PARTICLE-PARTICLE INTERACTIONS IN PARALLEL COMPUTATIONS

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Abstract. *Parallel implementation of vortex elements and temperature particles interactions is presented. The focus is to evaluate the performance of the Biot Savart Law when the interaction between vorticity and heat is computed. It is clear that if one wants to have a good resolution of the physical phenomena, when using numerical simulations, one has to use a suitable number of particles in computations. That requires greater memory and computational time. The purpose is to show the great potential of a Lagrangian-Lagrangian temperature particles method for the solution of mixed-convective heat transfer problems using parallel computation.*

Keywords: *Parallel implementation, FORTRAN using OpenMP, Vortex elements and temperature particles, Lagrangian description.*

1. INTRODUCTION

The interaction between vorticity and heat may occur in many situations of practical interest. The Lagrangian temperature particles method is an alternative to traditional mesh-based methods for solving differential equations that govern this kind of problem. Applications arise in many fields including astrophysics (gravitational interaction), chemistry, materials science, plasma dynamics (electrostatic interaction) and fluid dynamics (vortex interactions).

The development of Lagrangian vortex methods for low speed flow has been a fertile field of investigation for several decades. The essentials of Lagrangian vortex methods are: (i) numerical technique to solve the Navier-Stokes equations; (ii) suitable for Direct Simulation and Large-Eddy Simulation; (iii) uses vorticity (curl of the velocity) as a variable; (iv) computational elements move with the fluid velocity. Therefore, the purely Lagrangian methods offer a number of advantages over the more traditional Eulerian schemes (Chorin, 1973; Leonard, 1980; Lewis, 1999; Kamemoto, 2004; Alcântara Pereira et al., 2004): (i) computational elements only where vorticity is non-zero; (ii) no grid in the field; (iii) only 2D grid on vehicle surface; (iv) boundary conditions in the far field automatically satisfied.

Much of the early work on Lagrangian vortex methods was motivated by an interest in understanding the interactions between vorticity and heat for problems dominated by mixed-convective heat transfer. Ghoniem and Sherman (1985) presented a complete analysis of temperature particles with different properties and the vorticity generation due to the heat transfer process. The one-dimensional heat diffusion using random walk scheme (Chorin, 1973, 1978) was extensively investigated by the authors. Kamemoto and Miyasaka (1999) employed the core spreading model (Leonard, 1980) to simulate the forced convection heat transfer around a circular cylinder at high Reynolds numbers. They introduced the concept of discrete temperature elements with thermal core aiming to simulate a thin thermal layer along the body surface. Although they made an approximation that the temperature in the thermal layer was constant along the normal direction, the time-averaged Nusselt number distribution showed reasonable agreement with that of experiment for circular cylinder (Igarashi, 1984).

Two models for creating vortices from temperature particles to simulate natural convection were developed by Ogami (2001). A simplified energy equation was added to the incompressible Navier-Stokes equations by using Boussinesq approximation to account for the buoyancy force. The model 1 changed the strength of each vortex element during each time step of the simulation through a direct interpretation of the vorticity transport equation and consequently was a natural extension of the method of Ghoniem and Sherman (1985) to two-dimensional problems. This model is suitable for the regions where both vortex and temperature elements are overlapped. The model 2 considered that a vortex pair (one positive and one negative) could be generated from one temperature particle. This kind of idea was based on the fact that the slope of a temperature element is precisely approximated by the density distribution of two Gaussian particles with opposite strength. In addition to those two models, the diffusion velocity method (Ogami and Akamatsu, 1991) was used in order to handle heat and vorticity diffusion. In the one-dimensional field, the models were compared with analytic solution, and the accuracy and validity were clarified. In two-dimensions was presented the application sample with the natural convection and the interaction between vorticity and heat.

Alcântara Pereira and Hirata (2003) developed a Lagrangian-Lagrangian temperature particles method to simulate the mechanism of heat transfer in the separated flow region behind a circular cylinder. These authors considered the similarity between the energy equation and the vorticity transport equation for a two-dimensional and incompressible flow (Kamemoto and Miyasaka, 1999; Nakamura et al., 2001). Vortex and temperature elements were introduced into the flow field close to a wall surface to ensure boundary conditions of problem, however, no attempt to include interaction between vorticity and heat was made.

