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PARALLEL FINITE VOLUME METHOD SIMULATION OF THREE-DIMENSIONAL FLUID FLOW AND CONVECTIVE HEAT TRANSFER FOR VISCOPLASTIC NON-NEWTONIAN FLUIDS

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CONVECTIVE HEAT TRANSFER SIMULATION OF VISCOPLASTIC FLUIDS

ABSTRACT

Three-dimensional fluid mechanics and heat transfer for viscoplastic flows are described by FVM. The OpenMP approach has been implemented to parallelize the numerical code. Results for the elapsed times, speed-ups and efficiencies are presented. The code was used to describe the natural convection ($Ra=104$; 106) and the lid driven cavity ($Re=100$; 1000) processes with Bingham, Casson and Herschel-Bulkley fluids ($Bn=0.01$; 1.0). Results describing isotherms, velocity distributions and streamtraces, as a function of Ra , Re , Pr and Bn numbers are shown. The grid size analysis shows that different sizes are required to obtain precise results for Nusselt number and friction factor.

Keywords: three-dimensional; finite volume method; OpenMP; viscoplastic fluids; natural convection; mixed convection.

NOMENCLATURE

Bn	Bingham number, $Bn = \tau_y L / u_0 \eta_0$
Cp	Heat capacity [J/kgK]
C _f	Friction factor, $C_f = 2\dot{I}_w / Re$
g	Gravity acceleration, [m/s ²]
Gr	Grashof number, $Gr = g\beta\rho(T_H - T_C)L/\eta_0$
k	Consistency index [Pa*s ⁿ]
L	Characteristic length, [m]
m	Exponential growth parameter, [s/m]
M	Dimensionless exponential growth parameter, $M = m\sqrt{g\beta\Delta T/L}$
n	Non-Newtonian behavior index
Nu	Nusselt number, $Nu = hL/\lambda$
S	Source term
T	Temperature [K]
u, v, w	Velocity components [m/s]
U, V, W	Dimensionless velocity components, $U = u/u_0; V = v/u_0; W = w/u_0$
Ra	Rayleigh number, $Ra = \rho g\beta(T_H - T_C)L^3/\eta_0\alpha$
Pr	Prandtl number, $Pr = \eta_0 Cp/\lambda$
Re	Reynolds number, $Re = \rho Lu_0/\eta_0$
Ri	Richardson number, $Ri = g\beta(T_H - T_C)L/u_0^2$

x, y, z	Coordinate axis components [m]
X, Y, Z	Dimensionless coordinate axis components, $X=x/L$; $Y=y/L$; $Z=z/L$
<i>Greek</i>	
α	Thermal diffusivity [m^2/s]
β	Thermal expansion coefficient [$1/\text{K}$]
$\dot{\gamma}$	Deformation rate [$1/\text{s}$]
$\dot{\gamma}$	Rate strain tensor
Γ	Dimensionless diffusivity coefficient
$\dot{\Gamma}$	Dimensionless deformation rate, $\dot{\Gamma} = \dot{\gamma}L/u_0$
η	Viscosity of the fluid, [$\text{Pa}\cdot\text{s}$]
η_0	Plastic viscosity of the yielded fluid [$\text{Pa}\cdot\text{s}$]
H	Dimensionless viscosity, $H = \eta/\eta_0$
θ	Dimensionless temperature, $\theta = (T - T_C)/(T_H - T_C)$
λ	Thermal conductivity [W/mK]
μ_{yield}	Yield viscosity [$\text{Pa}\cdot\text{s}$]
ρ	Density [kg/m^3]
τ_y	unyielded stress [Pa]
τ	Shear stress tensor
Ω	Dimensionless convective factor
<i>Subscripts</i>	
C	Cold
H	Hot

1	Local value
Wall	Local gradient calculated at vessel walls
W	Local gradient calculated at vessel/duct walls
0	Reference value

INTRODUCTION

Viscoplastic fluids are those non-Newtonian fluids characterized by a yield-stress, defined as a threshold after what a fluid readily flows [1-2]. In general, yield-stress fluids are suspensions of particles or macromolecules, such as pastes, gels, foams, drilling fluids, food products, and nanocomposites.

Processes with viscoplastic fluids are of great importance in mining, chemical and food industry. For instance, several works have showed that rheological properties of fruit juices [3-4] and mining pulps [5-6] are well described by viscoplastic non-Newtonian models such as Herschel-Bulkley, Bingham and Casson. The applications of interest of our numerical experiments are related to the flow with viscoplastic non-Newtonian fluids due to changes in buoyancy forces caused by thermal effects and mixed convection effects.

Natural convection involving Newtonian fluids has been broadly investigated. Both experimental and numerical studies have been made; hence reliable benchmark results are available [7-12].

Nevertheless due to experimental difficulties, to the best of our knowledge, only numerical studies with non-Newtonian fluids of the classical natural convection process have been conducted [13, 14]. There is an extensive collection of works concerning with natural convection of non-Newtonian fluids, most of them based on the use of the Ostwald de Waele model, with and without liquid-solid phase change, being applied to describe food processing [15-18] and casting solidification [19-21]. Hossain and Reddy [22] studied the flow of a power law non-Newtonian fluid past an isothermal vertical slotted surface. They found that as the behavior index increases, both the friction factor and the Nusselt number increased. Also, a study of the Rayleigh-Bénard problem for a power law non-Newtonian fluid, confirmed the previous observation respect to the behavior index (n) of a shear-thinning fluids ($0 < n < 1$). Nevertheless for

shear-thickening fluids ($n > 1$) the opposite effect was observed [23]. Vola et al. [24] and Turan et al. [25] studied the natural convection process inside a square enclosure filled with a fluid of the Bingham type. In the former work, through a domain discretization by low order finite elements, the yield stress effect on temperature and velocity distribution was studied. The results obtained show that at higher yield stress values the apparition of rigid zones that modified the vortices position and the temperature distribution turns out to be controlled by thermal diffusion. Meanwhile, in the latter work the commercial software FLUENT was used to solve the coupled conservation equation of mass, momentum and energy. Related to the rheological properties of the fluid, for high values of the Bingham number (Bn), no significant flow was induced within the enclosure [26].

