5$ .

This test deforms the Gaussian hills, without creating new extrema on the fluid density since the wind is divergence free, and the final solution is equal to the initial condition. Figures illustrating this process are available in [35].

Figures 11 and 12 show the error convergence in  $L_{\infty}$  and  $L_2$  norms for the tracer concentration  $\phi$ . Similar to the previous test case, it is observed that all schemes with UNLIM achieve second-order accuracy, while for MONO, the order is reduced. Once more, the errors of the equi-edge grid are slightly smaller than those from the equiangular grid.

## 722 4.3. Flow deformation through a divergent wind

Finally, the divergent deformational test case from [35] is considered, where the time-dependent winds are given by

$$\begin{cases} u_{\lambda}(\lambda,\theta,t) = -u_0 \sin^2(\frac{\lambda+\pi}{2}) \sin(2\theta) \cos^2(\theta) \cos(\frac{\pi t}{T}), \\ v_{\theta}(\lambda,\theta,t) = \frac{u_0}{2} \sin(\lambda+\pi) \cos^3(\theta) \cos(\frac{\pi t}{T}), \end{cases}$$
(76)

where  $u_0 = \frac{\pi R}{2T}$ . The time step for N = 48 is adopted as  $\Delta t^{(0)} = 6400$  seconds, leading to a Courant number of approximately 0.91. The initial conditions

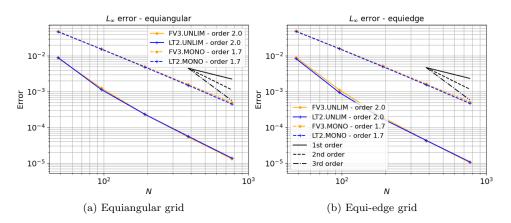


Figure 11:  $L_{\infty}$  error convergence for the tracer concentration  $\phi$  in the transport model using the two Gaussian hills as the initial condition and the divergence free deformational wind on equiangular (a) and equi-edge (b) grids after 12 days. Blue lines indicate the use of the LT2 scheme, while orange lines represent the FV3 scheme. Solid lines represent the results with the unlimited PPM (UNLIM) scheme, whereas dashed lines represent the results with the monotonic PPM (MONO).

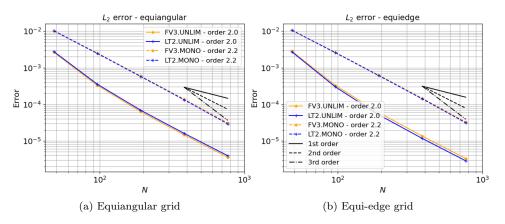


Figure 12: As Figure 11 but using  $L_2$  norm.

are again the two Gaussian hill (Equation (75)). Unlike the previous tests, this test introduces divergent wind. This test deforms the Gaussian hills, creating new extrema for the tracer density  $\rho\phi$ , and the final solution is equal to the initial condition. Figures illustrating this process are available in [35].

Figures 13a and 13b display the final error of the tracer concentration

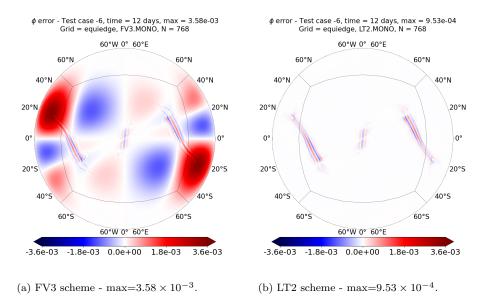


Figure 13: Transport experiment errors for the tracer concentration  $\phi$  using the two Gaussian hills and the divergent wind after 12 days, using the monotonic scheme (MONO) with FV3 (a) and LT2 (b) schemes on the equi-edge grid with N = 768.

 $\phi$  at a cube face for the equi-edge grid using the MONO scheme. Similar results on the equiangular grid are obtained and not shown here. The errors for the FV3 scheme are observed to be much larger, with the maximum error being four times that of the LT2 scheme. Significant errors are present in many cells for FV3, whereas the errors in the LT2 scheme are smaller and concentrated in some ripples.