The purpose of this paper is to show the potentialities of the Lagrangian temperature particles method developed by Alcântara Pereira and Hirata (2003) including the buoyancy force effect in parallel computations. The buoyancy force is analyzed by the using the model 1 presented by Ogami (2001). As example of tests, the new methodology developed here is applied to that problem of airplane wake dissipation (Hirata et al., 2002) in order to perform long-time simulations using vortex elements and temperature particles.

It is clear that numerical simulations with large numbers of particles require great computational power, thus involve large amounts of CPU time. Therefore, it is imperative to make use of a parallel implementation so that results can be obtained in a feasible time. In this paper was decided to use OpenMP parallel programming in the most CPU intensive parts of the computational code. OpenMP is a standard for shared-memory systems, which are the majority of modern computers. All the created threads have a private memory section, along with another portion that is shared among others threads. Since all the data is stored in a single machine, the data exchange between cores is faster than in distributed memory systems. Moreover, OpenMP's ease of use and short system setup time allows for a simple implementation. The use of a shared portion of memory requires different approaches to avoid race conditions. These create errors in the calculations and jeopardize any performance gains. The prevention of race conditions demand programmer's thinking on the variables dependencies. Whenever a variable value obtained by a thread is required by another thread; synchronization needs to be specified in order to guarantee the calculations happen in the correct order. Synchronizations represent idle cores waiting others to run down the code, shrinking efficiency. The calculations done in each thread need to be balanced between the cores to obtain better thread synchronization, thus maximum performance. See other details in the next Section.

2. THE LAGRANGIAN TEMPERATURE PARTICLES METHOD IN PARALLEL COMPUTATIONS

The governing equations with Boussinesq approximation for incompressible and two-dimensional flow of a Newtonian fluid with constant properties around a heated solid wall can be written as the following dimensionless form:

$$\nabla \cdot \mathbf{u} = 0 \ , \tag{1}$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \frac{Gr}{Re^2}\theta\,\mathbf{j} - \nabla p + \frac{1}{Re}\nabla^2 \mathbf{u}, \text{ where } \theta = \frac{T - T_\infty}{T_w - T_\infty}, \tag{2}$$

The governing equations, Eq. (1) and Eq. (2), respectively the continuity and the Navier-Stokes equations, are described in this paper with the vorticity transport equation by taking the rotational of the Navier-Stokes equations as follows:

$$\frac{\partial \omega}{\partial t} + (\mathbf{u} \cdot \nabla)\,\omega = Ri\frac{\partial \theta}{\partial x} + \frac{1}{Re}\nabla^2 \omega. \tag{3}$$

Equation (3) governs the dynamics of each vortex element.

The aerodynamic loads can be described from the Eq. (1) and Eq. (2) with the pressure Poisson equation derived by taking the divergence of Navier-Stokes equations (Shintani & Akamatsu, 1994).

For the present mathematical formulation the energy equation assumes the following form:

$$\frac{\partial \theta}{\partial t} + (\mathbf{u} \cdot \nabla)\theta = \frac{1}{Re\,Pr}\nabla^2 \theta \ . \tag{4}$$

Equation (4) governs the dynamics of each temperature particle.

In the above governing equations, Eq. (3) and Eq. (4), $\mathbf{u}$ is the velocity field, θ is the dimensionless temperature (being respectively T_w the solid wall temperature and T_∞ the far away fluid temperature) and $t = b^2/\Gamma$ is the dimensionless time (being b the length scale, Γ the circulation associated to the vortical structure and Γ/b the velocity scale, both of a physical problem). The dimensionless numbers, respectively, the Reynolds number, the Prandtl number and the Richardson number, are defined as:

$$Re = \frac{\Gamma}{\nu}, \tag{5}$$

$$\mathrm{Pr} = \frac{\nu}{\alpha}, \tag{6}$$

$$\mathrm{Ri} = \frac{\mathrm{Gr}}{\mathrm{Re}^2}, \tag{7}$$

where ν is the kinematic viscosity and α is the thermal diffusivity.