The lid-driven cavity problem is one of the most important forced convection benchmarks because of the simple driving of the flow by means of the tangential motion with constant velocity of a single lid. Several benchmark results are available for the two-dimensional lid-driven cavity problem without [27-31] and with heat transfer effects [32-34]. During the last years, with more accurate numerical methods, further three-dimensional calculations have become available; see e.g. Yeckel et al. [35], Ku et al. [36], Albensoeder et al. [37] and references herein. Dean et al. [38] presented a wide review about results and numerical methods concerning with forced Bingham fluids. Mitzoulis and Zisis [39] made a two-dimensional study through the finite element method of the lid driven cavity problem with a Bingham-Papanastasiou fluid for large Bingham values ($Bn > 1$). The authors found that increasing the unyielded zone decreases the vortex intensity and moves the vortex center closer to the lid. Dall'Onder dos Santos et al. [40], performed a numerical simulation of SMD viscoplastic fluids inside a two-dimensional lid-driven cavity through the finite element method. The authors found two non-symmetric unyielded regions attached to the bottom and upper walls. Mendu and Das [41], accomplished a two-dimensional study of a two facing lids cavity by the lattice Boltzmann method. The authors studied the effect of power law index and Reynolds number on fluid mechanics and on variation of the drag coefficient. They found that as the power law index increases, drag coefficient increases and hence a

higher computation time was required as n decreased. Syrakos et al. [42], numerically studied a two-dimensional lid driven cavity problem of a Bingham fluid, with Bn in the range 0-1000, by the finite volume method with a multigrid algorithm. The authors noticed that the convergence of the method becomes slow at high values of Bn , moreover the implementation of a multigrid method convergence was accelerated compared to the single-grid SIMPLE method.

Large scale Computational Fluid Dynamics (CFD) applications require predicting precise values for field variables which implies the execution of a great quantity of floating point operations. Thanks to recent technological advances, the performance in executing these operations can be improved by the use of fast and low-cost Graphics Processing Units (GPUs) [43, 44], multiple Central Processing Units (CPUs) and multiple memory units that are connected via an interconnection network to form a parallel computer [45, 46]. To use a parallel computer efficiently, the computational task must be divided into a set of subtasks that can be solved on multiple processors concurrently and a code to perform those tasks on the processors must be developed. The Open multi-Processing (OpenMP) library is a parallel programming model for shared memory multi-core processors that became a software standard as a result of a combined effort among hardware vendors and software developers. OpenMP was designed to provide a standard interface in FORTRAN and C/C++ programs for such a parallelization [46]. In a shared-memory environment, parallelization is possible without modifying the numerical method (preserving the resolution properties) even though attention must be paid in order to achieve a good parallel performance. OpenMP parallel computation can be carried out easily and effectively, because these cores are connected to the same Random Access Memory (RAM) [47]. The performance of OpenMP has been tested on different architectures of multicore-based shared memory. Wei et al. [48] by running the case of particle transport in a pipe flow study analyzed three different shared memory systems based on Non-Uniform Memory Access (NUMA) and Unified Memory Access UMA architectures. It was found that data locality is the key to reach a high performance, also on shared-memory systems. In the same sense, Nordén et al. [49] found that OpenMP is competitive with MPI on UMA and NUMA-

optimized architecture. Several authors share the idea about the poor scalability of OpenMP [46, 50] based on the work of Hoeflinger et al. [51], who claimed that through this method a good performance for a small number of processors (<16) could be achieved. They explored the cause of poor scalability and pointed out the importance of optimizing cache and memory utilization in numerical applications as well as the implementation of a set of language issues. To deal with the problem of the poor scalability of OpenMP many investigations into dual-level parallelism have been published [47, 50, 52, 53]. Despite of this widespread conception, a substantial computational time reduction for 3D unsteady flow simulations can be achieved by the implementation of OpenMP directives [54].

Natural convection inside a cubical cavity and mixed convection in a lid driven cavity of viscoplastic fluids (Bingham, Herschel-Bulkley and Casson) in three-dimensional domains are numerically studied by a FVM based OpenMP parallelized code. The remainder of the paper is organized as follows. In section 2, the physical situation and the mathematical model, including the constitutive models for viscoplastic fluids are outlined. In section 3, the computational implementation of the FVM based code designed for 3D non-Newtonian fluid simulation, called non-Newtonian fluid flow simulator (NFFS), is described. The OpenMP parallel implementation of the NFFS code is described in section 4. In section 5, results for validation and parallel performance of the NFFS code are shown. Original numerical results represented by distributions of temperature, velocity and streamtraces, and calculation of Nusselt number and friction factors obtained with second order accuracy are discussed.

PHYSICAL AND MATHEMATICAL MODELS

The geometry, the system of coordinates and the boundary conditions for the two cases of laminar flows induced by buoyancy effects and by mixed convection of a viscoplastic fluid inside a cavity are shown in Figure 1. The limiting case of a cubical cavity with four sides of equal length L is considered. The left and right vertical walls are differentially heated at isothermal temperatures of T_H and T_c , respectively, whereas the remaining walls are considered adiabatic.

The governing equations are formulated for an incompressible Non-Newtonian fluid with constant thermo-physical properties. Density for the gravitational term in the y-momentum equation is assumed to have a linear dependence on temperature changes according to the Boussinesq approximation.

The non-dimensional governing equations are then expressed as:

mass conservation equation:

$$\frac{\partial U}{\partial X} + \frac{\partial V}{\partial Y} + \frac{\partial W}{\partial Z} = 0 \quad (1)$$

momentum conservation equations

$$\Omega_u \left(U \frac{\partial U}{\partial X} + V \frac{\partial U}{\partial Y} + W \frac{\partial U}{\partial Z} \right) - \Gamma_u \nabla \cdot (H(\dot{\Gamma}) \nabla U) + \frac{\partial P}{\partial X} = 0 \quad (2)$$

$$\Omega_v \left(U \frac{\partial V}{\partial X} + V \frac{\partial V}{\partial Y} + W \frac{\partial V}{\partial Z} \right) - \Gamma_v \nabla \cdot (H(\dot{\Gamma}) \nabla V) + \frac{\partial P}{\partial Y} + S_v = 0 \quad (3)$$

$$\Omega_w \left(U \frac{\partial W}{\partial X} + V \frac{\partial W}{\partial Y} + W \frac{\partial W}{\partial Z} \right) - \Gamma_w \nabla \cdot (H(\dot{\Gamma}) \nabla W) + \frac{\partial P}{\partial Z} = 0 \quad (4)$$

energy conservation equation

$$\Omega_\theta \left(U \frac{\partial \theta}{\partial X} + V \frac{\partial \theta}{\partial Y} + W \frac{\partial \theta}{\partial Z} \right) - \Gamma_\theta \nabla \cdot (\nabla \theta) = 0 \quad (5)$$

The coefficients in the mathematical modeling adopt the parameters shown in Table 1, for each one of the two cases being studied. The dimensionless governing parameters, independent and dependent variables are:

$$X = \frac{x}{L}; Y = \frac{y}{L}; Z = \frac{z}{L} \quad (6)$$

$$P = \frac{pL}{\eta_0 u_0}; U = \frac{u}{u_0}; V = \frac{v}{u_0}; W = \frac{w}{u_0}; \theta = \frac{T - T_C}{T_H - T_C} \quad (7)$$

$$H = \frac{\eta}{\eta_0}; \dot{\Gamma} = \frac{L}{u_0} \dot{\gamma} \quad (8)$$

$$Ra = \frac{\rho g \beta (T_H - T_C) L^3}{\eta_0 \alpha}; Pr = \frac{\eta_0 C p}{\lambda}; Re = \frac{\rho L u_{y=L}}{\eta_0}; Ri = \frac{g \beta (T_H - T_C) L}{u_{y=L}^2} = \frac{Gr}{Re^2} \quad (9)$$

Viscoplastic materials are those that show no deformation up to a certain level of stress. Above this yield stress the material flows readily. Plasticity is common to widely different materials. Many molten metals, concentrated suspensions of solid particles in Newtonian liquids, fruit pulps, paints, some polymeric solutions, among others, exhibit plastic behavior. For instance, several studies have demonstrated that rheological properties of fruit juices are well described by Non-Newtonian models such as Hershel-Bulkley [55], Bingham and Casson [56], which are the fluids studied in the next sections.

