

# Accuracy, Stability, and Efficiency of Lattice Boltzmann Models in Simulating Non-Newtonian Flow

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1      Note: anything in red is just random garbage notes. You can ignore it for  
2      the most part.

## 3      **Abstract**

4      The Lattice Boltzmann method (LBM) is a computational method that can be  
5      used for simulating fluid flow. It is well-suited for complex flows such as non-  
6      Newtonian, free surface, and multiphase multicomponent flows. Non-Newtonian  
7      flows are the primary focus of this paper, as many practical engineering problems  
8      such as the flow of cement slurries and concretes, the filling of molds by molten  
9      metals and plastics, blood flows, etc., are best modeled as non-Newtonian fluids.  
10     LBM is a statistical mechanical approach for simulating fluid flow. Each time  
11     step consists of streaming particle distributions to neighboring nodes, and col-  
12     lisions of particle distributions at each node through a collision operator. The  
13     collision operator is of interest because it has a lot of control over the physics  
14     that are simulated, e.g. constitutive laws, interfacial dynamics, etc., and it has  
15     implications on numerical stability and computational efficiency. In this pa-  
16     per, various collision operators and methods for stability enhancement will be  
17     examined for their suitability for simulating non-Newtonian flows in terms of  
18     accuracy, numerical stability and computational efficiency. The structure of the  
19     paper will be as follows: blah, blah, blah.

## 20     **1      Introduction**

### 21     **1.1    Applications of Non-Newtonian Flow**

22     The dynamic viscosity of a fluid is a measure of its resistance to shear defor-  
23     mation. For many fluids, at a constant temperature, the dynamic viscosity can  
24     be considered as constant. These fluids are known as Newtonian fluids. Non-  
25     Newtonian fluids have an apparent dynamic viscosity, or apparent resistance  
26     to shear stress, that is variable—even at a constant temperature—and is often a  
27     function of strain-rate. There are a number of fluids in science and engineering  
28     applications that can be classified as non-Newtonian; pastes, slurries, molten  
29     plastics, polymer solutions, dyes, varnishes, suspensions, and some biomedical  
30     liquids such as blood all behave in a non-Newtonian manner [4]. Of all of the  
31     different non-Newtonian behaviors that exist, there are two models under which  
32     much of the behaviors may be idealized:

- 33     1. *Yield stress fluids.* Yield stress fluids, also known as Bingham plastics,  
34     do not flow until a threshold value of stress, referred to as its yield stress,  
35     is exceeded. Some examples of yield stress fluids are drilling muds, fresh  
36     cement slurries and concretes, and melted metal alloys [11]. Understand-  
37     ing the flow of cement slurries and concretes is important because they  
38     are used in the cementing of oil and gas wellbores, and in construction.

If the cement job for an oil and gas wellbore is not completed successfully then gases and fluids can leak through the wellbore to contaminate ground water or the atmosphere. The goal of understanding cement slurry and concrete flows during construction is to understand how construction forms can be completely filled as voids can lead to structural deficiencies [?]. Yield stress flow is relevant in many other disciplines and applications because of the many substances that exhibit yield stress behavior, e.g. pastes, paints, muds, molten plastics and metals, and blood [23]. As a consequence, simulating yield stress fluids can help engineers develop better pastes and paints, understand the flow and deformation of mud and clay in geotechnical engineering, understand blood circulation, and better manufacture metal and plastic parts.

2. *Power-law fluids.* Power-law behavior is more commonly known as *shear-thinning*—when the apparent viscosity decreases with increasing strain-rate—or *shear-thickening*—when the apparent viscosity increases with increasing strain-rate. Shear-thinning fluids are also known as *pseudo-plastics*, and some examples include polymer mixes and molten plastics. Shear-thickening fluids are also known as *dilatants*, and some examples include quicksand, a cornstarch and water mixture, and a silica and polyethylene glycol mixture.

Developing numerical methods for approximating these non-Newtonian flows is important because of how difficult, and often impossible, it is to derive analytical, closed-form solutions.

