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# OceanTracker 0.5: Fast Adaptable Lagrangian Particle Tracking in Structured and Unstructured Grids

Ross Vennell[1], Laurin Steidle[2], Malcolm Smeaton[1], Romain Chaput[1], and Ben Knight[1]

[1]Cawthron Institute, Nelson, New Zealand
[2]University of Hamburg, Germany

**Correspondence:** R. Vennell (ross.vennell@cawthron.org.nz)

**Abstract.** Particle tracking is frequently used to compute particle movements within hydrodynamic ocean models; however, modelling millions of particles is computationally challenging. OceanTracker is designed to minimise the time required to obtain results from particle tracking. Firstly, by being computationally fast, it enables users to scale to large numbers of particles, thus obtaining better statistics or exploring a wider range of cases within acceptable run times. Secondly, OceanTracker can calculate multiple particle statistics during the computational run, eliminating the time needed to post-process large volumes of recorded particle trajectories. The adaptability of OceanTracker's modular computational pipeline allows users to add and modify components which govern particle physics, behaviour, and statistics. The computational pipeline is entirely assembled from user-provided parameters, supplied as a text file or built using helper methods. Coders can easily modify existing components through code inheritance. Currently, OceanTracker supports hydrodynamic model output for unstructured grids (SCHISM, FVCOM, DELFT3D-FM) and structured grids (ROMS, NEMO/GLORYS). Computing the trajectories for more than a million particles with OceanTracker on a single computer core is 35 times faster than the OpenDrift code and twice as fast as the Ocean Parcels code, despite treating structured grids as unstructured. As a result, on a basic laptop computers it can model one million particles for one month in less than one hour, or many more particles on better hardware. OceanTracker's design allows multiple variations of particle tracking to be configured to run in parallel.

## 1 Introduction

Particle tracking is key to answering many scientific and practical questions about bio-physical transport in the ocean (Lynch et al., 2014; Van Sebille et al., 2018), such as movement of larvae, residence times (Lucas and Deleersnijder, 2020), or quantifying connectivity between regions, e.g. (Atalah et al., 2022). A major challenge is simulating millions of particles (Van Sebille et al., 2018). Large numbers enable better estimates of particle statistics, such as heat maps or connectivities. For example, when estimating connectivities between regions, where connectivity is weak, but the consequences are significant, such as for the spread of invasive species. Scaling also facilitates a much wider exploration of particle behaviours (e.g. light-dependent vertical velocities of larvae) and the sensitivity of results to parameters governing those behaviours.

Simulating millions of particles creates two challenges. Firstly, computing their trajectories in user, acceptable time frames. Secondly, the time required to post-process the trajectories to obtain the required particle statistics, along with the effort

required to manage large volumes of output (see Sec. 2.1). OceanTracker minimises user effort by addressing both of these challenges.

OceanTracker's computational speed makes it possible to scale particle numbers on modest computer hardware. Table 1 shows a range of hardware, all of which can compute one month of particle trajectories for 1 million particles in less than an hour on a single CPU. The comparison in Sec. 4.1 indicates that OpenDrift (Dagestad et al., 2018) would require 32 hours to accomplish the same task. The times in Table 1 for computers with more CPUs and memory are not significantly faster than the basic Laptop I. However, when more CPUs and RAM are available, OceanTracker enables the easy division of the required runs into separate cases, which can then be run in parallel to significantly reduce run times (see Sec. 4.2).

The second component of minimising a user's time and effort is reducing the time spent in post-processing. Having the computational speed to scale to millions of particles will produce large files containing the computed particle trajectories. The time needed to analyse these tracks to yield the required particle statistics becomes a major bottleneck for the user, along with the logistical issues of storing and accessing what may be terabytes of output for analysis. OceanTracker resolves both of these issues by recording particle statistics during the computational run, e.g. by counting particles inside grid cells "on-the-fly" to produce a heat map, or counting particles inside polygons to calculate connectivities between regions, as shown in Fig. 1 and Sec. 3.8. On-the-fly statistics address both the post-processing time and storage issues, as no particle trajectories need to be recorded, and the volume of the statistical outputs are independent of the number of particles released.

A key aspect of OceanTracker is the ability for users to easily adapt how particles behave and the statistics calculated. To achieve this, OceanTracker is built around the concept of a *computational pipeline*, which is broken into a series of steps, where each step performs a specific computational *role*, see Fig. 3. Each role many be undertaken by one or more components added by a user's configuration. The components are implemented as Python classes, which are dynamically added at runtime to a role. For example, multiple release group components with different release locations and schedules can be added to carry out the particle release role, all done within a single computational run. Similarly, multiple components can be added to carry out the on-the-fly statistics role in the same computational run. Other roles with the Computational pipeline included dispersion, suspension, or modifications to their trajectories due to behaviours (e.g. larvae settling within a polygon). Dynamically adding components to roles within the Computational pipeline enables flexibility in building the specific computations required by a user.

A challenge in having an adaptable computational pipeline is enabling both coders and non-coders to access the same level of adaptability. For both, OceanTracker's computational pipeline is entirely constructed from a user-supplied configuration that defines which components are added to roles with the computational pipeline. For each component, the configuration also gives the *parameters* which specify their individual settings, Sec. 3.1.1, e.g. the configuration of the component added to the resuspension role will set a critical friction velocity parameter, above which particles will resuspend. Fig. 4 provides a minimal example of this, showing the same run executed either through coding or, or from parameters supplied in one of two standard text file formats. Another advantage of the use of text file parameters is that it allows web-based particle tracking on-demand services to easily access the same level of computational pipeline adaptability, e.g. (Vennell et al., 2019).

Implementing an adaptable Computational pipeline built from components added by the user can a conflict with making fast code. For example, consolidating all particle operations in the computational pipeline within a single loop over all particles would be faster, i.e. performing all required computations for each particle one at a time. This approach increases efficiency, as the data required for each particle is likely to be in the faster chip memory cache if used more than once. It also avoids the need to create, read or write arrays in main memory of intermediate results. However, it is much harder to adapt a single loop over all particles when there are many operations with different variants. OceanTracker takes a middle ground, by breaking up the computational pipeline into a series of modular operations on all particles assembled into a sequence of operations within the roles illustrated in Fig. 3. This modular approach compromises speed, but significantly enhances adaptability.

A single particle tracking framework that works for both structured and unstructured grids simplifies the particle tracking process for users by having a uniform approach regardless of the hydrodynamic model used. Particle trackers for unstructured grids are rare due to the complexity involved in coding the movement and interpolations within the grid. A review of ocean Lagrangian analysis (Van Sebille et al., 2018) lists 11 particle trackers, of which only one "LIGHT in MPAS-O" is capable of working with unstructured grids. Those compatible with both types of grid are even rarer, e.g OpenDrift. A secondary goal for OceanTracker is to provide a single framework that auto-detects the type of grid from multiple hydrodynamic model formats and identifies useful optional variables, such as bottom stress used in particle re-suspension. This enables users to focus on the outcomes they need from particle tracking, rather than the details of the underlying hydrodynamic model.

Examples of OceanTracker's applications to date are:

- Backtracking to infer likely locations of the parents of settled mussel larvae. Approximately 600 million particles were released over ten years and tracked for their 6-week lifetimes. (Atalah et al., 2022).
- Investigating phytoplankton retention mechanisms in an estuary with populations that grow through particle splitting. One billion particles were released, with up to 1 million active at any one time.(Steidle and Vennell, 2023).
- Inferring the area within which the eDNA of a species may be detected from water samples (Pastor Rollan et al., 2024).
- Estimating the risk of invasive species from ballast water discharged from ships transiting coastal shipping routes from the release of 65 million particles (Smeaton et al., in prep).
- Determining pathways for the spread of diseases between aquaculture farms from connectivities between 500 farms based on 150 million particles (Knight BR, 2024).
- Online ocean plastics public engagement tool, allows users to drop virtual plastic and see where it travels to. Returns 20 particle trajectories in less than 1 sec from an on-demand particle tracker server (Vennell et al., 2019).

