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Intercomparisons of five ocean particle tracking software packages

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Abstract. Particle tracking is widely utilized to study transport features in a range of physical, chemical, and biological processes in oceanography. In this study, a new offline particle tracking package, Tracker, is introduced and its performance is evaluated in comparison to an online Eulerian dye, one online and three offline particle tracking software packages in a small high-resolution (200 m) model domain and a large coarser (1000 m) model domain. It was found that both particle and dye approaches give similar results across different model resolutions and domains when they were tracking the same water mass, as indicated by similar mean advection pathways and spatial distributions of dye and particles. The flexibility of offline particle tracking and its similarity against online dye and particle tracking make it a useful tool to complement existing ocean circulation models. Lastly, the new Tracker was shown to be a reliable particle tracking package to complement the Regional Ocean Modeling System (ROMS), and tradeoffs of performance, modifiability, and ease of use that can influence the choice of which package to use are discussed.

1 Introduction

Lagrangian particle tracking is a very common and useful tool, especially in the post-processing of existing oceanographic model runs (van Sebille et al., 2018), and is of great value in applied oceanography like pollutant dispersion (e.g., Havens et al., 2009; Nepstad et al., 2022), oil spills (e.g., Nordam et al., 2019), harmful algal blooms (e.g., Giddings et al., 2014; Rowe et al., 2016), planktonic larvae (e.g., Brasseale et al., 2019; Garwood et al., 2022), marine plastics (e.g., Onink et al., 2021), and search-and-rescue (e.g., Chen et al., 2012), to name a few. Particle trajectories can be computed "online" along with the velocity fields at every time step as a part of ocean circulation models, for instance, the built-in particle tracking module "floats" in the Regional Ocean Modeling System (ROMS, Shchepetkin and McWilliams, 2005; Melsom et al., 2022). The trajectories can also be computed "offline" using stored hydrodynamic model output (Dagestad et al., 2018). Generally, offline tracking is more frequently applied in the literature than online tracking.

Many offline particle tracking software packages have been developed for multiple applications in oceanography, e.g., OceanParcels (https://oceanparcels.org/), Ichthyop (https://ichthyop.org/), TRACMASS (Döös et al., 2013), PaTATO (Fredj et al., 2016), TrackMPD (Jalon-Rojas et al., 2019), OceanTracker (Vennell et al., 2021), Deft3D-PART (Deltares, 2022), Ariane (http://stockage.univ-brest.fr/~grima/Ariane/), and CMS (https://github.com/beatrixparis/connectivity-modeling-system). Several previous studies have compared one

Lagrangian particle tracking model with passive Eulerian dye experiments to evaluate how well the particle trajectories integrated in a Lagrangian framework can represent the dye spreading in an Eulerian framework (e.g., North et al., 2006; Wagner et al., 2019; Melsom et al., 2022; Nepstad et al., 2022). Yet few have compared different particle tracking models since the tracking codes are often developed to work with separate ocean models or forcing file formats. It is challenging to draw conclusions by comparing the output from each of them. Given the increasing popularity of particle tracking techniques in studying ocean transport features, it is useful to evaluate the performance of the popular particle tracking software that can be assessed in a uniform testbed, e.g., using the same ocean circulation model. Here, we utilized a well-established, realistic, circulation model LiveOcean (MacCready et al., 2021) to evaluate several publicly available and commonly used particle tracking software packages.

LiveOcean is built using ROMS and is a realistic numerical model of ocean circulation and biogeochemistry for the coastal and estuarine waters of the northern California Current System (https://faculty.washington.edu/pmacc/LO/LiveOcean.html). The model is run quasi-operationally, making three-day forecasts of currents and other water properties every day. It is widely used by a variety of stakeholders concerned with the effects of ocean acidification, hypoxia, harmful algal blooms, and larval transport on fisheries. Details of model configuration and validation are given in MacCready et al. (2021). LiveOcean has an offline particle tracking code written in python named "Tracker" (v1.1), which has been used to identify the source of estuarine inflow from continental shelves (Brasseale and MacCready, 2021) and track trajectories of the harmful species *Pseudo-nitzschia* in daily post-processing to assist resource managers to decide to open or close WA beaches for razor clam harvest in combination with beach sampling (https://faculty.washington.edu/pmacc/LO/p5_Phab_full_salt_top.html, Stone et al., 2022).

To further evaluate the performance of Tracker and conduct multiple particle tracking model evaluations, three offline tracking codes: LTRANS (Schlag and North, 2012), OpenDrift (Dagestad et al., 2018), and Particulator (Banas et al., 2009) were selected among other particle codes. We selected these three packages because they all can work with ROMS output, facilitating direct intercomparison. They span a representative range of common programming languages, Fortran, Python, and MATLAB, as well as a range of algorithm choices (Table 1). Besides intercomparisons among these offline particle tracking codes, online passive dye experiments are used as a benchmark to evaluate their performance. ROMS online particle tracking "floats" is also tested to supplement the comparisons. To facilitate the implementation of online dye and particle tracking, a new, nested hydrodynamic model that only covers the domain of Hood Canal (Figure 1b) was established using ROMS. The Hood Canal model has a horizontal resolution of 200 m and shares the same 30 vertical layers with LiveOcean. The northern open boundary is interpolated from the LiveOcean large domain while all other forcings (river and atmospheric forcings) come from the same sources as LiveOcean. Freshwater discharge from an additional eight tiny rivers (Figure 1b) was added to improve the simulated salinity field in Hood Canal.

In this short paper, we aim to make a series of tests of four offline and one online particle tracking software packages to evaluate to what extent they all produce the same answer and to what extent they can reproduce results consistent

https://doi.org/10.5194/gmd-2023-45
Preprint. Discussion started: 22 May 2023

Geoscientific Model Development
Discussions

with a passive dye. We also kept track of the computational efficiency and discussed ease of use of all tracking codes to provide practical guidance about tradeoffs for other researchers to decide which code to use.

