A CONTINUUM MODEL OF PLATELET
AGGREGATION: CLOSURE,
COMPUTATIONAL
METHODS AND
SIMULATION

by

Robert David Guy

A dissertation submitted to the faculty of
The University of Utah
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy

Department of Mathematics
The University of Utah
May 2004
Copyright © Robert David Guy 2004

All Rights Reserved
THE UNIVERSITY OF UTAH GRADUATE SCHOOL

SUPERVISORY COMMITTEE APPROVAL

of a dissertation submitted by

Robert David Guy

This dissertation has been read by each member of the following supervisory committee and by majority vote has been found to be satisfactory.

Chair: Aaron L. Fogelson

Paul C. Fife

James P. Keener

Graeme W. Milton

Jingyi Zhu
To the Graduate Council of the University of Utah:

I have read the dissertation of Robert David Guy in its final form and have found that (1) its format, citations, and bibliographic style are consistent and acceptable; (2) its illustrative materials including figures, tables, and charts are in place; and (3) the final manuscript is satisfactory to the Supervisory Committee and is ready for submission to The Graduate School.

Date

Aaron L. Fogelson
Chair, Supervisory Committee

Approved for the Major Department

Graeme W. Milton
Chair/Dean

Approved for the Graduate Council

David S. Chapman
Dean of The Graduate School
ABSTRACT

An existing continuum model of platelet aggregation in large arteries is presented. The blood and aggregating platelets are treated as a single fluid with varying material properties to account for links between platelets. There are two distinct spatial scales, the scale of the fluid and the much smaller scale of platelet–platelet interactions. Activated platelets interact to form elastic links on the smaller scale. These links influence the fluid flow by the addition of an extra stress.

The presence of two spatial scales makes the problem extremely difficult to analyze or to simulate. However, under the assumptions that the links act as linear springs with zero resting length and the breaking rate of the links is independent of the strain, the equations on the platelet scale can be eliminated in favor of an evolution equation for the stress tensor. In this dissertation, a closure model is presented that allows the breaking rate of a link to depend on its length while only working with variables on the fluid length scale. The closure model is compared with the full model using asymptotic analysis and computational tests.

The closure is used to explore the behavior of the model by simulating a growing aggregate on an injured vessel wall. These tests show that the model platelet aggregate is capable of covering an injury and redirecting the fluid. The results of the tests also reveal aspects of the model that need to be improved in future versions, such as the boundary condition at solid walls and the treatment of the aggregate as a single phase material. In creating these simulations, some computational challenges were encountered. The stability of an approximate projection method for solving the incompressible Navier-Stokes equations on a cell-centered grid is analyzed. The boundary conditions at the upstream and downstream boundaries are discussed, and a numerical method is proposed and analyzed.
Ты жена собака
CONTENTS

ABSTRACT ................................................................................ iv
LIST OF TABLES ...................................................................... ix
ACKNOWLEDGEMENTS ......................................................... x

CHAPTERS

1. INTRODUCTION .................................................................. 1

2. THE MODEL ....................................................................... 5
   2.1 Model Equations ............................................................... 5
       2.1.1 Elastic Links ............................................................ 6
       2.1.2 Forces from Links ...................................................... 8
       2.1.3 Platelets and Activator ............................................. 9
       2.1.4 Summary of Equations ........................................... 10
   2.2 Closure on Macro-scale .................................................. 11
       2.2.1 Constant Breaking ................................................... 12
       2.2.2 Other Closures ........................................................ 13
       2.2.3 Summary of Equations ........................................... 15
   2.3 Relationship to Polymeric Fluids ...................................... 15
       2.3.1 Linear Viscoelastic Models ...................................... 16
       2.3.2 Nonlinear Viscoelastic Models ................................. 17
       2.3.3 Transient Network Models .................................... 20

3. EVALUATING CLOSURES: STEADY SHEAR FLOW .......... 23
   3.1 Full Model ..................................................................... 23
       3.1.1 Short Bonds ............................................................ 25
       3.1.2 Long Bonds: Even Power Law Breaking ................... 27
       3.1.3 General Power Law Breaking .................................. 30
   3.2 Closure Model ............................................................... 30
       3.2.1 Breaking as a Function of Trace ............................... 31
       3.2.2 Breaking as a Function of Trace per Bond .................. 32
           3.2.2.1 Power Law Breaking ....................................... 34
           3.2.2.2 Exponential Breaking ...................................... 34
           3.2.2.3 Finite Energy .................................................. 37
   3.3 Comparison .................................................................... 37
       3.3.1 Asymptotic Comparison ......................................... 37
       3.3.2 Numerical Comparison .......................................... 41
   3.4 Conclusions .................................................................... 45
4. NUMERICAL SIMULATIONS OF THE MODEL

4.1 Nondimensionalization ........................................ 46
4.2 Time Stepping and Grid Structure ............................. 49
4.3 Platelets and Activator ....................................... 49
   4.3.1 Advection ............................................. 51
   4.3.2 Diffusion ............................................. 54
   4.3.3 Reaction ............................................. 54
4.4 Stress ..................................................... 55
   4.4.1 Two-Dimensional Fluids – Three-Dimensional Links ...... 55
   4.4.2 Platelet Pressure ..................................... 56
   4.4.3 Updating the Stress .................................... 57

5. NUMERICAL EXPERIMENTS .................................... 60

5.1 Grab and Pull Experiments .................................... 60
   5.1.1 Computational Tests .................................... 63
   5.1.2 Comparison with the Full Model ......................... 63
5.2 Growing Aggregate: Parallel Plate Flow ..................... 71
   5.2.1 Model at Solid Boundaries ............................... 73
   5.2.2 Initiating the Reaction ................................ 73
   5.2.3 Estimating Parameters .................................. 75
   5.2.4 Computational Tests .................................... 77
      5.2.4.1 Formation, Breaking, and Activation Rates ...... 77
      5.2.4.2 Longer Simulation .................................. 83
      5.2.4.3 Different Breaking Rate ........................... 86
   5.2.5 Summary of Experiments ................................. 88
   5.3 Discussion ............................................... 89

6. NUMERICAL SOLUTIONS OF THE INCOMPRESSIBLE
   NAVIER-STOKES EQUATIONS ................................ 92

6.1 Motivation .................................................. 92
6.2 Implementing Accurate Projection Methods .................. 94
   6.2.1 Temporal Discretization ................................ 95
   6.2.2 Spatial Discretization .................................. 96
   6.2.3 Nonlinear Terms ....................................... 99
   6.2.4 Comparison of Methods ................................ 100
6.3 Stability Analysis .......................................... 101
   6.3.1 Stability on MAC Grid .................................. 102
   6.3.2 Stability on a Cell-centered Grid: Approximate Projection .. 105
      6.3.2.1 Constant Extrapolation ........................... 106
      6.3.2.2 Higher Order Gradients ........................... 109
6.4 Numerical Tests ............................................ 111
   6.4.1 Model Problem ......................................... 111
   6.4.2 Navier-Stokes Test ...................................... 113
6.5 Discussion ................................................ 114
7. MODELING A PRESSURE DRIVEN FLOW ............................ 117
   7.1 Constant Pressure Drop ........................................... 118
   7.2 Pressure-Flux Relationship ....................................... 118
   7.3 Model Problem ....................................................... 120
       7.3.1 Problem Formulation ........................................... 120
       7.3.2 Steady State Solution ......................................... 121
       7.3.3 Numerical Schemes .............................................. 123
           7.3.3.1 Explicit Scheme .......................................... 123
           7.3.3.2 Implicit Scheme .......................................... 128
       7.3.4 Averaging Scheme .............................................. 128
           7.3.4.1 Weights Depend on Time Step ............................ 130
           7.3.4.2 Weights Independent of Time Step ....................... 131
       7.3.5 Numerical Tests: Oscillations ................................ 132
   7.4 Multiple Dimensions .............................................. 139
       7.4.1 Numerical Scheme .............................................. 139
       7.4.2 Nondimensionalization ......................................... 141
       7.4.3 Practical Time Step Restriction ............................. 142
       7.4.4 Numerical Tests ................................................ 144
   7.5 Summary ............................................................. 146

8. CONCLUSIONS ............................................................ 149

APPENDICES

A. MODEL DERIVATIONS ..................................................... 154

B. MULTIGRID ON CELL-CENTERED GRIDS ............................... 156

C. BREAKING RATE FOR GRAB AND PULL EXPERIMENT ............... 164

REFERENCES ............................................................... 166
LIST OF TABLES

3.1 Values of $A_m$ for $\alpha(r) = 1 - r^b$ ........................................ 40
3.2 Values of $A_m$ for $\alpha(r) = r(1 - r) \exp(br)$ .............................. 40
3.3 Computed values of $C_a$ ......................................................... 41
5.1 Parameters values used in grab and pull experiments ....................... 61
5.2 Parameters fixed throughout aggregate growth simulations ................ 76
5.3 Dimensionless parameters defined using parameters in Table 5.2 .......... 76
5.4 Values of $C_4$ and $G$ in experiments ....................................... 78
6.1 Ghost cell formulas and resulting gradients at left boundary ............... 106
6.2 Max norm of error in horizontal velocity, $u$ ................................... 114
6.3 Max norm of error in pressure .................................................. 115
6.4 $L_1$ norm of error in horizontal velocity, $u$ .................................. 115
6.5 $L_1$ norm of the error in pressure .............................................. 115
7.1 Minimum value of $\theta$ allowed by (7.68) for $\Delta t = 1/128$ ............ 143
B.1 Ghost cells weights for relaxation ............................................ 163
B.2 Ghost cells weights for interpolation .......................................... 163
B.3 Ghost cells weights for computing residuals ................................. 163
ACKNOWLEDGEMENTS

I would like to thank my supervisory committee members Paul Fife, Aaron Fogelson, Jim Keener, Graeme Milton, and Jingyi Zhu for helpful discussions while preparing this dissertation; Aaron Fogelson, my advisor, for all of his guidance, helpful discussions, encouragement, and time; Jim Keener for the many spontaneous conversations about math, science, and sports; my wife Oksana for all her love and support throughout my time as a graduate student; my family for all of the encouragement from the beginning; the many friends around the office who create a fun working environment. This work was supported in part by an NSF VIGRE grant and NSF grant #DMS-0139926 to Aaron Fogelson.
CHAPTER 1

INTRODUCTION

Hemostasis is the normal physiological response to blood vessel injury and is essential to maintaining the integrity of the vascular system. Hemostasis consists of two interacting processes, platelet aggregation and coagulation. The first involves cell-cell adhesion resulting in a platelet aggregate, and the second is an enzyme network that leads to the formation of a fibrin gel (clot) around the aggregating platelets. A malfunction of either process can lead to strokes, myocardial infarction, and other cardiovascular diseases. It is therefore important to understand these processes. This dissertation concerns modeling platelet aggregation.

The clotting response to vessel wall injury is essential to arrest bleeding and to heal the injury, but aggregates can also form on ruptured atherosclerotic plaques where the flow may be restricted because of the presence of the plaque. These aggregates can block the blood flow through the vessel, reducing oxygen transport to vital organs. Even if these clots do not immediately occlude the artery, they may embolize and become lodged elsewhere in the circulatory system.

Platelets are present in the blood in large numbers ($\approx 250,000/mm^3$) but only account for a small volume fraction ($\approx 0.3\%$). In the absence of injury, platelets circulate passively in the blood. In this state of passive circulation, the platelets are referred to as resting or nonactivated platelets. When the vessel wall is injured, proteins in the subendothelium, such as collagen, are exposed and react with nearby resting platelets. Platelets attach to the injured surface, and these attachments initiate the activation process, in which nonactivated platelets become activated platelets. Upon activation, platelets release chemicals into the plasma, which can activate other platelets even if they do not directly contact the injury. Once activated, platelets change shape from discoid objects to spiny spheres and express surface receptors that allow them to stick to one another to form a platelet aggregate.

A pair of activated platelets can be held together by the formation of molecular
cross-bridges, formed by the protein fibrinogen (or von Willebrand factor) binding to receptors on each of the platelets’ surfaces. The platelet surface contains approximately 50,000 receptors for fibrinogen, which are expressed only when the platelet is activated. In the model presented in this dissertation, platelet interactions are accounted for by the formation of links, which when stretched generate forces that act on the fluid.

The surrounding fluid plays a significant role in platelet aggregation. The flow transports platelets and chemicals, which are released from the surfaces of activated platelets. As platelets join the growing aggregate, the fluid must be redirected around the stationary platelets, generating stresses within the aggregate. These stresses may cause the inter-platelet links to break. As the aggregate grows and extends into the interior of the vessel the presence of the aggregate affects the flow.

Simultaneously modeling all of the processes of platelet activation, transport, and cohesion while also accounting for fluid dynamics and mechanics of the growing aggregate is a difficult problem. Many models focus on a subset of these processes. For example, there have been many models that considered the transport of chemicals and the distribution of fluid stresses around objects of fixed shape for flows in steady state [4, 15, 21, 22]. Sorensen et al. created a model to study the problem of chemical transport coupled with platelet deposition, but in this model the deposited platelets did not modify the fluid flow [37, 38].

Fogelson developed a computational model that tracks individual platelets [11]. Tracking the motion and interactions of individual platelets is computationally expensive, and so it is possible to construct simulations involving only a small number of platelets. In order to model aggregation on larger spatial scales, Fogelson developed a continuum model of platelet aggregation [12, 13], in which concentrations of platelets interact rather than individual platelets. It is this continuum model that is the basis for the work presented in this dissertation.

The details of the continuum model are presented in Chapter 2. In its most general form, the variables of the model depend on two spatial variables: one for the fluid scale and one for the much smaller platelet scale. The variable for the small spatial scale is used to describe the distribution of inter-platelet links. Integrals over the small scale of this distribution of links define stresses that feedback on the fluid. The presence of two spatial scales makes the model difficult to analyze and expensive to simulate. Under the assumptions that the links behave as linear springs and the breaking rate of the links is
independent of the length of the link, the dependence on the small scale can be eliminated. However, the assumption that link breaking is independent of the length of the link is very restrictive and leads to unphysical behavior.

One of the goals of the work presented in this dissertation is to propose and evaluate closure models so that the breaking rate is not constant, but the model equations close on the fluid scale. Eliminating the dependence on the small spatial scale yields a system for which exploring the model behavior is computationally tractable. Another goal of this work is to develop computational methods to simulate this closed system and to explore the behavior of the model in situations which have not yet been investigated.

The model and closure are presented in Chapter 2. Also in this chapter we discuss models of polymeric flow, for which the continuum model is a generalization. The continuum model was derived independently from the models of polymeric flow, but these models of interacting polymers provided the inspiration for the closure model proposed in this dissertation. The closure model is compared with results from the full model analytically in a simple flow and numerically for a more complex flow. The analytic comparison is made under steady shearing in the limit of large shear rate for a uniform concentration of activated platelets. This analysis is presented in Chapter 3.

Under more complex conditions, analysis of the model is not feasible, and so further evaluation of the closure model is done numerically. In Chapter 4 we detail the numerical methods used to construct simulations of the model. In Chapter 5 the results from numerical experiments are presented. Two types of experiments are performed. In the first set of experiments, we repeat a test from Wang and Fogelson [41] designed to illustrate the effects of a nonconstant breaking rate. In this work the authors developed numerical methods to simulate the full model. We use this test to numerically compare the predictions of the full model and the closure model. In the second set of numerical experiments, we use the closure model to explore the growth of an aggregate along the wall of a parallel plate flow chamber. In these experiments we explore some of the model parameters for which there are no known values. These tests are also performed to evaluate the model’s ability to simulate the growth of a platelet aggregate under conditions similar to a physiological environment.

Chapters 6 and 7 are somewhat separate from the preceding chapters. These two chapters concern numerical methods to solve the Navier-Stokes equations and the appropriate boundary conditions for simulating a pressure driven flow for which the computational
domain is only a portion of the physical domain being modeled. In each case the numerical stability of model problems is analyzed to understand the stability of more complicated problems. This stability analysis was performed after encountering numerical instabilities while constructing simulations of parallel plate flow.
CHAPTER 2

THE MODEL

In the continuum model, the concentrations of nonactivated platelets, activated platelets, and platelet activator are modeled. In the current implementation, the chemistry of activation is simplified. All sources of activation are lumped into the single quantity we call activator. Activator interacts with nonactivated platelets to produce activated platelets. The activated platelets interact with each other to form elastic links, which when stretched by velocity gradients, produce stresses that affect the fluid. The only feedback on the fluid from the platelets is through these stresses. The equations that govern the fluid flow are the incompressible Navier-Stokes equations,

\[
\begin{align*}
\rho (u_t + \mathbf{u} \cdot \nabla \mathbf{u}) &= -\nabla p + \mu \Delta \mathbf{u} + \mathbf{f}_b + \mathbf{f}_p \\
\nabla \cdot \mathbf{u} &= 0.
\end{align*}
\]  

(2.1) (2.2)

The two forcing terms, \( \mathbf{f}_b \) and \( \mathbf{f}_p \), represent general body forces and the body forces that result from platelet interactions, respectively.

In this chapter we derive the equations that govern the platelets, activator, and forces generated by aggregation. The model contains two separate spatial scales, that of the vessel and that of the platelet. In this form the we refer to the model as the full model. After presenting the full model, we explore ways of eliminating the dependence on the platelet scale.

The ideas for the closures presented in this chapter were inspired by similar models from nonNewtonian fluid dynamics. Though derived independently, the model is very similar to models of polymeric flow. These models are discussed, and the similarities and differences between polymer models and the platelet model are noted.

2.1 Model Equations

A continuum description of platelets is appropriate only when the spatial scale of the fluid is much larger than the size of individual platelets. Moderately sized arteries have
a diameter on the order of 1 mm, while the diameter of platelets is on the order of 1 \( \mu m \). A continuum description is appropriate for this situation. Let \( \epsilon \) denote the ratio of the length scale of the platelet to the length scale of the vessel. That is

\[
\epsilon = \frac{\text{platelet diameter}}{\text{vessel diameter}}. \tag{2.3}
\]

Note that \( \epsilon \ll 1 \), which is necessary in the model derivation.

The derivation presented here differs considerably from the original derivation presented in [12]. The resulting equations are identical, but the definitions of some of the variables differ by a scale factor. These scaling differences make no difference, except when interpreting the results obtained with the model.

### 2.1.1 Elastic Links

We define a function \( \bar{E}(x, r, t) \) that describes the links between activated platelets. Let \( z(x, t) \) be the total concentration of elastic links at \( x \). For a fixed point in space \( x \), \( \bar{E}(x, r, t) \) is the density of the concentration of links between the points \( x \) and \( x + r \), so that the total concentration of links connecting to the point \( x \) is

\[
z(x, t) = \int \bar{E}(x, r, t) \, dr. \tag{2.4}
\]

The units of \( \bar{E} \) are links per unit volume per unit volume. Let \( \phi_a(x, t) \) represent the concentration of activated platelets. Suppose that links form by simple mass action kinetics involving activated platelets with a formation rate, \( \bar{\alpha} \), that is a function of the separation of the platelets, and links break with a breaking rate, \( \bar{\beta} \), that may be a function of the length of the link. With these assumptions, the time derivative of \( \bar{E} \) is given by

\[
\frac{d\bar{E}}{dt} = \bar{\alpha} (|r|) \phi_a(x, t) \phi_a(x + r, t) - \bar{\beta} (|r|) \bar{E}. \tag{2.5}
\]

Note that this time derivative above is not the partial derivative, but the total time derivative.

Using the chain rule, the total time derivative of \( \bar{E} \) is

\[
\frac{d\bar{E}}{dt} = \frac{\partial \bar{E}}{\partial t} + \frac{dx}{dt} \cdot \nabla_x \bar{E} + \frac{dr}{dt} \cdot \nabla_r \bar{E}. \tag{2.6}
\]

The rate of change of the spatial variable \( x \) is just the velocity at \( x \), so that

\[
\frac{dx}{dt} = u(x, t). \tag{2.7}
\]
The variable \( r \) is also a spatial variable, but it denotes a location relative to \( x \). Let
\[
\xi = x + r,
\]
so that
\[
\frac{dr}{dt} = \frac{d\xi}{dt} - \frac{dx}{dt} = u(\xi, t) - u(x, t) = u(x + r, t) - u(x, t).
\]
(2.8)

Substituting (2.7) and (2.8) into (2.6) gives
\[
\frac{dE}{dt} = \frac{\partial E}{\partial t} + u(x, t) \cdot \nabla_x E + \left( u(x + r, t) - u(x, t) \right) \cdot \nabla_r E.
\]
(2.9)

Equating the right sides of equations (2.5) and (2.9) gives the evolution equation for \( E \)
\[
\frac{\partial \tilde{E}}{\partial t} + u(x, t) \cdot \nabla_x \tilde{E} + \left( u(x + r, t) - u(x, t) \right) \cdot \nabla_r \tilde{E} = \tilde{\alpha} (|r|) \phi_a(x, t) \phi_a(x + r, t) - \tilde{\beta} (|r|) \tilde{E}.
\]
(2.10)

So far this derivation has not used the fact that the length scale of platelets is much smaller than the length scale of the domain. In order to emphasize this difference in scales, we now rescale the distribution variable \( r \) so that
\[
r = \epsilon y.
\]
(2.11)

We define \( E \) as a rescaling of \( \tilde{E} \) by
\[
E(x, y, t) = \epsilon^3 \tilde{E}(x, r, t).
\]
(2.12)

The factor of \( \epsilon^3 \) is used so that the total concentration of links at a point given in equation (2.4) can be written in the new coordinate as
\[
z(x, t) = \int \tilde{E}(x, r, t) \, dr = \int E(x, y, t) \, dy.
\]
(2.13)

In the new coordinate, the formation and breaking rates are
\[
\alpha (|y|) = \epsilon^3 \tilde{\alpha} (|r|) \quad \text{and} \quad \beta (|y|) = \tilde{\beta} (|r|).
\]
(2.14)

By multiplying equation (2.10) through by \( \epsilon^3 \) and changing coordinates to eliminate the appearance of the variable \( r \), the evolution equation for \( E \) that results is
\[
\frac{\partial E}{\partial t} + u(x, t) \cdot \nabla_x E + \left( u(x + \epsilon y, t) - u(x, t) \right) \cdot \epsilon^{-1} \nabla_y E = \alpha (|y|) \phi_a(x, t) \phi_a(x + \epsilon y, t) - \beta (|y|) E.
\]
(2.15)
Expanding the functions $u(x + \epsilon y, t)$ and $\phi_\alpha(x + \epsilon y, t)$ about the point $x$, and retaining only the $O(1)$ terms in equation (2.15) gives the equation

$$
\frac{\partial E}{\partial t} + u(x, t) \cdot \nabla_x E + \left(y \cdot \nabla u(x, t)\right) \cdot \nabla_y E = \alpha(|y|) \phi_\alpha^2(x, t) - \beta(|y|) E.
$$

(2.16)

This equation is the final form that is used in the model.

### 2.1.2 Forces from Links

Equation (2.16) describes how the distribution of links evolves, but it is through the stretching of the links that body forces develop that feed back onto the fluid. We now derive an expression for the body forces due to links. Let $\mathbf{F}(r)$ be the force generated by a single link. The total body force due to links is

$$
\mathbf{f}_p(x, t) = \int E(x, r, t) \mathbf{F}(r) \, dr.
$$

(2.17)

We wish to express the integral in terms of the scaled coordinate $y$. The force is rescaled as $\mathbf{F}(r) = \epsilon^{-1} \mathbf{F}(y)$. Note that the dimensions of force are $[\text{mass}] [\text{length}] / [\text{time}]^2$. The factor of $\epsilon^{-1}$ accounts for a rescaling of this length dimension in the force. With the integral in terms of the scaled coordinate, the body force is

$$
\mathbf{f}_p = \epsilon^{-1} \int E(x, y, t) \mathbf{F}(y) \, dy.
$$

(2.18)

The presences of the $\epsilon^{-1}$ seems troubling. Note that if the integrand were an odd function in $y$, then the body force would be zero. The force, $\mathbf{F}(y)$, must be an odd function, and, as it turns out, the link distribution function is “almost” an odd function, making the body forces order one.

By its definition, $E$ must satisfy

$$
E(x, -y, t) = E(x - \epsilon y, y, t).
$$

(2.19)

Expanding the right side of this equation for small $\epsilon$ gives

$$
E(x, -y, t) = E(x, y, t) - \epsilon y \cdot \nabla_x E(x, y, t) + O(\epsilon^2),
$$

(2.20)

which explains the statement that $E$ is almost an odd function. Make the change of variables $y \to -y$ in equation (2.18), use the expansion (2.20), and use that $\mathbf{F}(-y) = -\mathbf{F}(y)$ to get

$$
\mathbf{f}_p = -\mathbf{f}_p + \int y \cdot \nabla_x E(x, y, t) \mathbf{F}(y) \, dy + O(\epsilon).
$$

(2.21)
Rearranging this equation and retaining only the leading order term gives

\[ f_p = \frac{1}{2} \int y \cdot \nabla_x E(x, y, t) F(y) \, dy. \]  \hspace{1cm} (2.22)

This equation can be used to compute the body forces for a given distribution of links.

We now give another useful form, which is more commonly used. Write the force per link in the form

\[ F(y) = S(|y|) \, y, \]  \hspace{1cm} (2.23)

where \( S(|y|) \) represents the stiffness of the link as a function of the length of the link.

The body force defined by equation (2.22) can be expressed as the divergence of the stress tensor

\[ \tau(x, t) = \frac{1}{2} \int E(x, y, t) S(|y|) \, yy^T \, dy, \]  \hspace{1cm} (2.24)

where \( yy^T \) represents the tensor product. One of the goals of this dissertation is to produce model equations that do not include any dependence on the small spatial scale. In section 2.2 we introduce an evolution equation for \( \tau \) that does not require explicit knowledge of \( E \) to compute the stresses.

### 2.1.3 Platelets and Activator

The equations that describe the concentrations of nonactivated and activated platelets account for advection, diffusion, and activation. Let \( \phi_n \) and \( \phi_a \) denote the concentrations of nonactivated and activated platelets, respectively, and let \( c \) denote the concentration of activator. The equations that govern the concentrations of these three quantities are

\[ \frac{\partial \phi_n}{\partial t} + u \cdot \nabla \phi_n = D_n \Delta \phi_n - R(c) \phi_n \]  \hspace{1cm} (2.25)
\[ \frac{\partial \phi_a}{\partial t} + u \cdot \nabla \phi_a = R(c) \phi_n \]  \hspace{1cm} (2.26)
\[ \frac{\partial c}{\partial t} + u \cdot \nabla c = D_c \Delta c + A R(c) \phi_n. \]  \hspace{1cm} (2.27)

We now describe the reasoning behind each of these terms.

Both platelets and activator are advected by the fluid. The activator diffuses with diffusion coefficient \( D_c \). Note that the nonactivated platelets diffuse, but activated platelets are assumed not to diffuse. The platelet diameter, about 1 \( \mu \text{m} \), is large enough that one would not expect Brownian motion to be a significant mechanism for transporting platelets. The motivation for including diffusion of platelets in the model comes from the observation that platelets undergo a random motion, which is thought to result from
collisions with red blood cells [43]. Red blood cells are much larger (≈ 7-8 μm in diameter), make up 45% of the volume of whole blood, and are very deformable [16]. The tumbling of the red blood cells causes a mixing of the blood, which causes the platelets to undergo a diffusion-like motion. However, as activated platelets form larger and larger aggregates, the effect of red blood cells on the motion of these aggregates should diminish. The change in diffusion is accounted for by allowing nonactivated platelets to diffuse and assuming that the diffusion of activated platelets is negligible in the model equations.

The final terms that need to be described are the reaction terms. In the presence of activator, nonactivated platelets become activated at a rate $R(c)$. In the model equations $R(c)\phi_n$ is subtracted from equation (2.25) and added to equation (2.26) to account for activation. When activated, platelets release the contents of dense granules that contain ADP [1]. Let $A$ denote the amount of ADP released per platelet upon activation. Because $R(c)\phi_n$ is the concentration of platelets activated per unit time, the term $AR(c)\phi_n$ is added to the right hand side of equation (2.27) to account for the release of additional activator. Note that we have assumed that ADP is the primary activator. Thrombin is a potent activator that is produced on the surface of activated platelets. The equations could easily be modified to include thrombin as well as ADP, as has recently been explored in [14]. For the purposes of this dissertation, it is sufficient to consider only activation by ADP.

Activation by ADP requires a threshold concentration to be reached before activation takes place [1]. The form of the activation function used in this dissertation is

$$R(c) = R_0 H (c - c_0),$$

where $R_0$ is the activation rate above threshold, $H$ is the Heaviside function, and $c_0$ represents the threshold concentration required for activation.

### 2.1.4 Summary of Equations

Before discussing the model further, we write the model equations together. The model equations are
\[
\begin{align*}
\rho (u_t + u \cdot \nabla u) &= -\nabla p + \mu \Delta u + f_b + \nabla \cdot \underline{\sigma} \quad (2.29) \\
\nabla \cdot u &= 0 \quad (2.30) \\
\frac{\partial E}{\partial t} + u \cdot \nabla E + (y \cdot \nabla u) \cdot \nabla_y E &= \alpha (|y|) \phi_a^2 - \beta (|y|) E \quad (2.31) \\
\underline{\sigma}(x, t) &= \frac{1}{2} \int E(x, y, t) S(\langle y \rangle) y y^T dy \quad (2.32) \\
\frac{\partial \phi_n}{\partial t} + u \cdot \nabla \phi_n &= D_n \Delta \phi_n - R_0 H (c - c_0) \phi_n \quad (2.33) \\
\frac{\partial \phi_a}{\partial t} + u \cdot \nabla \phi_a &= R_0 H (c - c_0) \phi_n \quad (2.34) \\
\frac{\partial c}{\partial t} + u \cdot \nabla c &= D_c \Delta c + A R_0 H (c - c_0) \phi_n. \quad (2.35)
\end{align*}
\]

In this form we refer to the model as the full model, because it contains two spatial scales. Below we discuss when the model can be expressed with only one spatial scale.

### 2.2 Closure on Macro-scale

The model equations presented so far depend on two spatial scales, which we refer to as the macro-scale for the fluid scale \((x)\) and the micro-scale for the platelet scale \((y)\). The presence of two spatial scales makes analyzing and simulating the model difficult. We would like to eliminate the dependence on the micro-scale, if possible. This would cut the number of spatial dimensions in half, and make analysis and simulations more tractable.

The only variable in the model that explicitly depends on the micro-scale is the link distribution \(E\), but it is the stress, which does not depend on \(y\), that affects the motion of the fluid. We now attempt to use the equation for \(E\) to derive an evolution equation for \(\underline{\sigma}\) in hope of eliminating the dependence on \(y\) in the model. To produce an evolution equation for \(\underline{\sigma}\), begin by multiplying equation (2.31) through by \(1/2 S(\langle y \rangle) y y^T\) and then integrating over all \(y\). After some manipulations presented in Appendix A,

\[
\underline{\sigma} + u \cdot \nabla \underline{\sigma} = \underline{\sigma} \nabla u + (\underline{\sigma} \nabla u)^T + a_2 \delta \underline{\sigma} \\
- \frac{1}{2} \int (y^T \nabla u y) |y|^{-1} S'(\langle y \rangle) E(x, y, t) y y^T dy \\
- \frac{1}{2} \int \beta (|y|) E y y^T dy,
\]

where \(\delta\) represents the identity tensor, and \(a_2\) is given by

\[
a_2 = \frac{2\pi}{3} \int_0^\infty \alpha(r) S(r) r^4 dr. \quad (2.37)
\]
There are two terms remaining that still depend on the micro-scale. The first can be eliminated by assuming that links behave like linear springs, so that $S'(|y|) = 0$. The assumption of constant stiffness is used for the remainder of this dissertation, and the stiffness is denoted by $S_0$. If it is assumed that the breaking rate, $\beta$, is not a function of the length of the link, then the integral involving the breaking rate becomes $\beta \sigma$. Using the assumptions that the stiffness is constant and the breaking rate is independent of the length of the link, the equation for the stress becomes

$$\sigma_{12} + u \cdot \nabla \sigma = \sigma \nabla u + (\sigma \nabla u)^T + a_2 \phi_0^2 \beta - \beta \sigma.$$  \hspace{1cm} (2.38)

We now discuss some possible forms of $\beta$.

### 2.2.1 Constant Breaking

In previous versions of the model [12, 13], in order to close the equations on the macro-scale, it was assumed that the breaking rate was constant, so that $\beta = \beta_0$. Using this assumption, links that are stretched considerably, and as a result are making a large contribution to the stress, have the same probability of breaking as links that are under very little strain. This behavior is not expected in physical reality, but it is not obvious that very long links will affect the results from the model. As it turns out, the assumption of constant breaking rate does lead to some unsatisfactory behavior in the model. This is demonstrated by two computations of the stress for a steady state velocity profiles.

Consider the situation of a steady state shear flow with a uniform concentration of activated platelets, denoted by $\phi_a = \phi_0$. Let $\gamma$ denote the shear rate, so that the velocity field is $u = (\gamma x_2, 0, 0)$. Under these conditions, the stress tensor due to links can be computed from equation (2.38). The resulting shear stress is

$$\sigma_{12} = \frac{\phi_0^2 a_2}{\beta_0^2} \gamma.$$ \hspace{1cm} (2.39)

Notice that the shear stress is a linear function of the shear rate. A useful rheological measurement of interest for non-Newtonian fluids is the shear viscosity [6, 25]. The shear viscosity is the ratio of the shear stress to the shear rate, so that

$$\mu_{\text{shear}} = \frac{\sigma_{12}}{\gamma}.$$

The shear viscosity computed using (2.39) is independent of the shear rate. If the breaking rate were to increase with the length of the link, then the shear viscosity would be expected
to decrease as the shear rate increases. This phenomenon is known as shear thinning. To relate this to platelet aggregation, imagine a layer of aggregating platelet which is being sheared by fluid flow parallel to the surface of the layer. We expect that if the aggregate is sheared harder, it would break up more readily and provide less resistance to the flow. As this computation shows, the constant breaking rate does not allow this behavior. The behavior of the full model during steady shear flow is analyzed in detail in Chapter 3.

For a second thought experiment, suppose that the velocity is a planar extensional flow, so that \( \mathbf{u} = (\gamma x_1, -\gamma x_2, 0) \) with a uniform concentration of activated platelets. Using equation (2.38) to solve for \( \sigma_{11} \) gives that

\[
\sigma_{11} = \frac{\phi_0^2 \sigma_2}{\beta_0 - 2\gamma}.
\]  

(2.40)

This computation shows that arbitrarily large stresses can be generated by forcing the flow at a finite velocity. These high stresses, which are clearly unphysical, result from the presence of arbitrarily long links.

These two computations show that the assumption of constant breaking leads to some unsatisfactory behavior of the model. In these two tests there was no feedback from the platelets to the fluid, the platelet concentration was uniform, and the concentration of platelets did not change. These tests do not give direct information about the behavior expected in circumstances more like those of a dynamically changing platelet aggregate. However, computational tests of the full model in more dynamic situations with nonconstant breaking rates were performed by Wang and Fogelson [41]. The results from these computational tests showed that a nonconstant breaking rate is necessary to produce certain realistic behaviors that are relevant in modeling platelet aggregation.

### 2.2.2 Other Closures

As discussed in the previous section, the assumption of a constant breaking rate closes the system on the macro-scale, but produces unphysical results. We would like to be able to allow the breaking rate to be variable, and still close the equations on the macro-scale. The system closes as long as the breaking rate is not a function of the micro-space scale. One option is to assume that the breaking rate is a function of macro-scale quantities only, but it is not clear on which quantities the breaking rate should depend.

