Recent Advances in Computational Simulation of Macro-, Meso-, and Micro-Scale Biomimetics Related Fluid Flow Problems

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Abstract

Over the last decade, computational methods have been intensively applied to a variety of scientific researches and engineering designs. Although the computational fluid dynamics (CFD) method has played a dominant role in studying and simulating transport phenomena involving fluid flow and heat and mass transfers, in recent years, other numerical methods for the simulations at meso- and micro-scales have also been actively applied to solve the physics of complex flow and fluid-interface interactions. This paper presents a review of recent advances in multi-scale computational simulation of biomimetics related fluid flow problems. The state-of-the-art numerical techniques, such as lattice Boltzmann method (LBM), molecular dynamics (MD), and conventional CFD, applied to different problems such as fish flow, electro-osmosis effect of earthworm motion, and self-cleaning hydrophobic surface, and the numerical approaches are introduced. The new challenging of modelling biomimetics problems in developing the physical conditions of self-clean hydrophobic surfaces is discussed.

Keywords: biomimetics, computational simulation, macro-, meso-, micro-scale, hydrophobic, surfaces

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1 Introduction

In the natural world, plants and animals have evolved over time to best adapt to the environment. For example, earthworms and other soil animals such as dung beetles can move efficiently in mud or moist soil without sticking to it. Sharkskin has built-in drag reduction which ensures that the shark can swim at very high speed. The lotus leaf can repel water and remove contaminants and clean its surface. The nests of termites are built with effective natural ventilation and air-conditioning, *etc.* Such interesting phenomena have drawn attention and a new subject area called biomimetics has been developed.

Biomimetics, which may be interpreted as “abstraction of good design from nature”^[1], could help to find solutions to improve technological designs and provide appropriate models for developing efficient and sustainable engineering functional surfaces for technological application. Plants and animals interact very effectively with the environment by exchanging energies

and mass flow across their cuticles of specific micro structures and functions to achieve energy balance and high efficiency. To mimic these in technological design, the interaction between the functional surfaces and the surrounding environments should be better understood, their physical nature should be effectively modelled and simulated. Indeed computational modelling can certainly supply efficient numerical experiments to get the best or optimised approaches, as long as the theoretical models can be developed. For example, conventional methods of CFD have been used for modelling a fish-like body moving in viscous liquid such as water^[2–4] and the explosive discharge of the bombardier beetle for the design of novel engine components^[5]. However for many biological functional surfaces of microstructures, good design of technological functional surfaces imitated from biological surface morphologies may not just be a simple geometrical analogy; the conditions of physical similarity need to be identified and satisfied; other numerical methodologies beyond the conventional CFD at micro or meso scales may be necessary. Thus,

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there is the need to develop physical and numerical models for transferring biological low adhesive super-hydrophobic surfaces for the design of self-cleaning surfaces of engineering materials.

By taking advantage of increasing computer power, CFD has been playing an increasingly important role in scientific numerical calculations and in industrial and engineering designs. CFD, as a major tool for solving transport equations (Navier-Stokes types equations), has been applied to almost all types of design of industrial processes or facilities involving fluid flows. Typical examples include numerical predictions of fluid flow in various engineering channels and flows across surfaces with different configurations, simulation of multiphase flow or mixing in reactors or combustion chambers, and flow and heat transfer in heat exchangers. In recent years, there has been a great deal of effort focused towards understanding the complex physics of fluid flow in different engineering domains, multiphase free surface flow and fluid interaction with different surfaces including biological interfaces. Meanwhile, scientist and engineers have started to explore novel numerical methods to predict the transport phenomena in sub-micro and nano-scale regimes due to its importance in development of next generation integrated circuits, ultra-fast laser processing, micro scale systems and a host of emerging technologies^[6].