Bingham Model

The well-known Bingham model called after E. C. Bingham, who first described the paint flows in this way in 1916, is described first. Broadly speaking, the fluid behaves as a Newtonian fluid under the influence of the shear stress $\tau > \tau_y$; when the yield stress falls below τ_y (unyielded region) a solid structure is formed. The Bingham model in tensorial form can be expressed as:

$$\bar{\tau} = \left(\frac{\tau_y}{\dot{\gamma}} + \eta_0 \right) \dot{\gamma}; |\tau| > \tau_y \quad (10a)$$

$$\dot{\gamma} = 0; |\tau| \leq \tau_y \quad (10b)$$

where $\dot{\bar{\gamma}}$ is the rate strain tensor whose components are defined by $\dot{\gamma}_{ij} = \partial u_i / \partial x_j + \partial u_j / \partial x_i$ and $\bar{\tau}$ the stress tensor. τ_y is the yield stress and η_0 the plastic viscosity of the yielded fluid. The scalar $\dot{\gamma}$ is function of the second invariant of the strain tensor, which is given by:

$$\dot{\gamma} = \left(\frac{1}{2} \dot{\bar{\gamma}} : \dot{\bar{\gamma}} \right)^{\frac{1}{2}} \quad (11)$$

O'Donovan and Tanner [57] proposed the bi-viscosity model as a convenient method of modeling materials with yield stress. This model (12), assumes that at very low shear rates the material behaves as a highly viscous liquid and that above a critical shear rate a transition in behavior occurs, namely yielding.

$$\bar{\tau} = \mu_{yield} \dot{\bar{\gamma}}; \dot{\gamma} \leq \frac{\tau_y}{\mu_{yield}} \quad (12a)$$

$$\bar{\tau} = \tau_y + \eta_0 \left(\dot{\bar{\gamma}} - \frac{\tau_y}{\mu_{yield}} \right); \dot{\gamma} > \frac{\tau_y}{\mu_{yield}} \quad (12b)$$

Beverly and Tanner [58] found that higher accurate results were based on a yield viscosity μ_{yield} equal to $1000\eta_0$. According to this argument, the dimensionless apparent viscosity is given by:

$$H(\dot{\gamma}) = 1 \times 10^3; \dot{\gamma} \leq 1 \times 10^{-3} Bn \quad (13a)$$

and after yielding, the fluid takes an apparent viscosity :

$$H(\dot{\gamma}) = \left(1 - \frac{1}{1 \times 10^3} \right) \frac{Bn}{\dot{\gamma}}; \dot{\gamma} > 1 \times 10^{-3} Bn \quad (13b)$$

where Bingham number Bn is a parameter that represents the ratio of yield stress to viscous stress, defined as follows:

$$Bn = \frac{\tau_y L}{u_0 \eta_0} \quad (14)$$

Herschel-Bulkley model

The Herschel-Bulkley model (1926) is also characterized by a yield stress. The difference with respect to the Bingham model is that the fluid behaves as a power-law fluid under the influence of the shear stress $\tau < \tau_y$. The Herschel-Bulkley model written in tensorial form can be expressed as:

$$\bar{\tau} = \left(\frac{\tau_y}{\dot{\gamma}} + k \dot{\gamma}^{n-1} \right) \bar{\dot{\gamma}}; |\tau| > \tau_y \quad (15a)$$

$$\bar{\dot{\gamma}} = 0; |\tau| \leq \tau_y \quad (15b)$$

where k corresponds to the consistency index and n is the behavior index. Papanastasiou [59] proposed an alternative approach to overcome the issue that represents yield stress, avoiding the discontinuity caused by the yield criterion. The modification involves the incorporation of an exponential term, permitting the use of only one equation for the entire flow curve, before and after yield (16).

$$H(\dot{\gamma}) = \dot{\gamma}^{n-1} + \frac{Bn}{\dot{\gamma}} \left[1 - \exp(-M \dot{\gamma}) \right] \quad (16)$$

with $M = m \sqrt{g \beta \Delta T / L}$, where m is an exponential growth parameter that allows an approximation of the Papanastasiou modified Herschel-Bulkley model to the Herschel-Bulkley model at low shear rates by imposing a large value to m. The bi-viscosity models and Papanastasiou's modification are empirical improvements designed primarily to achieve a convenient viscoplastic constitutive equation for numerical simulations [60].

Casson Model

This model was introduced by Casson (1959) for the prediction of the flow behavior of pigment-oil suspensions. The Casson model in tensorial form can be expressed as:

$$\bar{\tau} = \left(\sqrt{\eta_0} + \sqrt{\frac{\tau_y}{|\dot{\gamma}|}} \right)^2 \dot{\gamma}; |\tau| > \tau_y \quad (17a)$$

$$\dot{\gamma} = 0; |\tau| \leq \tau_y \quad (17b)$$

The dimensionless Casson-Papanastasiou model to approximate the rheological behavior of the fluid is given by:

$$H(\dot{I}) = 1 + 2 \left[\frac{Bn \left(1 - \exp \left(-\sqrt{M \dot{I}} \right) \right)}{|\dot{I}|} \right]^{1/2} + \frac{Bn \left(1 - \exp \left(-\sqrt{M \dot{I}} \right) \right)}{|\dot{I}|} \quad (18)$$

Boundary conditions

No-slip boundary conditions for velocities at the solid walls of the cavity are imposed. Heat transfer boundary conditions include uniform hot and cold temperature on the vertical left and right walls respectively

$$\theta(0, Y, Z) = 1; \theta(L, Y, Z) = 0 \quad (19)$$

and the adiabatic condition on the other walls

$$\left. \frac{\partial \theta}{\partial Y} \right|_{Y=0, Y=L} = \left. \frac{\partial \theta}{\partial Z} \right|_{Z=0, Z=L} = 0 \quad (20)$$

