A NUMERICAL METHOD TO ACCELERATE CFD OF BUOYANCY DRIVEN FLOWS WITH STRONG PROPERTY VARIATIONS

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1. INTRODUCTION

Simulating turbulent flows driven by buoyancy is a challenging computational task even assuming that the Oberbeck-Boussinesq (OB) approximation is valid and fluid properties are constant. However, the OB form of the Navier-Stokes (NS) equations can only provide reliable solutions if the temperature differences are quite small [1]. For practical problems of convective heat transfer with large temperature differences or using temperature-sensitive fluids, the variation of properties is often outside this range, leading to non-Oberbeck-Boussinesq (NOB) convection. In this challenging regime, usual symmetries are diminished, and the flow patterns become fluid-dependent [2, 3]. When one tries to model these property variations, the simulation cost increases drastically because the emerging Poisson equation for pressure has variable coefficients in space and time. To significantly accelerate these simulations, we have recently presented [2, 4, 5] an efficient methodology for variable property flows. Using a pressure-correction and a pressure-splitting scheme, the variable coefficient Poisson equation for the pressure is transformed into a constant coefficient equation which allows the application of Fast Direct Solvers (FDS). The method can accommodate strong temperature-dependent variations of thermophysical fluid properties for all terms of the conservation equations. The computational cost and the low-memory footprint of the method is demonstrated by presenting LES and DNS results for a differentially heated cavities using liquid metals, executed on CPUs and various low-end single GPU cards. When compared against NS-solvers using iterative pressure solvers, the presented method was found to accelerate LES and DNS simulations by speedup factors of $O(100)$ for CPU and $O(1000)$ for GPU architectures.

2. GOVERNING EQUATIONS & NUMERICAL METHOD

When the flow can be considered as incompressible and the properties of the medium vary with temperature, the governing equations take the form:

$$\frac{\partial \rho}{\partial \tau} + \frac{\partial u_j}{\partial x_j} = 0 \quad (1)$$

$$\frac{\partial u_i}{\partial \tau} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial P}{\partial x_i} + \frac{1}{\rho}\frac{Pr}{\sqrt{Ra}}\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right] + \frac{1}{Fr^2}\delta_{i,3} \quad (2)$$

$$\frac{\partial \Theta}{\partial \tau} + u_j \frac{\partial \Theta}{\partial x_j} = \frac{1}{\rho C_p}\frac{1}{\sqrt{Ra}}\frac{\partial}{\partial x_j}\left(k\frac{\partial \Theta}{\partial x_j}\right) \quad (3)$$

where u_i represent the velocity components along x, y and z directions and t is the non-dimensional time. P stands for the non-dimensional pressure and Θ the non-dimensional temperature. The scales used to non-dimensionalise these equations are the height (h) of the domain as the characteristic length scale and $V_o = a\sqrt{Ra}/h$ as the velocity scale where a is the thermal diffusivity. Using these scaels, $t_o = h/V_o$ becomes the time scale and $P_o = \rho V_o^2$ the pressure scale. Temperature is made non-dimensional as $\Theta = (T - T_{ref})/\Delta T$, where $\Delta T = T_h - T_c$ is the maximum temperature difference of the heated (T_h) and cooled (T_h) parts of the problem. T_{ref} denotes the reference temperature of the problem, $T_{ref} = (T_h + T_c)/2$. Using these scales, the characteristic dimensionless groups emerging are the Rayleigh ($g\beta\Delta T h^3 \nu^{-1}\alpha^{-1}$), Prandtl ($\nu\alpha^{-1}$) and Froude ($a\sqrt{Ra\, g^{-1}\, h^{-3}}$) numbers. All thermophysical fluid properties (ρ, μ, C_p, k) are non-dimensionalised using the value of

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each property at the reference temperature T_{ref}. The specific temperature-dependent property variation of any selected fluid can be defined using simple temperature dependent polynomials [2, 4].