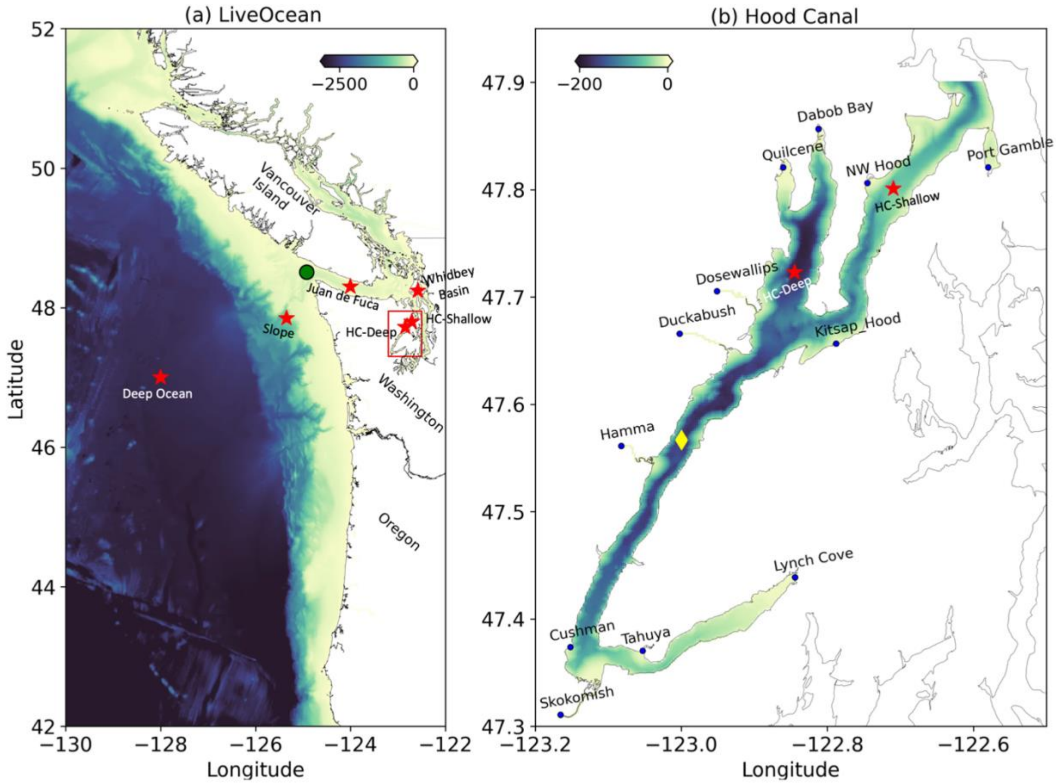

Figure 1: (a) LiveOcean and (b) Hood Canal model domains and bathymetry. In (a), the red stars represent sites selected for 1-D vertical well mixed condition tests. The green dot indicates the particle release location to test offline particle tracking codes in the LiveOcean domain. In (b), the yellow diamond indicates particle and dye release location using the Hood Canal model domain. The blue dots represent locations with river inputs.

2 Methods

2.1 Tracker

Tracker is developed to work with ROMS hydrodynamic outputs and uses a 4th-order Runge-Kutta solver for particle advection. Random displacement (as a modified random walk) is implemented in the vertical to represent the effects of turbulent mixing and prevent particles from unrealistically accumulating in low-diffusivity areas (Visser, 1997; North et al., 2006; Banas et al., 2009),

$$z_{n+1} = z_n + \frac{\partial AK_s}{\partial z} \cdot \Delta t + R\sqrt{2AK_s \cdot \Delta t}\,, \tag{1}$$

where z_n is the vertical particle position at time step n after the advection, Δt is the timestep, R is a normal distributed random function with a mean of 0 and a standard deviation of 1. AK_s is the vertical diffusivity evaluated at $(z_n + 0.5\frac{\partial AK_s}{\partial z}\Delta t)$, and the derivative $\frac{\partial AK_s}{\partial z}$ is evaluated at z_n (North et al., 2006). The vertical profile of eddy diffusivity

https://doi.org/10.5194/gmd-2023-45
Preprint. Discussion started: 22 May 2023

AK_s is smoothed using a 3-point Hanning window prior to calculating the vertical derivatives, similar to the smoothing technique applied in North et al., (2006). In addition, the surface and bottom AK_s are adjusted to be equal to the values one grid point in. The choice was motivated by the fact that we use a nearest-neighbour search algorithm and were concerned that particles close to the top or bottom might use a near-zero diffusivity.

To speed computation, Tracker uses pre-computed nearest-neighbour search trees to find velocities and other fields (e.g., diffusivity, temperature, and salinity) used for moving each particle forward. This was found to speed computation for the large grid size of the model domain. To test if Tracker can give trustworthy results, one important test is the preservation of vertical well mixed conditions (North et al., 2006). Another is the similarity to dispersion of an inert dye.

2.1.1 Well mixed condition test

Using the hourly-saved hydrodynamic output from LiveOcean, six sites in different dynamic settings from the deep ocean to the Salish Sea (Figure 1a) were selected to perform the well mixed condition (WMC) tests on Tracker with horizontal and vertical advection turned off and a random displacement model implemented for the z direction. For each site, 4,000 particles were seeded uniformly from the free surface to the bottom. The WMC tests were run for 12 hours with both a time-dependent diffusivity profile (from 2021.01.01 00:00:00 to 12:00:00) and a steady diffusivity profile (at 2021.01.01 00:00:00, Figure 2). The timestep for tracking particles in WMC tests is 300 s. The initially well-mixed particles are expected to remain uniform in a statistical sense regardless of the diffusivity profiles, in consistent with the Eulerian solution to the 1-D vertical diffusion equation with an initial uniform concentration and no flux boundaries (Visser, 1997; Rowe et al., 2016; Nordam et al., 2019). Metrics of success for WMC tests follow North et al. (2006) that particle numbers were compared to a “non-significant range” to test whether the WMC was satisfied.

2.2 Other offline particle tracking software packages

Here we briefly describe the three other offline particle tracking packages: LTRANS (North et al., 2006), Particulator (Banas et al., 2009), and OpenDrift (Dagestad et al., 2018), with more details about their configurations given in Table 1 and provided in respective references.

LTRANS is a well-documented tool written in Fortran 90, specifically for output from ROMS. It has broad applications in studying larvae transport (North et al., 2008), oil spills (North et al., 2011; Testa et al., 2016), coastal connectivity (Li et al., 2014), plastics (Liang et al., 2021), algae (Wang et al., 2022), etc. Particulator is written in MATLAB, mostly specific to output from ROMS, and has been used to study water pathways (Banas et al., 2015; Stone et al., 2018), and harmful algal bloom (Giddings et al., 2014). OpenDrift is written in Python and has flexibility to work with forcing data from different ocean models, including ROMS. It has rather wide-ranging applications in tracking particles with diverse properties, e.g., fish eggs (Melsom et al., 2022), Environmental DNA (Andruszkiewicz et al., 2019), oil, chemical tracers, sediment, capsized boats, icebergs, etc. (https://opendrift.github.io/index.html).

https://doi.org/10.5194/gmd-2023-45
Preprint. Discussion started: 22 May 2023

Geoscientific Model Development Discussions

Given the different interpolation schemes, numerical algorithms, how turbulent dispersion and encounters with model boundaries are treated, we limit our inter-model comparisons by only considering advection of passive (or neutrally buoyant) particles by the three-dimensional flow and vertical turbulent mixing (without surface windage and waves).

2.3 Online passive dye experiment and particle tracking

A passive dye experiment was conducted to determine if the particle-tracking model predictions agree with simulated diffusion. Dye can be considered the "truth" that particle tracking codes seek to replicate. However, this idea is complicated by the presence of numerical mixing which is intrinsic to model advection algorithms (Burchard and Rennau, 2008; Ralston et al., 2017). Numerical mixing increases the dispersion of tracers, as quantified by the decrease of their variance. In Broatch and MacCready (2022), numerical mixing was found to account for one-third of the total mixing of salinity in the LiveOcean Model inside the Salish Sea. While most model studies to not quantify numerical mixing, those that have, mostly limited to estuaries, show that it is significant. Thus, we expect in general that dye will experience greater horizontal and vertical dispersion than the particles, especially in regions with strong horizontal gradients.

