Deliverable 4.4.1, 4.4.2, and 4.4.3

# WP4

# Forecast numerical modeling for coastal extreme weather and flooding risk management

## Activity 4.4

## Set up of high resolution coastal dispersion model close to river outlet

## D4.4.3 Manual of the developed FLOWAdria Software

# PROJECT AND ACTIVITY DETAILS

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## 0. Introduction

Numerical simulations of hydrodynamical flows and fluid particle trajectories are based on the implementation of a modelling device which must be adapted to the specific case study. The dispersion of passive tracers in the marine waters, depending on the aspect ratio, can be classified in two major categories:

A) large-scale, quasi-2D dispersion in open sea without obstacles;

B) small-scale, 3D dispersion in coastal areas, e.g. around a river outlet, where natural and/or artificial obstacles may be present.

We will define "FlowADRIA" as the main modelling device having two independent operating modes: OpenSea (mode "A") and CoastalFlow (mode "B").

The modelling strategy for the two operating modes is different. Large-scale 2D transport and diffusion of passive particles at the sea surface across the whole Adriatic basin has two major contributions:

1- a time-evolving velocity field, defined on a spatial grid, typically 1-10 km and one-day resolution, which is mainly responsible of the advection of a tracer concentration, i.e. the evolution of the mean position (order-1 moment);
2- a sub-grid additional model which takes into account the missing velocity components, smoothed out by the finite resolution cut-off, which is responsible of the relative dispersion between particles (order-2 moment).

Notice the role of Point-2 is to restore the right dispersion rates at small and mesoscale, otherwise underestimated by the large-scale advecting model. To accomplish this task, the sub-grid additional model must be suitably calibrated on observational real drifter data.

Point-1, on the other hand, regards the description of surface ocean dynamics at basin scale (500-1000 km for the Adriatic Sea). Marine current data can be retrieved from established Ocean product providers and may come either from general circulation model outputs or from satellite remote sensing techniques. In this case, the computation of the trajectories is "off-line" with respect to the velocity field, i.e. firstly, all the necessary Eulerian data are stored and, secondly, the Lagrangian data are simulated.

Small-scale, 3D transport and diffusion simulations must be implemented simultaneously with the flow computation which depends on the considered case study, i.e. the computation of fluid particle trajectories is "on-line" with respect to the flow. The 3D operating mode allows to simulate hydrodynamical systems at very high resolution so it is no longer necessary to consider an additional sub-grid model since all significant contributions to the dynamics are supposed to be reproduced.

Furthermore, the 3D coastal flow model allows to simulate transport and dispersion of inertial tracers, e.g. sediments of various mass and size, which may be deposited on the seabed and change the geomorphology.

In the following sections the operating modes of the modelling device will be described in detail.

## 1. FlowADRIA OPEN SEA Mode

FlowADRIA Open Sea (hereafter OS) is the FlowADRIA's module that simulate the Lagrangian transport of passive tracers in open sea, entirely developed and mantained at ISMAR-Roma – GOS, formerly ISAC U.O.S. Lecce – GOS.

FlowADRIA OS is a parallel program, written in C/C++, developed to calculate Lagrangian transport of couples of passive tracers under the forcing of Eulerian ocean currents provided by several ocean models. It currently runs on 64/128 cores of a local high-performance computing system at ISAC U.O.S. Lecce.

Numerical simulations with FlowADRIA OS can be useful in a variety of use cases: transport of marine organisms, biological connectivity, pollutant discharge, oil spill, and search and rescue operations. Furthermore, simulation of particle's couples rather than single particles allows for simpler analysis of characteristics relative dispersion in ocean (Palatella et al. 2014; Lacorata et al. 2014; Maffucci et al. 2016; Torri et al. 2018; Lacorata et al. 2019).

Currently, depending on application framework, FlowADRIA OS can be forced by Eulerian ocean currents provided by a variety of ocean model, e.g. MFS (Mediterranean Forecasting System, all versions) for numerical experiments in Mediterranean Sea, Globcurrent (all versions) or GLORYS2V4 when trasport is considered in world's oceans. A '2D mode' for buoyant tracers is also available.