The numerical method is based on a fractional-step approach and finite differences on Cartesian, staggered grids. The Immersed Boundary Method (IMB) is used to describe the presence of solid boundaries and FDS solvers are employed to solve the derived Poisson equation. The momentum equations are discretised in space with 2nd order central differences. The temperature equation is discretised using the Hybrid Linear Parabolic Approximation (HLPA) scheme. Time marches with a 2nd order fully explicit Adams–Bashforth scheme or a semi-implicit Crank-Nicolson scheme. In LES mode, the turbulent sub-grid scales of motion are modelled by the Smagorinsky or the filtered structure function models.

The efficiency of the proposed method is mainly due to the capability of using robust FDS for pressure solution while the fluid properties in equations (1) – (3) are allowed to vary in space and time. This is achieved by using a pressure-splitting technique to transform the emerging variable-coefficient Poisson equation for pressure into a constant-coefficient equation. A comprehensive presentation of the numerical methodology and details on its implementation can be found in [4]. The extension of the method to gas flows using the low-Mach approximation can be found in [5]. Part of the method was originally developed for interfacial multiphase problems of immiscible fluids [8]. The extension of the method to multi-phase convective heat transfer with NOB conditions is under progress.

3. RESULTS

The method has been already validated for a wide range of parameters for heated channels, Rayleigh-Bénard convection [1], thermally driven cavities filled with liquids or gases [4, 5] and mixed convection in ventilated cavities [6]. To demonstrate the efficiency and the potential of the developed method, three different cases are presented in the following sections: (a) the OB flow in a differentially heated cavity (section 3.1), (b) a fully developed turbulent channel flow at $Pr = 0.025$, $Re_\tau = 150$ (section 3.2), and (c) the flow in a square cavity filled with Ga–In–Sn eutectic alloy (section 3.3).

3.1 Flow in a differentially heated cavity

In this section, a subset of results for the turbulent flow inside a square cavity filled with air are presented. The differentially heated cavity is square and the gravity field is assumed to act vertically downwards. The flow is assumed to be periodic along y-direction and the associated Rayleigh (Ra) varied in the range $Ra = 10^9 - 10^{11}$. To match the conditions of the DNS study of Sebilleau et al. [7], the OB approximation was used for property variations. Various grid sizes were used to simulate this case and the simulation cost in terms of physical memory and cpu times for each grid is presented in Table 1. Figure 1 shows the comparison for the first and the second order statistics against the reference DNS data for $Pr = 0.7$ and $Ra = 10^{11}$ [7].

Table 1: Memory requirements and wall-clock times for various grids executed on CPUs and single-GPU cards. The flow simulated was a differentially heated cavity at $Ra = 10^{11}, Pr = 0.7$ [7]. Execution times include the generation of 1st and 2nd order statistics.

Grid	Numerical Resolution			RAM	Total simulation time for 500 time units			
					CPU 2xE2860 Xeon™	GPU GTX-1050Ti	GPU GTX-2070S	GPU V100
	Nx	Ny	Nz	(GB)	(hrs)	(hrs)	(hrs)	(hrs)
G1	62	32	62	0.01	0.17	0.1	0.05	0.03
G2	98	48	98	0.1	0.42	0.1	0.05	0.03
G3	116	64	116	0.1	1	0.3	0.08	0.05
G4	166	96	166	0.3	6	2.1	0.5	0.34
G5	194	128	194	0.6	10	3.3	0.8	0.52
G6	272	128	272	1.1	50	16.7	4.2	2.8
G7	384	192	384	3.4	167	55.6	15.0	10.1