Typical simulations treat the impermeability condition on the solid wall by using or the method of panels or the method of images (Katz and Plotkin, 1991). Each nascent vortex element from the solid wall must be positioned at a shedding point placed near each pivotal point fixed on the wall. The strength of the nascent vortex element $\Delta\Gamma$ is obtained imposing the no-slip condition on the all pivotal points. Therefore, each panel has a pivotal point to ensure simultaneously the impermeability and the no-slip conditions.

The strength of each nascent temperature element is obtained through an interpretation for the Fourier law close to the heated body surface (Nakamura et al., 2001):

$$\frac{\partial q}{\partial t} = -\alpha \frac{\partial T}{\partial n}, \text{ where n denotes the normal direction to the surface.} \tag{8}$$

According to the model 1 of Ogami (2001) the intensity of each vortex element is increased by the amount $\Delta\Gamma^*$ due to direct interpretation from Eq. (3), such as:

$$\frac{\partial \omega}{\partial t} = \mathrm{Ri} \frac{\partial \theta}{\partial x}. \tag{9}$$

The foundation of Lagrangian-Lagrangian temperature particles method rests on the use of Eq. (3) and Eq. (4) to track a fluid based on the evolution of vorticity and temperature fields. The vorticity and energy equations are free of the computational instabilities associated with the convective term. Computational simulation requires the discretization in space and time of Eq. (3) and Eq. (4). The two-dimensional, incompressible unsteady flow around a heated solid wall uses an algorithm based on Eq. (3) and Eq. (4) that splits the advective-diffusive operators in the forms (Chorin, 1973):

$$\frac{D\omega}{Dt} = \frac{\partial \omega}{\partial t} + (\mathbf{u} \cdot \nabla)\omega = 0 , \tag{10}$$

$$\frac{\partial \omega}{\partial t} = \frac{1}{\mathrm{Re}} \nabla^2 \omega . \tag{11}$$

$$\frac{D\theta}{Dt} = \frac{\partial \theta}{\partial t} + (\mathbf{u} \cdot \nabla)\theta = 0 , \tag{12}$$

$$\frac{\partial \theta}{\partial t} = \frac{1}{\mathrm{Re\,Pr}} \nabla^2 \theta , \tag{13}$$

The temperature particles method represents the vorticity field by Lamb vortex elements (Kundu, 1990), whose transport by advection and diffusion is carried out in a sequence within the same time increment of Δt. In this context, the Lagrangian approach is used to simulate the vorticity advective process, governed by Eq. (10). The advective motion of each vortex element is determined by integration of each vortex point path equation, which here is solved using a second-order Adams-Bashforth scheme (Ferziger, 1981). The total velocity induced at each vortex element is computed considering the uniform flow, the solid wall and the vortex-vortex interaction (by using the Biot-Savart law).

The process of vorticity diffusion for each k^{th} vortex element, governed by Eq. (11), is simulated using a fractional random walk method introduced by Chorin (1973):

$$\varsigma_k(t) = \sqrt{\frac{4\Delta t}{\mathrm{Re}} \ln\left(\frac{1}{P}\right)} \left[\cos(2\pi Q)_x + \sin(2\pi Q)_y\right], \tag{14}$$

where P and Q are random numbers between 0 and 1.

The strength of each nascent temperature element is computed as (see Eq. (8)):

$$\Delta q_k = \frac{1}{RePr}\frac{T_k - T_\infty}{T_w - T_\infty}\frac{\Delta s_k \Delta t}{\varepsilon}, \tag{15}$$

where Δs_k is the elementary length of the solid wall, ε is the normal distance between the pivotal point k and the shedding point and Δt is the time increment. The temperature induced by each temperature particle is given by a Gaussian distribution:

$$T(r) = \frac{\Delta q}{\pi \sigma_T^2}\exp\left(-\frac{r^2}{\sigma_T^2}\right), \tag{16}$$ σ_T is the temperature core radius.

