M.C. Sukop
D.T. Thorne, Jr.
Lattice Boltzmann Modeling

Michael C. Sukop
Daniel T. Thorne, Jr.

Lattice Boltzmann Modeling

An Introduction for Geoscientists and Engineers

With 83 Figures

Springer

Dr. Michael C. Sukop
Florida International University
Department of Earth Sciences
University Park
Miami FL 33199
USA

Email: sukopm@fiu.edu

Dr. Daniel T. Thorne, Jr.
Georgetown College
Department of Mathematics,
Physics, and Computer Science
400 E College Street
Georgetown KY 40324
USA

Email: danny_thorne@georgetowncollege.edu

Library of Congress Control Number : 2005930890

ISBN-10 3-540-27981-4 Springer Berlin Heidelberg New York
ISBN-13 978-3-540-27981-5 Springer Berlin Heidelberg New York
2nd. corrected printing

Springer is a part of Springer Science+Business Media
Springer.com

Cover design: E. Kirchner, Heidelberg
Typesetting: camera-ready by author
Production: Almas Schimmel
Printing: Krips bv, Meppel
Binding: Stürtz AG, Würzburg

Printed on acid-free paper 30/3141/as 5 4 3 2 1

Preface

This book represents our effort to convey the understanding of Lattice Boltzmann Methods (LBM) that we have developed over the last 4 years. This understanding is incomplete; consultation of any of the other main texts and journal articles on the subject will reveal the depth of the topic and the level of mathematical and physical sophistication necessary for complete mastery. Nevertheless, we are able to accomplish remarkable things with LBM and we wish the same for our readers. This book is aimed at our peers who may be curious about the technique or simply wish to use it as a tool now and, like us, continue learning about it in greater depth in the future. Rather than the ‘last word’ on the techniques, we present first introductions. Criticism from those more knowledgeable on details of some of the methods is probably inevitable and deserved. We take responsibility for all errors in the text, but cannot be responsible for any results of applying the ideas or models we present.

MS and DT, Miami, Florida USA, July 22, 2005

MS wishes to thank Professor Dani Or of the University of Connecticut and the post-doc funding from NSF and NASA he provided for creating an environment where a beginner could invest the time needed to build a basic knowledge of LBM. The environment and support of the Earth Sciences department at Florida International University have similarly been essential to continuing this work and the completion of this book. I learned lattice gases as an aside during my Ph.D. with Professor Ed Perfect (now University of Tennessee) with funding from the University of Kentucky Research Challenge Trust Fund and the Center for Computational Sciences under the much appreciated guidance of Professor Craig Douglas. Dr. Liliana Di Pietro graciously hosted me at Institut National de la Recherche Agronomique (INRA) in Avignon, France and provided me with my first experiences with multiphase lattice gases; funding for that trip came from a University of Kentucky Dissertation Enhancement Award. Jessica Chau (UConn), Vasile Turcu, Seth Humphries (Utah State), and Teamrat Ghezzehei (Lawrence Berkeley National Lab) helped by listening to me and contributing from their mathematics and computer sciences backgrounds.

Jessica Chau also contributed to my earliest multicomponent model and the work on cavitation. Shadab Anwar (FIU) helped by testing the codes and running some of the simulations presented in the book. An early single component multiphase LBM FORTRAN code by Louis Colonna-Romano (Clark University and Worcester Polytechnic Institute) that I found on the Internet associated with Chen (1993) was instrumental in getting me started; vestiges of that code may still be visible in the current codes. Discussions with Frederik Verhaeghe of the Katholieke Universiteit Leuven in Belgium led to the correction of an error in our earlier codes. Jessica Chau (University of Connecticut), Yusong Li (Vanderbilt University), C. L. Lin (University of Utah), and Shadab Anwar (Florida International University), provided peer review. Three classes of students have thus far served as a testing ground for the material presented here; many more will follow and the book will be improved. Finally, my collaboration with DT at Florida International University and earlier at the University of Kentucky has been exceptionally valuable.

MS, Miami, Florida USA, July 22, 2005

DT thanks MS for the opportunity to join him in lattice Boltzmann methods research. MS is an excellent mentor and through collaboration with him I have not only explored an exciting new frontier of fluids modeling but grown much as a researcher in general. In addition, DT offers thanks to his erstwhile thesis advisor, Prof. Craig Douglas, for support, guidance and inspiration during my graduate school years, without which my path through life would have been unimaginably different and most surely would not have led here.