In parallel with the development of conventional CFD techniques, which are based on continuum theory using mainly the finite volume method (FVM) and finite element method (FEM) for solving Navier-Stokes equations, the meso- and micro-scale methods have recently been developed. As a typical meso-scale method, the lattice Boltzmann method (LBM) has many computational advantages^[7]. Residing on the mesoscopic level, the LBM simulates fluid flow by tracking the development of distribution functions of assemblies of molecules. In doing so, the LBM is able to incorporate the interaction of fluid particles, which is the physical origin of phase segregation and surface tension. The interfacial dynamics, which is essential for multiphase flow but difficult to deal with at the macroscopic level, can be readily modelled using the LBM by incorporating the interaction of fluid particles. In addition,

the LBM is computationally more efficient than molecular dynamics, as it avoids tracking individual molecules and the solution procedure is explicit and easy to implement and parallelize. Thus, the LBM has been developed into a promising numerical scheme for simulating complex fluid flows, phase separation or mixing, and dealing with complex interfaces. In terms of micro/nano-scale simulation, molecular dynamics (MD) method and direct simulation of Monte Carlo (DSMC) method have rapidly been developed and applied to simulate various complex physics problems, while the simulations covered both micro/nano-scale geometries and micro time scales^[8,9].

In recent years, significant progress has been made on coupling macro-scale simulation that is normally based on conventional CFD with molecular level simulation^[10,11]. The development of high performance computer (HPC) has promoted such coupling approaches and parallel calculations. This has made it possible to simulate numerically many difficult physics problems with complex biological interfaces. This article starts with a review of the author's recent work and advances in multi-scale modelling of fluids flow related problems at Nottingham University, and then raises the new challenge of modelling biomimetics problems in developing the physical conditions of self-clean hydrophobic surfaces.

2 CFD modelling of macro-scale biomimetic fluid flow and the built environment

Conventional CFD methods have been applied to simulate numerically biomimetic problems since the 1980s. Most popular numerical work^[2,3] model the motion of fish-like bodies in water based on turbulence theory of conventional fluid mechanics. Recent work at the University of Nottingham (Fig. 1) has demonstrated using the commercial CFD code FLUENT to simulate this type of biomimetic problem^[4]. Other examples of using commercial CFD code to study biomimetics problems include simulation of flapping^[12] and the explosive discharge of the bombardier beetle^[5,13].

Researchers at the University of Leeds are studying the bombardier beetle's unique natural "combustion" technique to see if it can be copied for use in the aircraft

Fig. 1 CFD simulation of fish-like body in water^[4].

Fig. 2 A bombardier beetle ejecting its water-steam jet at 100°C^[13].

industry. Understanding the bombardier beetle's jet-based defence mechanism (Fig. 2) may help to solve a problem that can occasionally occur at high altitude – reigniting a gas turbine aircraft engine which has cut out, when the outside air temperature is as low as -50° .

In addition, to learn from natural or animal architectures of natural ventilation, commercial codes such as PHOENICS and FLUENT have been used to study problems of climate in the built environment and urban planning. Fig. 3 shows recent results of the numerical simulation of environmental design of thermal ventilation of a new urban district in Dubai^[14]. The pressure and temperature distributions around the buildings could lead to further considerations of how to improve the local environmental designs. Fig. 4 shows the results of commercial CFD code of FLUENT used for evaluating the effect of air flow ventilation on “SARS” virus distribution in new sick buildings — Amoy garden, Hong Kong^[15]. Fig. 4a shows a map of garden and buildings; Fig. 4b shows the loss maintained in external sewage pipes and window-style air-conditioning systems; Fig. 4c

presents the results of a CFD simulation of wind velocity distribution at the fifth floor with wind speed at $5 \text{ m}\cdot\text{s}^{-1}$; while Fig. 4d shows the enlarged local distribution of Fig. 4c. It is clear that the wind curtain effect has resulted in the virus staying in the narrow gap of the buildings for locating the drainage pipelines, shown as the low pressure and velocity zones. The virus zones contribute greatly to the SARS outbreak as window style air-conditioning systems are well linked with these low-pressure zones. Numerical experiments are carried out much more easily and better results of environmental improvement can be obtained. Fig. 4e shows one of the improved results; the ventilation in the gap area is significantly improved by enlarging the gap from 1.5 m to 3 m.

