A Fast Monotone Discretization of the Rotating Shallow Water Equations

Guillaume Roullet¹, Tugdual Gaillard¹

¹Univ. Brest, CNRS, IRD, Ifremer, Laboratoire d'Océanographie Physique et Spatiale (LOPS), IUEM,

Brest, France

Key Points:

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7	• Use WENO reconstructions on the mass flux and on the nonlinear Coriolis term
8	• Reach low level of energy dissipation and high accuracy on material conservation
9	of potential vorticity
10	• Express the continuous equations with index coordinates, finite volume quanti-
11	ties, covariant and contravariant components of the velocity
12	• Minimize the number of operations and maximize the arithmetic intensity
13	• Achieve 2 GFlop per second per core with a pure Python code

Corresponding author: Guillaume Roullet, roullet@univ-brest.fr

14 Abstract

This paper presents a new discretization of the rotating shallow water equations and a 15 set of decisions, ranging from a simplification of the continuous equations down to the 16 implementation level, yielding a code that is fast and accurate. Accuracy is reached by 17 using WENO reconstructions on the mass flux and on the nonlinear Coriolis term. The 18 results show that the build-in mixing and dissipation, provided by the discretization, al-19 low a very good material conservation of potential vorticity and a minimal energy dis-20 sipation. Numerical experiments are presented to assess the accuracy, which include a 21 resolution convergence, a sensitivity on the the free-slip vs. no-slip boundary conditions, 22 a study on the separation of waves from vortical motions. Speed is achieved by a series 23 of choices rather than a single recipe. The main choice is to discretize the covariant form 24 written in index coordinates. This form, rooted in the discrete differential geometry, re-25 moves most of the grid scale terms from the equations, and keep them only where they 26 should be. The model objects appearing in resulting continuous equations have a nat-27 ural correspondence with the grid cell features. The other choices are guided by the max-28 imization of the arithmetic intensity. Finally this paper also proves that a pure Python 29 implementation is not only possible but also very fast, thanks to the possibility of hav-30 ing compiled Python. As a result, the code performs 2 TFlop per second using thousand 31 cores. 32

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Plain Language Summary

Using a simplified model of the ocean and atmosphere dynamics, this paper presents 34 a set of numerical and programming decisions that yields a code that is both fast and 35 accurate. The accuracy is assessed in terms of capacity of the code to maintain dynamic 36 structures over long periods of time while avoiding the emergence of numerical noise in 37 the solution. Accuracy is achieved by using a very accurate discretization on two deci-38 sive terms of the model equations. Speed is achieved by a series of choices ranging from 39 a simplification of the continuous equations down to the implementation level. This pa-40 per also proves that a pure Python code is a viable alternative to perform simulations 41 on high performance computing centers with as much as 2 TFlop per second using thou-42 sand cores. 43

44 1 Introduction

The rotating shallow water (RSW) equations are the perfect framework to test con-45 cepts, methods and ideas for later applications to more sophisticated atmospheric or oceanic 46 models. When it comes to numerical modeling, two goals are particularly important: speed 47 and accuracy. They are rather antagonistic for accuracy comes with higher order schemes, 48 which are computationally more expensive than low order ones, therefore penalizing speed. 49 However things are more subtle because a higher order discretization in time may allow 50 a larger time step, whereas a higher order discretization in space may increase the ef-51 fective resolution, allowing to use a coarser grid. The price of having high-order discretiza-52 tions may thus be largely compensated. In this paper we show how the WENO recon-53 struction (Jiang & Shu, 1996), a highly computationally demanding scheme, can be used 54 in a RSW model on both the continuity and the momentum equations to provide high 55 accuracy, while still allowing a very fast code. The merits are such that this numerical 56 method opens the way for a new class of sub-grid-scale closure. 57

Having a code running fast is a very valuable quality. For a given amount of com-58 putational resources, it allows for a longer time integration or a greater spatial resolu-59 tion. Achieving speed involves many design choices, rather than one, that include the 60 programming language, the algorithms implementation and the code design in general. 61 When measured in terms of floating point operations (Flop) per second, the speed is-62 sue rapidly touches to the hardware architecture. The question should be, for a given 63 computer, how close is the code speed to the maximum speed achievable on this com-64 puter. The maximum speed is given by the clock frequency but, if the code involves too 65 much data transfer between the memory and the CPU, the effective speed can be far from 66 this maximum. Indeed, according to the roof-line model (Williams et al., 2009), the speed 67 might be memory-bound or compute-bound, and that depends on the arithmetic inten-68 sity, which is the ratio of the number of Flop per float exchanged between the memory 69 and the core. To achieve the optimal speed, a code should be in the compute-bound re-70 gion, namely it should have a large enough arithmetic intensity, which means to perform 71 as many Flop on the data, once the data have been transferred to the core. This issue 72 is often overlook in atmosphere and ocean models. 73

Increasing the arithmetic intensity is not so easy. We are aware of at least three
techniques. First, this can be done by blending many operations into a few large loops,

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as opposed to having many loops each doing one operation. A typical example of code 76 following this approach is ROMS (Shchepetkin & McWilliams, 2005). This technique comes 77 at the expend of code readability and modularity, which makes code evolutions harder, 78 e.g. changing the time stepping. The second possibility is to use numerical discretiza-79 tions that require more Flop per grid point. A very good example of such demanding 80 computation is a high order WENO reconstruction (Shu, 1999), which loops back on 81 the question of accuracy. Indeed, replacing linear schemes with high-order non-linear schemes 82 not only increases the arithmetic intensity, but it also increases the model accuracy. This 83 is the main point of this paper. We elaborate on the benefits of WENO reconstruction 84 below. 85

The third technique is to simply reduce the number of Flop, and the associated data 86 transfer. This might sound odd but there is actually an obvious way, though neglected: 87 strip down the RSW equations to a minimal covariant form. The discretized RSW equa-88 tions, when written either in curvilinear coordinates or on non rectangular grids, are usu-89 ally cluttered with a lot of grid scale factors multiplications (lengths, inverse of lengths) 90 and areas). In this paper we show how these scale factors can be removed almost every-91 where in the vector invariant form of the RSW equations. The price is to slightly change 92 the objects the code manipulates. Without further explanations yet, the changes are the 93 following: use the array indices (i, j) as spatial coordinates, use finite volume quantities 94 carrying their area, replace the velocity components with the pairs of covariant and con-95 travariant components. These changes arise naturally from the discrete differential ge-96 ometry (Desbrun et al., 2006; Cotter & Thuburn, 2014), which identifies the basic ob-97 jects such as scalars, vectors, vorticity, as differential forms and which connects them with 98 the grid features, respectively cells, edges and vertices, while emphasizing the crucial dif-99 ference between the primal and the dual mesh. To avoid burying the ideas into an over-100 whelming formalism, we will start from known grounds and make the concepts emerge 101 naturally. For the reader tempted to know more we may suggest this very tutorial pa-102 per (Perot & Zusi, 2014). The obtained simplified form of the RSW equations has many 103 advantages. It is light, in terms of operations involved; it is fully adapted to a discretiza-104 tion on a logically rectangular C-grid; and, last but not least, it is covariant, in the sense 105 that the form is invariant under a change of coordinates. Thanks to the covariance the 106 space is really seen as an array of cells, even on the continuous equations. 107

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As already mentioned, the programming language is central. Until recently the climate-108 atmospheric-ocean community mostly relied on Fortran and MPI. Fortran has long been 109 considered as the ultimate language for HPC. Things are changing. New codes in Cython 110 or Julia (Ramadhan et al., 2020) are now popping up quite regularly. But pure Python 111 codes remain rare, mostly because Python is an interpreted language. This can now be 112 overcome thanks to the numba module (Lam et al., 2015) that allows to compile Python. 113 This paper proves that all the ideas presented so far can be implemented in a pure Python 114 code, while reaching 2.0 GFlop per second on a 2.5 GHz core, and 2.0 TFlop per sec-115 ond on the same architecture with a thousand cores. 116

Finally another possibility to increase the speed is to trade it with accuracy by using single precision floats, or even a blend of a single precision and BFloats (two bytes floats), which de facto reduces the memory traffic and the time of each Flop. This approach has been recently tested quite thoroughly (Klöwer et al., 2020).

Let us now turn on the accuracy aspect. Accuracy encompasses several properties. In this paper we are particularly interested in the ability: i) to have minimal energy dissipation, ii) to materially conserve the potential vorticity (PV), iii) to maintain noisefree PV, iv) to separate vortical motions from wave motions and v) to enforce clean lateral boundary conditions, either free or no-slip. We achieve these properties with essentially one key idea: use WENO reconstructions on the mass flux and the nonlinear Coriolis term, namely the two decisive terms that control these properties.