Nusselt number and friction factor calculations

Dimensionless heat transfer on the right and left walls were computed in terms of local and average Nusselt number by evaluating the dimensionless temperature gradients between the walls and the surrounding fluid according to the expressions (22) and (23). The local Nusselt number is expressed in terms of the non-dimensional temperature gradient:

$$Nu_l(Y, Z) = -\frac{\partial \theta}{\partial X} \Big|_{wall} \quad (21)$$

and the global Nusselt numbers at each plane is calculated through the equation:

$$\overline{Nu}_{H,C} = \int Nu_{H,C}(Z) dZ \quad (22)$$

Numerically, due to the large values of the velocity gradients of the non-Newtonian fluids near the walls the local Nusselt numbers were calculated using a second order error expression.

$$Nu_l(Y, Z) = -\left[\left(\frac{\theta_l - \theta_{H,C}}{\Delta X_l} \right) - \frac{\Delta X_l}{\Delta X_l + \Delta X_2} \left[\left(\frac{\theta_2 - \theta_l}{\Delta X_2} \right) - \left(\frac{\theta_l - \theta_{H,C}}{\Delta X_l} \right) \right] + O(\Delta X^2) \right] \quad (23)$$

The local friction factor in terms of dimensionless variables was calculated through the equation (24), in which $(\dot{\Gamma}_w)$ corresponds to the local dimensionless shear stress.

$$C_f = \frac{2}{Re} \dot{\Gamma}_w \quad (24)$$

Due to the rheological behavior of the fluids of interest, the velocity gradients of the local shear rate were calculated by a second order error expression. For the sake of completeness, the expression for the local dimensionless shear rate used in the moving wall (Y=1) was:

$$\dot{I}_w|_{Y=l} = \sqrt{\left(\left.\frac{\partial U}{\partial Y}\right|_{Y=l}\right)^2 + \left(\left.\frac{\partial W}{\partial Y}\right|_{Y=l}\right)^2} \quad (25)$$

with:

$$\left.\frac{\partial U}{\partial Y}\right|_{Y=l} = \left[\left(\frac{U_l - U_{Y=l}}{\Delta Y_l} \right) - \frac{\Delta Y_l}{\Delta Y_l + \Delta Y_2} \left[\left(\frac{U_2 - U_l}{\Delta Y_2} \right) - \left(\frac{U_l - U_{Y=l}}{\Delta Y_l} \right) \right] + O(\Delta Y^2) \right] \quad (26a)$$

$$\left.\frac{\partial W}{\partial Y}\right|_{Y=l} = \left[\left(\frac{W_l - W_{Y=l}}{\Delta Y_l} \right) - \frac{\Delta Y_l}{\Delta Y_l + \Delta Y_2} \left[\left(\frac{W_2 - W_l}{\Delta Y_2} \right) - \left(\frac{W_l - W_{Y=l}}{\Delta Y_l} \right) \right] + O(\Delta Y^2) \right] \quad (26b)$$

where U_l, W_l are the dimensionless velocities values for the two closest nodes to the top wall.

COMPUTATIONAL IMPLEMENTATION

The governing coupled non-dimensional non-linear second order partial differential equations (1)-(5) with the no-slip boundary conditions and thermal boundary conditions (19) and (20) were solved with the finite volume method, FVM, by using the SIMPLE algorithm [61]. A fifth power interpolation law was used to calculate the convective terms at the finite volume surfaces while the diffusion terms were determined by using linear interpolation functions for the dependent variables between the nodes with the staggered grids. Calculations in the first iterations were accomplished by assuming a Newtonian behavior in order to obtain a velocity field which permitted the apparent viscosity calculation [62]. Then, a pressure correction was introduced [61]. The resulting systems of algebraic equations were solved through the block Gauss-Seidel (backward/forward) iteration with regard to planes in Z-direction and an ADI (alternating directions iterative method) in each plane (TDMA algorithm). Under-relaxation was used during the iterative process in the calculation of the improved values for the dependent primitive

variables. The calculations were accomplished by using a workstation of 16 cores (4 Opteron 8347, 1.9GHz; 32 GB memory), in which the effect on overall performance of the number of processors being used was analyzed. The GNU Fortran compiler Gfortran and the Intel Fortran compiler IFORT under Linux platform were used for the compilation of the Fortran90 source codes.

OPENMP PARALLELIZATION

The four steps procedure performed by Hoeflinger et al. [51] to parallelize their combustion code was followed. In the first step, the serial version of the code NFFS-FVM was profiled and optimized in order to identify the more time consuming subroutines. This work was done by implementing the tools Coverage (-fprofile-arcs; -ftest-coverage) and Profiling (-pg), availables as options in conjunction with the Gfortran compiler. The more time consuming subroutines of NFFS-FVM code to be parallelized are described in Table 2, along with the percentages of the total running time of the program. According to these results, in the second step the Solve subroutine became the first target since it was the most time consuming subroutine and it is intensively called by MECFLU, CALCPH and SIMPLE subroutines. The TDMA algorithm consists of two steps: first, a set of algebraic operations are performed in three nested Do-loops, one for each Cartesian axis, this is the forward step and finally the solution is obtained by backward substitution. In the third step, two different approaches were evaluated in order to parallelize the Solve subroutine. The first approach required splitting the main loop into the forward and backward loops. The parallel region blocks are defined using the *!OMP Parallel directive*. In this strategy, referred here as the naive approach, the parallel code section is executed by all threads. Some data environment directives (*Shared, Private...*) were used to control the sharing of program variables that were defined outside the scope of the parallel region. The variables were defined as *Shared by the default* but when a *Private* variable was defined, a separate copy per thread of the variable was done. OpenMP is sometimes called ‘fork-join’ parallelism because multiple parallel threads (forks) are launched in parallel regions of the code and then are joined into a single thread (the master one) for serial processing in non-parallel region. Nevertheless this procedure caused an undesirable *data shuffling* which appears because the data

blocks are remapped onto threads.

The implemented strategy to remove the *data shuffling* issue implied a *handmade* splitting of the outer Do-loop. In order to do that, first the total number of threads should be obtained through the environment variable `OMP_GET_NUM_THREADS`, then each thread must be identified through the environment variable `OMP_GET_THREAD_NUM` which returns the thread number of the thread executing within its thread team. Load balancing refers to how evenly balanced the work load is among different processors. There are two ways to distribute the work for a good load balance. One alternative is the static decomposition carried out before the computation phase of the work. The second procedure is to distribute the work in a dynamic on demand fashion, as a processor becomes idle [50]. The former was chosen for this approach; therefore the junk size, which accounts the load balancing, is a constant value.

The implementation of the *handmade approach* allows that the threads can access to the same block of memory during the calculations, avoiding the *data shuffling* by the inversion of the index order for the backward substitution step. Therefore the TDMA algorithm calculations were done by using only one parallelization block. It is worth to notice that each array and constant used into the parallelized block must be explicitly defined as shared, private or first-private according to its function and range. In this approach, as a general rule the three-dimensional arrays were defined as shared variables meanwhile the constant values, such as the tuples i, j, k , were private variables. The synchronization directives include *barrier* or *critical*. A *critical* directive was used to restrict access to the enclosed code to only one thread at time; meanwhile a *barrier* directive caused a thread to wait until all other threads in the parallel region have reached the barrier. An implicit barrier exists at the end of the parallel region block. This is a very important point when threads are modifying shared variables.