The numerical experiments conducted in Fig. 4 indicate that a design tool based on the CFD simulations can be developed to predict a potential artificial disaster at the stages of designing and planning rather than to study on possible solutions of repairing or improvement after it has taken place.

Fig. 3 CFD simulation for Dubai environmental design^[14].

Fig. 4 CFD experiment of narrow gap effect on virus distribution in Amoy garden^[15].

3 The challenge and limitation in developing biomimetic functional surfaces

It is well known that the fundamental interactions between an organism and its environment occur at interfaces. This is the reason why biological surfaces became optimised multifunctional interfaces over millions of years of evolution. Different functions, for example the limitation of uncontrolled loss of water, protection from solar radiation, micro effect of induced turbulence on flow drag reduction, defence against pathogens, *etc.* lead to a great variety of complex three dimensional

surface structures at microscopic levels.

Materials scientists have long been interested in generating low or non-adhesive surfaces, but their only approach was by generating ultra-smooth interfaces. Since 1995, the discovery of super-hydrophobic micro- and nano-structured biological surfaces has led to remarkable innovation in this field^[16]. In recent years, research in biological functional surfaces has become one of the most important topics in biomimetics. Scientists today are increasingly searching out interesting animals and plants to gain design insights that will help them create novel materials and compounds. A few

examples of the transfer of biological morphologies of plants and animals to technological applications can be identified, which includes the structural colours of the Morpho butterfly, the anti-reflective glass and plastic surfaces based on the cornea model of nocturnally active moths, the riblet foils on airplanes similar to the shark-skin, and bionic roughness on the plough mouldboard copied from dung beetles' surface structures^[17–19]. These designs were derived using the scanning electron microscope (SEM) and the theory of geometrical similarity. Indeed this is very difficult because, in a microscopic view, biological surfaces often show an unexpected variety of complex three dimensional micro- and nano-structures. Many plants, such as the lotus leaves, are characterised by two levels of texture combined with hydrophobic surface chemistry. Barthlott *et al.* have pioneered research of the lotus-effect and designing water repellent functional surfaces for engineering materials^[20]. By observing water droplets resting on biological surfaces, it is found that due to the combination of micro roughness and hydrophobicity, water droplets roll off even at slight inclinations; and this property of super-hydrophobic (non-wettable) surfaces is defined as the ability of self-cleaning. The science behind this phenomenon is that the surface structure of micro roughness leads to an extreme reduction of both contact areas between the water droplet and the surface and between the contaminant particles and the surface, as shown in Figs. 5 and 6^[20].

Fig. 5 Mercury droplet on the adaxial leaf surface of *Colocasia esculenta* demonstrating the lotus-effect, Bar: 50 μm .

Biological anti-adhesive surfaces are of great technological interest nowadays. Scientists and engineers have made much effort to transfer or imitate the

biological functional surface structures to technological surfaces of engineering materials. During the past decade, significant studies on micro surface structures of different species have been made by scanning electron microscopy (SEM) and atomic force microscopy (AFM) to imitate engineering functional surfaces. However, most of these imitations are based on geometrical similarity; the properties of physical similarity are not properly confirmed. Although some macro physical performances may be verified through experimental measurements or tests, the actual physical similarity has not been applied to the imitations or designs. In fact, the complex microscopic morphologies of biological functional surfaces make any experimental verification of physical similarity of the imitations extremely difficult. Nevertheless, this could be realised by carrying out numerical experiments and taking advantage of increasing computer power. To verify the physical similarity of biomimetic designs, the important aspects of the models require innovative further study on:

- (1) Precise mathematical characterisation of visualised interactions between the functional surfaces and surrounding media such as water with contaminant particles.
- (2) More advanced understanding of the effect of surface morphology on the physics of media behaviours.

