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Some remarks about a community open source Lagrangian pollutant transport and dispersion model

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Abstract

Nowadays fishes and mussels farming is very important, from an economical point of view, for the local social background of the Bay of Naples. Hence, the accurate forecast of marine pollution becomes crucial to have reliable evaluation of its adverse effects on coastal inhabitants' health. The use of connected smart devices for monitoring the sea water pollution is getting harder because of the saline environment, the network availability and the maintain and calibration costs[2]. To this purpose, we designed and implemented WaComM (Water Community Model), a community open source model for sea pollutants transport and dispersion. WaComM is a model component of a scientific workflow which allows to perform, on a dedicated computational infrastructure, numerical simulations providing spatial and temporal high-resolution predictions of weather and marine conditions of the Bay of Naples leveraging on the cloud based[31] FACE-IT workflow engine[27]. In this paper we present some remarks about the development of WaComM, using hierarchical parallelism which implies distributed memory, shared memory and GPGPUs. Some numerical details are also discussed.

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Keywords: Lagrangian Methods, Numerical Interpolation, Cloud Computing, High Performance Computing, Scientific Workflow, Smart Devices, Internet of Things

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1. Introduction

The coastal water quality is crucial for fish and mussel farms. In particular potential seafood contaminations caused by inshore discharges or offshore spills in areas close to aquaculture farms can adversely affect the human health. Then a continuous monitoring of the pollutants emission into sea water is crucial. In this context, some computational models for air and water quality have been recently considered and implemented[23,36], while more specific grid computing based components have been developed for general environmental simulations[1,26]. Here, we are interested in the effects of the transport of potentially toxic substances, spilled out from some coastal point sources can reach the mussel farms and, because of the mussel-pollutant contact, promote the bioaccumulation in filter feeders organisms linked to

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the mussel-pollutant contact time. More specifically, in order to face this scenario, we have designed and implemented a three dimensional Lagrangian model, for the simulation and prediction of pollutant spills, transport and dispersion in both inshore and offshore environments, called WaComM[29] (Water Community Model). In this paper we provide some details about the way in which WaComM is implemented and configured in a weather-sea scientific workflow based on a model chain involving WaComM and the community numerical models WRF (Weather Research and Forecasting) and ROMS (Regional Ocean Modeling System). The rest of the paper is organized as follows: section 2 concerns the related work; in section 3 numerical issues and remarks about the Lagrangian model are given; section 4 provides further implementation details of WaComM; section 5 exhibits some preliminary computational evaluations; finally section 6 draws conclusions and presents future developments.

2. Related Work

The ROMS is a free-surface, terrain-following, primitive equations ocean model. ROMS characterizes and simulates the meso-scale and sub-mesoscale ocean and coastal water dynamics and is a widely used tool by the scientific community[38,39,43]. In our application, we force ROMS to get high-resolution atmospheric forecast and flow velocity on a curvilinear boundary-fitted grid. More in detail, ROMS is used to deploy a real-time forecast for the transport and deposition of water pollutants using the WaComM model.
WaComM implements a Lagrangian technique consistent with the advection-diffusion where the dispersion phenomenon is reproduced by imaginary numerical particles whose characteristics, as pollutant concentration and settling velocity, are assigned. At each time step, the computed position of each particle depends on the flow velocity, provided by the hydrodynamic model ROMS, and on a random jump representing the turbulence diffusion. Because of to the high number of particles, the model is computing intensive and parallelization is needed for its effectiveness in real world applications[6,14,17,25,32,33]. To this aim, we leverage on GVirtuS[28], a general-purpose virtualization service for high performance computing applications on cloud environments, which focuses on NVidia CUDA GPGPU virtualization and virtual clusters based on MPI. The RAPID GVirtuS incarnation[30] 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[35] 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[27]. FACE-IT is used as main computational playground for the implementation of the WaComM Lagrangian model running as an on-demand and routinely workflow. The mathematical model underlying LAMP3D[42] (Lagrangian Assessment for Marine Pollution 3D model) requires as input data the velocity which has to be available at each time t, and at each position of the particles as time varies, possibly. Data about the velocity, in its deterministic component, are provided by the ROMS. Since those values are known only on some a priori assigned grid points, not uniformly distributed, some kind of interpolation method must be used. Once the velocity field is interpolated everywhere, the Lagrangian model LAMP3D is coupled with a bidimensional implementation of the Princeton Ocean Model[24] in order to calculate the needed initial and boundary conditions. This model has been used as baseline for our WaComM development.