Using the Hood Canal model, a passive dye was introduced from a grid cell in the middle of water column of the channel (Figure 1b) and was tracked for 7 days starting from 2021.06.01 00:00:00. Before activating the dye module, the hydrodynamic simulations were run for the whole year of 2021 with daily saved restart files. An additional variable 'dye_01' was added to the restart file at 2021.06.01 00:00:00 with a concentration of 1 in the selected grid cell and 0 elsewhere. The timestep for dye transport is 40 s. The MPDATA advection scheme (Smolarkiewicz, 1984) was applied for dye, the same as temperature and salinity. This scheme effectively reduces numerical dispersion and prevent negative concentration values (Melsom et al., 2022).

To compare Eulerian dye and Largangian particles, 10^5 particles with a distribution of $100\times100\times10$ (longitude, latitude, vertical) were released from the same Hood Canal model grid cell at the same time as dye release for all four offline tracking codes. Particle tracking was driven by the hourly saved history files in each case. Each particle was associated with a particular mass ε_0 obtained as the ratio of the initial dye mass to the total particle number (i.e., 10^5). The timestep for offline particle tracking is 300 s. Previous experiments with Tracker showed this time step was required in LiveOcean in regions with strong currents and complex channel shape. Longer time steps would sometimes advect particles over narrow land regions instead of following curving channels. A slightly different seeding strategy was applied for ROMS online particle module for convenience. The 10^5 particles were distributed uniformly along the diagonal of the selected model grid cell. The timestep for online tracking is 40 s. Additional comparisons for the four offline particle packages were conducted using the large LiveOcean model domain and its hourly saved history file. 10^4 particles were evenly distributed within a 1 km × 1 km square at the free surface and in the middle water column near the mouth of the strait of Juan de Fuca (Figure 1a). Particles were tracked for 7 days from 2021.01.01 00:00:00 with a timestep of 300 s. In all experiments mentioned above, dye concentration and particle trajectory positions were saved hourly for further analysis.

To compare the mean pathways of dye and particles, their centers of mass were calculated as

$$M_{x\_dye}(t) = \frac{\sum_{i=1}^{N_{total\_grid}} x_{i\_dye} \cdot C_{i\_dye} \cdot V_i}{\sum_i C_{i\_dye} \cdot V_i}, \quad (2)$$

$$M_{x\_particle}(t) = \frac{\sum_{i=1}^{N_{total\_particle}} x_{i\_particle}}{N_{tot\_particle}}, \quad (3)$$

where N_{total_grid} is the total number of model grid cells, $N_{total\_particle}$ is the total particle number, C_{i_dye} is the dye concentration in model grid cell i, and V_i is the corresponding grid cell volume. The centers of mass in y and z dimensions were calculated with similar equations.

3 Results & Discussion

3.1 Well mixed condition tests

The vertical particle distributions from WMC tests for Tracker are shown in Figure 2. Results at other locations (not shown) gave similar results. The site with deeper depth passed WMC tests for both time-dependent and steady vertical diffusivity profiles. Occasional failures of WMC tests were found at the shallow site, specifically the vertical regions with low diffusivity and increasing gradient. Particles tend to cluster in low diffusivity regions, e.g., ~38 m in the site HC-shallow (Figure 2b, 2f). Previous studies suggested that demonstration of WMC was influenced by discontinuities in AK_s profiles, the interpolation scheme used to estimate AK_s and its vertical gradient, and the timestep of particle tracking (Brickman and Smith, 2002; North et al., 2006). Here we demonstrated that the 3-point Hanning window used to smooth AK_s profiles, the nearest neighbor interpolation scheme used to obtain AK_s, and a timestep of 300 s in Tracker generally passes the WMC test for sites from offshore deeper than 2,500 m to the Salish sea shallower than 40 m, however there are occasional failures. We proceed by assuming that the effects of such failures would in practice be smeared out as particles are moved rapidly by tidal advection through a wide range of conditions.

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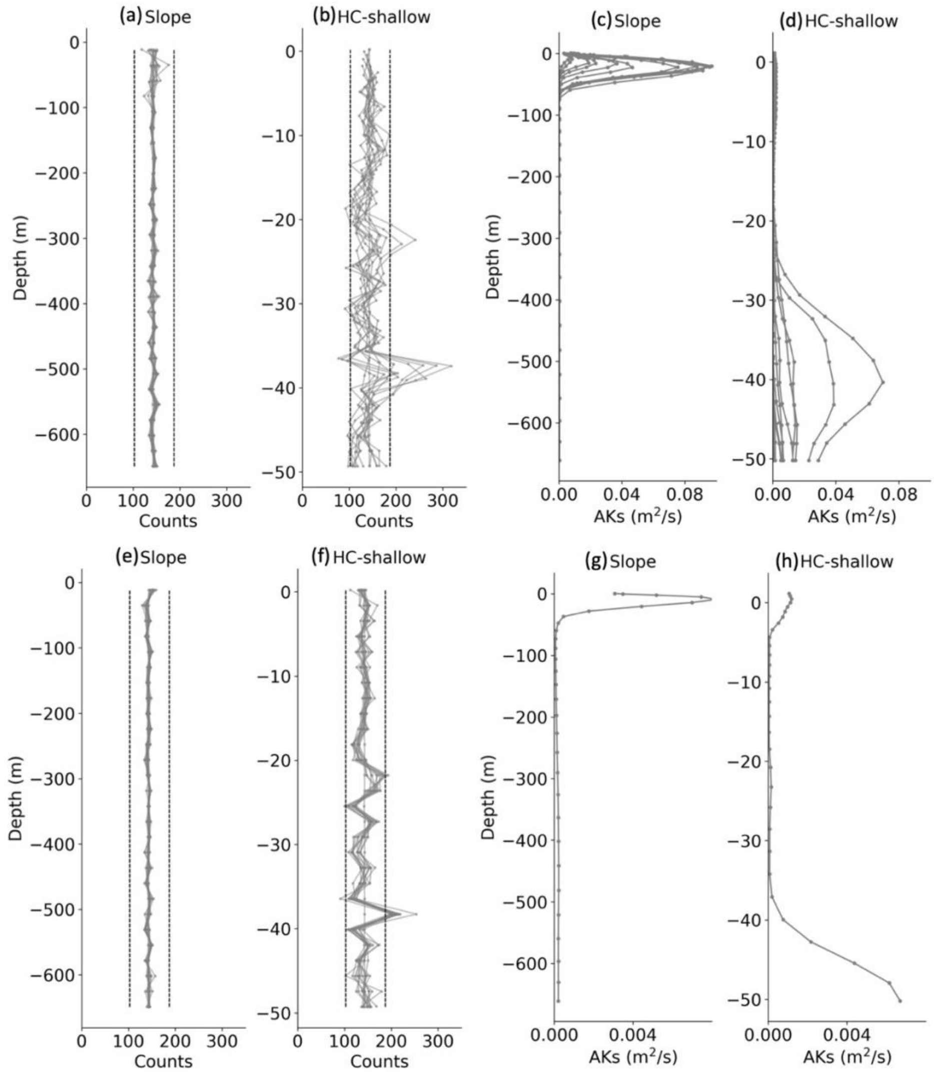