As discussed in section 2.3, this model is similar to models of polymeric fluids. In [36] a closure for a similar equation was proposed in which it is assumed that the breaking rate is a function of the trace of the stress tensor, so that
The energy of a link between \( x \) and \( x + \epsilon y \) is \( 1/2 S_0 |y|^2 \), and so integrating this expression against \( E \) over all \( y \) gives the total energy due to links at the point \( x \). The integral that defines the trace of the stress tensor is

\[
\text{Tr} (\sigma) = \frac{1}{2} \int ES_0 y_j y_j \, dy = \frac{1}{2} \int ES_0 |y|^2 \, dy,
\]

where we use the convention that repeated indices imply summation. The trace can therefore be interpreted as the total energy due to links at a point.

The equations for which this closure is used in [36] are similar to our model equations, but not identical. An important distinction is that in [36], the function that plays the role of \( E \) is constrained so that

\[
\int E \, dy = 1.
\]

For our model, this would mean that the total number of links at each point is the same, which is clearly not the case. Recall that the total number of links at a point is denoted by \( z \). Another reasonable closure explored in this dissertation is achieved by assuming that the breaking rate is a function of the ratio of the trace of the stress to the total number of links, so that

\[
\beta = \beta \left( \frac{\text{Tr} (\sigma)}{z} \right).
\]

Since the trace has the interpretation of the total energy due to links, the ratio of the trace to the total number of links can be interpreted as the average energy per link at a point. Exploiting the fact that the stiffness is constant, we may write

\[
\frac{\text{Tr} (\sigma)}{z} = \frac{1}{2} \int ES_0 y_j y_j \, dy = \frac{S_0}{2} \left< |y|^2 \right>,
\]

meaning that this ratio is proportional also to the average squared length of the links at a point.

In order to use a closure that depends on the concentration of links, an evolution equation for \( z \) must be derived. This is done in the same fashion as the equation for the stress. Integrating each term in equation (2.31) over all of \( y \) gives the equation

\[
z_t + \mathbf{u} \cdot \nabla z = a_0 \psi_0^2 - \beta z,
\]
where
\[ a_0 = 4\pi \int_0^{\infty} \alpha(r)r^2 \, dr, \]  
(2.44)
and we have assumed that the breaking rate is independent of the micro-scale link length.

Both of these closures seem reasonable. Their usefulness is evaluated on their ability to approximate the behavior of the full model. In Chapter 3, the stresses that result in steady shear flow are compared both asymptotically and numerically to the full model. These comparisons reveal how the form of the breaking rate in the closure can be chosen to best reproduce the behavior of a given breaking rate for the full model.

### 2.2.3 Summary of Equations

Assume that the model has been closed by letting the breaking rate be independent of the length of the link. The complete set of model equations is

\[
\rho (u_t + u \cdot \nabla u) = -\nabla p + \mu \Delta u + f_b + \nabla \cdot \sigma, \quad (2.45)
\]

\[
\nabla \cdot u = 0 \quad (2.46)
\]

\[
\sigma_t + u \cdot \nabla \sigma = \sigma \nabla u + (\sigma \nabla u)^T + a_2 \phi_n^2 \delta - \beta \sigma \quad (2.47)
\]

\[
z_t + u \cdot \nabla z = a_0 \phi_n^2 - \beta z \quad (2.48)
\]

\[
\frac{\partial \phi_n}{\partial t} + u \cdot \nabla \phi_n = D_n \Delta \phi_n - R_0 H (c - c_0) \phi_n \quad (2.49)
\]

\[
\frac{\partial \phi_a}{\partial t} + u \cdot \nabla \phi_a = R_0 H (c - c_0) \phi_a \quad (2.50)
\]

\[
\frac{\partial c}{\partial t} + u \cdot \nabla c = D_c \Delta c + A R_0 H (c - c_0) \phi_n. \quad (2.51)
\]

The formation rates of the stress and the concentration of links are related to the link formation function by

\[
a_2 = \frac{2\pi}{3} \int_0^{\infty} \alpha(r)S_0 r^4 \, dr \quad (2.52)
\]

\[
a_0 = 4\pi \int_0^{\infty} \alpha(r)r^2 \, dr. \quad (2.53)
\]

### 2.3 Relationship to Polymeric Fluids

The model presented in this section is similar to certain models that arise in models of polymeric fluid. Before discussing the details of these models we introduce some standard models of viscoelastic fluids. If the platelet concentration is constant in time and uniform in space and the breaking rate is constant, equation (2.47) reduces to a standard constitutive model that appears in general viscoelastic fluids. Therefore we begin this
discussion with a brief introduction to linear viscoelastic models, which leads naturally to nonlinear models that are similar to the constitutive equation for platelet stress under the conditions described above. We conclude this section with a brief discussion about transient network models, which are models used in polymeric fluids and are very similar to the model presented in this dissertation. This section summarizes ideas from [6, 7, 25].

2.3.1 Linear Viscoelastic Models

We begin by considering the shearing of a viscous fluid and the shearing of an elastic solid. Let \( u \) denote the velocity field of the fluid, and let \( w \) denote the displacement field of the elastic solid. The velocity of the viscous fluid is given by

\[
u_1 = \dot{\epsilon} y,
\]

where the shear rate, or strain rate, is denoted by \( \dot{\epsilon} \). The shear stress that results is

\[
\sigma_{12}^f = \mu \dot{\epsilon},
\]

where \( \mu \) is the viscosity. The displacement of the elastic solid is

\[
w_1 = \epsilon y,
\]

where \( \epsilon \) represents the strain. The shear stress in the solid is

\[
\sigma_{12}^s = G \epsilon,
\]

where \( G \) represents the elastic modulus.

Consider a fluid that supports both viscous stress and elastic stress. We can relate the shear stresses in (2.55) and (2.57) through the strain rate. Suppose that the strain and the strain rate are related by

\[
\frac{\partial \epsilon}{\partial t} = \dot{\epsilon}.
\]

Combining (2.55) and (2.57) gives

\[
\sigma_{12} + \lambda \frac{\partial \sigma_{12}}{\partial t} = \mu \dot{\epsilon},
\]

where

\[
\lambda = \frac{\mu}{G}.
\]
Note that if $\lambda \to 0$ a viscous fluid is recovered. This equation describes the shear stress for a shear flow. To describe more general flows, the scalar strain rate must be extended to a strain rate tensor. The strain rate tensor is

$$\dot{\varepsilon} = \nabla \mathbf{u} + (\nabla \mathbf{u})^T = 2\mathbf{D},$$

where $\mathbf{D}$ is the deformation rate tensor of the fluid. The constitutive equation for the stress tensor is

$$\sigma + \lambda \frac{\partial \sigma}{\partial t} = \mu \dot{\varepsilon}.$$  

(2.62)

This constitutive equation was proposed by Maxwell [31], and is considered the first constitutive equation used to describe viscoelastic fluids, and so such fluids are called \textit{linear Maxwell fluids}.

### 2.3.2 Nonlinear Viscoelastic Models

So far we have not shed light on the relationship between viscoelastic fluids and the model of platelet aggregation presented in this dissertation. In order to bridge this gap, we must introduce nonlinear Maxwell fluids. One way to move from the linear Maxwell fluid to the nonlinear models is to carefully examine what time derivative should appear in (2.62) rather than the partial time derivative. This approach requires a detailed discussion of convected coordinate systems and is beyond the scope of this dissertation, but a thorough discussion of this topic can be found in [6]. An equivalent way to move to the nonlinear models is to eliminate the time derivative by presenting an integral constitutive equation, and then modifying the definition of strain.

Equation (2.62) can be integrated to get

$$\sigma = \int_{t_0}^t \frac{\mu}{\lambda} \exp \left( (t' - t)/\lambda \right) \dot{\varepsilon}(t') dt'.$$

(2.63)

This integral shows explicitly how the fluid has a fading memory of past strain rates that affect the stress. This integral constitutive law can also be written in terms of past strain by integrating by parts. Fluids, unlike solids, do not have a natural reference configuration from which to define strain. We can define the strain as a function of two times, representing the strain between the configurations at those two times by

$$\varepsilon(t, t') = \int_{t'}^{t''} \dot{\varepsilon}(t'') dt''.$$  

(2.64)

Using this definition for the strain, (2.63) can be integrated by parts to get

$$\sigma = \int_{t_0}^t \frac{\mu}{\lambda^2} \exp \left( (t' - t)/\lambda \right) \varepsilon(t, t') dt'.$$

(2.65)
Recall that the elastic modulus is \( G = \mu/\lambda \), and so this integral can be written as

\[
\sigma = \int_{-\infty}^{t} \lambda^{-1} \exp\left(\frac{(t' - t)}{\lambda}\right) G \zeta(t, t') \, dt'.
\]  
(2.66)

This form shows that another interpretation of the constitutive law is that the fluid has a fading memory of strain.

If displacement gradients are small, the strain can be expressed as the symmetric part of the displacement gradient. This strain is referred to as linear strain. However, when displacement gradients are not small, linear strain is not the appropriate measure of strain. Consider a fluid particle whose position \( \mathbf{x}' \) at time \( t' \) was \( t \), and whose current position is \( \mathbf{x} \) at time \( t \). We introduce two different displacement gradient tensors

\[
F_{ij} = \frac{\partial x'_i}{\partial x_j},
\]  
(2.67)
and its inverse

\[
F^{-1}_{ij} = \frac{\partial x_i}{\partial x'_j}.
\]  
(2.68)

These two velocity gradients can be used to define two different strain tensors: the Cauchy strain tensor

\[
C_{ij} = \frac{\partial x'_m}{\partial x_j} \frac{\partial x'_m}{\partial x_j},
\]  
(2.69)
and the Finger strain tensor

\[
C^{-1}_{ij} = \frac{\partial x_i}{\partial x'_m} \frac{\partial x_j}{\partial x'_m}.
\]  
(2.70)

Each of these tensors provides a measure of strain. We do not discuss which strain should be used, but we use the Finger strain tensor because the constitutive law it produces is similar to the constitutive law that appears in the model of platelet aggregation.

Consider the integral form of the linear Maxwell fluid given by (2.66) with the strain measured by the Finger tensor, so that

\[
\sigma = \int_{-\infty}^{t} \lambda^{-1} \exp\left(\frac{(t' - t)}{\lambda}\right) G \zeta^{-1}(t, t') \, dt'.
\]  
(2.71)
To produce a differential constitutive law we take the total time derivative of both sides, including convection of the stress, to get

\[
\sigma_t + \mathbf{u} \cdot \nabla \sigma = G \lambda^{-1} \zeta^{-1}(t, t) - \int_{-\infty}^{t} \lambda^{-2} \exp\left(\frac{(t' - t)}{\lambda}\right) G \zeta^{-1}(t, t') \, dt'
\]  
(2.72)

\[
+ \int_{-\infty}^{t} \lambda^{-1} \exp\left(\frac{(t' - t)}{\lambda}\right) G \zeta^{-1}(t, t') \, dt'.
\]  
(2.73)
Note that using the definition of the Finger tensor, its time derivative is given by
\[
\dot{C}^{-1} = \nabla u C^{-1} + (\nabla u C^{-1})^T.
\tag{2.75}
\]
Using this relationship, equation (2.74) simplifies to
\[
\sigma_{\alpha t} + u \cdot \nabla \sigma = G \lambda^{-1} \dot{\sigma}_\alpha + \frac{1}{\lambda} \sigma_\alpha + \nabla u \sigma + (\nabla u \sigma)^T.
\tag{2.76}
\]
This equation is identical to the platelet stress constitutive equation if the concentration of activated platelets is uniform and the breaking rate is constant and if we define the relaxation time and elastic modulus by
\[
\lambda = \beta^{-1} \quad \text{and} \quad G = \frac{\phi_0 \beta}{\beta},
\]
where \(\phi_0\) represents the concentration of activated platelets. Under these conditions we see that the platelet model reduces to a standard model of a viscoelastic fluid.

Equation (2.76) can be rewritten in a form that is more commonly used to describe fluids of this type. Note that when the velocity gradient is zero, the steady state stress from equation (2.76) is
\[
\sigma = G \dot{\sigma}_\alpha\tag{2.77}
\]
which is like an extra pressure. So that the stress will be zero when the velocity gradients are zero, we can subtract off this pressure to define a new stress tensor by
\[
\tau = \sigma - G \dot{\sigma}_\alpha\tag{2.78}
\]
Using this definition for \(\tau\) and equation (2.76), we can write
\[
\tau_{\alpha t} + u \cdot \nabla \tau = \nabla u \tau + (\nabla u \tau)^T + G \dot{\tau} - \lambda^{-1} \tau.
\tag{2.79}
\]
Simply rearranging this equation we write
\[
\tau + \lambda \left( \tau_{\alpha t} + u \cdot \nabla \tau - \nabla u \tau - (\nabla u \tau)^T \right) = \mu \dot{\tau}.
\tag{2.80}
\]
In this form we see that this equation is very similar to the linear Maxwell equation (2.62). In fact, the terms multiplied by \(\lambda\) in equation (2.80) are analogous to the time derivative. Equation (2.80) is called the upper-convected Maxwell equation.

In the platelet model \(\sigma\) is the stress due to platelets only. There is additional stress arising from the viscosity of the fluid. Fluids of this type are not called Maxwell fluids,
rather they are Oldroyd-B fluids. The constitutive equation for Oldroyd-B fluids appears in two different forms. As we have done, stress in these fluids is the sum of two stresses: one that satisfies the upper convected Maxwell equation and another viscous contribution. Sometimes these two stresses are combined into a single stress, and an evolution equation similar to (2.80) can be used to describe the evolution of this stress.

We can interpret the continuum model for platelet aggregation as an Oldroyd-B fluid with an elastic modulus and viscosity depending on the activated platelet concentration. This interpretation is useful when selecting parameters for simulations. For example if $a_2$ and $\beta$ are changed proportionally, the elastic modulus of the aggregate does not change but its extra viscosity does.

### 2.3.3 Transient Network Models

In the previous section we showed a relationship between equation (2.47) for the platelet stress and equations that are used to describe viscoelastic fluids. The presentations of the linear Maxwell equation (2.62) and the upper convected Maxwell equation (2.80) were somewhat phenomenological. The equation for the platelet stress arises from assumptions about the movement and forces of small scale elastic links. Similar multiscale approaches have been used to model polymeric fluids [25]. The continuum model of platelet aggregation presented in this dissertation was first derived by Fogelson [12] independently of the polymer fluid literature, but as we discuss in this section, the continuum model is a generalization of a transient network model.

As the name implies, network models are used to describe fluids that consist of a solvent surrounding a network of polymer strands that interact only at junctions. Junctions can be chemical crosslinks or simply entanglements between polymer strands. These junctions break and reform as the network is deformed by the flowing solvent, and the stretching of strands produces elastic stresses. This network is represented by a distribution function $\psi(x, y, t)$ that describes the density of elastic links between points, which has the same meaning as the function $E(x, y, t)$ in the continuum model. In discussing polymer network models we use $\psi$ to represent the distribution of junctions rather than $E$ to distinguish from the platelet model.

So far our description of network models is no different from our description of the model of platelet interactions presented in this dissertation. However, there are distinct differences between these two models. In the platelet model, activated platelets are required in order to form elastic links, and the concentration of activated platelets
varies spatially and temporally. In models of networked polymer, the concentration of polymer is uniform in space and time, meaning the network is always present, while in the platelet model the network forms as time progresses. In most, but not all, models of networked polymer, it is assumed that if a junction breaks, it immediately reforms, but in a configuration not contributing to the stress. Therefore, the total number of junctions (the equivalent of $z$ in our model) is a constant.

Network theory was first proposed by Green and Tobolsky [19]. The work was inspired by rubber elasticity theory, which is also based on the idea of a network of crosslinked polymer that produce stress when deformed, but the rubber network does not break. Green and Tobolsky assumed a constant probability per unit time of a junction rupturing, and they assumed that junctions re-form instantaneously upon breaking, but they form in a configuration typical of equilibrium. They also assume that the polymer strands move with the fluid velocity, meaning that the Finger tensor is the appropriate measure of strain. These assumptions lead directly to the integral constitutive law (2.71). This theory was generalized by Lodge [30] to include multiple, independent relaxation times (breaking probabilities) to give the integral constitutive law

$$\varphi = \int m\left(t-t'\right)C^{-1}(t,t')dt',$$  \hspace{1cm} (2.81)

where

$$m\left(t-t'\right) = \sum_j \frac{G_j}{\lambda_j} \exp\left(-\left(t-t'\right)/\lambda_j\right).$$  \hspace{1cm} (2.82)

Equation (2.81) is often called the Lodge equation. These integral constitutive laws can be differentiated to produce differential constitutive laws, as was done in the previous section. These early network theories provide a structured framework to produce the Maxwell model.

Yamamoto [45, 46, 47] generalized the theory of Green and Tobolsky so that the formation rate and breaking rates are functions of the length that chains are stretched. The evolution equation for the distribution of links can be written as

$$\frac{\partial \Psi}{\partial t} + \mathbf{u} \cdot \nabla_x \Psi + (\mathbf{y} \cdot \nabla \mathbf{u}) \cdot \nabla_y \Psi = g\left(|\mathbf{y}|\right) - h\left(|\mathbf{y}|\right) \Psi,$$  \hspace{1cm} (2.83)

where $g$ and $h$ are the formation and breaking rate functions. As in previous network models, it is assumed that as soon as a junction ruptures it re-forms at a length characteristic of equilibrium. This assumption specifies the form of the formation rate function
in terms of the breaking rate function. To see this, let $\Psi_0$ represent the link distribution function at steady state under no flow. Equation (2.83) gives that

$$g (|y|) = h (|y|) \Psi_0. \quad (2.84)$$

Using (2.84), equation (2.83) reduces becomes

$$\frac{\partial \Psi}{\partial t} + u \cdot \nabla \Psi + (y \cdot \nabla u) \cdot \nabla_y \Psi = h (|y|) (\Psi_0 - \Psi). \quad (2.85)$$

In this form the re-formation assumption is made explicit. The relationship expressed in (2.84) shows that links form at equilibrium at a rate equal to the breaking rate of nonequilibrium strands.

Yamamoto’s model suffers from the same closure problem that was discussed in section 2.2. In order to close the model on the macro-scale, Phan-Thein and Tanner [36] proposed that the breaking rate depend on the trace of the stress rather than on the length of the link. This assumption was discussed at length in section 2.2.2. This model is often referred to as the PTT model after the authors’ initials. The PTT model was the inspiration for the closure proposed in this dissertation. As was discussed previously, the number of links in the platelet model is not constant, as it is in the PTT model, and so the trace of the stress divided by the number of links may be a more reasonable closure for the platelet model.

Network models for which the number of links is not constant have been proposed. Mewis and Denn [32] proposed a general model that modifies (2.85) by the addition of an extra breaking function so that

$$\frac{\partial \Psi}{\partial t} + u \cdot \nabla \Psi + (y \cdot \nabla u) \cdot \nabla_y \Psi = h (|y|) (\Psi_0 - \Psi) - p \Psi, \quad (2.86)$$

where $p$ is some function that should be zero at equilibrium. Tanaka and Edwards [39] modify the formation rate $g$ so that it depends on the number of chains in the network.

The platelet model is distinct from these theories that consider a variable number of links. In these models the number of links changes because of the deformation of an existing network. In the platelet model, the number of links changes with deformations, but it is also controlled by the number of activated platelets. The concentration of activated platelets changes in space and time and depends on the reaction between activator and nonactivated platelets.
CHAPTER 3
EVALUATING CLOSURES: STEADY SHEAR FLOW

As discussed in section 2.2, the continuum model can be closed by assuming that the breaking rate is a function of averaged quantities rather than the length of the bond. In order to evaluate the effect of closure approximations, asymptotic expressions for the stresses in a steady shear flow in the limit of large shear are derived for the full model and for closure models. These results are compared for different forms of the breaking rate function. In all cases the background flow is the two-dimensional, steady shear flow

\[ \mathbf{u} = (G x_2, 0, 0), \]

where \( G \) is the shear rate. The quantity that is used to compare the models is the shear viscosity, which is defined as

\[ \mu = \frac{\sigma_{12}}{G}. \]

Recall from section 2.2.1 that when the breaking rate is constant, the shear viscosity is constant. As is shown in this chapter, when the breaking rate is not constant, the shear viscosity decreases with increasing shear rate. This phenomenon is known as shear thinning.

3.1 Full Model

For the full model we are able to generate asymptotic results when the breaking rate is a polynomial function or a piecewise constant function of the length of the link. Before tackling the different forms of breaking, we present the relevant equations and nondimensionalize them.

Equation (2.31) for the link distribution function for a steady shear flow takes the form

\[ G y_2 \frac{\partial E}{\partial y_1} = \phi^2_0 \alpha(r) - \beta(r) E, \]

\[ (3.3) \]
where \( r = |y| \). Recall that the stress tensor due to links is

\[
\sigma_{ij} = \frac{1}{2} \int S_0 E y_i y_j \, dy.
\]

We will assume that the formation function \( \alpha(r) \) has compact support, meaning there is some distance beyond which no links form. Scale lengths by the size of the support of \( \alpha(r) \), denoted \( r_0 \). Let \( \beta_0 \) represent the characteristic breaking rate scale, and let \( \alpha_0 \) represent the characteristic formation rate. Scale \( E \) by \( 2 \alpha_0 / \beta_0 \) and the stress by \( S_0 \alpha_0 r_0^5 / \beta_0 \). Let \( \gamma = G / \beta_0 \) be the dimensionless shear rate. The dimensionless equations are

\[
\gamma y_2 \frac{\partial E}{\partial y_1} = \alpha(r) - \beta(r) E \quad (3.4)
\]

\[
\sigma_{ij} = \frac{1}{2} \int E y_i y_j \, dy, \quad (3.5)
\]

where we have used the same notation for dimensional and dimensionless functions.

Because of symmetry, the equation for \( E \) only need be solved for \( y_2 \geq 0 \), and so it is assumed below that \( y_2 \) is positive. For notational convenience, define

\[
r_z = \sqrt{z^2 + y_2^2 + y_3^2}.
\]

Define the functions \( \rho \) and \( b \) by

\[
\rho (y_1, y_2, y_3) = \frac{1}{\gamma y_2} \int_0^{y_1} \beta(r_s) \, ds
\]

\[
b = \sqrt{1 - y_2^2 - y_3^2} \quad (3.7)
\]

\[
b_1 = \sqrt{1 - y_3^2} \quad (3.8)
\]

Equation (3.4) can be integrated to give

\[
E = \begin{cases} 
\frac{1}{\gamma y_2} \exp (-\rho (y_1, y_2, y_3)) \int_{-b}^{y_1} \alpha (r_\xi) \exp (\rho (\xi, y_2, y_3)) \, d\xi & |y_1| \leq b \\
0 & \text{otherwise}
\end{cases}
\]

\[
(3.9)
\]

Split \( \sigma_{ij} \) into the stress due to short bonds and the stress due to long bonds, where “short” refers to some finite length. We define short bonds as those whose length is less than 1, which is the length of the support of the formation function.

\[
\sigma_{ij} = \sigma_{ij}^s + \sigma_{ij}^l = \frac{1}{2} \int_{|r|<1} E y_i y_j \, dy + \frac{1}{2} \int_{|r|\geq1} E y_i y_j \, dy.
\]

\[
(3.10)
\]
The stress is split into these two categories because short and long bonds give different asymptotic behaviors. In fact, for short bonds the form of the breaking rate need not be specified to determine the order of the leading order terms for the stress.

### 3.1.1 Short Bonds

First we explore the behavior of the stress due to short bonds. The results are especially relevant when there are no long bonds present, as would be the case if the bonds had a maximal length at which they break. We now show that each component of the stress due to short bonds is order $\gamma^{-1}$.

Using the expression given for $E$ in (3.9) and the definition of short bonds gives

$$
\sigma_{ij}^s = \int_{-1}^{1} \int_{0}^{b_1} \int_{-b}^{b_1} \frac{y_i y_j}{\gamma y_2} \exp(-\rho(y_1, y_2, y_3)) \alpha(r \xi) \exp(\rho(\xi, y_2, y_3)) d\xi dy_1 dy_2 dy_3.
$$

By combining the exponentials above and using the definition of $\rho$,

$$
\sigma_{ij}^s = \int_{-1}^{1} \int_{0}^{b_1} \int_{-b}^{b_1} \frac{y_i y_j}{\gamma y_2} \alpha(r \xi) \exp\left(-\frac{1}{\gamma y_2} \int_{\xi}^{y_1} \beta(r_s) ds\right) d\xi dy_1 dy_2 dy_3. \tag{3.11}
$$

Note that $\beta$ must be finite and bounded away from zero for short bonds. The formation rate must be finite, but it may go to zero. We could change the definition of short bonds, so that $\alpha$ is also bounded away from zero. Therefore without loss of generality, we take $\alpha$ and $\beta$ equal to one, because this does not change the order of the stress.

With $\alpha$ and $\beta$ set to one, equation (3.11) simplifies to

$$
\sigma_{ij}^s = \int_{-1}^{1} \int_{0}^{b_1} \int_{-b}^{b_1} y_i y_j \left(1 - \exp\left(-\gamma^{-1} \frac{y_1 + b}{y_2}\right)\right) dy_1 dy_2 dy_3. \tag{3.12}
$$

Note that for a finite value $K$,

$$
1 - \exp(-\gamma^{-1} K) = \gamma^{-1} K + O(\gamma^{-2}).
$$

It is tempting to expand the exponential in a Taylor series and claim the integrand is order $\gamma^{-1}$. This cannot be done because $(y_1 + b)/y_2$ is not bounded as $y_2$ goes to zero. We again split the domain of integration into two pieces so that

$$
\sigma_{ij}^s = \sigma_{ij}^{1s} + \sigma_{ij}^{2s},
$$

where

$$
\sigma_{ij}^{1s} = \int_{-1}^{1} \int_{A}^{b_1} \int_{-b}^{b} y_i y_j \left(1 - \exp\left(-\gamma^{-1} \frac{y_1 + b}{y_2}\right)\right) dy_1 dy_2 dy_3 \tag{3.13}
$$
and
\[
\sigma_{ij}^{2s} = \int_{-1}^{1} \int_{0}^{A} \int_{-b}^{b} y_i y_j \left( 1 - \exp \left( -\gamma^{-1} \frac{y_1 + b}{y_2} \right) \right) dy_1 dy_2 dy_3. \tag{3.14}
\]
It is true that both \(\sigma_{ij}^{1s}\) and \(\sigma_{ij}^{2s}\) are positive. This is easily seen for \(\sigma_{11}^{1s}, \sigma_{22}^{1s}\), and \(\sigma_{33}^{1s}\) because the argument of the exponential is always less than or equal to zero, and so the integrand is positive. The only nonzero shear stress is \(\sigma_{12}^{1s}\). To show that \(\sigma_{12}^{1s}\) is positive we rearrange the integral
\[
I_1 = \int_{-b}^{b} y_1 \left( 1 - \exp \left( -\gamma^{-1} \frac{y_1 + b}{y_2} \right) \right) dy_1,
\]
as follows
\[
I_1 = \int_{-b}^{b} -y_1 \exp \left( -\gamma^{-1} \frac{y_1 + b}{y_2} \right) dy_1 \\
= \exp \left( -\gamma^{-1} \frac{b}{y_2} \right) \int_{-b}^{b} -y_1 \exp \left( -\gamma^{-1} \frac{y_1}{y_2} \right) dy_1 \\
= \exp \left( -\gamma^{-1} \frac{b}{y_2} \right) \left( \int_{-0}^{0} y_1 \exp \left( -\gamma^{-1} \frac{y_1}{y_2} \right) dy_1 + \int_{0}^{b} -y_1 \exp \left( -\gamma^{-1} \frac{y_1}{y_2} \right) dy_1 \right) \\
= \exp \left( -\gamma^{-1} \frac{b}{y_2} \right) \left( \int_{0}^{b} y_1 \exp \left( -\gamma^{-1} \frac{y_1}{y_2} \right) dy_1 + \int_{0}^{0} -y_1 \exp \left( -\gamma^{-1} \frac{y_1}{y_2} \right) dy_1 \right) \\
= \exp \left( -\gamma^{-1} \frac{b}{y_2} \right) \int_{0}^{b} y_1 \left( \exp \left( -\gamma^{-1} \frac{y_1}{y_2} \right) - \exp \left(-\gamma^{-1} \frac{y_1}{y_2} \right) \right) dy_1.
\]
In this form, the integrand is clearly positive, which establishes that \(I_1\) is positive and therefore both \(\sigma_{ij}^{1s}\) and \(\sigma_{ij}^{2s}\) are positive.

The integrand appearing in the definition of \(\sigma_{ij}^{2s}\) is less than one, and the volume of the domain of integration is bounded by \(4A\). Therefore we have the bound
\[
\sigma_{ij}^{2s} \leq 4A.
\]
Combining this bound with the fact that \(\sigma_{ij}^{2s} \geq 0\) gives
\[
\sigma_{ij}^{1s} \leq \sigma_{ij}^{2s} \leq \sigma_{ij}^{1s} + 4A. \tag{3.15}
\]
Provided \(A\) is chosen appropriately, a constant for example, the exponential appearing in the integrand of \(\sigma_{ij}^{1s}\) may be expanded in a Taylor series about \(\gamma^{-1} = 0\), which shows that
\[
\sigma_{ij}^{1s} = O(\gamma^{-1}).
\]
In order to expand the integrand of (3.13) in a Taylor series, the argument of the exponential must remain bounded as \(\gamma \to \infty\). Suppose that \(A\) is chosen to depend
on $\gamma$. Choosing $A = \gamma^{-1}$ ensures that the argument of the exponential is bounded, and inequality (3.15) shows that $\sigma_{ij}^* = O(\gamma^{-1})$.

### 3.1.2 Long Bonds: Even Power Law Breaking

For $y_1 > b$ no new links form, and $E$ can be expressed as

$$E(y_1, y_2, y_3) = \exp(\rho(b, y_2, y_3)) \exp(-\rho(y_1, y_2, y_3)) E(b, y_2, y_3),$$

where $\rho$, defined by (3.7), involves an integral of $\beta$ over the first component. For long bonds we consider the special case where $\beta$ is an even polynomial of $r$ of degree $2m$. Specifically,

$$\beta = \kappa r^{2m} + l.o.t.$$

This choice allows the integral that defines $\rho$ to be evaluated. Let $P_j$ denote a polynomial of degree $j$. We can express $\rho$ as

$$\rho(b, y_2, y_3) = \frac{P_{2m+1}(b)}{\gamma y_2},$$

and

$$\rho(y_1, y_2, y_3) = \frac{\kappa y_1^{2m+1}}{\gamma y_2(2m+1)} + \frac{P_{2m-1}(y_1)}{\gamma y_2}. \quad (3.18)$$

With these substitutions for $\rho$, equation (3.16) becomes

$$E(y_1, y_2, y_3) = \exp\left(\frac{P_{2m+1}(b)}{\gamma y_2}\right) \exp\left(\frac{-\kappa y_1^{2m+1}}{\gamma y_2(2m+1)} - \frac{P_{2m-1}(y_1)}{\gamma y_2}\right) E(b, y_2, y_3).$$

(3.19)

Before proceeding with the computation of the stress, we present some technical lemmas. The first is Watson’s Lemma [23].

**Lemma 1 (Watson’s Lemma)** Let $g(t)$ be a function for which there exist positive constants $K$ and $b$ such that $|g(t)| < K \exp(bt)$ for large $t$. In a neighborhood of the origin, suppose that $g(t)$ can be represented by the series

$$g(t) = g_0 t^{\alpha_0} + g_1 t^{\alpha_1} + \ldots + g_m t^{\alpha_m} + R_{m+1}(t),$$

where the sequence $\{\alpha_n\}$ is a nonnegative increasing sequence, and there exists some $C$ such that

$$|R_{m+1}| < C t^{\alpha_{m+1}}$$

for all $t$ in the neighborhood. Let $\lambda$ be a real number greater than $-1$. For large, positive $x$ the following expansion holds

$$\int_0^\infty t^\lambda e^{-xt} g(t) dt \sim g_0 \frac{\Gamma(\lambda + \alpha_0 + 1)}{x^{\lambda + \alpha_0 + 1}} + g_1 \frac{\Gamma(\lambda + \alpha_1 + 1)}{x^{\lambda + \alpha_1 + 1}} + \ldots$$
The second lemma is a specific application of Watson’s Lemma.

**Lemma 2** Suppose that $\gamma$ and $K$ are positive constants and $P_{m-1}$ is a polynomial of degree $m-1$. Then for large $\gamma$ to leading order

$$\int_0^\infty y^\lambda \exp\left(-\gamma^{-1}(Ky^m + P_{m-1}(y))\right) \, dy \sim \frac{1}{m} K^{-\frac{\lambda+1}{m}} \Gamma\left(\frac{\lambda+1}{m}\right) \gamma^{\frac{\lambda+1}{m}}. \quad (3.20)$$

**Proof**: Let $I$ represent the integral in (3.20). Begin by making the change of variables

$$y = \gamma^{1/(m-1)} \left(\frac{1}{K}\right)^{1/m} u^{1/m}.$$

The integral $I$ becomes

$$I = A \int_0^\infty u^{(\lambda+1-m)/m} \exp\left(-\gamma^{1/(m-1)} u\right) \exp\left(-\gamma^{-1} Q_{m-1}\left(u^{1/m}\right)\right) \, du, \quad (3.21)$$

where

$$A = \frac{1}{m} \left(\frac{1}{K}\right)^{(\lambda+1)/m} \gamma^{(\lambda+1)/(m-1)},$$

and

$$Q_{m-1}\left(u^{1/m}\right) = P_{m-1}\left(\gamma^{1/(m-1)} \left(\frac{1}{K}\right)^{1/m} u^{1/m}\right).$$

It can be easily verified that

$$\left|\gamma^{-1} Q_{m-1}\left(u^{1/m}\right)\right| < K_1 u^{(m-1)/m} + K_2, \quad (3.22)$$

where $K_1$ and $K_2$ are positive constants. Replacing $\gamma^{-1} Q$ by either the upper or the lower bound in (3.21), allows the application of Watson’s Lemma, and either bound gives the same leading order. Using the lower bound,

$$I \leq A \int_0^\infty u^{(\lambda+1-m)/m} \exp\left(-\gamma^{1/(m-1)} u\right) \exp\left(K_1 u^{(m-1)/m} + K_2\right) \, du. \quad (3.23)$$

Watson’s Lemma can be applied to the integral in this inequality with $x = \gamma^{1/(m-1)}$ and $g(u) = \exp\left(K_1 u^{(m-1)/m} + K_2\right)$. The leading order term in the expansion of $g$ around the origin is 1. This would also be the case if the upper bound from (3.22) had been used instead. Since both bounds give the same leading order, we have

$$I \sim A \int_0^\infty u^{(\lambda+1-m)/m} \exp\left(-\gamma^{1/(m-1)} u\right) \, du \sim A \Gamma\left(\frac{\lambda+1}{m}\right) \gamma^{-\frac{\lambda+1}{(m^2-m)}},$$

and using the definition of $A$ completes the proof. □
Because we are primarily interested in computing the shear viscosity, we focus on the shear stress. The shear stress due to long bonds is

$$\sigma_{12}^l = \int_{-1}^{1} \int_{0}^{b_1} \int_{b}^{\infty} E(y_1, y_2, y_3) y_1 y_2 dy_1 dy_2 dy_3. $$

Substituting for $E$ using equation (3.19) gives

$$\sigma_{ij}^l = \int_{-1}^{1} \int_{0}^{b_1} \exp \left( \frac{P_{2m+1}(y_1)}{\gamma y_2} \right) y_2 E(b, y_2, y_3) I_1 dy_2 dy_3, \quad (3.24)$$

where

$$I_1 = \int_{b}^{\infty} y_1 \exp \left( \frac{-\kappa y^{2m+1}}{\gamma y_2 (2m+1)} - \frac{P_{2m-1}(y_1)}{\gamma y_2} \right) dy_1.$$  

The lower limit of $I_1$ may be extended to zero, altering the result by a term of order $\gamma^{-1}$. Lemma 2 can then be applied to this modified integral to give

$$I_1 \sim \frac{\kappa^{-2/(2m+1)}}{(2m+1)(2m-1)/(2m+1)} \Gamma \left( \frac{2}{2m+1} \right) \gamma^{2/(2m+1)} y_2^{2/(2m+1)}. \quad (3.25)$$

The general form of $E(b, y_2, y_3)$ is

$$E(b, y_2, y_3) = \frac{1}{\gamma y_2} \int_{-b}^{b} \alpha (r_\xi) \exp \left( \frac{-1}{\gamma y_2} \int_{\xi}^{b} \beta (r_s) ds \right) d\xi.$$ 

To leading order

$$E(b, y_2, y_3) \sim \frac{1}{\gamma y_2} \int_{-b}^{b} \alpha (r_\xi) d\xi, \quad (3.26)$$

where we have taken the exponential to be one to leading order, even though $y_2$ is not bounded away from zero. However, using the same arguments previously applied to such integrals for short bonds, it can be shown that this approximation is valid. Similarly, we take the exponential appearing in the integrand of (3.24) to be one to leading order by the same arguments, so that

$$\sigma_{ij}^l \sim \int_{-1}^{1} \int_{0}^{b_1} \frac{1}{\gamma} \int_{-b}^{b} \alpha (r_\xi) I_1 dy_2 dy_3, \quad (3.27)$$

Combining (3.27) and (3.25) gives the leading order behavior for long bonds

$$\sigma_{12}^l = C_m \gamma^{(1-2m)/(2m+1)} + o \left( \gamma^{(1-2m)/(2m+1)} \right), \quad (3.28)$$

where the constant $C_m$ is

$$C_m = \frac{\kappa^{-2/(2m+1)}}{(2m+1)(2m-1)/(2m+1)} \Gamma \left( \frac{2}{2m+1} \right) \frac{1}{2} \int_{r<1} y_2^{2/(2m+1)} \alpha(r) dy.$$
Because the shear stress due to short bonds is of higher order than (3.28), to leading order, the shear stress is

$$\sigma_{12} = C_m \gamma^{(1-2m)/(2m+1)} + o \left( \gamma^{(1-2m)/(2m+1)} \right),$$

and the shear viscosity, \( \mu = \sigma_{12}/\gamma \), is

$$\mu = C_m \gamma^{-4m/(2m+1)} + o \left( \gamma^{-4m/(2m+1)} \right).$$

(3.29)

### 3.1.3 General Power Law Breaking

More general power laws can be handled by assuming that for large \( y_1 \), the breaking rate can be approximated as

$$\beta \approx y_1^n.$$

This approximation results from assuming that the bonds are stretched only in the direction of shear. The leading order behavior of the shear stress can then be obtained using the same techniques used in the previous section to obtain

$$\sigma_{12} = C_n/2 \gamma^{(1-n)/(n+1)}.$$

This method of approximation is straightforward, but it does not allow for the computation of the next order term.

