Dear editor and two reviewers,

We appreciate your works on improving the quality of our manuscript. Many questions of yours propel us to do more inspections on our scheme LASM. Under the great driving force, we extend LASM to 3-D in these months, which we have planed to do in the next few months. Thank the editor for giving us so adequate time!

The following is our response to the two reviewers.

Response to #1 reviewer:

1. Questions: A price to pay in these models is that one needs to use an interparcel mixing algorithm when the density of parcels in an area becomes too large (and LASM needs a global mass fixer to map variables to a fixed grid!).

Answer: The interparcel mixing is needed because the parcel shape is not simulated very well or even not simulated at all. Therefore, it is not caused by the sparse density of parcels. If the density of parcels in an area is large, auto-refinement is needed to control the density of parcels, but in the current tests, even including a 3-D large-eddy simulation which is extremely turbulent, there is no need for considering refinement.

The global mass fixer is needed in some other Lagrangian schemes, such as HEL. ATTILA does not use the fixer, because it does not consider the mass conservation on the grids at all! The mass fixer can be dismissed if the tracer tendency is not calculated on the grids, so the remapped variables on the grids are just for diagnostics purpose.

2. Questions: The main novelty of this manuscript is the new mixing algorithm. Although the authors do not spend much space on the reactive species test case, the reviewer believes that provides new and interesting insights into physics-dynamics coupling with Lagrangian models.

Answer: More content for the physics-dynamics coupling is added. The two types of the tendency evaluation are discussed in section 2.3. The title is also changed to include 'physics-dynamics coupling'.

3. Questions: First of all, please provide more details on Figure 1 and 2. The reviewer does not clearly see what the authors are trying to explain with these Figures.

Answer: Figure 1 is used to show a case where the linear approximation of a parcel degenerated. If the parcel shape is simulated exactly, the skeleton points should on the ellipse in this case. In section 2.2, "The most direct symptom of this degeneration is that the positions of skeleton points (say s) deviate from the ones calculated from Hi (say s'). Fig. 1 demonstrates an example of degeneration, where the current shape of a parcel in red ellipse mismatches the skeleton points in green dots." The caption is improved.

Figure 2 compares the results of the deformation tests with different γ_m (i.e., the maximum permitted parcel filament degree). The second paragraph of section 3.1 explains this figure. When $\gamma_m = 2$, the parcels can not turn to be long, and excessive

mixing will distribute the tracer mass to the wrong places, which will cause the aliasing error. So a moderate value 5 is chosen for γ_m .

4. Questions: Secondly, testing the mixing algorithm on just a few idealized test cases seems to lack robustness testing. Do these tests span flow conditions found in realistic full model simulations? Could one compare the mixing algorithms in established models with the mixing algorithm in this manuscript? Could one do a turbulent flow and look at energy spectra for the tracers or some other mixing diagnostic (e.g., entropy measure as proposed in Lauritzen and Thuburn, 2011, QJRMS)?

Answer: We have conducted a 3-D large-eddy simulation to test LASM, which should be robust, since the flow is extremely turbulent. The parcel distribution is shown in Fig. 10 as the horizontally averaged number of parcels contained in the grid cells, and there is no trend during the simulation. We have calculated the entropy defined in Lauritzen and Thuburn (2011) for the deformation test, and the entropy is very small (0.00038) compared with ~0.01 in CSLAM (3rd-order with filter), but not zero since there is interparcel mixing.

5. Questions: The mixing algorithms have tunable parameters: what values would the authors settle on for "real-world" applications?

Answer: The conventional parameters are tabulated in Table 1. They may be needed to be adjusted in the "real-world" application.

6. Questions: Doing physics-dynamics coupling on the parcel grid leads to a noise-free solution while performing the coupling on the static mesh results in noise in Cl and Cl2. First of all, please provide details on the mapping from tracer grid to the static grid (Dong et al., 2014) and inform the reader how the tendencies are mapped from the static lat-lon grid to the Lagrangian grid. In particular, what variables are mapped: the product between mixing ratio and density or just mixing ratio? Is tracer mass conserved in the process?

Thereafter the authors are kindly asked to investigate further why doing the coupling on the static mesh leads to a noisy solution. Obviously the mapping from Lagrangian parcel space to the static mesh (and vice versa) preserves linear relations (since Cly is conserved!). Is it the mapping from parcel grid to lat-lon grid that results in noise, is it the mapping of tendencies from lat-lon to parcel grid that introduces noise, or both? Does the mass-fixer introduce noise? Could it be the large resolution difference between parcel grid (in areas of convergence) and 1 degree lat-lon grid?

The reviewer would like to see a much more comprehensive analysis and discussion of the physics-dynamics issue since that is one of the cruxes of Lagrangian models.

Answer: The density remapping formulas are shown in Eq. (9) and (10), and the mass tendency remapping from grids to parcels is shown in Eq. (21). The tracer mass is conserved in the process when evaluating the tendency on the parcels.

The noise solution when evaluating the tendency on the grids is caused by the negative density on the parcels, due to the inconsistency between parcels and grids, that is the tendencies are calculated based on the densities on the grids, which may be excessive

for the parcels. The problematic tendencies are disregarded in this study to avoid negative density. Because the chemical reaction is local, so the mass is still conserved in this case. When consider non-local processes (e.g., convection), the problematic tendencies should be redistributed to the right places to ensure mass conservation. We have rewritten section 2.3, and changed 3.3 accordingly.

7. Question: Section 2.4: This section reads as an internal planning document and should not be part of a journal paper.

Answer: This section has been deleted.

Response to #2 reviewer:

1. Question: One could have hoped that the updated mixing was derived from more physically based arguments than in the original LASM. However, I have troubles to see that this is generally the case. There seems to be a number of parameter settings that a set on an ad-hoc basis.

Answer: It is normal that every practical numerical scheme contains some kinds of artifacts. For example, the flux limiters or filters used in many Eulerian advection schemes to ensure positivity and monotonicity make those schemes nonlinear, which should be linear. The interparcel mixing added in LASM is inherited from the earlier Lagrangian schemes, such as STOCHEM (Stevenson et al. 1998) and ATTILA (Reithmeier and Sausen 2002). But because the parcels in LASM have shape, which is not the case in other Lagrangian schemes, some artifacts are needed to adjust the shape of some parcels that are not approximated well by the linear deformation matrix. The performance of the mixing was verified by some test cases, such as the deformation test case. It will be studied further when LASM is applied to real GCM.

2. Question: Another major issue is the cost of the scheme and in particular the cost of identifying the computational grid (or procedure) needed to perform the interparcel mixing. How can this parallelize on modern computers? How is the multi-tracer efficiency? A discussion of these issues is requested.

