INTERNATIONAL JOURNAL FOR NUMERICAL METHODS IN FLUIDS
Int. J. Numer. Meth. Fluids 2005; **47**:1245–1251
Published online 27 January 2005 in Wiley InterScience (www.interscience.wiley.com). DOI: 10.1002/fld.914

Numerical modelling of solid particle motion using a new penalty method

T. N. Randrianarivelo*,†, G. Pianet, S. Vincent and J. P. Caltagirone

TRansferts Ecoulements FLuides Energetique (*TREFLE*), *UMR CNRS 8508*, *Site ENSCPB 16 Avenue Pey Berland 33607 PESSAC Cedex*, *France*

SUMMARY

The present article reports on an original implicit tensorial penalty method (ITPM) for modelling solid particle motion in an incompressible flow. The basic idea is to decompose the viscous stress tensor of Navier–Stokes equation into contributions representing elongation, pure shearing and rotation. An artificial viscosity is associated to each stress contribution. The penalty method is used to impose different stress components thanks to a generalized augmented Lagrangian method implemented by introducing four Lagrange multipliers. An iterative Uzawa algorithm is finally used to achieve the numerical solution. The classical problems of Couette's flow between two coaxial cylinders and the settling of a particle in a tank filled with a viscous fluid have been chosen to demonstrate the capability of the new method. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: Navier–Stokes; penalty method; stress tensor; direct numerical simulation; multiphase flows; liquid/particle interactions

1. INTRODUCTION

Numerous problems motivated by applications from environment and engineering sciences involve multiphase flows with coupled stress interactions. In this regard, modelling of solid particle motion in a surrounding fluid has received a considerable research interest. The adoption of unstructured grid techniques for numerical modelling of such complex flow phenomena is known to be costly in terms of computational time. Numerical modelling using a fixed grid mesh is an interesting alternative. However, careful handling of different stress components should be employed for accurate distinction between the fluid and solid phases.

*Correspondence to: T. N. Randrianarivelo, TRansferts Ecoulements FLuides Energetique (TREFLE), UMR CNRS 8508, Site ENSCPB 16 Avenue Pey Berland 33607 PESSAC Cedex, France.
†E-mail: randrian@enscpb.fr

Contract/grant sponsor: Publishing Arts Research Council; contract/grant number: 98-1846389

Received 27 April 2004
Revised 2 September 2004
Accepted 14 September 2004

Several popular numerical modelling approaches permit to impose specific stresses in the motion equations, for example the immersed boundary (IB) method of Peskin [1], the Brinkman penalty technique of Arquis and Caltagirone [2] or the fictitious domain approach of Glowinski *et al.* [3]. All the above-mentioned methods are based on introducing extra terms in the Navier–Stokes equations in order to locally modify the motion equations according to the local characteristics of the media.

In the present work, a general formulation for solving incompressible multiphase flows involving gas, liquid and solid particles is proposed. The basic idea of our work is to consider all the media as fluid with specific rheological properties. In this way, a multiphase flow problem could be treated with a single set of equations.

The present article is organized as follows. The original decomposition of the stress tensor for Newtonian fluids and its numerical implementation is first presented. The application of the implicit tensorial penalty method (ITPM) to treat incompressibility stress and solid behaviour is described in Section 2. The problems of Couette's flow between two coaxial cylinders and the settling of a particle in a tank filled with a viscous fluid have been chosen to demonstrate the capability of the new method in the last section.

2. NEW FORMULATION OF THE STRESS TENSOR AND TENSORIAL PENALTY METHOD

The classical governing equations of an incompressible flow can be written as

$$\begin{aligned} \nabla \cdot \mathbf{u} &= 0 \\ \rho\left(\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u})\right) &= -\nabla p + \rho \mathbf{g} + \nabla \cdot \bar{\bar{\sigma}} + \mathbf{S}_t \end{aligned} \tag{1}$$

where $\mathbf{u}$ is the velocity, ρ the density, t the time, p the pressure, $\mathbf{g}$ the gravity vector, $\bar{\bar{\sigma}}$ the stress tensor, $\mathbf{S}_t$ an additional source term. The stress tensor $\bar{\bar{\sigma}}$ for a viscous Newtonian fluid (see Reference [4]) is written

$$\bar{\bar{\sigma}} = -p\bar{\bar{Id}} + \lambda \nabla \cdot \mathbf{u}\, \bar{\bar{Id}} + 2\mu \bar{\bar{D}} \tag{2}$$

where λ and μ are, respectively, the compression and dynamic viscosities and $\bar{\bar{D}} = \frac{1}{2}(\nabla \mathbf{u} + \nabla^t \mathbf{u})$ is the tensor of deforming rate and $\bar{\bar{Id}}$ the identity matrix.