### 3.2 Closure Model

We now compare the leading order behavior of the stresses for two closure approximations for the steady shear flow problem. The cases considered are (1) the breaking rate is a function of the trace of the stress and (2) the breaking rate is a function of the ratio of the trace of the stress and the total number of links. The trace of the stress is the total bond energy, and so the ratio of the trace to the number of bonds is the average energy per bond. Because the energy of a bond is proportional to the squared length of the bond, the ratio of the trace to the number of bonds is proportional to the average squared bond length. Before analyzing these cases the equations for the stress and number of bonds are presented and nondimensionalized.

The general breaking rate is denoted by \( \beta \), where it is assumed that \( \beta \) is not a function of the length of the link, so that the system closes on the macro-scale. Let the velocity
be the steady shear flow defined by (3.1). Equations (2.47) and (2.48) for the stress (in component form) and for the density of links at steady state are

\begin{align}
-2G\sigma_{12} &= \phi_0^2 a_2 - \beta \sigma_{11} \quad \text{(3.30)} \\
0 &= \phi_0^2 a_2 - \beta \sigma_{22} \quad \text{(3.31)} \\
0 &= \phi_0^2 a_2 - \beta \sigma_{33} \quad \text{(3.32)} \\
-G\sigma_{22} &= -\beta \sigma_{12} \quad \text{(3.33)} \\
0 &= \phi_0^2 a_0 - \beta z. \quad \text{(3.34)}
\end{align}

As before, scale the stress by \( S_0 \phi_0^2 \alpha_0 r_0^5 / \beta_0 \), where \( r_0 \) is the radius of the support of the formation function. Scale \( z \) by \( \phi_0^2 \alpha_0 r_0^3 / \beta_0 \), and let \( \gamma = G / \beta_0 \) be the nondimensional shear rate. The nondimensional system is

\begin{align}
-2\gamma \sigma_{12} &= a_2 - \beta \sigma_{11} \quad \text{(3.35)} \\
0 &= a_2 - \beta \sigma_{22} \quad \text{(3.36)} \\
0 &= a_2 - \beta \sigma_{33} \quad \text{(3.37)} \\
-\gamma \sigma_{22} &= -\beta \sigma_{12} \quad \text{(3.38)} \\
0 &= a_0 - \beta z, \quad \text{(3.39)}
\end{align}

where

\[ a_2 = \frac{2\pi}{3} \int_0^1 \alpha(r) r^4 \, dr \quad \text{and} \quad a_0 = 4\pi \int_0^1 \alpha(r) r^2 \, dr. \quad \text{(3.40)} \]

All quantities in this system are nondimensional, even though we use the same notation as in the dimensional system.

### 3.2.1 Breaking as a Function of Trace

Before specifying the form of the breaking rate function, it is useful to manipulate equations (3.35)-(3.38). Solving these equations for the stress in terms of \( \beta \) and \( \gamma \) gives

\begin{align}
\sigma_{11} &= \frac{\beta^2 + 2\gamma^2}{\beta^3} a_2 \quad \text{(3.41)} \\
\sigma_{22} = \sigma_{33} &= \frac{a_2}{\beta} \quad \text{(3.42)} \\
\sigma_{12} &= \frac{a_2}{\beta^2 \gamma} \quad \text{(3.43)}
\end{align}

and the shear viscosity is

\[ \mu = \frac{a_2}{\beta^2}. \quad \text{(3.44)} \]
Denote the trace by \( T \). The expression for the trace is

\[
T = \frac{3\beta^2 + 2\gamma^2}{\beta^3} a_2.
\]  

(3.45)

Solving equation (3.45) for \( \gamma^2 \) gives

\[
\gamma^2 = \frac{\beta^3 T}{2a_2} - \frac{3}{2} \beta^2.
\]  

(3.46)

As \( \gamma \to \infty \), equation (3.46) shows that at least one of \( \beta \) or \( T \) must also grow without bound. We will assume that \( \beta \) always grows without bound, but \( T \) may be bounded. For large enough \( \gamma \), the second term in equation (3.46) becomes small compared to the first. Ignoring this term gives

\[
\gamma^2 \approx \frac{\beta^3 T}{2a_2}.
\]  

(3.47)

Once the form of \( \beta \) is specified, equation (3.47) can be inverted to find the behavior of \( T \) in terms of \( \gamma \). Also using equation (3.47), the stress can be expressed in terms of \( T \) rather than \( \beta \). Equations (3.41)-(3.46) become

\[
\sigma_{11} \approx T - (2a_2)^{-1/3} \gamma^{2/3} T^{1/3} \approx T
\]  

(3.48)

\[
\sigma_{22} = \sigma_{33} \approx 2^{-1/3} a_2^{2/3} \gamma^{-2/3} T^{1/3}
\]  

(3.49)

\[
\sigma_{12} \approx 2^{-2/3} a_2^{1/3} \gamma^{-1/3} T^{2/3}
\]  

(3.50)

\[
\mu \approx 2^{-2/3} a_2^{1/3} \gamma^{-4/3} T^{2/3}.
\]  

(3.51)

If \( \beta \) is a function of the trace only, the trace will not go to zero as \( \gamma \) gets large. From (3.47), either the trace or the breaking rate must become unbounded. It is physically unreasonable that the breaking rate could become unbounded as the trace became small. Therefore the trace cannot approach zero as \( \gamma \) gets large. Thus, equation (3.51) shows that the shear viscosity decreases no faster than \( \gamma^{-4/3} \). Comparing with the viscosity computed using the full model given by (3.29), this is the rate of shear thinning when the breaking rate is a quadratic function of the length of the bond. This shows that breaking as a function of trace is incapable of producing all the shear thinning rates of the full model. Because of this limitation, we do not further analyze this model.

3.2.2 Breaking as a Function of Trace per Bond

In the previous section the breaking rate was assumed to be a function of the trace, which can be interpreted as the total energy due to links. Note from equation (3.39) that \( z \) is proportional to \( \beta^{-1} \). The total number of links must go to zero while the total energy,
equivalent to the trace, stays bounded away from zero if the breaking is just a function of the trace. This means that the energy per bond, \( T/z \), must grow without bound as the shear rate increases. This result is not physically reasonable.

In this section we consider the case where the breaking rate depends on the ratio of the trace to the number of bonds or the average squared length. The average squared link length is

\[
\langle r^2 \rangle = \frac{\int E y_i y_i \, dy}{\int E \, dy}.
\]

Using the nondimensional stress defined by (3.5) gives

\[
\langle r^2 \rangle = \frac{2T}{z}.
\]

In order to make the comparison with the full model, the closure breaking rate is assumed to be a function of \( 2T/z \). The specific forms of the breaking rate considered are the power law, the exponential, and the bounded trace per bond.

Equation (3.39) immediately relates the breaking rate and the number of links by

\[
\beta = \frac{a_0}{z}. \tag{3.52}
\]

Using this equation and equations (3.41)-(3.44), the stresses and the shear viscosity can be expressed as functions of the number of links and the shear rate as

\[
\begin{align*}
\sigma_{11} &= \frac{a_2}{a_0} \left( z + \frac{2\gamma^2}{a_0^2} z^3 \right) \tag{3.53} \\
\sigma_{22} = \sigma_{33} &= \frac{a_2}{a_0} z \tag{3.54} \\
\sigma_{12} &= \frac{a_2 \gamma}{a_0^2} z^2 \tag{3.55} \\
\mu &= \frac{a_2}{a_0^2} z^2. \tag{3.56}
\end{align*}
\]

Equation (3.47), can be written as

\[
\gamma^2 \approx \frac{a_0^2 T}{2a_2 z^3}. \tag{3.57}
\]

For the different forms of \( \beta \), we use equation (3.52) to find the trace as a function of \( z \). Then equation (3.57) can be inverted to find \( z \) as a function of \( \gamma \), and this expression for \( z \) is substituted into equations (3.53)-(3.56).
3.2.2.1 Power Law Breaking

Suppose the breaking rate is of the form

\[ \beta = 2^m \kappa \left( \frac{T}{z} \right)^m + \text{l.o.t.,} \]  

(3.58)

where \( \kappa \) and \( m \) are nonnegative constants. This form is chosen to compare with the even power law breaking rate in the full model. Using equation (3.52) to find \( T \) as a function of \( z \) gives

\[ T \approx \left( \frac{a_0}{2^m \kappa} \right)^{1/m} z^{(m-1)/m}. \]

Plugging into equation (3.57) and solving for \( z \) gives

\[ z \approx \left( \frac{(4a_2)^{-m} a_0^{m+1}}{\kappa} \right)^{1/(2m+1)} \gamma^{-2m/(2m+1)}. \]

The stresses and viscosity from equations (3.53)–(3.56) are

\[ \sigma_{11} \approx 2 \left( \frac{a_2^{m+1/3} a_0^m}{4^m \kappa} \right)^{1/(2m+1)} \gamma^{-2m/(2m+1)} \]  

(3.59)

\[ \sigma_{22} = \sigma_{33} \approx \left( \frac{a_2^{m+1/3} a_0^m}{4^m \kappa} \right)^{1/(2m+1)} \gamma^{-2m/(2m+1)} \]  

(3.60)

\[ \sigma_{12} \approx \left( \frac{a_2^{1/2} a_0^m}{4^m \kappa} \right)^{2/(2m+1)} \gamma^{-4m/(2m+1)} \]  

(3.61)

\[ \mu \approx \left( \frac{a_2^{1/2} a_0^m}{4^m \kappa} \right)^{2/(2m+1)} \gamma^{-4m/(2m+1)}. \]  

(3.62)

3.2.2.2 Exponential Breaking

Suppose that the breaking rate is

\[ \beta = \exp \left( 2\kappa T/z \right). \]

As for power law breaking, use equation (3.52) to find \( T \) as a function of \( z \), resulting in

\[ T = \frac{z}{2\kappa} \ln \left( \frac{a_0}{z} \right). \]

Substituting this expression for \( T \) into equation (3.57) gives

\[ \gamma^2 \approx \frac{a_0^3}{4\kappa a_2 z^2} \ln \left( \frac{a_0}{z} \right). \]  

(3.63)
Next this equation must be inverted to find $z$ as a function of $\gamma$. Before doing this, we introduce a change of variables

$$g^2 = \frac{4\kappa a_2}{a_0} \gamma^2; \quad w = \frac{a_0}{z}.$$ 

The equation we wish to solve is

$$g^2 = w^2 \ln(w).$$

We seek to solve this equation to leading order as $w \to \infty$. Begin by taking the logarithm of this equation to get

$$2 \ln(g) = 2 \ln(w) + \ln(\ln(w)). \quad (3.64)$$

Again to simplify notation, we introduce the change of variables

$$h = \ln(g); \quad x = \ln(w).$$

Using this change of variables, equation (3.64) becomes

$$2h = 2x + \ln(x). \quad (3.65)$$

For large $x$, $2x$ dominates the right size of equation (3.65), and so we may write

$$x = h + h_1, \quad h_1 = o(h).$$

This is substituted into equation (3.65) in order to find an expansion of $h_1$. After some minor manipulations,

$$h_1 = -\frac{1}{2} \ln(h) - \frac{1}{2} \ln \left(1 + \frac{h_1}{h}\right).$$

Because $h_1 = o(h)$, the second logarithm must go to zero as $h$ gets large, and so the two term expansion is

$$x = h - \frac{1}{2} \ln(h) + h_2, \quad h_2 = o(\ln(h)). \quad (3.66)$$

Note that these first two terms are large for large $h$. We must continue the expansion until the last term goes to zero for large $h$. This constraint is due to the change of variables. This expansion must be exponentiated when changing back to the original variables, and it transforms to a product of exponentials. The only way the error terms can be ignored is if the terms in the series are going to zero in the asymptotic limit,
so that when exponentiated they are multiplying the asymptotic approximation by one.
Substituting (3.66) into (3.65) to find \( h_2 \), we find after some manipulation
\[
h_2 = \ln(h) \quad + o \left( \frac{\ln(h)}{h} \right).
\]
Because \( h_2 \to 0 \), no other terms are needed to find the leading order behavior of the
original variables.

The expansion of \( x \) is
\[
x = h - \frac{1}{2} \ln(h) + \frac{\ln(h)}{4h} + o \left( \frac{\ln(h)}{h} \right).
\]
We now change back to the original variables. First change back to the variables \( w \) and \( g \) and exponentiate the series to get
\[
w = g(\ln(g))^{-1/2} \exp \left( \frac{\ln(\ln(g))}{4\ln(g)} + o \left( \frac{\ln(\ln(g))}{\ln(g)} \right) \right).
\]
The exponential can be expanded to get the leading order term in the series,
\[
w = g(\ln(g))^{-1/2} + O \left( \frac{g \ln(\ln(g))}{(\ln(g))^{3/2}} \right).
\]
Now changing back to the original variables of \( z \) and \( \gamma \),
\[
z = \left( \frac{a_0}{4\kappa a_2} \right)^{1/2} \gamma^{-1} \left( \ln(\gamma) - \frac{1}{2} \ln \left( \frac{a_0}{4\kappa a_2} \right) \right)^{1/2} + O \left( \frac{\ln(\ln(\gamma))}{\gamma (\ln(\gamma))^{1/2}} \right).
\]
Using this expression for \( z \), the stresses and viscosity from equations (3.53)–(3.56) are
\[
\sigma_{11} \approx 2 \left( \frac{a_0}{4\kappa a_2} \right)^{3/2} \gamma^{-3} \left( \ln(\gamma) - \frac{1}{2} \ln \left( \frac{a_0}{4\kappa a_2} \right) \right)^{3/2}
\]
(3.67)
\[
\sigma_{22} = \sigma_{33} \approx \left( \frac{a_2 a_0}{4\kappa} \right)^{1/2} \gamma^{-1} \left( \ln(\gamma) - \frac{1}{2} \ln \left( \frac{a_0}{4\kappa a_2} \right) \right)^{1/2}
\]
(3.68)
\[
\sigma_{12} \approx \frac{a_0}{4\kappa} \gamma^{-1} \left( \ln(\gamma) - \frac{1}{2} \ln \left( \frac{a_0}{4\kappa a_2} \right) \right)
\]
(3.69)
\[
\mu \approx \frac{a_0}{4\kappa} \gamma^{-2} \left( \ln(\gamma) - \frac{1}{2} \ln \left( \frac{a_0}{4\kappa a_2} \right) \right).
\]
(3.70)
3.2.2.3 Finite Energy

The final form of the breaking rate function we consider is one in which bonds can sustain only a finite energy. One example of such a breaking rate is

\[ \beta = \frac{\kappa}{W - \frac{T}{z}}. \]

where \( W \) represents some maximum energy. For the breaking rate to get large, to leading order

\[ T \approx Wz. \]

Plugging into equation (3.57) and solving for \( z \) gives

\[ z \approx \left( \frac{a_0 W}{2a_2} \right)^{1/2} \gamma^{-1}. \]

Finally using equations (3.53)–(3.56),

\[ \begin{align*}
\sigma_{11} & \approx \sigma_{22} = \sigma_{33} \approx \left( \frac{a_0 a_2 W}{2} \right) \gamma^{-1} \quad (3.71) \\
\sigma_{12} & \approx \frac{a_0 W}{2} \gamma^{-1} \quad (3.72) \\
\mu & \approx \frac{a_0 W}{2} \gamma^{-2}. \quad (3.73)
\end{align*} \]

Note that the shear viscosity is \( \mathcal{O} \left( \gamma^{-2} \right) \), as is the case in the full model when there are only short bonds, meaning all bonds break by some finite length.

3.3 Comparison

We now compare the shear viscosities produced from the full model and the closure model. For polynomial breaking rates we compare the asymptotic results for high shear. The comparison is made numerically for all shear rates and other breaking rate functions.

3.3.1 Asymptotic Comparison

We compare the asymptotic shear viscosity for the full model and the closure model for the power law models

\[ \beta_{\text{full}} = \kappa r^{2m} + l.o.t. \quad \beta_{\text{close}} = 2^m \kappa \left( T \right)^{m} + l.o.t. \quad (3.74) \]

We compute the ratio of the resulting shear viscosities given by (3.29) and (3.62). This ratio is

\[ \frac{\mu_{\text{full}}}{\mu_{\text{close}}} = \Gamma \left( \frac{2}{2m+1} \right) \left( \frac{2}{2m+1} \right)^{(2m-1)/(2m+1)} \frac{a_2/(2m+1)}{a_2^{1/(2m+1)} a_0^{2m/(2m+1)}}. \quad (3.75) \]
where
\[ a_{2/(2m+1)} = \int_{r<1} y_2^{2/(2m+1)} \alpha(r) \, dy. \]
Note that this ratio depends on the formation function \( \alpha \), and below we explore how strongly this ratio varies as the formation function changes.

Because of the radial symmetry of \( \alpha \), the integrals involving \( \alpha \) can be simplified to involve integrals over just \( r \), as was done in (3.40). Doing the same for \( a_{2/(2m+1)} \) gives
\[ a_{2/(2m+1)} = 4\pi \frac{(2m + 1)}{(2m + 3)} \int_0^1 r^{(4m+4)/(2m+1)} \alpha(r) \, dr. \] (3.76)
Using (3.40) and (3.76), we are then able to divide the ratio (3.75) into two parts, one independent of \( \rho \) and one which depends on \( \alpha \), giving
\[ \frac{\mu_{\text{full}}}{\mu_{\text{close}}} = \Gamma \left( \frac{2}{2m + 1} \right) \left( \frac{2}{2m + 1} \right)^{(2m-1)/(2m+1)} \frac{(2m + 1)}{(2m + 3)} 6^{1/(2m+1)} A_m, \] (3.77)
where
\[ A_m = \frac{\int_0^1 r^{(4m+4)/(2m+1)} \alpha(r) \, dr}{\left( \int_0^1 r^2 \alpha(r) \, dr \right)^{1/(2m+1)}} \]
The quantity \( A_m \) contains all the dependence of the ratio of viscosities on the formation function.

For simple forms of the formation function, polynomials for example, \( A_m \) can be computed explicitly. Rather than delve into such computations, we choose to explore how \( A_m \) varies for several reasonable choices for \( \alpha \) by evaluating \( A_m \) numerically. The two forms of alpha considered are
\[ \alpha(r) = 1 - r^b, \quad 0 \leq b < \infty, \]
and
\[ \alpha(r) = r(1 - r) \exp(br), \quad -\infty < b < \infty. \]
Recall that the length of links has been scaled so that for these two functions \( 0 \leq r \leq 1 \). Graphs of these functions for various values of \( b \) are displayed in Figure 3.1 and Figure 3.2. The computed values of \( A_m \) for a range of values of \( m \) and \( b \) are given in Table 3.1 and Table 3.2. These results show that \( A_m \) changes little over a wide range of geometries. The lower values arise when the formation function is concentrated near \( r = 0 \). When the formation function is concentrated around \( r = 1 \) or when \( m \) is large, the value of \( A_m \approx 1 \).
Figure 3.1: Formation rate function $\alpha = 1 - r^b$.

Figure 3.2: Formation rate function $\alpha = w r(1 - r) \exp(br)$, where $w$ is a weight used to normalize. Graphs for negative values of $b$ are not displayed, but are similar to those of positive $b$ reflected about the line $r = 0.5$. 
Table 3.1: Values of $A_m$ for $\alpha(r) = 1 - r^b$

<table>
<thead>
<tr>
<th>$m$</th>
<th>0</th>
<th>0.1</th>
<th>1</th>
<th>10</th>
<th>$\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.94</td>
<td>0.94</td>
<td>0.95</td>
<td>0.97</td>
<td>0.97</td>
</tr>
<tr>
<td>5</td>
<td>0.98</td>
<td>0.98</td>
<td>0.98</td>
<td>0.99</td>
<td>0.99</td>
</tr>
<tr>
<td>$\infty$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
</tbody>
</table>

Table 3.2: Values of $A_m$ for $\alpha(r) = r(1-r)\exp(br)$

<table>
<thead>
<tr>
<th>$m$</th>
<th>$b$</th>
<th>$-100$</th>
<th>$-10$</th>
<th>0</th>
<th>10</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.90</td>
<td>0.91</td>
<td>0.97</td>
<td>0.99</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>0.96</td>
<td>0.97</td>
<td>0.99</td>
<td>1.00</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>$\infty$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td></td>
</tr>
</tbody>
</table>

Now we compare the part of the ratio in (3.77) that is independent of the geometry of $\alpha$. The closure model results from replacing the squared length with the average squared length. We could instead replace the squared length by some multiple of the average squared length, the multiple being chosen so that the asymptotic behavior of the shear viscosity is identical to the full model. Call such a constant $C_a$, so that the closure model results from the substitution

$$r^2 \rightarrow C_a \langle r^2 \rangle.$$ 

This effectively modifies $\kappa$ in (3.74) for the closure breaking rate by multiplying it by $C_a^m$ so that

$$\beta_{close} = 2^m C_a^m \kappa \left( \frac{T}{z} \right)^m + l.o.t.$$

Assume that constant $A_m \approx 1$, meaning the closure is independent of the geometry of the formation function, and choose

$$C_a = \left( \frac{\mu_{full}}{\mu_{close}} \right)^{-(2m+1)/2m},$$

where the ratio of viscosities is taken from (3.77). This choice of $C_a$ would produce similar shear viscosities at high shear rates for the full model and the closure model. Some computed values of $C_a$ are given in Table 3.3 for different values of $m$. Notice that the value of $C_a$ is significantly different from 1 for small values of $m$, but seems to approach 1 for large $m$. 
Table 3.3: Computed values of \( C_a \)

<table>
<thead>
<tr>
<th>( m )</th>
<th>1</th>
<th>2</th>
<th>5</th>
<th>100</th>
<th>1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_a )</td>
<td>0.683</td>
<td>0.715</td>
<td>0.780</td>
<td>0.961</td>
<td>0.994</td>
</tr>
</tbody>
</table>

### 3.3.2 Numerical Comparison

First we verify our asymptotic shear viscosities (3.29) and (3.62) are correct when \( m = 1 \). These formulas were also verified for other \( m \), but the results are not presented. For simplicity, the formation rate used is

\[
\alpha(r) = \begin{cases} 
1 & r \leq 1 \\
0 & r > 1 
\end{cases}.
\]

We wanted the breaking rate to vary little over the support of the formation function, and be a power law for large \( r \). A simple breaking rate satisfying these requirements is

\[
\beta(r) = \begin{cases} 
1 & r \leq 1 \\
\frac{1}{r^2} & r > 1 
\end{cases}.
\]

We computed the shear viscosity numerically by first solving for \( E \) using (3.4) and then evaluating the integral (3.5) to find the stress. As can be seen in Figure 3.3, the asymptotic result agrees well with the numerical result. For the closed model, the breaking rate used is

\[
\beta(\langle r \rangle) = \begin{cases} 
1 & \langle r \rangle \leq 1 \\
\langle r^2 \rangle & \langle r \rangle > 1
\end{cases}.
\]

Figure 3.4 shows excellent agreement between the asymptotic result and the numerical result.

Next we compare the shear viscosity obtained from the full model and the closed model to each other for shear rates both large and small. Figure 3.5 shows the two shear viscosities plotted on the same graph. Note that both models show the same power law dependence on the shear rate, as predicted by the asymptotics, but the constant multiple is larger for the full model, also predicted by the asymptotics. The results are notably different around shear rate 1. The full model begins shear thinning at much lower shear rates than the closed model.

When the shear rate is zero, using the formation rate (3.78) and the breaking rate (3.79), the average bond length is

\[
\langle r^2 \rangle = \frac{3}{5}.
\]
Figure 3.3: Verification of the asymptotic shear viscosity (3.29) for the breaking rate function (3.79) for the full model.

Figure 3.4: Verification of the asymptotic shear viscosity (3.62) for the breaking rate function (3.80) for the closed model.
Figure 3.5: Comparison of the shear viscosity for the full model with breaking rate (3.79) and the closure model with breaking rate (3.80) for a large range of shear rates.

Rather than simply replace the squared length with the average squared length in (3.79) we try the closure breaking rate

$$\beta(\langle r \rangle) = \begin{cases} 
1 & \langle r^2 \rangle \leq 3/5 \\
1 + \langle r^2 \rangle - \left( \frac{3}{5} \right) & \langle r^2 \rangle > 3/5
\end{cases}.$$  \hspace{1cm} (3.81)

The shear viscosity resulting from this breaking rate is compared with the full model in Figure 3.6. This breaking rate shows much better agreement with the full model at low and moderate shear rate compared to the closure model with the breaking rate (3.80).

Finally we compare the shear viscosities produced by the exponential breaking rate. The formation rate used is again (3.78). For the full model the breaking rate tested is

$$\beta(r) = \begin{cases} 
1 & r \leq 1 \\
\exp(0.5(r^2 - 1)) & r > 1
\end{cases}.$$  \hspace{1cm} (3.82)

The result is compared with the shear viscosity produced by the closure model with breaking rate

$$\beta(r) = \begin{cases} 
1 & \langle r^2 \rangle \leq 3/5 \\
\exp\left(0.5\left(\langle r^2 \rangle - 3/5\right)\right) & \langle r^2 \rangle > 3/5
\end{cases}.$$  \hspace{1cm} (3.83)

The results are displayed in Figure 3.7. The asymptotic approximation is in excellent agreement with the closure model. The full model viscosity is slightly larger than that of
Figure 3.6: The closure model with breaking rate (3.81) is compared to the full model with breaking rate (3.79).

Figure 3.7: The closure model with breaking rate (3.83) is compared to the full model with breaking rate (3.82).
the closed model at high shear. Recall this was also the case with the power law breaking rate.

3.4 Conclusions

In order to evaluate closure models, we analyzed the behavior of the model when a uniform concentration of activated platelets is undergoing steady shearing. The two closures considered are (1) the breaking rate as a function of the trace of the stress, or total link energy and (2) the breaking rate as a function of the ratio of the trace to the number of links, or the average energy per bond. Based on an asymptotic analysis at high shear rates, we reject the closure of a breaking rate which depends only on the trace. This closure is limited in that it cannot reproduce all of the shear thinning rates obtained in the full model.

When the closure breaking rate is taken to be a function of the average energy per link, or average squared link length, the asymptotic analysis shows that the closure model shear thins at the same rate as the full model. The constant appearing in this leading order term is not the same for the two models, and it depends on the the form of the formation rate and breaking rate functions. However the dependence on the formation rate is weak.

The asymptotic results are relevant only for large shear rates. We numerically compute the shear viscosity for a wide range of shear rates to compare the full model and the closure model. The results show that simply replacing the squared length with average squared length produces a notable difference in the shear viscosities around shear rate one. The shear viscosity in the closure model began decreasing at a larger value of the shear rate than did the full model. In this particular test, the breaking rate in the full model tested was constant for links of length less than the formation radius and quadratic for links longer than the formation radius. Better results were obtained when it was assumed that the breaking rate in the closure model increased only when the averaged length exceeded the average length at which links form. We conclude that with an appropriate choice of closure model the behavior of the full model in a steady shear flow can be reproduced for all shear rates.
We now detail the methods used to produce numerical simulations of the model equations (2.45)-(2.51). We begin by nondimensionalizing the equations, and then discuss how the system is discretized in time and space. The remainder of this chapter focuses on the numerical solutions to the equations related to the platelets, activator, and the stress induced by platelet links. The method used to solve the Navier-Stokes equations is discussed in Chapter 6.

4.1 Nondimensionalization

Before solving the equations numerically, the model equations (2.45)-(2.51) are nondimensionalized. We begin by scaling the Navier-Stokes equations. Let $U$ represent the scale of the velocity and $L$ represent the length scale associated with the velocity field. The ratio $L/U$ defines the time scale. We scale the pressure and stress due to platelets by $\rho U^2$. Using these scalings, the nondimensional Navier-Stokes equations with the addition of the stress due to the platelets become

\begin{align*}
    u_t + u \cdot \nabla u &= -\nabla p + \frac{1}{\text{Re}} \Delta u + \nabla \cdot \sigma \\
    \nabla \cdot u &= 0,
\end{align*}

where

\[ \text{Re} = \frac{\mu}{\rho L U} \]

is the Reynolds number. We note that scaling the stress on the same scale as the pressure may not always be appropriate. Other possible scalings are discussed after the remainder of the nondimensionalization has been presented.

Let $\Phi$ and $\text{Ch}$ represent the scales of the platelet concentrations and the activator respectively. The platelet concentration scale is chosen based on the physical situation.
being simulated. For example if the simulation concerns blood flow *in vivo*, then $\Phi$ would correspond to the concentration of resting platelets in healthy plasma. The concentration of activator is chosen to be the activation threshold for ADP. The nondimensional platelet and activator equations become

\[
\frac{\partial \phi_n}{\partial t} + \mathbf{u} \cdot \nabla \phi_n = \frac{1}{\text{Pe}_n} \Delta \phi_n - C_1 H(c - 1)\phi_n \tag{4.3}
\]

\[
\frac{\partial \phi_a}{\partial t} + \mathbf{u} \cdot \nabla \phi_a = C_1 H(c - 1)\phi_n \tag{4.4}
\]

\[
\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = \frac{1}{\text{Pe}_c} \Delta c + C_2 C_1 H(c - 1)\phi_n, \tag{4.5}
\]

where the constants $C_1$ and $C_2$ are the nondimensional activation rate and activator release constants and $\text{Pe}_n$ and $\text{Pe}_c$ are the Peclet numbers of the nonactivated platelets and activator. The values of these nondimensional constants are

\[
C_1 = \frac{R_0 L}{U}, \quad C_2 = \frac{A \Phi}{\text{Ch}}, \quad \text{Pe}_n = \frac{LU}{D_n}, \quad \text{and} \quad \text{Pe}_c = \frac{LU}{D_c}.
\]

The nondimensional equations for the stress and the aggregation intensity function are

\[
\sigma_t + \mathbf{u} \cdot \nabla \sigma = \sigma \nabla \mathbf{u} + (\sigma \nabla \mathbf{u})^T + C_4 \phi_a^2 \delta - C_3 \beta \sigma \tag{4.6}
\]

\[
z_t + \mathbf{u} \cdot \nabla z = C_5 \phi_a^2 - C_3 \beta z, \tag{4.7}
\]

where $C_3$ is the dimensionless breaking rate, which is the ratio of the fluid time scale to the breaking time scale, and $C_4$ and $C_5$ are the dimensionless formation rates for the stress and the aggregation intensity. These nondimensional constants have the form

\[
C_3 = \frac{\beta_0 L}{U}, \quad C_4 = \frac{a_0 \Phi^2 L}{U \Sigma}, \quad C_5 = \frac{a_0 \Phi^2 L}{U Z},
\]

where $\Sigma$ and $Z$ represent the characteristic scales of the stress and aggregation intensity, respectively, and $\beta_0$ is the scale of the breaking rate function. The stress scale is $\Sigma = \rho U^2$, which was chosen to match the scale of the pressure. Another sensible scale for the stress is the value the stress takes when there is no flow and the activated platelet concentration is at the characteristic concentration. This scaling simply introduces another constant in the Navier-Stokes equations and affects how the breaking rate is computed.

The scale of the aggregation intensity is somewhat arbitrary because the only other equation where variable $z$ appears is in the computation of the average link energy.
One such scale that has been used to compare with previous simulations of the model [12, 13, 41] is

$$Z = \Phi^2 L^3.$$ 

Note that this scaling has the proper units, but it is independent of the formation and breaking rates and may not always be appropriate. However, in these previous versions of the model, the aggregation intensity did not appear in any of the other equations and was simply used as a visualization tool. With our choice of closure model, the aggregation intensity now influences other equations. Another possible scaling is

$$Z = \frac{a_0 \Phi^2}{\beta_0}.$$ 

This scale represents the steady state value of the aggregation intensity at the characteristic activated platelet concentration when there is no velocity. Again, the choice is somewhat arbitrary because the average bond energy may be rescaled. In order to reduce the number of nondimensional parameters in the model $z$ could be scaled so that $C_5 = C_4$. This is the scaling used when not comparing with results from other codes.

The breaking rate function $\beta$ depends on the ratio of $\text{Tr} \left( \sigma \right) / z$, which is the average energy per bond. The value of $\beta$ is nondimensionalized by a characteristic breaking rate scale, chosen so that under no flow conditions, the nondimensional breaking is $\beta = 1$. Suppose that the stress and aggregation intensity have been nondimensionalized as previously discussed. When there is no flow, equations (4.6) and (4.7) give that the average energy per bond is

$$w^* = \frac{\text{Tr} \left( \sigma \right)}{z} = \frac{3C_4}{C_5}, \quad (4.8)$$

where we denote this value by $w^*$ for convenience. As discussed in Chapter 3, the form of the breaking rate function used is such that the breaking rate is relatively constant when the energy per bond is below $w^*$. For example, a typical nondimensional linear breaking rate function used is

$$\beta \left( w \right) = \begin{cases} 1 & w \leq w^* \\ 1 + b \left( w - w^* \right) & w > w^* \end{cases}, \quad (4.9)$$

where $b$ is the nondimensional derivative of the breaking rate function. The breaking rate is the only equation in which $z$ affects any other variables. As discussed previously the scale of $z$ does not matter due to the way in which the breaking rate is scaled.
4.2 Time Stepping and Grid Structure

The entire system of equations is advanced in time by advancing the equations related to the platelets a full time step, computing the forces due to links, using these forces as input to advance the Navier-Stokes equations for a full time step, and then repeating the process. Using this method of time stepping means that effectively the fluid velocity and the platelet related variables are stored at different points in time. This is illustrated in Figure 4.1, where the fluid velocity is denoted by $u$ and the platelet variables are simply notated by $\sigma$.