3. Design

WaComM can be thought of as an evolution of the LAMP3D model, where we optimized the algorithms, by adding features as restarting and shared memory parallelization, in order to improve its performance on a high performance computing environment. In the following, the underlying mathematical model is described. Pollutants are modelled as inert Lagrangian particles, that trace the marine circulation without feedback interactions with sea current fields and other particles. Each particle is assumed to have: initial position $r_0 = r(0) = (x_0, y_0, z_0)$ at the initial time $t = t_0 = 0$; position $r(t) = (x(t), y(t), z(t))$ at time t ($t \geq t_0$); 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[37]. At each time t, given $U(r(t), t)$ for each position $r(t)$ (or an estimate of it), the final position of the particle $r(t_{k+1}) = r(t_k + \Delta t)$, at time $t_{k+1} = t_k + \Delta t$, shall be calculated by means

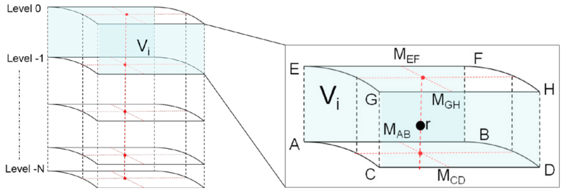

Fig. 1. Example of cell. The cells form the irregular grid where the values of U are known.

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 $r(t_k)$ denotes a starting position, at the starting time t_k, and $\Delta t > 0$ measures the 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 $[t_k, t_{k+1} = t_k + \Delta t]$ in the grid $\tau_{j,k} = t_k + j \cdot d\tau$ $(j = 0, \ldots, N)$, where $d\tau = \Delta t/N$ denotes the discretization time step. To this aim, the evaluations of $U(r(\tau_{j,k}), \tau_{j,k})$ and $\eta(r(\tau_{j,k}), \tau_{j,k})$ are required at each time τ_j. 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 a set of vertexes of a finite number of polyhedrons V_i (cells). These cells are all topologically homeomorphic to cubes and their union is the space domain of U. An illustration example of the form of such cells is in Figure 1. We remark that each 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[15,16]. However, here we deal with a structure of the grid, that is a smart subdivision of the domain in polyhedral structures, then we can take advantage of this fact by using some kinds of interpolants that exploit the geometry of the cells forming the mesh[11,12,13,20]. In this case we choose a simple trilinear interpolation approach using barycentric coordinates[12,21,22]. In particular, 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. More in detail, in order to estimate the value of $U(r(\tau_{j,k}), \tau_{j,k})$, we perform two trilinear interpolations at time steps t_k and t_{k+1}. In particular, by referring to notations in Figure 1, we execute the following computations: evaluate $U(M_{EF}(t_k), t_k)$ by using a linear interpolation model which gives the value: $\widetilde{U}(M_{EF}(t_k), t_k) = \lambda_E\, U(B(t_k), t_k) + \lambda_F\, U(B(t_k), t_k)$,, where λ_E and λ_F are the barycentric coordinates of M_{EF} with respect to E and F. Observe that this formula uses the known values $U(E(t_k), t_k)$ and $U(F(t_k), t_k)$; analogously, using the values $U(G(t_k), t_k)$ and $U(H(t_k), t_k)$, on the side GH, obtain the estimate $\widetilde{U}(M_{GH}(t_k), t_k)$; then, apply the linear interpolation model to the points M_{EF} and M_{GH} and obtain the estimate $\widetilde{U}(M_{EFGH}(t_k), t_k)$ of U at M_{EFGH}. Notice that the previous steps actually implements the bilinear interpolation on the top face of V_i; the same bilinear interpolation is also applied to the bottom face in order to get the estimate value $\widetilde{U}(M_{ABCD}(t_k), t_k)$; re-apply the linear interpolation model between the points M_{ABCD} and M_{EFGH} in order to compute the estimate $\widetilde{U}(r(t_k), t_k)$ of U at $(r(t_k), t_k)$. All the previous steps are re-used at time t_{k+1}, to get the estimate of $\widetilde{U}(r(t_{k+1}), t_{k+1})$ of U at $(r(t_{k+1}), t_{k+1})$, and, finally, values $\widetilde{U}(r(t_k), t_k)$ and $\widetilde{U}(r(t_{k+1}), t_{k+1})$ are linearly interpolated, with respect to the time variable to estimate $U(r(\tau_{j,k}), \tau_{j,k})$. At the end of each time interval, a scaled concentration field $C_{i,j,k}$ is obtained by simply counting the number of particles found within each grid cell (i, j, k).

4. Implementation

The modeling system can be used in an ex-ante fashion, as a decision support tool[26] 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 in witch the pollutants are spilled out from well known punctual coastal sources located in the bay of Naples. As suggested by the described numerical approach, the model WaComM is computing intensive and a parallelization strategy is necessary for its usage in real-world applications[19,40]. The problem size scales with the input data and it grows as the number of emission sources and emitted particles increases. Nevertheless, the computational load is largely influenced by the choice of the discretization time step, for integrating equation (1), which should be short enough to correctly represent the turbulent diffusion processes.

