Numerical and Implementation Issues in Food Quality Modeling for Human Diseases Prevention

A. Galletti[1], R. Montella[1,2], L. Marcellino[1], A. Riccio[1], D. Di Luccio[1], A. Brizius[2] and I. Foster[2]
[1]*Department of Science and Technology, University of Naples "Parthenope", Centro Direzionale, Isola C4, 80143, Napoli, Italy*
[2]*Computation Institute, University of Chicago, 5735 South Ellis Avenue, 60637, Chicago, IL, U.S.A.*

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Abstract: Monitoring nearshore sea water pollution using connected smart devices could be nowadays impracticable due to the aggressive saline environment, the network availability and the maintain and calibration costs. Accurate forecast of marine pollution is most needed to evaluate the adverse effects on coastal inhabitants' health when fishes and mussels farming economically characterizes the local social background. In an operational context, numerical simulations are performed routinely on a dedicated computational infrastructure producing space and temporal high-resolution predictions of weather and marine conditions of the Bay of Naples. In this paper we present our results in developing a community open source Lagrangian pollutant transport and dispersion model, leveraging on hierarchical parallelism implying distributed memory, shared memory and GPGPUs. Some numerical details are also discussed. This system has been used to develop an alarm system to help local authorities in making decisions regarding the collection of mussels. The model setup and the simulation results will be improved using FairWind, an under development system dedicated to coastal marine crowdsourced data gathering and sharing, based on smart devices and Internet of Things afloat.

1 INTRODUCTION

Human health can be adversely affected by pollutants emission into sea water, specially from seafood contamination caused by inshore discharges or offshore spills in areas close to aquaculture farms.

Fish and mussel farms are critically sensitive to coastal water quality, and thus require continuous monitoring to enforce food security and quality and to prevent any possible disease affecting human health.

The potentially toxic substances emitted from point sources can, in more or less short time, reach the mussel farms and promote, in relation to the mussel-pollutant contact time, the bioaccumulation in filter feeders organisms. Several studies have shown that pathogens, such as bacteria and enteric viruses, can be transmitted by mussels and the widespread habit of consuming raw or slightly cooked shellfish contributes to maintaining the incidence of hepatitis A cases in the southern Italy at high level (Croci et al., 2003).

On the other hand, nevertheless the availability of technologies for remote water quality monitoring system using wireless sensors (Haron et al., 2009), the livestock sampling and the microbiological spottily analysis fails if the goal is a consistent data time series needed by any process aimed to make inference with human health. The use of connected smart devices is fully feasible in a context where the farms are in a limited environment, while the challenges rise for fish and mussel farms in marine nearshore, but open waters: the extreme weather events, the aggressive saline environment, the network and energy availability and, last but not least, the need for continuous maintenance and sensors calibration could have a negative impact on the use of a technical solution fully based on the Internet of Things afloat approach.

To face the above depicted scenario, we designed and implemented WaComM (Water Community Model), a three dimensional Lagrangian model enforcing the decision support system and enabling the simulation and prediction of pollutant spills, transport and dispersion in both inshore and offshore environments (Giunta et al., 2005).

Here, we provide some details about the way in which the input data of our Lagrangian model are ob-

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tained. Moreover, we give some insights about the related parallel implementation.

In order to support the numerical model solution, we leverage on crowdsourced data acquired by the system called "FairWind" a smart, cloud-enabled, multifunctional navigation system for leisure and professional vessels. This system has been developed as an open technologies developing platform based on the Android operating system for smart devices.

In this context, the system is used to collect data from on board marine instruments such as, but not limited to, GPS, heading, pitch, roll, yaw and speed sensors, water temperature, depth and weather sensors. Collected data are sent on the land using grid file transfer technologies, and then processed in order to improve data quality and consistency.

Data, made available to the community as open data, are used to improve the model setup (i.e. high resolution coastal digital depth model) and will be used for model evaluation and improvement (surface temperature, surface current).