Figures 14 and 15 show the error convergence in  $L_{\infty}$  and  $L_2$  norms for the 739 tracer concentration  $\phi$ . These figures highlight a major significant distinction 740 between LT2 and FV3 schemes, unlike the previous tests. It is clear that FV3 741 with the unlimited PPM achieves only first-order accuracy, whereas LT2 with 742 the unlimited PPM achieves third-order accuracy, exceeding expectations of 743 second-order accuracy, for both equi-edge and the equiangular grids and error 744 norms. For the monotonic scheme, LT2 demonstrates second-order accuracy 745 in the  $L_2$  norm, while FV3 is only first-order. LT2 with the monotonic 746 scheme, exhibits smaller errors in the  $L_{\infty}$  norm compared to the FV3 scheme 747 for all grids. This discrepancy arises because the FV3 splitting is designed 748 for divergence-free flows, while LT2 is designed to be second-order regardless 749 of the flow characteristics. 750

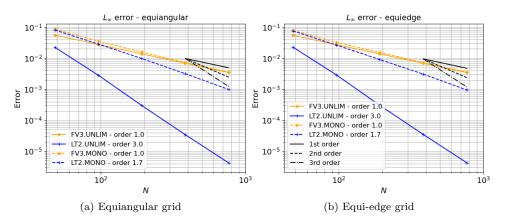


Figure 14:  $L_{\infty}$  error convergence for the tracer concentration  $\phi$  in the transport model using the two Gaussian hills as the initial condition and the divergent deformational wind on equiangular (a) and equi-edge (b) grids after 12 days. Blue lines indicate the use of the LT2 scheme, while orange lines represent the FV3 scheme. Solid lines represent the results with the unlimited PPM (UNLIM) scheme, whereas dashed lines represent the results with the monotonic PPM (MONO).

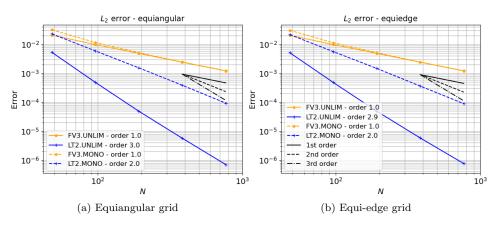


Figure 15: As Figure 14 but using  $L_2$  norm.

## 751 5. Concluding remarks

This work has revisited the FV3 transport scheme in all its details. This thorough examination has allowed for proposed modifications to improve the accuracy of the FV3 advection scheme, leading to a proposed scheme named LT2.

The FV3 transport scheme relies on applying 1D finite-volume fluxes,

namely the PPM, using a direction-splitting strategy. The proposed modifications to the 1D scheme aim to allow for a more accurate treatment in
handling metric terms and computing the departure points. Furthermore, the
FV3 scheme combines the 1D fluxes in such a way that the splitting error for
a constant scalar field and divergence-free wind is eliminated. In contrast,
the LT2 scheme does not have this property but introduces a second-order
error in this case.

To compare both schemes, this paper has considered a transport model on the sphere, where it is needed to solve two conservative transport equations: one for the tracer concentration and another for the fluid density. Subsequently, numerical simulations were conducted with both schemes on the equiangular and equi-edge cubed-sphere grids

The LT2 scheme showed to have slightly smaller errors than the FV3 769 scheme for divergence-free winds. Both schemes are second-order when no 770 limiter is employed and the wind is divergence-free. The major difference 771 between FV3 and LT2 is when the wind is not divergence-free. In this case, 772 FV3 is only first order, while LT2 is second-order. Even with a limiter, 773 LT2 is much more accurate than FV3 in this case, specially in the  $L_2$  norm. 774 This was demonstrated consistently throughout the simulations. Therefore, 775 the major conclusion here is that the LT2 scheme is more accurate regard-776 less of whether the wind is divergence-free or not, while FV3 is accurate 777 only for divergence-free winds. Additionally, although the LT2 scheme does 778 not possess the constancy-preserving property, it has been demonstrated to 779 accurately solve the constant scalar field case under divergence-free wind con-780 ditions, achieving second-order on the equi-edge cubed-sphere and close to 781 third order on equiangular cubed-sphere. Furthermore, the equiangular grid 782 was shown to be less sensitive to cube corners in the test where a Gaussian 783 hill passes through four cube corners. These last two results indicate that 784 the equiangular grid appears to be more accurate. 785

All the simulations presented in this paper used the duo-grid framework 786 of [23], which affects FV3's scalability. Optimization of the duo-grid inter-787 polation from [23] is a work in progress. Although this paper has focused on 788 the transport model, the ultimate goal is to use the LT2 scheme within the 780 full three-dimensional non-hydrostatic solver. In particular, the LT2 scheme 790 may be used to compute the fluid depth and the absolute vorticity fluxes 791 in the shallow-water equations that are solved in the three-dimensional non-792 hydrostatic solver along the Lagrangian surfaces [9] to update the horizontal 793 winds. 794