Using a WENO reconstruction on the nonlinear Coriolis term may seem odd be-128 cause the upwinding breaks the invariance under the time reversal symmetry, which un-129 avoidably introduces dissipation. The opposite strategy for accuracy is to seek a sym-130 plectic integrator (Brecht et al., 2019). There are in fact several good reasons for using 131 WENO. First, a close inspection of the RSW equations written in vector-invariant form 132 reveals the equal importance in the material conservation of PV of the mass flux and the 133 nonlinear Coriolis term, which is a vorticity flux. So if one applies a WENO reconstruc-134 tion on the mass flux, to provide mixing, it is appealing to proceed similarly on the non-135 linear Coriolis term to have a consistent discretization of the PV and to ensure maxi-136 mum symmetry between the two fluxes. We will show that this technique brings the afore-137 mentioned properties on the PV dynamics. Second, from the energy point of view, the 138 nonlinear Coriolis term should have a vanishing work, but if we consider the filtered ver-139

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sion of the RSW equations in vector-invariant form, following the LES filter technique 140 (Sagaut, 2006), then, once again, the nonlinear Coriolis term turns out to be the key player. 141 Indeed, the vector-invariant form transforms the momentum flux into the nonlinear Cori-142 olis term and the gradient of kinetic energy term. These two terms play a very differ-143 ent role on the energy equation. The gradient term becomes the divergence of the ki-144 netic energy flux whereas the nonlinear Coriolis term turns out to be the term respon-145 sible for the exchange of energy between the resolved grid scales and the sub-grid scales. 146 Therefore advocating for using the WENO reconstruction to compute this term. The 147 third, and last reason was originally formulated by Mullen et al. (2011). If we let the dif-148 ferential geometry guides our numerical choices, then the transport of the momentum 149 should be discretized in such way that it obeys the properties of the Lie derivative. This 150 pleads for upwinding the vorticity in the nonlinear Coriolis term. If one also demands 151 high order discretization and monotonicity, then a WENO reconstruction is a natural 152 solution. Note that WENO reconstructions have already been tested for shallow water 153 models (Xing & Shu, 2005; Noelle et al., 2007; Gallerano & Cannata, 2011) but it was 154 on the flux form of the momentum equation. Applying it on the nonlinear Coriolis term 155 is completely new to our knowledge. 156

From the more general perspective of large eddy simulations (LES) models, the idea 157 stems from the MILES approach (Boris et al., 1992). MILES was designed for three di-158 mensional models as an alternative to physically based explicit closures, typically the Smagorin-159 sky closure or one of its variant. In ILES the closure takes the form of a monotonic dis-160 cretization of the mass and momentum fluxes. Such closure is coined *implicit* (Margolin 161 et al., 2006) or *numerical* (Pope, 2004). A numerical closure is opposed to a physical or 162 purely physical closure for which there is a physical model supporting the closure. The 163 use a monotonic discretization on the nonlinear Coriolis term rather than on the momen-164 tum flux, can be seen as a variant of the MILES approach. This paper adds up to the 165 list of closures for LES models solving the RSW equations (Graham & Ringler, 2013). 166

This paper is organized as follows. In Section 2, we show how the continuous RSW equations can be strip down to a very simple form while still handling general curvilinear coordinates and being fully covariant. We discuss the material conservation of PV to motivate the discretization, which is presented in Section 3. In Section 4, implementation choices are described and the code speed is assessed. In Section 5, the accuracy

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¹⁷² of the code is tested with three experiments, each assessing one aspect. A summary is

¹⁷³ given in Section 6.

¹⁷⁴ 2 A fresh look at the RSW equations

The goal of this section is to present the RSW equations in the form that it is well suited for having a fast and accurate numerical model, namely

$$\frac{\partial \mathbf{u}}{\partial t} = -(\zeta^* + f^*) \,\mathbf{U}^{\perp} - \boldsymbol{\nabla} \left(g(h+b) + k\right) \tag{1}$$

$$\frac{\partial h^{\star}}{\partial t} = -\boldsymbol{\nabla} \cdot (h^{\star} \mathbf{U}) \tag{2}$$

$$\zeta^{\star} = \nabla \times \mathbf{u} \tag{3}$$

$$k = \frac{1}{2} \mathbf{u} \cdot \mathbf{U} \tag{4}$$

which is the vector invariant form slightly in disguise. Indeed, at this stage only four terms have their classical definition: h, the layer depth, g is the acceleration due to gravity, bthe bottom topography and k the kinetic energy density. The other terms require more context before being fully defined. In particular the meaning of the \star decorator and the use of two different terms **u** and **U** for the velocity will be explained. The $^{\perp}$ symbol on \mathbf{U}^{\perp} has its usual meaning, it designates the quarter turn counterclockwise rotated **U**.

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2.1 Index coordinates

We start by endowing the space with a mapping system. The most general way is 188 to use curvilinear coordinates (η_1, η_2) . They might be Cartesian (x, y), spherical (ϕ, θ) , 189 cylindrical (r, θ) , or any other. Among the other possibilities are the index coordinates 190 (i, j), associated with a logically rectangular grid. These coordinates, which are grid res-191 olution dependent, are natural to locate grid cell features such as centers, edges, and ver-192 tices because all the variables are mapped with only integers or half integers indices, de-193 pending on the variable staggering. But their most interesting property is that two ad-194 jacent points of the same feature in the direction either i or j are separated by either 195 di = 1 or dj = 1. Thus, the partial derivative $\partial \phi / \partial i$ of a field $\phi(i, j)$ is naturally dis-196 cretized as 197

$$\frac{\partial \phi}{\partial i} \to \phi[i+1,j] - \phi[i,j], \qquad (5)$$

with no division, because di = 1. By using index coordinates, a spatial derivative boils down to one subtraction. This is the first optimization and simplification of this paper. For the rest of this paper, we will use the index coordinates, therefore using (i, j) instead of (η_1, η_2) . The consequence is that the ∇ operator reads

$$\boldsymbol{\nabla} = \left(\frac{\partial}{\partial i}, \frac{\partial}{\partial j}\right),\tag{6}$$

and its discretized version only involves the two points differences (5).

Once the coordinates system is defined, the space must be equipped with a metric to measure the distance between two nearby points, say P_1 at (i, j) and P_2 at (i + di, j + dj). This is achieved with the first fundamental form

$$ds^2 = e_1^2 di^2 + e_2^2 dj^2 \tag{7}$$

where $e_1(i, j)$ and $e_2(i, j)$ describe the metric of the space. For the index coordinates system, (e_1, e_2) are the elementary distances between two points separated either by (1, 0)in the direction *i*, or by (0, 1) in the direction *j*. In other words, (e_1, e_2) are the grid cell lengths and they carry the length dimension. For other coordinates systems, e_1 and e_2 may not have the dimensions of a length, e.g. in the Cartesian coordinate case $(e_1, e_2) =$ (1, 1), or not have the same dimension, e.g. in the cylindrical coordinate case $(e_1, e_2) =$ (1, r).

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2.2 Finite volumes and contravariant components

To present the second optimization and simplification, let us recall how the equations in curvilinear coordinates are usually written. In particular, the continuity equation $\partial h/\partial t = -\nabla \cdot (h\tilde{\mathbf{u}})$, where $\tilde{\mathbf{u}} = (\tilde{u}, \tilde{v})$ is the velocity, reads

$$\frac{\partial h}{\partial t} = -\frac{1}{e_1 e_2} \left(\frac{\partial}{\partial i} (h \, \tilde{u} \, e_2) + \frac{\partial}{\partial j} (h \, \tilde{v} \, e_1) \right) \,. \tag{8}$$

This equation, though absolutely correct, is unnecessarily cluttered. The drawbacks are many. Beyond the code readability, it harms the code speed because it requires unnecessary multiplications and unnecessary data transfer from the memory to the CPU, as e_1 and e_2 are also bi-dimensional arrays in the general case. It also makes the interpolation of model variables more involved. (8) can be simplified into (2), viz.

$$\frac{\partial h^*}{\partial t} = -\frac{\partial}{\partial i}(h^* U) - \frac{\partial}{\partial j}(h^* V) \tag{9}$$

²²⁷ with no sacrifice, by simply defining

$$h^* = h e_1 e_2$$
, and $\mathbf{U} = (U, V) = (\tilde{u}/e_1, \tilde{v}/e_2)$. (10)

(9) now involves only two multiplications, that correspond to a genuine non-linearity of the RSW equations, and three additions/subtractions. The grid scale factors are gone. The price to pay is to accept working with the less intuitive variables (h^*, \mathbf{U}) rather than the usual "physical" $(h, \tilde{\mathbf{u}})$. The benefits are considerable: computationally, implementation wise and even conceptually. The simplification neither comes by chance or is a mathematical trick. (9) exposes the geometric nature of the objects we should manipulate. Let us comment on these two variables.