The rest of the paper is organized as follows: section 2 is about related work; section 3 focuses on the numerical issues driving the design of our Lagrangian model; section 4 is on details about the WaComM implementation with focus on parallel cores; section 5 is about the novel contribution of the crowdsourcing approach in this application research field; section 6 describes some preliminary computational evaluations; finally section 7 presents conclusions and future developments.

2 RELATED WORK

The Regional Ocean Modeling System (ROMS) is a free-surface, terrain-following, primitive equations ocean model widely used by the scientific community to characterize and simulate the meso- and sub-mesoscale ocean and coastal water dynamics (Haidvogel et al., 2000; Wilkin et al., 2005; Shchepetkin and McWilliams, 2003; Shchepetkin and McWilliams, 2005). In this application ROMS is forced by a high-resolution atmospheric forecast and provides the flow velocity on a curvilinear boundary-fitted grid.

ROMS was used to deploy a real-time forecast for the transport and deposition of water pollutants using the particle-tracking WaComM model, which implements a Lagrangian technique consistent with the advection-diffusion equation (Rodean, 1996).

In this kind of model, the dispersion phenomenon is reproduced by imaginary numerical particles; at each of these particles different characteristics are assigned, e.g. pollutant concentration and settling velocity.

At each time step, the particle position is calculated on the basis of the flow velocity, computed by the hydrodynamic model ROMS, and a random jump representing the turbulence diffusion.

GVirtuS (Montella et al., 2011) is a general-purpose virtualization service for high performance computing applications on cloud environments, focusing on NVidia CUDA GPGPU virtualization and MPI based virtual clusters.

The RAPID GVirtuS incarnation (Montella et al., 2016b) was used as GPGPU remoting provider for hierarchical parallelism, sending the instruction set kernel to the accelerating hardware, processing data on the device and then sending back results to the general purpose CPU.

The FACE-IT (Framework to Advance Climate, Economic, and Impact Investigations with IT) project (Pham et al., 2012) has been developed, and continues to be developed, to provide a cloud-based science gateway for the web-based access to a range of data projects, simulation models and analysis tools (Montella et al., 2015). FACE-IT builds on the Globus Galaxies platform, which has been developed over the past several years at the University of Chicago, initially in support of the Globus Genomics project (Madduri et al., 2015). FACE-IT is used as main computational playground for the implementation of the WaComM Lagrangian model running as an on-demand and routinely workflow (Montella et al., 2016a).

3 DESIGN

WaComM is the evolution of the LAMP3D model. We optimized the algorithms in order to improve its performance on high performance computing environment adding features as restarting and shared memory parallelization. The description of the underlying mathematical model is as follows.

Pollutants are considered as inert Lagrangian particles, tracing the marine circulation without feedback interactions with sea current fields and other particles. Each particle is assumed to have:

- position $r(t) = (x(t), y(t), z(t))$ at time t;
- initial position $r_0 = r(0) = (x_0, y_0, z_0)$ at the initial time $t = t_0 = 0$;
- velocity $v(r(t),t) = U(r(t),t) + \eta(r(t),t)$ at time t, where $U(r(t),t)$ denotes the deterministic velocity, and $\eta(r(t),t)$ is the stochastic fluctuation

arising from the Langevin equation model in order to describe the Brownian motion of particles (Rodean, 1996).

Given $U(r(t),t)$, or an estimate of it, for each position $r(t)$ and at each time t, the final particle position $r(t_{k+1}) = r(t_k + \Delta t)$, at time $t_{k+1} = t_k + \Delta t$, can be computed by means of the equation:

$$r(t_k + \Delta t) = r(t_k) + \int_{t_k}^{t_k+\Delta t} v(r(t),t)\,dt, \quad (k = 0, 1, \ldots), \tag{1}$$

where $r(t_k)$ is a starting position, at the starting time t_k, and $\Delta t > 0$ denotes a time interval length (in WaComM we set $\Delta t = 1\,h$).