The two-dimensional arrays or the three-dimensional arrays defined in one plane must be handled by only one thread in order to avoid other source of *data shuffling*. In the case of the handling of boundary data, the race condition should be avoided through the use of `!$OMP BARRIER`. The remaining more time consuming subroutines: MECFLU, CALCPH and SIMPLE were parallelized implementing the

previously explained *handmade approach*. The subroutines that calculate the power-law differencing scheme (DIFLOW), the non-Newtonian viscosity (NON_NEW), the coefficients and source terms of the Navier-Stokes equations (GAMSOR) and those that upgrade the boundary values for the velocities (BOUND) were readily integrated to the dynamic extent of the MECFLU subroutine parallel block. The same holds true for the CALCPH subroutine parallel block, including the subroutine returning the properties (PROPS) which must be used in applications with phase-change fluids. The parallelization of NFFS-FVM code and the interaction between the main subroutines is summarized in Figure 2.

ANALYSIS AND DISCUSSION OF RESULTS

Validation and verification of the NFFS-FVM code

To test the correctness and accuracy of the results obtained by the parallelized NFFS-FVM code, benchmark problems about natural convection ($Ra=10^3$ - 10^6 ; $Pr=0.71$) [9] and the forced convection lid driven cavity problem, ($Re=100$; 400; 1000) [36] in three dimensional cavities were replicated. The validation of the code was accomplished through comparison with experimental data for natural convection of air (Figure 3) with $Pr=0.71$ and $Ra=10^5$. In general, a highly accurate agreement between the results was achieved. Along with the validation and verification of the code, a grid size study with an adaptive grid refinement scheme was done for each case of interest, revealing as expected, that finer grids are needed when physics associated to the numerical experiment becomes more complex (Tables 3 and 4). In Table 3 a comparison of the obtained results for maximum values of two velocity components, the Nusselt number and the average Nusselt number with those reported by Fusegi et al. [9], for four values of the Raleigh number in the range 10^3 - 10^6 is shown. In general, percentage errors not greater than 3.5% were obtained. The verification of the NFFS-FVM code was done through a comparison of the U and V velocity profiles along the Y and X axes, respectively, with the benchmark results reported by Ku et al. [36]. As in the foregoing validation, the verification of the NFFS-FVM code was done along the grid size study for the three laminar Reynolds numbers (100, 400 and 1000). As it can be seen in Figure 4, there is an excellent agreement between the predicted velocity profiles for the studied Re numbers. According to

the mesh study a grid with 63^3 nodes was chosen for the lid driven cavity study for $Re=100$ and a grid of 101^3 for $Re=1000$.

Grid size study

A grid size study with an adaptive grid refinement scheme (Figure 5) was done prior to the parallel performance and to the results analysis based on the selected grids for the Newtonian cases obtained in the previous section. In each coordinate direction, the grid is divided in three zones: two zones close to the walls with length l which have a higher density of control volumes (one third of the total number control volumes, $NCV/3l$) and one zone in the middle with a minor density of control volumes ($NCV/(3(L-2l))$).

Natural convection

The natural convection study for the viscoplastic non-Newtonian fluids was performed for $Ra=10^4$ ($Pr=0.01$; $Bn=0.01$) and $Ra=10^6$ ($Pr=1.0$; $Bn=0.1$), therefore the Grashof number was kept constant between studies. Tables 4 and 5 depict the obtained results for three reference values: positive maximum U and V velocity components along the Y and X axes, respectively, and the Nusselt number, for different grid sizes. According to the Nusselt number in Table 4, the results obtained with the Herschel-Bulkley model ($n=0.95$) are more sensitive to grid size than those obtained for the Bingham and Casson models. Meanwhile the percentage error between the two finer grids for the Bingham and Casson models is less than 1%, for the Herschel-Bulkley model the deviation is higher. Such a difference can be qualitatively remarked after comparing the velocity profile U along the vertical axis (Y) for $X=Z=0.5$ in the Figures 6a and 6b. This explains the additional grid size study that was performed for the Herschel-Bulkley model. In the grid size study for the higher Rayleigh and Bingham numbers it can be noticed a weaker dependency of the results for the velocities. The percentage errors for the maximum velocity components U and V along the Y and X axes, respectively, are less than 0.15% between the two finer grids. The U velocity profiles along the vertical axis (Y) for $X=Z=0.5$ in the Figures 6c and 6d support such a statement. Nevertheless the Nusselt number dependency with respect to the grid size is more important as

it can be seen in Table 5, being greater for the Bingham (0.2%) and the Herschel-Bulkley (0.15%) fluids in comparison with the Casson fluid (0.06%).

Lid driven cavity

The adaptive grid size study for the non-Newtonian lid driven cavity with forced convective heat transfer was performed for a Bingham fluid, with $Bn=0.1$, for $Re=100$ and $Re=1000$. The variation of the Nusselt number ($X=0$) and the friction factors in selected surfaces ($X=0$; $Y=0$; $Y=L$) and the velocity profiles U and V along the Y ($X=Z=L/2$) and X ($Y=Z=L/2$) axis, respectively, were used as the base for the grid size study. The obtained Nusselt number and the friction factor for the selected grids are shown in Table 6.

The nodes are uniformly distributed between three regions of size defined by the closest regions to the walls, i.e. for the grid in Figure 5 with 81^3 nodes; the closest regions to the wall have a length of $l=0.25L$ ($d=25\%$). The Nusselt number was found to be a weaker function of the grid size; with a maximum observed percentage error between two consecutive grids of 1%. On the contrary, the friction factor is a stronger function of the grid size because velocity gradients are higher than temperature gradients adjacent to the walls, especially the friction factor calculated at $Y=1$ and $X=0$, which it was found to be exactly the same that the one obtained in the right surface ($X=1$). According to the obtained results in Table 6, a grid with 93^3 nodes and a refined region next to the wall with a length of $0.02L$ ($d=2\%$) must be used to obtain reliable results for the coefficient friction for a Bingham fluid. The velocity profiles U and V along the non-dimensional X and Y axes of a Bingham fluid with $Re=100$, $Pr=1$ and $Bn=0.1$, for different grid sizes, are shown in Figure 7. It can be seen that the velocity profile V along the X axis being influenced by buoyancy forces, is more sensitive to the grid size that the velocity profile U along the X axis. The velocity profile obtained with the grid of 103^3 nodes with a refined region next to the wall with a length $0.02L$ showed a change in trend observed with respect to the other velocity profiles. This change in trend of the V -profile is confirmed near to the wall at $X=0$ after comparing different sizes of the refined region next to the walls for the same grid size. These differences as well as the obtained results for friction factors confirm that different grids are required in order to obtain reliable results for the velocities

and therefore for velocity gradients. In the case of predicting velocities a grid with 93^3 ($d=5\%$) can be recommended as a reliable discretization of the domain in order to obtain accurate results for a Bingham fluid with $Re=100$, $Pr=1$ and $Bn=0.1$. The grid size study for the Bingham fluid with $Re=1000$ is shown in Figure 8 for the velocity profiles U and V along the X and Y axes, respectively. According to this study, a grid of 117^3 nodes is good enough in order to describe the fluid mechanics for this particular non-Newtonian fluid.