Like many other particle trackers, OceanTracker saves users' time by performing particle tracking "offline", based on the recorded output from a hydrodynamic model. In contrast, "online" particle tracking performs computations during the hydrodynamic model run. Hydrodynamic model run times are typically much longer than those of particle tracking. Thus, any new variations in particle tracking requires re-running the slow hydrodynamic model. As a result, offline particle tracking facilitates

| | Specifications | | | Minutes per modelled month | | |
|---|---|---|---|---|---|---|
| | CPU | RAM Gb | Freq. MHz | Read | Computation | Total |
| Laptop I | 4 | 8 | 1.6-3.9 | 7 | 41 | 48 |
| Laptop II | 10 | 16 | 1.7-4.7 | 4 | 23 | 27 |
| Desktop I | 8 | 32 | 3.7-4.4 | 8 | 32 | 40 |
| Desktop II | 32 | 128 | 3.7-4.5 | 4 | 25 | 30 |
| Work station | 36 | 256 | 2.7-3.7 | 8 | 39 | 47 |

**Table 1.** OceanTracker run times for modeling 1 million particles over a period of 1 month. The runs utilised a single core, a time step of 15 minute and Runge-Kutta 4 time integration. The 3D SCHISM hydrodynamic model included 79k nodes and 140k triangles.

faster exploration of variations in behaviours and the sensitivity of results to parameters, e.g. fall velocity. Some examples of offline ocean particle trackers are PARTRACK (Knight et al., 2009), LIGHT (Wolfram et al., 2015), OpenDrift (Dagestad et al., 2018), ROMSpath (Hunter et al., 2022) and Ocean Parcels (Delandmeter and Van Sebille, 2019). This paper outlines the features and structure of the latest version of the OceanTracker particle tracker (Vennell et al., 2021).

This paper provides an overview of its features in Sec. 2, including some example outputs in Fig. 1. Sec. 3 details its structure and describes how to configure the computational pipeline in Sec. 3.1.1. Additionally, Sec. 3.9 outlines integrated models which combines components within roles to achieve a higher level functionality, such as calculating Lagrangian coherent structures. Sec. 4 explores the features contributing to OceanTracker's speed and compares its performance to OpenDrift and Ocean Parcels.

## 2 Overview

This section highlights some of OceanTracker features that minimise user effort, its physics and an example use case is presented in Fig. 1.

### 2.1 Features reducing user effort

In addition to computational speed, OceanTracker incorporates an number of features that significantly reduce the time and effort required to obtain results from the analysis of particle trajectories. The most significant features are:

**Release groups:** Allows simultaneous release of multiple groups of particles, each with distinct locations and timing. This functionality enables users to obtain more comprehensive results from a single computational run, as shown in Fig. 1, Sec. 3.5 and Appendix A. This eliminates the need for setting up and managing multiple runs to explore different release scenarios.

**On-the-fly particle statistics:** OceanTracker enables the addition of multiple statistics components to a computational run based on counting particles within user specified grids or polygons. This enables the calculation of diverse statistics from the same set of particle trajectories during one computational run. For instance, it can generate different heat maps for moving

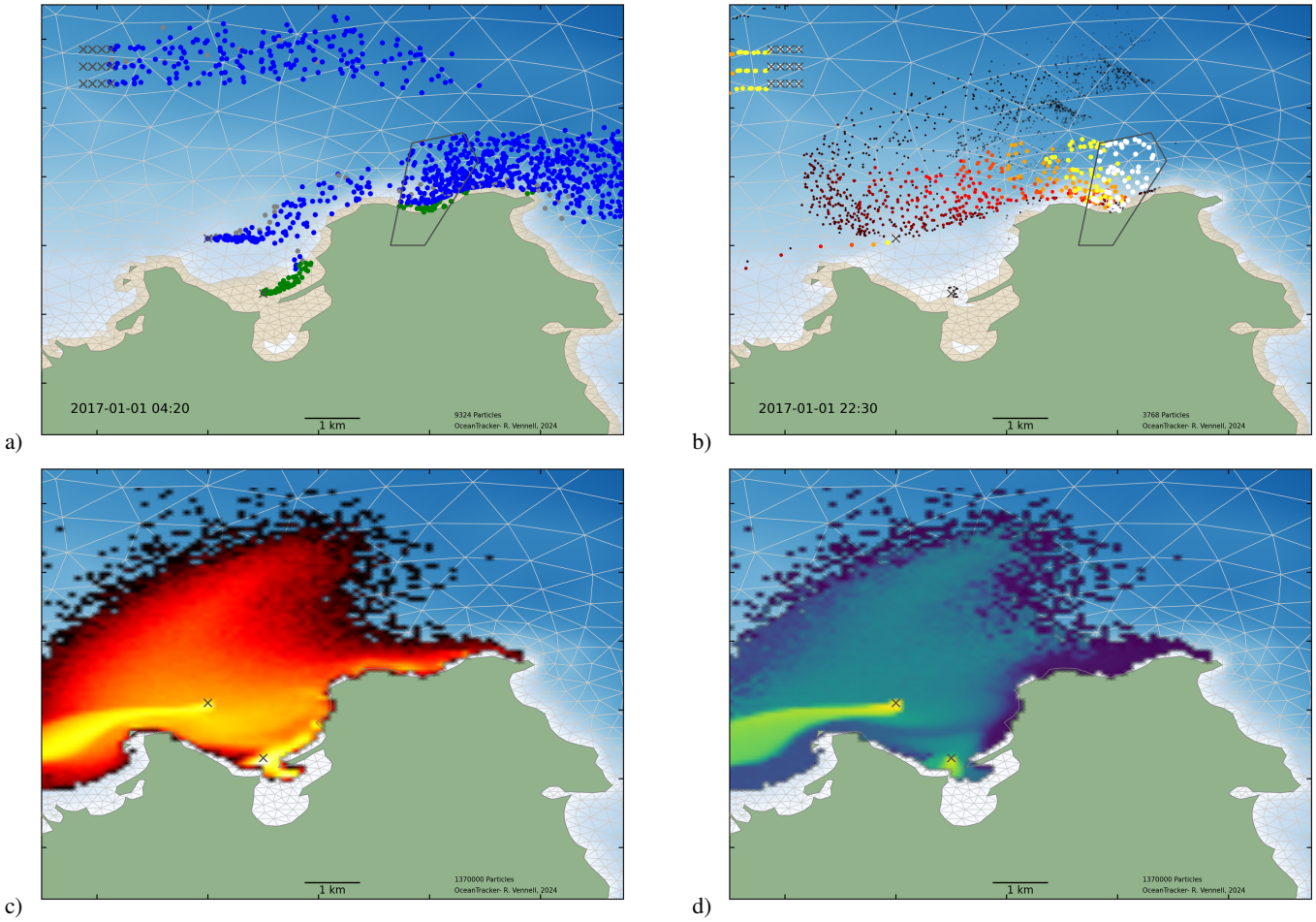



**Figure 1.** Examples of simultaneous point, polygon and grid particle release groups, Sec. 3.5. a) A snapshot of the particles: blue indicates particles are moving, grey signifies particles on the bottom that may later resuspend and green particles those stranded by an outgoing tide. Dry cells are shown in brown, with the blue shading indicating water depth. b) Particles sized and coloured according to a decaying particle property Sec. 3.2.2. c) Heat-map of log particle counts from a release of 1.3 million particles from a pair of point sources. d) Heat-map of decaying particle property on a logarithmic scale. The code to run this example is in Appendix A.

