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A particle distribution function approach to the equations of continuum mechanics in Cartesian, cylindrical and spherical coordinates: Newtonian and non-Newtonian fluids

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ABSTRACT

The evolution equations for the particle distribution functions are written in a divergence form applicable in three dimensions. From this set, it is shown that the continuity equation and the equations of motion are satisfied in Cartesian, cylindrical and spherical coordinates for all fluids when additional source terms are added to the equations of evolution in the latter two coordinate systems. If the body forces are present, a new set of source functions is required in each coordinate system and these are described as well. Next, the energy equation is derived by using a separate set of particle distribution functions. Modifications of the relevant equations to be applicable to incompressible fluids is described. The incorporation of boundary conditions and the description of the numerical scheme for the simulation of the flows employing the new approach is given. Validation results obtained through the modelling of a mixed convection flow of a Bingham fluid in a lid-driven square cavity, and the steady flow of a Bingham fluid in a pipe of square cross-section are presented. Next, using the cylindrical coordinate version of the evolution equations, numerical modelling of the steady flow of a Bingham fluid and the Herschel–Bulkley fluid in a pipe of circular cross-section have been performed and compared with the simulation results using the augmented Lagrangian method as well as the analytical solutions for the velocity field and the flow rate. Finally, some comments on the theoretical differences between the present approach and the existing formulations regarding Lattice Boltzmann Equations are offered.

1. Introduction

In the numerical modelling of the flows of Newtonian and non-Newtonian fluids, the finite element method (FEM) is the preferred option. However, it has become increasingly clear that FEM requires a lot of CPU and is not fast enough. This outcome has led to the development of two different numerical schemes: the first is based on the smoothed-particle hydrodynamics (SPH) method which has been applied to non-Newtonian moulding flow by Fan et al. [1], and to the simulation of solid bodies suspended in a shear flow of an Oldroyd-B fluid by Hashemi et al. [2]; and the second scheme is the Lattice Boltzmann equation (LBE) and its variant, namely the particle distribution function method.

Briefly, SPH works by dividing the fluid domain into a set of discrete elements, also referred to as particles. These particles have a spatial distance, known as the "smoothing length" h, over which their properties are "smoothed" by a kernel function. This means that the physical quantity of any particle can be obtained by summing the relevant properties of all the particles which lie within the range of the kernel. For example, using Monaghan's cubic spline kernel [3], the temperature at position $\mathbf{x}$ depends on the temperatures of all the particles within a radial distance $2h$ of $\mathbf{x}$.

The contributions of each particle to a property are weighted according to their distance from the particle of interest, and their density. Mathematically, this is governed by the kernel function, W. The kernel functions commonly used include the Gaussian function and the cubic spline. The latter function is exactly zero for particles further away than two smoothing lengths, unlike the Gaussian, where there is a small contribution at any finite distance away. That is, the cubic spline has the advantage of saving computational effort by not including the relatively minor contributions from distant particles. While the advantages of SPH are many, one drawback over grid-based techniques is the need for large numbers of particles to produce simulations of equivalent resolution.

In contrast with SPH, the particle distribution function method employed here depends on fifteen (resp. twenty two) particles only to

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mimic the continuity equation and the equations of motion (resp. the full set of continuity equation, the equations of motion and the energy equation) applicable to the motion of a fluid. No averaging process as in SPH is needed. As summarised by Huilgol and Kefayati [4], it is possible to derive the continuity equation and Cauchy's equations of motion for a compressible Newtonian fluid, when one uses the Bhatnagar-–Gross–Krook (BGK) approximation. In LBE, the derivations are based on expanding the particle distribution functions as a Taylor series in $\mathbf{u}$, retaining terms up to order $|\mathbf{u}|^2$, where $\mathbf{u}$ is the macroscopic velocity, with coefficients depending on the relaxation time and the grid spacing and the time step. Hence, when one considers incompressible Newtonian fluids, it is not surprising that the kinematic viscosity ν is relaxation time and grid-dependent, for it is given by [5]

$$\nu = \frac{(2\tau - 1)}{6}\cdot\frac{(\Delta x)^2}{\Delta t}, \tag{1.1}$$

where τ is the relaxation time, $\triangle x$ is the grid size and $\triangle t$ is the time step. Clearly, these restrictions on the viscosity make it difficult to model the flows of non-Newtonian, incompressible fluids. For a complete description of these matters, see Huilgol and Kefayati [4]. In addition to the problems arising from Eq. (1.1), Fu et al. [6–8], So et al. [9] and Kam et al. [10] have reiterated the difficulties in employing the LBE formulation in solving Navier–Stokes equations.

In order to overcome these inherent problems, new models for the particle distribution functions are needed. In the Finite Difference Lattice Boltzmann Method (FDLBM) due to Fu and So [6], the particle distribution function leads to the conservation of mass and the equations of motion applicable to incompressible fluids, when the flows are assumed to occur in a two dimensional setting underpinned by a D2Q9 lattice, using Cartesian coordinates only. These results were refined by Huilgol and Kefayati [4] through the use of vector analysis and linear algebra.