2.1. *An original formulation of stress tensor*

The aim is to reformulate the problem so as to include terms representing different natural contributions of the stress tensor dealing with compression, tearing, shearing and rotation. This decomposition facilitates the distinct penalty of each term in order to strongly impose the associated stress (see Reference [5]). In fact, these terms originally exist in the classical formulation. However, they are explicitly exhibited in the governing equations thanks to the new introduced formulation. The intermediate formulation of $\bar{\bar{\sigma}}$ is

$$\bar{\bar{\sigma}} = -p\bar{\bar{Id}} + \lambda\nabla\cdot\mathbf{u}\,\bar{\bar{Id}} + 2\mu(\nabla\mathbf{u} - \bar{\bar{\Omega}})$$

in which $\bar{\bar{D}}$ is removed by a combination of the second order tensor $\nabla\mathbf{u}$ and its asymmetrical part $\bar{\bar{\Omega}}$ [4]. The final form is

$$\bar{\bar{\sigma}} = (-p + \lambda\nabla\cdot\mathbf{u})\bar{\bar{Id}} + \kappa\bar{\bar{\Lambda}} + \zeta\bar{\bar{\Theta}} - \eta\bar{\bar{\Gamma}} \tag{3}$$

where $\nabla\cdot\mathbf{u}$ represents the compression term, $\bar{\bar{\Lambda}}$, $\bar{\bar{\Theta}}$ and $\bar{\bar{\Gamma}}$, respectively, represents the elongation pseudo-tensor, pure shearing and the rotation pseudo-tensor. The designation of pseudo-tensor is used since $\bar{\bar{\Lambda}}$, $\bar{\bar{\Theta}}$ and $\bar{\bar{\Gamma}}$ do not verify the classical tensorial properties of continuum mechanics. Artificial viscosity coefficients (κ, ζ, η) have been associated to each viscous stress. It should be noted that the values of λ, κ, ζ, η correspond to $-\frac{2}{3}\mu$, 2μ, 2μ, μ in the classical formulation. The stress tensor formulation of (3) can be explicitly written in a tensorial form in Cartesian co-ordinates as

$$\bar{\bar{\sigma}} = \begin{bmatrix} -p + \lambda\nabla\cdot\mathbf{u} & 0 & 0 \\ 0 & -p + \lambda\nabla\cdot\mathbf{u} & 0 \\ 0 & 0 & -p + \lambda\nabla\cdot\mathbf{u} \end{bmatrix} + \kappa \begin{bmatrix} \frac{\partial u}{\partial x} & 0 & 0 \\ 0 & \frac{\partial v}{\partial y} & 0 \\ 0 & 0 & \frac{\partial w}{\partial z} \end{bmatrix}$$
$$+\zeta \begin{bmatrix} 0 & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & 0 & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & 0 \end{bmatrix} - \eta \begin{bmatrix} 0 & \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} & \frac{\partial u}{\partial z} - \frac{\partial w}{\partial x} \\ \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} & 0 & \frac{\partial v}{\partial z} - \frac{\partial w}{\partial y} \\ \frac{\partial w}{\partial x} - \frac{\partial u}{\partial z} & \frac{\partial w}{\partial y} - \frac{\partial v}{\partial z} & 0 \end{bmatrix} \tag{4}$$

2.2. Generalized UZAWA algorithm for ITPM

In the adoption of an Eulerian–Eulerian approach, it is necessary to distinguish between different media Ω_i appearing in the domain. The ITPM can then be applied to penalize stress components in the domain, according to the media. A distribution function $C_i(M,t)$, also called volume fraction, has been associated to each phase. Values of the volume fraction in the domain are obtained solving an auxiliary advection equation, $\partial C_i/\partial t + \mathbf{u}\cdot\nabla C_i = 0$, using a volume of fluid (V.O.F.) method [6]. $C_i(M,t) = 1$ if M belongs to Ω_i and $C_i(M,t) = 0$ otherwise. The interface between different Ω_i is then defined as $C_i(M,t) = 0.5$. Fluid properties (density, viscosity, etc.) have been evaluated as functions of the value of volume fraction. The penalty method adopted for solving motion equations (1) and (3) is described as follows.