The first realization is that the velocity which fluxes the mass is \mathbf{U} , whose dimen-236 sions are T^{-1} . U turns out to be the contravariant form of the velocity in the index co-237 ordinates system. The second realization is the use of h^* . As the product of h with the 238 area $A = e_1 e_2$, h^* is naturally the *amount* of h, i.e. the finite volume version of h. The 239 discretized version of h^{\star} should be natural for every numerical modeler but its contin-240 uous version might be a bit more mysterious. It is worth an explanation. In the contin-241 uous equations, A is an infinitesimal surface area. In Cartesian coordinates, A would be 242 dx dy and h^* would be h dx dy. This might look awkward, but it is not, for there is a solid 243 underlying mathematical theory: the differential geometry. In this paper we have decided 244 to not use the artillery of differential geometry because it would overwhelm the discus-245 sion with too many concepts. However, it is with these concepts in mind that this work 246 has been carried out. The reader interested in the connection with the differential ge-247 ometry may look at these papers. The present paper is really aimed at numerical mod-248 elers. A consequence of h^* carrying its infinitesimal area is that it can be used as is in 249 a domain integration. For instance, the total volume is $V = \int h^*$. 250

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2.3 Covariant components

252 Similarly the momentum equations in curvilinear coordinates vector-invariant form253 usually read

$$\frac{\partial \tilde{u}}{\partial t} = (\zeta + f)\tilde{v} - \frac{1}{e_1}\frac{\partial}{\partial i}\left(g(h+b) + \frac{1}{2}|\tilde{\mathbf{u}}|^2\right)$$
(11)

$$\frac{\partial \tilde{v}}{\partial t} = -(\zeta + f)\tilde{u} - \frac{1}{e_2}\frac{\partial}{\partial j}\left(g(h+b) + \frac{1}{2}|\tilde{\mathbf{u}}|^2\right), \qquad (12)$$

where f is the Coriolis parameter and ζ is the vorticity

$$\zeta = \frac{1}{e_1 e_2} \left(\frac{\partial}{\partial i} (e_2 v) - \frac{\partial}{\partial j} (e_1 u) \right).$$
(13)

(12) can be transformed into (1), viz.

$$\frac{\partial u}{\partial t} = (\zeta^{\star} + f^{\star})V - \frac{\partial}{\partial i}\left(g(h+b) + k\right) \tag{14}$$

$$\frac{\partial v}{\partial t} = -(\zeta^* + f^*)U - \frac{\partial}{\partial j}\left(g(h+b) + k\right) \tag{15}$$

by defining

$$\mathbf{u} = (u, v) = (\tilde{u} e_1, \tilde{v} e_2), \qquad (16)$$

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$$f^{\star} = f e_1 e_2, \quad \zeta^{\star} = \frac{\partial v}{\partial i} - \frac{\partial u}{\partial j} \quad \text{and} \quad k = \frac{1}{2} \mathbf{u} \cdot \mathbf{U}.$$
 (17)

As in the continuity equation, no grid lengths are involved in either the gradient or the curl. The vector **u** has two interpretations: it is both a circulation element, and the covariant form of the velocity in the index coordinates system. By combining the definitions of **u** and **U** we have $(u, v) = (U e_1^2, V e_2^2)$. This relation can be written in tensor notation $\mathbf{u} = \mathbf{g} \mathbf{U}$, with

$$\mathbf{g} = \begin{pmatrix} e_1^2 & 0\\ 0 & e_2^2 \end{pmatrix} \tag{18}$$

the metric tensor. The dimensions of the covariant components are $L^2 T^{-1}$. Therefore 269 neither **u** or **U** have the dimensions LT^{-1} of a speed. The distinction between **u** and 270 U may seem quite artificial and formal at first. It turns out that they correspond to two 271 very different substances: \mathbf{u} is the momentum, the dynamical quantity that is transported 272 and that obeys a conservation law, whereas \mathbf{U} is the flux, the kinematic quantity that 273 transports things. ζ^* has the same dimensions as **u** and satisfies $\zeta^* = \zeta e_1 e_2$. Conse-274 quently ζ^{\star} can be seen either as an elementary circulation along a closed loop, or as the 275 usual vorticity times the area element, i.e. the finite volume version of ζ . Likewise, f^* 276 is the finite volume version of the planetary vorticity f. At this stage, (9-10, 14-17) are 277 in the form we use for the discretization. 278

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2.4 Potential vorticity

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A central diagnostic quantity of the RSW equations is $q = (\zeta^* + f^*)/h^*$, the potential vorticity, abbreviated PV throughout this paper. PV plays a central role in rotating flows for it allows to split the dynamics into a balanced part, captured by the PV evolution, and the unbalanced, the gravity waves, that propagate with vanishing net PV transport. Being a ratio of two finite volume quantities, q is a density, as opposed to a

finite volume quantity. It obeys $\partial q/\partial t + \mathbf{U} \cdot \nabla q = 0$, which expresses the material con-285 servation on fluid parcels. This conservation law is highly desirable at the numerical level. 286 It should be emphasized that the material conservation is much more demanding numer-287 ically than a global conservation. In practice, it means that the probability density func-288 tion of q remains stationary in time. Ensuring exact material conservation of this derived 289 quantity is possible on steady flows, e.g. the cases 2 and 3 of (Williamson et al., 1992), 290 but it is impossible on arbitrary flows, for a fundamental reason. Indeed, the material 291 conservation holds as long as there is no dissipation nor mixing, viz. for inviscid flows 292 but, sooner or later, mixing of PV kicks in. This is because of the tendency for the PV 293 to develop filaments that, under the flow deformation, elongate and get thinner with time, 294 a process known as the direct cascade of enstrophy. For RSW equations the enstrophy 295 density is $q^2 h$ and for inviscid flows, the total enstrophy, integrated over the domain, 296 $Z = \int q^2 h^*$ should be conserved. In a numerical model the direct cascade of enstro-297 phy should proceed as inviscidly as possible across the resolved scales until it reaches the 298 grid scale, at which point the numeric should be helped to parameterize the unresolved 299 cascade continuation. This parameterization usually boils down to dissipate the enstro-300 phy at the grid scale. In this paper we adopt the MILES approach consisting in using 301 monotonic upwinded reconstructions to provide the required dissipation of enstrophy. 302 But the tricky point is that q is essentially a by-product of the equations, there is no di-303 rect handle on the PV evolution. The PV dynamics is controlled only through the dy-304 namics of h^* and $\omega^* = \zeta^* + f^*$, the finite volume absolute vorticity. To complicate even 305 more, ω^* is also a derived quantity, but fortunately, the vector invariant form exposes 306 the ω^* dynamics in plain sight offering a way to consistently handle h^* and ω^* . 307

The numerical discretization we propose aims at having a PV material conserva-308 tion as good as possible. The material conservation is not a mere coincidence, it corre-309 sponds to a hidden symmetry of the equations: the invariance of the equations under a 310 relabeling of the parcels. Enforcing material conservation discretely is thus a way to sat-311 isfy this hidden symmetry of the equations. For that we adopt a slight change of per-312 spective on the role of q in the numerical integration. Instead of focusing on q, we fo-313 cus on ω^* . Indeed, in practice, the material conservation of PV derives from a subtle can-314 cellation in the momentum and the continuity equation between the vorticity flux $\omega^* \mathbf{U}$ 315 and the mass flux $h^{\star}\mathbf{U}$. Let us carefully examine how this cancellation works for this will 316 suggest a new way to discretize the RSW equations. 317

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To derive the material conservation of PV we apply the chain rule on

$$\frac{\partial q}{\partial t} = \frac{1}{h^{\star 2}} \left(h^{\star} \frac{\partial \omega^{\star}}{\partial t} - \omega^{\star} \frac{\partial h^{\star}}{\partial t} \right) \tag{19}$$

that reveals the very symmetrical role between the continuity equation and the the equa-320 tion for the absolute vorticity. The latter is derived by taking the curl of (1), namely 321

$$\frac{\partial \omega^{\star}}{\partial t} = -\boldsymbol{\nabla} \cdot \left(\omega^{\star} \, \mathbf{U}\right),\tag{20}$$

which expresses that the vorticity obeys a conservation law in flux form, exactly like h^* . 323 Substituting (20) in (19) yields 324

$$\frac{\partial q}{\partial t} = \frac{1}{h^{\star 2}} \left(-h^{\star} \nabla \cdot (\omega^{\star} \mathbf{U}) + \omega^{\star} \nabla \cdot (h^{\star} \mathbf{U}) \right)$$
(21)

$$= -\frac{1}{h^{\star 2}} \left[h^{\star} \mathbf{U} \cdot \boldsymbol{\nabla} \omega^{\star} - \omega^{\star} \mathbf{U} \cdot \boldsymbol{\nabla} h^{\star} + \underbrace{h^{\star} \omega^{\star} \boldsymbol{\nabla} \cdot \mathbf{U} - h^{\star} \omega^{\star} \boldsymbol{\nabla} \cdot \mathbf{U}}_{=0} \right]$$
(22)
$$= -\mathbf{U} \cdot \boldsymbol{\nabla} q.$$
(23)

$$= -\mathbf{U}\cdot\mathbf{\nabla} q.$$

We see that the material conservation arises because of the cancellation of the two terms 328 in (22), which follows from the identity 329

$$\boldsymbol{\nabla} \cdot (\phi^* \mathbf{U}) = \mathbf{U} \cdot \boldsymbol{\nabla} \phi^* + \phi^* \boldsymbol{\nabla} \cdot \mathbf{U}, \qquad (24)$$

where ϕ^* is either h^* or ω^* . On a C-grid, the discrete version of this identity can be made 331 exact provided the quantity ϕ^* , in the flux $\phi^* \mathbf{U}$, is interpolated at velocity point. 332