Numerical integration of (1) could be made in several ways; in our approach we use the Eulero method that considers a discretization of the time interval $[t_1, t_1 + \Delta t]$ in the grid

$$\tau_{j,k} = t_k + j \cdot d\tau, \qquad j = 0, \ldots, N$$

where $d\tau = \Delta t / N$ denotes the discretization step. To do this, at each time τ_j the evaluations of $U(r(\tau_{j,k}), \tau_{j,k})$ and $\eta(r(\tau_{j,k}), \tau_{j,k})$ are required. However, these values are provided by ROMS only at some discrete time instants, and on a discrete irregular three-dimensional grid. Such a grid can be thought of as the set of vertexes of a finite number of polyhedrons V_i (cells). These cells are all topologically homeomorphic to a cube and their union is the space domain of U.

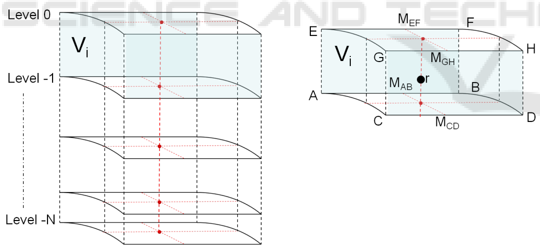


Figure 1: Example of cell. The cells form the irregular grid where the values of U are known.

An example of the form of such cells is in Figure 1. Notice that the irregular polyhedron is defined by assigning its eight vertexes.

Possible choices of interpolants, which do not need any information about the mesh (i.e. the so-called mesh-free methods) are the radial basis functions methods (Cuomo et al., 2013; Fasshauer, 2007). However, when some structure of the grid is assigned, i.e. when a smart subdivision of the domain in geometrical polyhedral structures is known, one can take advantage of this fact and so several kinds of interpolants, exploiting the geometry of the cells that form the mesh, can be defined (Galletti and Maratea, 2016; Cuomo et al., 2014a; Cuomo et al., 2014b; Cuomo et al., 2015). In this case we choose a simple trilinear interpolation approach using barycentric coordinates. In particular, by referring to the notations introduced in Figure 1, we compute velocities at any spatial location, e.g. at particle position r and desired time, by the linear interpolation of velocities made available by ROMS at the vertexes of any grid cell and regular time intervals.

In order to assign the stochastic fluctuations, WaComM relies on the standard 'K-theory', based on a diffusion coefficient which is estimated by preprocessed ROMS data. An exponential decay which uses the T90 parameter (the time required to degrade 90% of the biodegradable matter in a given environment) is applied to takes into account decaying processes. A sedimentation velocity, $w_{\text{sed}} = (0, 0, -w_{\text{sed}})$, is added to the deterministic component of velocity to simulate settling particles. At the end of each suitably chosen time interval, a scaled concentration field $C_{i,j,k}$ is computed by simply counting the number of particles found within each grid cell.

4 IMPLEMENTATION

The modeling system can be used in an ex-ante fashion, as a decision support tool to aid in the selection of the best suitable areas for farming activity deployment, or in an ex-post fashion, in order to achieve a better management of offshore activities. We tested the system on several case studies where pollutants are spilled out from well known punctual sources located along the coasts of Campania region.

As arguing from the numerical approach, the model is computing intensive and parallelization is needed for its usage in real-world applications. The problem size increases with the number of emission sources and the number of emitted particles. Moreover, the computing time is influenced by the integration time step which should be short enough to correctly represent the turbulent diffusion processes.

Although consistent results can be guaranteed using the sequential implementation of the WaComM model, the wall-clock performance actually makes the production unfeasible.

Hence, the growing need of on-demand results, which involves a large computational effort for WaComM, suggests to use general purpose GPUs in order to efficiently perform computing intensive tasks.

In particular, a GPU implementation is considered for the WaComM main cycles involved for the interpolation and evaluation steps of the 3D momentum and dispersion parameters. This concerns with a parallel design schema hierarchical and heterogeneous.

The implementation of the GPGPU enabled code is realized with the NVIDIA CUDA programming model, and using heterogeneously both the CPU and GPU (Ortega et al., 2016) supported by an MPI based distributed memory approach. Such an implementation considers a dynamical load balancing on the particle number.