We have implemented a generalized augmented Lagrangian approach first developed by Fortin [7] who considered the pressure p (referred as lg_1 in the present study) as a Lagrange multiplier which accumulates the constraint of incompressibility. Following this work, tensorial Lagrange multipliers $l\bar{\bar{g}}_2$, $l\bar{\bar{g}}_3$, $l\bar{\bar{g}}_4$ have been introduced to accumulate the corresponding constraints on Λ, Θ or Γ. The associated Lagrangian $L(\mathbf{u}, lg_1, l\bar{\bar{g}}_2, l\bar{\bar{g}}_3, l\bar{\bar{g}}_4)$ that should be minimized under several constraints is defined as

$$L(\mathbf{u}, lg_1, l\bar{\bar{g}}_2, l\bar{\bar{g}}_3, l\bar{\bar{g}}_4) = \int_\Omega \left(\rho\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u}\cdot\nabla\mathbf{u}\right) - \rho\mathbf{g}\right)\mathbf{u}\,\mathrm{d}\Omega$$
$$+ \int_\Omega \nabla\cdot((lg_1 - \lambda(\nabla\cdot\mathbf{u} - (\nabla\cdot\mathbf{u})^\infty))\bar{\bar{Id}})\,\mathbf{u}\,\mathrm{d}\Omega + \int_\Omega \nabla\cdot(l\bar{\bar{g}}_2 - \kappa(\bar{\bar{\Lambda}} - \bar{\bar{\Lambda}}^\infty))\,\mathbf{u}\,\mathrm{d}\Omega$$
$$+ \int_\Omega \nabla\cdot(l\bar{\bar{g}}_3 - \zeta(\bar{\bar{\Theta}} - \bar{\bar{\Theta}}^\infty))\mathbf{u}\,\mathrm{d}\Omega - \int_\Omega \nabla\cdot(l\bar{\bar{g}}_4 - \eta(\bar{\bar{\Gamma}} - \bar{\bar{\Gamma}}^\infty))\,\mathbf{u}\,\mathrm{d}\Omega \quad (5)$$

where $(\nabla\cdot\mathbf{u})^\infty, \bar{\bar{\Lambda}}^\infty, \bar{\bar{\Theta}}^\infty, \bar{\bar{\Gamma}}^\infty$ are reference values to impose when λ, κ, ζ and η admit significant orders of magnitude leading to penalty. A correct penalty is ensured choosing the values of the new viscosities such that the magnitude of $(\lambda\nabla\cdot\mathbf{u})\bar{\bar{Id}}$, $\kappa\bar{\bar{\Lambda}}$, $\zeta\bar{\bar{\Theta}}$ and $\eta\bar{\bar{\Gamma}}$ is 10^2–10^3 times the most important term (inertia, gravity, viscous force) in the Navier–Stokes equations.

The minimization of $L(\mathbf{u}, lg_1, l\bar{\bar{g}}_2, l\bar{\bar{g}}_3, l\bar{\bar{g}}_4)$ is realized using a generalized UZAWA algorithm. The solution procedures are described as follows:

- Source term in the Navier–Stokes equations (1) can now be written as $\mathbf{S}_t = \nabla\cdot((lg_1^n - \lambda\nabla\cdot\mathbf{u})Id) + \nabla\cdot(l\bar{\bar{g}}_2^n - \kappa\bar{\bar{\Lambda}}^\infty) + \nabla\cdot(l\bar{\bar{g}}_3^n - \zeta\bar{\bar{\Theta}}^\infty) - \nabla\cdot(l\bar{\bar{g}}_4^n - \eta\bar{\bar{\Gamma}}^\infty)$
- Knowing lg_1^0 and $l\bar{\bar{g}}_i^0$ for $i\in\{2,3,4\}$, Lagrange multipliers lg_i^{n+1} are computed as

$$lg_1^{n+1} = lg_1^n - \lambda\nabla\cdot\mathbf{u}, \quad l\bar{\bar{g}}_i^{n+1} = l\bar{\bar{g}}_i^n - \alpha_i\bar{\bar{T}}_i$$

with $\alpha_2 = \kappa$, $\alpha_3 = \zeta$, $\alpha_4 = \eta$ and $\bar{\bar{T}}_2 = \bar{\bar{\Lambda}}$, $\bar{\bar{T}}_3 = \bar{\bar{\Theta}}$, $\bar{\bar{T}}_4 = \bar{\bar{\Gamma}}$.