175 **Figure 2: 1-D vertical well mixed condition (WMC) tests at two sites (Figure 1a) in LiveOcean model domain and the associated profiles of vertical diffusivity (c-d, g-h). (a-b) WMC tests using time-dependent diffusivity profiles shown in (c-d). (e-f) WMC tests using steady diffusivity profiles in shown (g-h). All WMC tests were conducted for 12 hours with hourly output and a timestep of 300 s. The dashed lines in (a-b, e-f) indicate the non-significant range, outside which the WMC tests fail.**

https://doi.org/10.5194/gmd-2023-45
Preprint. Discussion started: 22 May 2023

3.2 Comparisons among particle tracking software packages using the Hood Canal model

3.2.1 Offline versus online particle tracking

Centers of mass of trajectories from all particle tracking codes, relative to the initial release location, are shown in Figure 3. Particles were initialized at the low tide and the tracking was followed by a flood tidal phase. A very good inter-model match was achieved for the first 5-6 hours during the flood tide. After this point, all models still tend to follow the same trend, but drift apart presumably because of these different interpolation and advection schemes and online or offline tracking. The differences increase with time since different particle locations sample different velocities and diffusivities.

Horizontal spreading of vertically integrated particle mass (Figure 4) and vertical distributions of particles (Figure 5) exhibit similar evolutions among all tracking codes. Particles from OpenDrift tend to be less spreading. Generally, results from online tracking stays in the middle of other offline tracking codes. Compared to offline tracking, online particle trajectory is updated every timestep along with the hydrodynamic model runs and vertical transport is better accounted (Ricker and Stanev, 2020). However, offline tracking provides more flexibility to incorporate forcings from more than one numerical model or observational databases. In offline mode, it is easier to modify algorithms to include user-defined processes (e.g., diel vertical migrations, settling and resuspension) and test parameters or different particle seeding strategies without rerunning the full ocean model, which can be computationally expensive (Dagestad et al., 2018; Hunter et al., 2022; Melsom et al., 2022). Simulation backward in time is also more easily performed offline. To the best of our knowledge, no studies so far have targeted backward tracking using online particle tracking models. On the other hand, updating trajectories in offline tracking could suffer from inaccuracies induced by interpolation scheme since it reads subsampled or averaged model outputs, which could smear out short-time and small-scale advective processes simulated by ocean circulation models (Wagner et al., 2019; Melsom et al., 2022).

3.2.2 Lagrangian particle tracking versus Eulerian passive dye

Using the Eulerian dye model prediction as a benchmark, we evaluate the performance of the Lagrangian particle tracking models. Like the comparisons among different particle tracking codes, the particle and dye models also agree well with each other within the first few hours following their initial release (Figure 3). The evolution of the center of mass from online particle tracking matches the best with the center of mass of dye. The horizontal center of mass of dye stays between all particle tracking models, while dye predicts somewhat deeper mixing than particle models, with the vertical center of mass being about 5-10 m deeper after 30 hours (Figures 3c). Greater vertical spreading of dye was also observed in the histogram (Figure 5). Dye fills the upper 20-140 m after 2 days while particles are still confined to a depth range of 50-90 m around their release depth. To obtain the histogram of vertical dye distribution, dye mass inside each model grid was converted to particle number via the constant ε_0 (defined in section 2.3).

The horizontal spread of vertically integrated dye and particle mass is shown in Figure 4. Generally, dye is also more widespread than particles in the horizontal. Low values of dye spread faster than particles and cover a greater area. However, the spread of high mass concentration exhibits a reasonable degree of similarity, indicating that the

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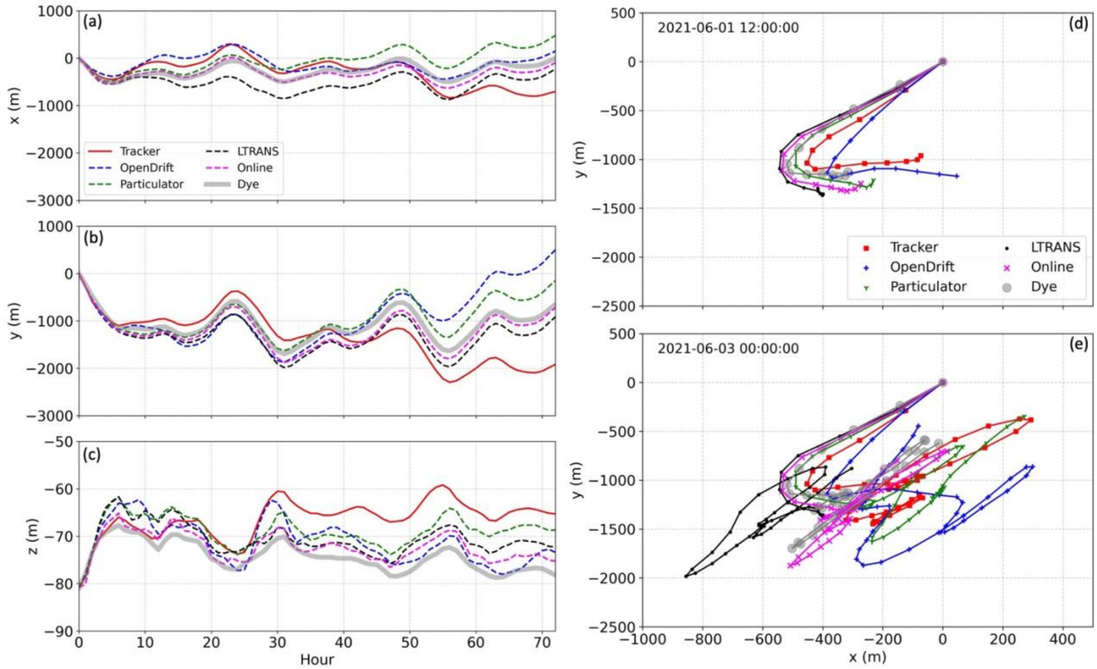
Preprint. Discussion started: 22 May 2023

Lagrangian particle-tracking models all yield similar simulations of vertical dispersion, although formulations for particles and dye transport differ largely in details (North et al., 2006). It is suggested (North et al., 2006; Wagner et al., 2019; Broatch and MacCready, 2022; Nepstad et al., 2022) that the vertically reconstituted diffusivity profile, vertical model grid resolution, total particle number, the temporal subsampling of velocity fields, and numerical mixing influencing dye concentration give rise to the deviations between particle tracking and inert dye component.