The discretization we propose is now clear: use monotonic high-order biased re-333 construction of ω^* and h^* to estimate the terms $\omega^* \mathbf{U}^{\perp}$, in the momentum equation, and 334 $h^*\mathbf{U}$, in the continuity equation. For the mass flux, this is the usual upwind interpola-335 tion. For the nonlinear Coriolis term the upwinding should be done in the direction of 336 the flux, namely \mathbf{U}^{\perp} , not in the direction of the momentum on which it applies. This 337 is the main originality of this paper. 338

3 Discretization 339

We now present the model discretization by going through three aspects: the space 340 and time discretizations; and the handling of the boundary conditions. 341

3.1 Space discretization 342

The model equations are discretized on a logically rectangular C-grid. In the C-343 grid there is a natural distinction between the *primal* grid and the *dual* grid (Figure 1a). 344

In this paper we chose to map the primal grid centers with integer indices and the dual 345 grid centers with half integer indices. The velocity components, both covariant and con-346 travariant, are defined on the edges of the dual grid, h^{\star} is defined at cell centers of the 347 primal grid and the vorticity terms ζ^* and f^* are defined at cell centers of the dual grid, 348 which are also the vertices of the primal grid. The rotated \mathbf{U}^{\perp} is defined on the edges 349 of the primal grid, which implies that its components are staggered compared to the com-350 ponents of U (Figure 1a). Following the C-grid terminology, we denote "u-point" and 351 "v-point" the place where u and v are discretized. 352

Because we use the index coordinates (i, j), the model equations are completely oblivious to e_1 and e_2 , the grid scale factors, which means that for u, v and h^* the space is seen as an array of regular indices, regardless of the underlying metric. Consequently the grid cells are truly squares, of size 1×1 in the index units. This also means that spatial interpolations, involved in the evaluation at non native locations, should be done on the regular grid of indices, not on the irregular grid of spatial locations.

Before giving the discretized equations we define three spatial operators. The first one is the finite difference operator

$$\delta_{i+1/2}[\phi] = \phi_{i+1} - \phi_i \tag{25}$$

estimating the along *i* partial derivative of ϕ at location i+1/2 assuming ϕ is discretized at integer locations along *i*. The converse is also needed $\delta_i[\phi] = \phi_{i+1/2} - \phi_{i-1/2}$ to estimate a partial derivative at location *i* using a quantity discretized at half integer locations. To designate an along *j* partial derivative we should use either $\delta_j[\phi]$ or $\delta_{i+1/2}[\phi]$.

The two others are interpolation operators, interpolating along direction i (or along the j direction, with the j index). The first one is the linear second order, or two points averaging

$$\overline{\phi}^{i+1/2} = \frac{1}{2} \left(\phi_i + \phi_{i+1} \right) \,, \tag{26}$$

and the second is the WENO reconstruction

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$$I_{i+1/2}[\phi^{\star}, U] = U \sum_{s \in S} c_s \, \phi_{i+s}^{\star} \,, \tag{27}$$

where S is the stencil of the reconstruction and c_s are the weights. In this paper we use *n*-order WENO reconstructions (Jiang & Shu, 1996; Shu, 1999), $n \in \{1,3,5\}$, whose stencils have n elements. The n = 1 case is the first order upwind interpolation and

we have either $c_0 = 1$ if U > 0, or $c_1 = 1$ if U < 0. In the n = 3, 5 cases the recon-375 struction is nonlinear because the weights c_s depend on $\{\phi_{i+s}, s \in S\}$. In any case $\sum_{s \in S} c_s =$ 376 1. Having an even number of points, the stencils are shifted in the upwind direction, which 377 depends on the sign of U. In the 5th order case, $S = \{-2, -1, 0, 1, 2\}$ if U > 0, and 378 $S = \{-1, 0, 1, 2, 3\}$ if U < 0. As defined, the interpolation operators use quantities 379 discretized at integer locations (ϕ_{i+s}) to estimate it at i+1/2. The reverse is also needed: 380 use quantities discretized at half integer locations to estimate it at i. In that case we would 381 write either $\overline{\phi}^i$ or $I_i[\phi^*; U]$. Note that (27) assumes that U is discretized at the location 382 where ϕ^{\star} is reconstructed. This will always be the case. For sake of completeness the 383 WENO reconstruction is detailed in the appendix. Note that (27) is referred as a *recon*-384 struction rather than an interpolation. Reconstruction is the word used when the quan-385 tity to be interpolated is a *finite volume* quantity, and interpolation is usually reserved 386 when the interpolated quantity is the density (e.g. h or ω), or equivalently the finite dif-387 ference quantity. In this paper, the WENO scheme is applied to h^* and ω^* , the finite 388 volume quantities. We therefore exclusively use the WENO reconstruction. 389

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With these notations defined, we can now give the discretized model equations. They read

 $U = u/e_1^2, \qquad V = v/e_2^2, \qquad B = g(b + h^*/A) + k,$ (28)

$$\nabla B \rightarrow (\delta_{i+1/2}[B], \delta_{j+1/2}[B])$$
 (29)

$$\mathbf{\nabla} \cdot (h^{\star} \mathbf{U}) \rightarrow \delta_i [I_{i+1/2}[h^{\star}, U]] + \delta_j [I_{j+1/2}[h^{\star}, V]]$$
(30)

$$\omega^{\star} = f^{\star} + \boldsymbol{\nabla} \times \mathbf{u} \quad \rightarrow \quad f^{\star} + \delta_{i+1/2}[v] - \delta_{j+1/2}[u] \tag{31}$$

$$k = \frac{1}{2} \mathbf{u} \cdot \mathbf{U} \quad \rightarrow \quad \frac{1}{2} \left(\overline{uU}^i + \overline{vV}^j \right) \tag{32}$$

$$\omega^{\star} \mathbf{U}^{\perp} \rightarrow (I_j[\omega^{\star}, V_m], -I_i[\omega^{\star}, U_m])$$
(33)

399 and

$$U_m = \overline{\overline{U}}^{ij+1/2}, \qquad V_m = \overline{\overline{V}}^{ji+1/2}.$$
(34)

The only place where the metric terms are used is in (28). The required metric terms are (e_1, e_2) , the edge lengths of the dual, at respectively u-points and v-points, and Athe primal cell area. In addition, and only during the initialization, A_v , the dual cell area, is needed to define $f^* = A_v f$.

Because of the rotation, the components of $\mathbf{U}^{\perp} = (-V, U)$ must be deduced from U through some averaging because U and V are discretized at (i + 1/2, j) and (i, j + 1/2, j)

- 1/2) whereas \mathbf{U}^{\perp} requires flipped locations. This is done with the four points averag-407 ing in (34). This averaging is one of the decisive ingredient of the TRISK discretization 408 (Thuburn et al., 2009; Ringler et al., 2010). 409
- The discretization (33) is the main originality of this paper. The WENO reconstruc-410 tion is usually applied on conservation laws written in flux form. In the case of the mo-411 mentum equation this is on the flux of momentum. Here, because of the vector invari-412 ant form, there is no momentum flux. But, as discussed earlier the nonlinear Coriolis term 413 is the vorticity flux and, as such, it can be computed with a WENO reconstruction. 414
- The idea of putting some kind of upwinding and monotonicity on the nonlinear Cori-415 olis term is not new. In some aspect, the anticipated PV method (APVM) (Sadourny 416 & Basdevant, 1985) implements it, although in a quite different fashion. APVM has been 417 compared to other sub-grid closures (Graham & Ringler, 2013) in the context of RSW 418 models. The APVM consists in expliciting the PV in the vorticity term ($\omega = qh$) and 419 in using a first order upwind interpolation of the PV in the local direction of the flow. 420 In the APVM there is no directional splitting. The APVM can be seen as a semi-lagrangian 421 method where the PV is estimated at the place where it was a time step earlier. As be-422 ing a first order interpolation, the APVM induces more enstrophy dissipation than the 423 method presented in this paper, while being energy-conserving. Also, contrary to our method 424 that is parameter free, the original APVM introduces a numerical parameter that must 425 be tuned with respect to the grid size and time step. A parameter-free extension of the 426 APVM has been proposed (Chen et al., 2011) for the small h deviations case, whose as-427 sumption our method does not require. Finally, the use of the finite volume ω^* makes 428 the APVM completely unnatural within the framework we propose. Indeed, it would re-429 quire to write $\omega^* \mathbf{U}^{\perp}$ as $q(h^* \mathbf{U}^{\perp})$. We would then use a centered discretization for the 430 mass flux $h^* \mathbf{U}^{\perp}$ and have the upwinding on the q term. This would completely break 431 the symmetry of treatment between the continuity and the momentum equation. With 432 this in mind, the discretization we propose appears oppositely quite natural, almost as 433 self emerging from the equations, without ad-hoc choice and parameter-free. 434
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For the kinetic energy term we use (32), which is a classical discretization. However, it is worth noting that the kinetic energy term could also be discretized with a WENO 436 reconstruction, as follows 437

$$\overline{uU}^{i} + \overline{vV}^{j} \to s_{u} I_{i}[uU, s_{u}] + s_{v} I_{j}[vV, s_{v}]$$
(35)

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with $s_u = \operatorname{sign}(\overline{U}^i)$ and $s_v = \operatorname{sign}(\overline{V}^j)$ inside the operator, to keep track of the upwinding directions at the grid center, and as prefactors, to ensure positivity even if $s_u < 0$ or $s_v < 0$. Doing so would seriously increase the number of FLOP per time iteration (see Section 4). Given the lack of obvious immediate benefit, we did not pursue this idea further.