Shallow-water numerical experiments were also conducted using both the 795 FV3 and LT2 schemes, along with the test cases from [47] and [49]. Some 796 of these experiments and their results are detailed in Chapter 6 of [50]. It 797 was observed that the LT2 scheme did not deteriorate the accuracy of the 798 shallow-water solver. Both schemes showed very similar results for these 799 shallow-water tests. This is expected, as most of the shallow-water equation 800 tests available in the literature have small or no wind divergence. We are 801 currently working on developing a test for the shallow-water equations where 802 divergence plays a key role in the solution dynamics to evaluate the LT2 803 and FV3 schemes in this case. In this scenario, it is expected that the LT2 804 scheme should produce a more accurate solution. The results considering 805 the shallow-water equations will be discussed in a follow-up work. One could 806 also consider comparing the LT2 and FV3 schemes using moist shallow-water 807 models (eg., [51, 52, 53]), where wind divergence impacts the dynamics of 808 the moisture variables. 809

Horizontal wind divergence plays a pivotal role in many phenomena on the 810 atmosphere such as in tropical cyclones, hurricanes and in the Intertropical 811 Convergence Zone [54]. For example, hurricanes are fueled by strong hori-812 zontal wind convergence at the Earth's surface, with strong horizontal wind 813 divergence occurring at high altitudes. Furthermore, horizontal wind diver-814 gence plays a vital role at convective scales, influencing the initiation and 815 development of convection, precipitation processes, and the vertical struc-816 ture of the atmosphere. Therefore, we expect that the LT2 scheme has the 817 potential to improve the forecast of these phenomena where wind divergence 818 is present, especially at convective scales. For example, LT2 scheme may be 819 used to conduct a study based on [55], where the impact of using different 1D 820 PPM schemes of FV3 on hurricane intensity prediction is investigated. This 821 study highlights how modifying the advection scheme may improve hurricane 822 intensity prediction and affect the eyewall convection location, and we expect 823 that the LT2 scheme could yield better results in this scenario. 824

### 825 CRediT authorship contribution statement

Luan F. Santos: Conceptualization, Formal analysis, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft, Writing - review & editing. Joseph Mouallem: Conceptualization, Methodology, Software, Resources, Supervision, Writing - review & editing. Pedro S. Peixoto: Conceptualization, Funding acquisition, Methodology, Project administration, Resources, Supervision, Writing - original draft, Writing review & editing.

## <sup>833</sup> Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

### 837 Data availability

The source code used in this work is available at https://github.com/ luanfs/FV3\_container. This code is based on the duo-grid version of FV3 implemented by [23]. Additionally, the code was executed using Docker, leveraging the containerized version of the SHiELD (System for High-resolution prediction on Earth-to-Local Domains) model developed by [56].

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#### 854 Disclaimer

The statements, findings, conclusions, and recommendations are those of the author(s) and do not necessarily reflect the views of the National Oceanic and Atmospheric Administration, or the US Department of Commerce.

## 858 Appendix A. Metric term relations

A straightforward computation using Equation (2) shows that the derivatives of the mappings  $\Gamma_p$  are explicitly given by:

$$d\Gamma_1(X,Y) = \frac{R}{(1+X^2+Y^2)^{3/2}} \begin{bmatrix} -X & -Y\\ 1+Y^2 & -XY\\ -XY & 1+X^2 \end{bmatrix},$$
 (A.1)

and similar formula holds for the other values of p. Thus, it follows that the metric tensor of  $\Gamma_p$  is explicitly given by

$$G_{\Gamma}(X,Y) = \frac{R^2}{(1+X^2+Y^2)^2} \begin{bmatrix} 1+X^2 & -XY\\ -XY & 1+Y^2 \end{bmatrix},$$
 (A.2)

and the metric term of  $\Gamma_p$  is given by:

$$\sqrt{\mathfrak{g}_{\Gamma}}(X,Y) = \frac{R^2}{(1+X^2+Y^2)^{3/2}}.$$
 (A.3)