Comparing online particle tracking and online passive dye experiment in ROMS, Lagrangian particle tracking tends to be more computationally demanding (Table 2). The average time for running hydrodynamics for one day in Hood Canal model is about 160 s using 200 cores on a Linux cluster. The running time increases a little to 196 s with dye module activated, and it increases to 1218 s when floats module was activated to track 10^5 particles. However, particle tracking, especially offline tracking, is more flexible, and dye calculations can be more costly in some instances. For example, multiple passive dyes are required to represent multi-component river-borne discharges (e.g., nutrients, pathogens, freshwater) but particles can carry all these properties in one trajectory tracking experiment (Banas et al., 2015). Particle tracking is also economical in disk space since only particle locations and associated water properties, e.g., salinity and temperature, are stored but dye is usually saved for the whole model domain (Melsom et al., 2022). In addition, particle tracking models can resolve particle displacement at sub-grid scales (Alosairi et al., 2020; Xiong et al., 2023) because dye is a grid cell property.

https://doi.org/10.5194/gmd-2023-45
Preprint. Discussion started: 22 May 2023

Geoscientific Model Development
Discussions



230 **Figure 3: The centers of mass in x, y, z directions obtained from offline and online particle tracking and passive dye experiments using Hood Canal model. (a-c) evolution of the centers of mass. (d-e) the centers of mass in x and y directions with particles tracked for (d) 12 hours and (e) 48 hours. Particles and dye were released inside Hood Canal at 2021.06.01 00:00:00 (Figure 1b).**

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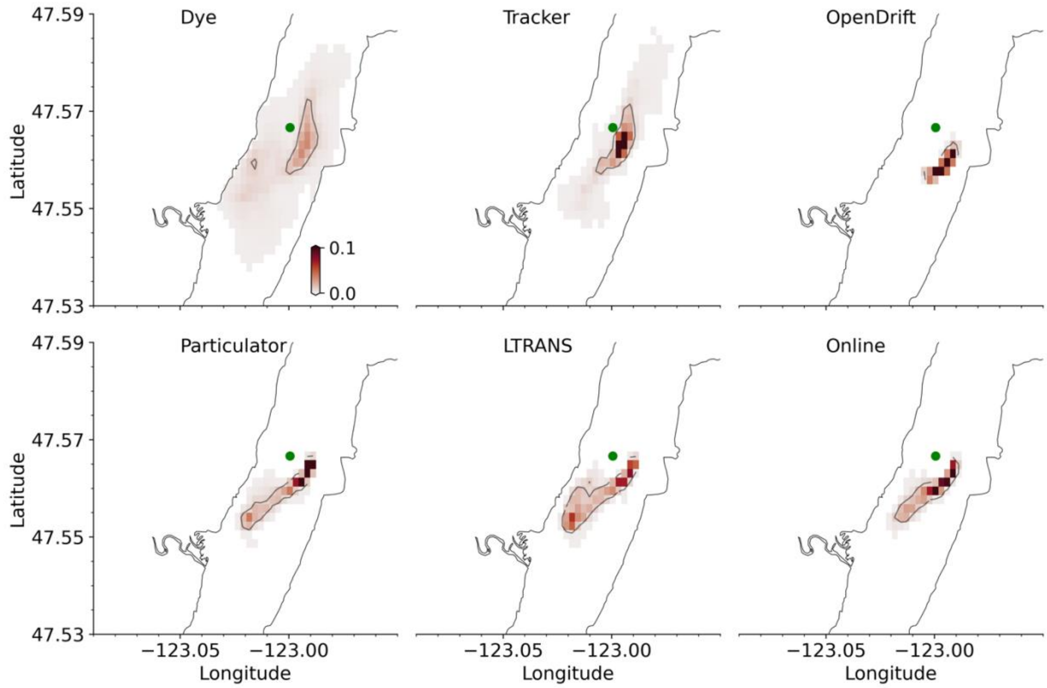
Preprint. Discussion started: 22 May 2023



235 **Figure 4: Snapshot of vertically integrated dye and particle mass (scaled to 0-1 by the initial dye or particle mass) after 1-day of simulation using the Hood Canal model. The green dot indicates the initial dye and particle release location. The black contour in each panel represents a value of 0.01.**

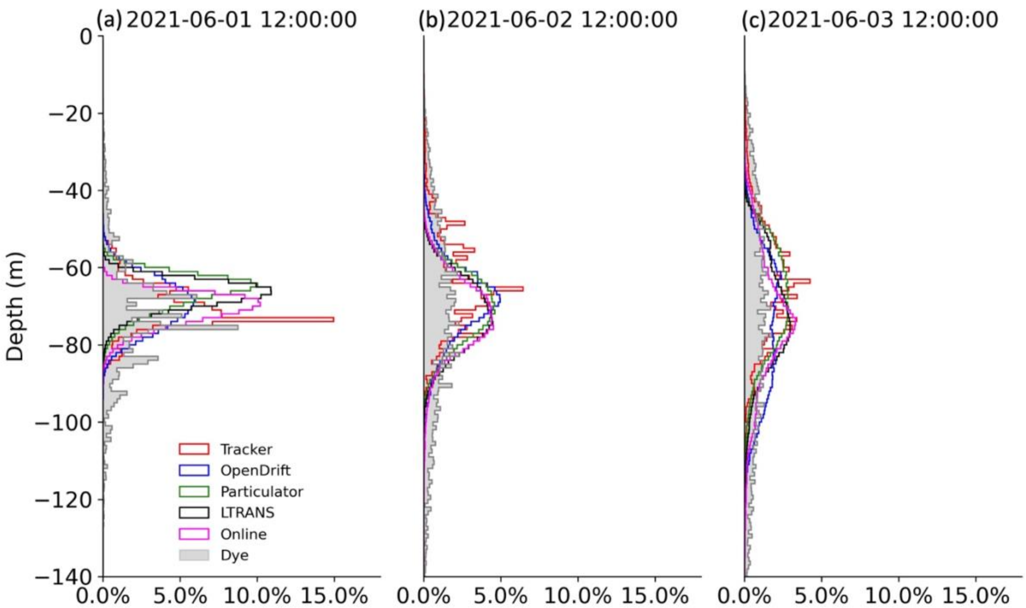


Figure 5: Histogram of vertical particle and dye distributions using Hood Canal model at 12, 36, and 60 hours after release. The effects of numerical mixing may be the cause of the greater vertical spread of dye vs. particles.