The computational domains in all of our simulations are rectangular. The domain is discretized in regularly spaced mesh points. It is important to note that we use a cell-centered discretization, meaning that functions on the mesh are stored at the center of cell defined by the mesh lines, rather than at the intersections of mesh lines. When functions on the mesh are stored at the intersection of mesh lines, we refer to this discretization as a vertex-centered grid. Examples of each type of discretization are displayed in Figure 4.2.

The use of the cell-centered grid is motivated by our choice of advection solver, which is discussed in detail in section 4.3.1. Two rows of ghost cells are used on the exterior of the domain so that stencils of spatial operators need not be modified near the boundaries. The values of the ghost cells are set depending on what operator is being applied and the boundary conditions.

We now discuss how the platelet variables are advanced in time, beginning with the equations for the platelets and activator and then the stress.

4.3 Platelets and Activator

The equations for the nonactivated platelets, activated platelets, and the activator all of a similar form: advection-diffusion-reaction equations. Rather that working with the

![Figure 4.1: The fluid velocity and the platelet velocity are stored at different discrete time points.](image)
exact form of the model equations, consider the general equation
\[
\frac{\partial \psi}{\partial t} + \mathbf{u} \cdot \nabla \psi = D \Delta \psi + R(\psi),
\]  
(4.10)

where \(\psi\) represents the vector of all quantities involved in the advection-diffusion-reaction equation. This general equation is sufficient for the purposes of this discussion.

We again employ time splitting to advance this equation in time. For each time step we first advect \(\psi\), then diffuse \(\psi\), and to complete the time step we update reaction terms. So for each time step we solve the series of equations

1. Advection
\[
\psi_t + \mathbf{u} \cdot \nabla \psi = 0,
\]  
(4.11)

2. Diffusion
\[
\psi_t = D \Delta \psi,
\]  
(4.12)

3. Reaction
\[
\psi_t = R(\psi).
\]  
(4.13)

We now discuss the methods employed to solve each of these equations.
4.3.1 Advection

The advection equations (4.11) are advanced using a high-resolution, conservative method developed by LeVeque [28] for incompressible flow. If the flow is incompressible, the advection equation

$$\psi_t + u \cdot \nabla \psi = 0$$  \hspace{1cm} (4.14)

can be written in the equivalent form

$$\psi_t + \nabla \cdot (u\psi) = 0.$$  \hspace{1cm} (4.15)

These two forms are referred to as *advective form* and *conservative form*, respectively. Mathematically these two forms are equivalent, but discretized, they can result in numerical solutions with slightly different characteristics. If the conservative form is discretized, the total amount of $\psi$ is conserved. Sometimes the advective form is preferred over the conservative form. For example, consider the case where $\psi$ is constant in some region of space, but the velocity field is not constant. The conservative form may produce a nonconstant $\psi$, but the advective form will preserve this structure. However, differencing the advective form does not guarantee that $\psi$ is conserved. LeVeque’s algorithm is a blend of the two forms of differencing, that has the desirable properties of advective differencing, but it is fully conservative.

The method requires that $\psi$ be discretized on a cell-centered grid. Let $\psi_{ij}^n$ represent the average of the function $\psi$ at time $t_n$ over the cell $[x_i-h/2, x_i+h/2] \times [y_j-h/2, y_j+h/2]$. The velocities are stored at the cell edges with normals parallel to their direction, as is done for the MAC grid discussed in section 6.2.2. See Figure 4.3 for an example of the grid structure. Let $F_{i-1/2,j}$ and $G_{i,j-1/2}$ denote the numerical fluxes across the left and bottom edge respectively.

We now describe the algorithm for finding $q_{ij}^{n+1}$ from $q_{ij}^n$. For simplicity, we assume that both components of the velocity are positive. The changes to the algorithm for velocity with arbitrary sign are straightforward and require considering in which direction information should propagate. The algorithm proceeds in a series of stages. The first stage corresponds to first order upwinding. The following stages update the fluxes to provide a more accurate solution. The algorithm can be described in terms of waves propagating, which has a nice geometric interpretation that we make use of when appropriate.
The time step begins with the quantities $\psi_{i,j}^+, F_{i-1/2,j}$, and $G_{i,j-1/2}$ all initialized to zero. These quantities are updated at each stage, and the formula

$$\psi_{ij}^{n+1} = \psi_{ij}^n + \psi_{ij}^+ - \frac{\Delta t}{h} \left( F_{i+1/2,j} - F_{i-1/2,j} + G_{i,j+1/2} - G_{i,j-1/2} \right)$$

(4.16)

is used to update $\psi$. In the first stage the quantity $\psi_{ij}^+$ is computed as

$$\psi_{ij}^+ = -\frac{\Delta t}{h} \left( u_{i-1/2,j} \left( \psi_{ij}^n - \psi_{i-1,j}^n \right) + v_{i,j-1/2} \left( \psi_{ij}^n - \psi_{i,j-1}^n \right) \right).$$

(4.17)

This step corresponds to first order upwinding in advective form. Note that if the discrete incompressibility condition

$$u_{i+1/2,j} - u_{i-1/2,j} + v_{i,j+1/2} - v_{i,j-1/2} = 0$$

(4.18)

is satisfied, then differencing the advective form is equivalent to differencing the conservative form. In order for this algorithm to be conservative, it is necessary that condition (4.18) hold. Using the interpretation of wave propagation, the term $\psi_{ij}^+$ is the addition to $q_{ij}$ during one time step due to the normal propagation of waves from the cell on the left and the cell on the bottom. In LeVeque’s terminology, this is called the increment wave.

The remaining steps in the algorithm update only the fluxes, and so they are guaranteed to be conservative. The addition in each stage makes the algorithm more accurate. The first stage only accounted for propagation of waves normal to cell edges. The second
stage of the algorithm accounts for transverse propagation. The fluxes at the top and right edge are updated by

\[ G_{i,j+1/2} = G_{i,j+1/2} - \frac{\Delta t}{2h} u_{i,j+1/2,j} v_{i,j+1/2} (\psi^n_{i,j} - \psi^n_{i-1,j}) \]  
(4.19)

\[ F_{i+1/2,j} = F_{i+1/2,j} - \frac{\Delta t}{2h} v_{i,j+1/2,j} u_{i,j+1/2,j} (\psi^n_{i,j} - \psi^n_{i,j-1}) . \]  
(4.20)

Accounting for transverse propagation does not improve the order of the accuracy of the algorithm, but it does improve the stability and reduces the error.

The first order terms derive from assuming a piecewise constant profile for \( \psi \) on each cell. To move to a second order scheme, a piecewise linear profile is assumed on each cell. Since the cell averages were propagated in the previous stages, we consider propagation of linear profiles with mean zero. A different linear profile is used for propagation in the two directions. For propagation in the \( x \)-direction the profile is constant in the \( y \)-direction and has slope \( \frac{1}{A} (\psi^n_{ij} - \psi^n_{i-1,j}) \Phi_{i-1/2,j} \), where \( \Phi_{i-1/2,j} \) is a flux limiter used to prevent oscillations near steep gradients of \( \psi \). The normal propagation of these linear profiles is the third stage of the algorithm. Let \( S \) represent the collection of second order corrections to the flux. At the left and bottom edges of the cell, the corrections are

\[ S_{i-1/2,j} = \frac{1}{2} | u_{i-1/2,j} | \left( 1 - \frac{\Delta t}{h} | u_{i-1/2,j} | \right) \left( \psi^n_{i,j} - \psi^n_{i-1,j} \right) \Phi_{i-1/2,j} \]  
(4.21)

\[ S_{i,j-1/2} = \frac{1}{2} | v_{i,j-1/2} | \left( 1 - \frac{\Delta t}{h} | v_{i,j-1/2} | \right) \left( \psi^n_{i,j} - \psi^n_{i,j-1} \right) \Phi_{i,j-1/2} \]  
(4.22)

The edge fluxes are then updated as

\[ F_{i-1/2,j} = F_{i-1/2,j} + S_{i-1/2,j} \]  
(4.23)

\[ G_{i,j-1/2} = G_{i,j-1/2} + S_{i,j-1/2} . \]  
(4.24)

At this point the solution is second order accurate, but the final stage accounts for transverse propagation of the second order corrections. The updates to the fluxes are

\[ G_{i,j+1/2} = G_{i,j+1/2} + \frac{\Delta t}{h} v_{i,j+1/2,j} S_{i-1/2,j} \]  
(4.25)

\[ G_{i-1,j+1/2} = G_{i-1,j+1/2} - \frac{\Delta t}{h} v_{i-1,j+1/2,j} S_{i-1/2,j} \]  
(4.26)

\[ F_{i+1/2,j} = F_{i+1/2,j} + \frac{\Delta t}{h} u_{i+1/2,j} S_{i,j-1/2} \]  
(4.27)

\[ F_{i+1/2,j-1} = F_{i+1/2,j-1} - \frac{\Delta t}{h} u_{i+1/2,j-1} S_{i,j-1/2} . \]  
(4.28)

Even though this does not improve the order of accuracy of the solution, LeVeque notes that the error is reduced and mild oscillations near discontinuities are reduced in his
computational tests. The final step in the algorithm is to compute $\psi_{ij}^{n+1}$ using equation (4.16).

### 4.3.2 Diffusion

The time discretization used for the diffusion equation (4.12) is the standard Crank-Nicholson scheme, which is second order accurate in space and time [34]. Discretizing equation (4.12) gives

$$\frac{\psi^{n+1} - \psi^n}{\Delta t} = \frac{D}{2} \left( L\psi^n + L\psi^{n+1} \right),$$

where $L$ is a discrete approximation to the Laplacian operator. At the interior points of the domain, the form of $L$ is the standard, second order accurate, five-point approximation to the Laplacian

$$(L\psi)_{i,j} = \frac{\psi_{i-1,j} + \psi_{i+1,j} - 4\psi_{i,j} + \psi_{i,j-1} + \psi_{i,j+1}}{\Delta x}.$$ (4.30)

Rearranging equation (4.29), we obtain the equation

$$\left( I - \Delta t \frac{D}{2} L \right) \psi^{n+1} = \left( I + \Delta t \frac{D}{2} L \right) \psi^n.$$ (4.31)

This equation is solved using a multigrid method [40], modified for the cell-centered grid structure. A full discussion of multigrid on cell-centered grids, including the handling of boundary conditions is presented in Appendix B. We use V-cycles with $\psi^n$ as the initial guess for $\psi^{n+1}$. The smoothing is done using $(1, 1)$ red-black Gauss-Seidel.

### 4.3.3 Reaction

Updating the reaction terms by solving equation (4.13) is easier than handling the advection and diffusion terms, because there is no spatial coupling of grid points in this equation. The problem reduces to solving a ODE at each point. Due to the simplicity of the reaction terms in equations (4.3)–(4.5), a stable, second order solve is straightforward.

If the concentration of activator at a point is subthreshold at the beginning of the time step, it will remain subthreshold during that time step. In this case, there are no reactions that take place at that grid point. If the concentration of activator is above threshold at the beginning of a time step, then the concentrations are updated at each grid point by

$$\phi_{n}^{n+1} = \exp (-C_1 \Delta t) \phi_{n}^{n},$$

$$\phi_{a}^{n+1} = \phi_{a}^{n} + \phi_{n}^{n} - \phi_{n}^{n+1},$$

$$c^{n+1} = c^{n} + C_2 (\phi_{n}^{n} - \phi_{a}^{n+1}).$$
This is clearly a second order method for updating the reaction terms.

4.4 Stress

We now describe how the stress and the aggregation intensity are advanced in time, and how the resulting body force is computed. All of the simulations in this dissertation are performed in two spatial dimensions. A two-dimensional velocity field is often interpreted as existing in three dimensions with all quantities independent of the third dimension. This raises the question of whether links form in two or three dimensions. We begin with a discussion of this question.

4.4.1 Two-Dimensional Fluids – Three-Dimensional Links

As it turns out, links can form in three dimensions, and because they form isotropically, the formation of links in the third dimension does not introduce fluid disturbances in this dimension. Suppose that the velocity field is of the form

\[ u = (u(x_1, x_2), v(x_1, x_2), 0), \]

so that the velocity gradient is

\[ \nabla u = \begin{bmatrix} u_{x_1} & v_{x_1} & 0 \\ u_{x_2} & v_{x_2} & 0 \\ 0 & 0 & 0 \end{bmatrix}. \]  

The three components of stress that contribute to the body force in the \( x_3 \)-direction are \( \sigma_{13}, \sigma_{23} \), and \( \sigma_{33} \). The equations that govern these components of the stress are given by using this form of the velocity gradient in equation (4.6) for the stress to get

\[
\begin{align*}
\frac{\partial \sigma_{13}}{\partial t} + \mathbf{u} \cdot \nabla \sigma_{13} &= u_{x_1} \sigma_{13} + u_{x_2} \sigma_{23} - C_3 \beta \sigma_{13} \\
\frac{\partial \sigma_{23}}{\partial t} + \mathbf{u} \cdot \nabla \sigma_{23} &= v_{x_1} \sigma_{13} + v_{x_2} \sigma_{23} - C_3 \beta \sigma_{23} \\
\frac{\partial \sigma_{33}}{\partial t} + \mathbf{u} \cdot \nabla \sigma_{33} &= C_4 \phi_a^2 - C_3 \beta \sigma_{33}.
\end{align*}
\]

The equations for \( \sigma_{13} \) and \( \sigma_{23} \) depend on each other, but do not depend on any other components of the stress. Since prior to aggregation, these two components of the stress will be zero, they remain zero for all time.

The third component, \( \sigma_{33} \), does not remain zero for all time, and so it produces a nonzero body force in the \( x_3 \)-direction, which it seems, may be incompatible with the
assumption that the flow is uniform in the $x_3$-direction. We show below that this nonzero body force is balanced by the pressure, and so it does not disturb the velocity field. As is discussed thoroughly in Chapter 6, the purpose of the pressure is to enforce the incompressibility constraint. This modification to the pressure does not affect the fluid velocity.

Before further discussing the pressure, we discuss how $\sigma_{33}$ is computed. If links are assumed to be forming in three dimensions, the value of $\sigma_{33}$ is necessary to compute the trace, which is used in the breaking rate. Note that the form of equation (4.38) for $\sigma_{33}$ is the same as equation (4.7) for the aggregation intensity, except that the formation rate is different. The aggregation intensity is computed for use in the breaking rate function and for visualization purposes. The value of $\sigma_{33}$ can be recovered from the value of the aggregation intensity by

$$\sigma_{33} = \frac{C_4}{C_5} z.$$  \hfill (4.39)

Therefore allowing links to form in three dimensions does not introduce any more computational work than when links only form in two dimensions.

### 4.4.2 Platelet Pressure

As mentioned in the previous section, the stress due to platelet links has a component that contributes to the pressure. Suppose that the velocity gradient of the flow is zero. In this special case, the equation for the stress is

$$\sigma_t + \mathbf{u} \cdot \nabla \sigma = C_4 \phi_a^2 \delta - C_3 \beta \sigma$$  \hfill (4.40)

Suppose that initially all the components of the stress are zero. No off diagonal elements of the stress can form, and the equation for each of the diagonal elements is the same. The stress is then just a scalar, and we write

$$\sigma = \pi \delta,$$  \hfill (4.41)

where $\pi$ represents a quantity we call the platelet pressure. The platelet pressure evolves by

$$\pi_t + \mathbf{u} \cdot \nabla \pi = C_4 \phi_a^2 - C_3 \beta \pi.$$  \hfill (4.42)

When the stress is just a scalar, the body force given by the divergence of this stress is just the gradient of the platelet pressure. The addition of this gradient to the momentum equation does not affect the velocity, only the fluid pressure, because the fluid is incompressible.
Now suppose that the velocity gradients are not zero. The stress is not equivalent to a pressure, but we can still define the platelet pressure according to equation (4.42). Let \( \tau \) be a stress tensor defined by
\[
\tau = \sigma - \pi \delta.
\]
(4.43)
If \( \nabla \cdot \tau \) is used in the momentum equation rather than \( \nabla \cdot \sigma \), the velocity remains unchanged and only the pressure is modified. Using equation (4.6) and (4.42), we find the equation for the evolution of \( \tau \) to be
\[
\tau_t + u \cdot \nabla \tau = \nabla u \tau + (\nabla u \tau)^T + \pi D - C_3 \beta \tau,
\]
(4.44)
where \( D \) is the fluid rate of deformation tensor defined by
\[
D = \nabla u + \nabla u^T.
\]
This equation is similar to the equation for the stress, except that the formation rate depends on the the product of the platelet pressure and the rate of deformation. Suppose that the platelet pressure is large, due to a high formation rate or low breaking rate, and the velocity gradients are small. In this case all the components of \( \tau \) are of similar size, but the diagonal elements of \( \sigma \) are much larger than the off diagonal elements. For this reason, we have found that \( \tau \) is sometimes better behaved numerically than \( \sigma \) when it is used as the platelet stress, especially near the edges of aggregates, where sharp gradients of \( \phi_3 \) and \( \sigma \) are encountered. However, for simulations involving solid boundaries, we have found that computing the forces using \( \sigma \) is better behaved than when using \( \tau \).

Even though \( \tau \) is used as the platelet stress, equation (4.44) is not solved. Instead equation (4.6) is solved for \( \sigma \), and then \( \tau \) is computed using (4.43). Keeping track of the platelet pressure does not require solving any additional equations. Note that equation (4.42) for the platelet pressure is identical to equation (4.38) for \( \sigma_{33} \), so that \( \tau = \sigma_{33} \). Just as \( \sigma_{33} \) is computed as a multiple of \( z \), so is \( \tau \). Therefore, only the quantities \( \sigma \) and \( z \) need be computed.

### 4.4.3 Updating the Stress

As is done for the platelet and activator equations, the equations for the stress and the activator are advanced in multiple stages. First homogeneous advection equations are advanced
\[
\begin{align*}
\sigma_t + u \cdot \nabla \sigma &= 0 \\
z_t + u \cdot \nabla z &= 0.
\end{align*}
\]
(4.45) (4.46)
The advection is performed as described in section 4.3.1. Two different approaches were applied to the remaining terms. One approach is to then advance the equation

$$\sigma_t = \sigma \nabla u + (\sigma \nabla u)^T,$$

and complete the time step by updating the reaction terms

$$\sigma + u \cdot \nabla \sigma = C_4 \phi_a^2 \delta - C_3 \beta \sigma \quad \text{(4.48)}$$

$$z_t = C_5 \phi_a^2 - C_3 \beta z. \quad \text{(4.49)}$$

This method of time splitting was used when the breaking rate was assumed to be constant. The three steps of the solve are referred to as the advection step, the stretching step, and the reaction step. Note that since the velocity gradients are treated as constants throughout the time step, there is no spatial coupling in the stretching and reaction steps, and in each step the equations are linear.

When the breaking rate is a function of the average bond energy, the equations can be stiff, depending on the form of the breaking rate. In this case we found that a different method of time stepping must be employed for stability. Also note that when a nonconstant breaking rate is used, the equations become nonlinear. We now discuss the method of time stepping that was used for all of the simulations presented in this dissertation. Each time step was taken in two stages rather than in three. The advection step is performed as the first stage, and the stretching and reaction steps were combined into a single step.

To begin the time step, the quantities $\sigma^n$ and $z^n$, are advected to produce the temporary quantities $\sigma^*$ and $z^*$. The remaining stretching and reaction terms are discretized as

$$\frac{\sigma^{n+1} - \sigma^*}{\Delta t} = \left( \frac{\sigma^{n+1} + \sigma^*}{2} \right) \nabla u + \left( \frac{\sigma^{n+1} + \sigma^*}{2} \right)^T \nabla u$$

$$+ C_4 \left( \frac{\phi_a^n + \phi_a^{n+1}}{2} \right)^2 \delta - C_3 \left( \frac{\beta^{n+1} \sigma^{n+1} + \beta^* \sigma^*}{2} \right) \quad \text{(4.50)}$$

$$\frac{z^{n+1} - z^*}{\Delta t} = C_5 \left( \frac{\phi_a^n + \phi_a^{n+1}}{2} \right)^2 - C_3 \left( \frac{\beta^{n+1} z^{n+1} + \beta^* z^*}{2} \right) \quad \text{(4.51)}$$

If $\beta$ is not a constant function, these equations are nonlinear, but they are decoupled in space, which significantly reduces the amount of work needed to perform the nonlinear solve. In two spatial dimensions, at each grid point there are four unknowns: $\sigma_{11}^{n+1}, \sigma_{12}^{n+1}, \sigma_{22}^{n+1}, \sigma_{23}^{n+1}$. 
\( \sigma_{22}^{n+1}, \) and \( z^{n+1}. \) Newton’s method is used to solve the system (4.50)-(4.51) at each grid point, using \( \sigma^* \) and \( z^* \) to initialize the iteration. If the iteration does not converge in some predefined number of iterations, the time step is cut in half and the initial iterate is set to the last value for which the iteration converged. This process is repeated until the solution is advanced to time \( n + 1 \) or until the time step is refined some critical number of times, in which case the solver fails. This time refinement is only done locally. That is, the refinement of time at a given grid location does not affect any other grid locations.
CHAPTER 5

NUMERICAL EXPERIMENTS

In this chapter the results of numerical experiments are presented. The first set of experiments involves the formation of an aggregate in a spatially periodic extensional flow, which is presented to demonstrate the effects of a nonconstant breaking rate. Results from the closure model are compared with results generated using the full model. The second set of experiments involves a growing aggregate on the wall in a pressure-driven, parallel plate flow. These experiments are presented to explore the model’s utility in simulating the development of an aggregate around an injured vessel wall.

5.1 Grab and Pull Experiments

The grab and pull experiment was designed by Wang and Fogelson [41] to test the effects of nonconstant breaking rates in the full model. Activator is introduced at the beginning of the test, and the aggregate begins to form. At some time all the activator is removed, and the aggregate is pulled in an effort to break the aggregate into pieces, which explains the name grab and pull experiments.

All quantities discussed are nondimensional, with the scalings described in Chapter 4. The values of some nondimensional parameters that remain fixed for all of the experiments are given in Table 5.1. The computational domain is the square $[-0.5, 0.5] \times [-0.5, 0.5]$ with periodic boundaries in both directions. Periodic boundary conditions were chosen to avoid the complications introduced by solid boundaries. Before adding platelet activator, the fluid velocity is

$$u = \sin (2\pi x) \cos (2\pi y)$$

$$v = -\cos (2\pi x) \sin (2\pi y).$$

This fluid velocity is used to compute the background force necessary to drive this steady flow at Reynolds number 25. This background force is applied throughout the computation. The computation begins with a uniform distribution of nonactivated platelets.
Table 5.1: Parameters values used in grab and pull experiments

<table>
<thead>
<tr>
<th>$C_1$</th>
<th>$C_2$</th>
<th>$C_3$</th>
<th>$C_4$</th>
<th>$C_5$</th>
<th>$P_e_n$</th>
<th>$P_e_n$</th>
<th>Re</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>20</td>
<td>1</td>
<td>$30\pi$</td>
<td>$2\pi$</td>
<td>$10^7$</td>
<td>$2 \cdot 10^5$</td>
<td>25</td>
</tr>
</tbody>
</table>

Activator is introduced within a circle of radius 0.15 centered on the stagnation point at the origin, and links begin to form. At time 0.1 the activation of new platelets is prevented.

After the aggregate has formed for some time, an additional background force is applied in such a way that the pulling force of the fluid in the $x$-direction is accentuated. This extra force is entirely in the $x$-direction and its value is

$$F_{\text{pull}} = F_{\text{max}} f_1(x) f_2(y),$$  \hspace{1cm} (5.3)

where $f_1$ and $f_2$ are constructed by linear combinations of hyperbolic tangent functions, and plots of these functions are displayed in Figure 5.1. In the tests presented here the maximum extra force is set to $F_{\text{max}} = 100$, which is about 18 times larger than the maximum value of the magnitude of the background force driving the flow.

![Figure 5.1](image-url)

Figure 5.1: The functions $f_1(x)$ and $f_2(y)$ are used to define the shape of the extra force used to pull at the aggregate.
Figure 5.2: Formation of an aggregate without extra background force to pull the aggregate. The aggregate forms and the fluid velocity is essentially zero inside the aggregate. The solid lines represent contours of the aggregation intensity and the dashed contour denotes the boundary where the activator is above threshold.
5.1.1 Computational Tests

For the first simulation, no extra forces are applied to the forming aggregate. Results from the simulation at several points in time are displayed in Figure 5.2. The solid lines are contours of the aggregation intensity ($z$) and the dashed line is the contour that represents the threshold level of platelet activator. The aggregate forms and essentially stops the flow inside the aggregate. The results are displayed for a constant breaking rate, but the results were identical for nonconstant breaking rates, indicating that the aggregate is able to resist the background forces without significantly straining the links.

When the extra pulling force is applied to the aggregate, the effect of a nonconstant breaking rate becomes apparent. For the next two tests the extra force is applied at the same time that activation is stopped, time 0.1. First this test is performed for a constant breaking rate, and plots from this simulation at several points in time are displayed in Figure 5.3. The vertical bars in these plots denote the regions in space where the pulling force is concentrated. The application of the pulling force deforms the aggregate, but the aggregate resists being pulled apart. Because the breaking rate is constant, the application of the pulling force does not change the rate at which links break.

In Figure 5.4 the results of the same test with a nonconstant breaking rate are shown. All of the parameters are identical to the previous test, except the breaking rate is

$$\beta(w) = \begin{cases} 
1 & w \leq w^* \\
1 + 8\left(\frac{w}{w^*} - 1\right) & w > w^*
\end{cases}, \quad (5.4)$$

where $w^*$ is chosen to be the value of the average link energy at which links form. As can be seen in Figure 5.4 the aggregate separates into two pieces after the addition of the pulling force. Links continue to form, as can be seen by the contours of the aggregation intensity. In contrast with the previous test, the addition of the extra force affects the rate at which links break, causing an increase in link rupture in the center of the aggregate. This test shows that a nonconstant breaking rate produces behavior that cannot be realized if only a constant breaking rate is used.

5.1.2 Comparison with the Full Model

The results of the grab and pull experiment presented so far for the closure model are consistent with the conclusions from [41]: the aggregate cannot be pulled apart with a nonconstant breaking rate. However, in order to make a more detailed comparison with the full model, we must quantify the results of the experiment. We define three
Figure 5.3: Grab and pull with a constant breaking rate. The activation is stopped and the extra force is applied at time 0.1. The solid lines represent contours of the aggregation intensity and the dashed contour denotes the boundary where the activator is above threshold. The vertical bars denote the location of the pulling force.
Figure 5.4: Grab and pull with the nonconstant breaking rate (5.4). The activation is stopped and the extra force is applied at time 0.1. The solid lines represent contours of the aggregation intensity and the dashed contour denotes the boundary where the activator is above threshold. The vertical bars denote the location of the pulling force.
measures based on the integrals of the aggregation intensity which provide a quantitative
description of the experiment.

The first quantity is the mean of the aggregation intensity along the line \( x = 0 \), which
is denoted by \( Z_0 \) and computed as

\[
Z_0(t) = \int_{-0.5}^{0.5} z(0, y, t) \, dy. \tag{5.5}
\]

This quantity characterizes the total number of links in the center of the aggregate.

The second quantity used to characterize the experiment quantifies the thickness of the
aggregate along the line \( x = 0 \). This quantity is denoted by \( Z_2 \) and computed by

\[
Z_2(t) = \frac{\int_{-0.5}^{0.5} y^2 z(0, y, t) \, dy}{Z_0}. \tag{5.6}
\]

The final quantity used for comparing the experiments measures the displacement of each
half of the aggregate from the center of the domain. This quantity is denoted by \( Z_x \) and
is defined by

\[
Z_x(t) = \frac{\int_{-0.5}^{0.5} \int_{-0.5}^{0.5} x z(x, y, t) \, dx \, dy}{\int_{-0.5}^{0.5} \int_{-0.5}^{0.5} z(x, y, t) \, dx \, dy}. \tag{5.7}
\]

The value of \( Z_x \) is like the center of mass of the links with a negative \( x \)-coordinate.

The two types of breaking rates considered for the closure model are linear in the
average energy per bond and exponential in the average energy per bond. The forms of
the breaking rate were chosen to be similar to those tested in Chapter 3. For the closure
model, the breaking rate is constant for values of the average energy per bond below the
value at which links form, and for the full model the breaking rate is constant for lengths
less than the maximum length at which links form. The specific forms of the breaking
rate function for the closure model are

\[
\beta(w) = \begin{cases} 
1 & w \leq w^* \\
1 + b(w/w^* - 1) & w > w^* 
\end{cases}, \tag{5.8}
\]

and

\[
\beta(w) = \begin{cases} 
1 & w \leq w^* \\
0.5 \left( 1 + \exp(2b(w/w^* - 1)) \right) & w > w^* 
\end{cases}. \tag{5.9}
\]

The parameter \( b \) represents the right derivative of the breaking rate at \( w^* \). The corre-
sponding breaking rates for the full model are

\[
\beta(r) = \begin{cases} 
1 & r \leq 1 \\
1 + b r(r^2 - 1) & r > 1 
\end{cases}. \tag{5.10}
\]
and

$$\beta(r) = \begin{cases} 
1 & r \leq 1 \\
0.5\left(1 + \exp(2b_f(r^2 - 1))\right) & r > 1 
\end{cases}$$  \hspace{1cm} (5.11)$$

For a given value of $b$ for the closure model, the corresponding value of $b_f$ is

$$b_f = \frac{\int_1^0 r^2 \alpha(r) dr}{\int_0^1 \alpha(r) dr} b.$$  \hspace{1cm} (5.12)

This formula for $b_f$ results from the scaling as is shown in Appendix C. The nondimensional formation rate used for the tests with the full model is

$$\alpha(r) = \begin{cases} 
1 & r \leq 1 \\
0 & r > 1 
\end{cases}$$  \hspace{1cm} (5.13)

The computations of the full model are performed using the code from [41] with the variable scales adjusted to match the scalings used in the closure model. The code for the full model and closure model not only differ in the computation of platelet stress, but also in the algorithm used to solve the Navier-Stokes equations. Therefore some of the observed differences in the results may originate from differences in the numerical solvers.

First the linear breaking rates are compared in Figures 5.5, 5.6, and 5.7. Plots of $Z_0$, $Z_2$, and $Z_x$ as functions of time for three different values of $b$ for both the closure model and the full model are displayed in Figures 5.5(a), 5.6(a), and 5.7(a), respectively. Note that only one curve is displayed for $b = 0$, because in the case of constant breaking the models should be the same. However there are slight differences in the implementations of the two codes, which are discussed later. As these three plots show, the results from the two models are different. For the lower value of $b$ ($b = 4$), the values $Z_0$, $Z_2$, and $Z_x$ were lower for the full model than for the closure model, and the difference between these values for the two models increased in time. This difference indicates that the links in the closure model broke less readily than in the full model for this breaking rate function.

For the higher value of $b$ ($b = 8$), the difference between the two models is less pronounced. The value of $Z_0$ computed using the two models is very similar, but the closure model predicted the lower values for this case. The values of $Z_2$ are larger for the closure model until around time 0.4 when the aggregate has essentially pulled apart. The values of $Z_x$ are also generally larger for the closure model, but these differences in $Z_2$ and $Z_x$ between the two models are small. The difference in $Z_x$ is on the order of several mesh widths.
Figure 5.5: $Z_0$ for the full model and closed model is compared for the linear breaking rate. (a) The time course of $Z_0$ for different value of $b$. Solid curves correspond to the closure model and dashed curves correspond to the full model. (b) $Z_0$ as a function of $b$ at time $t = 0.3$. 
Figure 5.6: $Z_2$ for the full model and closed model is compared for the linear breaking rate. (a) The time course of $Z_2$ for different value of $b$. Solid curves correspond to the closure model and dashed curves correspond to the full model. (b) $Z_2$ as a function of $b$ at time $t = 0.3$. 
Figure 5.7: $Z_x$ for the full model and closed model is compared for the linear breaking rate. (a) The time course of $Z_x$ for different value of $b$. Solid curves correspond to the closure model and dashed curves correspond to the full model. (b) $Z_x$ as a function of $b$ at time $t = 0.3$. 
This test was run for a range of values of $b$. We do not show the plots of $Z_0$, $Z_2$, and $Z_x$ in time for all of these tests. Instead, we plot these three values at time 0.3 as a function of $b$ for the two models. These plots are displayed in Figures 5.5(b), 5.6(b), and 5.7(b). The difference in the results for the constant breaking rate is evident in these plots. The difference is most notable in the value of $Z_2$. All three plots show a similar trend: the results from closure model and the full model are similar for small and large values of $b$, but differ most for the values in the middle of the range tested.

The exponential breaking rate was also tested. Plots of $Z_0$ and $Z_x$ for the two models for different values of $b$ are displayed in Figure 5.8. As with the linear breaking rate, the results are more similar for the higher value of $b$ ($b = 2$) than for the lower value of $b$ ($b = 1$). However, this difference is more dramatic for the lower value of $b$, the aggregate did not pull apart in the closure model but it did in the full model. For the higher value of $b$, the value of $Z_0$ is much higher in the closure model around time 0.2 than the value obtained with the full model. However, the aggregate pulls apart around the same time, which is shown by the similar times at which $Z_0$ becomes zero.

The behavior of the aggregate that results from using the closure model does not match the full model exactly. Of course, it is not expected that the closure model should reproduce the results obtained using the full model perfectly. The closure model seems generally to underestimate the breaking of links from the full model, but in most cases the qualitative behavior is similar. When the breaking rate increased sharply (large values of $b$) the quantitative predictions of the two models were similar. Because the models are identical for a constant breaking rate, the results are similar when breaking rate increases slowly. There is, however, a range of moderate increase in the breaking rate for which the behavior of the two models differs considerably for both the linear and exponential breaking rates. In this range the aggregate did not pull apart in the closure model as it did in the full model. This difference is more striking with the exponential model.

5.2 Growing Aggregate: Parallel Plate Flow

In this section we present simulations of aggregate growth on the wall of a parallel plate flow chamber. Our goal in performing these simulations is to explore the possible behaviors that result by varying the model parameters. The results of these simulations may provide insight into the model’s applicability to platelet aggregation on the wall of a damaged vessel. The simulations presented in this section are some of the first simulations
Figure 5.8: The full model and closure model are compared for an exponential breaking rate. Solid curves correspond to the closure model and dashed curves correspond to the full model. (a) The time course of $Z_0$. (b) The time course of $Z_x$.
of the continuum model involving solid walls. The first computational tests of the model with solid boundaries were performed by Nolen [35], but the tests were somewhat limited and the conclusions were not insightful.

Before presenting the computational results, we first discuss a known deficiency with the model at solid boundaries, which leads to the question of how the growth on the wall should be initiated. One goal in performing these simulations is to explore the behavior of the model in a physiological setting. To initiate the reaction, we propose a simple method to mimic an injured vessel wall. In the computational experiments, we vary the formation and breaking rates of links, the activation rate, and breaking rate function. The remaining parameters are estimated based on their values in large arteries.

### 5.2.1 Model at Solid Boundaries

At solid boundaries the typical boundary condition for the fluid is the no slip condition, which means that all components of the velocity vector are zero. In the model, activated platelets are transported only by the fluid velocity. Therefore, if platelets become activated on a no slip boundary, they remain at that location for all time. In an injured vessel, platelet aggregation is initiated by nonactivated platelets interacting with the injured wall. Platelets should not be able to bind to the wall except where the subendothelium is exposed. No such mechanism is accounted for in this model, and because of the no slip boundary conditions, activated platelets at the wall are permanently attached.