Fig. 6 Particle and water droplet roll off on smooth surface (left) and on micro roughness surface (right).

4 Modelling of droplets on hydrophilic and hydrophobic surfaces

The physical models of a biological surface interacting with its surrounding media will be increasingly important tools for transferring biological low adhesive and super-hydrophobic surfaces to technological applications. To date the studies on such models are still very

limited, numerical approaches have not been achieved effectively. To simulate the behaviour of a biological or imitated functional surface interacting with the environment, the surface with specific micro morphology and its surrounding media such as water with contaminant particles must be considered as one system. The interaction takes place at the interface of the biological or imitated solid surface and surrounding multiphase fluids.

In the present study at Nottingham, a water droplet at normal temperature surrounded by air spreads on partial wetting surfaces is studied and simulated^[21]. Naturally, the densities of two fluids (water and air) are at $\rho_L = 1 \times 10^3 \text{ kg} \cdot \text{m}^{-3}$ and $\rho_G = 1.29 \text{ kg} \cdot \text{m}^{-3}$ (density ratio is about 775), the initial surface tension between water and air is $\sigma_{LG} = 1 \times 10^{-3} \text{ kg} \cdot \text{s}^{-2}$. In the current approaches, the motion of water droplet on a hydrophilic surface with a hydrophobic stripe is simulated successfully using a new scheme of the lattice Boltzmann method^[21].

According to the Young's law^[22], when a liquid-gas interface meets a partial wetting solid wall, the contact angle, θ_w , measured in the liquid, can be calculated from a balance of surface tension forces at the contact line as

$$\cos \theta_w = \frac{\sigma_{SG} - \sigma_{SL}}{\sigma_{LG}}, \quad (1)$$

where σ_{SG} and σ_{SL} are the solid-gas and solid-liquid surface tension forces, respectively. In the LBM

scheme^[21], such a wetting angle is represented by wetting potential Ω as

$$\cos \theta_w = \frac{(1 + \Omega)^{3/2} - (1 - \Omega)^{3/2}}{2}. \quad (2)$$

For a given wetting angle in the range of $0 < \theta_w < \pi$, Ω has the form

$$\Omega = 2 \operatorname{sgn} \left(\frac{\pi}{2} - \theta_w \right) \left\{ \cos \left(\frac{\gamma}{3} \right) \left[1 - \cos \left(\frac{\gamma}{3} \right) \right] \right\}^{1/2}, \quad (3)$$

where $\gamma = \arccos(\sin^2 \theta_w)$ and $\operatorname{sgn}(\xi)$ gives the sign of ξ .

The method was first applied to a water droplet spreading on a uniform wetting or hydrophilic surface. As shown in Fig. 7, the droplet spreads as time marching and finally reaches the equilibrium shape; the contact angle approximates to the initially predicted value as $\theta_w = \pi/4$. Fig. 8 shows another case of droplet spreading on uniform wetting surface, the droplet finally reaches an equilibrium shape with contact angle at $\theta_w = \pi/2$.

The method was also applied to water droplet spreading on heterogeneous surfaces. As shown in Fig. 9, the behaviour of a small hemispherical water droplet spreads on a heterogeneous surface is simulated. The heterogeneous surface consists of a hydrophilic surface of contact angle $\theta_w = \pi/6$ and a narrow hydrophobic strip (width of 0.6 mm) located at the centreline of the surface of contact angle $\theta_w = 5\pi/6$. The droplet stretches over the area occupied by the hydrophilic surface in the early stages of the spreading due to the

Fig. 7 Droplet spreading on uniform hydrophilic surface, $\theta_w = \pi/4$, $t = 0 \sim 0.0675 \text{ s}$ ^[21].