3.3 Comparison among offline particle tracking software packages using the LiveOcean model

Additional comparisons just among the four offline particle tracking codes were conducted using the larger LiveOcean model domain. Particles were released from the free surface and the middle water column in the coastal area at 2021.01.01 00:00:00 (Figure 1a) and particle dispersal regions along the coast are with a horizontal grid resolution of ~1000 m (Figure 6h-i). The particle tracking period was dominated by southerly winds, favorable for northward and onshore near-surface currents over the shelf (Giddings et al., 2014). Thus, particles exhibit net northward transport, and the surface-released particles move closer to the coast (Figure 6h-i). Besides the center of mass, particle density, a ratio of the vertically integrated particle numbers in each horizontal grid cell to the respective grid cell area, was also calculated (Figure 7). A relatively good match in the center of mass among these tracking codes is evident for about 1 day of tracking (Figure 6). This suggests that the decorrelation time (Klocker and Abernathey, 2014) is about 1 day in this region. After that, the center of mass still follows a similar trend with the separation increases with time. The spatial coverages of particles in the horizontal and vertical also share similar patterns but exhibit somewhat different local accumulation patches (Figures 7-8). As we saw in the Hood Canal experiments, all four offline particle tracking codes have similar performance when they track the same water mass in the coarser model domain and in the shelf environment. Note, however in Figure 8 that there are real differences in the details of vertical particle distribution among the models after 2 days. These result in part from the details of the algorithms used for vertical dispersion, and in part from particles experiencing different mixing due to growing differences in location.

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Preprint. Discussion started: 22 May 2023

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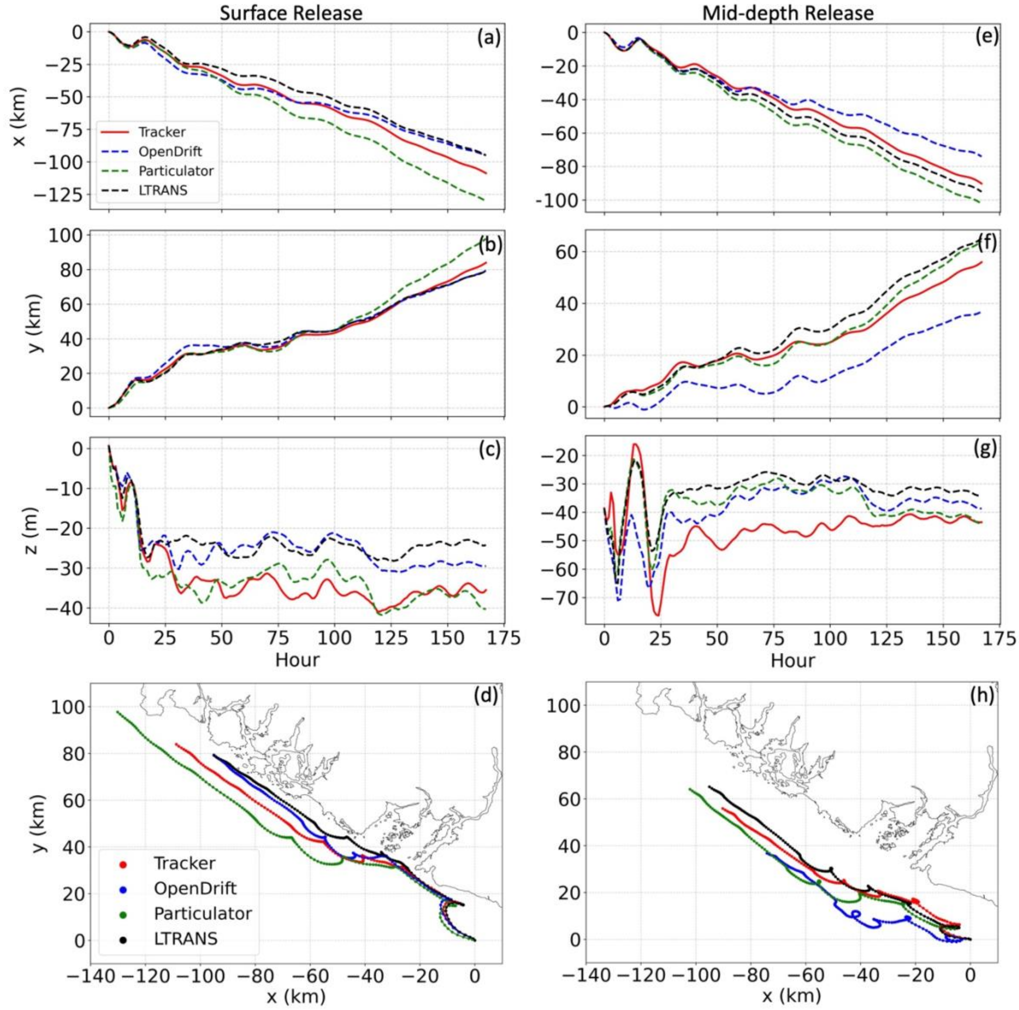

260 **Figure 6: The centers of mass in x, y, and z directions for all four offline particle tracking codes simulated in the LiveOcean model. (a-c) particles released from the free surface. (e-g) particles released from the middle water column. (d, h) centers of mass in x and y directions.**

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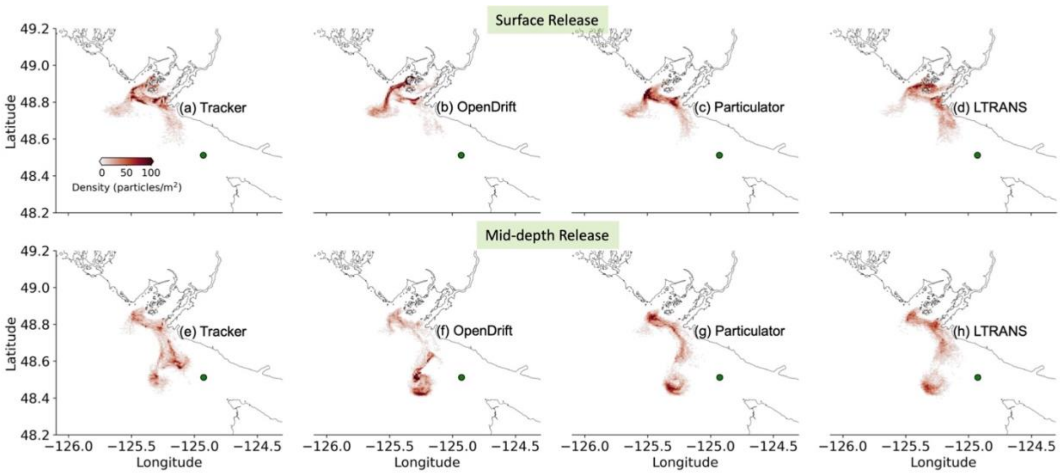

Figure 7: Vertical integral of particle densities for all four offline particle codes after 2 days of tracking in the LiveOcean model. (a-d) particles were released from the free surface, (e-h) particles were released from the middle water column. Green dots represent particle release location.