Answer: The search of the grid cells that are covered by a parcel is performed by a cover-tree algorithm (Beygelzimer et al., 2006), which is provided by a C++ machine-learning library (MLPACK). The time complexity of the search operation is O(log n), where n is the number of total grid cells. This number can be greatly reduced when run in parallel after the domain is decomposed into small ones. The multi-tracer efficiency of Lagrangian schemes is very high compared with Eulerian and semi-Lagrangian schemes, because different tracer species share a lot of information (e.g., trajectory, remapping coefficients). This statement has been verified by HEL (Kaas et al. 2013), see Fig. 13 there. This is also true for LASM. We have added a paragraph at the bottom of page 7.

3. Question: It is stated that the neighboring parcel shapes are unaffected by the mixing with them. But from a physical point of view one should expect that any mixing will tend to make the shape of the neighboring (as well as the actual) parcel more isotropic, i.e., the shape is actually influenced by the mixing.

Answer: The shape of the neighboring parcel is not changed, but the tracer density is affected by the mixing, so the mass is transferred among parcels. This resembles the diffusion in a Eulerian scheme, where the mesh cells are fixed. Only the degenerated parcel shape is changed to be more isotropic, and that parcel has the maximum weight (i.e., 1) when calculate the mean density. The reason for mixing in this way is to minimize the effects.

4. Question: A mass fixer is introduced. It should be discussed in a little more detail how this works. I presume it is only relevant for the Eulerian representation (i.e. on a regular grid) and not in the Lagrangian space of the parcels?

Answer: Yes, the mass fixer is used to ensure the tracer mass on the grids equals the one on the parcels, so it is only relevant for the Eulerian representation. The total mass on the parcels will be conserved all the time. Some paragraphs are appended in the end of section 2.1 to explain the mass fixer.

5. Question: It is unclear why a mass fixer in the grid representation is influencing the mass in parcel space. Couldn't one just fix the mass in Eulerian space without affecting that in parcel space. Or maybe I misunderstood. Please explain in more detail.

Answer: When evaluating the tendencies on the grids, the mass fixer will affect the masses on the parcels eventually, since the tendencies will be remapped back on the parcels. But as it is stated in section 2.3 and 3.3, it is better to evaluate the tendencies on the parcels. Then the mass fixer does not affect the parcel space.

6. Question: "... and respects the local flow properties". But the ATTILA mixing also respects local flow properties in terms of local deformation rate?

Answer: ATTILA does not respect the local flow properties. It only mixes the parcel centroids within one Eulerian grid cell. CLaMS (McKenna et al. 2002a) and HEL do respect the local flow properties by considering the deformation information.

7. Question: The re-shaping takes place after the mixing, and is independent of the degree of actual mixing. But what if no or insufficient mixing has actually occurred for parcel i because there were no or only rather distant neighbors. Then the parcel is re-shaped (to be more circular) even without being mixing. This seems physically inconsistent. If no mixing has taken place the physical parcel should keep its irregular shape until it can actually be mixed.

Answer: The parcel distribution is controlled by the flow, which is constrained by the fluid dynamics in turn. Therefore, the cases when the density of parcels is so low that a parcel has no neighbor should be very rare. We have conducted a large-eddy simulation to see what will happen when using extremely turbulent 3-D flow in the new section 3.4, and this did not happen. Reithmeier and Sausen (2002) ran ATTILA within ECHAM4 for 30 years, and the parcels were still well distributed. The auto-refinement algorithm may be designed in the future to improve the accuracy and performance, but for the time being, we would like to keep LASM as simple as possible.

8. Question: The γ_m value of 5 is apparently chosen on an ad-hoc basis. Such a large value implies that the domain of influence of a parcel is also large.

Answer: We have tested several values for γ_m , and 5 is a moderate value. γ_m does not imply that the domain of influence of a parcel is also large. It just measures how long a parcel is.

9. Question: It is unclear what is learnt from the right panel in Fig. 4. It could be deleted.

Answer: That figure is used to show that there are no ill-shaped parcels when using new mixing algorithm, compared with the old ones (the left one).

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An updated interparcel mixing algorithm in the Lagrangian advection scheme with shape matrix (LASM) v0.2: interparcel mixing, physics-dynamics coupling and 3-D extension

L. Dong¹, B. Wang^{1,2}, L. Liu², and Y. Huang^{3,4}

¹LASG, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China
 ²Ministry of Education Key Laboratory for Earth System Modelling, Center for Earth System Science (CESS), Tsinghua University, Beijing, China
 ³LACS, Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China
 ⁴University of Chinese Academy of Sciences, Beijing, China

Correspondence to: L. Dong (dongli@lasg.iap.ac.cn)

Abstract

The interparcel mixing algorithm in the Lagrangian advection scheme with shape matrix (LASM) is updated to make the scheme more robust. The linear degeneration criterion is replaced by the maximum deviation of the skeleton points so that the new algorithm is more effective in controlling the shape of parcels, which is vital for long time simulation. LASM is inherently shape-preserving without any complicated filter or limiter, so and it is linear. This fact contributes to the ability of LASM of preserving the sum of multiple tracers exactly on the parcels in LASM. A newly proposed terminator "toy"-chemistry test is also used to test LASM, which shows that LASM can preserve the weighted sum of two reactive chlorine-like species precisely. The physics-dynamics coupling (i.e., tendency evaluation type) is also discussed. A flow generated by a WRF large-eddy simulation is also used to test the 3-D extension of LASM.

1 Introduction

Lagrangian modeling approaches have long been recognized as a better alternative to the Eulerian or semi-Lagrangian ones for modeling the advection of tracers, due to their ability to reduce the numerical diffusion significantly, though some roadblocks need to be cleared. Therefore, more and more Lagrangian advection (or transport) schemes were proposed during the last two decades from different research communities. Based on the application objects, the research directions of the Lagrangian methods can be divided into four categories: (1) atmospheric dispersion modeling, (2) atmospheric chemical transport modeling, (3) cloud-resolving modeling, and (4) general circulation modeling. Lin et al. (2013) gave a panoramic view of the Lagrangian modeling of the atmosphere.

In the first category, the turbulent diffusion needs to be tackled thoroughly, because the temporal and spatial scales are relatively short and small respectively. These models are called Lagrangian Particle Dispersion Model (LPDM). The flow is decomposed into resolved mean and unresolved turbulent parts (the molecular diffusion is regularly ignored), where

the first part comes from the reanalysis or model output, and the latter part is described by the stochastic process (Thomson, 1987). Two of the representative schemes (or models) are HYSPLIT (Draxler and Hess, 1998) and FLEXPART (Stohl et al., 2005), which are used widely in the atmospheric emergency response, such as the volcanic ash cloud simulation. It is noteworthy that their turbulent diffusion formulations are different. Although the turbulent diffusion are both formulated in terms of the turbulent velocity components, FLEX-PART solves the Langevin equation with the assumption of a Markov process, but HYSPLIT uses an autocorrelation coefficient and a random component. Recently, FLEXPART was extended to WRF in Brioude et al. (2013). Another model is NAME III developed in UK Met Office (Jones et al., 2007).

