ParCFD'2020
32^{nd} International Conference on Parallel Computational Fluid Dynamics
May-11-13 2020, Nice FRANCE

HIGH PERFORMANCE COMPUTING OF BUBBLE COLLAPSE ON HETEROGENEOUS SUPERCOMPUTER

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Key words: High performance computing, compressible multiphase flow, shock waves, heterogeneous CPU-GPU computing, OpenACC

Abstract. SCB is an in-house fluid solver developed for computing two-phase compressible flows involving strong shocks and expansion waves. Taking into account that the proportion of the heterogeneous computing platforms becomes more and more important in HPC world, hybrid programming approach is becoming essential to use this kind of supercomputer. Based on this assessment, an approach combining MPI and OpenACC librairies has been implemented.

1 INTRODUCTION

A shock-induced bubble collapse is a very intense event and the simulation of such processes is very challenging. **SCB** is devoted to simulate stiff bubble collapses and compressible liquid gas flows by solving a hyperbolic system componed by four-equations. This system is derivated from the five-equation model proposed by Kapila et al. [4]. In a previous study [1], a programming approach combining MPI and OpenMP libraries has been successfully implemented in **SCB** and the high potential of the four-equation model has been showned on challenging 3D stiff cases as well as the scalability of **SCB**. In this study we present an extended version of the solver for GPU-accelerated clusters using OpenACC directives on a 3D reference case.

2 Model, numerical method and parallel paradigms

In the framework of homogeneous mixture model, one can assume that each phase is inviscid and compressible. Moreover, diffusive effects, mass transfer and surface tension are all neglected. In the following, subscripts l and g are related respectively to liquid and

gas phases. The void fraction is α. This four-equation model is built around 3 conservative equations (mass, momentum, total energy) and an additional transport equation for α:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{1}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u} + P\mathbf{1}) = \mathbf{0}, \tag{2}$$

$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho H \mathbf{u}) = 0, \tag{3}$$

$$\frac{\partial \alpha}{\partial t} + \mathbf{u} \cdot \nabla \alpha = K \ \nabla \cdot \mathbf{u}, \quad \text{where} \quad K = \frac{\rho_l c_l^2 - \rho_g c_g^2}{\frac{\rho_l c_l^2}{1-\alpha} + \frac{\rho_g c_g^2}{\alpha}} \tag{4}$$

Equations (1)-(4) are solved using the cell-centered finite volume method on a cartesian grid. The numerical flux and the non-conservative term are computed by using a HLLC scheme and the second order is obtained through the MUSCL-Hancock method. In previous work [1] the hybrid parallization of **SCB** mixing MPI and OpenMP are presented and a scalability up to 20000 cores are observed. While OpenMP provides the possibility, through a new set of directives, to use graphics-accelerator resources, the comparisons observed in the literature against OpenACC have convinced of the usefulness of this paradigm on GPU. Another advantage of OpenACC is its implementation close to OpenMP. Nevertheless attention must be paid when copying data from the host device to the accelerator device, to avoid unnecessary round-trips between devices.

3 Performance and results

The study consists of simulating the collapse of a bubble due to a incident shock wave near a solid wall, problem investigated in 2D by Johnsen and Colonius [2] and more recently in 3D by Werminger et al. [5]. A spherical air bubble with an initial radius R_0, located at coordinates $(x_{(b,0)}, y_{(b,0)}, z_{(b,0)})$, is immersed in water at temperature 293 K under the following initial conditions:

$$(\rho, \mathbf{u}, p) = \begin{cases} (998 \text{ kg/m}^3, \mathbf{0} \text{ m/s}, 10^5 \text{ Pa}) & \text{inside the liquid} \\ (1 \text{ kg/m}^3, \mathbf{0} \text{ m/s}, 10^5 \text{ Pa}) & \text{inside the gas} \end{cases} \tag{5}$$

To close the problem, material parameters for the stiffened gas EOS are set to:

$$(\gamma_l, p_{\infty_l}, C_{p_l}) = (6.68, 4.103 \cdot 10^8 \text{ Pa}, 1650 \text{ J/kg.K}), \text{ for the liquid phase} \tag{6}$$

$$(\gamma_g, p_{\infty_g}, C_{p_g}) = (1.4, 0 \text{ Pa}, 1487 \text{ J/kg.K}), \text{ for the gas phase.} \tag{7}$$