The advective motion of each temperature particle, governed by Eq. (12), is determined by integration of each temperature path equation, which here is solved using a second-order Adams-Bashforth scheme. The total velocity induced at each temperature particle is computed considering the uniform flow, the solid wall and the vortex-temperature interaction (by using the Biot-Savart law).

The process of heat diffusion for each k^{th} temperature particle, governed by Eq. (13), is simulated using the random walk method:

$$\varsigma_k(t) = \sqrt{\frac{4\Delta t}{RePr}\ln\left(\frac{1}{P}\right)}\left[\cos(2\pi Q)_x + \sin(2\pi Q)_y\right], \tag{17}$$

where P and Q are random numbers between 0 and 1.

Using the circulation definition, $\Gamma = \iint_A \boldsymbol{\omega}\cdot\mathbf{n}dA$, the Eq. (9) is discretized in the following form (the temperature-vortex interaction):

$$\Delta\Gamma^* = Ri\frac{\partial\theta}{\partial x}\Delta t\,\Delta A, \tag{18}$$ ΔA is the area occupied by the Lamb vortex element with core radius of σ.

The derivative on Eq. (19) is solved by derivative centered difference, such as:

$$\left.\frac{d\theta}{dx}\right|_i = \frac{\theta_{i+1} - \theta_{i-1}}{2\Delta x} - \frac{\Delta x^2}{6}\left.\frac{d^3\theta}{dx^3}\right|_i - \frac{\Delta x^4}{120}\left.\frac{d^5\theta}{dx^5}\right|_i - \ldots \tag{19}$$

The above equation is truncated in the first term, where Δx the i^{th} vortex core radius. All the temperature elements placed in the fluid domain are used to compute the dimensionless temperatures θ_{i+1} and θ_{i-1} in the neighborhood of the i^{th} vortex element.

Considering the vorticity-vorticity, the vorticity-temperature and the temperature-vorticity interactions (see Eq.(18)) represent around 99% of the CPU time in a typical numerical simulation, parallel sections were implemented inside the respective subroutines. Due to the inducted effect's independency from one particle to another, the calculations can efficiently be made in parallel. Each thread was provided the latest particles cloud position and intensity, thereafter select an arbitrary particle and calculate the cloud effects in it. This is the same method used in the serial code, but in this case each core evaluates a different particle, reducing the total time. This strategy proved itself extremely efficient, providing high CPU usage and near null thread idle time.

Thread generation and memory allocation produce a time overhead that although necessary, must remain at minimum levels. Since the performance gains do not repay the time spent in the section creation, parallel sections are not created for small loops. Consequently, in the presence of nested loops, the starting point of a parallel section has to be outside the outer loop to minimize intrinsic parallel overheads. Code scalability is common criteria to analyze not only the code's parallel efficiency but the rate of return on investment in additional hardware. The most commonly accepted definition is given by:

$$\text{speed up} = \frac{\text{run time on single processor}}{\text{run time on N processors}} . \tag{20}$$

Intrinsic parallelism overheads limit the amount of threads that provide performance improvement. At certain point the thread's quantity increase only returns a greater time to handle this higher number of threads.

3. RESULTS, CONCLUSIONS AND PERSPECTIVES

The problem to be exemplified is that of aircraft wake interactions with the ground during the landing and takes off operations. The main motivation is the reduction of elapsed time between subsequent operations that affects directly the safety of a landing (or take off) due to the aircraft wake that remains over the ground and that takes some time to dissipate or to be removed by lateral winds. Therefore, to avoid the flight of an aircraft in the wake of another one is the main concern in airport operation (Machol, 1993). To this observation one should mention Critchley and Foot (1991), "Accidents occur in subsequent operations, mainly in the 30 ~ 70 m range above ground level, when strong vorticity structures are interacting with the runaway ground", and Zheng and Ash (1996), "The free vortices, leaving the wing tips, have an intensity proportional to the aircraft size and develops for considerable distances".