This issue at no slip boundaries does not prevent us from performing simulations, but this problem should be addressed in future versions of the model. Currently a model that accounts for interactions with the wall is being explored [14]. Because we use a cell-centered discretization, there are no grid points on the physical boundaries of the domain. Therefore, no platelets should be able to reach the no slip boundary. However, as the simulations show, a significant degree of aggregation on the boundary can effectively bring the fluid velocity to zero, as though the aggregate were attached to the wall.

### 5.2.2 Initiating the Reaction

The lack of a proper model for the boundary raises the question of how to initiate the growth of the aggregate. One possibility is to use a reactive boundary condition for the nonactivated platelet concentration such as

$$\frac{\partial \phi_n}{\partial n} = R(x)\phi_n,$$

(5.14)
where \( R(x) \) is only nonzero where the wall is injured. These platelets that interact with the boundary do not leave the domain, rather they become activated platelets. These activated platelets should be introduced where they became activated: at the boundary. However, we do not store the concentration of activated platelets along the boundary, because of the choice of the cell-centered grid. These newly activated platelets cannot enter the domain via a flux, as can the nonactivated platelets, because activated platelets are transported only by the fluid, which has zero velocity along the boundary. We therefore abandon the idea of a reactive boundary in this implementation.

Another possible method to initiate the growth of the aggregate is to place activator in some region of space at the beginning of the simulation. This was the approach used in the grab and pull simulations. For parallel plate flow, this has the drawback that this initial burst of activator may wash away, or at least move downstream before significant aggregation takes place.

As we have noted, the method is lacking a proper treatment of the reactions of platelets with the solid wall. In order to simulate an injured zone along the vessel wall, we introduce a fixed region in space so that nonactivated platelets in this region become activated at some rate. We refer to this region as the injured zone, which is not just along the boundary, but it extends into the computational domain. This is a simplification of the approach taken in [14]. The reaction terms in the model equations (2.49)-(2.51) for the platelets and activator are modified to include activation in the injured zone. The modified equations are

\[
\frac{\partial \phi_n}{\partial t} + \mathbf{u} \cdot \nabla \phi_n = D_n \Delta \phi_n - \left( R_0 H (c - c_0) + R_{iz}(x) \right) \phi_n \tag{5.15}
\]

\[
\frac{\partial \phi_a}{\partial t} + \mathbf{u} \cdot \nabla \phi_a = \left( R_0 H (c - c_0) - R_{iz}(x) \right) \phi_a \tag{5.16}
\]

\[
\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D_c \Delta c + A \left( R_0 H (c - c_0) + R_{iz}(x) \right) \phi_n \tag{5.17}
\]

The form of the function \( R_{iz}(x) \) is

\[
R_{iz} = R_{iz\text{max}} \max \left( \left( 1 - 4(x - x_c)^2 - 80y^2 \right)^3, 0 \right), \tag{5.18}
\]

where \( x_c \) is the \( x \)-coordinate of the center of the injured zone and we have assumed that \( y = 0 \) is the location of the boundary and the values of \( x \) and \( y \) are nondimensional. The support of this injured zone is a half ellipse 1 unit long in the \( x \)-direction and extending approximately 0.12 units vertically. Note that the reaction rate decays rapidly away
from its center \((x_c, 0)\). We take \(x_c = 1.25\) for all of the simulations presented in this dissertation.

This injured zone approach introduces another parameter, the activation rate in the injured zone, which is not required to be the same as the activation rate due to activator. Recall that the nondimensional activation rate due to activator is denoted by \(C_1\) and is defined by the product of the time scale and the dimensional activation rate \(R_0\). Similarly, we define \(C_{iz}\) as the nondimensional activation rate due to activation of the injured zone. It is defined by the product of the time scale and \(R_{iz\text{max}}\).

### 5.2.3 Estimating Parameters

There are many parameters in the model. We do not wish to vary every parameter in these simulations, because there are far too many and because there is no need to vary some parameters such as the diffusion coefficients or the viscosity. We are able to estimate values for some of the parameters that remain fixed for all simulations. For some other parameters we estimate a range of reasonable values, and the values of the remaining parameters are unknown before beginning the simulations.

The separation between the parallel plates is chosen to be 0.1 cm for all simulations. This size is comparable to the scale of the moderate sized arteries, like those which supply the heart. The density of the fluid is always taken to be 1.0 g/cm. The viscosity of plasma (1.3 cP) is higher than that of water (1.0 cP) and the viscosity of whole blood is even higher than plasma. The viscosity of whole blood depends on the concentration of red blood cells, and because of the deformability of these cells the viscosity also depends on shear rate. We ignore the shear rate dependence of the viscosity for simplicity, and take the viscosity to be 4.0 cP. For all simulations the centerline velocity of the undisturbed flow is taken to be 10 cm/s, which is comparable to the velocity in large arteries.

The concentration of nonactivated platelets that is uniform at the beginning of the simulation and introduced upstream is taken to be the concentration \(\text{in vivo}\). This value is \(3 \cdot 10^5\) plt/mm\(^3\). Upon activation the release of ADP per platelet is taken to be \(2 \cdot 10^{-11}\) \(\mu\)mol/plt [2]. The threshold value for aggregation is taken to be 1.0 \(\mu\)M [44]. The diffusion coefficient for ADP is \(5 \cdot 10^{-6}\) cm\(^2\)/s [21] and for nonactivated platelets is \(10^{-7}\) cm\(^2\)/s [17].

This completes the description of parameters that we do not vary in our simulations. These values are summarized in Table 5.2. These values can be used to define all of the variable scales except for the scale of the aggregation intensity, which depends on
Table 5.2: Parameters fixed throughout aggregate growth simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>domain height</td>
<td>0.1 cm</td>
</tr>
<tr>
<td>fluid density</td>
<td>1.0 g/cm³</td>
</tr>
<tr>
<td>fluid viscosity</td>
<td>0.04 P</td>
</tr>
<tr>
<td>undisturbed centerline velocity</td>
<td>10 cm/s</td>
</tr>
<tr>
<td>platelet concentration upstream</td>
<td>3 \cdot 10^5 plt/mm³</td>
</tr>
<tr>
<td>ADP release</td>
<td>2 \cdot 10^{-11} µmol/plt</td>
</tr>
<tr>
<td>ADP threshold for activation</td>
<td>1.0 µM</td>
</tr>
<tr>
<td>ADP diffusion coefficient</td>
<td>5 \cdot 10^{-6} cm²/s</td>
</tr>
<tr>
<td>platelet diffusion coefficient</td>
<td>10^{-7} cm²/s</td>
</tr>
</tbody>
</table>

the link formation rate function, $\alpha$. Using these variable scales the Reynolds number, Peclet numbers, and dimensionless activator release can be computed. These values are displayed in Table 5.3.

We estimate a reasonable range for the activation rates, but no ranges are apparent for the formation and breaking rates. Suppose a platelet is traveling above the vessel surface and the shear rate is 1500 s$^{-1}$, which is on the high end of normal shear rates in the circulation system. If the injured zone is about 100 µm long, the platelet will travel over this zone in 1/15 s. We therefore estimate that the minimum activation rate is on the order of 10 s$^{-1}$, at least due to interaction with the wall. We estimate that the fastest a platelet could become activated is about 10 ms, which gives an upper bound on the activation rate of about 100 s$^{-1}$. These estimates provide a range of only two orders of magnitude to explore. Using the time scale of 0.01 s, the dimensionless activation rate

Table 5.3: Dimensionless parameters defined using parameters in Table 5.2

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reynolds number</td>
<td>$Re = \frac{\rho LU}{\mu} = 25$</td>
</tr>
<tr>
<td>platelet Peclet number</td>
<td>$Pe_n = \frac{LU}{D_n} = 10^7$</td>
</tr>
<tr>
<td>activator Peclet number</td>
<td>$Pe_c = \frac{LU}{D_c} = 2 \cdot 10^5$</td>
</tr>
<tr>
<td>activator released</td>
<td>$C_2 = \frac{A\Phi}{Ch} = 6$</td>
</tr>
</tbody>
</table>
from interaction with the wall, $C_{1iz}$, must be in the range 0.1 to 1.0. In the simulations we vary $C_{1iz}$ over this range and vary $C_1$ over the larger range 0.01 to 1.0.

We have no means of estimating the parameters related to formation and breaking. Rather than specify the link formation function and the stiffness, we simply experiment with the values of the dimensionless formation rate, $C_4$. For the breaking rate, we experiment with the nondimensional scale of the breaking rate function, $C_3$. We use the exponential breaking rate function, but we do experiment with the derivative of this function. As noted in section 4.1, the scaling of the aggregation intensity is arbitrary, and so we scale it so that its formation rate is identical to the formation rate of stress. This scaling eliminates the nondimensional constant $C_5$ from consideration.

The volume flux of the fluid is controlled by a pressure-flux relationship, as discussed thoroughly in Chapter 7. The prescribed pressure gradient across the domain is given by

$$G_p = \frac{12(1 - \theta)}{\theta \text{Re}} \frac{Q}{\text{Re}^\beta},$$

where $Q$ is the flux per unit length, or area flux, defined by

$$Q = \int_0^1 u(0, y) \, dy.$$  \hspace{1cm} (5.20)

The parameter $\theta$ represents the fraction of the actual domain that is represented by the computational domain. By varying its value while keeping the size of the computational domain fixed, effectively the sensitivity of the pressure drop in response to blockage is varied. We keep the value of $\theta$ fixed while exploring other parameters.

5.2.4 Computational Tests

In this section we present three sets of computational tests. In the first set we experiment with the formation, breaking, and activation rates. In the second test we take one of the parameters sets from the first set and run the computation for a longer time. In the final test we show the effect of changing the derivative of the breaking rate function. Results are reported in nondimensional quantities, though times are reported in seconds. To avoid confusion, dimensional quantities are always reported with units.

5.2.4.1 Formation, Breaking, and Activation Rates

We begin by experimenting with the activation rate parameters $C_1$ and $C_{1iz}$; the formation rate, $C_4$; and the scale of the breaking rate, $C_3$. In all these tests the breaking rate function is the exponential function (5.9) with a fixed value of $b = 2$. The value of $\theta$
in the pressure-flux relationship is 0.05. The results are organized by the values of $C_4$ and the ratio $G = C_4/C_3$. The value of $G$ is the number of links per squared concentration of platelets that would form at steady state under no flow conditions. For each pair of values of $C_4$ and $G$, we explore a range of activation rates for activation by ADP and for activation due to the injured zone. We discuss the results of tests for the five pairs of values of $C_4$ and $G$ listed in Table 5.4.

**Test 1: $C_4 = 0.1$, $G = 10$.** The computations were run to nondimensional time 50, real time 0.5 s. Only a small number of links formed over this time period, and the flow was only mildly disturbed by their presence for all of the activation rates tested. In all cases, the number of links that formed was less than 1% of the maximum number that could form under no flow conditions.

The velocity field and location of the threshold level of activator are plotted in Figure 5.9(a) for fast activation rates. It is difficult to see from the vector field, but the velocity is slightly distorted from its undisturbed state. The horizontal velocity profiles for several cross sections of the domain are displayed, for both the fast activation rates and slow activation rates. These plots show that the velocity has been modified due to the small concentration of links, but this distortion is small.

**Test 2: $C_4 = 0.1$, $G = 100$.** For the second test we increase $G$ by a factor of 10 and use the same formation rate as in Test 1. This computation was run until time 0.5 s for a range of activation rates. When the activation rate in the reaction zone was too low ($C_{1iz} \leq 0.1$), there was very little aggregation outside of a region concentrated near the boundary, and the velocity field was not significantly different from its undisturbed state. When the activation rate in the injured zone was increased an aggregate grew along the wall. Results are shown in Figure 5.10.

Contours of the aggregates are displayed in Figure 5.10 (a,b) for a fast activation rate in the injured zone ($C_{1iz} = 1$) and a slow activation rate in response to activator ($C_1 = 0.01$) at two different times in the computation. The plot at time 0.1 s shows that platelets have become activated and a small aggregate is beginning to grow on the wall. Note that the highest concentration of links is downstream from the injured zone.

<table>
<thead>
<tr>
<th>Name</th>
<th>Test 1</th>
<th>Test 2</th>
<th>Test 3</th>
<th>Test 4</th>
<th>Test 5</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_4$</td>
<td>0.1</td>
<td>0.1</td>
<td>1</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>$G$</td>
<td>10</td>
<td>100</td>
<td>10</td>
<td>10</td>
<td>1</td>
</tr>
</tbody>
</table>

**Table 5.4: Values of $C_4$ and $G$ in experiments**
Figure 5.9: In Test 1 there is very little link formation by time 0.5 s. The dashed line denotes where the activator concentration is above threshold. (a) The velocity field is not significantly modified from its initial state, even with the fast activation rates $C_1 = 0.5$ and $C_{1zx} = 1.0$. (b,c) The horizontal velocity profiles are displayed at different cross sections of the domain. The activation rates are (b) $C_1 = 0.01$ and $C_{1zx} = 0.1$ and (c) $C_1 = 0.5$ and $C_{1zx} = 1.0$. The velocity is not significantly modified by the small number of links.
Figure 5.10: Results from Test 2. (a,b) Fast activation rate in the injured zone, $C_{1iz} = 1$, and slow activation from activator, $C_1 = 0.01$. (c,d) Fast activation rate in the injured zone, $C_{1iz} = 1$, and fast activation from activator, $C_1 = 0.5$. (a) Plot at time 0.1 s; $z$ contours are 0.05, 0.08, and 0.2. (b) Plot at time 0.5 s; $z$ contours are 0.05, 1.0, 2.0, and 2.8. (c) Plot at time 0.1 s; $z$ contours are 0.04, 0.1, and 0.26. (d) Plot at time 0.5 s; $z$ contours are 0.05, 1.0, 2.0, and 2.8.
Activator is flowing downstream, but activation from this is slow, and so activator and activated platelets are flowing out of the domain. As can be seen from the plot from time 0.5 s, the aggregate continues to grow, both upstream and downstream. The highest concentration of links is further upstream than its previous location.

In Figure 5.10 (c,d) results are shown for a fast activation rate in the injured zone ($C_{1iz} = 1$) and a fast activation rate in response to activator ($C_1 = 0.5$) at the same times shown for the previous computation. At time 0.1s an aggregate is beginning to grow along the wall, downstream from the injured zone, as in the previous case with the slower activation rate. However, in contrast with the previous case, there is a higher concentration of activated platelets and more links have formed away from the center of the forming aggregate. This response is due to the faster activation rate. At the later time, the aggregate has grown along the wall from the front of the reaction zone all the way to the outflow boundary.

**Test 3: $C_4 = 1$, $G = 10$.** For the third test we increase the link formation rate by a factor of ten over its value from the previous two tests. The value of $G$ is the same value from Test 1. Results with a slow activation rate due to activator are displayed in Figure 5.11(a,b) for a moderate activation rate and fast activation rate in the injured zone, respectively. With this faster formation rate for links, the activated platelets are able to resist the flow quickly and prevent significant aggregation downstream. Note that the aggregate extends further downstream for the lower injury zone activation rate. When the activation rate in the injury zone is low, the first platelets to become activated do not form enough links to resist the flow. These platelets move downstream until they form a sufficient concentration of links to prevent flowing downstream.

The results for moderate and fast activation rates are shown in Figure 5.11(c,d), respectively. In both cases the growth downstream is substantial compared to the case of low activation previously discussed. The results with low activation rates showed that there was less aggregation downstream with a higher activation rate in the injured zone. Once the injured zone is covered by the aggregate, it is the activation rate from activator that controls further growth. When the activation rate is high in the fluid, more platelets become activated and release more activator. The result of this positive feedback is rapid growth of the aggregate. These results are shown at time 0.4 s, rather than at 0.5 s as in (a,b) because the significant aggregation at the outflow boundary eventually caused the solver to fail.
Figure 5.11: Results from Test 3 at time (a,b) 0.5 s and (c,d) 0.4 s. $z$ contours are 0.05, 2, 8.5, and 9.85. (a) Moderate activation in the injured zone ($C_{1iz} = 0.1$) and slow activation from activator ($C_1 = 0.01$). (b) Fast activation in the injured zone ($C_{1iz} = 1$) and slow activation from activator ($C_1 = 0.01$). (c) Fast activation in the injured zone ($C_{1iz} = 1$) and moderate activation due to activator ($C_1 = 0.1$). (d) Fast activation in the injured zone ($C_{1iz} = 1$) and fast activation due to activator ($C_1 = 1$).
Test 4: $C_4 = 10$, $G = 10$. For the fourth test we increase the link formation rate further while maintaining the same value of $G$. The results of this test for both slow and fast activation due to activator are displayed in Figure 5.12. When the activation rate by activator is low, the shape of the resulting aggregate is similar to the shape in Test 3, as can be seen by comparing Figure 5.11(b) to 5.12(a). The obvious difference between these two cases can be seen in the spacing of the contours of $z$, with more links forming in the middle of the aggregate when the formation rate is higher. There are more subtle differences at the upstream and downstream edge of the aggregate. The downstream edge appears smoother for the lower formation rate, and at the upstream edge there is more upstream growth along the boundary for the faster formation rate. This second feature is difficult to see in the plot, but the contour of the activator is clearly extending upstream for the faster formation rate.

When the activation rate from activator is increased, the differences in Test 3 and Test 4 are more distinct, as is seen by comparing Figure 5.11(d) and Figure 5.12(b). When the links form faster, the aggregate does not grow as rapidly downstream. Activated platelets form links quickly enough that they do not flow very far downstream before coming to rest. The upstream growth along the boundary that occurred with the lower activation rate is even more pronounced with this faster activation rate, to the point that the aggregate has reached the upstream boundary.

Test 5: $C_4 = 1$, $G = 1$. In Test 2, it appeared that a small number of links was able to resist the flow. For Test 5, we use the formation rate from Test 3, but increase the breaking rate, so that $G$ is smaller by a factor of 10 than in the previous two tests. In Figure 5.13, the results are shown for fast activation in the injured zone and slow activation from activator. With this lower value of $G$, the aggregate appears to be stretching slowly downstream. Enough links form to slow the flow considerably, but the aggregate does not seem to be able to hold its shape as it is pushed downstream.

5.2.4.2 Longer Simulation

The simulations in the previous section were run no longer than 0.5 s. The formation and breaking rates from Test 3 with slow activation from activator produced an aggregate that covered the injured zone, but did not grow substantially downstream. For this set of parameters ($C_4 = 1, G = 10, C_1 = 0.01, C_{1iz} = 1$), we run until time 2 s to see how the aggregate behaves on a longer time scale. Plots of the aggregate at four different
Figure 5.12: Results from Test 4 with fast activation in the injured zone \((C_{1iz} = 1)\). \(z\) contours are 1, 4, 8.5, and 9.85. (a) Slow activation from activator \((C_1 = 0.01)\) at time 0.5 s. (b) Fast activation from activator \((C_1 = 0.5)\) at time 0.4 s.

Figure 5.13: Results from Test 5 at time 0.5 s. Activation in injured zone is fast \((C_{1iz} = 1)\) and activation due to activator is slow \((C_1 = 0.01)\). \(z\) contours are 0.05, 0.4, and 0.80.
Figure 5.14: Growth simulation with parameters $C_4 = 1$, $G = 10$, $C_1 = 0.01$, and $C_{1iz} = 1$. $z$ contours are 1, 6, and 9.5. Plots of the aggregate at time (a) 0.5 s, (b) 1 s, (c) 1.5 s, and (d) 2 s.
time points are shown in Figure 5.14. The upstream portion of the aggregate is changing very little over this time period, but at the downstream edge, there is a trail of activator emanating from the aggregate that is slowly flowing downstream. By time 2 s, enough links have formed downstream to begin to redirect the flow.

5.2.4.3 Different Breaking Rate

In all of the simulations presented so far, the same breaking rate function was used. Here we present the results of a simulation that illustrates that the form of the breaking rate function can play a significant role in the growth of the aggregate. In order to demonstrate this effect, we perform two simulations in each of which the breaking rate function is the exponential function (5.9), but the value of \( b \) is 0.25 for one simulation and 4 for the other. For both simulations the activation rate in the injury zone is fast, \( C_{1iz} = 1 \), and the activation rate from activator is moderate, \( C_1 = 0.25 \). The formation rate of links is \( C_4 = 1 \) and the value of \( G = 25 \). The value of \( \theta \) in the pressure flux relationship is 0.2. All other parameters are identical to their values from the previous simulations. This parameter set was chosen so that the aggregate would grow vertically quickly, and links would be stretched significantly.

In Figure 5.15 the results of these computations at time 1 s are shown. The shape of the two aggregates is drastically different. When the links break more readily, the aggregate extends significantly downstream from the injured zone, and when the links can sustain more energy, the aggregate grows vertically into the domain. Also shown in Figure 5.15 is the aggregate at time 2 s for the case in which the links are more resistant to breaking. By this time the aggregate has grown large enough to completely block the flow across the domain.

As nonactivated platelets from upstream contact activator near the surface of the aggregate, they become activated and begin to form links. If the links that form are not able to resist the fluid stress, these activated platelet flow downstream. Plots of the energy per bond for these two simulations are displayed in Figure 5.16. For both cases the energy per bond is largest at the upstream end on the top of the aggregate. This is the location at which platelets from upstream are becoming activated. As can be seen in this plot, when the breaking rate increases more slowly with the energy per bond, the links that form can sustain more strain before breaking. When the links break more easily, these platelets detach and flow downstream, where they join the aggregate as it
Figure 5.15: Simulation to compare the effect of different breaking rate. Results are shown at time (a,b) 1 s and time (c) 2 s. \( z \) contours are 1, 5, 10, 15, 20, and 24. Breaking rate is the exponential (5.9) with (a,c) \( b = 0.25 \) and (b) \( b = 4 \).
Figure 5.16: Energy per bond shown at time 1 s. Breaking rate is the exponential (5.9) with (a) $b = 0.25$ and (b) $b = 4$.

grows downstream.

Note that the computational domain used for these simulations is longer than those used in previous computations. The parameters for these simulations were chosen so that the aggregate would grow quickly, and as a result when a shorter domain was used, the aggregate easily reached the outflow boundary. Even with the extended domain, when the breaking rate increased sharply with the energy per bond, the aggregate reached the outflow boundary, and the numerical solver failed due to large forces accumulating at this boundary. In order to compute for a longer time in this case, we artificially reduced the platelet forces near the outflow boundary.

5.2.5 Summary of Experiments

The results from the computational experiments show that a variety of behaviors are possible with the model depending on the parameter values. With the simple model of the injury zone, we were able to produce a simulation in which activated platelets quickly
cover the injury with further aggregate growth occurring more slowly (Test 3, fast injury zone activation and slow activator activation). When this parameter set was used to compute for a longer time, the activator flowing downstream eventually caused growth along the boundary away from the main aggregate.

When the activation rates were sufficiently fast, the aggregate had a tendency to grow upstream and downstream in an uncontrolled manner. Even when the growth seemed contained, the activator flowing downstream eventually caused an aggregate to develop downstream. These results illustrate the need to include a more detailed model of the chemistry involved. In the blood there are other activating chemicals besides ADP, and there are also inhibitors present that might prevent aggregation downstream, away from the injury.

The simulations in which the breaking rate was varied showed that the form of the breaking rate may be important in controlling the growth of the aggregate. When the breaking rate increased quickly with the energy per bond, platelets that were activated at the front of the aggregate were not able to resist the fluid stress, and they flowed downstream and attached where the fluid stresses were lower. When the breaking rate decreased more slowly with the energy per bond, platelets were able to attach at the front of the aggregate where the fluid stresses were high. The parameters used in these simulations were chosen to promote fast aggregation, and so these results are not meant to mimic the actual rate of growth of a platelet aggregate. However these results show that the mechanical strength of links is an important consideration in modeling platelet aggregates.

5.3 Discussion

In this chapter we presented two types of computational experiments. The first type was presented to demonstrate the effects of a nonconstant breaking rate and compare the predictions of the closure model against the full model. The results of these experiments showed that nonconstant breaking rates produce behavior that cannot be realized with a constant breaking rate. The results generated by the closure model do not match the results of the full model exactly. The qualitative results are generally similar, and when the breaking rate function increases slowly or sharply, the quantitative results are also similar. There is a range of moderate increase in the breaking rate function for which the two models differed. Further experiments must be performed in order to understand
why the models differ for this range of breaking rates.

The development of the closure model allowed us to perform a variety of numerical simulations exploring the behavior of the model, which were previously not feasible using the full model. To complete one grab and pull computation, the full model took just under two hours on a 360 Mhz Sun ultra-SPARC2\textsuperscript{TM} processor, but the closure model took just under one minute on the same processor, which is faster by a factor of 120. The longest simulation performed with the closure model (2 s real time or 100,000 time steps) took around 8 hours. Performing this simulation with the full model would take over a month to complete. The fastest processors available to us at the time could perform this computation about three times faster than this estimate. Even with this speed up, performing a vast number of simulations with the full model would take an extremely long time, not counting the number of runs that had to be rerun during the debugging stages of development.

These simulations show that several aspects of this model must be developed further in order to capture the behavior of actual platelet aggregates. The activation chemistry used in all of these simulations was extremely simple, and could easily be improved in future versions of the model. As was discussed previously, the no-slip boundary condition for the fluid at solid boundaries implies that activated platelets at the wall are permanently attached. In reality activated platelets should be transported along the wall until they are able to form a sufficient number of links with the wall to halt this motion. In the computations presented here, we simulated an injured vessel by designating a small region along a portion of the wall where platelets became activated. This method provided a reasonable way to control the location of the aggregation, but as many of the simulations showed there was often substantial growth of the aggregate both upstream and downstream from the injury zone. We conclude that a more detailed model of the interactions with the boundary must be included in future versions of the model.

In all of these simulations, the concentration of activated platelets inside the aggregate was no higher than the concentration of nonactivated platelets present in the plasma, which corresponds to a volume fraction of only 0.3%. Real platelet aggregates consist of densely packed cells, and so the aggregates which grew in the parallel plate simulations cannot represent actual aggregates. This problem with the model is closely related to the problem with the boundary conditions that we have discussed repeatedly. Note that the
Peclet number for platelet transport (see Table 5.3) is extremely large, indicating that platelets are primarily transported by advection. In order for platelets to accumulate to a high density, the platelets forming the aggregate must be stationary while the fluid advects more platelets to this location.

In the current version of the model, platelets move at the local fluid velocity. This assumption seems reasonable at very low volume fractions of platelets, but as the density of platelets increases the model should allow for the fluid to slip past stationary platelets. We believe that treating the blood and platelets as a single phase is restrictive, and multiple phase models should be investigated in the future. For example, in a two phase model the fluid and the platelets would each have a velocity field and the interactions between these two phases would arise as terms in the momentum equations of each fluid. Such a model would not restrict the platelet phase to satisfy the no slip boundary conditions, as in the current version of the model.
CHAPTER 6

NUMERICAL SOLUTIONS OF THE INCOMPRESSIBLE NAVIER-STOKES EQUATIONS

In this chapter we describe the method used to compute numerical solutions of the incompressible Navier-Stokes equations. We also address the accuracy and stability of the method. The particular form of the equations considered is

\[ \begin{align*}
\mathbf{u}_t + \mathbf{u} \cdot \nabla \mathbf{u} &= -\nabla p + \nu \Delta \mathbf{u} + \mathbf{f} \\
\nabla \cdot \mathbf{u} &= 0,
\end{align*} \]

where the nondimensional viscosity \( \nu \) is equal to \( \text{Re}^{-1} \). If one were to naively begin to design a numerical scheme, several challenges would quickly become apparent. Because of the advection terms, the equations are nonlinear. The nonlinearity does complicate the construction of a numerical scheme, but this complication can be handled in a variety of ways, which are discussed later. Another difficulty, which is more specific to these equations, comes from the lack of an evolution equation for the pressure. In incompressible flow the pressure does not evolve, rather, its value is determined to enforce the incompressibility constraint. This idea is the basis of a class of methods called projection methods. In this chapter we provide brief a discussion of projection methods, and discuss some issues related to their implementation.

6.1 Motivation

The following, well-known decomposition theorem helps clarify the role of the pressure in incompressible flow and motivates projection methods.

**Theorem 3 (Hodge decomposition)** Let \( \Omega \) be a smooth, bounded domain, and \( \mathbf{u}^* \) be smooth vector field on \( \Omega \). The vector field \( \mathbf{u}^* \) can be decomposed in the form

\[ \mathbf{u}^* = \mathbf{u} + \nabla \phi, \]

(6.3)
where
\[ \nabla \cdot \mathbf{u} = 0 \text{ in } \Omega, \quad \mathbf{u} \cdot \mathbf{n} = 0 \text{ on } \partial \Omega. \]

We present the elementary proof of the theorem because it is constructive, and thus provides a method for performing this decomposition which can be used to implement a projection method.

**Proof:** Taking the divergence of (6.3) gives the Poisson equation
\[ \Delta \phi = \nabla \cdot \mathbf{u}^*, \quad (6.4) \]
with the boundary condition given by the normal component of (6.3) on the boundary
\[ \frac{\partial \phi}{\partial n} = \mathbf{u}^* \cdot \mathbf{n} \text{ on } \partial \Omega. \quad (6.5) \]

Together equations (6.4) and (6.5) define a Neumann problem for \( \phi \), which has a unique solution, up to an additive constant, provided the solvability condition
\[ \int_\Omega \nabla \cdot \mathbf{u}^* \, dV = \int_{\partial \Omega} \mathbf{u}^* \cdot \mathbf{n} \, dS \quad (6.6) \]
is satisfied. Equation (6.6) is always satisfied, because this is simply the divergence theorem. This defines the gradient part of the decomposition, and the divergence free field is then defined by \( \mathbf{u} = \mathbf{u}^* - \nabla \phi. \)

The preceding proof describes a procedure for decomposing an arbitrary smooth vector field into a gradient field and a divergence free field. Let \( \mathcal{P} \) denote the projection operator that takes vector fields and projects them onto divergence free fields, so that
\[ \mathcal{P} (\mathbf{u}^*) = \mathbf{u}, \]
and
\[ (I - \mathcal{P}) (\mathbf{u}^*) = \nabla \phi. \]
Note that the gradient field and divergence free fields that have zero normal component on the boundary define orthogonal subspaces of \( L^2(\Omega) \). They are clearly subspaces, and orthogonal because
\[
\begin{align*}
\int_\Omega \nabla \phi \cdot \mathbf{u} \, dV &= \int_\Omega \nabla \phi \cdot \mathbf{u} + \phi \nabla \cdot \mathbf{u} \, dV \\
&= \int_\Omega \nabla \cdot (\phi \mathbf{u}) \, dV \\
&= \int_{\partial \Omega} \phi \mathbf{u} \cdot \mathbf{n} \, dS \\
&= 0.
\end{align*}
\]
The requirement that $\mathbf{u} \cdot \mathbf{n} = 0$ on the boundary may be relaxed so that $\mathbf{u} \cdot \mathbf{n} = g$, provided $g$ satisfies

$$
\int_{\partial \Omega} g \, dS = 0.
$$

(6.7)

If $\mathbf{u}$ is interpreted as a velocity field, then the condition (6.7) physically means that the total flux of fluid across the boundary of the domain is zero, which is a consequence of incompressibility. When the boundary conditions are nonhomogeneous, the projection no longer defines a decomposition into orthogonal subspaces. The decomposition also may be applied to periodic velocity fields, with an obvious modification to the proof.

Applying the projection operator to equation (6.1) gives the equation

$$
\mathbf{u}_t = \mathcal{P} \left( -\mathbf{u} \cdot \nabla \mathbf{u} + \nu \Delta \mathbf{u} + \mathbf{f} \right),
$$

(6.8)

in which the pressure has been eliminated. This form is equivalent to the original equations (6.1)–(6.2). The equivalence of these two forms of the equations clarifies the role of the pressure in enforcing incompressibility. The proof of the Hodge decomposition is suggestive of a scheme for advancing the velocity and pressure in time: advance the momentum equation (6.1) to determine an intermediate velocity which is not required to be divergence free. Then to find the velocity at the new time, project the intermediate velocity field onto the space of divergence free fields, and use the gradient part of the projection to update the pressure.

### 6.2 Implementing Accurate Projection Methods

The first projection methods were pioneered by Chorin [9, 10]. Chorin’s original method is first order accurate in space and time. The next generation of projection methods proposed various ways to obtain a velocity which is second order accurate in space and time, but a pressure that is only first order accurate [5, 42]. In the same time period, Kim and Moin [24] proposed a method in which the pressure is excluded from the computation, but with a modification to the boundary conditions, they obtain a second order accurate velocity field. Interestingly, they do mention how the pressure can be recovered from their computation, and this pressure turns out to be second order accurate, provided the result is interpreted at the proper temporal location [8].

Other variations of the original projection method have been utilized. One such modification that we will discuss in detail is the approximate projection method [3, 33].
The idea of the approximate projection method is to relax the condition that the velocity field be divergence free, rather the velocity field that results is approximately divergence free. The utility of such methods is discussed below when we consider the different spatial discretizations.

6.2.1 Temporal Discretization

A second order time discretization of the momentum equation (6.1) is

\[
\frac{u^{n+1} - u^n}{\Delta t} + g^{n+1/2} = -\nabla p^{n+1/2} + \frac{\nu}{2} (\Delta u^n + \Delta u^{n+1}),
\]

(6.9)

where \( g^{n+1/2} \) represents some approximation to the nonlinear, advection terms at the half time level, and we have set the external forces to zero for convenience. We discuss the form of \( g^{n+1/2} \) in a later section. Let \( q \) be some approximation for the pressure that can be computed from the variables at the current time level. The projection method seeks a solution to (6.9), by first solving the equation

\[
\frac{u^* - u^n}{\Delta t} + g^{n+1/2} = -\nabla q + \frac{\nu}{2} (\Delta u^n + \Delta u^*),
\]

(6.10)

for an intermediate velocity \( u^* \). The velocity \( u^* \) is a solution to the discrete momentum equation, but it is not divergence free. Using the Hodge decomposition theorem, we know that \( u^* \) can be decomposed as

\[
u^* = u^{n+1} + \Delta t \nabla \phi,
\]

(6.11)

where \( u^{n+1} \) is divergence free. The factor of \( \Delta t \) is not required, but its relevance is clarified in the discussion of the pressure. Proceeding as in the proof of the decomposition, the divergence of this equation and the normal component on the boundary give the Poisson problem

\[
\Delta t \Delta \phi = \nabla \cdot u^*,
\]

(6.12)

with Neumann boundary conditions

\[
\Delta t \frac{\partial \phi}{\partial n} = (u^* - u^{n+1}) \cdot \hat{n}.
\]

(6.13)

Once \( \phi \) is known, the divergence free velocity is then found by computing

\[
u^{n+1} = u^* - \Delta t \nabla \phi.
\]

(6.14)

Note that there are no prescribed boundary conditions for the intermediate velocity \( u^* \). Often the boundary conditions for \( u^{n+1} \) are used for \( u^* \). A thorough discussion on boundary conditions can be found in [8].
We now discuss the computation of the pressure following the approach of [8]. The variable \( q \) represents some approximation to the pressure at time level \( n + 1/2 \). Some choices for \( q \) that have been used in methods that produce a second order accurate approximation to the velocity are \( q = 0 \) [24], \( q = p^n \) [42], and \( q = p^{n-1/2} \) [5]. We consider the case \( q = p^{n-1/2} \); the formulas for the other cases can be derived by straightforward modifications to the following arguments. To derive a formula for updating the pressure, use equation (6.11) to eliminate the intermediate velocity in equation (6.10) to obtain
\[
\frac{u^{n+1} - u^n}{\Delta t} + g^{n+1/2} = -\nabla p^{n-1/2} - \nabla \phi + \frac{\nu \Delta t}{2} \Delta \nabla \phi + \frac{\nu}{2} (\Delta u^n + \Delta u^{n+1}). \tag{6.15}
\]
Comparison with equation (6.9) suggests defining
\[
\nabla p^{n+1/2} = \nabla p^{n-1/2} + \nabla \phi - \frac{\nu \Delta t}{2} \Delta \nabla \phi. \tag{6.16}
\]
Commuting the Laplacian and the gradient operators gives the pressure update formula
\[
p^{n+1/2} = p^{n-1/2} + \phi - \frac{\nu \Delta t}{2} \Delta \phi. \tag{6.17}
\]
Using equation (6.12), this can be written as
\[
p^{n+1/2} = p^{n-1/2} + \phi - \frac{\nu}{2} \nabla \cdot u^*. \tag{6.18}
\]
Often, one is only interested in the velocity field, and the accuracy of the pressure is not important, as long as the accuracy of the velocity field is sufficiently high. As it turns out, this pressure update formula produces a second order accurate pressure, but a more common pressure update formula is
\[
p^{n+1/2} = p^{n-1/2} + \phi. \tag{6.19}
\]
This update formula gives a first order accurate pressure, but maintains the second order accuracy of the velocity.