The Chemical Transport Models (CTM) consider a large number of tracer species and chemical reactions in the second category. One of the widely used Lagrangian CTMs is STOCHEM (Collins et al., 1997; Stevenson et al., 1997, 1998; Utembe et al., 2010). Chemical Lagrangian Model of the Stratosphere (CLaMS) (McKenna et al., 2002b, a) is a more sophisticated CTM with a featured flow deformation based interparcel mixing. Hoppe et al. (2014) implemented CLaMS into ECHAM/MESSy Atmospheric Chemistry model (EMAC), and compared it with the standard flux-form semi-Lagrangian (FFSL) transport scheme in EMAC. In their results, the transport barriers at the edge of the polar vortex are better simulated in CLaMS. Another Lagrangian CTM is CiTTyCAT (Pugh et al., 2012). The boundaries between the above two categories are actually blurred, for example STOCHEM is incorporated in NAME III.

The third category includes the works on the cloud simulation in Lagrangian way. The clouds are divided into warm clouds and ice clouds. Shima et al. (2009) proposed a named the so called super-droplet method (SDM) aimed at for simulation of warm clouds. Each super-droplet represents a multiple number of real droplets with the same attributes and position. Sölch and Kärcher (2010) introduced a novel Lagrangian Cirrus Module (LCM), where the ice phase is simulated by a large number of simulation ice particles (SIPs) . Compared with the tradition bulk and bin schemes that contain heavily parameterized microphysics and radiative processes, LCM has less numerical diffusion, and the simulated

processes are more consistent without imposing thermodynamic equilibrium assumptions. Furthermore, Unterstrasser and Sölch (2014) added SIP splitting and merging operations to increase the efficiency of LCM. and mechanisms for an adaptive control of the SIP number are included (Unterstrasser and Sölch, 2014).

The fourth research effort comes from the general circulation modeling (GCM) community. The current research topic is the Lagrangian advection scheme in the dynamical core, that is to replace the Eulerian or semi-Lagrangian schemes by the Lagrangian ones. The turbulent diffusion is not considered, which is left to other physical parameterizations. The pioneer works were done by Reithmeier and Sausen (2002), which proposed Atmospheric Tracer Transport In a LAgrangian model (ATTILA). ATTILA was incorporated in ECHAM4 atmospheric GCM (AGCM) in Stenke et al. (2008), and positive results were gained compared with the standard semi-Lagrangian scheme, because ATTILA is able to maintain steeper and more realistic gradients. In Kaas et al. (2013), a hybrid Eulerian-Lagrangian Eulerian-Lagrangian scheme (HEL) was proposed, which has some similarities to particle in cell (PIC) methods. In HEL, one Eulerian scheme is running in parallel with the Lagrangian scheme, and their results are merged each time step. Lagrangian Advection scheme with Shape Matrix (LASM), which was proposed in Dong et al. (2014) and is the research object of this study, also belongs to this category. LASM conserves the tracer total mass strictly in the sense of parcels, which is similar to ATTILA. Stenke et al. (2009) used ATTILA in a fully coupled Chemistry-Climate Chemistry-Climate Model (CCM), so the fourth category is also blurred with the second one, and may be even with the first one in the future to form a unified scheme.

The major roadblock of the Lagrangian schemes is the aliasing error, which manifests itself as noises in the tracer density distribution. During the advection, the discrete parcels (or called particles, mass packets in other works) are assumed to be isolated from each other. When the flow is nonlinearly deformative, the shape of parcels will be deformed or elongated into filaments, or even be split into parts. Most Lagrangian advection schemes do not explicitly simulate the parcel shape, and assume the parcel represents the mean state of a compact volume around it. This assumption of the parcel shape is generally not valid, so large aliasing error will occur when remapping the tracer density onto the mesh of a GCM, if no interparcel mixing is considered. Different researchers designed different interparcel mixing algorithms to reduce or eliminate such errors. For example, ATTILA redefines the parcel boundaries by simply bringing the mass mixing ratio *c* of a species in a parcel closer to an average background mixing ratio, or called "interaction by exchange with mean", which is similar in STOCHEM (Stevenson et al., 1998). More advanced algorithms are devised in CLaMS that uses a Lyapunov exponent to measure for the deformation in the flow and inserts or merges parcels based on this exponent, and in HEL that incorporates the deformation rate of the flow and mixes tracers in a directionally biased way. Different from them, LASM explicitly describes the parcel shape by a linear deformation matrix, so a parcel can be rotated and stretched, not just translated. By doing this, the flow deformation plays an important role in the remapping process. Meanwhile, an adaptive mixing algorithm incorporating the directionally biased idea in HEL is proposed, but it is not through the mesh. In summary, any successful Lagrangian advection scheme must has an effective interparcel mixing algorithm, due to the limited resolution.

This work mainly updates the interparcel mixing algorithm in LASM (reported in Sect. 2.2) to make it more robust, and several tests are used to verify the performance of LASM in Sect. 3, including a also discusses the problems when considering physical or chemical tendencies of tracers. A new terminator "toy"-chemistry test (?) (Lauritzen et al., 2015) for the CTMs (reported in Sect. 3.3). The conclusions are drawn in Sect. 4. is conducted to verify different tendency evaluation types. To ensure the applicability of LASM in 3-D, we make several modifications, and use the turbulent flow of a standard WRF large-eddy simulation to drive LASM.

2 LASM details

The basic formulation of LASM (e.g., linear deformation matrix, skeleton points) was introduced in Dong et al. (2014), and only key ideas are restated below. The interparcel mixing algorithm is redesigned to overcome the potential problems in the old one. The

(2)

physics-dynamics coupling is also discussed, where the tendency evaluation type is the most important topics in LASM. The necessary changes are made to extend LASM into 3-D.

2.1 Key ideas

The continuous fluid is discretized into parcels in finite number N_p . The centroids of parcels are $\{x_{0i}, i = 1, \dots, N_p\}$. The shape of parcel i is approximated by a linear deformation matrix \mathbf{H}_{i} , so in 2-D cases, the parcels are represented as ellipses that can be translated, rotated and stretched. A spatial coordinate x can be transformed into a local coordinate system with x_{0i} as the origin:

$$\boldsymbol{x} = \boldsymbol{x}_{0i} + \boldsymbol{\mathsf{H}}_i \boldsymbol{y}, \tag{1}$$

$$oldsymbol{y} = oldsymbol{\mathsf{H}}_i^{-1}(oldsymbol{x} - oldsymbol{x}_{0i}),$$

where y is the local coordinate for x. To avoid the problems caused by the poles on the sphere, the above calculation is currently transferred onto a local stereographic projection plane with x_{0i} still as the origin:

$$\widetilde{x} = \mathbf{H}_i y, \tag{3}$$
$$y = \mathbf{H}_i^{-1} \widetilde{x}, \tag{4}$$

$$y = \mathsf{H}_i^{-1}\widetilde{x},$$

where \tilde{x} is the projected coordinate for x. In 2-D cases, four skeleton points are associated with each parcel for sensing the deformation of the flow, and H_i is determined by those points. The SVD (singular value decomposition) technique is used to decompose H_i as

$$\mathbf{H}_{i} = \mathbf{U}_{i} \mathbf{S}_{i} \mathbf{V}_{i \sim}^{T}, \tag{5}$$

where S_i is a positive diagonal scaling matrix with the diagonal elements in descending order, and \mathbf{U}_i and \mathbf{V}_i are matrices for rotation. The product of the diagonal elements of \mathbf{S}_i is the determinant of \mathbf{H}_{i} .