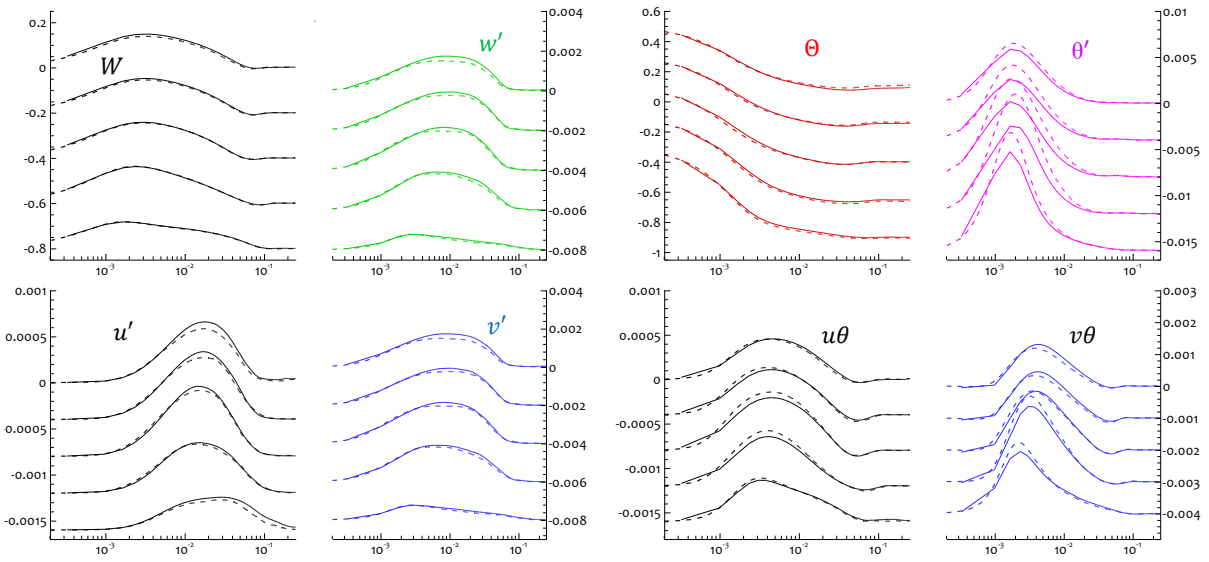

Figure 1: First and second order statistics from an LES simulation in a differentially heated cavity at $Ra = 10^{11}$, $Pr = 0.71$ against the DNS data (dashed lines) of Sebilleau et al. [7]. From bottom to top, each line corresponds to horizontal profiles at different vertical locations $(z/h) = 0.1, 0.2, 0.3, 0.4$ and 0.5. The simulation used ~28 million cells (grid G7 in Table 1).

3.2 Fully developed channel flow at Pr=0.025

To examine the simulation cost and the performance of realistic liquid metal flows, a set of simulations are presented for the liquid metal turbulent flow in a heated channel. The simulated liquid had a Pr number of 0.025 and the friction Re number was set to 150. The channel had dimensions of $(5, 3, 2)\delta$ along the streamwise, spawise and vertical directions, respectively. Figure 2 shows the comparison for the first and the second order statistics against the reference DNS data of Kasagi & Ohtsubo [9] for three different numerical resolutions.

3.3 Flow in a differentially heated cavity filled with GaInSn

In this section, a subset of results for the turbulent flow inside a square cavity filled with GaInSn are presented. The differentially heated cavity has an aspect ratio $\Gamma = \mathrm{H/W}$ where H is the height of the cavity and W is the distance between the hot and cold plates. The gravity field is assumed to act vertically downwards and the flow is assumed to be periodic along y-direction. The associated Rayleigh (Ra) number varied in the range $Ra = 5\mathrm{x}10^4 - 5\mathrm{x}10^7$, according to the DNS and experimental study of Zwirner et al. [10]. The flow was simulated using the actual property variations of the liquid eutectic alloy GaInSn where Pr varies in the range $Pr = 0.01 - 0.03$ [11]. Various grid sizes were used to simulate this case and the predicted values of Nusselt numbers for each case are presented in Table 2.

Table 2: Flow in a differentially heated cavity filled with GaInSn. Comparison of the predicted Nu numbers against the DNS and experimental data of Zwirner et al. [10].

