# Direct Simulation of Fluid Transport at Solid Interfaces with a Multiscale Lattice-Boltzmann Finite-Volume Method

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**Abstract:**
It is shown that the combined use of a mesoscopic lattice Boltzmann solver with finite-volume techniques, both enriched with local-refinement (multiscale) capabilities, permits to describe transport phenomena at fluid-solid interfaces to a degree of detail which may help dispensing with empirical correlations.

**Zusammenfassung:**
Es wird gezeigt, dass die kombinierte Benutzung eines mesoskopischen Lattice-Boltzmann-Solvers mit Finite-Volumen- Methoden, beide durch die Möglichkeit einer höheren örtlichen Auflösung verstärkt, es erlaubt, Transportphänomene zu beschreiben.

**Résumé:**
On montre que l'usage combiné d'une méthode mésoscopique Lattice-Boltzmann avec des techniques Volumes-Finis, les deux enrichies d'un maillage plus précis, permet de décrire des phénomènes de transport sur les interfaces fluide-solide, avec un niveau de détail tel qu'on peut éviter l'usage de corrélations empiriques.

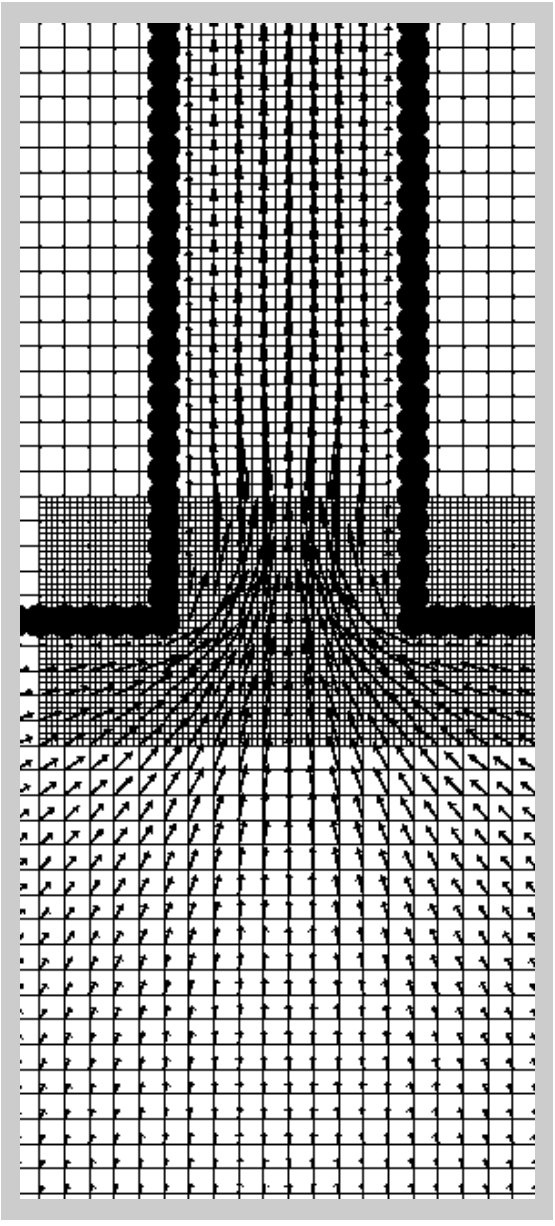
**Key words:** Hydrodynamics, transport phenomena, Lattice Boltzmann