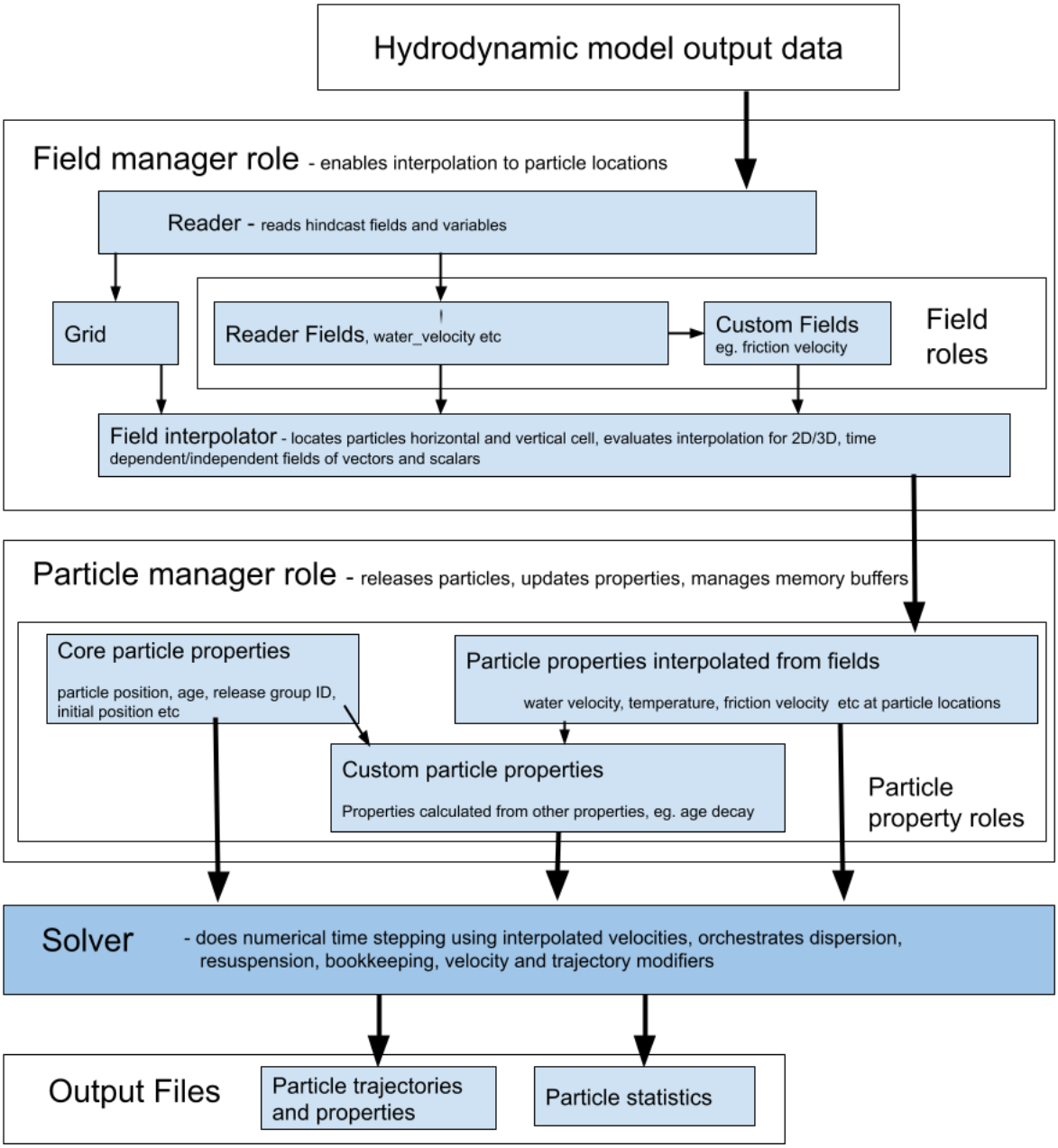



**Figure 2.** Outline of data flow through the two main data structures, fields and particle properties, from hydrodynamic model files to output. These data structure roles are outlined in Sec. 3.2. Each have "managers" to orchestrate operations on the variants of each data structure, to deliver particle properties to the solver.

particles and those on the bottom, and calculate connectivities between areas defined by polygons, all within the same run. On-the-fly statistics are calculated separately for each release group, e.g. individual heat maps for each release site, or connectivities between releases within multiple polygons and another set of polygons.

**Multiprocessing:** OceanTracker leverages multiple computer cores allowing users to run multiple scenarios in parallel. It simplifies multiprocessing by orchestrating all cases within a unified set of user parameters and organises the output in a consistent structure.

**Coding productivity** New functionality for tailored applications can be added to OceanTracker using the widely used Python language NumPy package (Harris et al., 2020). For complex computationally intensive operations Numba was used (Lam et al., 2015). A major advantage of Numba is that users do not need to learn new coding syntax, such as C, to speed for intensive operations. More on Numba in Sec. 4.

**Self-managing particle buffer**: Particle properties such as current location or status are stored in memory buffers. Theses expand dynamically as more particles are released, thus the user does have to specify the maximum number of particles they will use in advance. In addition, as particles are killed the memory buffers are consolidated by removing dead particles from memory, minimising the total memory required.

### 2.2 Physics

OceanTracker users can also enhance particle physics by adding components to the velocity modifiers role (eg. sinking velocities) or the trajectory modifiers role (e.g. particle splitting or larval behaviours) as outlined in Sec. 3.6 and Sec. 3.7. The core physical processes include:

**Dispersion role:** A random walk mechanism simulates dispersion due to sub-hydrodynamic grid scale processes (Lynch et al., 2014). By default, constant turbulent eddy viscosities are applied. If vertical 3D turbulent viscosity profiles are available in the hydrodynamic model files, these profiles are interpolated profile to calculate the vertical random walk instead, necessitating a vertical velocity correction (Ross and Sharples, 2004). Note that, the random walk is not applied as a step change in position, but as an equivalent additional velocity applied to each Runge-Kutta (RK) sub-step in the velocity modifiers loop, see Fig. 3 and Sec. 3.6.

**Re-suspension role:** Particles on the bottom may re-suspend if flows are strong enough. Whether and how far re-suspending particles jump above the sea bed depends on the friction velocity (equation 9.28 in Lynch et al. (2014)). Thus, particles are more likely to re-suspend and jump higher, in stronger flows. The friction velocity is calculated from the near seabed velocity assuming a logarithmic velocity profile, or the bottom-stress field if it can be found in the hydrodynamic model output.

**Tidal stranding role:** Particles in dry hydrodynamic model cells remain stationary until the cell becomes wet again. Dry cells flags are set from data in the hydrodynamic model. If this data is not available, then a cell is dry if the total water depth at the cell's center is less than a user given minimum value.

### 2.3 Other features

Along with the above core user replaceable physics roles, other functionalities include:

**Backtracking:** OceanTracker supports reverse time simulations, which can be useful for identifying potential sources of particles arriving at a given location. (Thygesen, 2011). Note that dispersion is not time-reversible, and this operates the same in the forward direction time, producing outputs, like heat maps, that offer a probabilistic view of sources.

**Nested grids:** To enable particle tracking beyond the open boundaries of a single hydrodynamic grid, OceanTracker can nest multiple inner grids within a broader scale outer grid. Particles exiting the open boundary of an inner grid are transferred to the outer grid, and particles on the outer grid which move inside an inner grid, are transferred to that grid. Each particle is aware of its current grid, allowing field values to be interpolated from the relevant grid. The inner and outer grids may consist of any combination of structured or unstructured grids.

### 2.4 Example

Fig. 1 presents some basic examples of OceanTracker outputs from a 3D simulation. This example shows point, polygon and regular grid particle releases within the same computational run, add discussed in Sec. 3.5. The snapshot in Fig. 1a) displays particles coloured according to their status, moving (blue), stranded by the tide (green) or on the bottom (grey).

Heat maps can illustrate the decay and dispersion of a pollutant from its source. To construct heat maps using particle tracking, sufficient particles must fall within each grid cell to ensure spatially smooth heat maps. The efficiency of OceanTracker allows for the release of millions of particles, enabling the direct creation of heat maps without the need for additional radial smoothing of particle counts. In Fig. 1c, 1.3 million particles were sufficient to produce a detailed heat map. This heat map was generated by counting particles into grid cells on the fly, thereby avoiding the need to record large volumes of particle trajectories. Fig. 1d) illustrates a heat map of the average value of a user-added exponentially decaying particle property.

