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# Fully resolved simulation of particle deposition and heat transfer in a differentially heated cavity

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#### ABSTRACT

In this paper a fictitious domain method is used to study the motion of particles in a differentially heated cavity. A collision strategy is implemented which is validated using the problem of two freely falling particles with natural convection taking place from the leading hot particle. The motion of the particles in a differentially heated cavity is considered where the vertical walls are subject to a temperature difference  $\Delta T$  whereas horizontal walls are assumed to be adiabatic. Depending on the fluid Grashof number different flow regimes and two critical Grashof numbers are identified. Sustained motion of the suspended particles is also studied and different behaviour is observed compared to the limiting case of tracer particles where simulations are usually performed using one-way coupled point-particle assumptions. Finally the effects of the particles can adversely influence the heat transfer rate. However, if hot particles are effectively removed from the wall, e.g. by increasing the Grashof number, wall heat transfer properties can still be enhanced.

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#### 1. Introduction

Understanding the fundamentals of particle motion in a cavity can benefit many environmental and industrial applications. The main concern in this paper is the motion induced by the natural convection due to a temperature gradient which is particularly important in the environmental systems, chemical and biochemical reactors. For example, in clean rooms, understanding the patterns of motion is crucial for controlling the concentration and effective removal of the environmental pollutants such as dust, aerosol particles and chemical vapours. Another important application of flow induced in enclosures due to an internal or external heat source, is the prediction of heat loss in solar collectors (Buchberg et al., 1976) and double-glazed windows (Korpela et al., 1982). In addition, assessing the risk and environmental impacts of severe accidents in chemical or nuclear reactors is only possible by understanding the deposition and removal mechanisms of micron-sized particles from a buoyancy induced flow in large enclosures (Puragliesi et al., 2011; Kissane, 2008).

A fundamental study of any of the aforementioned applications naturally reduces to the particle motion is a differentially heated cavity. A differentially heated cavity (DHC) is defined here as an

\* Corresponding author. Tel.: +44 234444556666. *E-mail address:* John.Shrimpton@soton.ac.uk (J.S. Shrimpton). enclosure filled with a fluid with a temperature dependent density, where the vertical walls are kept at two different, fixed temperatures denoted by  $T_h$  and  $T_c$  and the horizontal walls are assumed to be adiabatic. Fluid motion in a DHC has been studied extensively and many benchmark solutions are available, e.g. De Vahl Davis (1983) studied the 2D cavity problem and provided benchmark solutions for the laminar region for Rayleigh numbers between  $10^3$  and  $10^6$ . More recently accurate results were provided by Le Quere (1991) using a pseudo-spectral method for Rayleigh numbers between  $10^6$  and  $10^8$  by solving the Navier–Stokes and energy equations written in primitive variables.

Puragliesi et al. (2011) studied the particle transport in a buoyancy driven flow in a DHC. They studied the turbulent flow at two different Rayleigh numbers ( $Ra = 10^9$  and  $10^{10}$ ) using a Boussinesq approximation to include the density variation by the temperature gradient. They included the drag, gravity, buoyancy, lift and thermophoretic forces on the particle to calculate its motion. An Eulerian–Lagrangian (EL) approach is used to simulate the particle motion with a one-way coupled point-particle assumption. They found out that particle deposition is mainly caused by gravitational settling and the deposition mainly takes place at the bottom wall for particles with diameters larger than 10 µm.

Similar to Puragliesi et al. (2011); Akbar et al. (2009) used a one-way coupled point-particle assumption for the simulation of particle motion in a DHC. However they used lower Rayleigh

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numbers in the range of  $10^2$  to  $8 \times 10^5$ , and also considered the effects of the Brownian motion. They suggested that for the Rayleigh numbers larger than  $10^4$  only one large recirculation pattern is observed for the motion of the particles. However for smaller *Ra* most particles disperse toward the walls while some of them are trapped in a recirculation zone. They may however, leave the recirculation zone due to Brownian motion at a very low rate. They also confirmed that the thermophoretic and Brownian motion are only important for sub-micron particles.

Heat transfer augmentation in a DHC was investigated by Tiwari and Das (2007) for nano-particles and they reported a non-linear increase in the average wall Nusselt number by increasing the volume fraction. Recently Kuerten et al. (2011) reported that the average wall Nusselt number can increase for millimetre size particles similar to the nano-particles. They reported enhancements as large as 100% for heavy inertial particles.

All the aforementioned studies are performed using a pointparticle assumption with one- or two-way coupling strategies. This approach cannot be classified as a full direct numerical simulation (DNS) since in either case inter-phase momentum and thermal transfers are modelled. The effects of particles on the motion of fluid is assumed to be negligible in a one-way coupled simulation. In the case of a two-way coupled simulation, an undisturbed flow field is assumed to calculate the forces (Haeri and Shrimpton, 2011, 2012a) which is then fed back to the Navier–Stokes (NS) equations using an averaging process. Therefore these methods are DNS only in the sense of the fluid motion. In this paper a fictitious domain method (FDM) (Haeri and Shrimpton, 2013b) is used for the simulation of the particulate phase where no additional assumption is required for the calculation of the particle motion.