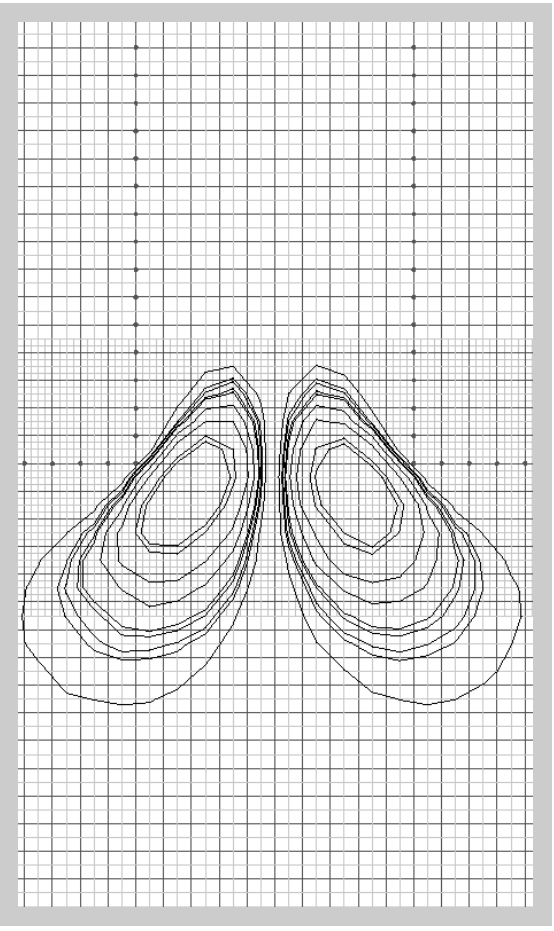
## 1 INTRODUCTION

Transport phenomena at fluid-solid interfaces play a major role in many emerging applications in material science, micro-engineering and biology [1]. Central to all of these applications is the quantitative assessment of the rate of absorption at fluid-solid interfaces of chemical species (typically reactive pollutants) carried by a fluid flow. A typical example in point are catalytic reactors, in which the absorbed species are converted into harmless reaction products via heterogeneus catalytic reactions. The rate of absorption of the pollutant, which controls the overall conversion efficiency of the catalytic device, depends crucially on the fine-scale details of fluid motion in the near-wall region. It is therefore clear that the microstructural conformation of the solid wall plays a major role in fixing the amount of pollutant absorbed at the solid interface. Since the micro-scale details of the wall geometry are not accessible to a macroscopic direct simulation for lack of computational resolution, their effects on the conversion efficiency are generally represented in a statistical sense, through the specification of average properties. Particularly important is the wall roughness, defined as the mean elevation of the wall profile, $\bar{h}$, relative to the global scale $H$ of the flow domain $\epsilon = \bar{h}/H$. Chemical absorption is then expressed via semi-empirical correlations between the major control parameters of the problem, namely the Reynolds number $Re = UH/\nu$, and the Péclet number $Re = UD/D$, where $U$ is a typical flow speed, $\nu$ the kinematic viscosity of the fluid carrier and $D$ the molecular diffusivity of the chemical species. Central to this analysis is the Darcy-Feisbach friction factor, defined as the relative amount of kinetic energy lost on frictional drag to the walls $f = 2\Delta P/\rho U^2$. Here $\rho$ is the fluid mass density and $\Delta P$ is the pressure loss between the inlet and outlet sections of the flow domain. The friction factor is typically a function of the Reynolds number and the wall roughness $\epsilon$. Such a dependence is tabulated in the so-called Moody charts, which form the basis of most practical calculations [2].

*Figure 9 (left): Blow-up of the inlet region of the monolithic converter, with a typical flow configuration at Re = 250. The solid circles represent wall sites. Note that three regions of refinement 1:1 (far-inlet), 1:4 (near-inlet), and 1:2 (thin-channel) have been used.*

*Figure 10 (right): Contour lines of the strain $S_{xy}$ in the inlet region of the monolythic converter for the same case as Fig. 9. Note that the contour lines (from $1.5 \times 10^{-3}$ to $10^{-4}$) do not suffer any visible discontinuity at the grid interface.*





of the thin channel. We performed a series of simulations at $Re$ = 90, 180, 250, 300 using 10 grid points along the vertical direction and 700 along the channel length (no-grid refinement). Without grid refinement, none of these cases could be completed successfully. With local grid refinement, we obtained $A$ = 48.1, 48.4, 49.8, 50 and $B$ = 0.35, 0.345, 0.31, 0.304. The coefficient $A$ is very close to the analytical value for a plane Poiseuille flow ($A$ = 48). Besides the numerical values, which compare reasonably well with experimental data in similar (but not exactly the same) conditions ($A \sim 43$, $B \sim 0.42 - 0.5$; [24]) it is important to observe that these coefficients show the expected independence of the Reynolds number $Re = \mathrm{ud}/\nu$ to a fairly acceptable degree of accuracy. This is in agreement with experimental findings, and lends further support to the physical consistency of the present method. In this work we have examined flows at low-moderate Reynolds numbers, for which no significant three-dimensional effects are expected. However, appreciable three-dimensional effects would surely arise in the presence of explicitly three-dimensional corrugations, such as those adopted to increase the mixing efficiency of micro-reactors [25]. Extending the present methodology to three-dimensional situations is an important task for future research. Another important task for future research is the improvement of the inter-grid boundary conditions. The basic requirement of these inter-grid boundary conditions is to impose continuity of the conserved quantities as well as that of their fluxes, across the interface. In the Filippova-Haenel's approach used here, continuity of the fluxes is imposed perturbatively, by expressing the non-equilibrium component of the distribution function via first-order space-time derivatives of the local equilibrium.

This provides pretty reasonable results, not only for the flow field itself, but also for more sensitive observables, such as the strain $S_{xy} = (\partial_y u + \partial_x v)/2$ (Fig. 10). However, the perturbative nature of this procedure may well require improvements whenever the local Knudsen number at the grid interfaces is no longer negligible. A non-perturbative formulation of the intergrid boundary conditions represents an interesting topic for further research.

## 5 CONCLUSIONS AND FUTURE DIRECTIONS

The lattice Boltzmann method shows increasing promise of representing a valuable tool for the computational analysis of multiscale fluid flow problems [26]. To this purpose, the native LB method requires substantial boosts in geometrical flexibility, to straddle across different scales, as well as in physical versatility, to accomodate additional physics besides fluid flow. Coupling of LB methods with existing transport algorithms within a grid-refined framework represents just one out of many possible strategies to accomplish the aforementioned task. The results presented in this work provide encouraging evidence that lattice Boltzmann solvers, coupled to a standard Finite-Volume treatment of scalar transport, both enriched with local-refinement capabilities, may prove very effective for the direct simulation of transport phenomena in low-Reynolds fluids. Much more validation and application work is clearly needed to put the present methodology on a firmer basis and extend its range of applications. In particular, three-dimensional extensions, non-perturbative formulations of inter-grid boundary conditions, and use of more sophisticated boundary conditions for arbitrarily shaped boundaries, appear of utmost importance to address real-life problems. Work along these lines is currently underway [27, 28].

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[1] Despite the 'Integer' in the title of the paper, the method is perfectly well suited to floating-point implementations.





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