More in detail, the distributed memory parallelization has been introduced in the hourly inner cycle of WaComM in order to enhance the performance. Such a cycle computes the path of each particle and, since no interaction between particles is assumed, each particle path can be virtually tracked independently of the others. As explained in the design section, the interpolation stage is time consuming. The problem size scales with the input data (the resolution of the momentum, the sea current 3D vector components - U, V, W - and the vertical T-diffusion - AKT - grid). Then, previous discussion justifies even more the shared memory parallel approach for the evaluation of the interpolation model.

5 DATA CROWDSOURCING

In the field of ocean modeling, the need for computational and storage resources is currently satisfied by the availability of cloud based services that reduce the total cost of ownership and accelerate the democratization of science (Foster, 2011). Nevertheless, to have more robust and accurate models, there is a need for detailed, high resolution, spatio-temporal data for initialization and validation. While data can be hard to obtain from traditional sources, due the lack of available public data in some coastal areas, the challenges of surveying large areas and other technical constraints, this data can be easily obtained using internet of things based crowdsourcing tools like FairWind

(Montella et al., 2016c).

FairWind is an integrated, multifunctional, navigation software based on open technologies designed and developed by a very interdisciplinary team in order to maximize the benefits and the advantages. It is a marine single board computer device leveraging a custom-built infrastructure on top of stable and well documented mobile and cloud technologies.

From the marine electronics point of view, the most remarkable innovation introduced by FairWind are the Boat Apps that extend the FairWind basic features, integrating with already present onboard instruments and straightforwardly interacting with industrial or self - made internet of things based instruments. The board dataset, collected by FairWind, is a scientifically intriguing source of huge amounts of geolocated data (big-data) about marine coastal environment (weather and sea conditions, surface sea currents, water temperature, water depth, etc.), boat engine status, boat performances (speed, heading, pitch, roll), presence of board water and waste management, fuel consumptions and, above all, safety at sea and search and rescue systems (Figure 2).

Data is collected on board and, when possible, sent to cloud storage and computing facilities using reliable, affordable, and safe technologies such as the Globus data transport services. Users can choose what data to share in a named or anonymous way. Operationally, once data is collected, it will be analyzed and processed in order to extract sensor calibration using big-data algorithms, evaluated with a quality model comparing it with data acquired by trustful equipment and, finally, made available as open data for ocean model initialization and/or validation.

6 EVALUATION

This section describes the WaCoMM model use case for the Campania Region (Italy), applied to prevent the consumption of contaminated food harvest in mussel farms. This farms have, generally, a long lines organization in which the mussels are attached to submerged ropes hung from a back-bone supported by large plastic floats.

In 2006, the Campania Region published the "*Guidelines for mussel farms: classification and monitoring system of mussels production and relaying areas*" to delineate the guideline to mussel farms monitoring.

This document identified the skills to perform the analysis provided by the *Experimental Zooprophylactic Institute of Southern Italy* (IZSM) for mussels samples and by the *Campania Regional Environmental Protection Agency* (ARPAC) for water samples. The *in situ* analysis also included the compulsory microbiological parameters: *Escherichia Coli* and *Salmonella spp*. In accordance with the current European legislation (2073/2005EC), the concentration of *E. Coli* and *Salmonella spp* in mussels must be less than 230 MPN/100g (Most Probable Number per 100 grams) and zero respectively.

The considered mussels rows (MF_{PT} in Figure 3) are located about 500 m distance to the coast in Punta Terone-Capo Miseno and cover an area of about 257 m^2, with a depth of about 20 m. In this case, the reared mussels are mostly *Mytilus Galloprovincialis*. The MF_{PT} mussels are allowed to be placed on the market for human consumption directly, without fur-