<sup>864</sup> It follows from the chain rule in Equation (6) that:

$$d\Psi_p(x,y) = d\Gamma_p(\beta(x),\beta(y)) \cdot \operatorname{diag}(\beta'(x),\beta'(y)), \qquad (A.4)$$

where diag( $\beta'(x), \beta'(y)$ ) is a diagonal  $2 \times 2$  matrix with diagonal entries given by  $\beta'(x)$  and  $\beta'(y)$ . The tangent vector basis { $\partial_x \Psi_p, \partial_y \Psi_p$ } satisfies:

$$\partial_x \Psi_p(x, y) = \beta'(x) \cdot \partial_X \Gamma_p(\beta(x), \beta(y)), \qquad (A.5)$$

$$\partial_y \Psi_p(x, y) = \beta'(y) \cdot \partial_Y \Gamma_p(\beta(x), \beta(y)).$$
(A.6)

<sup>867</sup> Finally, the metric term  $\sqrt{\mathfrak{g}_{\Psi}}$  is expressed in terms of  $\sqrt{\mathfrak{g}}_{\Gamma}$  as

$$\sqrt{\mathfrak{g}_{\Psi}}(x,y) = \beta'(x)\beta'(y)\sqrt{\mathfrak{g}}_{\Gamma}\big(\beta(x),\beta(y)\big) \tag{A.7}$$

$$= \beta'(x)\beta'(y)\frac{R^2}{\left(1+\beta(x)^2+\beta(y)^2\right)^{3/2}}.$$
 (A.8)

# Appendix B. Relations between wind representation on the cubedsphere and on latitude-longitude coordinates

We consider the latitude-longitude mapping  $\Pi : [-\pi, \pi] \times [-\frac{\pi}{2}, \frac{\pi}{2}] \to \mathbb{S}_R^2$ ,  $\Pi = (\Pi_1, \Pi_2, \Pi_3)$ , given by:

$$\Pi_1(\lambda,\theta) = R\cos\theta\cos\lambda,\tag{B.1}$$

$$\Pi_2(\lambda,\theta) = R\cos\theta\sin\lambda,\tag{B.2}$$

$$\Pi_3(\lambda,\theta) = R\sin\theta. \tag{B.3}$$

<sup>872</sup> Using this mapping, the unit tangent vectors may be computed as:

$$\boldsymbol{e}_{\lambda}(\lambda,\theta) = \begin{bmatrix} -\sin\lambda\\ \cos\lambda\\ 0 \end{bmatrix}, \quad \boldsymbol{e}_{\theta}(\lambda,\theta) = \begin{bmatrix} -\sin\theta\cos\lambda\\ -\sin\theta\sin\lambda\\ \cos\theta \end{bmatrix}.$$
(B.4)

A tangent vector field u on the sphere may be then written in terms of  $e_{\theta}$ and  $e_{\lambda}$  as:

$$\boldsymbol{u}(\lambda,\theta) = u_{\lambda}(\lambda,\theta)\boldsymbol{e}_{\lambda}(\lambda,\theta) + v_{\theta}(\lambda,\theta)\boldsymbol{e}_{\theta}(\lambda,\theta), \qquad (B.5)$$

where  $u_{\lambda}$  is the zonal component and  $v_{\theta}$  is the meridional component. The latitude-longitude representation is related with the normalized contravariant representation (Equation (10)) by the expression:

$$\begin{bmatrix} u_{\lambda}(\lambda,\theta) \\ v_{\theta}(\lambda,\theta) \end{bmatrix} = \begin{bmatrix} \langle \boldsymbol{e}_{x}, \boldsymbol{e}_{\lambda} \rangle & \langle \boldsymbol{e}_{y}, \boldsymbol{e}_{\lambda} \rangle \\ \langle \boldsymbol{e}_{x}, \boldsymbol{e}_{\theta} \rangle & \langle \boldsymbol{e}_{y}, \boldsymbol{e}_{\theta} \rangle \end{bmatrix} \begin{bmatrix} \mathsf{u}(x,y,p) \\ \mathsf{v}(x,y,p) \end{bmatrix}, \quad (B.6)$$

which holds since  $e_{\lambda}$  and  $e_{\theta}$  are orthogonal. This formula is just a basis conversion.

# Appendix C. Relation between time-averaged fluxes and departure points

In the following theorem, it is proven how the time-averaged flux is related to a spatial integral over a interval depending on departure points.