All spatial dimensions are defined relatively to the initial radius R_0. The computational domain is $[L_x \times L_y \times L_z] = [8R_0 \times 12R_0 \times 12R_0]$ and the position of the bubble is located at $(x_{(b,0)}, y_{(b,0)}, z_{(b,0)}) = (6R_0, 0, 0)$. The incident shock wave normal to x-direction is initialized at position $x_{sh} = 4.85R_0$. Performance tests has been investigated in 2D and 3D, with respectively 1 Million (1M) and 4 Million (4M) cells in 2D and 1 Billion (1B)

and 4 Billion (4B) cells in 3D. All the tests were carried out on the French supercomputer Jean Zay [3], composed with accelerated node with each one 2 Intel Cascade Lake 6248 and 4 Nvidia Tesla V100. The executable has been generated with PGI Fortran compiler (version 19.7).

Grid	CPU Time	GPU time	Gain
1M	691.00	34.60	19.97
2M	2770.0	102.79	26.94

Table 1: Comparison of computational time between one core Intel Xeon Gold 6248 and NVidia Tesla V100 card

The first tests were performed to establish the gain between a GPU card compared to a CPU core (Table 1). The gain is at least around 20 times. These rather good preliminary results must be confirmed in other 3D tests which require the use of efficient parallelism. And above all, care must be taken to ensure that scaling remains good enough when using multiple GPUs (Figure 1).

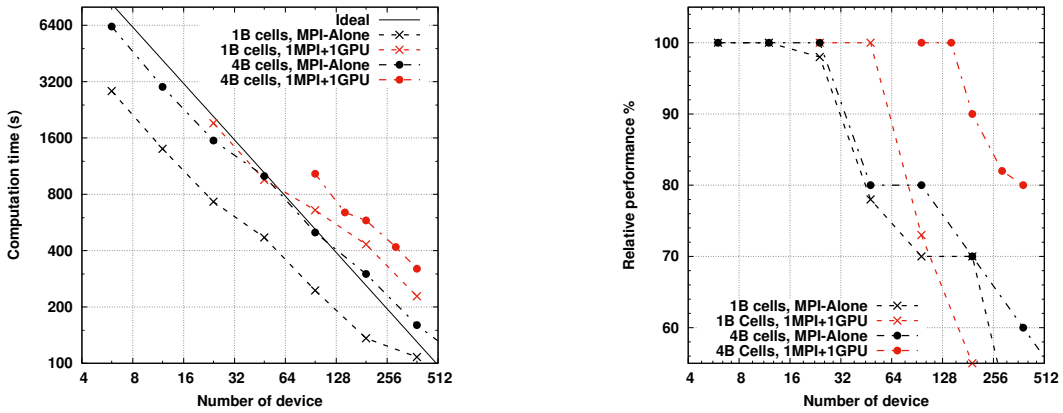

Figure 1: Multi-CPU/GPU. MPI-Alone: Only mpi processes for parallel computation. 1MPI+1GPU: hybride parallel computation. Device represents either 1 CPU (e.g. 20 mpi processes) or 1 GPU card attached to 1 mpi process. Scaling curve (left). Efficiency curve (Right).

Scalability with only MPI and MPI+GPU are quite similar as long as the size of the problem remains moderate (1B), with higher efficiency when using multi-GPU. When the problem size becomes larger (4B), the multi-GPU version maintains an efficiency of more than 80%, while it can decrease drastically with MPI-Alone. Finally, it appears that a GPU card delivers a performance which is at least equivalent to a dozen CPU cores.

4 Conclusions

A hybrid well-suited MPI+OpenACC implementation is developed. Moreover a performance study assesses the potential of the proposed approaches. Results indicate that OpenACC paradigm is mature and provides a good efficiency. Therefore it seems to be a

relevant choice for hybrid implementation with MPI library. Then, a shock-induced bubble collapse is computed and a very close agreement with existing results is illustrated.

Acknowledgments

This research was supported by the French National Research Agency ANR (project 18-CE46-009). Computations have been performed on the supercomputer facilities of the HPC resources of GENCI under allocations A0072A10981.

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