### 6.2.2 Spatial Discretization

We discuss regular (equally spaced) finite difference spatial discretizations of a rectangular domain. All of these discretizations partition the domain into some number of equal sized squares. The discretizations differ in where on the domain the discrete data are located. Two standard discretizations are the vertex (or node)-centered grid and the cell-centered grid. On the vertex-centered grid, all discrete variables are located on the
vertices of the squares. For the cell-centered grid, all data are located at the centers of
the squares. See Figure 6.1 for examples of both grids.

In order to perform a discrete projection, we proceed as in the proof of the Hodge
decomposition. Let \( u_{i,j} = (u_{i,j}, v_{i,j}) \) be a discrete velocity at the grid point indexed by
\((i,j)\), and let \( \phi_{i,j} \) be a discrete scalar located at the same grid point. Let \( D \) and \( G \) be
the discrete divergence and gradient operators, on either grid. Second order accurate
operators are

\[
(Du)_{i,j} = \frac{u_{i+1,j} - u_{i-1,j}}{2h} + \frac{v_{i,j+1} - v_{i,j-1}}{2h},
\]

(6.20)

and

\[
(G\phi)_{i,j} = \left( \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2h}, \frac{\phi_{i,j+1} - \phi_{i,j-1}}{2h} \right).
\]

(6.21)

To decompose the discrete velocity \( u^* \) into a discretely divergence free field and a discrete
gradient field, we seek \( u \) and \( \phi \) such that

\[
u^* = u + \Delta t G\phi
\]

(6.22)

\[
Du = 0.
\]

(6.23)

Applying \( D \) to both sides of (6.22), and using (6.23) we obtain the equation

\[
Du^* = \Delta t DG\phi = \Delta t L^w \phi.
\]

(6.24)

This equation can be solved to find \( \phi \), which then defines \( u \) using (6.22).

![Figure 6.1: Examples of (a) vertex-centered grid and (b) cell-centered grid. All data are located at the black dots.](attachment:figure6.1.png)
The operator $L^w$ represents a discrete approximation to the Laplacian. The superscript $w$ is used to denote the fact that the stencil for the operator is wide. The form of $L^w$ at point $i,j$ is

$$
(L^w \phi)_{i,j} = \frac{\phi_{i-2,j} + \phi_{i+2,j} - 4\phi_{i,j} + \phi_{i,j-2} + \phi_{i,j+2}}{4h^2}.
$$

The wide stencil for the discrete Laplacian creates some difficulties that are absent when working with the more standard, compact Laplacian

$$
(L \phi)_{i,j} = \frac{\phi_{i-1,j} + \phi_{i+1,j} - 4\phi_{i,j} + \phi_{i,j-1} + \phi_{i,j+1}}{h^2}.
$$

For example, suppose that the domain is periodic in both directions. When solving equation (6.24) the problem decouples into four separate subgrids on each of which $i$ and $j$ are either even or odd. This decoupling can give rise to instabilities because of differences between the grids. If the domain is not periodic, then these grids are coupled near the boundary. The wide stencil requires modification at two rows adjacent to the boundary, which also makes implementing a multigrid method more difficult.

Another grid structure which is commonly used for projection methods is the MAC (or staggered) grid, which was introduced by Harlow and Welch [20]. On the MAC grid the horizontal velocities are stored at vertical edges, the vertical velocities are stored at horizontal edges, and scalar quantities are stored at cell centers. An example is displayed in Figure 6.2. The discrete divergence is

$$
(Du)_{i,j} = \frac{u_{i+1/2,j} - u_{i-1/2,j}}{h} + \frac{v_{i,j+1/2} - v_{i,j-1/2}}{h},
$$

and the discrete gradient is $G \phi = (G_1 \phi, G_2 \phi)$, where the first component is defined by

$$
(G_1 \phi)_{i-1/2,j} = \frac{\phi_{i,j} - \phi_{i-1,j}}{h},
$$

and the second component is defined by

$$
(G_2 \phi)_{i,j-1/2} = \frac{\phi_{i,j} - \phi_{i,j-1}}{h}.
$$

Applying this divergence to the equation (6.22), with the gradient being the MAC gradient, gives the equation

$$
Du^* = \Delta t DG \phi = \Delta t L \phi.
$$

The operator $L$ is again a discrete approximation to the Laplacian, but it has the compact stencil given in (6.26). When solving equation (6.30), there is no decoupling of grids and handling the boundary conditions is straightforward.
Figure 6.2: Example of the MAC grid discretization. Velocities fields are stored at the edges of the cell perpendicular to the component of the velocity, and pressure (and other scalars) are stored at the cell centers.

The projection may seem more natural on the MAC grid, but it is sometimes useful to use a vertex- or cell-centered grid. As we discuss later, a popular method for computing the nonlinear terms requires that the velocities be on a cell-centered grid. Either of these other grid structures requires the use of the wide Laplacian to enforce the divergence free constraint. If, however, the constraint that the velocity be exactly divergence free is relaxed so that it is required that the velocity be only approximately divergence free, the use of the wide Laplacian can be avoided. Such methods are referred to as approximate projections, for obvious reasons. Suppose that a vertex- or cell-centered grid is being used. In the projection step equation (6.30) is solved instead of equation (6.24). The velocity $u$ that results is not exactly divergence free, but its divergence is order $h^2$ because this is a second order discretization of equation (6.4).

### 6.2.3 Nonlinear Terms

The nonlinear, advective terms can be approximated in a variety of ways. In Chorin’s original method [9, 10], the momentum equation (6.10) is solved using an ADI scheme with the nonlinear terms approximated as

$$u^n \cdot \nabla u^*.$$  

(6.31)

Of course this is only first order accurate in time and must be modified to get a second order scheme. Van Kan [42] uses the approximation
\[ \frac{1}{2} (u^n \cdot \nabla u^* + u^* \cdot \nabla u^n), \]  
which results in a second order scheme, and still only requires linear solves.

Another popular method of computing the nonlinear terms is to extrapolate them in time from past velocities. The simple method used by Kim and Moin is

\[ (u \cdot \nabla u)^{n+1/2} = \frac{3}{2} (u^n \cdot \nabla u^n) - \frac{1}{2} (u^{n-1} \cdot \nabla u^{n-1}) + O(h^2). \]  

Another very different extrapolation method was used by Bell \textit{et al.} [5], which is particularly useful for high Reynolds number flow. This method is based on high-resolution upwinding methods, which require that the cell-centered grid be used. As discussed previously, this grid structure complicates the projection step, and so this situation is ideal for an approximate projection.

A recent variation on the method of using high order upwinding is to employ time splitting to treat the advection separately [26]. In this approach, the cell-centered velocity is advected by an exactly divergence free edge velocity. At the beginning of the time step, the homogeneous advection equation

\[ u_t + u^e \cdot \nabla u = 0, \]  
is advanced one time step using the method described in [29], as implemented in the software package [27]. The cell-centered velocity is then used in place of \( u^n \) in the momentum equation to solve for \( u^* \). Because the advection is treated separately, this momentum equation is linear. The intermediate velocity is then averaged to the cell edges, and a MAC projection is performed to get the new cell edge velocity that is divergence free. The cell-centered velocity is then obtained by averaging the gradient from the MAC projection to the cell centers, and subtracting this average gradient from \( u^* \).

### 6.2.4 Comparison of Methods

A recent paper by Brown \textit{et al.} [8] removes much of the confusion surrounding the boundary conditions and the pressure in projection methods. In particular they analyze the accuracy of both the velocity and pressure for various combinations of pressure approximations, pressure update formulas, and boundary conditions on the intermediate velocity. Their analysis is done for a system with discrete time and continuous space. Using an approximate projection method, they generate numerical results that support their analysis. So as long as the spatial operators are discretized to sufficiently high order,
the results from [8] predict that full second order accuracy in the velocity and pressure are attainable.

We briefly summarize their results on the accuracy of projection methods. As discussed previously, let \( q \) represent the approximation to the pressure that is used in the momentum equation. The three methods considered are

1. Projection Method I (PM I) – The pressure gradient is lagged in the momentum equation, \( q = p^{n-1/2} \). The pressure is updated by \( p^{n+1/2} = p^{n-1/2} + \phi \).

2. Projection Method II (PM II) – The pressure gradient is again lagged in the momentum equation, \( q = p^{n-1/2} \), but the pressure is updated by \( p^{n+1/2} = p^{n-1/2} + \phi - \frac{\nu \Delta t}{2} \Delta \phi \).

3. Projection Method III (PM III) – The pressure gradient is not present in the momentum equation, \( q = 0 \). The pressure is not updated, rather is is computed by \( p^{n+1/2} = \phi - \frac{\nu \Delta t}{2} \Delta \phi \).

The time accuracy of each method is analyzed using normal mode analysis. Suppose that the intermediate velocity satisfies the boundary conditions that are prescribed for the velocity at the next time step. Then this analysis predicts that PM I gives globally second order velocities in time, but the pressure contains a numerical boundary layer making it only globally first order accurate. PM II is predicted to be globally second order accurate in both the velocity and the pressure. In order to achieve second order accuracy for PM III, the tangential component of the intermediate velocity on the boundary must be modified to depend on \( \phi \) from the previous time step.

We have found that projection method II is extremely sensitive to the spatial discretization, becoming unstable with certain discretizations. In this paper we further explore the stability of the methods analyzed in [8] by considering the spatial discretization. Specifically we will compare the stability properties of the three projection methods PM I–III using an exact projection on a MAC grid and an approximate projection on a cell-centered grid.

### 6.3 Stability Analysis

In order to explore the stability of the various discretizations, we consider a seemingly trivial problem: the time-dependent, one-dimensional Stokes equations with homogeneous boundary conditions on the velocity and no external body forces. Although this problem
seems trivial, it describes how one-dimensional perturbations evolve when solving the time dependent Stokes equations. Consider a perturbation from \((u, p) = 0\) to the horizontal velocity and the pressure that only varies in the \(x\)-direction. The system analyzed here describes how this error propagates in projection methods depending on the discretization. The discrete time system for projection methods I and II is

\[
\frac{u^* - u^n}{\Delta t} = -\partial_x p^{n-1/2} + \frac{\nu}{2} \partial_{xx} (u^* + u^n) \tag{6.35}
\]

\[
\Delta t \partial_{xx} \phi = \partial_x u^* \tag{6.36}
\]

\[
u^n + 1 = u^* - \Delta t \partial_x \phi \tag{6.37}
\]

\[
p^{n+1/2} = p^{n-1/2} + \phi - \chi \frac{\nu}{2} \partial_x u^* , \tag{6.38}
\]

where \(\chi\) is 0 for PM I or 1 for PM II. In order for a discretization to be stable, the solution to this system must decay to zero for any initial data.

Projection method III is treated separately because the pressure from one time step does not affect the velocity or the pressure at the next time step. This simplifies the stability analysis considerably, because we only need to study how errors propagate in the velocity. The discrete time system for PM III is

\[
\frac{u^* - u^n}{\Delta t} = \frac{\nu}{2} \partial_{xx} (u^* + u^n) \tag{6.39}
\]

\[
\Delta t \partial_{xx} \phi = \partial_x u^* \tag{6.40}
\]

\[
u^n + 1 = u^* - \Delta t \partial_x \phi \tag{6.41}
\]

\[
p^{n+1/2} = \phi - \frac{\nu}{2} \partial_x u^* , \tag{6.42}
\]

### 6.3.1 Stability on MAC Grid

We first discretize space using the MAC discretization, which means that the velocities are stored at cell edges and the pressure is stored at the cell centers. Divide the domain into \(N\) cells of equal size, and so the width of each cell is \(h = 1/N\). There are \(N\) unknowns for the pressure (one for each cell) and \(N - 1\) unknowns for the velocity (\(N + 1\) cell edges with two of the values given). The discrete Laplacian applied to the velocity, \(L_d\), is defined in the usual manner

\[
(L_d u)_j^{1/2} = \frac{u_{j-3/2} - 2u_{j-1/2} + u_{j+1/2}}{h^2}, \tag{6.43}
\]

where the subscript \(d\) signifies that the velocity satisfies homogeneous Dirichlet boundary conditions. The discrete divergence operator is defined as

\[
(D u)_j = \frac{u_{j+1/2} - u_{j-1/2}}{h}. \tag{6.44}
\]
For both of these operators, the boundary conditions $u_{1/2} = u_{N+1/2} = 0$ are used to define the operators at locations adjacent to the boundary. The gradient operator is just the negative of the adjoint of the divergence,

$$G = -D^T,$$  \hfill (6.45)

and the Laplacian used in the projection is

$$L_n = DG,$$  \hfill (6.46)

where the subscript $n$ signifies that this Laplacian reflects the homogeneous Neumann boundary conditions used in the projection. Note that there are no boundary conditions implied by $G$. With these discrete operators, equations (6.35)–(6.38) for PM I and PM II are discretized to

$$\frac{u^* - u^n}{\Delta t} = -Gp^{n-1/2} + \frac{\nu}{2}L_d (u^* + u^n)$$  \hfill (6.47)

$$\Delta t L_n \phi = Du^*$$  \hfill (6.48)

$$u^{n+1} = u^* - \Delta t G \phi$$  \hfill (6.49)

$$p^{n+1/2} = p^{n-1/2} + \phi - \chi \frac{\nu}{2} Du^*.$$  \hfill (6.50)

In order to analyze the stability of this system, we diagonalize the equations (6.47)–(6.48), eliminate the intermediate variables to find the linear operator that advances velocity and pressure in time, and then find the eigenvalues of this operator. For $j = 1 \ldots (N - 1)$ and $m = 0 \ldots (N - 1)$, the $j^{th}$ component of the $m^{th}$ eigenvector of $L_d$ is

$$s_j^{(m)} = \sin (m \pi h j),$$  \hfill (6.51)

with corresponding eigenvalue

$$\lambda^{(m)} = -\frac{4}{h^2} \sin^2 \left( \frac{m \pi h}{2} \right).$$  \hfill (6.52)

The form of the eigenvalues of $L_n$ is the same as for $L_d$, but the eigenvectors are

$$c_j^{(m)} = \cos \left( m \pi h (j - 1/2) \right),$$  \hfill (6.53)

for $m = 0 \ldots (N - 1)$ and $j = 1 \ldots N$. The discrete divergence and gradient map these sets of eigenvectors to each other in the following manner

$$D s_j^{(m)} = \frac{2}{h} \sin \left( \frac{m \pi h}{2} \right) c_j^{(m)},$$  \hfill (6.54)
\[ G c^{(m)} = -\frac{2}{h} \sin \left( \frac{m \pi h}{2} \right) s^{(m)}. \]  

Let \( S \) be the orthonormal matrix with column \( m \) given by the normalized \( s^{(m)} \), and let \( C \) be the orthonormal matrix with column \( m = 1 \ldots (N - 1) \) given by the normalized \( c^{(m)} \), and column \( N \) given by the normalized \( c^{(0)} \). Make the changes of coordinates 
\[
\begin{align*}
    u &= S^T \tilde{u}, & u^* &= S^T \tilde{u}^*, & p &= C^T \tilde{p}, & \phi &= C^T \tilde{\phi}
\end{align*}
\]

in equations (6.47)-(6.48). Then multiplying equations (6.48) and (6.50) on the left by \( C \) and equations (6.47) and (6.49) by \( S \), we diagonalize the equations.

The \( m \)th set of equations is
\[
\begin{align*}
    \frac{\tilde{u}^*_m - \tilde{u}^*_m}{\Delta t} &= 2 \frac{\sin \left( \frac{m \pi h}{2} \right)}{h} \tilde{p}^{n-1/2}_m - 2 \nu \frac{\sin^2 \left( \frac{m \pi h}{2} \right)}{h^2} \tilde{\phi}^*_m + \left(\tilde{u}^*_m + \tilde{u}^*_m\right) \\
    - \frac{4 \Delta t}{h^2} \sin^2 \left( \frac{m \pi h}{2} \right) \tilde{\phi}^*_m &= 2 \frac{\sin \left( \frac{m \pi h}{2} \right)}{h} \tilde{u}^*_m \\
    \tilde{u}^*_m &= \tilde{u}^*_m + \frac{2 \Delta t}{h} \sin \left( \frac{m \pi h}{2} \right) \tilde{\phi}^*_m \\
    \tilde{p}^{n+1/2}_m &= \tilde{p}^{n-1/2}_m + \tilde{\phi}^*_m - \nu \frac{\sin \left( \frac{m \pi h}{2} \right)}{h} \tilde{u}^*_m.
\end{align*}
\]

Equation (6.57) can be solved for \( \tilde{u}^* \), and equation (6.58) can be solved for \( \tilde{\phi}^*_m \). After eliminating \( \tilde{u}^* \) and \( \tilde{\phi}^*_m \), for each \( m \) we obtain a 2x2 matrix \( X_m \) which maps \((\tilde{u}^*_m, \tilde{p}^{n-1/2}_m)^T\) to \((\tilde{u}^*_m+1, \tilde{p}^{n+1/2}_m)^T\). The eigenvalues of these matrices determine the stability of the discretization. Solving equation (6.58) for \( \tilde{\phi}^*_m \) and substituting this into equation (6.59), we see that 
\[ \tilde{u}^*_{m+1} = 0. \]  

This means that errors introduced at some time step in the velocity or pressure do not propagate to the velocity at the next time step. The first row of \( X_m \) is entirely zero for all \( m \), which means that \( X_m \) is lower triangular, and so to determine the stability, we need to examine only \( x_{22} \).

After some algebraic manipulations using equations (6.57)-(6.60), we find 
\[ x_{22} = \frac{(1 - \chi) \frac{2 \nu \Delta t}{h^2} \sin^2 \left( \frac{m \pi h}{2} \right)}{1 + 2 \frac{\nu \Delta t}{h^2} \sin^2 \left( \frac{m \pi h}{2} \right)}. \]

If PM II is used (\( \chi = 1 \)), then all the eigenvalues of \( X_m \) are zero, and \( X^2_m = 0 \) for any \( m \). Because \( x_{21} \neq 0 \), errors introduced in the velocity at a time step appear in the pressure
of the following time step, but do not appear in either the velocity or pressure in the time step after that. For PM I \((\chi = 0)\), the method is still stable, because all the eigenvalues are less than one in magnitude.

Equations (6.58) and (6.59) are the same for projection method III. Again \(a_{m}^{n+1} = 0\), and because the pressure does not propagate, it need not be considered for stability. Therefore all three projection methods are stable on the MAC grid.

### 6.3.2 Stability on a Cell-centered Grid: Approximate Projection

We now consider the case of an approximate projection on a cell-centered grid. In this case the pressure and velocity are both stored at the cell centers. The discrete space and time system is similar to (6.47)-(6.50), but the operators must be appropriately modified near the boundary. A common way of handling boundary conditions on cell-centered grids is to use “ghost cells,” which are cells outside the physical domain whose value is set so that the difference operators need not be modified near the boundary. For example, the ghost cell value for the velocity at the left boundary is set to be \(u_{1} = -u_{1}\), which corresponds to linearly extrapolating the velocity from the physical boundary condition and the first interior point. The ghost cell value for \(\phi\) at the left boundary is set by \(\phi_{-1} = \phi_{1}\), which is a discretization of the homogeneous Neumann boundary condition that \(\phi\) satisfies.

For projection methods I and II, there is some ambiguity as to how the pressure gradient is computed at the cell adjacent to the physical boundary, because there are no boundary conditions for the pressure. For projection method I, the pressure gradient does not need to be computed from the pressure; it can simply be updated. In this case the computed pressure is forced to have constant normal derivative in time near the boundary, as a consequence of the boundary conditions used in the projection.

For projection method II, there is ambiguity near the boundary whether one chooses to update the gradient or the pressure. Updating the gradient requires computing the Laplacian of the gradient of \(\phi\). The normal component of the gradient is zero on the boundary, and this can be used in computing the Laplacian of the normal component of the gradient near the boundary. However, there are no boundary conditions for the tangential component of the gradient of \(\phi\). On the other hand, if the pressure is to be updated, it must then be differenced, but there are no boundary conditions for the pressure for use in a difference formula. It seems that either a one-sided difference must
be used near the boundary, or a lower order error must be introduced.

We analyze the case in which the pressure is updated and then differenced. Suppose that centered differencing is used to compute the gradient away from the boundary. One way to think of the gradient near the boundary is to use ghost cell values as for the velocity, but because there are no physical boundary conditions for the pressure, the value must be extrapolated using data only from the interior cells. Then the standard centered difference operator can be applied at the first interior cell to compute the gradient, but the resulting gradient is effectively a one-sided derivative whose form is determined by the manner in which the ghost cell value has been set. Some possible polynomial extrapolations and the resulting gradients are given in Table 6.1. We refer to these gradients as gradient 0, gradient 1, and gradient 2, to denote their accuracy (or order of polynomial extrapolation used for the ghost cells).

6.3.2.1 Constant Extrapolation

We repeat the procedure used to analyze the stability on the MAC grid, but only for the case of constant extrapolation. This gradient is used for analysis because the resulting system can be diagonalized, while this is not true for the other gradients. Also note that with this choice of extrapolation, the gradient applied to the pressure is the same gradient applied to \( \phi \) because the constant extrapolation formula is identical to the discretization of the homogeneous Neumann boundary condition. Even though our analysis is restricted to just one of the many possible gradients, it is still very informative because it gives information about how the stability is affected by using an approximate projection and the high order pressure correction. All of the gradients are identical at the interior points, and so because they differ only at points near the boundary, they can be viewed as perturbations of one another.

The operator \( L_n \) is the same operator used on the MAC grid. The eigenvalues of \( L_d \) are given by (6.52), but the eigenvectors on the cell-centered grid are

<table>
<thead>
<tr>
<th>type</th>
<th>ghost cell formula</th>
<th>gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>constant</td>
<td>( p_0 = p_1 )</td>
<td>( (p_2 - p_1)/2h )</td>
</tr>
<tr>
<td>linear</td>
<td>( p_0 = 2p_1 - p_2 )</td>
<td>( (p_2 - p_1)/h )</td>
</tr>
<tr>
<td>quadratic</td>
<td>( p_0 = 3p_1 - 3p_2 + p_3 )</td>
<td>( (-p_3 + 4p_2 - 3p_1)/2h )</td>
</tr>
</tbody>
</table>
for \( m = 1 \ldots N \) and \( j = 1 \ldots N \). The discrete divergence is computed by centered differencing everywhere, with the ghost cell values outside the domain set by \( u_0 = -u_1 \) to correspond to the homogeneous Dirichlet boundary conditions. This divergence operator applied to the eigenvectors of \( L_d \) gives
\[
Ds^{(m)} = \frac{1}{h} \sin (m\pi h) e^{(m)}.
\] (6.64)

The discrete gradient is also computed by centered differencing everywhere, with the ghost cells set by \( \phi_0 = \phi_1 \), which can be interpreted either as discretizing the homogeneous Neumann boundary condition or as constant extrapolation. This discrete gradient acting on the eigenvectors of \( L_n \) gives
\[
Ge^{(m)} = -\frac{1}{h} \sin (m\pi h) s^{(m)}.
\] (6.65)

Again define the matrices \( S \) and \( C \) as for the MAC grid, and make the transformations
\[
u = S^T \hat{u}, \quad u^* = S^T \hat{u}^*, \quad p = C^T \hat{p}, \quad \phi = C^T \hat{\phi}.
\] (6.66)

The \( m \)th set of equations is
\[
\frac{\hat{u}_m - \hat{u}_m^n}{\Delta t} = \frac{1}{h} \sin (m\pi h) \hat{p}_m^{n-1/2} - \frac{2\nu}{h^2} \sin^2 \left( \frac{m\pi h}{2} \right) (\hat{u}_m^* + \hat{u}_m^n) \]
\[
- \frac{4\Delta t}{h^2} \sin^2 \left( \frac{m\pi h}{2} \right) \hat{\phi}_m = \frac{1}{h} \sin (m\pi h) \hat{\phi}_m
\] (6.67)
\[
\hat{u}_m^{n+1} = \hat{u}_m^n + \Delta t \frac{1}{h} \sin (m\pi h) \hat{\phi}_m
\] (6.68)
\[
\hat{p}_m^{n+1/2} = \hat{p}_m^{n-1/2} + \hat{\phi}_m - \frac{\nu}{2h} \sin (m\pi h) \hat{u}_m^n.
\] (6.69)

From this system we eliminate the intermediate variables \( \hat{u}_m^* \) and \( \hat{\phi}_m \), and obtain, after algebraic manipulations,
\[
\begin{bmatrix}
\hat{u}_m^{n+1} \\
\hat{p}_m^{n+1/2}
\end{bmatrix} =
\begin{bmatrix}
\frac{(1 - a)}{(1 + a)} s^2 & \frac{scba}{(1 + a)} \\
\frac{-sc(1 - a)(1 + \chi a)}{ba(1 + a)} & \frac{s^2 + a(1 - \chi c^2)}{(1 + a)}
\end{bmatrix}
\begin{bmatrix}
\hat{u}_m^n \\
\hat{p}_m^{n-1/2}
\end{bmatrix},
\] (6.71)

where
\[
a = \frac{2\nu \Delta t}{h^2} \sin^2 \left( \frac{m\pi h}{2} \right), \quad b = \frac{h}{\nu}, \quad s = \sin \left( \frac{m\pi h}{2} \right), \quad c = \cos \left( \frac{m\pi h}{2} \right).
\]

Let the matrix that maps \( (\hat{u}_m^n, \hat{p}_m^{n-1/2})^T \) to \( (\hat{u}_m^{n+1}, \hat{p}_m^{n+1/2})^T \) be denoted by \( X_m \).
We now compute the eigenvalues of each $X_m$ to show that they are less than one in magnitude, making the scheme stable for both the standard pressure update and the higher order correction. The trace and determinant of $X_m$ are

$$\text{Tr}(X_m) = \frac{2s^2 + a(1 - s^2)(1 - \chi)}{(1 + a)}, \quad \text{det}(X_m) = \frac{(1 - a)s^2}{(1 + a)} \quad (6.72)$$

The characteristic polynomial for $X_m$ is

$$\lambda^2 - \text{Tr}\lambda + \text{det} = 0. \quad (6.73)$$

The roots of this equation are either real, or a complex conjugate pair. If the roots are complex, then their squared magnitude is equal to the determinant, which is less than one. Therefore if the roots are complex, they must have magnitude less than one. Now suppose that the roots are real. The graph of the characteristic polynomial is just a parabola with its vertex at $\text{Tr}/2$, which is positive. This implies that there must be at least one positive root, and if it is less than one, then the smaller root must be greater than negative one. It is sufficient to examine only the larger root. Note that it is also sufficient to consider the case of $\chi = 0$ (PM I), because the trace is larger than for $\chi = 1$ (PM II).

For the case $\chi = 0$, the larger eigenvalue is given by

$$\lambda = \frac{1}{2} \left( \frac{(2 - a)s^2 + a}{(1 + a)} + \sqrt{\left(\frac{(2 - a)s^2 + a}{(1 + a)^2}\right)^2 - 4\frac{(1 - a)s^2}{(1 + a)}} \right). \quad (6.74)$$

Simplifying under the square root gives

$$\lambda = \frac{1}{2(1 + a)} \left( p_1(s^2) + \sqrt{p_2(s^2)} \right), \quad (6.75)$$

where

$$p_1(r) = (2 - a)r + a,$$

and

$$p_2(r) = (2 - a)^2r^2 + 2(a^2 + 2a - 2)r + a^2.$$ 

Note that $s$ is in the range $[0, 1]$. If $a \leq 2$, then both $p_1$ and $p_2$ attain their maximum on $[0, 1]$ at 1. And so,

$$\lambda \leq \frac{1}{2(1 + a)} \left( p_1(1) + \sqrt{p_2(1)} \right) = 1 \quad \text{for} \quad a \leq 2. \quad (6.76)$$
Now consider the case of \( a > 2 \). It turns out that the maximum value of \( \lambda \) is again obtained at \( s^2 = 1 \), but it is a little more difficult to show this. Denote \( s^2 \) by \( r \). A straightforward computation shows that
\[
\frac{\partial^2 \lambda}{\partial r^2} = \frac{-2(2a - 1)(a - 1)}{(p_2(r))^{3/2}} < 0, \quad \text{since } a > 2,
\]
which means that the derivative of \( \lambda \) with respect to \( r \) is a decreasing function. The minimum value of the derivative of \( \lambda \) is obtained at \( r = 1 \), which is
\[
\left. \frac{\partial \lambda}{\partial r} \right|_{r=1} = \frac{1}{2a} > 0.
\]
Together (6.77) and (6.78) imply that \( \lambda \) is an increasing function of \( r \) on \([0, 1]\), and so we have shown that
\[
\lambda \leq \frac{1}{2(1+a)} \left( p_1(1) + \sqrt{p_2(1)} \right) = 1 \quad \text{for } a > 2.
\]
Therefore all the eigenvalues are less than or equal to one in magnitude, and both PM I and PM II are stable.

Showing projection method III is stable is very easy. We can use the results from above by assuming that \( \hat{p}^{n-1/2} \) is zero. Therefore, the element of \( X_m \) in the first row and column is all that is needed to determine the stability. This element is always less than 1 in magnitude, and therefore PM III is also stable.

### 6.3.2.2 Higher Order Gradients

As we proved in the previous section, setting the ghost cell values for the pressure using constant extrapolation produced a stable scheme for all projection methods. This analysis did not consider the accuracy of such an approach. The gradient that results is zeroth order accurate near the boundary, and as we shall see later in a numerical test, the pressure is not second order accurate for PM II. A more accurate extrapolation, and hence gradient, must be used near the boundary to produce a second order scheme. For PM III, the pressure gradient never needs to be computed, and so the discussion that follows only applies to PM I and PM II.

When using a different gradient for the pressure, we were unable to diagonalize the resulting system as was done when constant extrapolation was used. All of the gradients are identical to the one analyzed away from the boundary, but differ at grid points adjacent to the boundary. We consider other gradients as localized perturbations to the
gradient that was analyzed in the previous section. We can gain insight into the stability of these schemes by examining how sensitive the previous scheme is to perturbations.

In the previous section, we showed that the eigenvalues were an increasing function of the parameter $s^2 \in [0, 1]$. Recall that

$$s = \sin \left( \frac{m\pi h}{2} \right),$$

and so $s$ near 1 corresponds to $m$ near $1/h = N$. The eigenvalues are thus an increasing function of the frequency, $m$, of the eigenfunctions. We examine the structure of the matrices $X_m$ for large $m$. In particular, we examine $X_{N-1}$, so that $mh = 1 - h$, and we expand $X_{N-1}$ in a Taylor series for small $h$ to obtain

$$X_{N-1} = \begin{bmatrix} -1 + \left( \frac{\nu \Delta t \pi^2 + 4}{4\nu \Delta t} \right) h^2 & \frac{\pi}{2 \nu} h^2 \\ \frac{\nu \pi}{2} \chi + \left( \frac{3\pi - \chi (\nu \Delta t \pi^2 + 6\pi)}{12\Delta t} \right) h^2 & 1 - \frac{\chi \pi^2}{4} h^2 \end{bmatrix} + O(h^4).$$

(6.81)

This expansion reveals a significant difference between the cases $\chi = 0$ and $\chi = 1$. Suppose first that $\Delta t = O(h)$ and $\nu$ is $O(1)$. With these assumptions, if $\chi = 0$, the matrix is almost diagonal, but if $\chi = 1$ there is an $O(1)$ off diagonal element. This large off diagonal element makes the matrix significantly more sensitive to perturbations.

As an example of how the off diagonal element affects stability, consider the matrix

$$A = \begin{bmatrix} -1 + \delta_1 & 0 \\ d & 1 - \delta_2 \end{bmatrix}. \tag{6.82}$$

Now suppose that this matrix is perturbed in the upper right element, so that

$$\tilde{A} = \begin{bmatrix} -1 + \delta_1 & \epsilon \\ d & 1 - \delta_2 \end{bmatrix}. \tag{6.83}$$

If

$$\epsilon > \frac{\delta_2 (1 - \delta_1)}{d}, \tag{6.84}$$

then $\tilde{A}$ has an eigenvalue greater than one. If $d$ is small, then $\epsilon$ would have to be large to produce an eigenvalue greater than one. As $d$ gets larger, the perturbations that force an instability become smaller. If $d$ is $O(1)$, then perturbations of size $\delta_2$ can produce an instability. Applying this to the matrix $X_{N-1}$ with $\chi = 1$, shows that perturbations of order $h^2$ could produce an instability.

Projection method II with constant extrapolation for the pressure ghost cell values produces a stable scheme, but is significantly more sensitive to perturbations than projection method I. This analysis suggests that PM II will become unstable when higher
order extrapolations are used to set the ghost cells of the pressure, unless we choose those extrapolating formulas carefully. This is shown to be the case in the following section.

6.4 Numerical Tests

We perform two numerical tests. First we test the stability of the model problem for different choices of pressure gradients for both projection methods I and II. We test all of the gradients (gradient 0, gradient 1, and gradient 2) given in Table 6.1, and one more second order gradient, which we will refer to as gradient 2a. We derive the formula for gradient 2a by linearly extrapolating the gradient near the boundary, rather than extrapolating the pressure. The resulting gradient is second order accurate at every point, and has the form

\[(Gp)_{1} = \frac{-2p_{1} + p_{2} + 2p_{3} - p_{4}}{2h},\]  

(6.85)

If the ghost cells are set using the formula

\[p_{0} = 2p_{1} - 2p_{3} + p_{4},\]  

(6.86)

this gradient can then be computed by using the standard centered difference near the boundary. This method of setting the ghost cells extrapolates the pressure to third order, but it is very different than quadratic polynomial extrapolation in that a different set of grid points is used in the extrapolation formula. After exploring the stability using the model problem, we then explore both the stability and accuracy when these gradients are used in the full Navier-Stokes equations.

6.4.1 Model Problem

We proved that the model problem is stable if gradient 0 is used to compute the pressure. We test the stability of the model problem using the gradients 1, 2, and 2a for a large range of time steps and viscosities. For different values of the cell width \(h\), we varied the time step and viscosity between \(h^{3}\) and \(h^{-3}\). We began the computation with zero pressure, but with a random velocity, normalized to have 2-norm equal to 1. We use a random velocity, because it is likely to contain all frequencies. To determine the stability we run the computation until it is clear that the perturbation is growing or decaying.

For projection method I, all gradients produced stable schemes. For projection method II, only gradient 2 (quadratic polynomial extrapolation for the ghost cells) became unstable, while all the other gradients were stable for all time steps and viscosities tested.
Gradient 2 was stable for very small viscosities and time steps, but was very often unstable. Our analysis predicted that the higher order pressure correction is sensitive to perturbations at high frequencies, and apparently this sensitivity can produce instability depending on the gradient. However it was not clear why gradient 2 produced an unstable scheme, while the other gradients were stable.