## 3 OceanTracker structure

At a high level particle tracking code, takes the Eulerian water velocity field from a hydrodynamic model, interpolates these velocities to provide Lagrangian velocities at particle locations, and then numerically integrates these to predict particle trajectories. Beyond this, there are multiple other processes and computations that must be done at each time step. For example, the physical processes of dispersion, resuspension and tidal stranding, along with multiple bookkeeping processes. OceanTracker decomposes these processes into a series of components that fulfil specific roles. These components are executed in sequence as part of the *computational pipeline* outlined in Fig. 3 (see Sec. 3).

At a high level, Fig. 2 illustrates the data flow in OceanTracker from hydrodynamic model files to outputs, via its two main data structures 'fields' and 'particle properties' (see Sec. 3.2). Fields store data from the hydrodynamic model, such as water velocity, salinity, wind stress, as well as derived fields calculated from other fields, such as friction velocity. Particle-proprieties hold data for each particle, which could include its current location, status or a value interpolated from a field. These data structures enable access to and operations on their data. At a higher level these data structures are collectively "managed" as outlined in Sec. 3.3.

### 3.1 Computational pipeline

The high-level flow of data and computations are implemented by the computational pipeline. This system is constructed from components assigned to specific *roles* within the pipeline which implement required tasks. From a user's perspective, the adaptability of OceanTracker comes from the ability to add components and their settings within each role to create the Computational pipeline specific to their needs. The main time stepping loop proceeds in sequence through each role, executing the computation of components within each role. These components are constructed as Python classes, which are dynamically added to the computational pipeline during setup. The computational pipeline proceeds sequentially by simply calling the "update" method of each component within a role. Some roles, such as dispersion and re-suspension, allow only one class to be added. Others allow multiple classes to be added to that role, which are then looped over, updating all before progressing to the next role in the computational pipeline. For example, multiple trajectory modifiers which can combine to give the required particle behaviour, such as initially floating then later settling on the bottom.

#### 3.1.1 Building a computational pipeline.

The computational pipeline can be fully assembled using parameters from a text file or a Python dictionary, eliminating the need to code to run OceanTracker, e.g. Fig. 1b), c). However, coders may find it easier to create complex simulations using a 'helper' wrapper for OceanTracker. This allows coders to build their parameter dictionary using keyword arguments, by using two provided methods "settings" and "add class", see Fig. 1a). These helper methods build a Python parameter dictionary which adheres to the same structure as the JSON text file format shown in Fig. 1c). Whether built in code or from a text file this parameter dictionary is passed to OceanTracker to execute.

There are top level user configurable settings, such as time step, output folders etc, and within each role each component can have its own configuration settings. The configuration for each selected component typically includes the name of the Python class that the user is choosing to add to a role.

Most component settings have default values defined within the Python class, while a few must be specified by the user. Settings provided by the user are automatically checked for type and value range appropriateness.

#### 3.1.2 Computational steps.

Time stepping within the Computational pipeline is broken into a series of roles, each containing one or more components which implement that role, see Fig. 3. "Core" roles, such as resuspension or tidal stranding, only have one component to implement that role and have a default component if none is specified by the user. Others may have multiple components, each performing a different version of that role. For example, the particle properties role, may contain a user added a component which both calculates the distance travelled by each particle and another which determines which of a set of polygons each particle is currently inside.

The updating of each component is automated within the time stepping of the computational pipeline, with updates grouped by role, see Fig. 3. The order in which the roles are updated reflects their temporal dependence on the data from other roles.

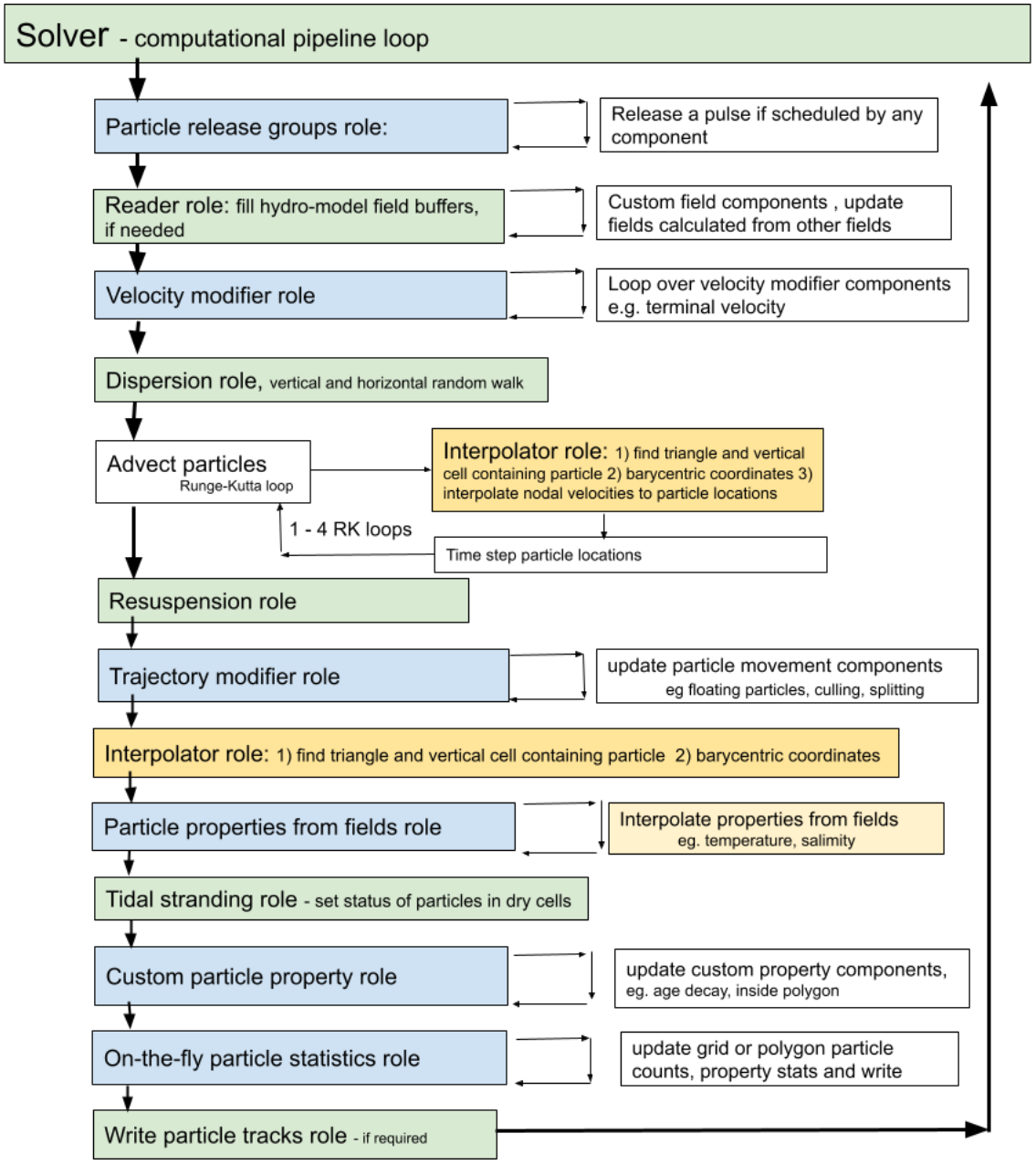



**Figure 3.** Flowchart illustration how components are updating ordered within the roles of the computational pipeline as part of the time stepping of the Solver role to advect particles. These operation roles are outlined in Sec. 3.2 and are implemented by components built as Python classes. Green are "core roles" which only containing one component, blue roles may contain one or more components which are looped through. For large runs, the most computational expensive steps are 1.) finding the cell containing each particle and 2.) evaluating the field interpolation. These steps are coloured yellow.

a) python

```python
from oceantracker.main import OceanTracker
# make instance of oceantracker
ot = OceanTracker()

# add  settings
ot.settings(output_file_base='minimal_example',
            root_output_dir='output',
            time_step= 120.)
# reader for hindcast files, format is auto detected
ot.add_class('reader',
             input_dir= '..\\demos\\demo_hindcast',
             file_mask=  'demoHindcastSchism*.nc')
# add  (x,y,z) locations where particles are released
# note: can add multiple release groups
ot.add_class('release_groups', name ='my_release_points',
             points= [[1595000., 5482600.,-1.],
                      [1599000., 5486200.,-2.]],
             release_interval= 3600, pulse_size= 10)
# start computation
ot.run()

```

b) yaml

```yaml
output_file_base: minimal_example
root_output_dir: output
time_step: 120.0
reader:
  input_dir: "..\\demos\\demo_hindcast"
  file_mask: "demoHindcastSchism*.nc"
release_groups:
  my_release_point:
  points: [[1595000,5482600],
           [1599000,5486200]]
  release_interval: 3600
  pulse_size: 10
```

c) json

```json
{
  "output_file_base": "minimal_example",
  "root_output_dir": "output",
  "time_step": 120.0,
  "reader": {
    "input_dir": "..\\demos\\demo_hindcast"
    ,
    "file_mask": "demoHindcastSchism*.nc"
    },
  "release_groups": {
    "my_release_point": {
      "points": [[1595000,5482600],
                 [1599000,5486200]],
      "release_interval": 3600,
      "pulse_size": 10}
  }
}
```

**Figure 4.** Minimal example of building a computational pipeline by a) Coding, using the 'helper' wrapper to build a Python parameter dictionary, or as user supplied parameters within a text file following the b) YAML or c) JSON standard.

