TURBULENT OSCILLATORY FLOW OVER RIPPLES AT HIGH REYNOLDS NUMBERS FOR PETA-SCALE SIMULATIONS

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INTRODUCTION

Surface waves in the coastal zone induce oscillatory flow motions in the vicinity of the seabed. These wave-induced coastal flows interact with the sandy seabed and modify the bed shape by generating coherent small-scale bed structures, which are generally known as ripples. The presence of ripples in oscillatory flows is important due to the impact they have on the seabed roughness and how they affect the near-bed boundary layer hydrodynamics. Simulations of higher and more real-scale Reynolds number (*Re)* require the use of supercomputers in order to obtain results in a reasonable amount of time. However, the constant evolution of the computing facilities makes the development of parallel algorithms a rather difficult task. The objective of the proposed research is to advance in the comprehension of coastal processes utilizing high performance computing (HPC) for the numerical simulation of the three-dimensional, turbulent flow, which is induced in the coastal zone by wave propagation. In particular, our CFD code (SimuCoast) has been developed using a hybrid MPI+OpenACC execution model that increases its scalability and allows it to engage the vast majority of high-end supercomputers. Special attention has been paid in the parallelization strategy of the Poisson solver that is the most computational demanding operation.

METHODOLOGY

The discretization of the Navier-Stokes equations is done on a Cartesian staggered grid following the methodology proposed in Grigoriadis et al. (2012). The numerical methodology is based on the extension of the immersed boundary method proposed by Balaras (2004) for representing the sea bottom. Additionally, an adaptive mesh refinement is utilized for the numerical solution of the equations. Large eddy simulation (LES) was used for simulating turbulence. In this approach, the flow structures are separated into the large eddies, which are explicitly solved, and the small eddies, which are parametrized with the use of an eddy-viscosity subgrid scale (SGS) model.

HPC IMPLEMENTATION

SimuCoast is written in Fortran using an object oriented implementation approach. Hence, the code facilitates the programming of new math and physical models, and encapsulates the complexity of the parallelization strategy. The parallel strategy consists in using a two-level hybrid MPI+OpenACC parallelization (see Figure 1).

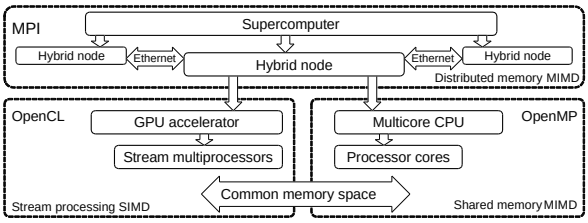

Figure 1 - Levels of parallelism and programming models exploited by SimuCoast in a hybrid supercomputer.

The inter node implementation consists in a distributed memory approach with communications that transfer the information between processors by means of the MPI protocol. The communication episodes are performed in a non-blocking way that reduces part of the communication costs and increases the scalability code. The intra-node computing is based in the OpenACC standard in order to exploit the different computing units of the nodes (multicore CPUs or accelerators). This approach facilitates the utilization of hybrid nodes since its portability is simplified to just changing the compilation flags of OpenACC, reducing the programming costs of re-writing large parts the code for using the accelerators.

The algorithm is based in the fractional step method for decoupling the pressure and the velocities. The solution of the Navier-Stokes equations is represented as loops that sweep the computing domain (Cartesian grid) for applying discretized operators. The iterations within these loops are independent to each other, and thus can be easily parallelized using OpenACC.

On the other hand, the Poisson equation needs to be solved once per time integration step and becomes the main bottleneck of the simulation. Our Poisson solver is composed by a combination of the Fourier decomposition for the two directions (x and y) with periodic boundary conditions and a direct solver for the z-direction (Borrell 2011). The improvements in the solver have empowered our code (up to 60 times of acceleration), making it capable of running peta-scale simulations.