In the above context, the free vortices, starting at the wing tips, are here defined by $\Gamma = \pm W/(\rho b U_a)$, where W is the aircraft weight, b is the wingspan and U_a is the approaching velocity. Therefore, from the wing tips free vortices are emanating with intensity $\pm \Gamma$; each vortical structure is represented as a pair of free vortex cloud (each with 100 discrete Lamb vortices with elementary intensity $\pm\Gamma/100$). The vortex clouds are first generated using a random walk procedure (Lewis, 1999), which start with all the vortices concentrated at a single point and ends when the outermost vortex reaches 0.1b (Hirata et al., 2002).

Aiming at assessing the method capability to predict the main quantitative features of the flow was chosen one value of the Reynolds for all cases, that is Re=75,000. The Prandtl number was fixed as Pr=1.0. The airport runway was represented by M=120 pivotal points, with a temperature of 273K, while the air is at 293K. The method of images (Katz and Plotkin, 1991) was employed to represent the airport ground plane. During each time step, M news vortex elements and M news temperature particles were generated at a distance $\varepsilon=\sigma=\sigma_T=0.001$ on a straight-line, passing by the control point and normal to the solid wall; these new vortex elements and temperature particles were added to the fluid domain. All runs were performed with 800 time steps of magnitude $\Delta t=0.05$. The Richardson numbers were: 0.0, 0.01, 0.1 and 1.0. Figure 1 summarizes all trajectories of free vortices from wing tips simulated with parallel processing. The experimental result pointed in the Tab. (1) was published by Liu and Srnsky (1990). The numerical trajectories of the free vortices are in good agreement with the experimental result. One can clearly observe that the computed trajectory of the primary vortex structure does try to follow the experimental results, even for long time simulation. Because the mixed convection was simulated in this research, it was possible to identify a moderate variation of the right free vortex trajectory, in special for $Ri = 1.0$.

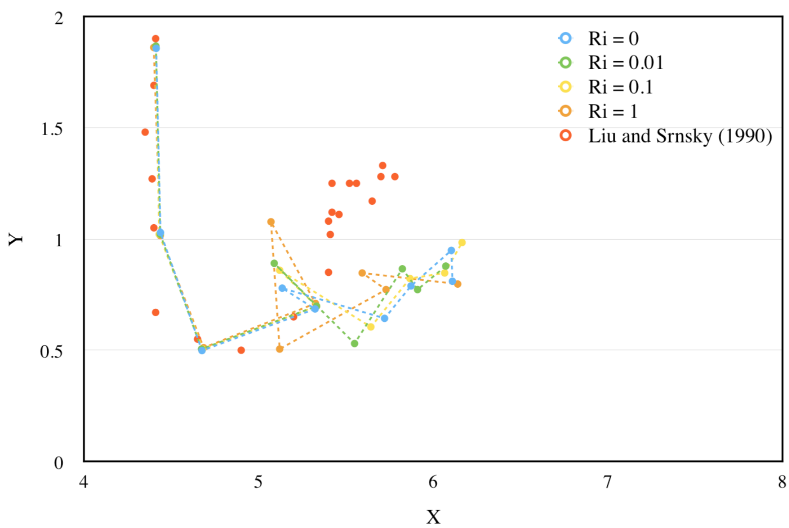
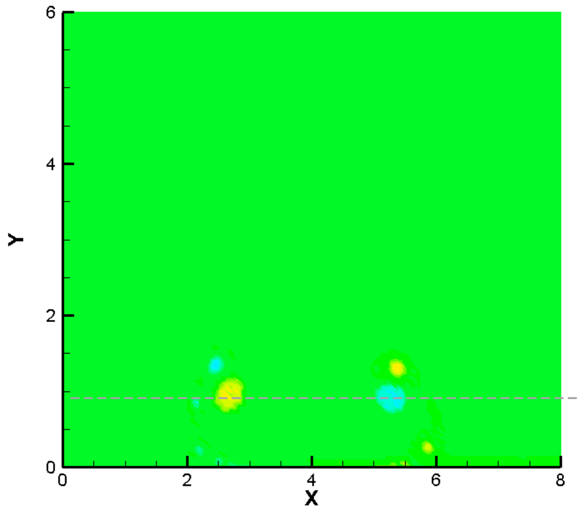