DT, Miami, Florida USA, July 22, 2005

Table of Contents

1 Introduction

Lattice Boltzmann models (LBM) have a remarkable ability to simulate single and multiphase fluids. A rich variety of behaviors, including unsteady flows, phase separation, evaporation, condensation, cavitation, solute and heat transport, buoyancy, and interactions with surfaces can readily be simulated. Persistent metastable states can be realized.

This book is intended primarily as a basic introduction that emphasizes intuition and the most simplistic conceptualization of processes. It largely avoids the more difficult mathematics and physics that underlie LB models. The model is viewed from a particle perspective where collisions, streaming, and particle-particle/particle-surface interactions constitute the entire conceptual framework. The beauty of these models resides in this simplicity. The particular multiphase models we develop here evolved primarily from the landmark papers of Shan and Chen (1993, 1994). These models are not perfect and their shortcomings have been explored in the literature. Nevertheless, they are exceptionally powerful and, because of their largely intuitive 'bottom up' nature, are particularly well suited to this kind of introduction.

Much of the material contained here can be extracted from the open literature and a number of pioneering books, including Succi (2001), Wolf-Gladrow (2000), and Rothman and Zaleski (1997). Chen and Doolen (1998) presented a review paper. However, beginners and those with more interest in model application than detailed mathematical foundations should find this book a powerful 'quick start' guide. We focus on 2-dimensional models, though extension to 3 dimensions is not particularly difficult. We work simultaneously with the fundamental equations and their computer implementation to illustrate the practical use of the equations. The reader should be aware of our approach to presenting code. Code is presented in small pieces throughout the text and is designed only to be human readable. It is pseudo-code, although it resembles C (as it is adapted from our actual implementation). Shortcuts in syntax (e.g., abbreviated variable indexing like `fij` for `f[j][i]`, and the abbreviation `foo+=bar` for `foo=foo+bar`) are employed generously to keep the code snippets brief and line-lengths short as well as to optimize for readability. Our intention is to convey the nature of the implementation clearly so that the reader is well equipped to begin an implementation of their own and/or browse and modify/extend an existing implementation. Readers interested in the details are encouraged to examine the working code.

We provide code on the Internet (LB2D_Prime) and offer exercises that focus on confirming the code's ability to match analytical or observed results; this helps to instill confidence and point out deficiencies in the simple LBM models we introduce. We include pertinent references to guide readers to more specialized sources. The field is expanding and evolving rapidly however and many papers have not been mentioned. Figure 1 shows the exponential growth in the number of papers published since 1992.

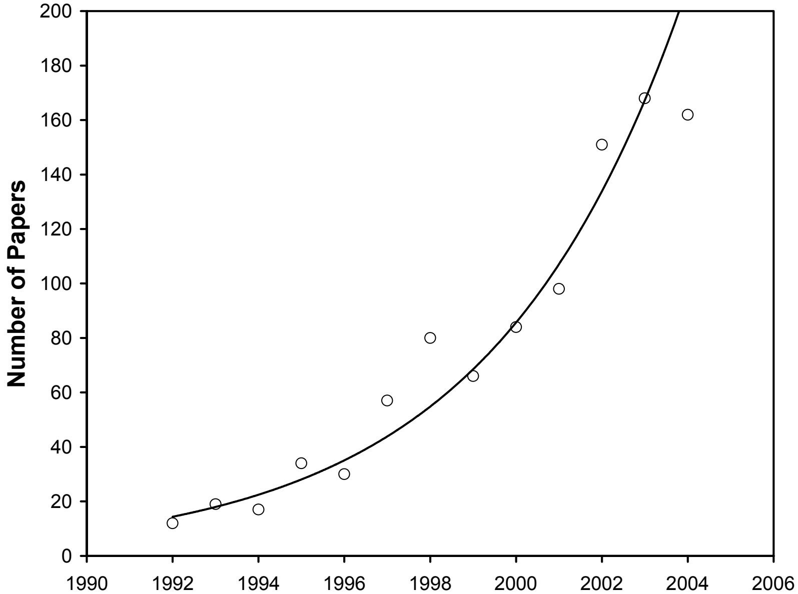

Figure 1. Growth in number of papers with 'lattice Boltzmann' as a 'topic' (search of article titles, abstracts, and keywords) in the Web of Science database 1992 - 2004. Solid line is fitted exponential growth curve. 2004 data may be incomplete.