RESULTS

The numerical results of this study were performed on the thin nodes of the Aris supercomputer of the Greek research & technology network (GRNET), this is a tier-1 system of the Partnership for Advanced Computing in Europe (PRACE). Each node is composed by two Intel Xeon E5-2680v2 10-core processors interconnected by a network Infiniband FDR1. The numerical experiments consist in two stages: first the validation of the code, and second, the analysis of the parallel performance of the code.

We validated our code with the experimental case of Fredsoe et al. (1999). HPC implementation allowed us to work with a denser grid than the one of Grigoriadis et al. (2012) and, consequently, achieving better results for the velocity profiles (Fig. 2).

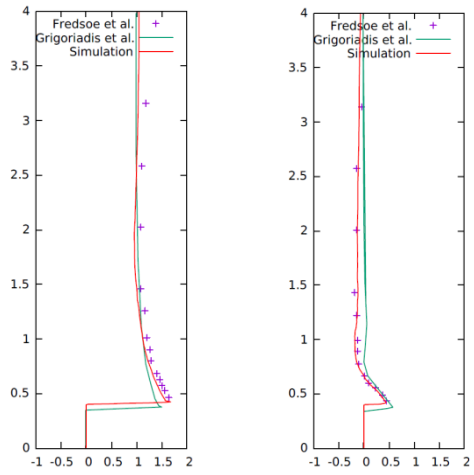

Figure 2 – Profiles of phase-averaged streamwise velocity at the ripple crest (left: $\omega t = 0$, right: $\omega t = 270$).

The same flow was also simulated for a substantially higher Reynolds number of $Re=2\times10^5$ which verified the good scalability of our code. Figure 3 depicts that the parallel efficiency of the code is up to 80% when using a grid of 100,000,000 cells and engaging 64 computing nodes (1280 CPU-cores).

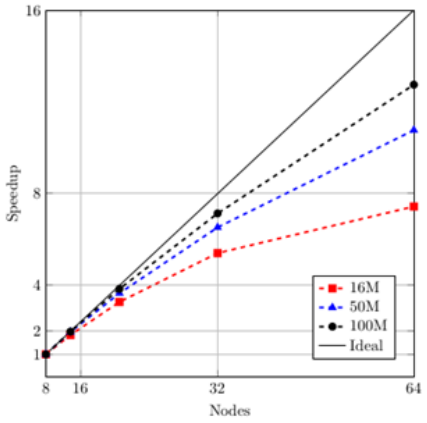

Figure 3 – Strong speedup of the performed simulations for three different grid sizes.

The direct Poisson solver for cases with two periodic boundary conditions was compared with a commonly used iterative solver, the Preconditioned Conjugate Gradient (PCG). In cases with more than 50 million cells, it was observed that the direct solver accelerates the Poisson equation in more 60 times (Fig. 4).

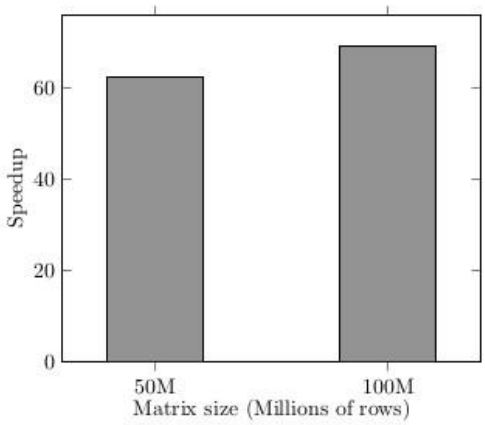

Figure 4 – Average acceleration of direct solver 2FFT+TDMA compared with an iterative PCG solver

ACKNOWLEDGEMENTS

This work was funded by the matching contribution (5231) of GSRT to the Initial Training Network SEDITRANS, implemented within the 7th Framework Programme of the European Commission, and was also supported by computational time granted from the Greek Research & Technology Network (GRNET) in the National HPC facility - ARIS - under project ID CoastHPC.

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