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# Lattice Boltzmann Modeling of Complex Flows for Engineering Applications



# Lattice Boltzmann Modeling of Complex Flows for Engineering Applications

**Andrea Montessori**

*University of Rome 'Roma Tre'*

**Giacomo Falcucci**

*University of Rome 'Tor Vergata', School of Engineering and  
Applied Physics, Harvard University*

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# Preface

Nature continuously presents to our eyes a huge number of complex and multi-scale phenomena, that, in many cases, involve the presence of one or more fluids, flowing, merging and evolving around us. Since its appearance on the surface of Earth, Mankind has tried to exploit and tame fluids for his purposes, probably starting with Hero's machinery to open the doors of the Temple of Serapis in Alexandria, to arrive at modern propulsion systems and actuators.

Today we know that fluid mechanics lies at the basis of countless scientific and technical applications from the smallest physical scales (nanofluidics, bacterial motility, diffusive flows in porous media), to the largest (from energy production in power plants, to oceanography and meteorology): it is essential to deepen the understanding of fluid behavior across scales, for the progress of Mankind and for a more sustainable and efficient future.

Since the very first years of the Third Millennium, the Lattice Boltzmann Method (LBM) has known an exponential growth of applications, especially in fields connected with the simulation of complex and soft matter flows. LBM, in fact, has shown remarkable versatility in different fields of applications, from nanoactive materials, to free surface flows, from multiphase and reactive flows to the simulation of the processes inside engines and fluid machinery. LBM is based on an optimized formulation of Boltzmann's Kinetic Equation, which allows for the simulation of fluid particles, or rather quasi-particles, from a mesoscopic point of view, thus allowing the inclusion of more fundamental physical interactions in respect to the standard schemes adopted with Navier–Stokes solvers, based on the continuum assumption.

In this book, we present the most recent advances of application of the LBM to complex flow phenomena of scientific and technical interest, with particular focus on the multi-scale modeling of heterogeneous catalysis within nano-porous media and multiphase, multicomponent flows.



# Acknowledgments

In this book, we propose an overview of the most relevant results that we obtained through the Lattice Boltzmann Method since our PhD fellowships.

We feel that we owe our gratitude to Prof. Sauro Succi, our mentor: with his continuous support over the years, he has inspired our scientific growth and encouraged us to achieve the methodological results gathered in this book. Besides him, we wish to thank a large number of Scholars who have contributed to our scientific enrichment: Prof. Efthimios Kaxiras, from Harvard University; Prof. Stefano Ubertini (University of Tuscia), Prof. Michele La Rocca (University of Rome ‘Roma Tre’), Prof. Gino Bella (University of Rome ‘Tor Vergata’) and Prof. Elio Jannelli (University of Naples ‘Parthenope’).

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Together with them, we wish to thank our families, for the continuous support they gave us and for the inspiration that they provided every day.

# Author biographies

## Andrea Montessori

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Andrea Montessori, PhD, is a Postdoc researcher in the Department of Engineering at the University of Rome ‘Roma Tre’ in Italy. He obtained his PhD (cum laude) in Engineering in 2017 from the University of Rome ‘Roma Tre’ with the thesis ‘Lattice Boltzmann approach to complex fluid phenomena across scales’. He has developed the Lattice Boltzmann Model for the simulation of complex fluid dynamics phenomena, including multiphase and multicomponent flows, reactive and nonequilibrium flows, and transport phenomena in 2D nanomaterials. He is involved in the IMASC project as a collaborator and was a visiting scholar at Harvard University in 2015. He has published more than 20 papers on Lattice Boltzmann models for fluid dynamics phenomena across scales of motion.

## Giacomo Falcucci

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Giacomo Falcucci, PhD, is Assistant Professor of Fluid Machinery, Energy and Environmental Systems at the University of Rome ‘Tor Vergata’ and Visiting Scholar of Computational Physics at the John A. Paulson School of Engineering and Applied Sciences of Harvard University. He obtained his PhD in Mechanical Engineering in 2009 from the University of Rome ‘Roma Tre’. He has developed novel numerical methods based on the Lattice Boltzmann Equation for the study of non-ideal fluids; his research activity is focused on the numerical and experimental investigation of Internal Combustion Engines, Fuel Cells, Alternative Energy Systems, and complex Fluid–Structure interaction phenomena for Energy Harvesting. In 2010, he was Visiting Professor of Heat Transfer at the Polytechnic School of Engineering of NYU. He is the author of more than 60 scientific works.