The use of WENO for the kinetic energy term may look surprising, at least for the 444 reader not familiar with the differential geometry. The differential geometry identifies 445 the spatial derivative in the flow direction of a quantity as the Lie derivative of its as-446 sociated differential form (Frankel, 2011). The Cartan identity splits the Lie derivative 447 in two terms, each one participating to the transport in a very specific way. For the mo-448 mentum, the associated differential form is \mathbf{u} , and these two terms are the nonlinear Cori-449 olis term and the gradient of kinetic energy of the vector-invariant form. Each term can 450 be seen as a composition of two basic operations of the differential geometry: the exte-451 rior derivative and the interior product, respectively a generalization of the ∇ operator, 452 and of the inner product. In the discretized equations we presented, the exterior deriva-453 tive shows up as the finite difference operators $\delta_i[\cdot]$ and $\delta_j[\cdot]$, whereas the interior prod-454 uct shows up as the WENO reconstruction operators $I_i[\cdot]$ and $I_j[\cdot]$. The idea of using 455 Cartan identity to discretize the transport of a vector field was pioneered by Mullen et 456 al. (2011), who also showed that a WENO reconstruction improves the accuracy, com-457 pared to the upwind first order reconstruction. Here we somehow generalize these results 458 to the full RSW equations. 459

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3.2 Time stepping

The code clearly separates the time scheme in one generic module. The implementation of a time scheme is very close to a textbook presentation. This is made possible because space and time discretizations are independent. The model variables are split into two groups: the prognostic variables $\phi = (u, v, h^*)$, obeying an explicit time evolution equation, and the diagnostic variables $\Phi = (\zeta^*, U, V, p)$. Formally, the code handles $s = (\phi, \Phi)$ the model state, as a collection of all variables, that obeys $\partial s/\partial t = L(s)$, with L the model operator. To better expose the prognostic and the diagnostic parts L



Figure 1. a) The classical C-staggering with locations for scalars (orange circles), vector components (blue circles) and vorticity (purple circles). The features (vertices, edges, faces) are colored in purple for the primal grid and orange for the dual grid. b) Illustration of the vorticity upwinding. Away from the boundaries, the vorticity flux (red arrow) at the v-point (red circle) is computed as the product of U (blue arrow), interpolated with a four points averaging (dotted blue arrows), and ω^* reconstructed along i using the five points stencil $(L_2, L_1, L_0, R_0, R_1)$. If cell A is masked, the stencil is shortened (L_1, L_0, R_0) ; if both cell A and cell B are masked, the stencil is (L_0) . In that latter case, if U were to the left, the vorticity would be reconstructed with the stencil (R_1, R_0, L_0) .

468 can be expanded into

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$$\frac{\partial \phi}{\partial t} = \mathsf{R}[\phi, \Phi] \tag{36}$$

$$\Phi = \mathsf{D}[\phi], \tag{37}$$

with R the right hand side for the prognostic variables and D the diagnostic relations for
Φ. Currently the code proposes two time schemes: the Leap-Frog Adams Moulton scheme
(LFAM3) (Shchepetkin & McWilliams, 2005) and the 3rd order stably strongly preserving Runge Kutta scheme (Gottlieb et al., 2001) (RK3)

$$s^{(1)} = s^n + \Delta t \,\mathsf{L}[s^n] \tag{38}$$

$$s^{(2)} = s^{n} + \frac{1}{4}\Delta t \left(\mathsf{L}[s^{n}] + \mathsf{L}[s^{(1)}]\right)$$
(39)

$$s^{n+1} = s^n + \frac{1}{6}\Delta t \left(\mathsf{L}[s^n] + \mathsf{L}[s^{(1)}] + 4\,\mathsf{L}[s^{(2)}]\right), \tag{40}$$

where Δt is the time step and s^k the model state at time step k. Both are third order in time. The LFAM3 is a predictor corrector scheme with only two calls to the right-hand side L per time iteration, whereas RK3 requires three calls to the right-hand side. RK3 is the model default choice.

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3.3 Boundary conditions at lateral boundaries

RSW models are quite often tested either in bi-periodic domains or on the whole 483 sphere, more rarely in domains with lateral boundaries. For oceanic applications, han-484 dling the lateral boundaries is a necessity. The other reason to present the lateral bound-485 ary conditions is that they fit particularly well with the choice of upwinding the vortic-486 ity in the nonlinear Coriolis term. The no-flow is enforced at no cost thanks to the C-487 grid but interestingly, the free-slip and the no-slip boundary conditions appears very nat-488 urally as conditions on the vorticity, which directly impact the normal component of flux 489 of vorticity at the boundary. 490

Solid boundaries can be either at the domain boundary or inside the domain. For 491 the latter case, we use a mask system $m_{i,j}$. A cell (of the primal grid) is solid if $m_{i,j}$ 492 0, fluid if $m_{i,j} = 1$. The no-flow boundary condition is imposed at each edge of the pri-493 mal grid where one adjacent cell is solid. It simply consists in setting u = 0 or v = 0494 at this edge. This is the standard technique. The real point of attention is on defining 495 ζ^* at points sitting along the boundary. The curl expression (31) cannot be immediately 496 used because the dual cell is not fully fluid. However, ζ^* conserves its physical mean-497 ing of being both the amount of vorticity in this partial cell, and the circulation along 498 the boundary of this partial cell. The latter offers the natural way to define ζ^{\star} , which 499 completely depends on the slip condition. In the free-slip case, $\zeta^* = 0$ at points along 500 the boundary. In the no-slip case, we keep compute ζ^* with (31) but we set u = 0 and 501 v = 0 for all edges, not fully in the fluid. For a straight boundary, say along i at j =502 0 and the fluid being for j > 0, this definition yields $\zeta_{i,0}^{\star} = -u_{i,1/2}$, which expresses 503 that a right-going flow generates a negative vorticity. The use of the differential forms 504 remove, once again, all the metric terms from the relation. The no-slip boundary con-505 dition behaves as a source of vorticity localized at the boundary. Interestingly, once this 506 vorticity is generated, it might be transported into the fluid by the nonlinear Coriolis 507 term. Let us see how. 508

For cell edges close to the boundary, the five points stencil of the the WENO 5^{th} 509 does not fit in. To overcome this issue, the code implements a varying stencil width with 510 the following policy: use the widest biased stencil, i.e. either one, three or five points, 511 fitting within the fluid cells. The one point stencil is the upwind first order interpola-512 tion. For the three points stencil, we use the third order WENO reconstruction (Shu, 513 1999) (explicited in Appendix A). The consequence is that the outward vorticity flux 514 at the edge next to the boundary is computed with a first upwind scheme, that adds a 515 little bit more of dissipation. In the free-slip case, since $\zeta^{\star} = 0$ at the boundary there 516 is no outward flux. 517

Instead of imposing the velocity at the boundary, and therefore the vorticity, we may want to impose the normal stress. In that case, it requires to introduce a viscosity to relate the stress to the velocity. We did not pursue this idea further as it is beyond the scope of the paper.

522 4 Speed

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4.1 Implementation choices

Performances on both the quality of the solutions and the speed were the top pri-524 orities in the code design. To achieve speed, a compiled language is required. Until re-525 cently this imposed the use of Fortran or C or a blend of Python and C (Pressel et al., 526 2015). The Julia language is currently used on several projects (Ramadhan et al., 2020; 527 Klöwer et al., 2020), whose chief advantage is to be a compiled language. Here we chose 528 another route. The code is entirely written in Python, without sacrificing speed. This 529 is possible thanks to the numba module. Numba (Lam et al., 2015) uses the LLVM com-530 piler (Lattner & Adve, 2004) to compile Python code. The bulk of the code is interpreted 531 Python, but all the computational functions are compiled. In practice, to compile a func-532 tion amounts in specifying its signature, namely the types of its inputs and outputs. In-533 side a function, and contrary to the pythonic policy, the loops can be explicitly devel-534 oped; the compiler takes care of them. Note that since Julia's compiler is also LLVM, 535 it makes the use of Julia less decisive for HPC. 536

The second element of speed is to systematically duplicate all arrays. Arrays are thus stored in [k,j,i] and in [k,i,j] conventions, the k index being for the layer index. The motivation is to always do finite differences with the convention where the data

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are contiguous in memory. Thus, the computation of the spatial derivative $\partial/\partial j$ or of 540 the along j-interpolation is done with the [k,i,j] convention. Data contiguity allows 541 a better usage of the L1-cache, which is the fastest. The price of duplicating is to per-542 form transpose operations to exchange the data from one convention to the other. For-543 tunately, the transpose operation is very fast as it is highly optimized. In practice the 544 transpose operation is done 20 times per time stage, which represents 16% of the total 545 time. Another advantage of this approach is to easily guarantee the numerical isotropy. 546 The two directions i and j are treated absolutely equivalently because there is only one 547 function for both operations. This is particularly convenient for the WENO reconstruc-548 tion. The WENO reconstruction, even though requiring many more operations than the 549 linear interpolation, is not much slower. 550

A third element of speed is of course the use of the covariant equations with the index coordinates that turn spatial differentiations into subtractions. The number of multiplications is minimal. The only computation involving many multiplications is the WENO reconstruction.