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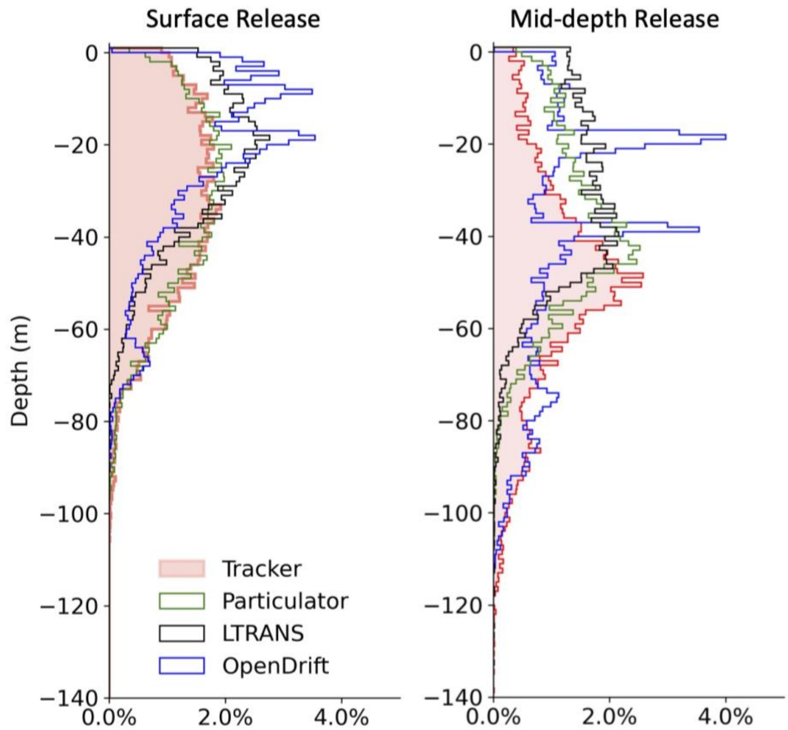

Figure 8: Histogram of vertical particle distribution for all four offline particle codes after 2 days of tracking in the LiveOcean model. Left panel: particles released from the free surface; right panel: particles released from the middle water column.

3.4 Computation time

Although all tested offline particle tracking codes share similar predictions compared with online particle tracking and Eulerian dye, especially for the first few days, computation efficiency is another important metric for their performance evaluation. The computation time for each offline tracking code was recorded using both the small domain of the Hood Canal model and the large domain of the LiveOcean model (Figure 9; Table 3). Each particle model was run to track neutrally buoyant particles for 25 hours with a timestep of 300 s. Particle locations and temperature and salinity at each particle's location were saved hourly. The total particle number was varied from 10^0 to 10^6. The computation time tests were conducted using an Apple M1 Pro for Particulator and OpenDrift, and a Linux machine for LTRANS. We recorded the computation time of Tracker both on the laptop and the Linux machine.

The two tracking codes, Tracker and OpenDrift, that were written in Python, have very close computation costs when tested on the Linux machine (Figure 9). Their computation time increases with increased particle number, with the largest increase when running 1 million particles. The performance of Tracker on a laptop is faster by a factor of 2-3 compared to the Linux machine, perhaps because of different file access speeds between solid-state and RAID drives

https://doi.org/10.5194/gmd-2023-45
Preprint. Discussion started: 22 May 2023

Geoscientific Model Development
Discussions
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used to store the model output. The LTRANS, written in Fortran, runs fast with a small number of particles but the computation requires a much longer time than other codes with increased particle number and even becomes prohibitive when tracking one million particles in the large LiveOcean domain with a grid dimension of $1302\times662\times 30$. Generally, more time is required to track particles in a larger model domain than a smaller one for all offline tracking codes. One interesting finding is that for Particulator, written in MATLAB, the computation time is only weakly influenced by the total particle number and the code can run very fast with the one million particles. The interpolation and advection scheme, algorithm structures, and programming languages could all affect the computation cost (Table 2). It is beyond the scope of this paper to explore the detailed tradeoffs between these factors, and instead hope the performance results may be one piece of information scientists can use when choosing a particle tracking package and designing an experiment.

https://doi.org/10.5194/gmd-2023-45
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Geoscientific Model Development
Discussions

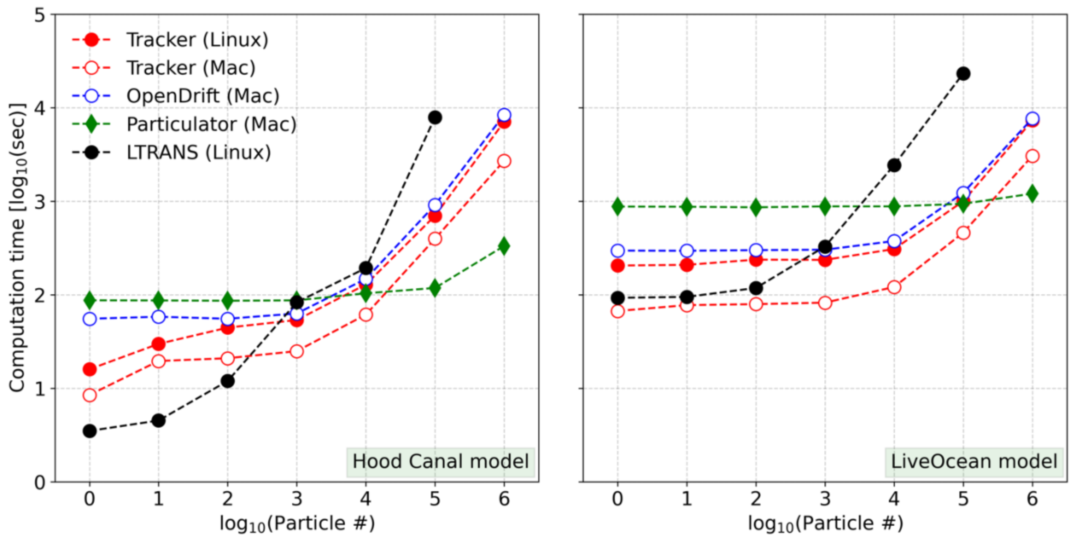

Figure 9: Computation time for tracking particles for 25 hours with a timestep of 300s for all four offline particle tracking codes. The total particle number increases from 10^0 to 10^6. The computation time for LTRANS was obtained on a Linux machine, while the computation time for Particulator and OpenDrift was obtained on Apple M1 Pro. Tracker was tested both on Linux machine and Mac. The computation cost for LTRANS with 1 million particles is prohibitive on the Linux machine when testing it with the large LiveOcean domain; for the small Hood Canal domain, the computation time of LTRANS is about 25 hours estimated from the timestamp of the hourly output files that were saved separately.

https://doi.org/10.5194/gmd-2023-45
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4. Conclusions

In this work, we introduced a new offline Lagrangian particle tracking model, Tracker, and tested its ability to preserve the vertical well mixed conditions. We also evaluated its performance compared with online Eulerian dye, one online and three offline particle tracking codes using a high-resolution (200 m) ocean circulation model. Additional comparisons were performed for all four offline tracking codes in a larger model domain with a horizontal grid resolution of ~1000 m in the particle tracking region.