(8)

The parcel Parcel *i* carries an amount of masses $\{m_i^s, s = 1, ..., N_s\}$ and densities $\{\rho_i^s, s = 1, ..., N_s\}$ for each tracer species, where N_s is the total number of tracer species. The centroid and densities volume of parcel *i* are updated by

$$\frac{\mathrm{d}\boldsymbol{x}_{0i}}{\mathrm{d}t} = \boldsymbol{V}, \tag{6}$$

$$\frac{\mathrm{d}\rho_{i}^{s}}{\mathrm{d}t} \frac{\mathrm{d}V_{i}}{\mathrm{d}t} = -\rho V_{i}^{s} \nabla \cdot \boldsymbol{V}, \underline{s} = 0, N_{s}, \tag{7}$$

where V is normally the gridded velocity field from the external models or data. In this study, V is on the lat-lon mesh or rectangular Cartesian mesh, and is interpolated onto the parcels by using bilinear interpolation.

The volume V_i of parcel *i* is defined by the first species:

$$V_i = \frac{m_i^0}{\rho_i^0},$$

and it should be the same for other species. On the other hand, the volume V_i should be equal to the determinant of \mathbf{H}_i . Generally, they are different, so the determinant of \mathbf{H}_i is reset to V_i by scaling \mathbf{S}_i , and \mathbf{H}_i is reconstructed from Eq. (5) each time step.

The anisotropic remapping between tracer parcels After the calculation of volume, the densities of all the species on parcel *i* are gained as:

$$\rho_i^s = \frac{m_i^s}{V_i}, s = 1, \dots, N_s,$$

where ρ_i^s and the model grids is the same as in Dong et al. (2014) m_i^s are the density and mass of tracer species *s* on parcel *i*. The tracer density is remapped between parcels and

model grids with the following formulas

$$\rho_{\mathcal{L}}^{s} = \frac{1}{\sum_{j \in S_{I}} \psi_{j}^{I}} \sum_{i \in S_{I}} \psi_{i}^{I} \rho_{i}^{s},$$

where ρ_I^s is the density on the grid *I*, except for S_i is the index set of connected grids for parcel *i*, S_I is the index set of connected parcels for grid *I*, and ψ_i^I is the shape function value evaluated on grid *I* with respect to parcel *i* (the body coordinate is noted as y_i^I)

$$\psi_i^I = \psi(\boldsymbol{y}_i^I). \tag{11}$$

 $\psi(\boldsymbol{y})$ is defined in Eq. (7) in Dong et al. (2014).

Since ψ_i^I is shared by all the tracer species, most of the calculations need to be done once for all the species, so the multi-tracer efficiency is high in LASM, which is the same as in HEL (Kaas et al., 2013). The searching of connected grids for each parcel is based on the cover-tree algorithm (Beygelzimer et al., 2006), and it is the most cost part of LASM. In the future, when parallelize LASM, this cost can be reduced when the domain is decomposed into small ones.

At the initial time step, the density is remapped from grids to parcels by using Eq. (9), and the total mass on the global mass fixer on the mesh. The fixer is used to ensure that the total tracer parcels is rescaled to the one on the grids only for the first step. After rescaling, the parcel volume is reset, so the deformation matrix and skeleton points are. Then the density on the parcels is remapped to grids each time step by using Eq. (10), and the total mass on the grids is conserved rescaled to ensure the consistency between parcels and grids. This mass fixer seems to be artificially, but it should be noted that the mass is already is noteworthy that the total mass is conserved exactly on the parcels in

(9)

(10)

LASMduring the simulation, which is different from the traditional non-conservative semi-Lagrangian schemes. Therefore, it is arguable that the mass fixer can be dismissed in LASM. By contrast, ATTILA in ECHAM4 (Reithmeier and Sausen, 2002) also does not consider the mass fixer . On the other hand, the at all.

The mass fixer will sabotage the desired features of the Lagrangian schemesaffect some properties on the grids. For example, without the mass fixer, the constant sum of three discontinuous tracers in the deformation test case (Lauritzen and Thuburn, 2012) is exactly preserved on the grids in LASM (not shown), which is hardly achieved by the Eulerian and semi-Lagrangian schemes due to the use of nonlinear shape-preserving filters, but when. When using mass fixer, this feature is lost in LASM, although property is lost on the grids, but the error is much smaller. relatively small. It should be noted that these properties will not be affected on the parcels.

By now, the trajectories <u>of parcels</u> and densities of <u>parcels tracers</u> are calculated, and the densities are remapped onto the grids. The next important ingredient of LASM is the interparcel mixing algorithm, which is updated as follows.

2.2 Interparcel mixing

Due to the discretization of the continuous fluid, an initial compact parcel cannot keep its integrity under the deformation of the flow. Some part of it needs to be exchanged with other parcels to form some kind of interparcel mixing, which will improve the degree of linear approximation of the parcel shape.

Previously, a parcel with index *i* is judged to be mixed or not according to a disorder degree \mathcal{D}_i , which is the ratio between the maximum and mean angles of the maximum angle to the mean angle, where the angles are between the major axes of the parcel and its surrounding or neighbor parcelsneighbor parcel. When \mathcal{D}_i is greater than a given threshold, the parcel *i* is mixed with its neighbors by distributing tracer masses to them, and its major axis is shrunk by a fixed factor 0.05. The volumes of the neighbor parcels are increased accordingly. \mathcal{D}_i is a good indicator of the flow condition, but this criterion and mixing manner rule failed in some cases, and caused extremely large and small parcels to

exist in a barotropic test case .- (see Fig. 4a). In this study, a more effective criterion and mixing manner rule are designed to better control the shape of parcels. A transition function

$$f(x_0, y_0, x_1, y_1, x) = \begin{cases} y_0 & x \le x_0 \\ (y_1 - y_0)(4 - 3t)t^3 + d_0 & x_0 < x \le x_1 , t = \frac{x - x_0}{x_1 - x_0} \\ y_1 & x > x_1 \end{cases}$$

is used to construct some thresholds.