Fig. 8 Droplet spreading on uniform moderate surface, $\theta_w = \pi/2$, $t = 0 \sim 0.0415 \text{ s}$ ^[21].

adhesive force of the surface; meanwhile, it rapidly contracts inward along the hydrophobic strip. With the development of time, the droplet spreads further on the hydrophilic area, contracts inward along the hydrophobic strip, and finally breaks up into two smaller droplets. The newly formed droplets continue spreading until an equilibrium state is reached. For a uniform hydrophilic surface separated by a hydrophobic strip, the spreading dynamics of the droplet is affected by three parameters, namely, the width of the hydrophobic strip, the gravity and the wetting property of the hydrophilic surface^[23]. A further examination and analysis of the effects of these three parameters on spreading and break-up of the droplet will be conducted in the near

future.

5 Applications of the meso-scope lattice Boltzmann method (LBM)

On modelling of flow relevant to biomimetics, a recent work in studying on electroosmotic driving flow within the micro thin liquid layer near an earthworm body surface is shown in Fig. 10^[24]. It is interesting to note that the variation of electroosmosis force causes two vortices, formed at $t = 0$, move correspondingly along the earthworm body surface at $1 \text{ mm} \cdot \text{s}^{-1}$ within a micro thin liquid layer of 400 nm in thickness. The moving vortices can probably improve the effect of anti soil adhesion.

Fig. 9 Water droplet spreading on a heterogeneous surface, $t = 0 \sim 0.154 \text{ s}$ ^[21].

Fig. 10 LBM simulation of electroosmotical driven flow within the liquid micro layer near an earthworm surface.

The LBM was developed since the 1980s when it was mainly employed to solve Navier-Stokes equations indirectly^[25]. Only since 1991 when Gunstensen *et al.* developed the chromodynamic model^[26], has the LBM been used to simulate multiphase fluid flow problems. Since then, a few multiphase LBM models have been introduced; they are the pseudo-potential model^[27,28], the free energy model^[29] and the index-function model^[30]. In general, at present two basic types of LBM model have formed the framework for LBM modelling of phase separation. The first is the model of Shan and Chen^[27, 28], in which a simple, effective interaction potential is proposed to describe the fluid-fluid interaction. In most approaches, interface formation is introduced phenomenologically by modelling the Boltzmann collision operator to impose phase separation. The work by Shan and Chen has attempted to relate phase separation to microscopic interactions. The second approach is to incorporate the fluid-fluid interactions into a body force term in the Boltzmann equation. This LBM approach removes second order artifacts in the pressure tensor and is found to produce more realistic interfacial interactions^[31].

Preliminary work using the LBM for modelling coalescence of bubbles and droplets dominated by surface tension have been done by Takada *et al.*^[32], Inamuro *et al.*^[33], and recent at Nottingham University^[34]. In the current approaches at Nottingham, a three-dimensional 15-velocity (D3Q15) model is applied, the velocity distribution functions of two bubbles or particles are used in the lattice Boltzmann equations. One is used for calculating an order parameter which distinguishes the two phases; the other is used for calculating the velocity of a two-phase fluid without a pressure gradient. The velocity satisfying the continuity equation can be obtained by using the relation between velocity and pressure corrections which are determined by solving the Poisson equation. The coalescence of bubbles or drops with density ratio up to 1000 can be simulated. On simulating droplets spreading on partial wetting surfaces, in addition to the author's recent work shown in Figs. 7 to 9, other relevant works are reported in Ref. [35].

6 Applications of microscopic molecular dynamic (MD) method

Well-known model fluids in MD include the “hard spheres fluid”, the “square well fluid” and the “Lennard-Jones (L-J) fluid”. One of the L-J fluid important features is its realism^[36]. Also as it can show vapour-liquid, solid-liquid and solid-vapour transitions, the critical point and the triple point, the L-J is often used as a reference for modelling properties of real fluids.