For example, custom particle properties may be calculated from field particle properties and are therefore updated after the interpolated field properties. The solver class implements the time stepping by managing the classes within the computational pipeline and the associated bookkeeping functions. By default, fourth order RK time integration is used, while first and second order RK are also available.

The first step involves looping over the release groups and releasing a single pulse for any scheduled release at the current time step and then find each newly released particle's current horizontal and vertical cell. Next, the solver checks if the reader field time buffers contain the required time steps: if not, the reader fills the buffers and any custom fields are calculated from the newly read time steps. In addition to the water velocity from the hydrodynamic model, the user may add additional particle velocities as "velocity modifiers", such as a fall velocity for denser than water particles. Next, random walk dispersion is added as an equivalent velocity, see Sec. 2.2. Particles are then advected by RK integration based on the velocity due to both the water velocity and any velocity modifiers. At each sub-step, their current horizontal and vertical cells and Barycentric coordinates are updated, so that each particle's velocity can be interpolated to their locations.

This is followed by, applying re-suspension and any trajectory modifiers, which add any additional movements to the particles or their status, e.g. settling in a polygon or culling. To calculate the properties of the moved particles, their current horizontal and vertical cells and Barycentric coordinates are updated again. Then, all field-derived particle proprieties are looped over and updated by interpolation; the status of each particle is changed if it is in a dry cell. The subsequent steps involve updating any custom particle properties, calculating any particle statistics that have been added to the computational pipeline, and then writing out time series of particle trajectories and particle properties if requested

### 3.1.3 Mechanisms enabling computational pipeline adaptability

The approaches that enable computational pipeline adaptability within OceanTracker are:

**Dynamic importing:** For all roles the Python classes that implement a specific component within a role are dynamically imported at run time. This enables users to flexibly build a computational pipeline. To do this, a user names the class using a "class name" setting of the component they wish to add to a role, see Sec. 3.1.1. The class name is a string which mimics standard Python class referencing used to import packages within a module. Core roles have default class names, and all in-built OceanTracker classes can be imported using a shortened version, the name of the Python class. Users can also use the class name setting to import their own versions of Python classes from their working directory to add to the computational pipeline at run time. This enables them to alter the way core components function, such as the solver or dispersion, or add additional on-the-fly statistics or novel particle properties.

**Inheritance:** New variants of a component are easily created by inheriting the base class for its role, or one of its children, and overwriting some of the methods to alter its computation. Commonly, this would involve overwriting the update method to meet specific needs. Children of a class inherit their parent's configuration settings and can redefine, remove or add new settings. For example, the polygon particle release class inherits most of its operations and settings from its parent point release.

**Internal naming:** This allows coders to refer to a component's class instances data and methods with a given name, without knowing where the instance reference is located within the code. To ease accessing reader fields from within the code, essential

fields used standardized names, such as "water velocity" or "water depth". These names are mapped to variables within the hydrodynamic model files by the reader, for vector fields this may require mapping to more than one file variable to an internal name, see Sec. 3.4. Both the reader fields and any custom fields have particle properties of the same name automatically created and interpolated at each time step, which a coder can access by name. Any optional components can also be named by the user, to allow easy referencing with their code.

## 3.2 Data structures computational pipeline

OceanTracker's two main data structures are fields and particle properties, see Fig. 2. This section outlines these data roles, while Sec. 3.3 describes their management.

### 3.2.1 Field role

The spatial fields stored within the hydrodynamic model's files are the foundation of offline particle tracking. These are stored and accessed using the "field" data structure, see Fig. 2. The water velocity field is a crucial spatial field for particle tracking, but there may be many other relevant fields, such as water depth, tide or wind-stress. OceanTracker automatically detects whether fields are 2D or 3D, time-dependent or independent or scalar or vector and manages they appropriately. There are also grid variables associated with the fields, including nodal locations, triangulation and cell adjacency.

Fields are read from files as detailed in Sec. 3.4. Additionally, custom fields can also be integrated into the computational pipeline. These fields are derived on the fly by calculation from existing fields. For example, a friction velocity field can be computed from the 3D velocity field near the sea-bed and used to determine whether a particle can be re-suspended by the flow. Custom fields are calculated using their update method, which is used to automatically executed after the primary fields have been read from the hydrodynamic model files.

### 3.2.2 Particle property role

'Particle properties' store the values for each particle and enable high level operations on these values as shown in Fig. 2b. These properties have different types, depending on how they are updated each time step and may be scalars or vectors.

**Field particle properties** store field values at each particle location, such as water velocity. Field particle properties. They are updated by interpolating the field data structure with the same internal name.

**Custom particle properties** store values calculated from other particle properties. For example, the "inside-polygons" class uses the location particle property to determine which user given polygon contains each particle.

**Core particle properties** are not updated using their class update method, but are managed by the main code. Examples include particle location and bookkeeping particle properties, such as particleID and release groupID numbers.

Some examples of currently available custom particle properties are:

**Age decay** models an exponentially decaying particle load, such as bacteria, based on the core "age" particle property

**Inside polygon** records which of a given set of polygons, a particle is currently inside. This is used calculate polygon connectivity statistics, or to allow larvae to settle when over a reef.

**Total water depth** represents the sum of tidal elevation and water depth. This property is useful for particles whose behaviour differs in different water depths, such as larvae that only settle in shallow water, even if a cell is not completely dry .

### 3.3 Manager roles in the computational pipeline

Instances of field and particle properties store, update, and manage access to individual fields or proprieties. Higher level operations on all the individual instances are orchestrated by "managers" which automate key processes, see Fig. 2.

**Fields group manager role** This orchestrates the setup, reading, updating and interpolation of fields, along with setting up the required grid variables, such as nodal locations, triangulation and the adjacency matrix. It also manages the process of finding each particle's current horizontal and vertical cell and updates the status of dry cells. By default, the fields group manager automatically adds a particle property with the same internal name as the field to the computational pipeline, to be interpolated from that field at each time step.

**Particle group manager role** This orchestrates the release of particles and the updating of all three types of particle properties. It also manages the dynamic memory buffers which hold the individual particle property values, expanding them as needed when particle numbers grow and culling computationally dead particles that are no longer of interest. Additionally, if required, this manager handles the writing of time series of particle trajectories and properties.

### 3.4 Reader role

The primary function of the reader to convert hydrodynamic model file variables into standardised internal formats. These variables may be split between different files and vector components may be stored as different variables. The reader builds a catalogue of all file variables and which files contain them. It then maps the file variables to standard internal variable names. Field variables are categorised as time varying, vector or 3D. For vector variables, e.g. water velocity, several file variable names can be mapped to a single internal vector variable, allowing vector fields to be treated as a single variable within computations.

To ensure files for time varying variables are read in the correct order, files are sorted into time order based on their time variable. Thus, is not reliant on a file naming conventions to determine file order. Each variable has its own list of files, which enables the reader to seamlessly accommodate hydrodynamic models where variables are split between files, which is the case for e.g. SCHISM version 5 output files and GLORYS output files, which are used in the NEMO modelling framework.

