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Modeling of natural convection with Smoothed Particle Hydrodynamics: Non-Boussinesq formulation

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ABSTRACT

A new variant of the Smoothed Particle Hydrodynamics (SPH) simulations of the natural convection phenomena is introduced. In many situations, where the density may vary significantly under the influence of temperature non-uniformities, the classical Boussinesq approximation fails. To characterize such situations, the Gay-Lussac dimensionless number is useful as a measure of density variations in non-isothermal flows. The novel points of the proposed modeling beyond the Boussinesq regime include the proper implementation of the buoyancy force and a smart connection between particle volume and incompressibility constraint. To examine the correctness of the new approach, numerical results are confronted with available reference data.

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1. Introduction

Natural convection phenomena, due to their relevance to many scientific and technical issues such as nuclear reactor systems, foundry devices, geophysical and astrophysical processes, etc., have been intensively studied in the literature. In particular, due to geometrical simplicity, square and rectangular wall-heated cavities have been widely explored. The most-cited benchmark solutions were provided by de Vahl Davis [1] using second-order central difference scheme. He performed simulations of steady-state natural convection in a horizontally-heated square cavity at the Rayleigh numbers up to $Ra = 10^6$. His studies were continued by numerous researchers to extend the range up to $Ra = 10^8$ by Le Quéré [2] and $Ra = 10^{11}$ by Lage and Bejan [3]. Evolution of the CFD methods led to benchmark solutions performed using other approaches such as Discrete Singular Convolution (DSC) [4] and the Lattice Boltzmann Method (LBM) [5].

All the above-mentioned papers are based on the Boussinesq approximation. However, the natural convection is often driven by large temperature differences leading to considerable density variations. In these cases the Boussinesq approximation fails. This situation takes place in foundry processes and astrophysical MHD simulations. In the literature, papers dealing with the non-Boussinesq regime are rare. The square side-heated cavity simulations of natural convection caused by large density variations were performed in the compressible Eulerian approach by Pesso and Piva [6], Vierendeels et al. [7] and Backer and Braack [8].

In the present work, a new technique for Smoothed Particle Hydrodynamics (SPH) simulations of natural convection phenomena beyond the Boussinesq regime is proposed. The SPH is a fully Lagrangian, particle-based method for fluid-flow computations. In the early stage it was developed by Monaghan [9] for some astrophysical phenomena, but nowadays, the SPH is increasingly often used for flows with interfaces and common in geophysical and astrophysical applications. The main advantage over Eulerian techniques is no requirement of the grid. Therefore, it is a natural approach to simulate multiphase flow phenomena as well as flows in complex geometries. In the present work we consider only incompressible flows (no density dependence on the hydrostatic pressure). This constraint is assured using weakly compressible technique, where the standard set of governing equations is closed by a suitably-chosen, artificial equation of state. An introduction to the SPH method is presented in Section 2.

As briefly recalled in Section 2 below, field quantities as density and temperature in SPH are modeled exactly at moving particles. As shown in Section 3.1, an implementation of the Boussinesq approximation in SPH is straightforward. It is done by extending the Navier–Stokes equation with an additional term. The SPH simulations under Boussinesq approximation were presented by Cleary and Monaghan [10]. The novel SPH approach for performing simulations in the non-Boussinesq regime is described in Section 3.2. The key points of this technique are the proper implementation of the buoyancy force and a smart connection between particle volume and incompressibility constraint, cf. Section 4.

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2. SPH formulation

2.1. Basic ideas

The main idea behind the SPH is to introduce kernel interpolants for flow quantities so that the fluid dynamics is represented by particle evolution equations, cf. [9–11] for a review. The SPH method is composed of two approximations. The first is interpolation of the field quantities at the point. To construct it, an integral interpolant $\widetilde{A}(\mathbf{r})$ of any field $A(\mathbf{r})$ is used

$$\widetilde{A}(\mathbf{r}) = \int_{\Omega} A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}',h)d\mathbf{r}', \tag{1}$$

where the integration is over all the domain Ω. Here, $W(\mathbf{r},h)$ is a weighting function (kernel) with a parameter h (smoothing length) that can be treated as a characteristic dimension of kernel. Generally, the kernel should posses the symmetrical form

$$W(\mathbf{r},h) = W(-\mathbf{r},h) \tag{2}$$

and enjoy following properties:

$$\lim_{h\to 0} W(\mathbf{r},h) = \delta(\mathbf{r}), \tag{3}$$

where $\delta(\mathbf{r})$ is the Dirac delta, and should be normalized so that

$$\int_{\Omega} W(\mathbf{r},h)d\mathbf{r} = 1. \tag{4}$$

The additional condition is that $W \in \mathbb{C}^n$ (where $n \geqslant 1$) and it is at least as many times differentiable as the field A. There are numerous possibilities to choose the kernel. To reduce the computational effort and properly implement the boundary conditions (Section 2.3), we decided to use the compact quintic spline kernel [12]:

$$W(\mathbf{r},h) = \begin{cases} \frac{7}{4\pi h^2}\left(1-\frac{|\mathbf{r}|}{2h}\right)^4\left(\frac{2|\mathbf{r}|}{h}+1\right), & \text{for } |\mathbf{r}| \leqslant 2h, \\ 0, & \text{otherwise.} \end{cases} \tag{5}$$