2.3. Numerical solution

Implicit finite volumes on a fixed Cartesian staggered grid are used to discretize the motion equations. The time derivatives are approximated by an Euler scheme of first order whereas the spatial fluxes are interpolated by centred schemes of second order. The resulting linear system is solved by an iterative procedure of conjugate gradient for non-symmetric matrix BiCGSTAB II [8], preconditioned with an incomplete Gauss factorization ILU [9].

The piecewise linear interface construction [6] method has been utilized to solve the advection equation of the volume fraction $C_i(M,t)$.

3. VALIDATIONS AND APPLICATIONS

3.1. Couette's flow

The simulation of the fundamental Couette's flow between two coaxial cylinders ($R_\mathrm{i} \leqslant R_\mathrm{e}$) on Cartesian grid has been chosen to verify the accuracy of ITPM. The rotation of the inner completely solid cylinder of radius R_i, drives the viscous fluid contained in the annular zone of the two cylinders. Since the inner solid is moving with a constant angular velocity Ω_0, this zone is characterized by a constant rotation pseudo-tensor and a non-deformable property. This offers us the opportunity to impose the rotation pseudo-tensor $\bar{\bar{\Gamma}}$ using ITPM. This behaviour

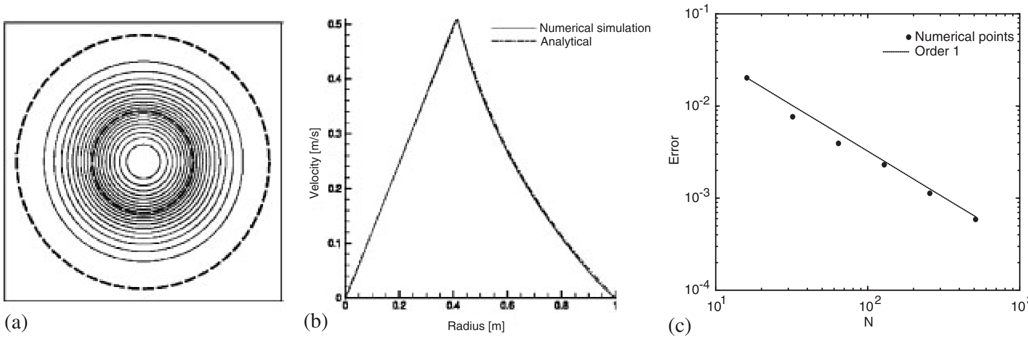

Figure 1. Couette flow between two coaxial cylinders: (a) Streamlines (128×128 Cartesian grid); (b) velocity profile; and (c) space convergence study.

of solid motion has been modelled by assigning a value equal to 10^9 to the rotation viscosity η. Incompressibility has been achieved using a variable augmented Lagrangian technique developed in Reference [10]. The flow field is characterized by circular streamlines both in solid and fluid areas (Figure 1(a)). The comparison with the analytical velocity profile is depicted on Figure 1(b). A space convergence study has been carried out and demonstrates order 1 (Figure 1(c)).

3.2. Settling of solid particles in Stokes' regime

We have also considered a spherical solid particle initially dropped without initial velocity in a cylindrical tank filled with a viscous fluid. Under the influence of gravity, the particle is instantaneously accelerated and falls in the viscous fluid to reach its terminal settling velocity, u_{ts}, when gravity forces balance drag force. Analytical Stokes' solution, characterized by a Reynolds number $Re_p = 2\rho_f R_p u_{ts}/\mu_f \leqslant 1$, is available for an infinite medium. However, Stokes' velocity is modified as

$$u_{ts} = \frac{2}{9}\frac{(\rho_p - \rho_f)}{\mu C_w} g R_p^2 \tag{6}$$

as soon as wall effects are not negligible. R_p is the particle radius, μ the fluid viscosity and C_w a correction factor taking into account wall interactions. C_w depends on the ratio between particle radius R_p and tank radius. Several studies have been carried to determine C_w. Comparisons of our numerical values of C_w with literature data are presented in Figure 2 showing the agreement between the present numerical computations and the exact theory of Haberman [11]. The order of space convergence is equal to 1.3.