Figure 2. Walltime per time iteration T rescaled with $N/(n_x n_y)$. On the left for the monocore case as a function of the domain size $n_x n_y$ and on the right the weak scaling, where the number of cores N is increased from N=1 up to N=1024, while the domain size per core $n_x n_y=10^4$ is kept constant. In blue are the performances for the supercomputer and in orange for a notebook (see text for the CPU specs).

4.2 Speed assessment

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With these choices, the code (Roullet, 2021) is very fast. With the default 5^{th} or-556 der WENO, and the SSP-RK3 time scheme, the code speed is about $0.3 \,\mu s$ per iteration 557 per grid point (Figure 2). The performances have been measured on a notebook (Intel[®]) 558 CoreTM i7-6600U at 2.6GHz) and Rome (AMD[®] EPYC 7502 at 2.5GHz) a supercom-559 puter hosted at TGCC (Saclay, France). Timing has been averaged over thousand time 560 iterations and excludes the I/O. The code has an almost perfect weak scaling (Figure 2b). 561 We may wonder how close is the code speed to the peak CPU performances. To answer 562 it we need to determine how many floating operations are done per grid cell and per time 563 iteration. 564

To estimate how far this speed is from the maximum peak performance of the CPU, 565 we count all the floating point operations (Table 1). The current implementation uses 566 840 Flop per time step and per grid point. With the minimum time T = 400 ns on the 567 Rome supercomputer, this gives 2.1 GFlop s^{-1} , which corresponds to 84% of the CPU 568 clock frequency. It is not overstated to say that this implementation is close to the max-569 imum hardware limits. Interestingly, with 708 Flop, the WENO reconstruction is the ma-570 jor contributor, representing 84% of the total Flop. By using a linear interpolation (up-571 wind 5^{th}), the reconstruction involves only 108 Flop¹ and therefore only 240 Flop per 572 time step. Naively we could expect the code to be 840:240=3.5 time faster. This is not 573 the case. In practice the linear interpolation gives $T \approx 350 \ ns$ corresponding to 0.7 GFlop s^{-1} . 574 The reason is clear. In this case the code speed is limited by the memory access, which 575 makes the CPU waiting for data. By increasing the arithmetic intensity, the use of WENO 576 puts the code into the compute-bound region, which maximizes the Flop per second. 577

578 5 Accuracy

The merits of the numerical choices are tested with three experiments, each testing one aspect: the merging of two vortices, the interaction of a dipole in an elliptical domain with free and no-slip condition, a dam break experiment in an annulus. The experiments are set in quite intense nonlinear regimes, although not going up to either shock wave formation or dry bed emergence.

 $^{^1\,\}mathrm{Corresponding}$ to 3 stages, 2 functions, 2 directions, 5 multiplications and 4 additions.

Function	Term	#M	#A
Continuity	WENO 5^{th}	64	54
	$\mathrm{d}(h^{\star}\mathbf{U})$	2	4
Vorticity flux	WENO 5^{th}	64	54
	\mathbf{U}^{\perp}	2	4
	Coriolis	2	4
	$\omega^{\star} \mathbf{U}^{\perp}$	2	2
Bernoulli	grad	0	4
Diagnostics	U	2	0
	ζ^{\star}	0	3
	$\mathbf{u} \cdot \mathbf{U}/2$	3	3
	$g(h^\star + h_b^\star)/A$	2	1
Total per stage		143	133
SSP RK3	stage 1	1	1
	stage 2	2	2
	stage 3	3	3
Total per time	435	405	

Table 1. Number of floating operations a breakdown

^aFloating points operations involve multiplications (#M) and additions/subtractions (#A). The numbers are given per grid point and per call to the function. For the RK3 time stepping, which is the default, the total number per time step is the three times the total per stage plus the operations in the time scheme itself.

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5.1 Merging of two vortices

This first set of experiments tests the sensitivity of the conservation laws on the model resolution. The experiments consist in the time evolution of two Gaussian vortices initially in geostrophic balance. The two vortices, of radius $\sigma = 0.07$, are separated by a distance $d = 1.4 \sigma$; specifically

$$h(x, y) = H + h_0 \left(G(x - d/2, y; \sigma) + G(x + d/2, y; \sigma) \right) ,$$

with $h_0 = 0.2$, H = 1 and $G(x, y; \sigma) = \exp[-(x^2 + y^2)/(2\sigma^2)]$. The domain is square, 590 with an edge length L = 1. We use the free-slip boundary condition. The two physi-591 cal parameters are g = 1 and f = 5 which yield a Rossby deformation radius R =592 $\sqrt{gH}/f = 0.2$, that sets the vortices in the submessive range. The speed scale is $gh_0/(f\sigma)$, 593 which yields a Rossby number of $Ro = gh_0/(f\sigma)^2$, namely $Ro \approx 1.6$, again typical of 594 the submessescale regime. The vortices are anticyclones because $h_0 > 0$. The flow is in-595 tegrated up to time t = 10. The domain is meshed with N^2 grid cells of uniform size. 596 N is varied from N = 100 to N = 3,200, by a succession of doubling. 597

The two vortices are close enough to merge, as revealed by the presence of single 598 core of negative PV in the center at t = 10 (Figure 3), instead of two initially. The de-599 tails of the merging sequence depend on the resolution, among which the amount of fil-600 aments and the balancing time. But quite clearly, and fortunately, the solution converges 601 with increasing N. The cases N = 1,800 and N = 3,200 are almost indistinguishable 602 by eye. A striking property is the absence of noise on the PV fields, for all resolutions. 603 This is a consequence of the implicit dissipation and mixing provided by the MILES ap-604 proach. A second striking feature is the capability for the code to produce and maintain 605 very thin filaments. Of course the case N = 3,200 is quite extreme for such a trivial 606 flow but nevertheless it is worth emphasizing. Not only are the filaments thin, they can 607 also be intense in terms of PV difference with the background state. This results in the 608 shear instability of a few filaments, as seen on the N = 1,800 case. 609

To better assess the convergence with the resolution we diagnosed the cumulative global dissipation (Fig. 4a-b) for both the energy $\epsilon_E = (E_0 - E)/E_0$ and the enstrophy $\epsilon_Z = (Z_0 - Z)/Z_0$, where the superscript 0 denotes the value at t = 0. The global energy E is defined as $E = \int eh^* - E_b$, with the energy density

$$e = \frac{1}{2}\mathbf{u} \cdot \mathbf{U} + \frac{1}{2}gh\,,\tag{41}$$

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Figure 3. Snapshots of potential vorticity at t=10, after the vortices merged, for four resolutions $n_x n_y = 100^2$, 200^2 , 800^2 , $3,200^2$. Only a quarter of each domain is displayed. The parameters are g=1, H=1, f=5. The anticyclones were initially Gaussian, in geostrophic balance, with a layer depth h=1.3 at their center.

and the background potential energy $E_b = \int (gH^2/2) dx dy$. E_b is removed from $\int eh^*$ 615 because it is the part of the energy that cannot be dissipated. This is the energy of the 616 rest state. Still, the total amount of energy dissipated is fairly small: $\epsilon_E \sim 2\%$ for N =617 100 and $\epsilon_E \sim 4.10^{-5}$ for N = 3,200, which is approaching perfect conservation. The 618 code actually reaches the point where the question becomes theoritical: during a vor-619 tex merging event should the energy dissipation go to zero in the limit of infinite reso-620 lution? The present experiments suggest that not but this would deserve a more thor-621 ough study, beyond the scope of this paper. The case of the enstrophy dissipation (Fig. 4b) 622 is very different. In all cases there is a finite amount of dissipation but the increase of 623 resolution delays the time at which the dissipation really starts, as well as it increases 624 the equilibration time. In the N = 100 case, the merging process is almost completed 625 as indicated by the plateau, at the largest resolution, there is still a lot of enstrophy to 626

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Figure 4. Energy (a) and enstrophy (b) dissipated as a function of time and resolution (color) for the vortex merging experiment. The energy of the rest state $gH^2/2$ has been removed from E and E_0 . (c) probability density function of potential vorticity at t = 0 (blue), t = 2 (red) and t = 10 (orange) for the merging experiment at the 3,200² resolution.

be dissipated. It is not clear whether all resolutions yield the same amount of enstrophy dissipation. Again this requires a more thorough study that we postpone for a later
paper.