The obtained results for Nusselt number and friction factor are shown in Table 7. It can be observed that the effect of the grid size and the length of the zone near to the walls (d) is more important to calculate the Nusselt number when $Re=1000$ than in the previous case ($Re=100$), this is explained because of the convective force becomes more intense. A grid with 117^3 is good enough to precisely determine the Nusselt number. The percentage deviation between the two finer grids with $d=10\%$ is only 0.3% . Again, friction factor is a more important function of grid size. Meanwhile the observed percentage deviation between the calculated Nusselt numbers for the finer (133^3) and the coarser (73^3) grids is around 2% , for the friction factor this deviation is 23% and 9% for the friction factor calculated at planes $X=0$ and $Y=0$, $Y=1$, respectively. The effect of the length of the closest region to the wall (d) on the Nusselt number and friction factors is studied for the grid with 117^3 nodes. The grid parameter d has not a noticeable effect in the shape of the velocity profiles as it can be seen in Figure 8, and the differences between the obtained results for Nusselt number shown in Table 7 do not exceed 0.2% . The decrease of d raises the percentage error of the friction factors calculated at the three walls, therefore to concentrate control volumes over $NCV/2.4L$ is not required in this case. According to these observations, a grid with 1173 ($d=10\%$) is good enough in order to describe the fluid mechanics and to obtain reliable results for the Nusselt number and a grid with 1333 ($d=10\%$) for the calculation of friction factors for $Re=1000$.

Parallel Performance Analysis

Broadly speaking, the parallelization strategy of the *handmade* approach, described in Figure 9, involves splitting the three-dimensional computational domain into blocks along the Z-direction and assigning each block to a thread or processor using OpenMP directive. Each block consists of several planes along the Z directions [45]. Since threads do not share information during runtime; the interface values used by each thread correspond to non-actualized values. This condition of the *handmade* approach is not a source for a lack of correctness of the results; nevertheless more threads working imply a higher number of iterations to achieve the imposed convergence criteria.

The parallel performance analysis of the NFFS-FVM code is done for both 3D natural convection and 3D lid driven cavity processes with a Newtonian fluid as a function of the Rayleigh and the Reynolds number respectively, with suitable grid sizes. The parallel performance of a parallelized code is generally analyzed in terms of two important concepts the speed-up (S) and the parallel efficiency (PE). Speed-up is defined as the ratio of the CPU time taken to solve these problems on a single-processor to the CPU time taken to solve a multi-processor version of the code. The efficiency of the parallel code is defined as the ratio of the speed-up to the number of processors used, therefore it represents the fraction of total time that processor is involved in doing useful computation [45, 46]. In Figure 10 the speed-ups for the NFFS-FVM code and the SOLVE and MECFLU subroutines for both 3D processes are shown. Meanwhile for the 3D Newtonian natural convection process good scalability results were obtained for ≤ 12 processors (PE=80%), for the 3D lid driven cavity problem the parallel efficiency decreased to 70-75%. In general, the obtained speed-ups are lower than the number of processors because of load balancing, task scheduling between processes, synchronization steps and communications will dominate and become the limiting factor of computational efficiency. In some cases, it can be seen that for $Ra=10^3$ (grid size 33^3) speed-up is super-linear, which means parallel efficiency (PE) is higher than 100%. This result is a consequence caused because each processor needs less memory to store the local problem, and cache memory can be used in a more efficient way [46]. The lower efficiency of the NFFS-FVM code with the

lid driven cavity process can be explained because the more efficiently parallelized CALCPH subroutine, for the calculation of the temperature coefficient matrix, is not implemented. Since our main goal is the simulation of non-Newtonian fluid mechanics processes, the performance analysis of the NFFS-FVM code for the 3D non-Newtonian natural convection process was done and it is shown in Figure 11. As for the Newtonian case, good scalability of results were obtained for ≤ 12 processors (PE=80-85%) for the rheological models of interest. Coverage is the percentage of the program that can be made parallel, according to the performance analysis and the PE's obtained. The coverage of our code was found to be high and according to speed-ups we can assure that the elapsed times with the original code were diminished by one order of magnitude, which is good enough for the kind of applications we are interested in.

Phenomenological description

Natural convection

The description of the fluid mechanics for the natural convection of the Bingham fluid is shown in Figure 12 for both studied Rayleigh numbers ($Ra=10^4$; 10^6). It is shown only for the Bingham fluid because of the observed similarities between the results for the three non-Newtonian models investigated. The results for the lower Rayleigh number exhibit the existence of the expected main vortex centered in an axis along the middle of the cavity. The secondary flows are identified as those fluid patterns away from the main centered vortex. These secondary flows are observed in the upper and lower edges of the cavity near to $X=0$ and $X=L$ (Figure 12a). The three-dimensional representation of the natural convection process allows observing how the secondary flows then pass through the center of the main centered vortex. To a higher Rayleigh number the fluid streamtraces adopt different patterns showing a main fluid recirculation region that takes the shape of the cavity, without the presence of secondary flows along the edges. For $Ra=10^6$ the fluid mechanics becomes more complex and three recirculation centers of fluid along the middle of the cavity parallel to the X-axis are founded.

A detailed description of the fluid mechanics in planes along the Z-axis is shown in Figure 13. It can be identified the main centered vortex and five secondary recirculation centers of fluid at the corners for $Ra=10^4$, two of them in the right lower corner of the cavity and the one that is compressed against the corner becomes more intense as the Z position approaches to L. For $Ra=10^6$, there are three recirculation centers of fluid along the middle of the cavity, one in the center and two pointing to the opposite direction. These recirculation centers of fluid become less intense as the Z position approaches to L. The distribution of the temperature in the three-dimensional domain can be seen in Figure 14 for the Bingham fluid. As it was mentioned before, the Grashof number ($Gr=10^6$) is kept constant between the numerical experiments, nevertheless the temperature distribution in both cases is completely different. For $Ra=10^4$ and $Bn=0.01$, the effect of thermal diffusion is important mainly in the upper side of the cavity, by the contrary for $Ra=10^6$ and $Bn=0.1$ the process is mainly governed by the fluid convection since the isotherms in most of the cavity are horizontal and almost perpendicular to the isothermal surfaces. The differences between the temperature profiles for the different rheological models can be appreciated in Figure 15. At low Rayleigh number, $Ra=10^4$, (Figure 15a) there are no appreciable differences between the temperature profiles, however when the Rayleigh number becomes higher, $Ra=10^6$, (Figure 15b) some differences can be noticed near to the walls. The temperature profile for the Casson model present a deviation near to the hot wall at $X=0$ in the lower part of the cavity meanwhile the temperature profile for the Herschel-Bulkley model present a deviation close to the cold wall near to the top part of the cavity.