Case		Numerical Resolution			Nu number [10]	Present
	Ra	Nx	Ny	Nz	Nu_H	Nu_H
1	$5x10^4$	62	32	62	2.76	3.00
2	$5\mathrm{x}10^5$	98	48	98	5.05	5.32
3	$5x10^6$	116	64	116	9.05	9.46
4	$5x10^7$	166	96	166	19.82	19.90

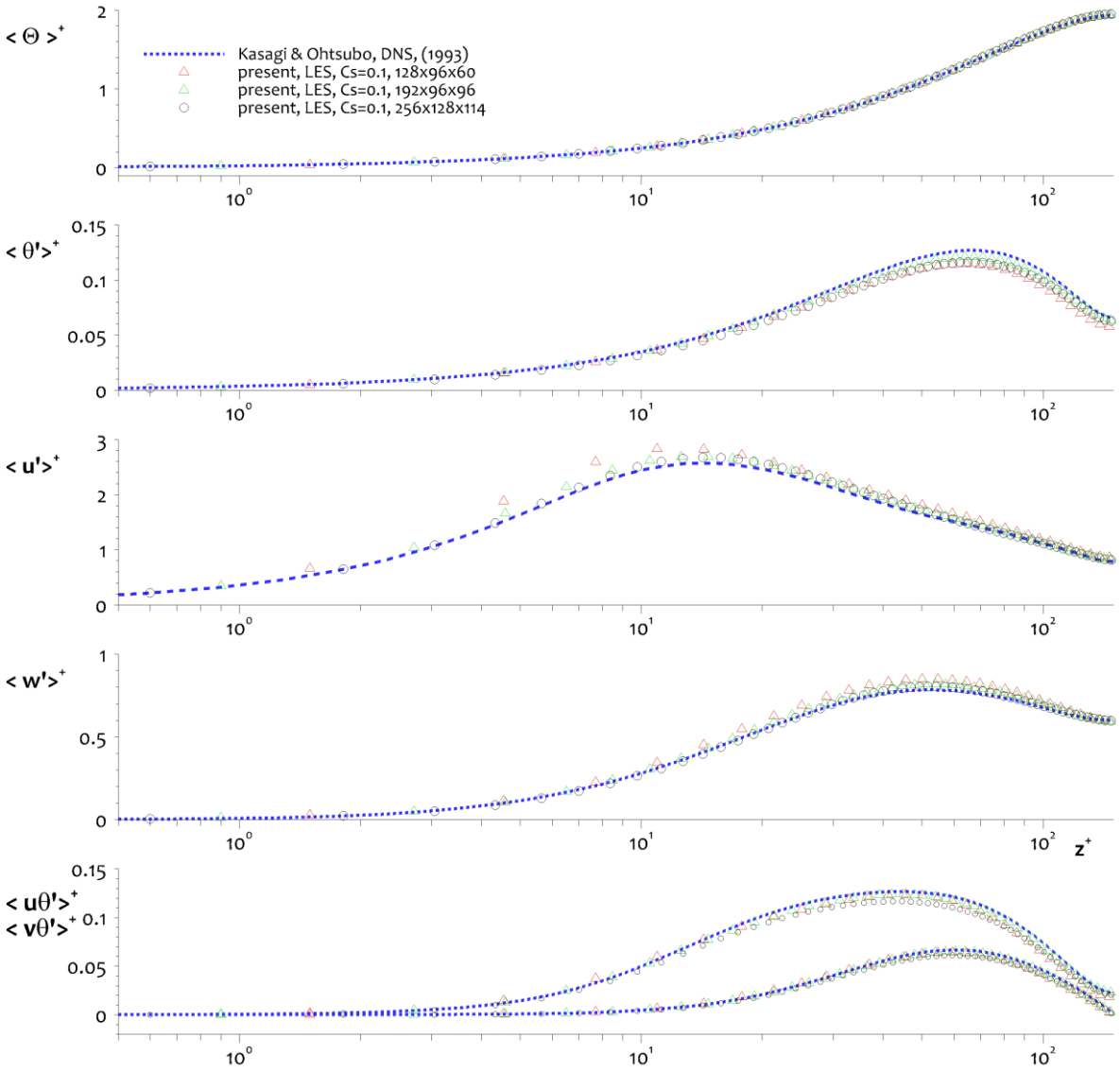

Figure 2: First and second order statistics from an LES simulation in a heated channel at $Re_\tau = 150$, $Pr = 0.025$ against the DNS data (dashed lines) of Kasagi & Ohtsubo [9]. The simulation used ~3.7 million cells ($256\ x\ 128\ x\ 114$).