Finally to assess the material conservation of PV we plot the probability density 630 function of PV in the N = 3,200 case for t = 0, t = 2 and t = 10 (Fig. 4c). At t = 2631 the enstrophy dissipation has not yet started (Fig. 4b) meaning the flow is still inviscid, 632 even though the vortices are already producing filaments (not shown). The pdf of PV 633 is remarkably close to its t = 0 value. Material conservation is very well ensured. At 634 t = 10 the pdf departs from its initial value. This is due to the mixing at the grid-scale. 635 Interestingly the PV on the cyclonic part (the initial vortices are slightly shielded with 636 a ring of cyclonic PV) remains quite well conserved. This confirms the visual impression 637 of the snapshot (Fig. 3), the cyclonic PV does not filament, therefore it does not mix, 638 therefore its pdf should remain constant in time, as it does. 639

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5.2 Vortex-wall interaction

In this set of experiments we test how the code performs on handling boundary conditions. The experiments consist in the time evolution of a vortex dipole with either the free-slip or the no-slip boundary condition (Figure 5). In order to have a variety of boundary shapes at the grid scale, the domain is elliptical, whose major and minor axis lengths are respectively 2 and 1. The grid is $1,600 \times 800$ with square grid cells. The experiments are started at t = 0 with two Gaussian vortices initially in geostrophic balance at the center of the domain. The two vortices, of radius $\sigma = 0.1$, are separated by a distance

 $_{648}$ $d = 1.1 \sigma$; specifically

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$$h(x,y) = H + h_0 \left(G(x - d/2, y; \sigma) - G(x + d/2, y; \sigma) \right)$$

with $h_0 = 0.15$ and H = 1. The two physical parameters are g = 1 and f = 5.



Figure 5. Potential vorticity snapshots of the dipole-wall interaction in the free-slip case at t = 12 (a) and no-slip case at t = 12 (b) and t = 40 (c). (d) Evolution of the energy and the enstrophy in the no-slip case. The resolution is $1,600 \times 800$. The initial position of the dipole center is at (1, 0.5).

In either cases, the dipole starts to move along the minor axis Southward, while 651 a weak trail of opposite PV, due to the vortex shield, moves Northward. As the dipole 652 approaches the wall, the dynamics starts to differ between the free-slip and the no-slip 653 boundary conditions. In the free-slip case, the dipole splits and each vortex continues 654 its journey, following the wall, in an inviscid manner, according to the mirror rule (Fig. 5a). 655 The PV remains materially well conserved, even close to the boundary. In particular there 656 is no spurious source or sink of PV near the wall. The no-slip case differs dramatically 657 (Fig. 5b). The phenomenology is well documented even though it is usually studied in 658 the context of the two dimensional Euler equations (Keetels et al., 2007; Farge et al., 2011). 659 The dipole generates a thin ribbon of opposite PV along the wall. As the dipole splits, 660 this ribbon detaches from the wall and gets entrained in the domain where it wraps around 661 each vortex. This halts the vortex drift along the wall. Instead, the vortices describe a 662

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loop and hit the wall again, generating another ribbon of PV that is later detached. The 663 rebonds continue causing the initial vortices to remain trapped near the collision point. 664 The series of layer detachments seed the flow with PV ribbons. The ribbons width and 665 the magnitude of their vorticity depend on the numerical resolution. For this experiment, 666 the ribbons are strong enough to experience shear instability causing them to roll up into 667 small vortices. The domain is thus progressively filled with a swarm of small scales vor-668 tices (Fig. 5c). The dipole-wall interaction is fundamentally dissipative. It dissipates en-669 ergy but it creates enstrophy (Fig. 5d). After the first collision (t = 8), the dissipated 670 energy $(E_0 - E)/E_0 \approx 310^{-4}$, whereas the created enstrophy $(Z - Z_0)/Z_0 \approx 30\%$. 671 During the following collisions, the dissipated energy increases steadily up to $6\,10^{-4}$ at 672 t = 40. The enstrophy behaves differently: it globally increases with time but with os-673 cillations. As the PV distribution becomes more and more random, the amount of cre-674 ated enstrophy plateaus at roughly 30%. In comparison, in the free slip case and at t =675 40, $(E_0 - E)/E_0 \approx 3 \, 10^{-6}$, and $(Z - Z_0)/Z_0 \approx -2 \, 10^{-3}$, which again shows the code 676 ability to preserve global invariants, even though the numerics has a build-in mechanism 677 for dissipation. 678

The solution at t = 40 has become quite turbulent (Fig. 5c), suggesting a fairly 679 large Reynolds number. Determining the Reynolds number is a challenging task because 680 there is no explicit viscosity in the model. The dissipation is solely handled by the WENO 681 reconstructions, in a highly implicit manner. This is a classical issue with the implicit 682 approach (Zhou et al., 2014). A possibility is to diagnose an effective numerical viscos-683 ity $\nu = Z^{-1} dE/dt$, based on the fact that for a true viscous operator the energy dis-684 sipation rate is related to Z by $dE/dt = -\nu Z$. From this numerical viscosity we can 685 form an equivalent Reynolds number $Re = E^{1/2}/(H\nu)$. With this metric, the Reynolds 686 number at t = 40 is $Re \sim 3.10^9$. 687

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5.3 Dam-break problem

In this last experiment we focus on the gravity waves dynamics, and its relation with the PV, on a dam-break experiment. To illustrate the code ability to handle curved coordinates we use an annulus domain with inner radius $r_0 = 1$ and outer radius $r_1 =$ 2. The coordinates (i, j) represent respectively the radial and the orthoradial directions. The metric tensor reads $\mathbf{g} = \text{diag}(dr^2 r^2 d\theta^2)$, where dr and $r d\theta$ are the grid lengths in the *i* and *j* direction. The discretization is uniform in dr and $d\theta$, with respectively

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and 200 grid points in *i* and 1,600 in *j*. The initial state is $h = H + h_0 \tanh(y/\sigma)$ and $\mathbf{u} = 0$, with $y = r \sin \theta$, $h_0 = 0.15$, H = 1 and $\sigma = 0.05$. The two physical parameters are g = 1 and f = 5. The imbalance at t = 0 generates inertia-gravity waves and



Figure 6. Snapshot of layer depth (a) and potential vorticity (b) at t=1.5 resulting from a dam-break located along y=0, with amplitude $\Delta h=0.3$. The other parameters are g=H=1 and f=5. Cylindrical coordinates are used to define the model metric. The resolution is $200 \times 1,600$.

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four Kelvin waves, two along each boundary. The Kelvin waves have a clear signature 698 on h (Fig. 6a), propagating along the boundaries with the boundary on their right (be-699 cause f > 0), with a trapping width consistent with $R_d = 0.1$. Their propagation speed 700 is close to $c = \sqrt{gH} = 1$ as a visual estimate tells: at t = 1.5 the Kelvin waves prop-701 agating along the inner boundary have moved of roughly a quarter turn. The agreement 702 is not perfect because the regime is nonlinear enough, introducing nonlinear corrections 703 in the wave speed. The structure of the inertia-gravity waves is more complicated. There 704 is a net asymmetry between the waves propagating on the shallower part $H - h_0$ and 705 the deeper part $H+h_0$. On the shallower part, the waves have clear nonlinear effects, 706 as revealed by the series of small scales ripples and suggestive of shock wave dynamics. 707 As there is no particular numerical treatment to handle the correct dissipation at shocks, 708 there is no warranty that these ripples should be there, although they might be solitons. 709 Having such small scales patterns on h is really due to the 5th order WENO reconstruc-710 tion on the mass flux. Switching to a first order interpolation removes all these signals 711 and makes h very smooth. 712

In contrast, the PV field has a very simple structure (Fig. 6b). At t = 1.5, the 713 geostrophic currents, resulting from the geostrophic adjustment and localized along the 714 initial discontinuity, have started to transport PV. This is the reason for the PV jump 715 to be deformed near the boundaries. The PV field is remarkably free of any wave sig-716 nal, except at the shock waves places where the PV exhibits the same ripples structure 717 than the wave. These ripples are indicative of dissipation in action, breaking the invis-718 cid assumption and the material conservation. Interestingly these PV ripples propagate 719 with the waves so that their rectifying effect on the PV is much smaller. With this col-720 orscale the net effect is invisible but a magnified colorscale reveals thin striations at few 721 places. These small amplitude striations are the clear evidence that dissipation occurred 722 which yielded local creation and destruction of PV. We will not go into more details as 723 the study of wave-PV coupling is far beyond the scope of this paper. However we be-724 lieve the numeric we propose is very promising to study these questions. 725