The parcel shape is approximated by a linear deformation matrix H_i as aforementioned. When the flow is linearly or quasi-linearly deformative, or the sizes of parcels are small enough compared with the deformation scale, this approximation is sufficient so that the parcels are free to sense the flow deformation. Meanwhile, the ratio between the major and minor axis length γ_i (i.e., the filament degree) is limited to a maximum value γ_m to keep the parcel compact, because long parcels will cause extensive computation for searching connected grids. Otherwise, the linear approximation may quickly degenerate, and this causes poor remapping, since the parcel shapes are not well simulated. The most direct symptom of this degeneration is that the positions of skeleton points (say *s*) deviate from the ones calculated from H_i (say *s'*), see. Fig. 1 for an example demonstrates an example of degeneration, where the current shape of a parcel in red ellipse mismatches the skeleton points in green dots. The deviation is calculated by

$$d = \frac{D(s, s')}{L},\tag{12}$$

where function D(.,.) is the spherical distanceon the sphere, and *L* is the half length of the major axis of the parcel. By defining in this way, *d* is a dimensionless number, and independent on the underlying domain (e.g., Earth radius). When the maximum deviation d_{max} of the skeleton points is greater than a given threshold d^* , \mathbf{H}_i is not regarded as a good approximation to the real shape of parcel *i*. The threshold is determined by

 $d^* = f(r_0, d_0, r_1, d_1, r), r = \underline{r_{\vee i}} \gamma_i,$

where d_0 (0.5) and d_1 (0.1) are the looser and stricter thresholds, r_0 (1) and r_1 (5) are the transition range, r_{vi} is the ratio between the volume of parcel *i* and the mean volume of it and its neighbors. In summary, the more elongated and larger parcel will have a stricter threshold.

Another difference from the old mixing algorithm is that the neighbor parcel shapes are not changed, so those parcels will not be disturbed by the mixing. The parcel This is similar with Eulerian schemes, where the mesh is fixed. Parcel *i* is not simply shrunk, and its volume is kept unchanged. The tracer density of the parcels is changed in the following mannerrule, which is similar with the ones used in Stevenson et al. (1998) and Reithmeier and Sausen (2002)STOCHEM (Stevenson et al., 1998) and ATTILA (Reithmeier and Sausen, 2002), but it is not through the mesh -(i.e., mix parcels within a grid cells), and respects the local flow properties .Note to a great extent. Note that the tracer species index is omitted for simplicity. Firstly, a weight w_j for the neighbor parcel *j* is calculated as before (see Eq. 18 in Dong et al., 2014), and the parcel *i* has a unit weight. The neighbor parcel that is closer to the parcel *i* along the major axis has a larger weight, so the weight is directionally biased as HEL. Then the mean density of parcels weighted by w_j is

$$\overline{\rho}_i = \frac{1}{\sum_{k \in S_i} w_k V_k} \sum_{j \in S_i} w_j m_j, \tag{13}$$

where m and V are the mass and volume respectively, S_i is the parcel index set of parcel i and its neighbors. The density of each neighbor parcel is restored to $\overline{\rho}_i$ as

$$\rho_j^* = \rho_j + C_{mj} \left(\overline{\rho}_i - \rho_j \right), \tag{14}$$

where $C_{mj} = w_j C_m$, and C_m is a restore coefficient that controls the mixing degree. C_m should be related to the time step size, and needs to be tuned accordingly. It can also be variant along the vertical spatial direction. The density of parcel *i* is calculated under the

constraint of mass conservation as

$$\rho_{i}^{*} = \frac{M_{i} - \sum_{j \in S_{i}, j \neq i} \rho_{j}^{*} V_{j}}{V_{i}}$$

= $\rho_{i} + C_{m} (\overline{\rho}_{i} - \rho_{i}).$ (15)

It can be seen that the parcel *i* is just restored to $\overline{\rho}_i$ with the coefficient C_m , and the mass on the parcels is exactly conserved during the mixing.

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After the density mixing calculation, the shape of parcel *i* is changed through reducing γ_i . . In (i.e., the filament degree). In the 2-D cases,

Before mixing:
$$\frac{S_0}{S_1} \frac{S_{max}}{S_{min}} = \gamma_i, S_{\underline{0}max} S_{\underline{1}min} = V_i,$$
(16)

After mixing:
$$\frac{S_0^*}{\underline{S_1^*}} \frac{S_{max}^*}{\underline{S_{min}^*}} = \alpha \gamma_i, S_{\underline{0}max}^* S_{\underline{1}min}^* = V_i, \qquad (17)$$

where S_0 and S_1 S_{max} and S_{min} are the diagonal elements of S_i , the new ones are

$$S_{max}^* = \sqrt{\alpha} S_{max},\tag{18}$$

$$S_{\min}^* = \frac{1}{\sqrt{\alpha}} S_{\min}, \tag{19}$$

and α is a reduction factor, and is determined by reshaping coefficient

$$\alpha = \frac{f(\gamma_0, \alpha_0, \gamma_1, \alpha_1, \gamma_i)}{\sqrt{(1 - \frac{\gamma_i}{\gamma_m}) + \frac{\gamma_i}{\gamma_m} \alpha_m}} \begin{cases} \gamma_i > \gamma_m, \\ \gamma_i \le \gamma_m, \end{cases}$$
(20)

where $\gamma_0 = 1$, $\alpha_0 = 1$, $\gamma_1 = 5$ and $\alpha_1 = 0.5 \alpha_m$ is the maximum value. This setup will make the shape of parcel *i* closer to circle in 2-D cases. After some simple manipulation,

$$S_0^* = \sqrt{\alpha} S_0,$$

$$S_1^* = \frac{1}{\sqrt{\alpha}} S_1.$$

Then the deformation matrix H_i is updated, and the skeleton points are reset accordingly. This reshaping rule is the most artificial part of LASM, which may be revised in the future, but from the results of the following tests, this rule does not have vital defect. The mixing in the Lagrangian schemes is driven by the flow deformation, whereas the inherent mixing in the Eulerian and semi-Lagrangian schemes is driven by the tracer density gradient, which is similar to the molecular diffusion. Currently, the above interparcel mixing is only for the computational aspect, but when the physical mixing is required, the similar form can be utilized with different parameters (Stevenson et al., 1998). For example, the disorder degree D_i can be used as a trigger of the turbulent mixing. In addition, the

2.3 Tendency evaluation

In the real applications, some other processes will calculate the tendencies for different tracer species. There are two types of tendency, which are both implemented in LASM.

stochastic turbulent diffusion in LPDM may be incorporated in the future to unify them.

The tendency in the first type resides on the Eulerian mesh of an existing model, such as the physics parameterizations (e.g., convection, microphysics) in an AGCM. The gridded tendencies need to be remapped onto the parcels, and the remapping formula is the same as the one for the tracer density in LASM. mass tendency is chosen to be remapped to ensure mass conservation

$$\Delta m_i^s = \frac{1}{\sum_{J \in S_i} \psi_i^J} \sum_{I \in S_i} \psi_i^I \Delta m_I^s.$$

In other Lagrangian schemes, the tendency on a mesh cell is distributed evenly to each parcel contained in that cell (Stevenson et al., 1998; Reithmeier and Sausen, 2002). The tendency in the second type is computed directly. It is noteworthy that there may be inconsistency between parcels and grids, which will cause negative masses on the parcels, which is more natural, such as the chemical reactions in a CTM. especially when the density is near zero, because the tendency is calculated based on the densities on the grids, and may be excessive for the parcels. When this happens, the parcels will disregard the tendencies in this study. Because the chemical reaction is local, the total mass will be conserved even so. In the future, extra procedures should be designed to redistribute

(21)

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the problematic tendencies reasonably to ensure mass conservation when the tendency is non-local (e.g., convection).