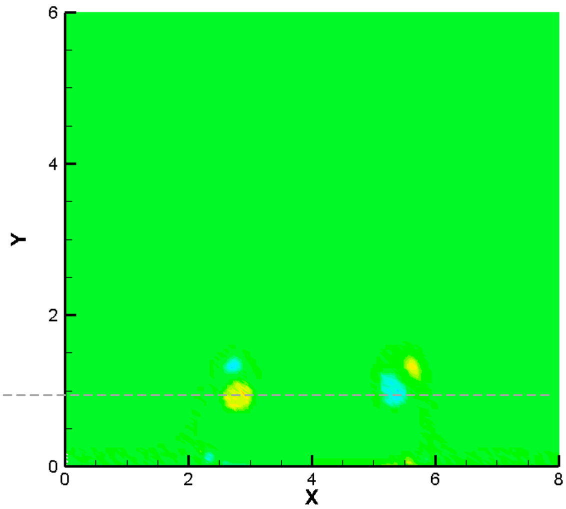
Figure 1. Trajectories of the free vortices from wing tips with $Re = 75,000$ and $Pr = 1.0$.

Figure 2(a) details the instantaneous vorticity distribution of the primary vortex structures at $t = 17.5$ with $Ri = 0.0$ (forced convection). The referred time step corresponds at the instant when the right primary vortex structure reaches its higher elevation after collide with the ground plane. Figure 2(b) presents the same time step, now with $Ri = 1.0$. In general, one could observe in the Fig. (1) an interesting phenomenon that is identified in the calculated trajectory starting from point very close to the ground, when after that the trajectory takes a steep upward direction until $t = 17.5$ and follows a steep descent to ground plane direction; from there on the trajectory more or less try to follows the experimental results. There is no information about real climate conditions of experimental result provided by Liu and Srnsky (1990).

Figure 3 presents a comparison between results with and without parallel processing. The gain obtained was very expressive. A typical simulation of this paper spent around 160 hours, without parallel processing, by using the following configuration: Two 2.4 GHz Quad Core Xeon E5620, 16Gb 1066 MHz DDR3 ECC SDRAM. For the same case, when it was used parallel processing the time was of 28.4 hours. The vortex-vortex and vortex-temperature interactions were subroutines that spend higher computational cost, because they involve the Biot-Savart law. Another one was the subroutine to compute the buoyancy force effect (Eq. (19)), i.e., the temperature-vortex interaction.



(a) with forced convection ($Ri = 0.0$)



(b) with mixed-convective heat transfer ($Ri = 1.0$)

Figure 2. Instantaneous vorticity distributions of airplane wake near the ground plane at $t = 17.5$ ($Re = 75{,}000$ and $Pr = 1.0$).

Figure 4 shows that the time distribution inside each kind of particle-particle interaction is different for parallel and serial code. It has been caused by an improper parallel section inside the temperature-vortex interaction subroutine, necessary to compute the buoyancy force effect (Eq. (18)). A total time of 42 hours were spent inside these interactions in the serial code, that were reduced to 13 hours using OpenMP. Although a total speedup of 5.75 times is acceptable using a 8 core computer, the aforementioned parallel code must be reviewed to improve its scalability. It will be imperative when run in distributed memory systems with great amount of cores (next investigation).