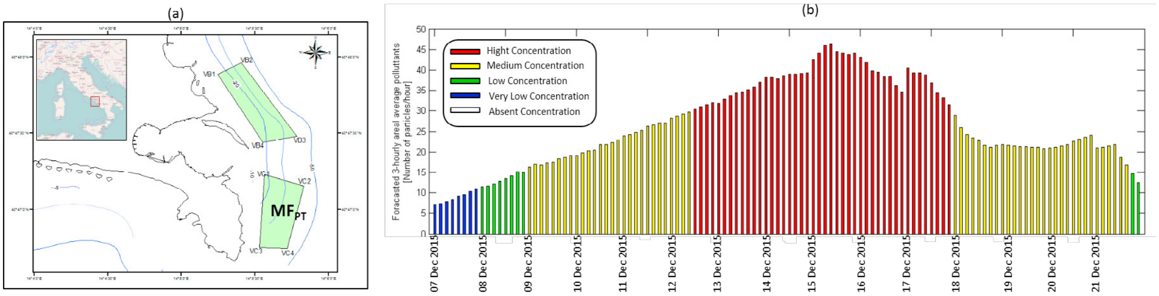

Fig. 2. Left: Mussel farms locations in the Bay of Pozzuoli. Right: Forecasted averaged particles concentration timeseries in the study area of Punta Terone-Capo Miseno.

Particularly, the interpolation stage is time consuming, as explained in section 3. Then a sequential implementation of the WaComM makes the production unfeasible and 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, for the WaComM main cycles (involved for the interpolation and evaluation steps of the 3D momentum and dispersion parameters) a GPU implementation is used, adopting a parallel design schema hierarchical and heterogeneous. The GPGPU enabled is based on the NVIDIA CUDA programming model and uses both the CPU and GPU with an MPI based distributed memory approach[34]. In detail, the MPI parallelization has been introduced in WaComM hourly inner cycle in order to enhance the performance .

5. Evaluation

In this section we explain a WaComM model test case carried out in Gulf of Naples (Campania Region, Italy). In the study area (Lat$_{\text{min}}$=40.48N, Lat$_{\text{max}}$=40.95N; Lon$_{\text{min}}$=13.91E, Lon$_{\text{max}}$=14.52E), the mussel farms (*Mytilus Galloprovincialis* specie) 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, so that the mytilus quality is more influenced by the sea pollutants spilled out by coastal sources linked to human activities. Among the many mussel farm in Gulf of Naples, the presented test case focuses on MF$_{PT}$ farm (Figure 2(a)) located about 500 m distance to the coast in Punta Terone-Capo Miseno, covering an area of about 257 m^2, with the ropes length of about 20m. In this context, WaComM model is included in a scientific workflow to ingest the forecast input data needed to initialize the simulation and track particles trajectories. In detail, the Weather Research and Forecasting Model (WRF) simulates the weather conditions to forcing the ROMS model (spatial resolution about 80m), which gives the sea conditions to drive the WaComM model lagrangian particles. The pollutant sources are considered as coastal points, spilling out 100 particles for each simulation hour. In this test we used 50 particle sources (all sources officially identified by local authorities). Figure 2(b) shows the results of numerical simulations from December 7th-21st 2015, in a zoomed spatial computational domain area including the mussel farm MF$_{PT}$. The output was stored at hourly interval. The particles concentration is grouped in five classes: high, medium, low, very low and absent, to link the number of particles with the human dangerousness. The comparison between WaComM numerical simulations and microbiological analysis showed a remarkable similarity in trends that confirmed the possibility to use the system as a decision maker tool in mussel farm management or other applications correlated with sea quality.

6. Conclusions

The human activities strongly affect the quality coastal marine waters with some effects which can heavily compromise the equilibrium of aquatic ecosystems and the human health. 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. In particular we showed main details about the numerical approach to compute the path of each particle of the model. WaComM is under continuous active development and 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 leveraging on general purpose accelerators[18]. To enhance the system reliability more checks with microbiological are needed in order to support consistent epidemiological studies on mussels and a better knowledge of the originated enterogastric diseases[41]. In order to ensure more reliable solutions of the numerical model, it would be advisable to conduct a crowdsourcing sample to collect atmospheric and marine physical data acquired from on board marine instruments with *internet of things* (IoT) techniques. Examples of IoT applications can be found in the cultural heritage, where ad hoc classification techniques (see[3,4,5,7,8,9,10]) have proven to be effective. In our context IoT data, acquired from on board marine instruments such as, for example, pitch, GPS, heading, roll, yaw and speed sensors or water temperature, depth and weather sensor, are collected and sent by means of grid file transfer technologies and, finally, processed to improve consistency and prediction quality of the output.

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