Many engineering problems are concerned with fluid flow and heat transfer in micro-scale systems such as micro cooling of electronic components and micro heat exchangers. Fig. 11 indicates the contact structure of triple phase of vapour-liquid-solid during evaporation and boiling. The MD simulation method helps to get microscopic insight to the region near the triple phase interface. The influence of long-range intermolecular forces between solid and liquid on the ultra-thin liquid film can be evaluated from the microscopic point of view. The existence of ultra-thin liquid film, with a thickness of several molecular layers, is initially verified from a nanoscopic viewpoint. In this way, it is investigated from a physical-chemical perspective instead of fluid-dynamical perspective to get some findings about the effect of solid heating wall on liquid film in a completely wetting system. Thus, the phenomena of heat and mass transfer in the region near the triple-phase contact line can be studied by changing the fluid atom numbers in the system, the heating solid wall temperature, and the simulation cell size.

Fig. 11 Triple phase contact structure.

In the present investigation at Nottingham, a system with L-J fluid confined between two solid walls is studied using nonequilibrium molecular dynamics (NEMD) simulations. Fig. 12 shows the liquid film of a 1200 argon atoms system under different temperature conditions. When the heating temperature is as high as 210 K, the liquid film still exists but its thickness

is decreased to the order of only one layer of argon atoms^[37]. Liquid particles in the film are absorbed on the solid wall because of the strong intermolecular forces in the completely wetting system. Similar MD modelling for CO₂ in the vicinity of dry out region in microchannel heat sink has also been carried out recently^[38].

Fig. 12 Snapshots of 1200 Ar molecules system with different heating temperatures (only the heating wall and nearby fluids are shown).

7 Coupling continuum to molecular dynamics simulation

The major technical difficulty in constructing such methods lies in coupling these very different descriptions of fluids at MD-continuum interface. Two descriptions in the overlap region are coupled and must be consistent, and the physics quantities, including density, momentum and energy, and their fluxes, must be continuous. The boundary conditions needed for continuum equations can be straightforwardly obtained by averaging the corresponding quantities from the particle description over the local region and over time. However, the reverse problem, generating microscopic particle configurations from known macroscopic quantities such as density, momentum, and energy, is non-trivial and must necessarily be non-unique. The problem is magnified when there is a flux of particles between continuum and discrete regions. In general, there is also a time coupling issue since the integration time step for continuum N-S equations is normally several orders of magnitude larger than that in the MD region.

Several coupling schemes have been developed. O'Connell & Thompson^[39] noted that it is important to have a finite overlap region to avoid sharp density oscillations and allow the two solutions to relax before they are coupled together. They used a relaxation method to force the average MD velocity in the region to follow the continuum solution. This introduces an ar-

bitrary relaxation rate, but the more important limitation of their approach is that it does not include mass flux at the MD-continuum interface. This limited the geometries they could consider, but their approach successfully reproduced a set of one-dimensional flows. Other recent progresses on the coupling are reported in Ref. [40–42]. At Nottingham, a numerical scheme of multi-domain coupling, typically the method of boundary uniqueness treatment, has been successfully developed and validated^[43]. These have paved the way for further work of micro-continuum coupling.

8 Conclusions

In this article, the state-of-the-art technology of numerical modelling of macro-, meso- and micro- scales including the author's recent work is reviewed. The potential of computational fluid dynamics modelling for biomimetic problems and recent advances are particularly discussed. Computational fluid dynamics at different scales has been shown to be useful for simulating and studying biomimetic problems concerning with fluid-fluid interfaces contacting with functional solid surfaces. Conventional CFD methods, typically the commercial codes, can be applied to a variety of biomimetic problems. The meso-scopic lattice Boltzmann method (LBM) seems to be an attractive method for dealing with surface tension dominated liquid-solid interface problems which are relevant to many topics of developing functional surfaces such as self-cleaning

surfaces. Moreover, the micro-scale molecular dynamics (MD) simulation is a method enabling us to gain an insight into surface tension dominated fluid flow problems typically at the interfaces of different phases; nevertheless, effective coupling strategies of continuum and molecular dynamics simulation must be applied.

Acknowledgement

This work is supported by the UK Engineering Physical Science Research Council (EPSRC) under EP/D500125/1 and also by the International Cooperation Key Project of Ministry of Science and Technology of China (Grant No. 2005DFA00805).

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