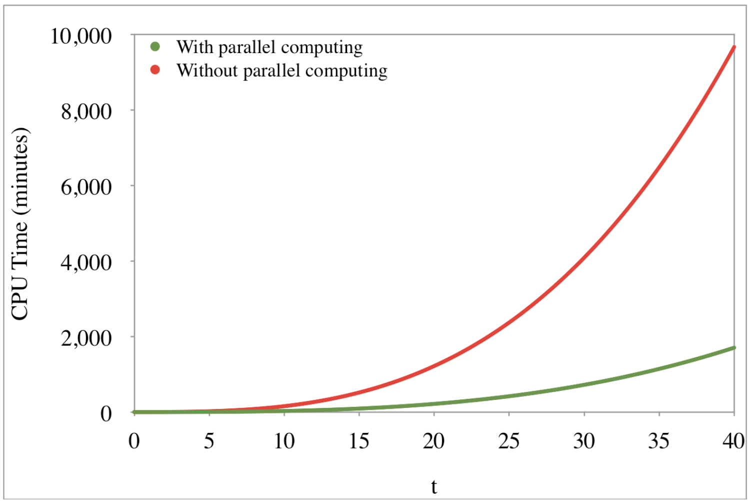
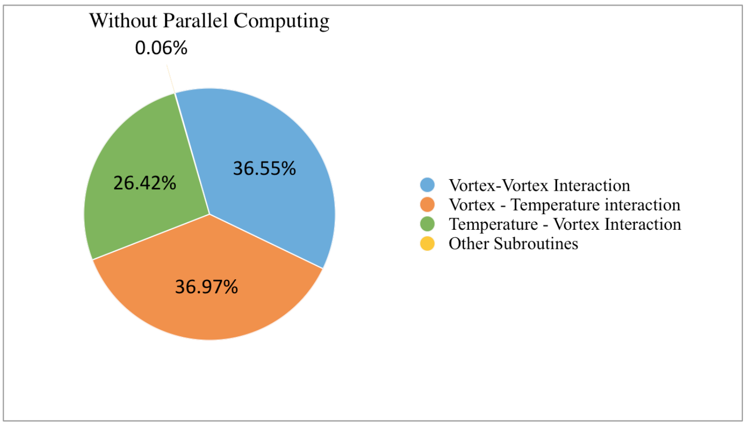
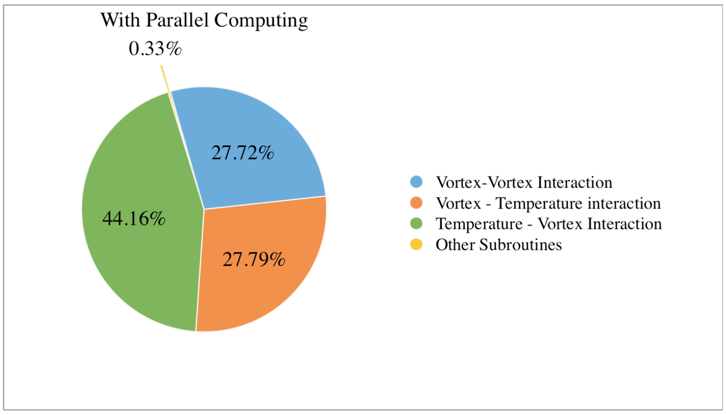


Figure 3. Parallel processing performance between dimensionless times of t=0 until t=40.



(a)



(b)

Figure 4. Percentage of the final CPU time for the particle-particle interactions.

The main objective of the work with the implementation of a temperature particles method for the analysis of unsteady and mixed-convective heat transfer of a typical flow has been achieved. The new methodology was tested for the airplane wake dissipation problem and showed able to provide good estimates for trajectories of vortices in a physical sense.

Future works will investigate the sensitivity of the methodology to the various simplifications used in creating an efficient scheme, and attempt to demonstrate a close connection to experimental predictions over a range of different flows in fluid mechanics and heat transfer.

The focus will to analyze problems involving both Vortex Induced Vibrations (VIV) and mechanisms of ground effect with mixed-convective heat transfer. The transport of heat associated with aerodynamics of bluff bodies is of great importance in engineering. Many areas of fluid mechanics and heat transfer are involved in understanding this kind of flows.

The experience from previous studies was added with the present research, allowing one to analyze complex situations where there is relative motion between bodies. These extend the applicability of the present Lagrangian-Lagrangian temperature particles method in parallel computations. The use of global as well local quantities combined to the near field flow pattern observations are useful to understand the complex mechanisms that lead the origin and the time evolution of the aerodynamic loads. As mentioned in the Section 2, the aerodynamic loads can be calculated using an integral formulation derived from the pressure Poisson equation (Shintani & Akamatsu, 1994). The methodology developed in this paper is greatly simplified by the utilization of the Lagrangian method associated with parallel processing. The characteristics, programming methodology and performance of parallel processing systems appear in different manners. However, the availability of suitable parallel computers to run long simulations is always an issue to be investigated and clarified by researchers.

4. ACKNOWLEDGEMENTS

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