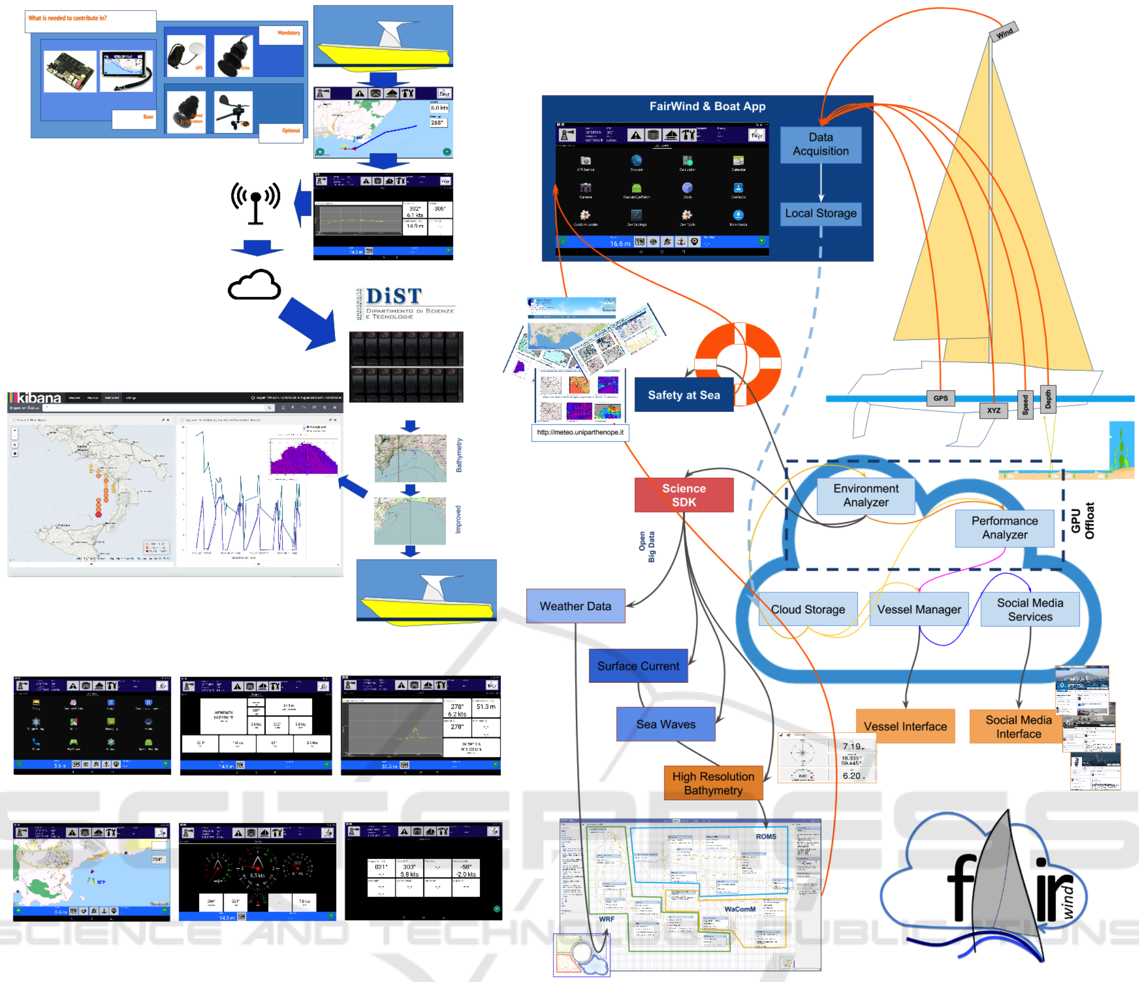


Figure 2: Smart devices in a context of internet of things afloat make data crowdsourcing affordable. FairWind equipped professional and leisure boats can contribute to model setup improvement and data assimilation.

ther treatment in a purification centre or after relaying (class type A). This makes the mussels quality very important to human diseases prevention.