Lid driven cavity with forced convective heat transfer

In this study, the importance of the natural convection relative to the forced convection is kept as a constant in both cases ($Ri=0.1$). The streamtraces for the three-dimensional lid driven cavity process are shown in Figure 16 for $Re=100$ and $Re=1000$. In both cases a broad recirculation of fluid inside the cavity is observed, however for $Re=1000$ the recirculation is more intense and the recirculation axis is located at a lower position. Because of this effect, secondary flows appear next to the lower edges of the cavity, as it is shown in Figure 16b. Also, it can be observed that the streamtraces of these secondary

flows pass through the recirculation center in a curling shape. A more detailed description of the fluid mechanics is shown in Figure 17 as a set of slices along the Z-axis. It can be noticed how the recirculation axis is located lower in the Y-axis for $Re=1000$ and how its position changes according to the Z-position. For $Re=100$ the position of the recirculation axis is practically independent of the Z-position showing a weak dependency of the third dimension in the results. As it was expected, the fluid mechanics behavior for the non-Newtonian fluids investigated becomes more complex when the Re is higher; the secondary recirculation regions of fluid are remarkable in the lower corners of the cavity which corresponds to the secondary flows identified with the streamtraces in Figure 16.

The temperature distribution for $Re=100$ and $Re=1000$ in the three-dimensional domain is shown in Figure 18. The effect of the buoyancy forces measured by the Grashof number, which is higher for $Re=1000$ ($Gr=10^5$), is observed after comparing the shape of the isotherms, which are more deformed when the Grashof number is higher. This effect can be seen in more detail in Figure 19 as well as the effect of the three-dimensionality. For $Re=100$, the shape of the isotherms is practically independent of the Z-position, by the contrary, the shape of the isotherms for $Re=1000$ change dramatically especially when the Z-position approaches to L .

CONCLUSIONS

A three-dimensional study allows identifying secondary flows that are very important to understand the physics behind a particular process with viscoplastic fluids, especially when the convective forces are increased ($Ra=10^6$, $Re=1000$). There were no noticeable differences between the characteristics of fluid mechanics and heat transfer of the studied viscoplastic rheological models keeping a constant Bingham number. But differences in the calculated Nusselt numbers, friction factors and isotherms distributions for the Herschel-Bulkley fluid respect to the Bingham and Casson's at high values of the Rayleigh number ($Ra=10^6$) in the natural convection process were found.

From the computational point of view, it was found that a single mesh is not always good enough to fully describe the fluid mechanics and heat transfer by convection and to calculate with a required accuracy fundamental engineering parameters of interest such as friction factor for non-Newtonian fluids. The use of a very refined grid with a high concentration of nodes close to the walls and numerical approximations to calculate the gradients with errors of the order of $(\Delta X)^2$ is required for Bingham, Casson and Herschel-Bulkley fluids.

A parallelization approach based on shared memory (OpenMP) was successfully implemented on a FVM based code for the prediction of fluid mechanics and heat transfer with both Newtonian and Non-Newtonian fluids. The implemented parallelization strategy required a careful management of the tasks to be distributed between the threads as well as of the variables in both the dynamic and static extent. None variable was defined as shared by default. Good scalability was found for ≤ 12 cores which is acceptable in this type of applications.

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Table 1. Values of boundary condition and coefficients for the mathematical modeling.

Numerical Experiment	T_{ref}	$u_{y=L}$	u_0	$\mathcal{Q}_{\vec{U}, \vec{V}, \vec{W}}$	$\Gamma_{\vec{U}, \vec{V}, \vec{W}}$	$S_{\vec{V}}$	S_θ	Γ_θ
Natural Convection	T_H	0	$\sqrt{g\beta L \Delta T}$	$\sqrt{\frac{Ra}{Pr}}$	1	$\sqrt{\frac{Ra}{Pr}}\theta$	$\sqrt{Ra \cdot Pr}$	1
Lid Driven Cavity	T_C	1	$u_{y=L}$	1	$\frac{1}{Re}$	$Ri \cdot \theta$	1	$\frac{1}{Re \cdot Pr}$

Table 2. More time consuming subroutines of the NFFS-FVM code.

Subroutine	Description	% Time
SOLVE	Solution of the system of equations by TDMA	50.44
MECFLU	Subroutine for the three velocity components coefficient matrix calculations. The subroutine SOLVE is called three times.	28.12
CALCPH	Subroutine for the temperature coefficient matrix calculations. The subroutine SOLVE is called once.	6.53
SIMPLE	Subroutine for the pressure coefficient matrix calculations. The subroutine SOLVE is called once.	5.72
DIFLOW	Subroutine for the calculation of the power-law differencing scheme	4.52

Table 3. Maximum velocities and Nusselt values calculated for the natural convection and the results obtained for Fusegi et al. [9].

Rayleigh Number	Grid	U_{max}	V_{max}	Nu_{max}	Nu
10^3	33^3	0.1326 (0.1314)	0.1324 (0.132)	1.4252 (1.42)	1.0892 (1.105)
10^4	45^3	0.1974 (0.2013)	0.2216 (0.2252)	3.6335 (3.652)	2.2526 (2.302)
10^5	57^3	0.143 (0.1468)	0.2454 (0.2471)	7.9751 (7.795)	4.6163 (4.646)
10^6	69^3	0.0815 (0.08416)	0.2581 (0.2588)	17.7831 (17.67)	8.8766 (9.012)

Table 4. Adaptive grid size study for the natural convection of viscoplastic fluids ($Ra=10^4$, $Pr=0.01$, $Bn=0.01$).

<i>Rheological Model</i>	<i>Bingham</i>			<i>Casson</i>			<i>Herschel-Bulkley</i>		
<i>Reference value</i>	U_{max}	V_{max}	Nu	U_{max}	V_{max}	Nu	U_{max}	V_{max}	Nu
45^3	0.7804	0.8173	1.4688	0.7698	0.8066	1.4597	0.7978	0.833	1.4859
57^3	0.8129	0.8463	1.4943	0.8020	0.8355	1.4847	0.8319	0.8645	1.5141
69^3	0.8380	0.8691	1.5136	0.8266	0.8576	1.5035	0.8587	0.8914	1.5357
81^3	0.8581	0.8890	1.5288	0.8460	0.8759	1.5181	0.8807	0.9123	1.5533
93^3	-	-	-	-	-	-	0.8990	0.9293	1.5677

Table 5. Adaptive grid size study for the natural convection of viscoplastic fluids ($Ra=10^6$, $Pr=1$, $Bn=0.1$).

