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# High Order Multiscale Methods for Advection-Diffusion Equation in Highly Oscillatory Regimes: Application to Surfactant Diffusion and Generalization to Arbitrary Domains

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**Abstract.** In this paper, we propose high order numerical methods to solve a 2D advection diffusion equation, in the highly oscillatory regime. We use an integrator strategy that allows the construction of arbitrary high-order schemes leading to an accurate approximation of the solution without any time step-size restriction. This paper focuses on the multiscale challenges in time of the problem, that come from the velocity, an $\varepsilon$-periodic function, whose expression is explicitly known. $\varepsilon$–uniform third order in time numerical approximations are obtained. For the space discretization, this strategy is combined with high order finite difference schemes. Numerical experiments show that the proposed methods achieve the expected order of accuracy, and it is validated by several tests across diverse domains and boundary conditions. The novelty of the paper consists of introducing a numerical scheme that is high order accurate in space and time, with a particular attention to the dependency on a small parameter in the time scale. The high order in space is obtained enlarging the interpolation stencil already established in [44], and further refined in [46], with a special emphasis on the squared boundary, especially when a Dirichlet condition is assigned. In such case, we compute an *ad hoc* Taylor expansion of the solution to ensure that there is no degradation of the accuracy order at the boundary. On the other hand, the high accuracy in time is obtained extending the work proposed in [19]. The combination of high-order accuracy in both space and time is particularly significant due to the presence of two small parameters—$\delta$ and $\varepsilon$—in space and time, respectively.

**AMS subject classifications**: 35J15, 65M06

**Key words**: High order discretization, time multi-scale, advection-diffusion equation, surfactant, oscillating trap, arbitrary domains.

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# 1 Introduction

In this paper, we develop numerical schemes to solve a model of the diffusion of particles within a fluid in the presence of an oscillating flow, caused by the oscillation of a specific body or trap. This topic has practical applications, particularly in understanding the relationship between living cell membranes (acting as traps) and diffusing particles (for example vital substances). In such an application, an important factor would be the rate at which these substances are captured by the trap. To investigate the capture rate, a biomimetic model was created [1–3], where an oscillating air bubble emulates a fluctuating cell, and the flow of charged surfactants represents the diffusing substances (see Fig. 1(a)). In this specific model, the surfactants consist of anions and cations with different configurations: the cations are hydrophilic, while the anions have a hydrophilic head and a hydrophobic tail, leading to their absorption at the air-water interface. The investigation of shape oscillations of drops immersed in a fluid with surfactants has been largely investigated, because of the multiple applications in nuclear physics, meteorology and chemical engineering [4,5,9]. In [6], the authors study the parameters that influence the oscillation frequency of an interface, with and without surfactants.

When studying the diffusion of particles in a moving fluid, it is fundamental to refer to advection-diffusion equations, that are important in many branches of engineering and applied sciences [7,8,10,11]. In this type of equations, two main terms appear: a non-dissipative, advective, hyperbolic term and a dissipative, diffusive, parabolic one. Numerical methods generally perform well when diffusion dominates the equation. However, when advection prevails, undesirable phenomena, such as spurious oscillations or excessive numerical diffusion, may happen, and some stability property needs to be satisfied [15]. One possible approach to solve this issue is the implementation of fine mesh refinement, e.g., satisfying a suitable stability condition on the mesh Péclet number [12]

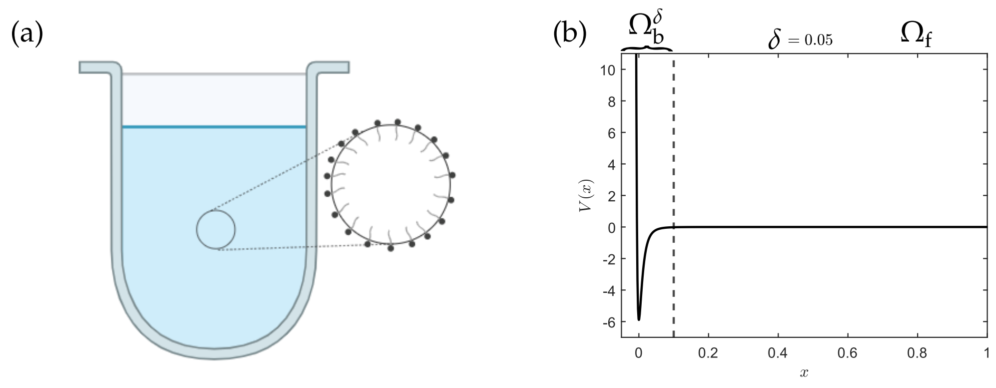


Figure 1: (a): Experimental setup of the diffusion-trapping of surfactants in presence of a trap. The zoom-in on the right shows the composition of the anions when they are stuck at the surface of the air bubble: the hydrophobic tails are inside the air bubble, while the hydrophilic heads lay on the surface. (b) Scheme of the potential $V(x)$, defined in Eq. (1.2), where $\delta$ is the thickness of the attractive-repulsive layer.