Depending on the applications, simulations can be done either forward in time or backward in time.

Numerical tracers can be released all together at the same time or continuously in time at fixed rate ('plume' release).

An important feature of FlowADRIA OS is the implementation of a Kinematic Lagrangian Model (KLM), a deterministic velocity field, analytically defined in terms of spatial derivatives of a given stream function, which gives rise to chaotic Lagrangian trajectories. KLM is a parameterization of the velocity field components poorly resolved by ocean models because of finite space and time resolution. Parameters needed for KLM tuning are generally calculated from the analysis of large buoy datasets (Palatella et al. 2014; Lacorata et al. 2014;).

Two external ASCII files are needed in order to run FlowADRIA OS, together with a list of forcing ocean current files:

- a ‘starting conditions’ file, where initial positions and starting times of particle’s couples are specified. If ‘plume’ release is selected starting times are ignored. Due to parallel design of the program, the number of simulated couples must be multiple of the used cluster’s cores.
- a ‘simulation parameters’ file, where parameters like internal timestep, time direction, release rate in ‘plume’ case, KLM parameters and so on.

### 1.1. FlowADRIA OS details

To simulate Lagrangian transport of passive tracers FlowADRIA OS requires a list of NetCDF files with Eulerian current fields covering the whole simulation length and a set of particle’s starting positions.

When a virtual particle is located at the point $\boldsymbol{X}(t) = \boldsymbol{x}$, its position at time $t + \Delta t$ is given by

$$\boldsymbol{X}(t + \Delta t) = \boldsymbol{X}(t) + \int_t^{t+\Delta t} \boldsymbol{v}(\boldsymbol{x}(\tau), \tau) d\tau$$

where $\boldsymbol{v}(\boldsymbol{x}(t)$ is the Eulerian current velocity in **x** at time t.

To estimate the particle displacement FlowADRIA OS uses a simple first-order Euler forward method, so the approximation $\boldsymbol{X}(t + \Delta t) = \boldsymbol{X}(t) + \boldsymbol{v}\big(\boldsymbol{x}(t)\big)\Delta t$ is used. To guarantee a good accuracy of calculated trajectories timestep $\Delta t$ must be small enough; usually, the internal timestep used by FlowADRIA OS for calculate tracers evolution is not greater than 120 seconds.

Since Eulerian current fields are provided by numerical model outputs, on a discrete grid (about 10 km order) and a discrete time interval (daily or weekly), the evaluation of $\boldsymbol{v}(\boldsymbol{x}(t))$ at each timestep is made interpolating the current fields in space and time.

FlowADRIA OS calculates at same time the evolution of couples of tracers and uses a kinematic Lagrangian model (KLM), a deterministic velocity field defined in terms of spatial derivatives of a stream function, to simulate mesoscale turbulent pair dispersion.

When motion is on surface only KLM is defined as a 2D multiscale lattice of horizontal convective cells (see Lacorata et al. 2014 for a detailed explanation and for parameters meaning):

$$U_{KLM}(x, y, t) = \sum_{n=1}^{N_m} A_n \sin[k_n x - k_n \varepsilon_n \, sin(\omega_n t)] \cos\,[k_n y - k_n \varepsilon_n \, sin(\omega_n t + \theta_n)]$$

$$V_{KLM}(x, y, t) = -\sum_{n=1}^{N_m} A_n \cos[k_n x - k_n \varepsilon_n \, sin(\omega_n t)] \sin\,[k_n y - k_n \varepsilon_n \, sin(\omega_n t + \theta_n)]$$