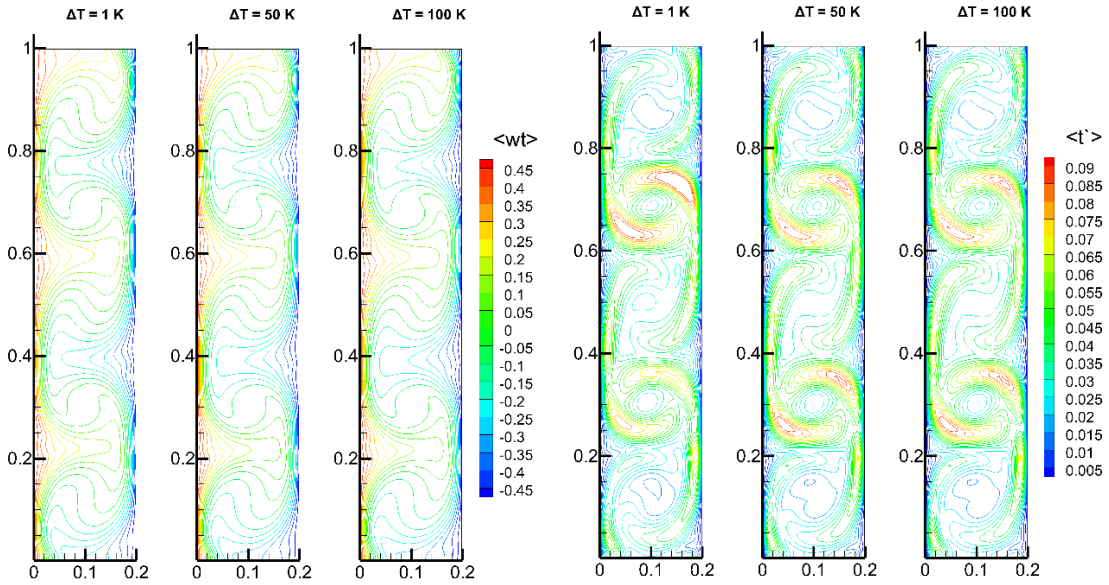

Figure 3:Effect of temperature difference ΔT on the predicted rms variation of the temperature field for a DHC with Γ=5, at $Ra = 4{,}12x10^7$. A liquid GaInSn was used as the medium, considering all property variations around a reference temperature of 399 ºK. These statistics have been collected form 2D LES simulations using a numerical grid of 96x292 cells, using (a) $\Delta T = 10\ K$, . (a) $\Delta T = 50\ K$ and (c) $\Delta T = 100\ K$.

4. CONCLUSIONS

A numerical method that can significantly accelerate simulation of buoyancy driven flows is presented. The efficiency of the method in terms of the computational effort emerges from the utilisation of FDS pressure and the low-memory footprint required. For NOB simulations, the present implementation of the proposed method requires ~115 MB of physical memory (RAM) per million nodes. The overhead with respect to their constant-property OB counterpart simulations was as low as ~20 – 25%. The method was also found to be compliant with recent advances in GPU architectures and was successfully ported to GPUs using the directive-based OpenAcc parallel programming model. Even using inexpensive desktop GPU cards, speedup factors of ~10 were reached with respect to CPU executions. The cost of each time step was measured as low as $\sim 5 - 10$ milliseconds per million nodes, using a single gaming GPU card such as GTX-2070S. This translates to simulation speeds that reach $\sim 7500 - 15000$ (time steps/hr) with a numerical grid of 50 million nodes.

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