For the applications in an AGCM, only the first type tendency can be used currently, since the mainstream physics parameterizations are all defined on the vertical columns of the mesh, for example ATTILA in ECHAM4 (Stenke et al., 2008). Nevertheless, there are some researches (Shima et al., 2009; Andrejczuk et al., 2010; Sölch and Kärcher, 2010; Unterstrasser and Sölch, the microphysics, which constructed numerical schemes to simulate cloud and precipitation in the Lagrangian framework The tendency in the second type is computed directly on the parcels, which is more natural and no inconsistency will occur. In the CTMs, it is easier to compute the tendencies in this type, because the chemical reactions take place on the parcelscan be described by the box model (Brunner, 2013). Several Lagrangian CTMs in this type exist, such as STOCHEM, CLaMS (McKenna et al., 2002a), etc., but NAME III calculates the chemistry on a fixed three-dimensional chemistry grid (Jones et al., 2007). Grewe et al. (2014) also investigated how the tendency should be evaluated. proposed a theoretical parcel reshaping for the finite mass method (FMM). When applying FMM in the 3-D atmosphere-chemistry models, a reshaping procedure is needed to construct the real density, because the parcel density is not real at the centroid position. In contrast, although LASM is based on FMM, the parcels in LASM carry the real density, so there is no need to reshape. There are also some researches (Shima et al., 2009; Andrejczuk et al., 2010; Sölch and Kärcher, 2010; Unterstrasser and Sölch; the microphysics, which constructed numerical schemes to simulate cloud and precipitation in the Lagrangian framework. In the future, more parameterization schemes may be designed on the fully Lagrangian framework.

The two types of the tendency are both implemented in LASM , and their influence on the simulation results of a newly proposed test case with chemical reactions is shown in Sect. The effects of the two type tendencies will be compared in a newly proposed terminator "toy"-chemistry test in section 3.3.

2.4 Roadmap of LASMAlthough LASM is a numerical scheme, it will be beneficial to do strict version control on its implementation following Extension to 3-D

LASM can be extended to 3-D by handling the following three factors: 1) the rigid boundary condition in the vertical direction (the horizontal boundary conditions are periodic); 2) the initial shape of the parcels; 3) the reshaping rule after mixing.

The rigid boundary condition is implemented by ensuring the vertical velocity is zero on the boundary. This is trivial in this study, since the flow is given by the external sources (e.g., WRF-LES simulation). The parcel centroids will never move outside the domain, if the time step size is not too large, but the parcel ellipsoid may penetrate through the boundary. To avoid potential problems, all the parcels within the boundary grid cells will be reset to sphere, and mixed accordingly. Similarly, ATTILA relocates air parcels in the software engineering practices. The following list is the future roadmap of LASM. More features will be added step by step. Application in an AGCM in 2.5-D mode with the vertical formulation unchanged. Parallel acceleration with the help of OpenMP and MPI. Handle the horizontal boundaries for application in an OGCM. Fully boundary layer after one time step, due to the rapid turbulent mixing (Reithmeier and Sausen, 2002; Stenke et al., 2008).

The interparcel mixing algorithm described above checks the parcel filament degree γ , and ensure $\gamma < \gamma_m$. In the 3-D setup with different vertical coordinates. Application in an CTM. Incorporate dynamics into 2-D LASM to form a barotropic dynamical core. Incorporate dynamics into applications, the horizontal and vertical space scale may differ greatly. For example, the axis span of a sigma terrain-following vertical coordinate is 1, but the horizontal axis span is hundreds of kilometers, so the initial parcels are like thin pies, which will confuse the algorithm. Therefore, the simulation domain is transformed to a logical one with equal axis spans in each direction. This transformation involves the flow velocity and the coordinates of grids and parcels.

When reshaping the mixed parcels, there is one more element S_{mid} in the scale matrix **S** in 3-DLASM to form a baroclinic dynamical core. Incorporate stochastic processes to form a dispersion model. S_{max} and S_{min} are changed as in Eq. (18) and (19), and S_{mid} is

(22)

$$S_{mid}^{*} = S_{max}^{*} - \frac{S_{max} - S_{mid}}{S_{max} - S_{min}} (S_{max}^{*} - S_{min}^{*}).$$

The three elements are scaled to ensure $S^*_{max}S^*_{mid}S^*_{min}$ equals the parcel volume. If $\gamma^* = \frac{S^*_{max}}{S^*_{min}} > \gamma_m$, the above procedures will be looped until $\gamma^* \leq \gamma_m$.

We utilize the 3-D Large-Eddy Simulation (LES) in WRF to construct a turbulent flow to verify this extension. The results are analyzed in section 3.4.

3 Test cases

In this section, three test cases four tests are used to verify the modifications updates of LASM. The first two cases are the same as used in Dong et al. (2014). The third one is newly proposed in **?**Lauritzen et al. (2015), which extends the previous inert scalars to reactive species. The fourth one uses a more turbulent 3-D flow generated by WRF-LES. The conventional parameters of LASM is tabulated in Table 1.

3.1 Deformation flow test

The deformation flow test was first proposed in Nair and Lauritzen (2010), and further extended in Lauritzen et al. (2012), which contains four large scale deformation flow formulas to challenge the advection schemes. In this study, we repeat the case with non-divergent flow to test the basic performance of the new interparcel mixing algorithm. The spatial resolution of the mesh is $1.5^{\circ} \times 1.5^{\circ}$, the parcel number is 22640, and the normalized flow period T is 5.

The effects of changing γ_m are shown in Fig. 2, which shows the mixing ratio distribution of the slotted cylinders at t = T/2 and t = T, and in and Table 2, which lists the correlation diagnostics with and without mass fixer. With the decreasing of γ_m , the parcels, which are under heavily stretching and shearing, cannot turn to be too long, and their tracer

masses will be mixed with the neighbor parcels. Fig. 2 shows the changes of mixing ratio distribution of the slotted cylinders at t = T/2 and t = T. When $\gamma_m = 2$, the filament structures of the slotted cylinders break up at t = T/2. This resembles the aliasing error shown in Fig. 13 in Dong and Wang (2012), and in Fig. 7 in Kaas et al. (2013), but with a different reason. The excessive mixing caused by the small γ_m distributes the tracer mass to the wrong places. Thus, γ_m should not be too small to let the aliasing error happen. The correlation diagnostics shown in Table 2 are evaluated on the parcels. As expected, the real mixing diagnostics l_r is also larger when γ_m is small, but the "range-preserving" unmixing diagnostics l_{μ} is smaller because of the extensive interparcel mixing. All the "overshooting" unmixing diagnostics l_o are zero in LASM, while other high-order Eulerian or semi-Lagrangian schemes need filter to achieve this requirement. In spite of this, it does not mean γ_m should be as large as possible. For example, in the following terminator "toy"chemistry test, when the tendencies for the tracers are considered, the larger γ_m causes the burr edge along the terminator as shown in Fig. 7. Therefore, the moderate value 5 for γ_m is used in LASM. By comparing Fig. 2 (the third row with $\gamma_m = 10$) with Fig. 12 in Dong et al. (2014) (the third row), it can be seen that the new algorithm is a little better to keep the final shape of the slotted cylinders, and l_r is $\frac{1.59 \times 10^{-4}}{1.97 \times 10^{-4}}$ in the new algorithm, which is 3.54×10^{-4} 3.34×10^{-4} in the old one.