In all of the schemes, high frequency oscillations dominated in the pressure and the velocity after a few time steps. This is not surprising, because we showed that the eigenvalues were an increasing function of the frequency of the eigenvectors. For all the gradients except gradient 2, these oscillations decayed in time. When gradient 2 became unstable, the high frequency oscillations grew near the boundary in both the velocity and the pressure. An example is displayed in Figure 6.3. This particular computation was run with \( N = 32 \) cells, time step \( h/2 \), viscosity 1, and a parabola as the initial velocity. The velocity and pressure are plotted after 200 time steps.

To see what is different about gradient 2 at high frequencies, we compare the different gradients near the boundary and compare them against each other and to the actual gradient which they approximate. Rather than just considering the basis of cosine functions, we consider both \( p = \cos(2m\pi x) \) and \( p = \sin(2m\pi x) \), which can also be used as a basis. The results for high frequencies are plotted in Figure 6.4 for \( h = 1/128 \). Notice that when applied to the high frequency cosine functions, all of the discrete gradients

![Figure 6.3: The (a) velocity and (b) pressure are plotted after 200 time steps for the model problem using gradient 2. The computation was run with \( N = 32 \) cells, time step \( h/2 \), viscosity 1, and a parabolic profile as the initial velocity.](image)
produce a value that has smaller magnitude than the actual derivative near the boundary. The value of gradient 2 is notably larger than the other discrete gradients. Gradients 1 and 2a are of similar magnitude with gradient 2a slightly larger. For the sine functions, gradient 2a produces the smallest and most accurate value. Again the value produced by gradient 2 is notably larger than the other gradients. Considering the other discrete gradients as a perturbations of gradient 0, these plots show that gradient 2 produces a larger perturbation to gradient 0 than does gradient 1 or gradient 2a at high frequencies. These results give some explanation as to why gradient 2 produced an unstable scheme.

6.4.2 Navier-Stokes Test

We now test the significance of the results of the model problem by solving the Navier-Stokes equations. We use a test problem from Brown *et al.* [8] for forced flow. The solution is

\[
\begin{align*}
  u &= \cos (2\pi (x - \omega)) \left(3y^2 - 2y\right) \\
  v &= 2\pi \sin (2\pi (x - \omega)) \left(y^3 - y^2\right) \\
  p &= -\frac{\omega'}{2\pi} \sin (2\pi (x - \omega)) (\sin (2\pi y) - 2\pi y + \pi) \\
      &\quad - \nu \cos (2\pi (x - \omega)) (-2\sin (2\pi y) + 2\pi y - \pi)
\end{align*}
\]

with \(\omega = 1 + \sin (2\pi t^2)\). From this solution, the force which drives the flow is calculated. The viscosity is set to one. Periodic boundary conditions are used in the \(x\)-direction.
and Dirichlet boundary conditions are used in the $y$-direction. The numerical solution is compared with the actual solution at time $t = 0.5$. The time step used for each computation is $\Delta t = h/2$, where $h$ is the grid spacing. The nonlinear terms are handled explicitly using the method of Kim and Moin [24], given in equation (6.33).

The max norm of the errors are displayed in Table 6.2 for the horizontal velocity, $u$, and in Table 6.3 for the pressure. Tables 6.4 and 6.5 give the $L_1$ norm of the errors for the velocity and pressure respectively. The errors in the vertical velocity, $v$, are similar to those of $u$ and are not displayed. For projection method I, all the gradients give essentially equivalent results. The velocity is second order accurate in both the $L_1$ and maximum norm, and the pressure is second order accurate in the $L_1$ norm, but appears to be order $3/2$ accurate in the maximum norm.

For projection method II, gradient 2 was sometimes unstable, and all the other gradients were stable. This agrees with the numerical results for the model problem. Gradients 1 and 2a showed full second order accuracy in the pressure, but gradient 0 showed order $3/2$ accuracy. The method using gradient 2 became unstable as time and space were refined. The instability showed up in these refined cases, not because of the smaller time step or space step, but because more time steps were taken. To test this we reran the computation with $h = 1/128$ for more time steps, and the solver failed to converge at time step 418, around time $t \approx 1.63$.

### 6.5 Discussion

We have discussed the ideas behind projection methods for solving the incompressible Navier-Stokes equations. A recent paper by Brown et al. [8] clarified issues surrounding the boundary conditions, the pressure, and the accuracy of projection methods. They

<table>
<thead>
<tr>
<th>method</th>
<th>gradient</th>
<th>$128 \times 128$</th>
<th>$256 \times 256$</th>
<th>$512 \times 512$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM I</td>
<td>0</td>
<td>9.86E-04</td>
<td>2.40E-04</td>
<td>5.93E-05</td>
<td>2.02</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>9.86E-04</td>
<td>2.40E-04</td>
<td>5.93E-05</td>
<td>2.02</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>9.86E-04</td>
<td>2.40E-04</td>
<td>5.93E-05</td>
<td>2.02</td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>9.86E-04</td>
<td>2.40E-04</td>
<td>5.93E-05</td>
<td>2.02</td>
</tr>
<tr>
<td>PM II</td>
<td>0</td>
<td>9.30E-04</td>
<td>2.34E-04</td>
<td>5.87E-05</td>
<td>2.00</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>9.30E-04</td>
<td>2.33E-04</td>
<td>5.86E-05</td>
<td>2.00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.55E-03</td>
<td>3.69E-01</td>
<td>nan</td>
<td>–</td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>9.30E-04</td>
<td>2.33E-04</td>
<td>5.86E-05</td>
<td>2.00</td>
</tr>
</tbody>
</table>
Table 6.3: Max norm of error in pressure

<table>
<thead>
<tr>
<th>method</th>
<th>gradient</th>
<th>$128 \times 128$</th>
<th>$256 \times 256$</th>
<th>$512 \times 512$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM I</td>
<td>0</td>
<td>2.33E-02</td>
<td>7.78E-03</td>
<td>4.03E-03</td>
<td>1.55</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>2.27E-02</td>
<td>8.61E-03</td>
<td>4.61E-03</td>
<td>1.49</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.31E-02</td>
<td>7.86E-03</td>
<td>4.37E-03</td>
<td>1.52</td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>2.29E-02</td>
<td>8.16E-03</td>
<td>4.42E-03</td>
<td>1.51</td>
</tr>
<tr>
<td>PM II</td>
<td>0</td>
<td>2.51E-02</td>
<td>1.20E-02</td>
<td>5.91E-03</td>
<td>1.44</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>9.90E-03</td>
<td>2.38E-03</td>
<td>5.86E-04</td>
<td>2.03</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.02E-02</td>
<td>3.22E+00</td>
<td>nan</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>9.94E-03</td>
<td>2.38E-03</td>
<td>5.88E-04</td>
<td>2.03</td>
</tr>
</tbody>
</table>

Table 6.4: $L_1$ norm of error in horizontal velocity, $u$

<table>
<thead>
<tr>
<th>method</th>
<th>gradient</th>
<th>$128 \times 128$</th>
<th>$256 \times 256$</th>
<th>$512 \times 512$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM I</td>
<td>0</td>
<td>1.78E-04</td>
<td>4.43E-05</td>
<td>1.10E-05</td>
<td>2.01</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1.77E-04</td>
<td>4.39E-05</td>
<td>1.09E-05</td>
<td>2.01</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.78E-04</td>
<td>4.40E-05</td>
<td>1.10E-05</td>
<td>2.01</td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>1.77E-04</td>
<td>4.39E-05</td>
<td>1.09E-05</td>
<td>2.01</td>
</tr>
<tr>
<td>PM II</td>
<td>0</td>
<td>1.73E-04</td>
<td>4.35E-05</td>
<td>1.09E-05</td>
<td>2.00</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1.73E-04</td>
<td>4.35E-05</td>
<td>1.09E-05</td>
<td>2.00</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>2.00E-04</td>
<td>4.17E-03</td>
<td>nan</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>1.73E-04</td>
<td>4.35E-05</td>
<td>1.09E-05</td>
<td>2.00</td>
</tr>
</tbody>
</table>

Table 6.5: $L_1$ norm of the error in pressure

<table>
<thead>
<tr>
<th>method</th>
<th>gradient</th>
<th>$128 \times 128$</th>
<th>$256 \times 256$</th>
<th>$512 \times 512$</th>
<th>rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM I</td>
<td>0</td>
<td>5.56E-03</td>
<td>1.30E-03</td>
<td>3.19E-04</td>
<td>2.04</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>5.58E-03</td>
<td>1.30E-03</td>
<td>3.18E-04</td>
<td>2.05</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>5.59E-03</td>
<td>1.31E-03</td>
<td>3.18E-04</td>
<td>2.05</td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>5.59E-03</td>
<td>1.30E-03</td>
<td>3.18E-04</td>
<td>2.05</td>
</tr>
<tr>
<td>PM II</td>
<td>0</td>
<td>1.61E-03</td>
<td>4.44E-04</td>
<td>1.30E-04</td>
<td>1.88</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1.32E-03</td>
<td>3.16E-04</td>
<td>7.77E-05</td>
<td>2.03</td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.18E-03</td>
<td>2.06E-01</td>
<td>nan</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2a</td>
<td>1.32E-03</td>
<td>3.16E-04</td>
<td>7.77E-05</td>
<td>2.03</td>
</tr>
</tbody>
</table>
may be the first to show full second order accuracy in the pressure. However, their analysis did not consider the stability of these schemes. We have extended their results by analyzing stability. We showed that on the MAC grid, all schemes are stable. However when an approximation projection is used, PM II is susceptible to instabilities, depending on how the gradient is computed near the boundary.

This work was inspired by our observation of instabilities while experimenting with an approximate projection method. In implementing PM II by computing the pressure, it is required to choose a difference formula for the pressure at points adjacent to the boundary. For a scheme that is supposed to be second order accurate pointwise, a natural choice for differencing the pressure is the second order, one sided difference using the three points closest to the boundary, which in this paper we refer to as gradient 2. As we demonstrated in this paper, this gradient also produced an unstable scheme. It appears that using a first order gradient (gradient 1) near the boundary is sufficient to produce a stable, second order accurate scheme. However, the only gradient for which we proved the scheme is stable is gradient 0, which did not show second order accuracy. We prefer gradient 2a, because, unlike gradient 1, it damps high frequency errors of the form that appeared when the scheme was unstable, as displayed in Figure 6.3. We did not prove that this scheme is stable, but we have been using a code with gradient 2a for some time, and have not noted any instabilities related to the projection method.

We have focused on approximate projection methods on cell-centered grids. This is because cell-centered grids are particularly useful if high order upwinding is used for the nonlinear terms, and is more commonly used than the vertex-centered grid. An approximate projection on a vertex-centered grid was used for the numerical tests in [8], and no instabilities arose. As we showed, the instabilities arose from the manner in which the pressure was differenced near the boundary. On a node-centered grid, the pressure is computed at the boundary, and so no extrapolation is required to difference the pressure. For this reason, we conjecture that the instability that we demonstrated is unique to the cell-centered grid.
CHAPTER 7

MODELING A PRESSURE DRIVEN FLOW

Consider a long pipe with pressure heads at each end. In a small section of the pipe
the channel is partially occluded. This section is to be the computational domain of
a simulation. This situation is illustrated in Figure 7.1. The problem addressed here is
determining the boundary conditions at the inlet and outlet of the computational domain.
One possibility is prescribing a constant pressure drop across the computational domain.
A second possibility is to relate the flux to the pressure drop, and use this relation to
derive a boundary condition. These two approaches are discussed below.

Before discussing different boundary conditions, some notation is established. Suppose
that when the tube is unobstructed, the pressure drop is known and the resulting flow
is a Poiseuille flow. Let $\Delta P$ represent the pressure drop across the whole tube, and
let $L$ represent the length of the tube. Let the radius of the tube be $a$. Divide the
tube into three pieces: upstream from the obstructed region, the obstructed region, and
downstream from the obstruction. Let $L_1$, $L_2$, and $L_3$ represent the length of each section
so that $L_1 + L_2 + L_3 = L$, and let $\Delta P_1$, $\Delta P_2$, and $\Delta P_3$ represent the pressure drops in each
section so that $\Delta P_1 + \Delta P_2 + \Delta P_3 = \Delta P$. Let $Q$ denote the flux through a cross-section
orthogonal to the walls of the tube. Assume that the fluid is incompressible, making $Q$ a
constant everywhere.

Figure 7.1: The computational domain is only a small section of the physical
domain.
7.1 Constant Pressure Drop

Suppose the pressure drop across the computational domain is to be prescribed. One reasonable approach is the suppose that the pressure drop per unit length is constant. This gives the condition

\[ \Delta P_2 = \frac{L_2 \Delta P}{L}. \]

To explore the validity of this assumption, we consider a simple problem. Suppose that the viscosity in the obstructed region is larger than in the other two regions, but there is no obstruction. The higher viscosity is meant to model an increase in flow resistance in this region. Increased resistivity could also be modeled by supposing the radius of the tube is smaller. Also suppose that each segment is long enough so that a steady parabolic profile is obtained in each section. The flux in each section is

\[ Q = \frac{\Delta P_j \pi a^4}{8L_j \mu_j}, \]

where \( \mu_j \) represents the viscosity of section \( j \). This shows that the pressure drop per unit length cannot be constant in each segment. If the viscosity is larger in the obstructed region, the pressure drop per unit length must also be larger in this segment. This simple example illustrates that the pressure drop per unit length in the obstructed region cannot be taken to be the same as in the unobstructed region. Some other value may be appropriate, but if the severity of obstruction changes, this value must be changed. It is therefore inappropriate to prescribe a constant pressure drop.

7.2 Pressure-Flux Relationship

Clearly the flux at the inlet of the computational domain is not constant. Because this is a pressure driven flow, an obstruction will cause a decrease in the flux. We now derive a relationship between the flux and the pressure drop.

Suppose that as part of the computation, either the flux or the pressure drop is measured and used to prescribe the other. Assume that in the sections upstream and downstream from the obstructed region the flow is a fully developed parabolic flow. The total length \( L \) and the total pressure drop \( \Delta P \) are both known. The following equations hold.
\[ Q = \frac{\Delta P_1 \pi a^4}{8L_1 \mu} \]
\[ Q = \frac{\Delta P_3 \pi a^4}{8L_3 \mu} \]
\[ \Delta P = \Delta P_1 + \Delta P_2 + \Delta P_3 \]
\[ L = L_1 + L_2 + L_3. \]

Eliminating \( \Delta P_1 \) and \( \Delta P_3 \) gives the expression
\[ Q = \frac{(\Delta P - \Delta P_2) \pi a^4}{8\mu (L - L_2)}. \] (7.1)

The quantities \( \Delta P, L, \) and \( L_2 \) are known. This formula could be used in two ways. The flux could be measured and used to predict the pressure drop, or the pressure drop could be measured and used to predict the flux.

Prescribing the flux or pressure drop alone does not provide enough boundary data. When prescribing the pressure drop, often homogeneous Neumann boundary conditions are imposed on the velocity. This approach amounts to assuming that the viscous stresses are zero at the inlet and outlet of the domain, and all stresses on these boundaries result from the pressure. A simple approach to prescribing the flux is to assume that the velocity profile at the inlet is parabolic, with the prescribed volume flux and to assume that the outlet has zero viscous stress. Implementations of these boundary conditions are discussed further when we present numerical tests.

A few special cases of this flux formula are checked to make sure it produces the expected results. Suppose there is an impermeable membrane in the obstructed region. At steady state the flux should be zero and the pressure drop across the membrane should be \( \Delta P \). This agrees with the formula. As a second special case, suppose that there is no obstruction. The pressure drop in the obstruction should be
\[ \Delta P_2 = \frac{L_2 \Delta P}{L}. \]

In this case the flux is expected to be
\[ Q = \frac{\Delta P \pi a^4}{8\mu L}. \]

With a little algebra, this can be shown to be true.

The relationship (7.1) applies to flow in a cylindrical pipe. The derivation could have been done for flow between parallel plates. In this case what we call flux, \( Q \), is not the
volume flux, but it is the area flux. Suppose that \( a \) represents the separation between the plates. The flux is defined to be

\[
Q = \int_0^a u \, dy.
\]

The formula analogous to (7.1) for parallel plates is

\[
Q = \frac{(\Delta P - \Delta P_2)a^3}{12\mu(L - L_2)}.
\]  \hspace{1cm} (7.2)

This formula is useful, because numerical calculations are often performed in two spatial dimensions.

### 7.3 Model Problem

A flux-pressure drop relationship similar to (7.1) has been used before by Fogelson (personal communication) and has sometimes exhibited numerical oscillations and instability. To understand the nature of these phenomena, a one-dimensional, linear model problem is used. First the model equation are discussed, and then various numerical treatments of the flux-pressure relationship are explored.

#### 7.3.1 Problem Formulation

Consider an unsteady flow between parallel plates, which are aligned with the \( x \)-direction and are separated by a distance \( a \). Suppose the flow is in the \( x \)-direction, so that the velocity is \((u,0)\), and let \( p \) denote the pressure. Using the fact that the fluid is incompressible,

\[
u_x = -v_y = 0,
\]

shows that \( u \) is independent of \( x \), which forces \( p_x \) also to be independent of \( x \). Because the vertical velocity is zero, the pressure cannot be a function of \( y \). Let \( G \) be the constant value of \( p_x \). The momentum equation for \( u \) takes the form

\[
\rho u_t = \mu \Delta u_{yy} - G, \quad u(0) = u(a) = 0.
\]  \hspace{1cm} (7.3)

The pressure gradient must be related to the pressure drop by

\[
G = -\frac{\Delta P_2}{L_2},
\]

where the notation of the previous section is used: \( \Delta P_2 \) is the pressure drop across the length \( L_2 \).
Suppose that the pressure gradient is related to the flux by

\[ G = \alpha Q - \beta, \quad (7.4) \]

for some positive constants \( \alpha \) and \( \beta \). The values of these constants correspond to physical parameters as in (7.2), but this is not relevant to this discussion. Substituting the pressure gradient from equation (7.4) into equation (7.3) gives

\[ \rho u_t = \mu u_{yy} - \alpha \int_0^a u \, dy + \beta, \quad u(0) = u(a) = 0. \quad (7.5) \]

This is the model problem that will be analyzed.

Before beginning the analysis, the problem is nondimensionalized. The space scale is chosen to be the distance separating the plates, \( a \), and the time scale is chosen to be \( T = \rho a^2/\mu \). This is the time scale of the viscous relaxation to steady state. Finally, scale the velocity by \( \frac{\beta}{T} \), which has the effect of making the pressure gradient \(-1\) when \( \alpha = 0 \). The nondimensional problem is

\[ u_t = u_{yy} - s \int_0^1 u \, dy + 1, \quad u(0) = u(1) = 0, \quad (7.6) \]

where \( s = \alpha a^3/\mu \).

### 7.3.2 Steady State Solution

The steady solution of equation (7.6) is the parabolic profile

\[ u_{ss} = \frac{6}{12 + s} y(1 - y). \]

To analyze the stability of this steady state, first shift the steady state to zero by introducing the change of variables

\[ U = u - u_{ss}. \]

This new velocity satisfies the equation

\[ \dot{U}_t = U_{yy} - s \int_0^1 U \, dy, \quad U(0) = U(1) = 0. \quad (7.7) \]

Consider a solution of the form \( U = e^{\kappa t} \hat{U}(y) \). If it can be shown that \( \kappa \leq 0 \), then this steady state is stable. For a solution of this form, equation (7.7) becomes

\[ \hat{U}_{yy} - \kappa \hat{U} - s \int_0^1 \hat{U} \, dy = 0, \quad \hat{U}(0) = \hat{U}(1) = 0. \]
Values of $\kappa$ are found by first solving the equation
\begin{equation}
\ddot{U} - \kappa \dot{U} - s Q = 0, \quad \dot{U}(0) = \dot{U}(1) = 0,
\end{equation}
and then determining which values of $\kappa$ admit a solution that satisfies
\begin{equation}
Q = \int_0^1 \dot{U} \, dy.
\end{equation}

For $\kappa > 0$, the solution to equation (7.8) is
\begin{equation}
\dot{U} = \frac{sQ \left( e^{y\sqrt{\kappa}} + e^{(1-y)\sqrt{\kappa}} - (e\sqrt{\kappa} + 1) \right)}{\kappa (e\sqrt{\kappa} + 1)}.
\end{equation}

Evaluating the integral of this solution, the constraint (7.9) becomes
\begin{equation}
Q = \frac{sQ \left( 2\kappa \left( e^{\sqrt{\kappa}} - 1 \right) - \kappa^{3/2} \left( e^{\sqrt{\kappa}} + 1 \right) \right)}{\kappa^{5/2} (e\sqrt{\kappa} + 1)}.
\end{equation}

Dividing both sides of this equation by $Q$ and rearranging gives the equation
\begin{equation}
2s\kappa \left( e^{\sqrt{\kappa}} - 1 \right) - s\kappa^{3/2} \left( e^{\sqrt{\kappa}} + 1 \right) - \kappa^{5/2} \left( e^{\sqrt{\kappa}} + 1 \right) = 0,
\end{equation}
which determines the eigenvalues. We now show that there are no positive eigenvalues.

Let $z = \sqrt{\kappa}$. Equation (7.12) can be simplified to
\begin{equation}
z^2 \left( e^z + 1 \right) \left( 2s \tanh \left( \frac{z}{2} \right) - sz - z^3 \right) = 0.
\end{equation}
The terms $z^2$ and $(e^z + 1)$ are always positive for any $z$. Let $g$ denote the function
\begin{equation}
g(z) = 2s \tanh \left( \frac{z}{2} \right) - sz - z^3.
\end{equation}

Note that $g(0) = 0$, and the derivative of $g$ is
\begin{equation}
\frac{dg}{dz} = -s \left( \tanh \left( \frac{z}{2} \right) \right)^2 - 3z^2,
\end{equation}
which is less that zero for all $z > 0$. This shows that $g(z) < 0$ for $z > 0$ and there are no positive solutions to (7.12). Therefore the steady state is stable.
7.3.3 Numerical Schemes

The numerical stability of two time stepping schemes for equation (7.7) are analyzed. In both the schemes presented, the viscous term is treated with a Crank-Nicholson type discretization because it is unconditionally stable and second order accurate in time [34]. The first scheme treats the pressure-like term explicitly in time, meaning that the pressure gradient is a function of the flux at the last time step. This strategy is referred to as the explicit scheme. The region of stability for the parameter $s$ is calculated for the explicit scheme. The second scheme analyzed treats the pressure term similarly to the viscous term. This implicit scheme is shown to be unconditionally stable. The presence of decaying oscillations is more difficult to analyze. These oscillations are acceptable provided they are “small,” and the definition of small is not clear. Some numerical results are presented to help understand when to expect these oscillations.

Before beginning the analysis of the individual schemes, some notation is introduced. Suppose the domain is discretized by $N + 2$ equally spaced points with the first and last points on the boundary. Let $h = 1/(N + 1)$ denote the spacing between the points, so that the discrete points are $y_j = jh$ for $j = 0 \ldots N + 1$. Discretize time into intervals of length $k$. Let $v^n_j$ denote the discrete evaluation of the continuous function $v(y, t)$, such that $v^n_j = v(jh, nk)$. The only functions we consider are those that satisfy the boundary conditions $v(0, t) = v(1, t) = 0$. This is assumed unless otherwise stated. Let $v^n$ denote the vector of length $N$ formed from the interior points of $v^n_j$ for $j = 1 \ldots N$.

Let $e$ denote the vector of length $N$ with every entry equal to 1. A discrete approximation to the integral can be written as

$$\int_0^1 v(y, nk) \, dy \approx h \sum_{j=1}^N v^n_j = he^T v^n.$$ 

Let $E$ be the rank one matrix defined by $E = ee^T$. The discrete, one-dimensional Laplacian used is the standard second order approximation

$$\partial_{yy} v(jh, nk) \approx \frac{v^n_{j-1} - 2v^n_j + v^n_{j+1}}{h^2}.$$ 

Let $L$ denote the matrix with $-2$’s on the main diagonal and 1’s on the super and sub diagonals.

7.3.3.1 Explicit Scheme

For the explicit scheme, the pressure gradient is computed from the flux of the last time step. The discretization is
\[
\frac{v^{n+1} - v^n}{k} = \frac{1}{2h^2} \left( L v^n + L v^{n+1} \right) - shE v^n. \tag{7.14}
\]

The linear system to solve to advance in time is

\[
\left( I - \frac{k}{2h^2} L \right) v^{n+1} = \left( I + \frac{k}{2h^2} L - skhE \right) v^n. \tag{7.15}
\]

To simplify notation define the parameter \( \delta \) and by

\[
\delta = \frac{k}{2h^2}.
\]

Equation (7.15) becomes

\[
(I - \delta L) v^{n+1} = (I + \delta L - skhE) v^n.
\]

Assume for the moment the matrix \( I - \delta L \) is invertible (this will be shown later). Define the matrix \( B \) by

\[
B = (I - \delta L)^{-1} (I + \delta L - skhE). \tag{7.16}
\]

Given the solution at time level \( n \), the solution at time level \( n+1 \) is given by \( v^{n+1} = B v^n \).

**Theorem 4 (Explicit Scheme Stability)** The discretization (7.14) gives a stable scheme if and only if \( \chi \leq 2 \), where \( \chi = skhN \).

**Proof**: First we examine the eigenvectors and eigenvalues of \( L \) and \( E \). The only nonzero eigenvalue of \( E \) is \( N \) with eigenvector \( e \). Denote the eigenvectors of \( L \) by \( w_m \) and the corresponding eigenvalues by \( \mu_m \). It is easily checked that the eigenvectors are

\[
(w_m)_j = \sin (m \pi j h),
\]

with eigenvalues

\[
\mu_m = 2 \cos (m \pi h) - 2,
\]

for \( m = 1, \ldots, N \). Note that the eigenvectors are mutually orthogonal. All the eigenvalues satisfy the inequality

\[
-4 < \mu_m < 0, \tag{7.17}
\]

and so the eigenvalues of \( I - \delta L \) satisfy the inequality

\[
1 < 1 - \delta \mu_m < 1 + 4 \delta. \tag{7.18}
\]

This shows that \( I - \delta L \) is invertible and all the eigenvalues are greater than one.
First suppose that $\chi \leq 2$. We show that for any vector $u$, $||Bu||^2 \leq ||u||^2$, where $|| \cdot ||$ denotes the vector 2-norm. This gives that the explicit scheme is stable. First divide the vector $u$ into its projection onto $e$ and onto the subspace orthogonal to $e$, so that

$$u = \alpha_1 e + \alpha_2 e^\perp,$$

where $e \cdot e^\perp = 0$. Because these vectors are orthogonal,

$$||u||^2 = |\alpha_1|^2 ||e|| + |\alpha_2|^2 ||e^\perp||^2.$$

Using that $e$ and $e^\perp$ are eigenvectors of $E$ with eigenvalues $N$ and 0 respectively,

$$Bu = (I - \delta L)^{-1} ((1 - \chi) I + \delta L) \alpha_1 e + (I - \delta L)^{-1} (I + \delta L) \alpha_2 e^\perp. \quad (7.19)$$

Now split $e$ and $e^\perp$ into their projections onto the eigenspaces of $L$, so that

$$e = \sum_{m=1}^{N} \beta_m w_m, \quad \text{and} \quad e^\perp = \sum_{m=1}^{N} \gamma_m w_m. \quad (7.20)$$

Plugging these expansions into the right side of equation (7.19) and taking the squared norms gives

$$||Bu||^2 = \left| \alpha_1 \sum_{m=1}^{N} \beta_m \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} w_m + \alpha_2 \sum_{m=1}^{N} \gamma_m \frac{1 + \delta \mu_m}{1 - \delta \mu_m} w_m \right|^2 \quad (7.21)$$

Using orthogonality, this inequality can be written as

$$||Bu||^2 \leq |\alpha_1|^2 \sum_{m=1}^{N} |\beta_m|^2 \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 ||w_m||^2
+ |\alpha_2|^2 \sum_{m=1}^{N} |\gamma_m|^2 \left| \frac{1 + \delta \mu_m}{1 - \delta \mu_m} \right|^2 ||w_m||^2. \quad (7.22)$$

Maximizing these ratios,

$$||Bu||^2 \leq |\alpha_1|^2 \max_m \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 \sum_{m=1}^{N} |\beta_m|^2 ||w_m||^2
+ |\alpha_2|^2 \max_m \left| \frac{1 + \delta \mu_m}{1 - \delta \mu_m} \right|^2 \sum_{m=1}^{N} |\gamma_m|^2 ||w_m||^2. \quad (7.23)$$
Using orthogonality and the expansions (7.20) gives

\[ ||Bu||^2 \leq |\alpha_1|^2 \max_m \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 ||e||^2 + |\alpha_2|^2 \max_m \left| \frac{1 + \delta \mu_m}{1 - \delta \mu_m} \right|^2 ||e_m^1||^2. \] (7.24)

Examine the two quantities that are being maximized. It follows from the inequality (7.17) that

\[ \left| \frac{1 + \delta \mu_m}{1 - \delta \mu_m} \right| \leq 1 \] (7.25)

for all \( m \). As for the other term being maximized, first note that

\[ \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} = \frac{2 - \chi}{1 - \delta \mu_m} - 1. \]

By assumption, \( \chi \) satisfies the inequality

\[ 0 \leq \chi \leq 2. \]

Using this inequality and inequality (7.18) give

\[ -1 \leq \frac{2 - \chi}{1 - \delta \mu_m} - 1 \leq \frac{2}{1 - \delta \mu_m} - 1 \leq 1, \]

and therefore for all \( m \),

\[ \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right| \leq 1. \] (7.26)

Combining the inequalities (7.24), (7.25), and (7.26), gives

\[ ||Bu||^2 \leq |\alpha_1|^2 ||e||^2 + |\alpha_2|^2 ||e_m^1||^2 = ||u||^2. \]

This shows that if \( \chi = skhN \leq 2 \), then the explicit scheme is stable.

To show that the explicit scheme is unstable for \( \chi > 2 \), we show that the norm of \( B \) is greater than one. In general, this does not imply instability, but because \( B \) is symmetric (this is verified below), instability is implied. Symmetric matrices have real eigenvalues and the eigenspaces are orthogonal, and so the singular values are just the absolute values of the eigenvalues [18]. Therefore if we show that the norm of \( B \) is greater than one, then there must be an eigenvalue greater than one in absolute value, and the scheme is unstable.

First we show that \( B \) is symmetric. Both \( L \) and \( E \) are symmetric, and so \( B \) is formed as the product of the two symmetric matrices \((I - \delta L)^{-1}\) and \((I + \delta L - skhE)\). In order for \( B \) to be symmetric, these two matrices must commute. Split this product up as

\[ B = (I - \delta L)^{-1} (I + \delta L - skh(I - \delta L)^{-1} E). \] (7.27)

The first product commutes because the two matrices have the same eigenvectors. The second product also commutes. Recall that \( E \) is a matrix of all ones, which clearly
commutes with symmetric matrices. Therefore \( B \) is symmetric because it is the product of two symmetric matrices that commute.

To complete the proof we show that if \( \chi > 2 \), the norm of \( B \) is greater than one. To show this, it is sufficient to find a vector whose norm is increased by multiplication by \( B \). This vector is the vector of all ones, \( e \). Since \( e \) is an eigenvector of \( E \) with eigenvalue \( N \),

\[
Be = (I - \delta L)^{-1}(1 - \chi I + \delta L) e
\]

Expand \( e \) in terms of the eigenvectors of \( L \), so that

\[
e = \sum_{m=1}^{N} \beta_m w_m.
\]

The squared norm of \( Be \) can be written as

\[
||Be||^2 = \left| \left| (I - \delta L)^{-1}((1 - \chi)I + \delta L) e \right| \right|^2
\]

\[
= \left| \left| \sum_{m=1}^{N} \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \beta_m w_m \right| \right|^2
\]

\[
= \sum_{m=1}^{N} \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 |\beta_m|^2 ||w_m||^2,
\]

using the orthogonality of the eigenvectors of \( L \). Minimizing over the eigenvalues gives

\[
||Be||^2 \geq \min_m \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 \sum_{m=1}^{N} |\beta_m|^2 ||w_m||^2 = \min_m \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 ||e||^2. \quad (7.28)
\]

Rearrange the factor in front of \( ||e||^2 \) as

\[
\min_m \left| \frac{1 - \chi + \delta \mu_m}{1 - \delta \mu_m} \right|^2 = \min_m \left| \frac{2 - \chi}{1 - \delta \mu_m} - 1 \right|^2.
\]

Because \( 2 - \chi < 0 \) and \( 1 - \delta \mu_m > 0 \), the two terms inside the absolute value are both negative, and so

\[
\min_m \left| \frac{2 - \chi}{1 - \delta \mu_m} - 1 \right|^2 > 1. \quad (7.29)
\]

Combining this inequality with (7.28) shows that

\[
||B|| > 1 \quad \text{for } \chi > 2.
\]

This completes the proof that the explicit scheme is stable if and only if \( \chi \leq 2 \).
7.3.3.2 Implicit Scheme

The implicit scheme treats the integral term similar to the viscous term. The discretization is

\[
\frac{v^{n+1} - v^n}{k} = \frac{1}{2h^2} (Lv^n + Lv^{n+1}) - \frac{sh}{2} (Ev^n + Ev^{n+1}).
\]  

(7.30)

The linear system to solve to advance in time is

\[
(I - \delta L + \frac{skh}{2} E) v^{n+1} = (I + \delta L - \frac{skh}{2} E) v^n.
\]

(7.31)

We now show that this scheme is unconditionally stable.

**Theorem 5 (Implicit Scheme Stability)** The implicit time stepping scheme (7.30) is unconditionally stable.

**Proof:** Let \( \lambda \) be an eigenvector of \( \delta L - (skh/2) E \). Because all the eigenvalue of \( \delta L \) and \( (-skh/2) E \) are less than or equal to zero, \( \lambda \) must also be less than or equal to zero. Thus the matrix \( (I - \delta L + skh/2E) \) is invertible. The solution at time \( n+1 \), \( v^{n+1} \), is given by

\[
v^{n+1} = (I - (\delta L - \frac{skh}{2} E))^{-1} (I + (\delta L - \frac{skh}{2} E)) v^n = C v^n.
\]

The scheme is unconditionally stable because the spectral radius of \( C \) is

\[
\rho(C) = \max_m \left| \frac{1 + \lambda_m}{1 - \lambda_m} \right| \leq 1,
\]

where the last inequality holds because \( \lambda_m < 0 \) for all \( m \).

7.3.4 Averaging Scheme

Another numerical treatment of the model problem is explored. This treatment differs from the previous two in that it is not a discretization of the model problem. The time stepping strategy of this third scheme, which will be referred to as the averaging scheme, is to compute the pressure gradient as an average of all past fluxes. This method was used by Fogelson because is seemed to show improved stability and less numerical oscillations than the explicit scheme. This scheme is not analyzed here, but some numerical results on the one-dimensional problem are presented. Again, the averaging scheme is not a discretization of the model problem. From the numerical scheme, the model of the pressure-flux relationship is recovered and its applicability is discussed.
The scheme is first presented as implemented by Fogelson; that is as an explicit time stepping scheme for the discrete problem. Let $\omega_1$ and $\omega_2$ be two nonnegative numbers such that $\omega_1 + \omega_2 = 1$. Introduce a variable representing the average fluxes over past times denoted by $Q_{\text{avg}}^n$. In the model problem, the pressure is assumed to be given as a function of the averaged flux rather than the flux at a single time step. The discrete system is

$$\frac{v^{n+1} - v^n}{k} = \frac{1}{2h^2} (Lv^n + Lv^{n+1}) - sQ_{\text{avg}}^n$$  \hspace{1cm} (7.32)

$$Q_{\text{avg}}^{n+1} = \omega_1 he^T v^{n+1} + \omega_2 Q_{\text{avg}}^n$$ \hspace{1cm} (7.33)

We explore how the stability of this scheme compares to the stability of the explicit scheme. The system (7.32)–(7.33) can be written in matrix form as

$$\begin{pmatrix} I - \delta L & 0 \\ -\omega_1 he^T & 1 \end{pmatrix} \begin{pmatrix} v \\ Q_{\text{avg}} \end{pmatrix}^{n+1} = \begin{pmatrix} I + \delta L & -ske \\ 0^T & \omega_2 \end{pmatrix} \begin{pmatrix} v \\ Q_{\text{avg}} \end{pmatrix}^n$$

The matrix that gives the solution at the next time from the previous time is

$$X = \begin{pmatrix} I - \delta L & 0 \\ -\omega_1 he^T & 1 \end{pmatrix}^{-1} \begin{pmatrix} I + \delta L & -ske \\ 0^T & \omega_2 \end{pmatrix}$$

In order to determine if the averaging scheme is stable, we numerically calculate the spectral radius of the matrix $X$ for a range of $\omega_1$ and $s$ values.