## 1.2 Lattice Boltzmann Method for non-Newtonian Flow

Analytical solutions rarely exist for even the simplest non-Newtonian flows because of the complexity that a non-linear constitutive relationship entails. It is generally more practical to approximate non-Newtonian flows using numerical methods. However, the non-linear constitutive equation—typically of the form  $\tau = \mu_{app}(\dot{\gamma})\dot{\gamma}$ , where the apparent viscosity,  $\mu_{app}$  is a function of the strain rate—results in certain challenges for numerical methods as well. Determining the apparent viscosity and shear rate of a flow will often require an iterative solution, a general Picard-type algorithm is:

1. Start with initial guess for the apparent viscosity,  $\mu_k = \mu_0$ .
2. Solve for the flow using the current value of apparent viscosity,  $\dot{\gamma}_k = \tau_k / \mu_k$ .
3. Update the apparent viscosity,  $\mu_{k+1} = \mu(\dot{\gamma}_k)$ .
4. Return to Step 2 until convergence is met.

Numerical solutions work by discretizing the equations that govern the physics of interest. When the solution for fluid flow problems vary in space and time,

77 a numerical approximation requires breaking the problem up into discrete loca-  
78 tions and discrete time steps. The significance of approximating a solution by  
79 discretizing the governing equations is that the iterative solution for the consti-  
80 tutive equation must be solved at each discrete location for each discrete time  
81 step, which becomes computationally expensive. The lattice Boltzmann method  
82 (LBM) is a numerical method for fluid flow that has the unique advantage that  
83 computing the strain rate is local to each node. This means that although  
84 an iterative solution is still required to determine the local strain rate and ap-  
85 parent viscosity, each iterative solution can be done in parallel, by a separate  
86 process, as they are independent of each other. Because hardware architectures  
87 have shifted from single, sequential processing systems to parallel processing  
88 systems, the local nature of the stress-strain-rate relationship in LBM gives it  
89 a distinct advantage for simulating non-Newtonian flows over other numerical  
90 methods.

91 The lattice Boltzmann method has been studied and successively applied to  
92 modeling various non-Newtonian flows. Chai et al. [6], Chen et al. [7], Fallah  
93 et al. [9], Tang et al. [20], Vikhansky [21], Wang and Ho [22] developed LBM  
94 models for simulating yield stress flows. The LBM model results agreed well  
95 when compared to analytical solutions for Bingham plastic Poiseuille flow, and  
96 values from literature for lid-driven cavity flows—showing the feasibility of using  
97 LBM models for yield-stress flows. LBM models for power-law fluid flows [5, 6,  
98 23, 24], and blood flows using the K-L, Casson, and Carreau-Yasuda constitutive  
99 relationships [1], have also been successfully developed and verified.

100 LBM does however, have its drawbacks. LBM can be considered as a type  
101 of finite-difference scheme for the continuous Boltzmann equation, and as such,  
102 has numerical properties in common with finite-difference schemes. One such  
103 consideration associated with this view, is the potential for numerical inaccura-  
104 cies and instabilities [2, 13, 16, 17]. Stability concerns are just as prevalent,  
105 if not more prevalent, in simulating non-Newtonian flows because the strong  
106 nonlinear relationship between shear stress and strain-rate can lead to high  
107 non-equilibrium fluctuations. Various schemes and strategies for incorporat-  
108 ing the physics of non-Newtonian flows and yet maintaining a stable numerical  
109 method have been developed and studied. The simplest approach for simulating  
110 a shear-rate dependent viscosity, used in [5, 7, 9, 18–20], is to make the relaxation  
111 time—which is proportional to apparent viscosity—variable and dependent on the  
112 local strain rate. A potential issue with the stability of the variable relaxation  
113 time approach is that as the relaxation time,  $\tau$ , approaches  $1/2$  the viscosity ap-  
114 proaches zero; and alternatively, if the relaxation time is much greater than one,  
115 the accuracy and stability of the method also degrades [14]. In order to ensure  
116 that the variable relaxation times did not approach values leading to numerical  
117 instabilities, [10, 18, 19] set upper and lower bounds on allowable relaxation  
118 times. Although bounding the relaxation time was shown to be effective in  
119 terms of stability, it is also nonphysical and can lead to approximations that are  
120 inaccurate, not because of round-off error or numerical instability, but because  
121 the relaxation time does not reflect the proper constitutive relationship of in-  
122 terest. Another scheme for incorporating non-Newtonian effects into LBM is to