3.3. Unsteady 3D simulations of a sphere settling in a tank

Further simulations have been carried out for the unsteady behaviour of a sphere settling in a tank. Comparisons have been made with PIV measurements [12] of a settling sphere with Re_p ranging from 1.5 to 31.9. Experimental and numerical particle velocities are compared in Figure 3(a). Concerning the $Re_p = 31.9$ case, a slice of the flow field is extracted when the sphere's centre is one diameter away from the tank's bottom, and a comparison of the

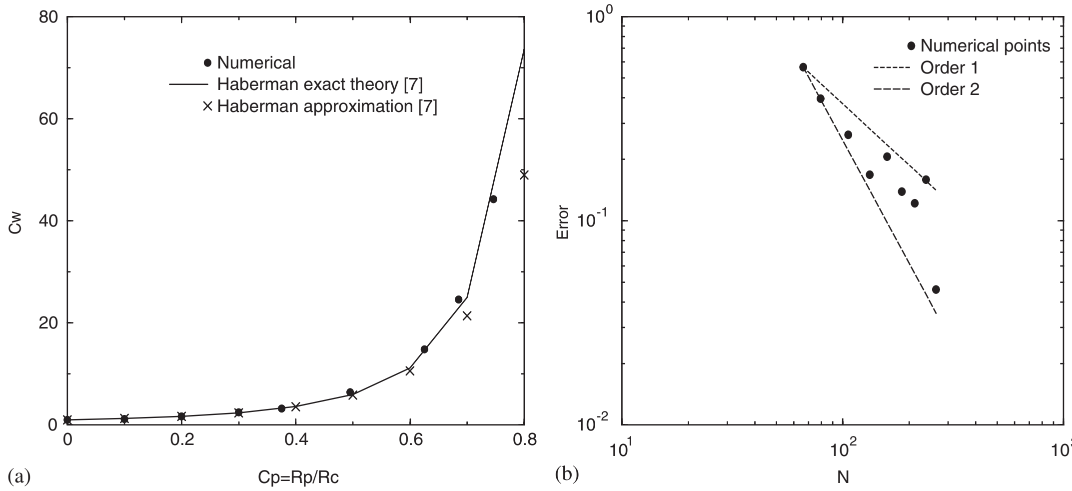

Figure 2. Settling of solid particle ($Re \ll 1$): (a) Comparison of present computed C_{w} with Haberman data; and (b) space convergence study.

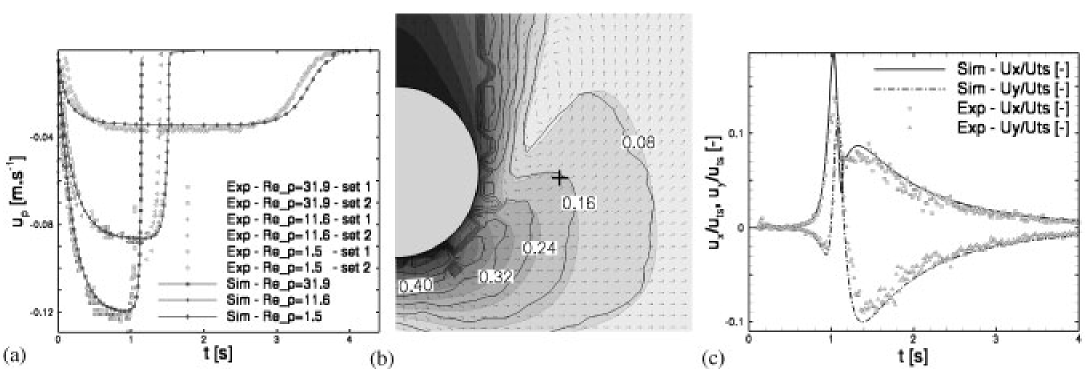

Figure 3. Settling of solid particle ($Re > 1$): (a) Particle velocity (E = experimental, S = simulation); (b) flow field $|u|/u_{\mathrm{ts}}$, $Re_{\mathrm{p}} = 31.9$, Experimental (lines) and Numerical (grey levels); and (c) fluid timeseries on a monitoring point (cf. black cross from (b)), $Re_{\mathrm{p}} = 31.9$.

velocity magnitude field $|u|/u_{\mathrm{ts}}$ is shown in Figure 3(b). Figure 3(c) represents the velocity components u_x/u_{ts} and $u_{\mathrm{y}}/u_{\mathrm{ts}}$ as functions of time on a monitor point. These results show that particle transient motion as well as fluid behaviour are well predicted by the ITPM method.