726 6 Conclusions

In this paper we have presented a fast and accurate discretization for the RSW equa-727 tions. Accuracy, measured in terms of potential vorticity dynamics and conservation laws, 728 is achieved by adapting the MILES approach (Boris et al., 1992) to the vector-invariant 729 form of the RSW equations. The decisive step is to use a 5th order WENO reconstruc-730 tion on both the mass flux and the nonlinear Coriolis term. Currently the method re-731 quires a logically rectangular C-grid. The generalization to the cubed sphere is possi-732 ble, the difficulty lays in handling the vorticity interpolation at the grid cells next the 733 cube edges. The generalization to hexagonal grids is more challenging because the vor-734 ticity points are not immediately aligned with \mathbf{U}^{\perp} , but the recent developments on WENO 735 reconstructions for unstructured grids (Tsoutsanis et al., 2011) pave the way to a clean 736 solution. Speed is achieved with a series of choices rather than a single recipe, yet with 737 a pure Python code. Though not the main point of this paper, we clearly proved that 738 Python has become a serious option for HPC, rivaling with Fortran. In the perspective 739 of using trained neural networks as parameterization for models, having a kernel in Python 740 is an advantage. The code reaches typically 2 GFlop per second per core on a classical 741 CPU architecture, which is above half the theoretical peak performance. The choices are: 742 a reformulation of the continuous equations, the use of the Numba module to compile 743 the most demanding functions, and the duplication of all arrays in two memory layouts 744

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to increase the arithmetic intensity by ensuring data contiguity in all functions. The re-745 formulation is based on the introduction of h^{\star} and ω^{\star} , the finite volume version of h and 746 the vorticity ω ; the use of index coordinates (i, j); and the introduction of **u** and **U**, 747 respectively, the covariant and the contravariant velocity. The grid lengths are used at 748 only two places, to compute **U** from **u** with the metric tensor **g**, and to relate h to h^* . 749 Everywhere else grid lengths are gone. Finite differences boil down to subtractions with 750 no multiplication or division, which reduces the number of Flop and the amount of data 751 transfered between the CPU and the memory. 752

With these choices, the floating points operations associated with the WENO re-753 constructions represent 85% of the total number of operations and, thanks to data con-754 tiguity, these operations are done at the CPU clock frequency, without being penalized 755 by memory access. This particular combination of a large fraction of the total Flop with 756 the data available in the fastest L1 cache is responsible for the overall code speed. 757

From the physical point of view, the numerical solutions show remarkable prop-758 erties: the PV field does not exhibit any noise at the grid scale, the material conserva-759 tion is excellent as far as the flow does not require enstrophy dissipation. The energy dis-760 sipation is vanishingly small with increasing resolution, even in the case where a finite 761 amount of enstrophy is dissipated. The code handles arbitrary shaped domains with both 762 free-slip and no-slip condition. The boundary condition on momentum is done quite nat-763 urally through the definition of the vorticity along the boundary, which is used to esti-764 mate the nonlinear Coriolis term. The no-slip boundary condition generates enstrophy, 765 as expected, whereas it dissipates energy. In that case, by interacting with the bound-766 ary, an initially smooth PV field continuously develops fine scale structures, causing the 767 flow to become turbulent. Finally we have shown on a dam-break experiment that the 768 PV field remains very smooth even when small scale waves propagate. The build-in nu-769 merical dissipation allows the code to handle shock waves without blow-up even though 770 it remains to be proven that this implicit dissipation satisfies the proper entropy con-771 dition on shock waves. 772

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This paper has shown a new way of implementing the MILES approach in a RSW model. Several generalizations can be contemplated, some of them already mentioned 774 earlier, but the real generalization is to adapt this idea to the full three dimensional equa-775 tions, in the non-hydrostatic regime. The extension is simple: use the WENO reconstruc-776

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tion to each sub-term of the vortex-force term. The hope is that it provides enough buildin dissipation to handle the direct cascades of both enstrophy and energy, and it acts as
a substitute for an explicit subgrid-scale closure. This idea has already been turned in
a real LES code, that shows comparable performances to the code presented in this paper.

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Appendix A WENO reconstruction

We now specify the $I_{i+1/2}[\phi, U]$ operator, that computes the flux $U\phi$ at location i+1/2. Because the operator is applied to finite volume quantities exclusively, it is strictly speaking a *reconstruction*, rather than an *interpolation*. We use the original WENO reconstruction (Jiang & Shu, 1996; Shu, 1999), also denoted WENO-JS. We express it in terms of Legendre polynomial (Balsara et al., 2016). We assume without loss of generality U > 0 and we start with the fifth order case, which is the general case.

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A1 5th order case

The fifth order reconstruction is based on the three stencils $S_1 = \{i-2, i-1, i\}$, $S_2 = \{i-1, i, i+1\}$ and $S_3 = \{i, i+1, i+2\}$ relative to cell index *i*. The reconstruction reads

$$I_{i+1/2}[\phi, U] = U\left(w_1\tilde{\phi}_1 + w_2\tilde{\phi}_2 + w_3\tilde{\phi}_3\right)$$
(A1)

794 with

$$\tilde{\phi}_k = \phi_i + \phi_k^{(1)} P_1(1/2) + \phi_k^{(2)} P_2(1/2) , \qquad (A2)$$

$$w_k = \frac{\alpha_k}{\alpha_1 + \alpha_2 + \alpha_3}$$
 and $\alpha_k = \frac{\gamma_k}{(\beta_k + \epsilon)^2}$ (A3)

where $P_1(x) = x$, $P_2(x) = x^2/2 - 1/24$ are the Legendre polynomials on the [-1/2, 1/2]interval, and w_k are the nonlinear weights associated with the stencils S_k . The discretiza-

tion is completed with the definitions of the smoothness indicator

$$\beta_k = \left(\phi_k^{(1)}\right)^2 + \frac{13}{12} \left(\phi_k^{(2)}\right)^2 \,, \tag{A4}$$

the value of first $(\phi_k^{(1)})$ and second $(\phi_k^{(2)})$ moments associated with the stencil S_k

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$$\phi_1^{(1)} = (\phi_{i-2} - 4\phi_{i-1} + 3\phi_i)/2$$
 and $\phi_1^{(2)} = (\phi_{i-2} - 2\phi_{i-1} + \phi_i),$ (A5)

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$$\phi_2^{(1)} = (-\phi_{i-1} + \phi_{i+1})/2$$
 and $\phi_2^{(2)} = (\phi_{i-1} - 2\phi_i + \phi_{i+1}),$ (A6)

$$\phi_3^{(1)} = (-3\phi_i + 4\phi_{i+1} - \phi_{i+2})/2 \quad \text{and} \quad \phi_3^{(2)} = (\phi_i - 2\phi_{i+1} + \phi_{i+2}), \quad (A7)$$

and the linear weights

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$$\gamma_1 = 1/10, \quad \gamma_2 = 3/5, \quad \gamma_2 = 3/10.$$
 (A8)

The regularization factor is set to $\epsilon = 10^{-8}$. These linear weights are the original ones proposed by Shu. They are the ones that makes the whole reconstruction fifth order at locations where ϕ is smooth.

The adaptation of this reconstruction to the case of the vorticity, namely $I_i[\omega, V]$, is straightforward. Because of the vorticity being discretized at half integers indices, the only change is to replace the ϕ_i terms with $\omega_{i-1/2}$ in the above formulas.

Close to boundary we use a 3rd order WENO reconstruction (Shu, 1999), if either $\{i-2\}$ or $\{i+2\}$ is outside of the domain but the $\{i-1, i, i+1\}$ cells are inside the domain. We downgrade to the 1st order reconstruction if either $\{i-1\}$ or $\{i+1\}$ is outside the domain. For sake of completeness we explicit the formula in these two cases.

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A2 3rd and 1st order cases

The third order case (Shu, 1999) reads

$$I_{i+1/2}[\phi, U] = U(w_1\tilde{\phi}_1 + w_2\tilde{\phi}_2)$$
(A9)

with $\tilde{\phi}_k = \phi_i + \phi_k^{(1)} P_1(1/2),$

$$w_k = \frac{\alpha_k}{\alpha_1 + \alpha_2}, \qquad \alpha_k = \frac{\gamma_k}{(\beta_k + \epsilon)^2}, \qquad \beta_k = \left(\phi_k^{(1)}\right)^2, \tag{A10}$$

 $\gamma_1 = 1/3, \ \gamma_2 = 2/3, \ \phi_1^{(1)} = \phi_i - \phi_{i-1} \text{ and } \phi_2^{(1)} = \phi_{i+1} - \phi_i.$

825 The first order case is simply

$$I_{i+1/2}[\phi, U] = U\phi_i \,. \tag{A11}$$

827 Acknowledgments

This work was supported by the French National program LEFE (Les Enveloppes Flu-

ides et l'Environnement) and also by the recurrent annual funding provided by the LOPS

- parent agencies UBO, CNRS, IRD and Ifremer. This recurrent funding is an important
- tool of the French research system that helps fundamental research. The work used HPC
- resources from GENCI-TGCC (Grant 2020-A0090112051). The code is available from
- https://doi.org/10.5281/zenodo.4968737.

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