The reader loads fields into memory buffers as they are needed. For time-dependent variables it reads multiple time steps into buffers, if the time steps required by the RK computation are not already in the loaded. By default, the buffer maintains 24 hydrodynamic model time steps in memory.

If needed, the reader converts the non-nodal values to values at the nodes of the triangles through interpolation. Readers and interpolators based on a hydrodynamic model's native grid, that do not need to do this conversion, could be developed in the future. To facilitate automation, the reader stores all fields in 4D arrays with dimensions (corresponding to time, node, z-depth and vector components).

Currently SCHISM, FVCOM, DEFLT3D-FM, NEMO/GLORYS and ROMS hydrodynamic model formats are supported (Zhang et al., 2016; Lai et al., 2010; Deltares, 2014; Moore et al., 2011). For the unstructured SCHISM and DEFLT3D-FM grids, which can have a mixture of triangular and quad cells, any quad cells are divided into triangles.

#### 3.4.1 Interpolator role

The interpolator serves as the link between the hydrodynamic model's fields held by the reader and the corresponding particle properties. After determining each particle's current triangle, horizontal and vertical cell, the interpolator converts field data values to values at each particle's location, which are then stored as particle properties. In the horizontal, OceanTracker currently uses linear interpolation in unstructured triangular grids from nodal values, utilizing a particles' Barycentric coordinates within their current triangle. Linear interpolation is applied within vertical layers and between time steps, except for the water velocity within the seabed layer. Here, vertical interpolation is based on a logarithmic layer, ensuring that particles near the seabed experience more realistic horizontal velocities, which is crucial for newly re-suspended particles.

The interpolator supports linear interpolation with three vertical grids, starting with Sigma grid (ROMS) and fixed z levels (Deft-3D FM, NEMO/GLORYS), which apply the same vertical grid at all locations. It also supports grids with spatially varying layer thicknesses, e.g. SCHISM and FVCOM. This includes SCHISM's LSC vertical grid, where the number of vertical layers varies spatially.

### 3.5 Particle release groups role

A "particle release group" introduces new particles into the computational pipeline. Each release group generates new particles at specified locations, which are released at designated times, in specified pulses sizes. Multiple release groups can be added, each with its specific locations and release schedule. The current release types include:

**Point release** spawns particle from a set of specified locations and depths. A optional radius setting allows particle releases randomly within a circular area around each point.

**Polygon release:** Particles are spawned at random locations within a user-defined given 2D polygon.

**Grid release:** spawns particles from points of a regular grid.

Particles will not be released in any locations outside the domain, see Fig. 1a). Also, by default, particles are not released within cells that are currently dry due to the tide. For all types it is possible to restrict releases to be randomly distributed within a given vertical layer, or to locations with water depth in a given range, e.g. for seaweed propagules whose parents only live in the shallow areas within a release polygon.

### 3.6 Velocity modifiers role

Additional bio-physical processes can add to the water velocity experienced by each particle. These are incorporated into the computational pipeline as "velocity modifiers", where the effects of each are added to the water velocity for use in the time integration (Fig. 3). An example of an in-built modifier is:

**Terminal velocity:** The modifier adds the terminal sinking or buoyant velocity to the ambient water velocity, either as a uniform value or a particle specific value drawn from a normal distribution.

### 3.7 Trajectory modifiers role

"Trajectory modifiers" are bio-physical processes that alter the movement of particles at each time step or their status. Examples of in-built modifiers include:

**Settlement:** Allows larvae to settle on reefs defined by polygons. The trajectory is modified by changing its status to “stationary”.

**Floating:** Sets each particle’s vertical position to that of the free-surface height at its current location.

**Culling:** At each time step, this component sets the status of a random fraction of particles for a given status (e.g. on the bottom) to be dead, allowing them to be removed from subsequent computations.

**Splitting:** This splits particles in two to simulate reproduction, at a set rate or probability. This can rapidly generate very large numbers of particles which need to be contained by a culling mechanism (Steidle and Vennell, 2023)

### 3.8 On-the-fly particle statistics roles

Scaling up particle numbers to millions can create large volumes of particle track data. The on-the-fly particle counting statistics approach produces a data output volume independent of the number of particles released. Currently, there are four main types of spatial particle statistics:

**Gridded:** Used to produce heat maps. These count particles inside cells of a regular grid at a user-specified time interval.

**Polygon:** Calculates the physical connectivity matrix between each release group and areas bounded by given polygons.

Both types record particle counts from each release group separately and have two variants.

**Time series:** Counts particles at specified time intervals, providing time series of heats-maps or connectivities.

**Age bins series:** Counts particles within each spatial bin into age bins, to produce age-based heat maps or connectivities. This has applications in tracking the age distribution of particles in specific areas.

It is also possible to limit which particles are counted, for example, only counting particles in a given vertical "z" range or only those lying on the bottom. Users can add multiple on-the-fly statistics components, all calculated from the same particles during the computational run, such as adding a particle statistic counting particles in different depth ranges. In addition to particle statistics, average values of particle properties within the spatial counting bins can also be calculated on-the-fly, such as water temperature or distance travelled.

An additional in-built statistic is **Residence time:**, which calculates time series of the average time that particles released within a polygon reside within that polygon (Lucas and Deleersnijder, 2020).

### 3.9 Integrated models

Many use cases require users to combine multiple roles to create higher level functionality. OceanTracker supports this aggregation of roles into a single component for reuse. These integrated models only require the parameters essential for executing their higher level function; the model manages the intricacies of assigning classes to appropriate roles to complete the overall function. Currently, there is one integrated model:

**On-the-fly Lagrangian Coherent Structures:** These structures identify regions of convergence or divergence within a fluid flow over time. OceanTracker calculates time series of Finite-Time Lyapunov Exponents (FTLE) (Haller, 2015; Harrison and Glatzmaier, 2012), which can be used to derive characteristics of Lagrangian Coherent Structures. The FTLE calculation uses the largest Eigenvalue of the strain tensor after specified lag times. This process involves releasing particles on a regular grid and calculating the distances between adjacent released particles. The user only needs to designate one or more grid locations and the required time lags. The integrated model sets up new regular grid releases at regular time intervals and calculates the FTLE on-the-fly for each grid and lag, eliminating the need to record and post process large volumes of particle trajectories.

## 4 Computational speed

The primary features contributing to computational speed of OceanTracker are:

**Finding cell:** In unstructured grids, significant computational time is spent determining the horizontal and vertical cells containing a particle. OceanTracker uses the particle history to improve the speed of its cell search. Short triangle and vertical walk algorithms improved the search speed by an order of magnitude, as outlined in (Vennell et al., 2021).

**Calculate once, use many:** To avoid repetition in performing key computational tasks, a particle's current triangle, barycentric coordinates, vertical cell and fraction of the vertical cell are recorded at each time step. These values then used repeatedly to interpolate multiple fields to the particle's location. Adopting this, 'calculate once, use many times' methodology significantly improves the efficiency of interpolations (Vennell et al., 2021).

**Dynamic Particle Buffer:** Particle proprieties are stored in memory buffers, which expanded as needed to accommodate newly released particles. System performance and memory utilisation can be optimised by periodically culling dead particles. For instance, setting a maximum particle age for a release group, beyond which they are no longer relevant, interest, will remove theses older particles from computations. When more than 20% are dead, particle memory buffers are compacted by removing dead particles.

**Uniform sigma-grid:** For 3D SCHSIM and FVCOM, models the search for the vertical cell is the most time-consuming step as their fractional layer thicknesses vary spatially. Thus, the vertical search for each particle's cell is done within different layer thicknesses. Optionally for these models, the vertical cell search can be made 5 times faster by vertically interpolating to spatially uniform sigma-layer fractional thicknesses. With uniform fractional thicknesses, finding the vertical cell is significantly quicker using rounding within a pre-calculated layer map, followed by a single correction step. For large numbers of particles, the time spent re-interpolating to this near-native vertical grid when reading the hydrodynamic model's files, is small

compared to the time saved by the faster vertical cell search. ROMS uses uniform S-grids, thus can directly can exploit the faster approach to vertical cell search at no additional effort.