4. CONCLUSION AND PROSPECTS

A new implicit tensorial penalty method (ITPM) has been presented for modelling solid particle motion in flows with a single set of equations. Stress tensor $\bar{\bar{\sigma}}$ has been first decomposed into compression, elongation, shearing and rotation contribution, respectively, noted $\nabla \cdot \mathbf{u}, \bar{\bar{\Lambda}}, \bar{\bar{\Theta}}$ and $\bar{\bar{\Gamma}}$. Four viscosities $\lambda, \kappa, \zeta, \eta$ have been associated to each contribution. The distinction between fluid and solid regions is then realized with a distribution function. A generalized augmented Lagrangian approach associated to an iterative Uzawa algorithm has been implemented to solve governing equations. The classical Couette flow between two coaxial cylinders problem has been chosen to test the imposition of a constant rotation of a solid. The settling of solid particle in confined configurations for a large range of Reynolds number has been studied.

ACKNOWLEDGEMENTS

This work was supported by Publishing Arts Research Council under grant number 98–1846389

REFERENCES

1. Peskin CS. Numerical analysis of blood low in the heart. *Journal of Computational Physics* 1977; **25**:220–252.
2. Arquis E, Caltagirone JP. Sur les conditions hydrodynamiques au voisinage d'une interface milieu fluide-milieu poreux: application la convection naturelle. *Comptes Rendus de l'Académie des Sciences Série II b* 1984; **299**:1–4.
3. Glowinski R, Pan TW, Periaux J. A fictious domain method for external incompressible viscous flow modeled by Navier–Stokes equations. *Computer Methods in Applied Mechanics and Engineering* 1994; **112**:133–148.
4. Ryhming I. *Dynamique des Fluides*. Presses Polytechniques: Romanes, 1985.
5. Caltagirone JP, Vincent S. Tensorial penalty method for solving Navier–Stokes equations. *Comptes Rendus de l'Académie des Sciences Paris, Série II b* 2001; **329**:607–613.
6. Youngs DL. Time-dependent multimaterial flow with large fluid distortion. In *Numerical Methods for Fluid Dynamics*, Morton KW, Baines MJ (eds). Academic Press: New York, 1982.
7. Fortin M, Glowinski R. *Méthodes de lagrangien augmenté. Application à la résolution numérique de problèmes aux limites*. Dunod: Paris, 1982.
8. Vincent S, Caltagirone JP. A one cell local multigrid method for solving unsteady incompressible multi-phase flows. *Journal of Computational Physics* 2000; **163**:172–215.
9. Gustafsson I. *On First and Second Order Symmetric Factorization Methods for the Elliptic Difference Equation*. Chalmers University of Technology, 1978.
10. Vincent S, Caltagirone JP, Lubin P, Randrianarivelo TN. An adaptative augmented Lagrangian method for three-dimensional multi-material flows. *Computers and Fluids* 2004; **33**:1273–1289.
11. Haberman WL, Sayre RM. *David Taylor Model Basin Report No. 1143*, U.S. Navy Dept., Washington, D.C., 1958.
12. ten Cate A, Nieuwstad CH, Derksen JJ, Van den Akker HEA. Particle imaging velocimetry experiments and lattice-Boltzmann simulations on a single sphere settling under gravity. *Physics of Fluids* 2000; **14**(11):4012–4025.
13. Happel J, Brenner H. *Low Reynolds Number Hydrodynamics*. Kluwer Academic Publishers: Dordrecht, 1963.
14. Khadra K, Angot P, Parneix S, Caltagirone JP. Fictious domain approach for numerical modelling of Navier–Stokes equations. *International Journal for Numerical Methods in Fluids* 2000; **34**:651–684.