It is also of interest to consider the nature of the published papers. Figure 2 gives the Web of Science Subject Categories for the papers published 1992-2004 that have lattice Boltzmann in their titles, abstracts, and/or keywords: most have appeared in physics and computer sciences. In our opinion, the distribution is likely to shift towards more applied areas (geosciences and engineering) as the power of these models is recognized.

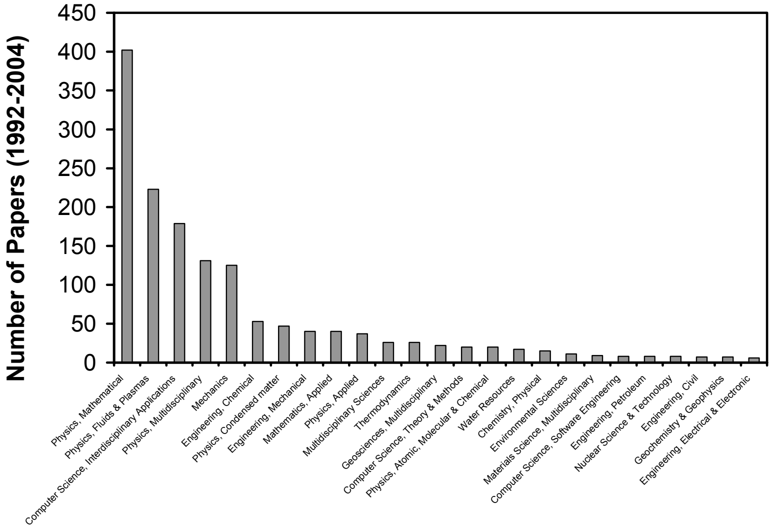

Figure 2. Web of Science Subject Categories for papers published 1992 - 2004 with lattice Boltzmann as a topic. Most papers so far have been published in Physics and Computer Science.

We begin our introduction to lattice Boltzmann models with a review of basic fluid mechanics concepts that are used later in the book. Cellular automata and lattice gases are covered briefly in the next chapter. Then we give a simplified introduction to Boltzmann gas concepts; it provides a basis for the 'stream and collide' mechanisms that are central to lattice gas models (the forebears of LBM) and LBM. Chapter 4 presents the core equations and computational aspects of LBM including a variety of boundary conditions. Chapter 5 introduces single component single phase LBM as the basis for extension to single component multiphase (SCMP LBM) in Chapter 6 and multi-component multiphase (MCMP LBM) models in Chapter 7. Solute transport is treated in Chapter 8 and Chapter 9 focuses on LBM for porous media at the macroscopic scale. Example simulations are included at each stage of model extension to illustrate increasingly sophisticated capabilities.

Another exciting use of LBM is for the simulation of shallow flows with the shallow water equations. We do not delve into this material as it has been covered in a recent book by Zhou (2003). We also do not touch on particle flows (e.g., Ladd 1993, 1994a,b; Ladd and Verberg 2001; Cates et al. 2004; Cook et al. 2004; Dupin et al. 2004).

Lattice Boltzmann models serve as exceptional numerical laboratories for a large number of physical and physicochemical processes. The ability to probe the simulations in detail for density and pressure gradients for example, has lead us to far deeper understanding of numerous phenomena than we would have achieved otherwise. While we expect quantitative results from lattice Boltzmann methods, the learning value of playing with 'toy' models must not be underestimated.

Here we present elementary examples of a broad range of applications to illustrate the enormous potential of LBM. Assimilation of LBM into mainstream scientific computing in geosciences and engineering will require extension of the models to larger applications that integrate databases and visualization as is characteristic of modern ground water models for example.

1.1 Review of Basic Fluid Mechanics

While some of our readers will need no introduction to or review of fluid mechanics, our experience indicates that for many it is worthwhile to review the most fundamental ideas on the behavior and quantitative treatment of fluids. This review is very minimalist in scope and focuses only on topics that are essential to basic understanding of LBM or will be the subject of LBM simulations in subsequent chapters. More advanced physical chemistry needed for single component multiphase models and other topics are reviewed in later chapters.

1.1.1 Momentum

One fundamental concept that will be needed is that of momentum. The momentum $\mathbf{p}$ is defined as $\mathbf{p} = m\mathbf{u}$ with m the mass and $\mathbf{u}$ the velocity.