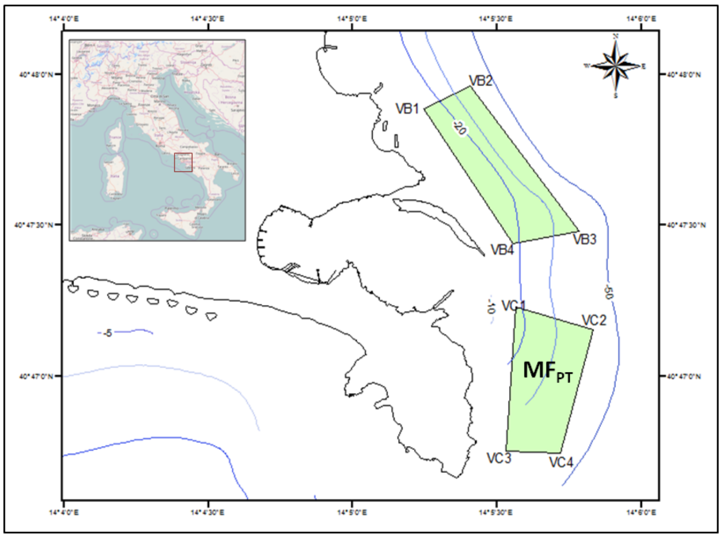
In some cases flooding events can bring too much pollutants to shellfish farms, banning them from harvesting.

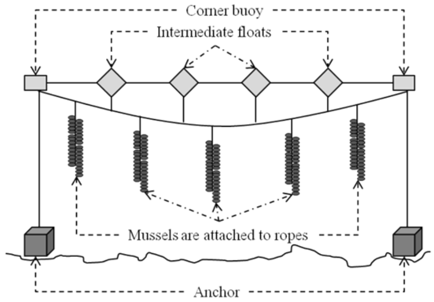
In this context, a forecasting system of the meteorological and hydrodynamic circulation, coupled with the WaComM model, can be a valid support to the mussel farm management.

WaComM is included in a scientific workflow to ingest the forecast input data needed to initialize the simulation and track particles trajectories.

The *Weather Research and Forecasting Model* (WRF) (Skamarock et al., 2001) simulates the weather conditions for driving the ROMS model. The WRF model has already been used to simulate weather conditions on the Campania region (Barone et al., 2000; Ascione et al., 2006). WaComM model domain is $715\times712\times11$ grid points (Lat_{min}=40.48N, Lat_{max}=40.95N; Lon_{min}=13.91E, Lon_{max}=14.52E). The pollutant sources in the Gulf of Naples are considered as points all along the coast, spilling out 100 particles for each simulation hour. Actually we used 50 particle sources. Our system has been tested comparing the numerical forecast and mussel microbiological analysis. The simulation spanned the time interval 07/12/2015 Z00 – 21/12/2015 Z23 and the output was stored at a hourly interval. On days 09/12/2015 and 21/12/2015 the local authorities carried out the microbiological analysis on *Mytilus Galloprovincialis* in Punta Terone mussel farm. Results showed a concentration of *E. Coli* much greater than the legal limits in the first day (5400 MPN/100g) and lower in the second day (45 MPN/100g); *Salmonella spp* was absent in both samples.

The mean wind direction started blowing from NW from 7 to 9 December 2015; in this period parti-





Mussel farm MF$_{PT}$		
Vertex	Latitude	Longitude
VC1	40°47'10''.14	14°05'30''.66
VC2	40°47'05''.64	14°05'46''.80
VC3	40°46'41''.10	14°05'42''.49
VC4	40°46'41'.64	14°05'28'.62

Figure 3: Mussel farms locations in the Bay of Pozzuoli. The studied mussel farm is in Punta Terone (MF$_{PT}$) area.

cles spilled out by sources in the eastern part moved towards the center, while particles emitted by sources in the western part remained close to the coast (see Figure 4). After, the mean wind shifted to NE and all particles moved towards the center of the gulf with a progressive increase in the concentration of the tracer in the area surrounding the two mussel farms with a maximum value on day 15/12/2015. Subsequently, the rotating ocean currents contributed to the dispersion of the tracer away from the mussel farms. This picture is also confirmed by microbiological analysis carried out on *Mytilus Galloprovincialis* mussels (Figure 5). The comparison between numerical forecast and microbiological analysis showed a remarkable similarity in trends, although this kind of analysis have to be performed in a more extensively fashion. That confirmed the possibility to use the system as a decision maker tool for applications correlated with sea quality and as a support system for experimental observations and controls.