We show that the mean advection pathways and spatial distributions of dye and particles are reasonably similar when they were tracking the same water mass. The spreading of Eulerian dye is more dispersive with a wider distribution of low concentrations. Similar inter-model comparisons were observed in both small (fine) and large (coarser) model domains. The passive dye was solved in a fixed Eulerian framework that addresses the advection and diffusion equation which might suffer from spurious numerical mixing. The Lagrangian particle tracking model employs a movable frame of reference. Online tracking may be expected to give more accurate results because it uses a much shorter time step between velocity fields but lacks flexibility compared to offline tracking. In our experiments, results from online particle tracking were not obviously different from that of any of the offline tracking packages. Although offline tracking is influenced by subsampled model output, parameterization of vertical turbulence mixing, and interpretation scheme, its flexibility and reliability against passive Eulerian dye and online tracking make it a useful and cost-effective tool in tracking transport pathways in oceanography. Finally, the reasonable preservation of well-mixed conditions and similar performance against other particle tracking codes and passive dye achieved by Tracker suggest that it is a reliable particle tracking package to use with ROMS. All tests in this study used a ROMS grid aligned along lines of constant latitude and longitude. In principle, Tracker should work on a more general grid, but this has not been tested.

Code availability

The source code for Tracker is hosted on Github at https://github.com/parkermac/LO/tree/v1.1/tracker; The associated Zenodo DOI and data files are at https://doi.org/10.5281/zenodo.7783639. The source code for other particle tracking packages can be found: OpenDrift: https://opendrift.github.io/; LTRANS: https://northweb.hpl.umces.edu/LTRANS.htm; Particulator: https://github.com/neilbanas/particulator.

Author contribution

PM is the primary developer for Tracker and the LiveOcean model. JX developed the Hood Canal model and carried out all the particle tracking and dye release experiments. JX drafted the manuscript and PM contributed to the review and editing.

Competing interests

The authors declare that they have no conflict of interest.

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Geoscientific Model Development Discussions

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Geoscientific Model Development Discussions
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Table 1. Configurations for different particle tracking codes.

	Tracker	OpenDrift	Particulator	LTRANS	ROMS online floats
Programming language	Python	Python	MATLAB	Fortran	Fortran
Time step	Self-defined	Self-defined	Self-defined	Self-defined	Same as baroclinic time step
Vertical turbulence	Random displacement	Random displacement	Random displacement	Random displacement	Random displacement
Land boundary	Move particles on land to the middle of the nearest wet rho point	• Stranding: particles deactivated • Previous: particles moving back to previous locations • None: particles not interacting with land	AvoidLand: particles carried onto land will wait there until flow can carry them away.	Particles reflected off the land boundary with an angle the same as the approach angle. The reflect distance equals the distance that particles exceeded the boundary.	Particles avoid crossing land boundary
Open boundary	Not specified, remove particles outside boundary in post-processing	Particles deactivated outside the domain (or absorbing boundary)	Particle stops if it will be transported outside the domain in the next timestep and wait there until flow moves it around inside the domain	• Reflective boundary: treated the same way as land boundary. • Sticking boundary: stop moving	Particles outside open boundary are deactivated
Vertical boundary	Reflect vertically back into the domain by a distance that the particle exceeds the boundary	• Bottom boundary: lift_to_seafloor, deactivate, previous, or resuspended • Surface boundary: reflective or stick to surface	Particles move outside the surface (or bottom) will be put back in sigma = 0 (or -1)	Reflect vertically back to the domain with the same distance that particles exceed the boundary	• ifdef float_sticky: floats that hit the surface are reflected; floats that hit the bottom get stuck; • undef float_sticky: floats that hit the surface or bottom are reflected
Advection scheme	4th-order Runge-Kutta	Euler, 2nd-order Runge-Kutta, 4th-order Runge-Kutta	2nd-order Runge-Kutta	4th-order Runge-Kutta	4th order Milne predictor and 4th order Hamming corrector
Interpolation scheme	Nearest neighbor	Bilinear	Bilinear	Water-column profile scheme for 3D and bilinear for 2D variables	• Inside masked cells: linear & nearest neighbor • Outside masked cells: bilinear
Backward tracking	Able to include	Yes	Able to include	Yes	Not able to do backtracking
Ease of use	• Read ROMS history file • No compilation required, easy to set up python environment • Flexible to define the initial particle release location and add user-defined functions • Running platform independent	• Needs to concatenate grid information to ROMS history file • No compilation required, easy to set up python environment • Flexible to define the initial particle release location, modify existing modules, and write user-defined modules. • Running platform independent	• Read ROMS history file • No compilation required but MATLAB is a commercial software • Flexible to define the initial particle release location • Running platform independent	• Read ROMS history file but each file must have at least 3 timesteps • Take time to compile source code • Flexible to define the initial particle release location • Run on Linux machine • Require a long time run for large number of particles	• Require experience to compile ROMS source code and set up HPC environment • The initial particle release location seems to be not very handy/flexible to specify • Run on Linux machine in parallel mode
Source code	https://github.com/parkermac/LO/tree/main/tracker	https://opendrift.github.io/	https://github.com/neilbanas/particulator	https://northweb.hpl.umces.edu/LTRANS.htm	https://www.myroms.org/wiki/floats.in

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Geoscientific Model Development Discussions
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Table 2. Computation time (second) for ROMS simulations conducted for 1 day.

Cases	Average* computation time
Hydrodynamic run	160
Hydrodynamic run + passive dye	196
Hydrodynamic run + online particle tracking (100,000 particles)	1218

*Averaged from 2021.06.01 to 2021.06.07

** All cases were run on UW's Hyak supercomputer with 200 cores.

Table 3. Computation time (second) for different particle tracking software packages using the Linux machine or Mac with a small Hood Canal model domain and a large LiveOcean model domain. All cases were run for 25 hours with a timestep of 300 s and hourly output with particle locations, and temperature/salinity recorded by each particle.

Particle number	Hood Canal model					LiveOcean model				
	Tracker (Linux)	Tracker (Mac)	OpenDrift (Mac)	Particulator (Mac)	LTRANS (Linux)	Tracker (Linux)	Tracker (Mac)	OpenDrift (Mac)	Particulator (Mac)	LTRANS (Linux)
1	16.0	8.5	55.5	87.4	3.5	205.8	67.2	297.2	878.8	92.9
10	29.9	19.6	58.3	87.1	4.5	209.2	77.6	295.8	875.0	95.1
100	44.6	21.0	55.5	86.4	12.0	237.9	79.5	300.7	863.3	118.4
1,000	53.8	25.0	63.2	87.3	83.2	236.6	82.5	303.8	883.0	328.7
10,000	129.1	61.5	148.2	103.9	193.5	308.9	121.3	376.1	882.7	2437.3
100,000	701.0	398.0	915.7	118.4	7931.8	1001.9	462.0	1234.0	941.8	23325.7
1000,000	7093.0	2715.2	8419.8	333.0	/	7309.3	3063.7	7678.2	1208.0	/