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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

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