**Numba:** Particle tracking requires complex operations with nested loops making per-particle decisions. These would be computationally slow in Phyton. For example, the triangle walk to find each particle's horizontal and vertical cell requires calculating its barycentric coordinates using multiple nested loops, while making particle by particle decisions, such as whether a particle is within the bottom layer that requires special treatment. To make complex looping and decisions 100s of times faster OceanTracker uses the Python extension Numba (Lam et al., 2015). Numba understands a large subset of Python and NumPy code, only requiring a decorator to speed critical code. Numba can outperform NumPy by eliminating the need to create temporary array memory for intermediate results. Thus, Numba's computational speed is similar to those of C or Cython. Numba complies functions when first called and the complied code is reused on subsequent calls. A disadvantage of using Numba is that compilation of the many Numba functions adds 20-30 sec. to OceanTracker's start-up processes. Optional caching of the complied Numba code to disk between runs minimises this delay.

**Parallelization:** Optionally OceanTracker can employ an embarrassingly-parallel approach to execute cases simultaneously, where cases run independently of each other as described in (Vennell et al., 2021). This is achieved by providing shared parameters that apply to all cases, along with a list of parameters specific to each case. For instance, while all cases share the same on-the-fly-statistics, each parallel case might release particles at different locations.

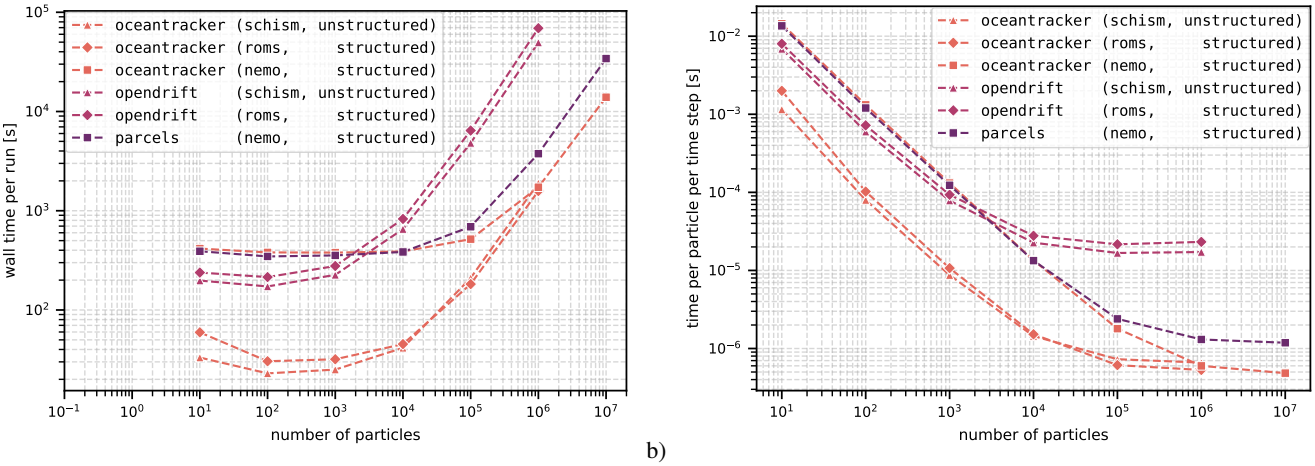
### 4.1 Speed comparisons

The following section compares the computational performance of OceanTracker with its closest alternative, OpenDrift (Dagestad et al., 2018). A similar comparison has been reported in Vennell et al. (2021). Since that publication the code base has undergone a significant overhaul. Previously relying on NumPy and SciPy for critical computational steps, it now uses Numba. This transition has facilitated the implementation of far more particle-specific decisions processes that enhances the realism of their movement, as outlined in Sec. 2.2.

The performance comparisons uses tree 3D hydro-dynamic models. The first is a high resolution unstructured mesh estuarine model described in Steidle and Vennell (2023) and built using SCHISM (Zhang et al., 2016). This model features 32,000 horizontal nodes and employs terrain-following coordinates for the vertical grid, with up to 20 levels. Its spatial resolution varies from 5m and 1400m. The second model is a regular grid ROMS model presented in López et al. (2020), consisting of about 250,000 nodes and 40 z-grid type vertical levels with a uniform horizontal resolution of 7 km. The third model is large NEMO model, which uses GLORYS as their hydrodynamics component, of the baltic sea, based on (Kärnä et al., 2021), containing about 600,000 horizontal nodes and 56 z*-grid type vertical levels.

All models have a temporal resolution of 1 h. By default Oceantracker and OpenDrift are compared using a fourth order Runge-Kutta advection and a dispersion step while the comparison to Parcels using the NEMO data set are performed using advection only, due to a lack of a native 3D dispersion method in Parcels.

The computational experiments were performed on the desktop computer I of table Table 1, which is equipped with an Intel(R) Core(TM) i5-10500 CPU @ 3.10GHz and 16 GB RAM. The computations covered 10 model days using 5 minute




a) b)

**Figure 5.** Comparison of the computational speed of OceanTracker, OpenDrift for structured (ROMS) and unstructured (SCHISM) grids, and Parcels for structured (NEMO/GLORYS) grids. a) Compares the total run time measured as wall time. b) shows the normalized computational time time per particle per RK4 time step.

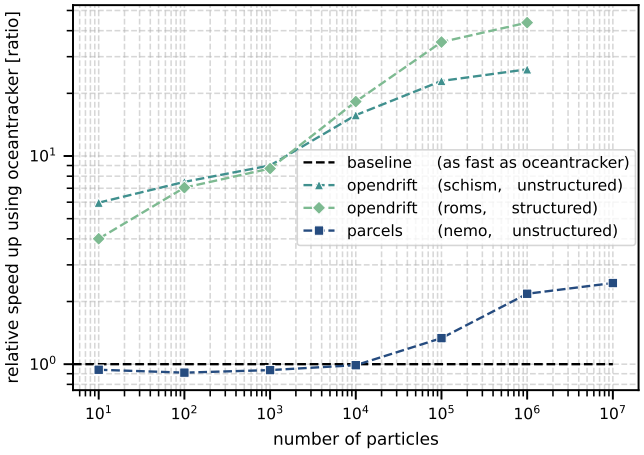



**Figure 6.** Comparison of the relative speed up from OceanTracker compared to OpenDrift and Parcels for the different data sets and particle sizes. The black baseline represents performance equal to OceanTracker where ratio equals 1

time steps, resulting in a total of 2880 time steps. Particles were released at 30 locations, with total particle numbers varying from 1000 to one million particles per model run. All computations were done on a single core. The source code that has been used to perform this speed tests is publicly available (see section Code Availability).

Figure 5a) displays the total run time across OceanTracker and OpenDrift on both structured and unstructured grids and Parcels for structured grids. Figure 5b) illustrates the scaling of both models in terms of time per particle per RK4 time step. Which indicates that OceanTracker can process nearly a million particles per second on a single desktop core.

For the SCHISM and ROMS data set, model setup times are the main contributor to OceanTracker's run time for particle counts up to 10000 particles. For these small numbers, OpenDrift's minimum run time was approximately 2 minutes, while OceanTracker's completed these runs in 30 seconds. For particle counts exceeding 10,000 setup times become negligible for both models. In 1 million particle simulations OceanTracker is up to 35 times faster than OpenDrift as shown in figure 6, resulting in total run times of 15 hours for OpenDrift and half an hour for Oceantracker.

OceanTracker treats structured grids as unstructured grids by triangulating them, whereas OpenDrift uses a native reader for the structured ROMS grids. Surprisingly, the native ROMs reader of OpenDrift does significantly enhance its performance with unstructured grids. Also, OceanTracker does not experience a significant speed penalty for treating structured grids as unstructured.

For the NEMO/GLORYS case, which uses a large data set with over 3 million spatial nodes, model setup times and reading the data remains the dominant cost for cases with particle counts of below 100,000. For the larger particle counts over 1,000,000 ocean tracker performs approximately twice as fast as Parcels, making it the fastest general purpose particle tracker for both structured and unstructured grids to our knowledge.