Next, in the Thermal Finite Difference Discrete Flux Method (TFDDFM) proposed by Fu et al. [8], their approach was extended to three dimensional problems using a D3Q15 lattice. The resulting equations are capable of incorporating body forces; moreover, a new set of particle distribution functions was employed to obtain the balance of energy equation. These results were reformulated in [4] using simple results from vector analysis and linear algebra, once again. The important point to note is that the previous restrictions on the pressure and the viscosity are eliminated in these derivations [4,6,8], meaning that one is free to choose a constitutive equation. That is, one can model a Newtonian fluid, or power law fluids, or viscoelastic and viscoplastic fluids. However, the derivations in [4,6,8] are suitable for Cartesian coordinates only.

In the present work, we unify and extend the derivation of the conservation of mass equation and Cauchy's equations of motion to Cartesian, cylindrical and spherical coordinates using linear algebra, vector and dyadic analysis, in a 3D format. While the methodology follows some of the features of the earlier work [4], the evolution equation for the particle distribution function is written in a divergence form with the addition of a new set of source functions; see Section 2. In Section 3, it is shown that this new set of particle distribution functions delivers the relevant equations applicable to flows in Cartesian, cylindrical and spherical coordinates. In Section 4, additional source functions to incorporate body forces are described and, in Section 5, the energy equation is derived employing a new set of particle distribution functions. In Section 6, the simple modifications necessary for the equations to be applicable to incompressible fluids are listed. Next, in Section 7 some comments on the incorporation of Dirichlet and stress boundary conditions, and validation results, based on the works which have appeared, are presented. Further, in Section 8, using the cylindrical coordinate version of the evolution equations, numerical modelling of the steady flow of a Bingham fluid and the Herschel–Bulkley fluid in a pipe of circular cross-section have been performed have been performed and compared with the simulation results using the augmented Lagrangian method as well as the analytical solutions for the velocity field and the flow rate. Finally, in the Concluding Remarks, some comments on the theoretical differences between the present approach and the existing formulations regarding Lattice Boltzmann Equations are offered.

It has to be noted that additional source functions have been employed in modelling non-swirling, axisymmetric flows of incompressible Newtonian fluids in cylindrical coordinates; for example, see the review by Huang and Lu [11], which has been extended to every axisymmetric flow in the review by Zhang et al. [12]. In these two reviews, the derivations are based on expanding the particle distribution functions as a Taylor series in $\mathbf{u}$, retaining terms up to order $|\mathbf{u}|^2$, where $\mathbf{u}$ is the macroscopic velocity. In the derivation employed here, the expansion occurs as a Taylor series in the microscopic particle velocity $\boldsymbol{\xi}_\alpha$, retaining terms up to $|\boldsymbol{\xi}_\alpha|^2$. As shown in Appendix A, it is not easy to compare the two methods of derivation. Leaving this aside, in the reviews [11,12], one finds that two time partial derivative time scales may be needed in some models. Or, two different sets of source terms are needed in recovering the Navier–Stokes equations. In the present work, only one relaxation time is needed and only one set of source functions is needed in cylindrical and spherical coordinates and none in Cartesian coordinates. Additionally, there are other differences between the source functions in [11,12] and those needed here to model the flows in cylindrical coordinates; see Section 3.2.

Finally, it has to be emphasised here that the evolution equations deal with all fluids, compressible of incompressible, and apply to every coordinate system employed regularly in fluid dynamics. Some of the dyadic products and related material used in the body of the paper, along with direct verifications that the equations of motion are correctly derived in cylindrical and spherical coordinates, are provided in Appendix B.

2. Particle distribution function

First of all, the evolution equation is usually written as follows:

$$\frac{\partial f_\alpha}{\partial t} + \boldsymbol{\xi}_\alpha\cdot\nabla f_\alpha = -\frac{1}{\varepsilon\,\tau}(f_\alpha - f_\alpha^{eq}), \tag{2.1}$$

where $\boldsymbol{\xi}_\alpha$ are the lattice vectors, modelled after the D3Q15 lattice and defined in Table 1 below, and ε is a small parameter to be prescribed when numerical simulations are considered, τ is the collision relaxation time, and f_α^{eq} is the equilibrium distribution function. One notes that in numerical modelling, the product $\varepsilon\tau$ is replaced by a suitably chosen non-dimensionalised time step.

In order to consider three dimensional flows, whether they be in Cartesian or cylindrical or spherical coordinates, the evolution Eq. (2.1) has to be modified. That is, the evolution equation for the particle

Table 1
Subscripts and microscopic velocities.

Value of α	ξ_α/σ
0	$\mathbf{0}$
1	$\mathbf{e}_1$
2	$\mathbf{e}_2$
3	$-\mathbf{e}_1$
4	$-\mathbf{e}_2$
5	$\mathbf{e}_3$
6	$-\mathbf{e}_3$
7	$\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3$
8	$-\mathbf{e}_1+\mathbf{e}_2+\mathbf{e}_3$
9	$-\mathbf{e}_1-\mathbf{e}_2+\mathbf{e}_3$
10	$\mathbf{e}_1-\mathbf{e}_2+\mathbf{e}_3$
11	$\mathbf{e}_1+\mathbf{e}_2-\mathbf{e}_3$
12	$-\mathbf{e}_1+\mathbf{e}_2-\mathbf{e}_3$
13	$-\mathbf{e}_1-\mathbf{e}_2-\mathbf{e}_3$
14	$\mathbf{e}_1-\mathbf{e}_2-\mathbf{e}_3$