**Theorem 1.** Assume that q and u are  $C^1$  functions and that q satisfies Equation (29), then:

$$\int_{t^n}^{t^{n+1}} (u\sqrt{\mathfrak{g}}q)(x_{i+\frac{1}{2}},s) \, ds = \int_{x_{i+\frac{1}{2}}^d(t^n,t^{n+1})}^{x_{i+\frac{1}{2}}} (\sqrt{\mathfrak{g}}q)(x,t^n) \, dx.$$
(C.1)

Proof. To start with, the variable  $\varphi = \sqrt{\mathfrak{g}}q$  is introduced to simplify the notation. Let us consider the mapping  $s \in [t^n, t^{n+1}] \to x^d_{i+\frac{1}{2}}(t^n, s)$ . Integrating  $\varphi$  at time  $t^n$  over all the range of  $x^d_{i+\frac{1}{2}}(t^n, s)$  for  $s \in [t^n, t^{n+1}]$  yields:

$$\int_{x_{i+\frac{1}{2}}^{d}(t^{n},t^{n+1})}^{x_{i+\frac{1}{2}}}\varphi(x,t^{n})\,dx = -\int_{t^{n}}^{t^{n+1}}\varphi\big(x_{i+\frac{1}{2}}^{d}(t^{n},s),t^{n}\big)\partial_{s}x_{i+\frac{1}{2}}^{d}(t^{n},s)\,ds, \quad (C.2)$$

which follows from the variable change integration formula, recalling that  $x_{i+\frac{1}{2}}^{d}(t^{n},t^{n}) = x_{i+\frac{1}{2}}$ . Hence, it suffices to prove that:

$$\varphi(x_{i+\frac{1}{2}}^d(t^n, s), t^n) \partial_s x_{i+\frac{1}{2}}^d(t^n, s) = -(u\varphi)(x_{i+\frac{1}{2}}, s).$$
(C.3)

<sup>891</sup> Firstly,  $\partial_s x_{i+\frac{1}{2}}^d(t,s)$  is computed using the Leibniz rule for integration in <sup>892</sup> Equation (37), which leads to

$$\partial_{s} x_{i+\frac{1}{2}}^{d}(t,s) = -\left(u(x_{i+\frac{1}{2}},s) + \int_{t}^{s} \partial_{s} u\left(x_{i+\frac{1}{2}}^{d}(\tau,s),\tau\right) d\tau\right)$$
  
$$= -u(x_{i+\frac{1}{2}},s) - \int_{t}^{s} \partial_{x} u\left(x_{i+\frac{1}{2}}^{d}(\tau,s),\tau\right) \partial_{s} x_{i+\frac{1}{2}}^{d}(\tau,s) d\tau.$$
(C.4)

Taking the derivative with respect to t of Equation (C.4), one gets:

$$\partial_t \partial_s x^d_{i+\frac{1}{2}}(t,s) = \partial_x u \left( x^d_{i+\frac{1}{2}}(t,s), t \right) \partial_s x^d_{i+\frac{1}{2}}(t,s).$$
(C.5)

One check upon inspection that the trajectory  $x_{i+\frac{1}{2}}^d$  that solves Equations (C.4) and (C.5) is given by:

$$\partial_s x_{i+\frac{1}{2}}^d(t,s) = -\exp\left(\int_t^s \partial_x u\left(x_{i+\frac{1}{2}}^d(\tau,s),\tau\right) d\tau\right) u(x_{i+\frac{1}{2}},s).$$
(C.6)

Secondly, to obtain  $\varphi(x_{i+\frac{1}{2}}^d(t^n,s),t^n)$ , we compute  $\varphi$  along the trajectory given by  $x_{i+\frac{1}{2}}^d(t,s)$ , and then take its time derivative:

$$\frac{d}{dt}\varphi(x_{i+\frac{1}{2}}^{d}(t,s),t) = \partial_{t}\varphi(x_{i+\frac{1}{2}}^{d}(t,s),t) + (u\partial_{x}\varphi)(x_{i+\frac{1}{2}}^{d}(t,s),t) 
= -\partial_{x}u(x_{i+\frac{1}{2}}^{d}(t,s),t)\varphi(x_{i+\frac{1}{2}}^{d}(t,s),t),$$
(C.7)

where we used that  $\varphi$  satisfies Equation (29) and that  $x_{i+\frac{1}{2}}^d(t,s)$  solves Equation (32). One check upon inspection again that  $\varphi$  that solves Equation (C.7) is given by:

$$\varphi\left(x_{i+\frac{1}{2}}^d(t,s),t\right) = \exp\left(-\int_t^s \partial_x u\left(x_{i+\frac{1}{2}}^d(\tau,s),\tau\right)d\tau\right)\varphi(x_{i+\frac{1}{2}},s).$$
(C.8)

Equation (C.3) can be obtained by multiplying Equation (C.6) by Equation (C.8) at  $t = t^n$ , which concludes the proof.

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