7 CONCLUSION

The quality of coastal marine waters depends strictly on the impact of human activities. Urban settlements, industries, agriculture, livestock farming and weather conditions produce effects which, individually or together, can heavily compromise or even disrupt the equilibrium of aquatic ecosystems.

In this paper we presented our research efforts in designing and developing WaComM, a community water quality model, with the main aim, but not limited to, to develop a forecast system and perform operational numerical predictions in the context of mussel farms management, in order to prevent *E. Coli* and *Salmonella* human diseases with a strong effort in data dissemination for local management decision support (Montella et al., 2007).

WaComM is under continuous active development.

From the implementation point of view a deep refactoring is needed in order to better exploit the hierarchical parallelism. The current implementation leverages on a naive application designed load balancing (Laccetti et al., 2013). A Portable, Extensible Toolkit for Scientific Computation (PETSc) approach could enhance the overall perforance and, above all, the problem scalability (Carracciuolo et al., 2015).

A short-term goal of our project is to extend the studied area to the whole coasts of the Campania Region in order to promote its use as an effective tool dedicated to improve the management of coastal farms. In order to achieve this target, we need to improve the robustness of the WaComM model and the scalability of the offline coupling system.

From the scientific point of view, we will enhance the simulation quality with data collected using the FairWind technology as depicted above improving the data acquisition from boat sensor as interconnected smart devices using the Internet of Things afloat technologies. This issue is a source of novelty even because the whole FairWind ecosystem is based on the SignalK marine data interchange open protocol (http://signalk.org). The proposed system is extensible in order to collect data from other sensors as, but not limited to, surface ph and salinity sensors that could improve the simulation quality and the model validation process and, finally, if supported by