Another observation from Table 2 is that: when the mass fixer on the grids is used, the unmixing and overshooting diagnostics (l_u and l_o) are not all zero. Therefore, we turn off the mass fixer, because the tracer total mass is already conserved on the parcels, and the mass fixer causes the losing of desired features (e.g., linear, shape-preserving) in LASM.

The effects of changing C_m are shown in Fig. 3. By increasing C_m , the mixing degree is enlarged, especially when $C_m = 0.1$. In the current study, the value 0.001 is chosen, which is the same as STOCHEM and ATTILA.

3.2 Barotropic test

The barotropic test provides more realistic flow, though no analytical solution is available. The same finite difference barotropic model is used to drive LASM as in Dong et al. (2014). The spatial resolution is $1.5^{\circ} \times 1.5^{\circ}$, and the time step size is 20 s to ensure the stability of the model. The initial conditions and topography are as subcase 2 in Dong et al. (2014), but in this study, the time step size Δt for LASM is increased to 1800 s to decrease the cost. The mixing coefficient C_m is changed to 0.01, due to the enlarging of Δt .

Firstly, we check the validity of the new criterion that judges the linear degeneration. The comparison between the old and new criterion is shown in Fig. 4. In the old one, many extremely large and small parcels appear, but they are eliminated in the new one. Therefore, the new criterion is better, and should replace the old one. Secondly, two triggers for the interparcel mixing are compared. The first one is *minimum mixing*, that is the linear degeneration of the parcel shape triggers the mixing. The second one is *all mixing*, that is the mixing is active each time step for each parcel, but only the shapes of the degenerated parcels are changed.

The results at day 4 are in Fig. 5. Clearly, all mixing causes substantial diffusion than minimum mixing When $C_m = 0.001$, the differences between minimum mixing and all mixing are imperceptible, due to the large Δt . After having increased C_m to 0.01, the diffusion in all mixing becomes visible. Based on this comparison, LASM manifests its ability of customizable mixing, and more physics-based triggers can be devised with the information available in LASM to fulfill different needs. Another notice is that C_m should be adjusted according to different application scenarios.

3.3 Terminator "toy"-chemistry test

This test (?) (Lauritzen et al., 2015) consists of transporting two reacting chlorine-like species (and X and X₂) in the deformation flow. Although the chemical reactions are nonlinear, the weighted sum $X_T = X + 2X_2$ (i.e., linear correlation) is preserved, even when the reactions are discretized. In addition, one of the reactions ($CI_2 \xrightarrow{k_1} 2CIX_2 \xrightarrow{k_1} 2X$) is photolytic so that the reaction rate k_1 is terminator-"like" terminator-like" and will produce very steep gradients in the chlorine species near the terminator. Only the schemes that are semi-linear can preserve the linear tracer correlation (i.e., X_T). Many Eulerian or semi-Lagrangian schemes satisfy the semi-linear constraint when the shape-preserving filters are not applied, but in

the real cases, such schemes must be limited by the filters to avoid adverse oscillations that may cause instability, so the linear correlation between the two species is **lostcompromised**. On the other hand, the Lagrangian schemes have the intrinsic property of being linear, so no complicated (maybe nonlinear) filter or limiter is needed to ensure the monotonicity. The linear property is the sufficient condition for the semi-linear property (Lauritzen and Thuburn, 2012). For example, LASM can preserve the constant sum of three tracers, which is more challenging than two tracers.

Except the scheme itself, the tendency evaluation and physics-dynamics coupling types also affect the results, such as the tendency evaluation type. In LASM, the tendencies of and X and X_2 are evaluated on the parcels and grids respectively. The spatial resolution of the lat-lon mesh is $1^{\circ} \times 1^{\circ}$. The time step size Δt is 1800s both for the chemistry and advection processes, because there is no need to use a smaller Δt in LASM, so the physics-dynamics coupling type is as ftype = 1 in ?. The results for , and X, X₂ and X_T at day 6 are shown in Fig. 6. Firstly, the constant is preserved exactly in both cases X_T is preserved very well when the tendencies are evaluated on the parcels, whereas there are errors in X_T when on the grids. The results of CAM-FV and CAM-SE can be referred in Fig. 3 in **?**Lauritzen et al. (2015), which indicates that X_T is disturbed in those schemes caused by the used shape-preserving filters. Secondly, it is obvious that the results with the tendencies evaluated on the parcels (i. e., when evaluating tendencies on the chemical reactions occur on the parcels) are better grids, small negative densities will occur near the terminator line. This is caused by the inconsistency between parcels and grids. Currently, LASM ignores the problematic gridded tendencies to avoid the negative densities. In Fig. 8, the cross sections of and X₂ at 45° S exhibit that LASM is shape-preserving inherently without any complicated and nonlinear filter, and the sharp gradients are simulated well near the terminator. By contrast, CAM-SE shows Gibbs phenomena when no filter or limiter is used (see Fig. 5 in ?)(see Fig. 5 in Lauritzen et al., 2015).

In summary, it is better to evaluate the tendencies on the parcels in LASM. For CTM application, the chemical reaction can be easily calculated on the parcels, and the

interparcel mixing in LASM will also improve the representation of the parcels relative to the earlier Lagrangian models (Henne et al., 2013).

3.4 3-D WRF-LES test

All the previous tests are in 2-D, so there are still concerns about the behavior of LASM in 3-D. This test will use the 3-D flow outputted from WRF-LES, which is extremely turbulent. The parameters for the LES are the standard ones in WRF, with $100 \text{ m} \times 100 \text{ m} \times 50 \text{ m}$ spatial resolution in a Cartesian domain and $\Delta t = 1 \text{ s}$. The time duration is 2 hours. The advection scheme in WRF belongs to the upwind-based finite difference method. The flux operators are fifth-order operators for the horizontal flux calculations and a third-order operator for the vertical flux calculation (Shamarock et al., 2008). The positive-definite limiter is also used to avoid negative tracer masses (Shamarock, 2006; Shamarock and Weisman, 2009).

Since WRF uses a terrain-following hydrostatic-pressure vertical coordinate η , the span of η is 1, which is too small compared with the horizontal axis span 3900 m, the coordinate system is linearly transformed into a logical one where all the axis spans are 1, so is the velocity field. An idealized tracer with initial cubic distribution is advected by both of the schemes. LASM is driven offline with a larger $\Delta t = 30$ s, and the parcel number is the same as the grid number of WRF.