KLM parameters, internal timestep, snapshot printing timestep and other input needed by FlowADRIA OS are listed in the 'simulation parameters' file with the following structure:

```
TIMESTEP 60.
KINEMATIC_THRESHOLD3D 0.95
KINEMATIC_THRESHOLD 2D 0.95
ALIVE_THRESHOLD 0.8
SNAPSHOT 3600
IFILE_START 0
BUOYANT 1
PLUME 1
TIME_END_PLUME 5184000
BACKTRAJECTORY 0
FLAG3D 0
LSTART3D 20
LEND3D 500
FACT3D 1.414
Eps3D 1e-04
VERTICAL_DECAY -1000
FLAG2D 1
LSTART2D 20000
LEND2D 120000
FACT2D 1.414
ENSTROPHY 3.e-9
VDEP 0.00
ABSORPTIONTOP 0
ABSORPTIONBOTTOM 0
ABSORPTIONLATERAL 1
```

Start conditions of particles (e.g. positions and ages in days) are listed in an ASCII files. After the first row, where is stated the number of couples that have to be simulated, each column shows: longitude and latitude for first and second particle of the couple, starting age (in days) and starting time (in seconds).

If the particles are not buoyant, the file specifies starting depths also in further two colums.

When in 'simulation parameters' file "PLUME = 1" is set, the last column is ignored and the particles are released at fixed rate until time assigned at "TIME_END_PLUME" (in seconds) is reached.

```
25600
14.4229  42.5914  14.4329  42.5914  0  0
14.4775  42.5524  14.4875  42.5524  0  0
14.4334  42.6021  14.4434  42.6021  0  0
14.4095  42.5867  14.4195  42.5867  0  0
14.4328  42.6327  14.4428  42.6327  0  0
14.4745  42.586   14.4845  42.586  0  0
14.4657  42.6658  14.4757  42.6658  0  0
14.4116  42.618   14.4216  42.618  0  0
14.484  42.552   14.494  42.552  0  0
...
```

Program is written in C/C++ and parallel tasks are carried out using OpenMPI, an open source Message Passing Interface implementation.

The computational time required by a FlowADRIA OS simulation depends on many factors, such as the number of particles involved, the length of the simulation. For example, using an internal timestep of 120 seconds and a snapshot of 1 hour, a typical numerical simulation with FlowADRIA OS, with ~25000 particle's couple, using 64 CPU, requires about 4 hours to produce trajectories over one year.

Trajectories are locally saved in ASCII format files, one for each CPU involved in the parallel simulation, with eight or ten colums (in 2D and 3D mode respectively). The columns show: simulation absolute time (s), couple ID, first particle longitude (degrees in -180:180), first particle latitude (degrees in -90:90), first particle depth (only in 3D mode, in meters), second particle longitude, second particle latitude, second particle depth (only in 3D mode), couple's age (in days), couple's starting time (in seconds).

```
0          0    14.5431   42.5066          14.5427  42.5057          0      0
3600  0  14.5466   42.5032          14.5461  42.5024          0.0423611  0
7200  0  14.5501   42.4999          14.5495  42.4991          0.0840278  0
10800 0  14.5536   42.4967          14.5529  42.4959          0.125694   0
14400 0  14.557    42.4936          14.5562  42.4929          0.167361   0
14400 1  14.6991   42.5572          14.7001  42.5574          0.0173611  12960
18000 0  14.5604   42.4907          14.5596  42.4899          0.209028   0
18000 1  14.7066   42.5527          14.7076  42.5529          0.0590278  12960
21600 0  14.5638   42.4878          14.5629  42.4871          0.250694   0
21600 1  14.7141   42.5482          14.7151  42.5484          0.100694   12960
...
```

When a particle leaves the domain, delimited by the forcing Eulerian current fields, or reaches the coastline, it is removed from the pool and its last position is saved.

**Figure 1.1.** plot of a couple' trajectories starting near Pescara. Colorbar shows the age in days of the particles during their path.

Depending on the requested analysis, the trajectories produced by a numerical simulation can be processed offline in different ways, e.g. calculating presence probability in space and time or adding effects of temperature or nutrient to evaluate their likelihood (Maffucci et al. 2016).