Conservation of mass and momentum are central to fluid mechanics and lattice Boltzmann models. Conservation of mass simply means that mass is not lost or created in the system under consideration. Conservation of momentum is well illustrated by the toy known as Newton's Cradle (Figure 3). Momentum attained by the moving ball just prior to its collision with the stationary balls is transmitted through the row of balls and converted back to motion of the ball on the opposite end of the row.

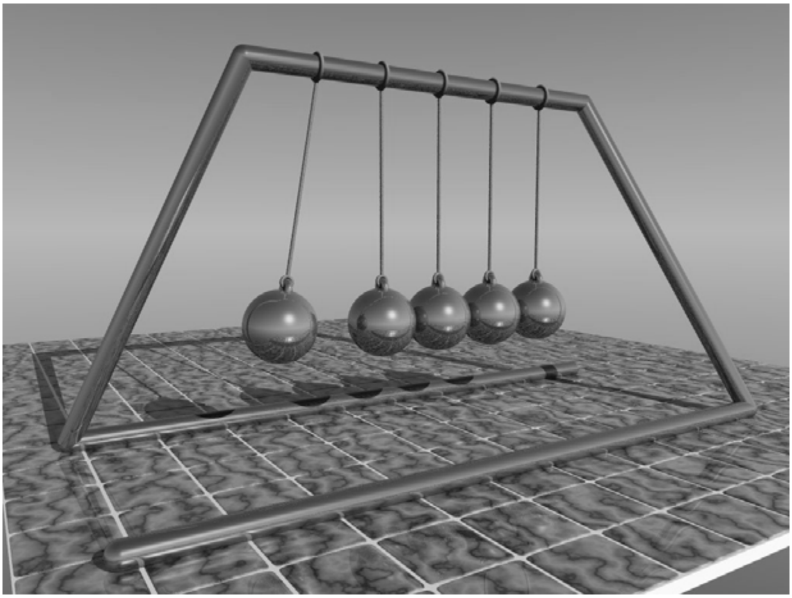

Figure 3. Newton's Cradle toy illustrates momentum conservation. (Rendering courtesy of Mark Hanford)

Not surprisingly, momentum is closely related to force. Newton's Second Law of Motion gives the force **F** as **F** = *m***a**, where **a** is the acceleration. Acceleration is the time rate of change of velocity or $d\mathbf{u}/dt$, so force can be written as

$$\mathbf{F} = m\frac{d\mathbf{u}}{dt} = \frac{d\mathbf{p}}{dt}. \quad (1)$$

1.1.2 Viscosity

The viscosity is a measure of the resistance to flow. Air has a very low viscosity relative to honey. Newton's Law of Friction relates the shear stress τ to the velocity gradient in a Newtonian fluid:

$$\boldsymbol{\tau} = \mu \frac{d\mathbf{u}}{dx}. \tag{2}$$

The coefficient of proportionality is the dynamic viscosity μ. The kinematic viscosity is the dynamic viscosity divided by the fluid density μ/ρ. It is commonly denoted by ν and has dimensions of L^2T^{-1}. The kinematic viscosity can be thought of as a diffusion coefficient for momentum since

$$\boldsymbol{\tau} = \mu \frac{d\mathbf{u}}{dx} = \mu \frac{\rho}{\rho} \frac{d\mathbf{u}}{dx} = \nu \frac{d\mathbf{p}}{dx} \tag{3}$$

which is analogous to Fick's First Law of diffusion where a unit volume is implicit in the denominator of the rightmost term. This analogy is quite clear in the similarities between LBM simulations of fluids and solute transport that we will examine later.

1.1.3 Reynolds Number

The Reynolds Number (*Re*) is a non-dimensional number that reflects the balance between viscous and inertial forces. It is given by $Re = u\,L/\nu$ where u is the fluid velocity, L is a characteristic length, and ν is the kinematic viscosity. Low velocity, high viscosity, and confined fluid conditions lead to a low *R*e, the dominance of viscous forces, and laminar flow. If Re << 1, the flow is known as Stokes or creeping flow (Figure 4). Such flow is traditionally thought to be common for liquids in many porous media due to small pore sizes.