We first discuss the mathematical formulation and the numerical method succinctly. Although the method is based on a FDM which has been extensively validated elsewhere (Haeri and Shrimpton, 2012b, 2013a,b), a collision strategy is implemented and validated in this paper using the problem of two particles settling in a cavity with an aspect ratio of larger than one. In addition the linear solver is accelerated on GPGPU (General-purpose graphics processing unit) using cuSPARSE and cuBLAS libraries and the speed-up results are presented. Particle transport in a buoyancy driven cavity is then examined using the FDM. However, it should be noted that all the simulations in this paper are restricted to 2D cavities. Particles are initially at rest on the bottom of the cavity and we have identified three different regimes depending on the Grashof number. In the sustained circulation regime, it is found that a strong circulation area forms near the hot wall due to the body forces generated from the particles falling away from the hot wall. In addition the gravitational force prevents the particles to migrate to the weaker circulation areas near the cold wall. It is tested to confirm that this motion is independent of the initial configuration of the particle by simulating a randomly injected initial configuration. Finally effects of particles on the heat transfer properties of the hot wall is studied and it is found that sluggish motion of large particles due to buoyancy and inertial effects can have a negative influence on the local value of the wall Nusselt number. However it is found that effective circulation of the particles, e.g. by increasing the Grashof number, can still enhance the wall Nusselt number.

#### 2. The numerical method

#### 2.1. Governing equations

The numerical method has been explained and validated extensively elsewhere (Haeri and Shrimpton, 2012b, 2013a,b). However since a collision strategy is implemented and validated in this paper, the numerical method is discussed succinctly here. If we let  $\Omega_p$  and  $\Omega_f$  be the immersed particle and the fluid domain respectively and  $\Omega = \Omega_p \cup \Omega_f$  be the domain including both the fluid and the particle, it is possible to extend the governing equations on the fluid domain (which will be the Navier–Stokes equations) to the particle domain by constraining the motion inside the particle domain to a rigid motion (Patankar et al., 2000), i.e. by enforcing

$$\frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) = 0 \quad \text{in} \quad \Omega_p.$$
(1)

Then the flow on the whole computational domain  $\Omega$ , is governed by the following continuity, momentum and energy balance equations:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \mathbf{u}_j}{\partial \mathbf{x}_j} = \mathbf{0},\tag{2}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial \sigma_{ij}}{\partial x_j} + f_{B,i} + f_{FD,i},\tag{3}$$

$$\frac{\partial \rho c_p T}{\partial t} + \frac{\partial \rho u_j c_p T}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \kappa \frac{\partial T}{\partial x_j} \right), \tag{4}$$

where

$$\sigma_{ij} = -P\delta_{ij} + \tau_{ij}, \quad \tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \tag{5}$$

and  $f_{FD,i}$  is a body force to impose the rigid motion. The buoyancy effects are presented by  $f_{B,i}$ , the fluid pressure by P and  $u_i$  is the fluid velocity. The mixture density, heat capacity and thermal conductivity are represented by  $\rho$ ,  $c_p$  and  $\kappa$  respectively. Mixture properties are defined by

$$\varphi = \Theta_p \varphi_p + (1 - \Theta_p) \varphi_f, \tag{6}$$

where  $\varphi = \{\rho, c_p, \kappa\}$  and subscripts *p* and *f* are used to refer to the particle and fluid properties at some reference temperature respectively. Also note that the tensor notation is used in this paper; for example a variable with subscript *f*, *i* is vector variable in fluid domain. and  $\Theta_p$  is a step function that takes the value of one in  $\Omega_p$  and zero otherwise. In the current method the particles are defined by an explicit stair-step grid (material grid hereafter) which freely moves on the background Eulerian grid where the solution is sought. Fig. 1 shows the material grid points used to define the particle. Using this explicit grid, particle volume fractions on the background Eulerian grid can efficiently be calculated by using the discrete delta functions (Haeri and Shrimpton, 2013b)

$$\Theta_p(\mathbf{x}) = \sum_{m=1}^{N_m} \delta_h \left( \frac{\mathbf{x} - \mathbf{X}_m}{h} \right) \upsilon_m \quad \forall \mathbf{x} \in g_h,$$
(7)

where  $N_m$ ,  $v_m$  and  $g_h$  are the number of material control volumes, volume of the m-th material CV and the support of the discrete delta function respectively. Also note that  $\mathbf{X}_m$  refers to the position of the *m*-th material grid point. The discrete delta function,  $\delta_h$ , is defined by

$$\delta_h(\mathbf{r}) = \frac{1}{h^d} \prod_{i=1}^d \phi(r_i),\tag{8}$$

where *d* is the dimensionality of the Eulerian grid, *h* is the Eulerian grid spacing and  $r_i = (x_i - X_{m,i})/h$ . There are several choices for the function  $\phi(r)$  in Eq. (8), one such function with reasonable smoothing and computational efficiency (Haeri and Shrimpton, 2012b) is the following function first suggested by Roma et al. (1999):

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