The second approximation of the SPH technique is discretization of space. This is done through dividing the domain into a fine-grained representation (particles). Each particle carries the properties of the field. The integral interpolant (1) becomes then the summation interpolant

$$\langle A\rangle(\mathbf{r}) = \sum_b A(\mathbf{r}_b)W(\mathbf{r}-\mathbf{r}_b,h)\Omega_b, \tag{6}$$

where $\mathbf{r}_b$ and Ω_b denote the position and volume of the particle b. The SPH task consists in computing the interpolant at each particle (say, a), so that Eq. (6) may be rewritten into the form

$$\langle A\rangle_a = \sum_b A_b W_{ab}(h)\Omega_b, \tag{7}$$

where $\langle A\rangle_a = \langle A\rangle(\mathbf{r}_a)$, $A_b = A(\mathbf{r}_b)$ and $W_{ab}(h) = W_{ba}(h) = W(\mathbf{r}_b - \mathbf{r}_a, h)$.

An additional quality of the SPH reveals when it comes to differentiation of the fields. In accordance with (1), the smoothed gradient of a scalar field $A(\mathbf{r})$ (for vector fields the procedure is analogous) assumes the form

$$\widetilde{\nabla A}(\mathbf{r}) = \int_{\Omega} \nabla A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}',h)d\mathbf{r}'. \tag{8}$$

Taking advantage of the integration by parts rule and using the kernel symmetry, Eq. (8) is transformed into

$$\widetilde{\nabla A}(\mathbf{r}) = A(\mathbf{r}')W(\mathbf{r}-\mathbf{r}')|_{\partial\Omega} + \int_{\Omega} A(\mathbf{r}')\nabla' W(\mathbf{r}-\mathbf{r}',h)d\mathbf{r}'. \tag{9}$$

Generally, the first r.h.s. term does not necessarily vanish for finite systems. The common practice is to neglect it and deal with the boundaries explicitly. The SPH discretization of (9) results in

$$\langle \nabla A\rangle_a = \sum_b A_b \nabla_a W_{ab}(h)\Omega_b. \tag{10}$$

Since the nabla operator acts only on the kernel, the SPH gradient of the field is dependent only on the values of the fields at particles, not gradients.

The way of obtaining higher derivatives is straightforward. For example, the Laplace operator which acts on the field $A(\mathbf{r})$ has the form

$$\langle \Delta A\rangle_a = \sum_b \sum_c A_c \nabla_a W_{ab}(h)\nabla_b W_{bc}(h)\Omega_b\Omega_c. \tag{11}$$

However, due to the accuracy and efficiency requirements, commonly used form is built as a combination of the finite difference approach and the SPH approximation [10].

2.2. Governing equations

The full set of governing equations for incompressible viscous flow is composed of the Navier–Stokes equation

$$\frac{d\mathbf{u}}{dt} = -\frac{1}{\varrho}\nabla p + \nu\nabla^2\mathbf{u} + \mathbf{g}, \tag{12}$$

where ϱ is the density, $\mathbf{u}$ the velocity vector, t the time, p the pressure, ν the kinematic viscosity, $\mathbf{g}$ the gravitational acceleration, and the continuity equation

$$\frac{d\varrho}{dt} = -\varrho\nabla\cdot\mathbf{u}, \tag{13}$$

that in the incompressible regime takes the divergence-free form $\nabla\cdot\mathbf{u} = 0$. Taking heat transfer into account, the system is extended by the energy equation (here, in the simplified form, as in [6])

$$\varrho c_p \frac{dT}{dt} = \nabla\cdot(k\nabla T), \tag{14}$$

where T is temperature, c_p is the specific heat and k is conductivity. Since the SPH is fully Lagrangian, we extend the above system by relation

$$\frac{d\mathbf{r}}{dt} = \mathbf{u}. \tag{15}$$

Additionally, it is important to note that writing SPH approximations of the field quantities, we assume that $\langle A\rangle_a \simeq A_a$. This relationship expresses no distinction between the computed field and its SPH approximation.

2.2.1. Continuity equation

Utilizing relation (10), the SPH formulation of the continuity Eq. (13) arises to the following form

$$\frac{d\varrho_a}{dt} = -\varrho_a \sum_b \mathbf{u}_b\cdot\nabla_a W_{ab}(h)\Omega_b. \tag{16}$$

It is important to note that various ways to express divergence exist. For example, using the identity

$$\nabla\cdot\mathbf{u} \equiv \frac{1}{\varrho}(\nabla\cdot(\varrho\mathbf{u}) - \mathbf{u}\cdot\nabla\varrho), \tag{17}$$

combined with (16), leads to a different SPH form

$$\frac{d\varrho_a}{dt} = \sum_b \varrho_b \mathbf{u}_{ab}\cdot\nabla_a W_{ab}(h)\Omega_b, \tag{18}$$

where $\mathbf{u}_{ab} = \mathbf{u}_a - \mathbf{u}_b$. The advantage of the above form over (16) is the symmetry with swapping particles a and b. Therefore, in practice, it is more accurate to use (18).

However, since forms (16) and (18) do not conserve the total mass of particles explicitly, we decided to use an alternative

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