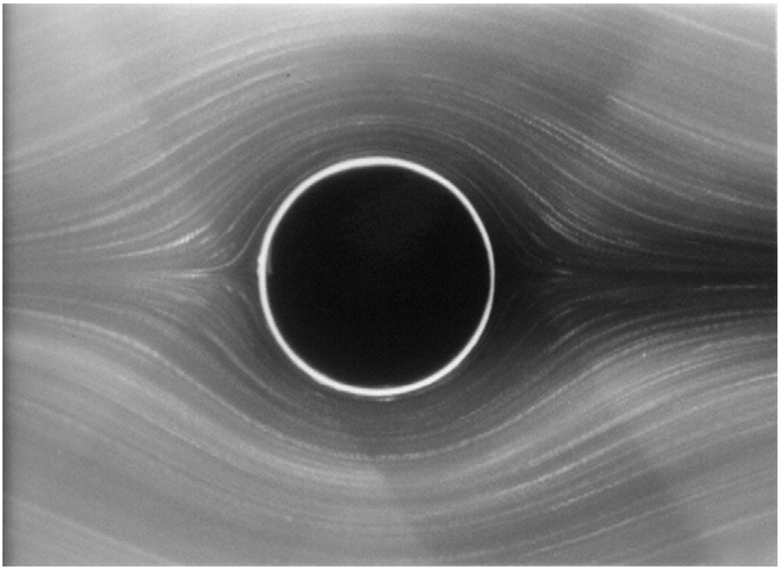

Figure 4. Stokes or creeping flow at low Reynolds number, Re ≈ 0.16 (Photograph by S. Taneda, with permission of the Society for Science on Form, Japan).

Higher velocities, larger length scales, or less viscous fluids lead to larger Reynolds numbers and the dominance of inertial forces over viscous forces. Under high Reynolds numbers the flow can become unstable (i.e., the onset of turbulence). Lattice Boltzmann models handle a range of Reynolds numbers very effectively and we will illustrate this later. The first departure from creeping flow is accompanied by a phenomenon known as flow separation and the formation of eddies as seen in Figure 5.

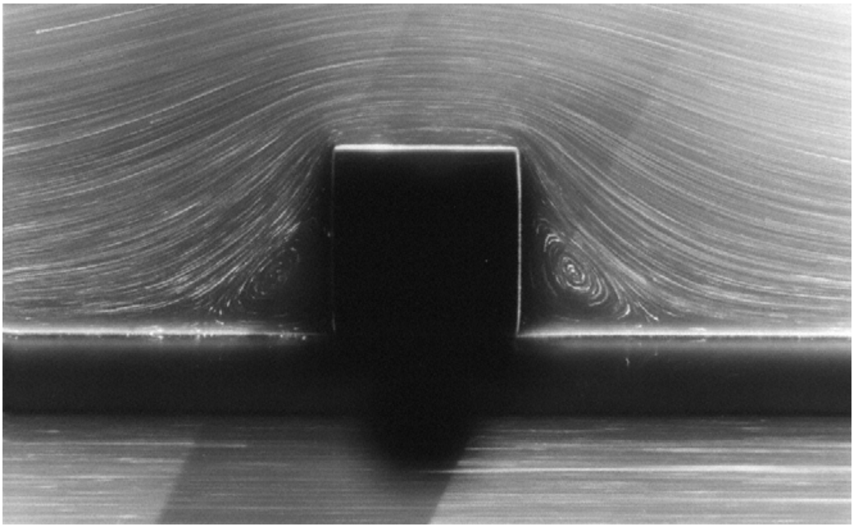

Figure 5. Separation at Re = 0.020 (Taneda (1979) with permission).

As the Reynolds number increases, unsteady and turbulent flows can ensue. We will investigate higher Reynolds number flows in Chapter 5.

1.1.4 Poiseuille Flow

An important and simple type of flow is that which occurs in a pipe or a slit between two parallel surfaces. These are called Poiseuille flows after the Frenchman Jean Léonard Marie Poiseuille (1797–1869) (Sutera and Skalak, 1993). In a slit or pipe, the velocities at the walls are 0 (no-slip boundaries) and the velocity reaches its maximum in the middle. As illustrated in Figure 6, the velocity profile in a slit of width $2a$ is parabolic and given by

$$u(x) = \frac{G^*}{2\mu}(a^2 - x^2) \qquad (4)$$

where G^* can be the (linear) pressure gradient $(P_{in} - P_{out})/L$ or a gravitational pressure gradient (for example, in a vertical pipe $G^* = \rho g$). We will consider entry length effects later.