## 2. FlowADRIA COASTAL Mode

For our simulations, we used open source code Delft3D (http://oss.deltares.nl/web/opendelft3d) , a modelling package which consists of several modules to compute amongst other the flow (FLOW), and the morphology (MOR, included in FLOW) in coastal waters. The FLOW module solves the depth-averaged or 3D shallow water equations on a rectilinear or curvilinear grid. The system of equations consists of the horizontal momentum equations, the continuity equation, the transport equation, and a turbulence closure model. The vertical momentum equation is reduced to the hydrostatic pressure relation as vertical accelerations are assumed to be small compared to gravitational acceleration and are not taken into account. Under the so-called "shallow water assumption" the vertical momentum equation reduces to the hydrostatic pressure equation. Under this assumption vertical accelerations due to buoyancy effects or sudden variations in the bottom topography are assumed negligible compared to gravitational acceleration and are not taken into account. The resulting expression is: $\partial P/\partial z = -\rho g h$. This makes the Delft3D-FLOW model suitable for modelling hydrodynamics in shallow seas, coastal areas, estuaries, lagoons, rivers, and lakes. It aims to model flow phenomena of which the horizontal length and time scales are significantly larger than the vertical scales. In order to solve the systems of equations, several boundary conditions are required: bed, free surface and lateral boundary conditions. Along closed boundaries the velocity component perpendicular to the closed boundary is set to zero (a free-slip condition). At open boundaries one of the following types of boundary conditions must be specified: water level, velocity (in the direction normal to the boundary), discharge, or linearised Riemann invariant (weakly reflective boundary condition, Verboom and Slob, 1984). For the transport boundary conditions we assume that the horizontal transport of dissolved substances is dominated by advection. This means that at an open inflow boundary a boundary condition is needed. Delft3D-FLOW is a numerical model based on finite differences. To discretise the 3D shallow water equations in space, the model area is covered by a rectangular, curvilinear, or spherical grid. It is assumed that the grid is orthogonal and well-structured. The variables are arranged in a pattern called the Arakawa C-grid (a staggered grid). In this arrangement the water level points (pressure points) are defined in the centre of a (continuity) cell; the velocity components are perpendicular to the grid cell faces where they are situated (see Fig. 2.1).

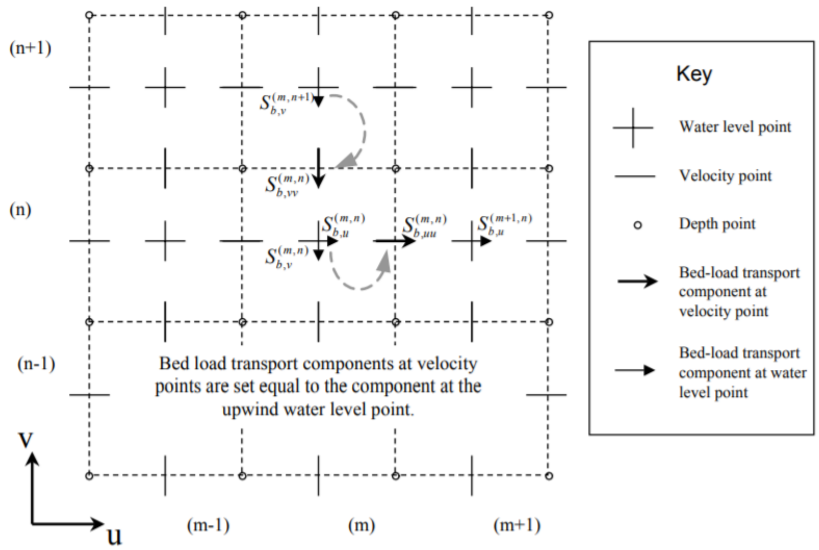


**Figure 2.1.** The Delft3D staggered grid showing the upwind method of setting bed-load sediment transport components at velocity points. Water-level points are located in the centre of the sediment control volumes.

In the online sediment version of Delft3D-FLOW, sediment is added to the list of constituents that can be computed by the transport solver. Up to five sediment fractions may be defined. Each fraction must be classified as “mud” or “sand” as different formulations are used for the bed-exchange and settling velocity of these different types of sediment. For sand sediment fractions the approach of van Rijn (1993) is applied. Also the magnitude of the bed-load transport on a horizontal bed is calculated using a formulation provided by van Rijn.

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