The results in the 3-D Cartesian domain after 1.5 hours for both LASM and WRF are depicted in Fig. 9. It is obvious that LASM has far less numerical diffusion than WRF, see the contour levels of the cloud-like tracer distributions on the upper levels. Meanwhile, there are a lot of structures on the lower levels in LASM, whereas the tracer are diffused heavily in WRF. The animation for both of WRF and LASM can be found in the supplement files.

One major concern about LASM is the cluster and rarefaction of parcels. For example, is it possible that a parcel has no or only distant neighbors? It should be noted that the distribution of the parcels is controlled by the flow, which is constrained by the fluid dynamics in turn. In Reithmeier and Sausen (2002), their results showed that the trajectories of the parcels during the 30 years control run remain well distributed (see Fig. 10 there). The

similar figure for LASM are drawn in Fig. 10, which shows that the horizontally averaged number of parcels contained in the cells has no significant trend. LASM will also crash when a parcel has no neighbors in this study, but this never happens in the tests. In spite of this, the adaptive refinement of parcels is still valuable for achieving better accuracy and performance, and this will be studied in the future.

4 Conclusions

The interparcel mixing algorithm in LASM is updated through by replacing the criterion of the linear degeneration of the parcel shape and the mixing mannerrule. The new criterion is a more direct indicator for the degeneration symptom, so the parcel shape is better controlled. In the new mixing manner, the restore coefficient C_m is used to adjust the mixing degree. rule, the densities of the involved parcels are restored to a mean density.

Several tests are utilized to verify the updates, including a newly proposed terminator "toy"-chemistry test. The results reveal that the new algorithm is effective and less arbitrary. It is noteworthy that LASM is a linear scheme, so it can preserve the sum of multiple tracer species and also the weighted sum of two reactive chlorine-like species exactly species exactly on the parcels and accurately on the grids. Two triggers for the interparcel mixing are compared, and LASM shows the great flexibility so that different triggers can be devised in the future to address different needs.

The two tendency evaluation types are discussed and tested. The first one, which evaluates the tendency on the parcels, is the most natural type. Some processes are trivial to be calculated in this type, such as the chemical reaction and microphysics. The other one, which evaluates the tendency on the grids, can cause negative values on the parcels, which should be carefully handled.

LASM is also extended to 3-D by handling the rigid boundary condition, adjusting the initial parcel shape, and changing the reshaping rule after mixing. The flow outputted by the WRF-LES is used to verify this extension of LASM, and the results of LASM and WRF

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indicate that LASM has far less numerical diffusion. The parcel distribution also shows that there is no cluster and rarefaction of parcels.

Code availability

The codes of LASM are managed by using GIT and hosted in on GitHub. The repository URL is https://github.com/dongli/LASM. There are also two repositories, GEOMTK (https://github.com/dongli/geomtk) and BARAOTROPIC-MODEL (), used by LASM as submodules, and BAROTROPIC-MODEL (https://github.com/dongli/barotropic-model) for generating 2-D barotropic flow. You can download all of them by invoking the following command commands in a shell: Four

\$ git clone --recursive https://github.com/dongli/lasm \$ git clone https://github.com/dongli/barotropic-model

Five external libraries (Udunits, Boost, Armadillo, NetCDF and MLPACK) are also needed to be installed. You can install them by using a package manager called PACKMAN (https: //github.com/dongli/packman) developed by the authors.

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Table 1. The correlation results with and without mass fixer for different values conventional parameters of γ_m LASM used in the deformation test case 4.tests.

Symbol	Meaning	Values
γ_m	tr-Maximum parcel filament degree	$t_{\overline{u}} 5_{\overline{\Sigma}}$
$\overset{d^*}{\underset{\sim}{\longrightarrow}}$	to Maximum skeleton point deviation bias	0.1
β_{1}	Ir Radial mixing weight coefficient	l_u -1
β_{2}	lo-Lateral mixing weight coefficient	1000
2 - <u>C</u> m	4.65×10^{-4} Restore coefficeint	0 -0.001
$lpha_m$	O-Maximum reshaping coefficient	0.5

Table 2. The correlation results evaluated on the parcels for different values of γ_m in the deformation test case 4.

γ_m	$5.36 \times 10^{-4} l_r$	$4.22 \times 10^{-6} l_{y}$	$5.22 \times 10^{-4} l_8$
5 2	2.50×10^{-4} 2.08 $\times 10^{-4}$	$0-7.50 \times 10^{-10}$	0
5	$1.98 imes 10^{-4}$	$\frac{2.60 \times 10^{-4}}{6.62 \times 10^{-9}}$	$1.01 imes 10^{-6} \ 9.89 imes 10^{-5} \ 0$
10	$\frac{1.59 \times 10^{-4}}{1.97 \times 10^{-4}}$	$0-7.68 \times 10^{-9}$	$0.1.62 \times 10^{-4} \ 5.31 \times 10^{-8} \ 0$
100	$\frac{1.20\times10^{-4}}{1.96\times10^{-4}}$	$0.8.78 \times 10^{-9}$	$0.1.19 \times 10^{-4} \cdot 2.56 \times 10^{-8} \cdot 0^{-8}$



Figure 1. A case of linear approximation degeneration of a parcel. The red ellipse is the current shape of the parcel, and the green points are the skeleton points of the parcel. The green points are not on the red ellipse indicates that the parcel shape is not approximated well by the linear deformation matrix.

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Figure 2. Deformation test case results with different γ_m . The left column is the slotted cylinders at t = T/2, and the right column is at t = T.

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Figure 3. Deformation test case results with different mixing coefficient C_m at t = T.



Figure 4. Comparison of the parcel shapes between the old and new interparcel mixing algorithms in a barotropic test case. Two extremely small and large parcels in the old algorithm are spotted by the red ellipses. In the new algorithm, there is no such ill-shaped parcels.



Figure 5. Comparison between minimum mixing and all mixing at day 4. All mixing means the interparcel mixing is triggered each time step for each parcel. The mixing coefficient C_m has two different values 0.001 and 0.01.



Figure 6. Contour plots of X, X_2 and X_T at day 6 for two types of tendency respectively. Solid black line is the location of the terminator line.



Figure 7. Contour plots of X at day 6 for two values of γ_m respectively. Solid black line is the location of the terminator line.



Figure 8. Cross section of X, X₂, and X_T at day $\frac{1}{1}$ with the tendencies evaluated on the parcels. Results are normalized by 4×10^{-4} (the initial value of X_T.

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Figure 9. 3-D volume-rendered advection results driven by the flow outputted by WRF-LES. The left figure is simulated by LASM, and the right one is by the advection scheme in WRF.

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Figure 10. Evolution of the parcel distributions during the WRF-LES simulation. Shown is the horizontally averaged number of parcels contained in the grid cells. Each line represents a level.