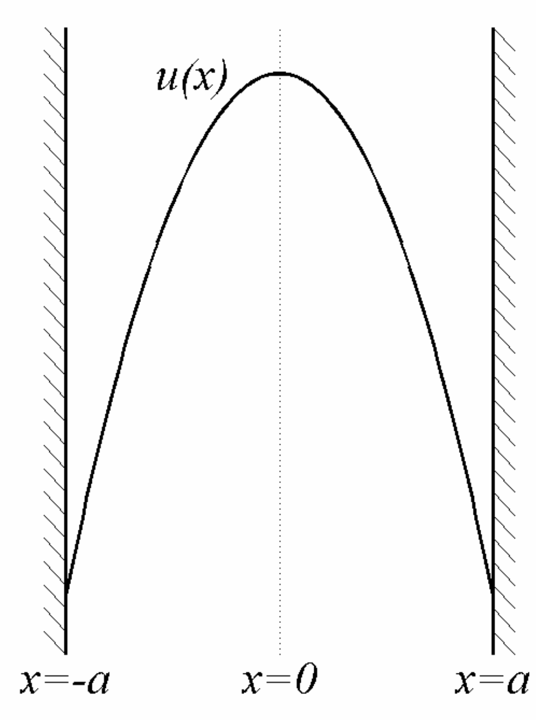

Figure 6. Poiseuille velocity profile.

It is useful to know that the average velocity in a slit is 2/3 of the maximum, or, since the maximum velocity is attained at $x = 0$,

$$u_{average} = \frac{2}{3}\frac{G^*}{2\mu}a^2 . \tag{5}$$

1.1.5 Laplace Law

There is a pressure difference between the inside and outside of bubbles and drops. The pressure is always higher on the inside of a bubble or drop (concave side) – just as in a balloon.

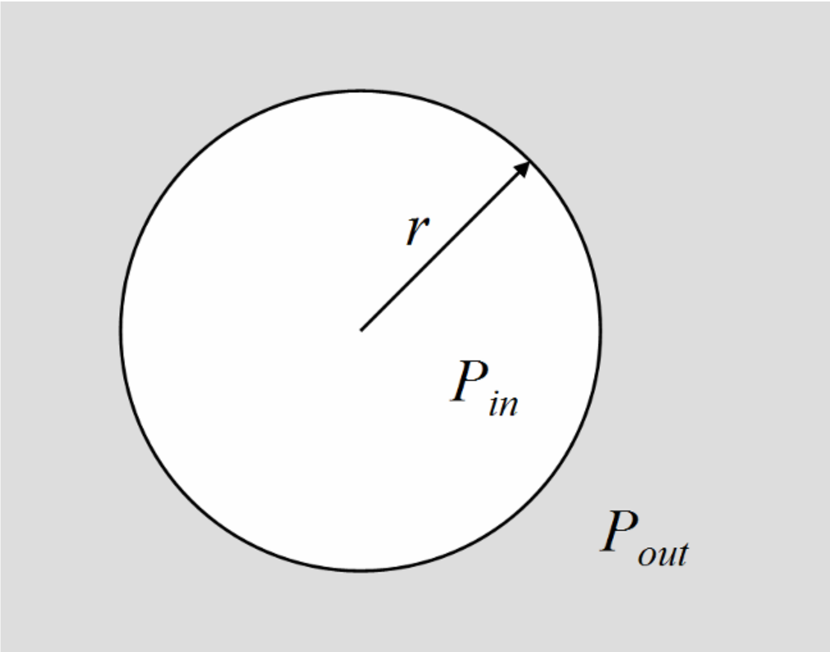

Figure 7. Definition diagram for Laplace Law. The difference in pressure inside and outside of a drop or bubble is inversely related to the radius r.

The pressure difference $\Delta P = |P_{outside} - P_{inside}|$ depends on the radius of curvature r and the surface tension σ for the fluid pair of interest. For two-dimensional drops and bubbles there is only one possible radius of curvature and

$$\Delta P = \frac{\sigma}{r}. \tag{6}$$

This Laplace Law indicates that ΔP is linear with respect to curvature $1/r$. We will use this later to estimate the surface tension in lattice Boltzmann simulations. The Laplace Law applies to both interfaces between a liquid and its own vapor (where σ is known as the surface tension) and between different fluids (like oil and water; where σ is referred to as the interfacial tension).