<i>Rheological Model</i>	<i>Bingham</i>			<i>Casson</i>			<i>Herschel-Bulkley</i>		
<i>Reference value</i>	U_{max}	V_{max}	Nu	U_{max}	V_{max}	Nu	U_{max}	V_{max}	Nu
69^3	0.0687	0.2182	8.9268	0.0687	0.2120	8.8032	0.0689	0.2256	9.0945
81^3	0.0686	0.2192	8.9277	0.0686	0.2126	8.8099	0.0688	0.2258	9.1124
93^3	0.0686	0.2190	8.9464	0.0685	0.2125	8.8153	0.0688	0.2262	9.1254
101^3	-	-	-	-	-	-	0.0688	0.2258	9.134

Table 6. Adaptive grid size study for lid driven cavity with heat transfer of a Bingham fluid ($Re=100$, $Pr=1$, $Ri=0.1$ and $Bn=0.1$).

Grid	$\overline{Nu} _{X=0}$			$C_f _{X=0}$			$C_f _{Y=0}$			$C_f _{Y=1}$		
	15%	5%	2%	15%	5%	2%	15%	5%	2%	15%	5%	2%
63^3	2.438	2.440	2.424	0.0469	0.0711	0.0761	1.871×10^{-3}	1.957×10^{-3}	1.939×10^{-3}	0.309	0.414	0.4587
82^3	2.448	2.449	2.450	0.0556	0.0681	0.078	1.824×10^{-3}	1.856×10^{-3}	1.930×10^{-3}	0.339	0.391	0.4342
93^3	-	2.445	2.451	-	0.0737	0.0836	-	1.912×10^{-3}	1.926×10^{-3}		0.4132	0.4566
103^3	-	-	2.447	-	-	0.0836	-	-	-		-	0.4449

Table 7. Adaptive grid size study for the lid driven cavity with heat transfer of a Bingham fluid (Re=1000, Pr=1, Ri=0.1 and Bn=0.1).

<i>Grid</i>	$\overline{Nu} _{X=0}$	$C_f _{X=0}$	$C_f _{Y=0}$	$C_f _{Y=1}$
73^3	-6.702	4.384×10^{-3}	1.490×10^{-3}	4.753×10^{-2}
103^3	-6.777	5.108×10^{-3}	1.572×10^{-3}	5.000×10^{-2}
117^3 (d=2%)	-6.788	7.228×10^{-3}	1.560×10^{-3}	5.887×10^{-2}
117^3 (d=5%)	-6.797	6.237×10^{-3}	1.593×10^{-3}	5.459×10^{-2}
117^3 (d=10%)	-6.795	5.470×10^{-3}	1.600×10^{-3}	5.140×10^{-2}
133^3	-6.815	5.644×10^{-3}	1.627×10^{-3}	5.200×10^{-2}

Figure 1. Physical three-dimensional domain of the numerical experiments.

Figure 2. Parallelized blocks of the code for the numerical solution of a Non-Newtonian fluid flow.

Figure 3. Grid Size study and validation of the NFFS-FVM code for the natural convection process of air ($Pr=0.71$; $Ra=10^5$).

Figure 4. Grid Size study and verification of the NFFS-FVM code for the lid driven cavity process (a. Re=100; b. Re=400 and c. Re=1000).

Figure 5. Two-dimensional view of an adaptive grid of 81^3 nodes with $d=25\%$.

Figure 6. Grid Size study for the natural convection process of viscoplastic fluids for $Ra=10^4$, $Pr=0.01$ and $Bn=0.01$ (a. Bingham; b. Herschel-Bulkley) and for $Ra=10^6$, $Pr=1$ and $Bn=0.1$ (c. Bingham; d. Herschel-Bulkley).

Figure 7. Grid Size study for the lid driven cavity with heat transfer process of a Bingham fluid ($Re=100$, $Pr=1$, $Ri=0.1$ and $Bn=0.1$). In the left column, the relative length of the zone near to the walls (d) is 25% for all the grids but for 103^3 ($d=2\%$). The right column corresponds to a grid size of 93^3 nodes.

Figure 8. Grid Size study (relative length of the zone near to the walls is 10%) for the lid driven cavity with heat transfer process of a Bingham fluid ($Re=1000$, $Pr=1$, $Ri=0.1$ and $Bn=0.1$).

Figure 9. Graphical representation of the implemented handmade approach for the OpenMP parallelization of the NFFS-FVM code.

Figure 10. Obtained speed-ups for the code NFFV-FVM (a) and the subroutines SOLVE (b) and MECFLU (c) for the simulation of the 3D natural convection process (left column) and the 3D lid driven cavity (right column).

Figure 11. Obtained speed-ups for the code NFFV-FVM (a) and the CALCPH subroutine (b) for the simulation of the 3D natural convection process with a non-Newtonian fluid ($Ra=10^4$, $Pr=0.01$, $Bn=0.01$).

Figure 12. Streamtraces of the 3D natural convection process with a Bingham fluid (a. $Ra=10^4$, $Pr=0.01$, $Bn=0.01$ and b. $Ra=10^6$, $Pr=1$, $Bn=0.1$).

Figure 13. Slices of the streamtraces of the 3D natural convection process with a Bingham fluid along the Z-axis ($Ra=10^4$, $Pr=0.01$, $Bn=0.01$ and $Ra=10^6$, $Pr=1$, $Bn=0.1$).

Figure 14. Temperature distribution in the 3D natural convection process with a Bingham fluid (a. $Ra=10^4$, $Pr=0.01$, $Bn=0.01$ and b. $Ra=10^6$, $Pr=1$, $Bn=0.1$).

Figure 15. Temperature distribution in the middle plane $Z=0.5$ at different Y positions for the Bingham (solid lines), Casson (dotted lines) and Herschel-Bulkley (dashed lines) rheological models (a. $Ra=10^4$, $Pr=0.01$, $Bn=0.01$ and b. $Ra=10^6$, $Pr=1$, $Bn=0.1$).

Figure 16. Streamtraces of the 3D lid driven cavity process with a Bingham fluid $Bn=0.1$, $Ri=0.1$, and $Pr=1$ (a. $Re=100$ and b. $Re=1000$).

Figure 17. Slices of the streamtraces of the 3D lid driven cavity process with a Bingham fluid along the Z-axis ($Ri=0.1$, $Pr=1$, $Bn=0.1$).

Figure 18. Temperature distribution in the 3D lid driven cavity process with a Bingham fluid $Bn=0.1$, $Ri=0.1$ and $Pr=1$ (a. $Re=100$ and b. $Re=1000$).

Figure 19. Slices of the temperature distribution of the 3D lid driven cavity process with a Bingham fluid along the Z-axis ($Ri=0.1$, $Pr=1$, $Bn=0.1$).