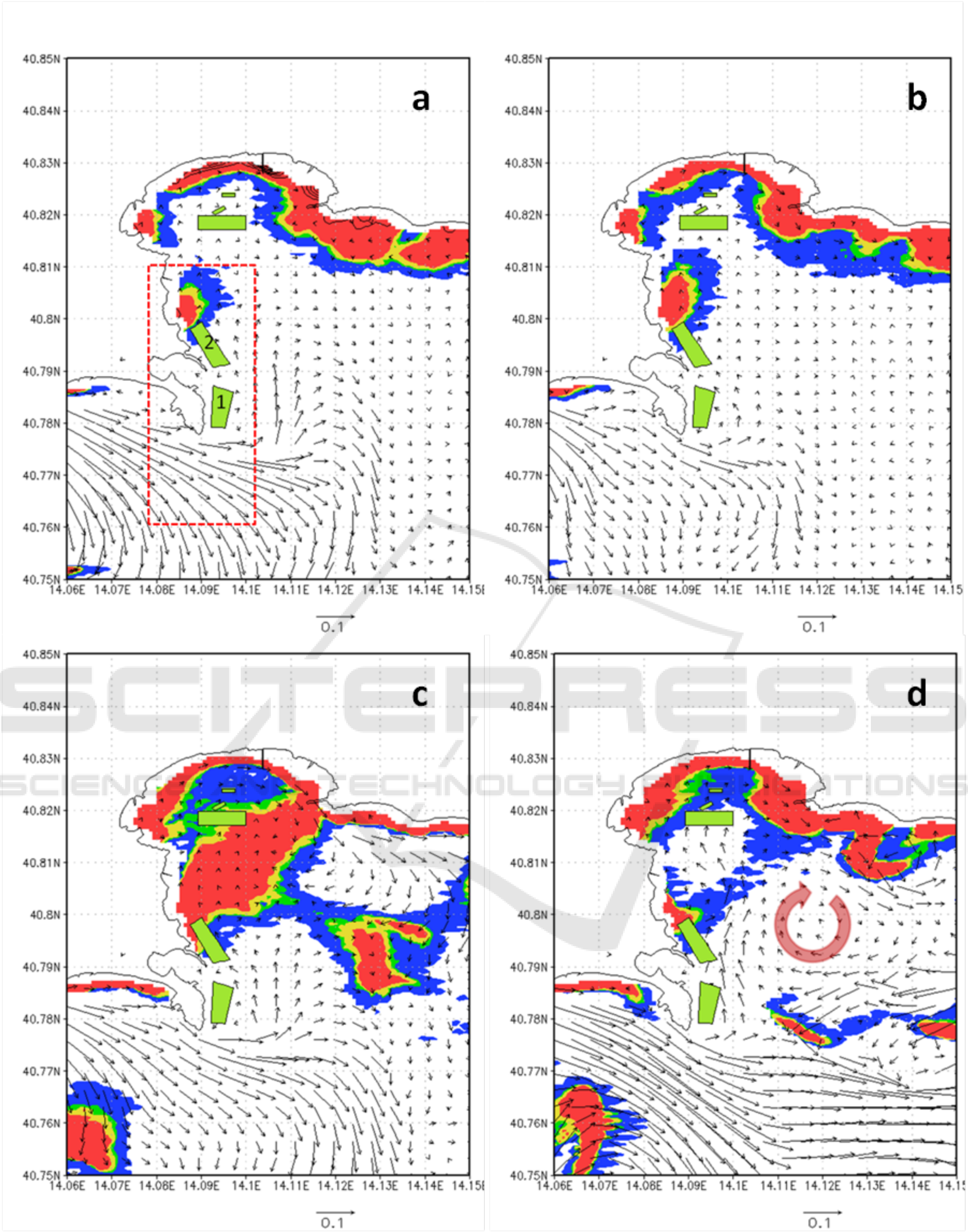


Figure 4: Sea surface currents (vectors) and pollutants concentration (red=high; yellow=medium; green=low; blue=very low; white=absent) in in Gulf of Pozzuoli (Campania Region, Italy) in days 08/12/2015 Z12 (figure A), 09/12/2015 Z12 (figure B), 15/12/2015 Z12 (figure C) and 20/12/2015 Z23 (figure D). The red dotted line is the area of Study with mussel farms in Punta Terone (number 1 in figure A) area.

a ground true based on better microbiological analysis and consistent epidemiological studies on mussels originated enterogastric diseases (Suffredini et al., 2014), enhance the overall system trustability.

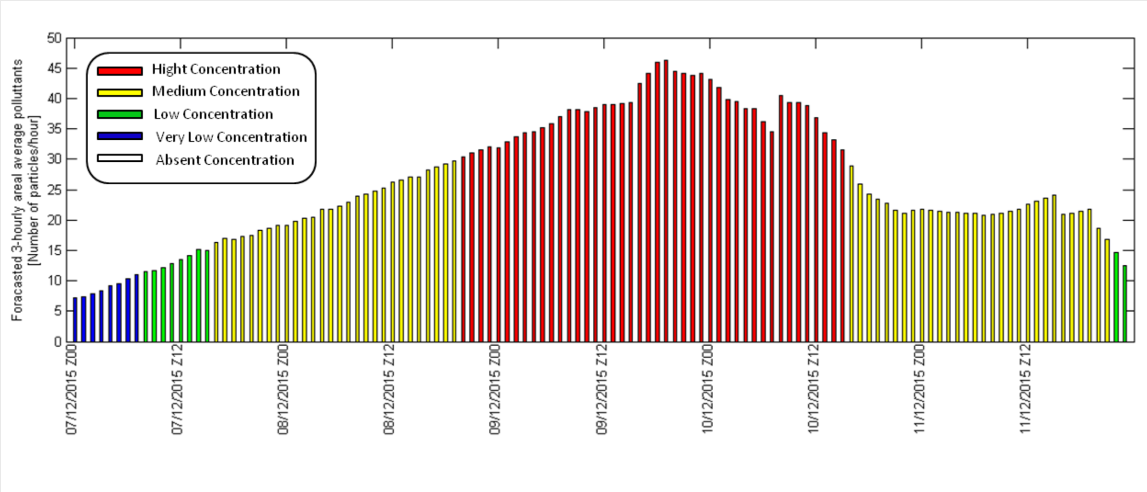


Figure 5: Forecasted averaged particles concentration timeseries in the study area.

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