### 4.2 Multi-processing scaling.

Fig. 7 shows that for a small grid, speed scales almost linearly with the number of processors, with 25 processors yielding nearly 25 times the speed. For large hydrodynamic model output, the time required to access field data from disk and main memory results in sub-linear scaling, as illustrated in Figure 7b. This data access bottleneck, suggested that restructuring the code to allow processors to share hydrodynamic model data or how it ordered in memory (Kehl et al., 2023) could improve how speed scales with the number of processors.

## 5 Discussion

Vennell et al. (2021) found OceanTracker to be significantly faster than OpenDrift for unstructured grids. Fig. 5 demonstrated there is a similar speed advantage for OceanTracker over OpenDrift on structured grids. This is surprising, as typically cell finding in structured grids is much faster, as it can be done by simple rounding of coordinates. This suggests that the speed difference is not mostly due to differences in their cell finding algorithm, but to some other aspects of their approaches.

For unstructured grids, the original OceanTracker was over two orders of magnitude faster than OpenDrift (Vennell et al., 2021). The latest version of OceanTracker is an order of slower than its predecessor. However, the latest version has much improved physics Sec. 2.2. This enhancement has required in more costly computations of particle by particle decisions regarding their movement. These decisions result in slower branching code, but yield more realistic physics.

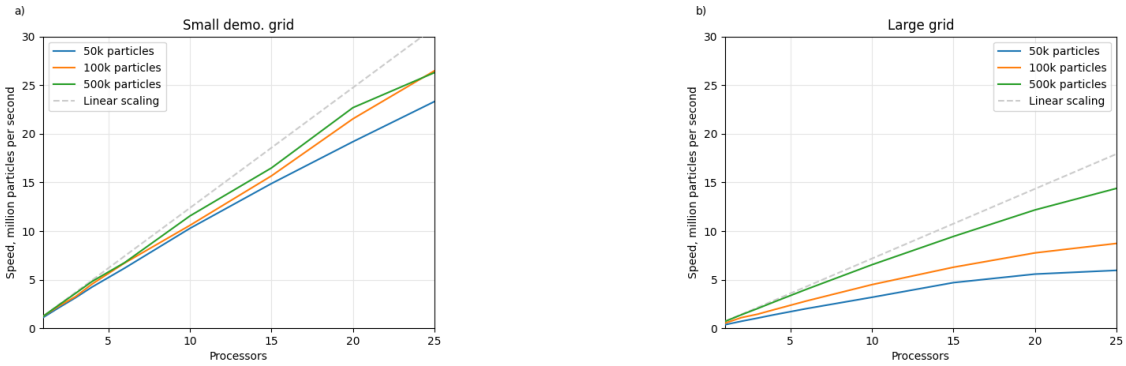



**Figure 7.** Scaling of computation speed of cases run in parallel mode. Speed is the total number of particles across all processors simulated per second of total run time. Colors show results for 50,000 to 500,000 particles released in single pulse on each processor. As reference, dashed line shows linear scaling of a single 500k pulse. a) Small demo grid, 12 nodes. b) Large grid Cook Strait NZ, 180k nodes (Vennell et al., 2021)

OceanTracker's implementation is a compromise between speed and adaptability, which imposes limitations. One is illustrated in Fig. 3, where core particle properties, such as a water velocity, location, current horizontal and vertical cell are updated at every RK sub-step. However, velocity and trajectory modifiers are updated only once per full RK step. This approach assumes that modifiers vary slowly enough in space and time, that they can be treated as constant within the full RK time step. This assumption limits the acceptable time step size, requiring users to choose a small enough computational time step that these modifiers can be treated as constant.

A recommended accuracy test for particle trackers is a circular flow of known period (Van Sebille et al., 2018). A 2D synthetic eddy test was performed, with a 1 $ms^{-1}$ peak flow at a 10km radius and 12 hour period. For 15 minute RK4 time steps the deviation of particles released 10km from the center was less than 0.3m from their initial radius after 10 days.

## 6 Summary

OceanTracker provides a comprehensive ocean particle tracking framework compatible with both structured and unstructured grids. Its speed allows users to scale to larger numbers of particles on modest computer hardware within acceptable run times. This capability facilitates enhanced particle statistics and broader exploration of variations in particle behaviours. Integrating the calculation of particle statistics directly within computational runs significantly reduces the time required to derive needed statistics. In addition, on-the-fly-statistics produce more manageable data volumes, as their size does not depend on the number of particles released, Sec. 3.8. The ability to add multiple release groups and statistics also reduces user efforts, by enabling multiple outcomes within the same computational run. Adaptability in building a Computational pipeline is enabled by a modular approach to roles within the computational pipeline using the techniques outlined in Sec. 3.1.3.

Future improvements to enhance OceanTracker's speed might include greater use of "Single Instruction Multiple Data instructions" on conventional CPUs (SMID). Additional optimisation should be possible by adapting expensive computational kernels to take advantage of GPUs. Table 1 indicates around 20% of run time is spent in reading the hydrodynamic model's files. An asynchronous reader sharing it memory with parallel particle computational processes could minimise this impediment. Reading costs could also be reduced by chunking or restructuring the data in memory (Kehl et al., 2023).

*Code availability.* OceanTrackers source code is available at https://github.com/.oceantracker/oceantracker/, Demonstrations and user guide at https://oceantracker.github.io/oceantracker/. The code is released under the MIT license. The code to perform the speed tests and their output are available at https://doi.org/10.25592/uhhfdm.14172

*Author contributions.* Vennell and Steidle are core code developers and primarily responsible for writing this paper. Smeaton, Chaput and Knight contributed to development of specific components of the code, extensive code testing and the structure of the paper.

*Competing interests.* The contact author has declared that neither of the authors has any competing interests.

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## Appendix A: Code for Fig. 1

```
# code to run particle tracking for Fig 1

from oceantracker.main import OceanTracker # load
ot= OceanTracker() # create an instance to build parameter dictionary= ot.params

# add settings
ot.settings(output_file_base='OTpaper_exmaple_A',  root_output_dir='output', time_step= 600.)

 # add reader to acces the hyrdo-model
ot.add_class('reader',  input_dir=r'oceantracker\demos\demo_hindcast',
                  file_mask=  'demoHindcastSchism*.nc')  # file mask to search for
# add a point release
```

```
ot.add_class('release_groups',name = 'my_point_release', class_name='PointRelease',
        points= [[1595000, 5482600, -2], [1594000, 5484200, -2]], # (x,y,z) of release points
        release_interval= 600, pulse_size= 5000)
# add polygon release at random depths between two z values
ot.add_class('release_groups',  name = 'my_polygon_release',  class_name='PolygonRelease',
        points=[[1597682., 5486972], [1598604, 5487275], [1598886, 5486464],
                [1597917., 5484000], [1597300, 5484000], [1597682, 5486972]],
        release_interval= 600,  pulse_size= 50, z_min= -2., z_max = 0.5)
# add grid releasing at random depths between two z values
ot.add_class('release_groups',  name = 'my_grid_release', class_name='GridRelease',
        grid_center=[1592000, 5489200], grid_span=[500, 1000], grid_size=[3, 4],
        release_interval= 1800,  pulse_size= 2, z_min= -2, z_max = -0.5)
# add a decaying particle property,# with exponential decay based on age
ot.add_class('particle_properties', name ='a_pollutant', class_name='AgeDecay',
            initial_value= 1000, decay_time_scale = 7200.) # exponential decay time scale 2hours
# add a gridded particle statistic to use as heat map
ot.add_class('particle_statistics', name = 'my_heatmap', class_name= 'GriddedStats2D_timeBased',
        grid_size=[120, 121],  release_group_centered_grids = True, update_interval = 600,
        particle_property_list = ['a_pollutant'],  status_min ='moving', z_min =-10.)
ot.add_class('resuspension', critical_friction_velocity=0.01) #set value for particle resupension

# run OT and return file name useful in plotting
case_info_file= ot.run()
```

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