use a constant relaxation rate, typically unity, and to instead incorporate the local shear-rate effect into equilibrium distribution functions. This means particle distribution functions will always relax toward equilibrium at the same rate, but that the definition of equilibrium is modified to represent the correct stress-strain-rate relationship. The equilibrium distribution function is derived for the specific constitutive relationship of interest using the Chapman-Enskog multi-scale expansion. The equilibrium distribution function for Bingham plastic flow was derived, implemented, and verified in [22]; and the equilibrium distribution functions for power-law fluids and Carreau fluids were derived, implemented, and verified in [26]. The strategy of using an equilibrium distribution function that incorporates the local shear-rate effect has the advantage that, because the relaxation time is constant (at unity), the local relaxation time will not approach values that are too small or too large, and so there is no reason to bound the relaxation time in a way that is nonphysical. Wang and Ho [23] developed another constant-relaxation time LBM scheme for non-Newtonian flows by splitting the effects of constitutive relationship into Newtonian and non-Newtonian parts—for example, considering the plastic viscosity and yield stress for a Bingham plastic separately—then incorporating the Newtonian part in the usual way, namely scaling the relaxation time to achieve the macroscopic (Newtonian) viscosity, and incorporating the non-Newtonian part as a source of momentum, i.e. as an external forcing term, that is dependent on local shear-rate. Although the constant-relaxation time strategies present interesting alternatives, the variable relaxation time scheme is used in the present study because of its simplicity and flexibility.

Much work has been done (not specific to non-Newtonian flows) to investigate and develop ways to enhance the stability of lattice Boltzmann methods. Sterling and Chen [16, 17] investigated the stability of LBM with the linear Bhatnagar–Gross–Krook (BGK) collision operator on 7-velocity and 9-velocity 2D lattices and a 15-velocity cubic lattice. The investigation was performed by linearizing all nonlinear terms about global equilibrium values and applying a von Neumann stability analysis on the resulting linearized equations. The spatial dependence of stability was analyzed by taking the Fourier transform of the linearized equations. Sterling and Chen concluded that the linear stability of LBM models depends on the mass distribution parameters, the mean velocity, the relaxation time, and the wave number. Worthing et al. [25] extended the stability analysis performed by Sterling and Chen, and instead of linearizing the LBM equations by expanding about global equilibrium values, Worthing et al. does something else. Their analysis discover both physical and nonphysical instabilities, and that setting the BGK relaxation time,  $\tau = 1$  provides the optimal accuracy in time. Expand a little more about what they did and its significance here.

Although much work has been done to characterize the stability of LBM models, these analyses have the following limitations to their applicability:

- von Neumann stability analysis, and linear stability analysis in general requires modifying the governing equations of the model so that they are

168 linear. This linearization cannot be done without introducing some error  
169 into the analysis.

170 • Much of the analysis that exists in literature is done about a uniform  
171 flow [15, 25].

172 • Analyses are most often carried out assuming periodic boundary condi-  
173 tions. Periodic boundary conditions are advantageous for stability analysis  
174 because the analysis is generally done by a Fourier analysis on the prop-  
175 agation of error. The periodicity of Fourier modes allows the periodic  
176 boundary conditions to automatically be satisfied. Such an analysis, how-  
177 ever, does not generalize well to instances when modes of the system are  
178 heavily influenced by the boundary conditions [25].

179 • The analyses are general and do not delve into any of the nuances of  
180 non-Newtonian flows.

181 Bawazeer wrote a thesis on the stability and accuracy of the lattice Boltzmann  
182 method. Perhaps I'll read it. I think Jonas Latt did too.

183 To improve upon the stability of LBM models, d'Humieres [8] developed  
184 a multiple-relaxation-time (MRT) collision operator, that takes place in mo-  
185 ment space and allows each moment to relax at a different rate. Lallemand  
186 and Luo [13] used von Neumann stability analysis to investigate the dispersion,  
187 dissipation, isotropy, Galilean invariance, and stability of the newly constructed  
188 LBM-MRT model. They concluded LBM with the MRT collision operator was  
189 more stable, but with increased computational expense, than what is still often  
190 used, the BGK collision operator. Note that although this increased compu-  
191 tational expense was decided to be not too significant for Newtonian flows ( $\approx$   
192 10-20% [13]), the issue may be magnified for non-Newtonian flows because an  
193 iterative solution for the constitutive equation can require that certain aspects  
194 of the collision operator be performed at each iteration (the strain rate tensor  
195 is determined from the non-equilibrium distribution function which must be  
196 mapped into momentum space when using the MRT collision operator). Both  
197 the BGK [1, 20, 23, 24] and MRT [6, 7, 9] collision operators have been used  
198 successfully to simulate non-Newtonian flows. Chen et al. concluded that the  
199 MRT collision operator was more stable for Bingham plastic flow and allowed  
200 the use of a more accurate approximation to the Bingham plastic constitutive  
201 relationship.

202 ELBM and entropic filtering stuff goes here. The price of entropic lattice  
203 Boltzmann models for fluid flow is living with a bounded transport coefficient.  
204 Entropically stabilized collision operators ensure that entropy always increases,  
205 i.e. that the second law of thermodynamics is never violated. For BGK, this  
206 means that the relaxation time is bounded from below in certain instances [3].  
207 "it may be argued that we are relinquishing some control over the transport  
208 coefficients" and "of course, making  $\tau$  a nontrivial function of the incoming state  
209 will impact the hydrodynamic equations derived from the model" [3]. "stability  
210 is guaranteed"? Define Lyapunov functional or Lyapunov stability condition.

211 The goal of this paper is to numerically study the implications of accuracy,  
212 stability, and efficiency for some of the different strategies for simulating non-  
213 Newtonian flows using LBM. The intention of the study is to aid scientists and  
214 engineers in understanding which strategy to choose given their priorities and  
215 applications of interest so as to maximize the advantages LBM has in simulating  
216 non-Newtonian flow. Advantages, such as LBM's potential to scale well in  
217 parallel, can be much less realized if the collision operator is too computationally  
218 expensive, or if numerical instabilities ensue. A numerical study can help to  
219 determine approximate numerical values, domains, and boundary conditions in  
220 which one LBM scheme may be more advantageous than another so that LBM  
221 may be used in a computationally efficient and stable manner.

## 222 **2 Lattice Boltzmann Method**

### 223 **2.1 Overview**

224 Some overview of Lattice Boltzmann Method stuff [12].



225	<b>2.2</b>	<b>The Boltzmann Equation</b>
226	<b>2.3</b>	<b>Boundary Conditions</b>
227	<b>2.4</b>	<b>Applied Forces</b>
228	<b>2.5</b>	<b>Collision Operator</b>
229	<b>2.5.1</b>	<b>Bhatnagar–Gross–Krook</b>
230	<b>2.5.2</b>	<b>Multiple Relaxation Time</b>
231	<b>2.5.3</b>	<b>Entropic Collisions and Entropy Balance</b>
232	<b>3</b>	<b>Stability Analysis</b>
233	<b>3.1</b>	<b>von Neumann Stability Analysis</b>
234	<b>3.2</b>	<b>Matrix Method of Stability Analysis</b>
235	<b>3.3</b>	<b>Other Possible Approaches</b>
236	<b>4</b>	<b>Numerical Study</b>
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238	<b>4.2</b>	<b>Lid-driven Flow</b>
239	<b>5</b>	<b>Conclusion</b>
240		<b>Acknowledgements</b>
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