For different values of $\omega_1$ the maximum value of $s$ such that the spectral radius is less than or equal to one is found using a bisection algorithm. The results from this computation are displayed in Figure 7.2. The value of $s$ has been normalized by the maximum value of $s$ that gives stability for the explicit scheme, $s_0 = 2/(khN)$. Note that when $\omega_1 = 1$, the explicit scheme is recovered. These results were generated with $N = 64$, $k = 0.1$, and $\mu = 1$. The computation was repeated for different values of these parameters and the results were identical. The critical value of $s$ increases as $\omega_1$ decreases. As $\omega_1$ goes to zero the critical value of $s$ grows without bound. This is to be expected because if $\omega_1 = 0$, the flux does not affect the pressure and the problem reduces to the diffusion equation. The value that Fogelson used in practice was $\omega_1 = 0.1$, at which point the critical value of $s$ is a factor of 19 larger than in the explicit scheme.

We now examine the scheme more carefully to determine what it is modeling. It remains to be seen how this problem is related to the model problem. Let $Q(t)$ be a function representing a flux. For simplicity assume that $Q(t) = 0$ for $t \leq 0$. Let $\{Q^n\}$ be the sequence obtained by sampling $Q(t)$ at discrete points in time, such that $Q^n = Q(nk)$,
where $k$ is the time step. From this sequence, we can define the sequence of average fluxes, \{Q^{n}_{\text{avg}}\} recursively by
\[ Q^{n}_{\text{avg}} = \omega_{2} Q^{n-1}_{\text{avg}} + \omega_{1} Q^{n}, \]
and it is not hard to show that
\[ Q^{n}_{\text{avg}} = \sum_{j=0}^{n-1} \omega_{1} \omega_{2}^{j} Q^{n-j}. \quad (7.34) \]

From taking the limit as the time step goes to zero, a continuous time flux average, $Q_{\text{avg}}(t)$, can be recovered if the limit exists. Two cases are considered: (1) the weights depend on the time step, (2) the weights are independent of the time step.

### 7.3.4.1 Weights Depend on Time Step

First suppose that the weights depend on the time step. Multiply and divide by $k$, make the substitution $\omega_{2} = e^{-\lambda k}$, and use that $\omega_{1} = 1 - \omega_{2}$ in equation (7.34) to get
\[ Q^{n}_{\text{avg}} = \frac{1 - e^{-\lambda k}}{k} \sum_{j=0}^{n-1} e^{-\lambda kj} Q^{n-j}. \quad (7.35) \]
Taking the limit in equation (7.35) as \( k \to 0 \) while \( nk = t \) remains constant gives

\[
Q_{\text{avg}}(t) = \lambda \int_0^t e^{-\lambda \tau} Q(t - \tau) \, d\tau.
\]  

(7.36)

This shows what continuous function the discrete sequence \( Q_{\text{avg}}^n \) is approximating. The average is taken over all past fluxes with exponentially decaying weights over past times.

Equation (7.36) provides insight into what this numerical scheme is modeling. In the averaging model the pressure gradient and average flux, rather than the flux, are related by a linear function. The pressure gradient has a “fading memory” of past fluxes. This interpretation is reminiscent of the history integrals that appear in viscoelasticity. The parameter \( \lambda \) characterizes the inverse of the time scale of this memory. Note that as \( \lambda^{-1} \to 0 \), the explicit model problem is recovered. One interpretation of the averaging model is that the flux upstream and downstream do not instantaneously equilibrate.

### 7.3.4.2 Weights Independent of Time Step

Return to equation (7.34) and consider the case where the weights are independent of the time step. We will eventually take the limit in (7.34) as the time step, \( k \), goes to zero with \( nk = t \) constant. First, let \( T \) be some fixed time before \( t \), and let \( N \) be the integer defined by \( N = \lfloor T/k \rfloor \). Split the sum in (7.34) into two parts as follows

\[
Q_{\text{avg}}^n = \sum_{j=0}^{N} \omega_1 \omega_2^j Q_{\text{avg}}^n - j + \sum_{j=N+1}^{n-1} \omega_1 \omega_2^j Q_{\text{avg}}^n - j
\]

\[
= \sum_{j=0}^{N} \omega_1 \omega_2^j Q(nk - jk) + \sum_{j=N+1}^{n-1} \omega_1 \omega_2^j Q_{\text{avg}}^n - j
\]

\[
= \sum_{j=0}^{N} \omega_1 \omega_2^j Q(t - jk) + \sum_{j=N+1}^{n-1} \omega_1 \omega_2^j Q_{\text{avg}}^n - j
\]

(7.37)

In the first sum above the quantity \( t - jk \) is less than \( t - T \). The original sum was split into these two pieces to allow for a Taylor series expansion of \( Q(t - jk) \) about time \( t \), and introducing \( T \) controls the size of the interval where the Taylor series is used.

First it is shown that the second of the two sums in (7.37) is exponentially small as \( k \to 0 \).

\[
\left| \sum_{j=N+1}^{n-1} \omega_1 \omega_2^j Q_{\text{avg}}^n - j \right| \leq \omega_1 \max_{0 \leq t \leq T} |Q(t)| \sum_{j=N+1}^{n-1} \omega_2^j = \omega_1 \max_{0 \leq t \leq T} |Q(t)| \frac{\omega_2^{n+1} - \omega_2^N}{1 - \omega_2}.
\]
As $k \to 0$, $n, N + 1 \to \infty$, and therefore this term is exponentially small. Now examine the first sum in (7.37). Expanding $Q(t - jk)$ about time $t$ gives

$$
\sum_{j=0}^{N} \omega_1^{j} Q(t - jk) = \sum_{j=0}^{N} \omega_1^{j} \left( Q(t) - jkQ'(t) + O(k^2) \right). 
$$

(7.38)

These sums can be computed to find the coefficients in the expansion as

$$
\sum_{j=0}^{N} \omega_1^{j} Q(t - jk) = C_1 Q(t) - kC_2 Q'(t) + O(k^2),
$$

(7.39)

where

$$
C_1 = \frac{1 - \omega_2^{N+1}}{1 - \omega_2},
$$

(7.40)

and

$$
C_2 = \omega_1 \frac{N \omega_2^{N+2} - (N+1) \omega_2^{N+1} + \omega_2}{(1 - \omega_2)^2}.
$$

(7.41)

As $k \to 0$, $N \to \infty$, and the terms such as $\omega_2^N$ are exponentially small. This shows that

$$
\sum_{j=0}^{n-1} \omega_1^{j} Q^{n-j} = Q(t) - k \frac{\omega_2}{\omega_1} Q'(t) + O(k^2).
$$

(7.42)

Therefore, if the weights are independent of the time step, the quantity of $Q_{avg}$ is a first order approximation to $Q$. Equation (7.42) gives the leading order term for the error. This expression shows that in practice, $\omega_1$ should not be $O(k)$ if $Q_{avg}$ is to approximate $Q$.

### 7.3.5 Numerical Tests: Oscillations

So far we have only explored the stability of various schemes for the model problem. We now use numerical tests to explore nonphysical oscillations in the methods. Numerical oscillations arise from negative eigenvalues of the update matrix. Requiring that all the eigenvalues be positive imposes too stringent a requirement on the time step. If the oscillating modes decay rapidly and do not contribute much to the solution, their presence is acceptable. The definition of “acceptable” depends on the application. We present some numerical tests to help understand when to expect these oscillations in the various schemes.

Suppose that a constant pressure gradient is applied to the fluid so that the flow is a steady Poiseuille flow. Then, the applied pressure gradient is relaxed to zero exponentially at the start of the computation, and the flux is monitored. This is the physical situation...
used as a test for oscillations. The model problem is nondimensionalized differently than for the stability analysis. The velocity is scaled so that at steady state the flux is one.

The model problem for parallel plate flow (two-dimensional) is

\[ u_t = \nu u_{yy} - s \int_0^1 u \, dy + (12\nu + s) \exp(-\lambda t), \tag{7.43} \]

with initial condition

\[ u(y, 0) = 6y(1 - y), \tag{7.44} \]

and boundary conditions

\[ u(0, t) = u(1, t) = 0. \tag{7.45} \]

The kinematic viscosity appearing in this equation is defined to be \( \nu = \mu/\rho \). Using the explicit scheme discretization, this problem becomes

\[ \left( I - \frac{k\nu}{2h^2}L \right) u^{n+1} = \left( I + \frac{k\nu}{2h^2}L - kh\lambda E \right) u^n + k(12\nu + s) \exp(-\lambda n). \tag{7.46} \]

Define the parameter \( \delta \) by

\[ \delta = \frac{k\nu}{2h^2}. \tag{7.47} \]

If \( s = 0 \), the eigenvalues of the update matrix, \((I - \delta L)^{-1}(I + \delta L)\), are known to be

\[ \frac{1 + \delta\mu_m}{1 - \delta\mu_m}, \tag{7.48} \]

where

\[ \mu_m = 2\cos(m\pi h) - 2. \]

Note that if \( \delta < 1/4 \), then all of the eigenvalues (7.48) are positive. Let \( \delta_0 = 1/4 \) denote the value of \( \delta \) below which the eigenvalues of the update matrix with \( s = 0 \) are guaranteed to be positive. Let \( s_0 = 2/(Nkh) \) denote the value of \( s \) below which the explicit scheme is stable.

For our numerical tests the time step is fixed at \( k = 0.01 \), and the number of grid points is fixed at \( N = 50 \). For different values of \( \lambda \), our results are reported by giving the values of \( \delta \) and \( s \) as multiples of \( \delta_0 \) and \( s_0 \). The higher the value of \( \delta \), the larger the viscosity. For low values of \( \delta \), numerical oscillations were not evident, even for \( s \) near \( s_0 \).

For the explicit scheme results are displayed for \( \delta = 100\delta_0 \) in Figure 7.3 and for \( \delta = 1000\delta_0 \) in Figure 7.4. Four different values of \( \lambda \) are used: 10, 50, 100, and \( \infty \). Oscillations were not prevalent for values of \( \lambda \) less than those displayed, suggesting that large values of \( s \) can be used without the worry of oscillations if the background force is
Figure 7.3: Explicit scheme with $\delta = 100\delta_0$ and (a) $\lambda = 10$, (b) $\lambda = 50$, (c) $\lambda = 100$, (d) $\lambda = \infty$. In all cases oscillations can be avoided by a modest reduction in $s$. 

Figure 7.4: Explicit scheme with $\delta = 1000\delta_0$. (a) $\lambda = 10$, (b) $\lambda = 50$, (c) $\lambda = 100$, (d) $\lambda = \infty$. Oscillations can be avoided by a modest reduction in $s$ in (a) and (b), but require a more substantial reduction in cases (c) and (d). In these cases the flux is changing rapidly because of the high viscosity. The time step is inappropriate for this situation, regardless of the value of $s$ or the method used.
not changing rapidly. For each value of $\lambda$, three different values of $s$ are used. The values of $s$ are different for different values of $\lambda$ and $\delta$. These values were chosen to show the different degrees of oscillations that can result. The larger the value of $s$, the more likely it is that oscillations result. In general, the results show that the value of $s$ only needs to be reduced by at most a factor of 2 from the critical value $s_0$ to eliminate oscillations. The exceptions are for very large $\delta$ and $\lambda$. When $\delta$ is very large, the flux changes very rapidly in response to the changes in the background force. When $\lambda \geq 100$, the time scale of the change in the background force is faster than the time step, and the time step should be reduced, regardless of the value of $s$.

The implicit scheme is unconditionally stable, but for comparison purposes, the values of $s$ are given in terms of $s_0$. The results from the test problem are displayed in Figure 7.5 with $\delta = 1000\delta_0$. The same values of $\lambda$ that were used for the explicit scheme are tested for the implicit scheme. Note that the implicit scheme not only allows greater values of $s$, but oscillations are also less likely to occur with values of $s$ that give oscillations in the explicit scheme. Again the case $\lambda = \infty$ shows that the time step is too large regardless of the scheme for the pressure-flux relationship.

The results of tests using the averaging scheme are shown in Figure 7.6. The results are displayed for $\delta = 100\delta_0$ using the same values of $\lambda$ that were used for the explicit and implicit schemes. These tests are organized slightly differently than for the explicit and implicit schemes. For each value of $\lambda$ a different value of $s$ is chosen and the results are displayed for three values of $\omega_1$: 0.25, 0.50 and 0.75. The results show that the averaging scheme does eliminate high frequency oscillations from the flux, however, small values of $\omega_1$ may introduce larger and lower frequency oscillations. These effects are more drastic when the background force changes rapidly. Rapid changes in the flux are not felt immediately by the pressure, because the pressure is being controlled by the average flux. Even though the stability of the averaging scheme is increased as $\omega_1$ decreases, these results suggest that small values of $\omega_1$ should be avoided.

The implicit scheme is the least likely of the three schemes to show oscillations for a given value of $s$. However, as we discuss in the next section, the implicit scheme is easy to implement on this model problem, but difficult to implement in multiple dimensions. Avoiding oscillations in the explicit scheme does not require a drastic reduction in the time step. The averaging scheme does remove high frequency oscillations from the explicit scheme, but when the value of $\omega_1$ is too small, rapid changes in the flux produce
Figure 7.5: Implicit scheme with $\delta = 1000\delta_0$ and (a) $\lambda = 10$, (b) $\lambda = 50$, (c) $\lambda = 100$, (d) $\lambda = \infty$. The implicit scheme is not only unconditionally stable, but it reduces numerical oscillations present in the explicit scheme.
Figure 7.6: Averaging scheme with $\delta = 100\delta_0$ and (a) $\lambda = 10$, $s = 0.95s_0$, (b)$\lambda = 50$, $s = 0.95s_0$, (c)$\lambda = 100$, $s = 0.75s_0$, (d)$\lambda = \infty$, $s = 0.50s_0$. High frequency oscillations are eliminated, but lower frequency oscillations are introduced for small values of $\omega_1$. 
unacceptably large unphysical oscillations. Therefore small values of $\omega_1$ should not be used. If larger values of $\omega_1$ are used, the increase of time step allowed by the averaging scheme is minimal compared to the explicit scheme, as can be seen in Figure 7.2. We conclude that the explicit scheme is the better choice if implementing the implicit scheme is not practical.

7.4 Multiple Dimensions

We now discuss one method for coupling the pressure and flux while solving the full Navier-Stokes equations. We use a projection method, discussed in Chapter 6, to solve the Navier-Stokes equations. The nonlinear terms are handled explicitly in time, employing time splitting to treat these separately. We limit our discussion and simulations to two spatial dimensions, although the treatment of boundary conditions extends naturally to three dimensions. The use of a projection method restricts the choice of methods for relating the pressure and flux. Implementing an implicit method cannot be easily done using a projection method. This is because the momentum equation is solved for an intermediate velocity, which is not required to be divergence free. The flux at the next time step is not known until after performing the projection. Therefore only the explicit and averaging methods are practical for use with a projection method. We test the explicit method to determine the relevance of the stability restriction in a physical setting. Based on the results from the previous section, we do not use the averaging method.

7.4.1 Numerical Scheme

The flow is between two solid parallel plates. No slip boundary conditions apply at the top and bottom wall. We aim to construct a numerical scheme that allows the pressure drop to be prescribed. Suppose that the plates are located at $y = 0$ and $y = a$, and suppose that the computational domain extends from $x = 0$ to $x = L_2$. We define the pressure drop, $\Delta P_2$, across the domain as

$$\Delta P_2 = \frac{1}{a} \int_0^a p(0, y) - p(L_2, y) \, dy.$$ 

Imagine splitting the physical pressure into two pieces: a linear function in the $x$-direction and the remainder of the pressure. We write this physical pressure as

$$p = \bar{p} + Gx. \quad (7.49)$$
The momentum equation can be written as

$$\rho (u_t + u \cdot \nabla u) = -\nabla \bar{p} - G e_x + \mu \Delta u + f_b,$$  

(7.50)

where $e_x$ is the unit vector in the $x$-direction. The value of $G$ is related to the pressure drop by

$$G = -\frac{\Delta P_2}{L_2},$$  

(7.51)

and its value is prescribed based on the flux. Rearranging equation (7.2) using the definition of $G$ gives

$$G = \frac{12\mu(L - L_2)}{a^3L_2}Q - \frac{\Delta P}{L_2},$$  

(7.52)

Because $G$ is accounting for the pressure drop, the numerical scheme must be constructed so that

$$\int_0^a \tilde{p}(0, y) - \tilde{p}(L_2, y) \, dy = 0.$$  

(7.53)

Our method respects this constraint.

A typical boundary condition applied at outflow boundaries is homogeneous Neumann conditions on all components of the velocity. An interpretation of this condition is that the flow has equilibrated so that it is no longer changing in the $x$-direction. The boundary condition $u_x = 0$ is also equivalent to the statement that there are no normal viscous forces at the outlet. We apply the homogeneous Neumann boundary conditions at both the inlet and the outlet to the intermediate velocity field, so that

$$u_x^* = 0 \text{ and } v_x^* = 0.$$  

(7.54)

Let $\phi$ denote the projection variable as in Chapter 6. On the solid walls the homogeneous Neumann boundary condition is applied to $\phi$, as before. For the inlet and outlet the boundary condition $\phi = 0$ is used. Note that these boundary conditions for the intermediate velocities and for $\phi$ ensure that the projection is orthogonal. The value of $\tilde{p}$ plays the role of the pressure, so that after the projection it is updated as

$$\tilde{p}^{n+1/2} = \tilde{p}^{n-1/2} + \phi - \chi \frac{\nu}{2} \nabla \cdot u^*,$$  

(7.55)

where $\chi$ is either 0 or 1 depending on whether the higher order pressure correction is desired. If $\chi = 0$, then the boundary conditions for $\phi$ ensure that the $\tilde{p}$ does not change on the inlet and outlet of the domain. In this case if the constraint (7.53) is satisfied initially, it will be satisfied for all time. This is also true if $\chi = 1$. Because $u_x^* = 0$ on
these boundaries, \( \nabla \cdot \mathbf{u}^* = v_y^* \), and because \( v^* = 0 \) on the no slip boundaries it follows that

\[
\int_0^a \nabla \cdot \mathbf{u}^*(0, y) \, dy = \int_0^a v_y^*(0, y) \, dy = v^*(0, a) - v^*(0, 0) = 0. \tag{7.56}
\]

Therefore, regardless of which pressure updating scheme is used, our numerical scheme ensures that the constraint (7.53) is satisfied.

### 7.4.2 Nondimensionalization

When there is no obstruction, the pressure gradient is \(-\Delta P/L\), and the steady state velocity profile is

\[
u = \frac{\Delta P}{2\mu L} (a - y). \tag{7.57}
\]

We scale the velocity by the centerline velocity of this undisturbed state, so that

\[
U = \frac{a^2 \Delta P}{8\mu L} \tag{7.58}
\]

is the velocity scale. Lengths are scaled by the separation distance between the plates, \( a \); time is scaled by \( a/U \); and the flux is scaled by \( Ua \). The Reynolds number is

\[
\text{Re} = \frac{\rho Ua}{\mu} = \frac{Ua}{\nu},
\]

where \( \nu = \mu/\rho \) is the kinematic viscosity. The pressure is scaled by \( \rho U^2 \), and so the pressure gradient is scaled by \( \rho U^2/a \). Using these scales to nondimensionalize equation (7.52), the relation between the force due to the pressure drop and the flux is

\[
\frac{\rho U^2}{a} \hat{G} = \frac{12(L - L_2)}{a^3 L_2} aU \hat{Q} - \frac{\Delta P}{L_2}, \tag{7.59}
\]

where \( \hat{G} \) and \( \hat{Q} \) represent nondimensional quantities. Using equation (7.58) to eliminate \( \Delta P \) and rearranging this equation gives

\[
\hat{G} = \frac{12(L - L_2)}{L_2 U a} \hat{Q} - \frac{8L \nu}{L_2 U a}. \tag{7.60}
\]

We define the nondimensional parameter \( \theta \) by

\[
\theta = \frac{L_2}{L}, \tag{7.61}
\]

which represents the fraction of the entire domain, which is represented by the computational domain. Equation (7.60) can be expressed in terms of just two nondimensional parameters as

\[
\hat{G} = \frac{12(1 - \theta)}{\theta \text{Re}} \hat{Q} - \frac{8}{\theta \text{Re}}. \tag{7.62}
\]
Dropping the hats, the nondimensional system of equations is
\[
\begin{align*}
\boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} &= -\nabla \tilde{p} - Ge_x + \frac{1}{\text{Re}} \Delta \boldsymbol{u} + f_b \\
\nabla \cdot \boldsymbol{u} &= 0 \\
Q &= \int_0^1 u(0, y) \, dy \\
G &= \frac{12(1 - \theta)}{\theta \text{Re}} Q - \frac{8}{\theta \text{Re}}.
\end{align*}
\] (7.63)
(7.64)
(7.65)
(7.66)

### 7.4.3 Practical Time Step Restriction

Having scaled the Navier-Stokes equations and the pressure-flux relationship, we now explore the severity of the time step restriction of the explicit method for the pressure-flux relationship for different physical situations. The stability bound for the one-dimensional, model problem applied to the pressure-flux relationship (7.66) is
\[
\Delta t < \frac{\theta \text{Re}}{6hN(1 - \theta)}. 
\] (7.67)

Note that this was derived for a node-centered grid, for which \( h = 1/(N + 1) \), making \( hN \approx 1 \). For a cell-centered grid, \( h = 1/N \), and it can be shown that the same stability bound holds. For our numerical tests in two-dimensions we use a cell-centered grid, and so \( hN = 1 \). In this case, the stability bound simplifies to
\[
\Delta t < \frac{\theta \text{Re}}{6(1 - \theta)}. 
\] (7.68)

Often the advection terms are handled explicitly when solving the Navier-Stokes equations, as discussed in Chapter 6. These explicit treatments of the advection terms are restricted by the CFL condition,
\[
\Delta t \leq \frac{h}{\max(\|\boldsymbol{u}\|)}.
\] (7.69)

We now compare the two time step restrictions (7.68) and (7.69) for different Reynolds numbers.

In the nondimensionalization, the velocity is scaled so that the undisturbed centerline velocity is 1. If the flow is disturbed due to a partial occlusion, the velocity may increase. For the purposes of estimating the severity of the CFL time step restriction (7.69), suppose that \( \max(\|\boldsymbol{u}\|) = 2 \). Suppose that the grid spacing is \( h = 1/64 \). For this scenario, the maximum time step allowed by the CFL condition is \( \Delta t = 1/128 \). For different Reynolds numbers, we determine the minimum value of \( \theta \) that would allow this time step and
satisfy the explicit scheme restriction (7.68). The results of this comparison are displayed in Table 7.1.

Recall that the value of $\theta$ is the fraction of the actual domain represented by the computational domain. For extremely small values of $\theta$ this model may not be appropriate. A more reasonable approach may be to prescribe a constant flux. A lower bound for a reasonable value of $\theta$ is on the order of 0.01. For Reynolds numbers on the order of 100, Table 7.1 shows that the CFL restriction is more severe than the pressure-flux restriction for applicable values of $\theta$. At very low Reynolds numbers, the pressure-flux restriction is more severe than the CFL condition for a large range of $\theta$ values. For Reynolds numbers in between these two extremes, the pressure-flux restriction is relevant for small values of $\theta$.

Recall that this comparison was made assuming that the maximum velocity is 2. If the velocity changes, which restriction is more severe, may change. In general, at high Reynolds numbers, the CFL condition controls the time step and at low Reynolds numbers the pressure-flux controls the time step. For intermediate values of the Reynolds number, the more severe restriction depends on the physical situation. Note that for extremely small Reynolds numbers, the explicit scheme requires that the time step be very small. In this case it may be appropriate to ignore the inertial terms and treat the flow as a Stokes flow, or zero Reynolds number flow. A different nondimensionalization for Stokes flow should be used in this case. For very small Reynolds numbers, it is more appropriate to scale the pressure by $\mu U/a$ rather than $\rho U^2$, because the viscous terms dominate the inertial terms. The resulting pressure-flux relationship analogous to (7.66) is

$$G_S = \frac{12(1 - \theta)}{\theta} Q_S - \frac{8}{\theta},$$

(7.70)

where we have used the subscript S to note that this relationship is for Stokes flow. For zero Reynolds number flow, the CFL condition does not apply, and the only time step restriction results from the pressure-flux relationship. Note that the equations are linear, meaning more numerical methods are available, and the implicit scheme may be practical to implement in this case.

| $\text{Table 7.1: Minimum value of } \theta$ allowed by (7.68) for $\Delta t = 1/128$ |
|---|---|---|---|---|
| $\text{Re}$ | 0.1 | 1 | 10 | 100 |
| $\theta$ | 0.319 | 0.045 | 0.0047 | 0.000047 |
7.4.4 Numerical Tests

We now perform a numerical test of the full Navier-Stokes equations to explore whether the explicit scheme produces numerical oscillations in the situation of a growing blockage. We also explore the role of the two stability restrictions for different Reynolds numbers. All quantities discussed in this section are nondimensional. The computational domain extends from $y = 0$ to $y = 1$ in the vertical direction, and $x = 0$ to $x = 4$ in the horizontal direction. At the beginning of the simulation, the flow is a steady Poiseuille flow. An extra blockage force is added in the $x$-direction to simulate a growing obstruction. This force has the form

$$f_{\text{block}} = -h(x)\left(1 - \tanh(8(y - 0.5t + 0.25))\right)\left(1 - \exp(-t)\right),$$  \hspace{1cm} (7.71)

where

$$h(x) = \frac{F}{4} \left(\tanh(8(x - 1)) - \tanh(8(x - 2))\right),$$  \hspace{1cm} (7.72)

and $F$ is chosen so that there is zero velocity at steady state.

The domain is discretized by a uniform mesh of spacing $h = 1/64$. We consider $\theta = 0.01$, and run the computation for the four Reynolds numbers: 0.1, 1, 10, and 100. The advection terms are handled by first updating the homogeneous advection equation

$$\mathbf{u}_t + \mathbf{u}^n \cdot \nabla \mathbf{u} = 0,$$

and then solving the momentum equation without the advection terms. The advection is performed using a high-resolution, conservative method developed by LeVeque [28] for incompressible flow, and is discussed thoroughly in Section 4.3.1. The advection algorithm is stable, provided the CFL restriction (7.69) is met. The computation uses a variable time step that is 90% of the minimum of the two time step restrictions (7.68) and (7.69).

First it was verified that the stability bound (7.68), which was derived for the one-dimensional model problem, holds for the two-dimensional Navier-Stokes equations. Indeed this is the case. The flux and the maximum time step allowed by the each constraint are displayed in Figure 7.7. At the lowest Reynolds number, 0.1, the time step constraint from the pressure-flux relationship was always at least an order of magnitude smaller than the CFL constraint, and often is even more restrictive. For the highest Reynolds number tested, 100, the CFL constraint was more restrictive, even as the flux got very small. For Reynolds numbers 1 and 10, the more restrictive time step constraint depended on how blocked the domain becomes. When the domain was partially occluded, the maximum
Figure 7.7: The fluxes and the time step restrictions are plotted for the test problem using the Navier-Stokes equations in two dimensions with a growing blockage. The four Reynolds numbers considered are (a) $Re = 0.1$ (b) $Re = 1$ (c) $Re = 10$ (d) $Re = 100$. The CFL condition is more restrictive for higher Reynolds numbers and the explicit handling of the pressure-flux relationship is more restrictive at low Reynolds numbers.
velocity increased around the blockage, and the CFL condition was more restrictive. When most of the domain was blocked, the velocity became very small, and the explicit scheme stability bound became the more restrictive.

None of the numerical simulations showed oscillations in the flux. The minimum value of the parameter $\delta$, discussed when numerically testing for oscillations in the model problem, was about 3.4 or 13.6$\delta_0$. This value is below the values of $\delta$ that were prone to oscillations in the model problem. Note that if $\Delta t$ is some multiple of the stability bound (7.68), then it is proportional to the Reynolds number, and $\delta = \Delta t/(2Reh^2)$ is then independent of the Reynolds number. In this case, the presence of oscillations is also independent of the Reynolds number, and the only way to obtain a large value of $\delta$ is to use an extremely fine spatial mesh or a value of $\theta$ close to 1. If $\theta$ is close to 1, then most of the actual domain is being represented by the computational domain, and a better modeling approach would be to choose the computational domain to correspond with the actual domain.

7.5 Summary

In this chapter we have considered the problem of modeling a pressure driven flow when only a portion of the actual domain is represented by the computational domain. Assuming a steady profile outside the computational domain, we derived a relationship between the pressure drop across and the flux through the computational domain. We analyzed the stability of two numerical schemes: one treats the relationship between the pressure and flux explicitly in time and the other uses an implicit treatment. We derived a stability bound for the explicit scheme and proved that the implicit scheme is unconditionally stable.

A third scheme, called the averaging scheme, was also considered. The assumption behind the averaging scheme is that the pressure depends on the time averaged flux rather than the flux. A discrete version of this method was presented, and it was shown that in different limits this scheme has different interpretations. If the averaging weights depend on the time step, the the average flux is the average over past fluxes weighted by a decaying exponential weight. If the weights stay fixed as the time step goes to zero, the average flux is a first order approximation to the actual flux, provided the weighs are chosen appropriately.

The presence of numerical oscillations in the three schemes was explored numerically.
The explicit scheme was the most prone to numerical oscillations, but only for large viscosities and rapidly changing forces. Using identical parameter values as the explicit scheme, the implicit scheme did not show notable high frequency oscillations. The averaging scheme eliminated the high frequency oscillations, but introduced larger amplitude, lower frequency oscillations when the current value of the flux was weighted too little in the average. To obtain a substantial enlargement of the stability region compared with the explicit scheme, the weight must be small. Based on these numerical tests, we do not recommend using the averaging scheme with small weight. With a weight close to one, the stability is similar to the explicit scheme, and so we conclude that it is not worth using in this case either.

The implicit scheme showed the best performance on the model problem, which was in one spatial dimension. When considering multiple dimensions, the implementation of the implicit scheme is difficult. It is not clear how this could be done using the projection method that we used to solve the Navier-Stokes equations. If the explicit scheme stability bound on the time step were restrictive for a given physical situation, it may be worth investigating implementing the implicit scheme. After scaling the equations for a two-dimensional flow, we showed that only at low Reynolds numbers is the stability bound restrictive on the time step. For high Reynolds numbers, the CFL condition imposed by the advection terms was the more restrictive bound. For moderate Reynolds numbers the physical situation dictated the more restrictive bound. In our simulation of a growing obstruction at moderate Reynolds numbers, which restriction was smaller changed in time, as the velocity speed up and then slowed down.

None of the numerical simulations showed any oscillations in the flux, meaning that the explicit scheme can be used in the physical situations of interest in this dissertation without introducing numerical oscillations. For the problems considered in this dissertation, the Reynolds numbers are not extremely small, and so the explicit scheme is sufficient.

Note that our derivation of the relationship between the pressure and the flux assumed that the flow upstream and downstream is at steady state. It remains to be explored how to include that the flow upstream and downstream need not be steady. Suppose, for example, that pulsatile flow is the undisturbed flow problem. In this case the steady flow pattern is clearly not a Poiseuille flow. Since pulsatile flow is not considered in this dissertation, this issue is not explored further here. In the future this issue should be
explored.
CHAPTER 8

CONCLUSIONS

Understanding the mechanisms of platelet aggregation is an important problem. One particularly difficult aspect of constructing models of aggregate formation is accounting for the interactions between the fluid, the platelets, and the platelet activating chemicals. In this dissertation, we present work on a model, developed by Fogelson [12, 13], appropriate for modeling platelet aggregation on the scale of large arteries. Concentrations of nonactivated platelets, activated platelets, and platelet activator are transported by the fluid. Concentrations of activated platelets interact to form protein links that when stretched by the flow, produce stresses that affect the fluid motion.

Link formation, breaking, and stretching occur on a spatial scale much smaller than that of the flow. The elastic links are accounted for by a distribution function that depends on two sets of spatial variables, so that at each point in the fluid there is a distribution of links over a spatial scale much smaller than the fluid scale. The stresses that affect the fluid arise from integrals of this link distribution function. The presence of two spatial scales makes the model difficult to analyze and expensive to simulate. The model closes on the fluid scale if it is assumed that links are linear springs and the breaking rate is independent of the strain. The assumption of a constant breaking rate is restrictive, and leads to undesirable behavior in the model.

One of the accomplishments of this dissertation is the investigation of a closure model, so that the system closes on the fluid scale, but the breaking rate is not restricted to be constant. The continuum model is a generalization of a type of model that has been applied to networks of crosslinked polymers, although it was derived independently. The closure model presented in this dissertation was inspired by closure models that have been applied to models of crosslinked polymers. One important distinction between polymer models and the continuum model is the changing concentrations of activated platelets and of elastic links.

The ability of the closure model to capture the behavior of the full model is tested
both analytically and numerically. We calculated the stresses using asymptotic analysis for the case of a uniform concentration of activated platelets undergoing a steady shear flow, in the limit of high shearing. Comparing the shear viscosity of the full and closure models, we showed that the two models predicted the same rate of shear thinning (same power law behavior). We numerically compared the shear viscosity over a wide range of shear rates, and the closure model was able to match the behavior of the full model very well.

To further evaluate the closure, we numerically compared its behavior to that of the full model in a more complex setting. In these numerical experiments, activator is added around the stagnation point of a spatially periodic extensional flow. At some later time in the simulation, after some links have formed, an extra force is applied in an effort to pull the aggregate apart. The results from the closure model agreed with the full model qualitatively. That is, the aggregate does not pull apart when the breaking rate is constant, but as the derivative of the breaking rate increases, the aggregate can be ruptured. We introduced some measures to quantify the results of the experiment. When the derivative of the breaking rate was large or small, the predictions of the two models agreed quantitatively, but for moderate values of the derivative, the two models differed. It is not expected that the behaviors in the two models should match perfectly for all breaking rates. However, the reason the two models differed when they did is not clear. More tests must be performed in order to understand these differences.

The development of a closure model has enabled us to explore the model computationally more extensively than was previously possible. For example, simulating the closure model was performed 120 times faster than the full model. Numerically solving even the closed system of equations is a nontrivial computational problem. To solve the equations we employ operator splitting, so that the different terms in the equation are handled separately. For example, solving an advection-reaction-diffusion equation is done by using an advection solver, reaction solver, and diffusion solver.

Advection is handled using a high resolution algorithm involving slope limiters. This algorithm is second order accurate for smooth data, but does not smear sharp interfaces, as would a simpler algorithm such as the standard first order upwinding. Equations involving inverting the Laplacian that arise from diffusion and in the Navier-Stokes solver are performed using multigrid, which is $O(n)$ where $n$ is the number of mesh points. Also, because multigrid is iterative in nature, when the diffusion coefficients are very small, the
The closure model makes the evolution equation for the stresses and aggregation intensity nonlinear. In an early version of the solver, we used the stress and aggregation intensity from the previous time step to compute the breaking rate. However, we found that the equation can be very stiff, and so we implemented a nonlinear solver to deal with the nonlinear breaking rate. Because of the chosen operator splitting, these nonlinear systems decoupled spatially, making for a small system to solve at each grid point.

The numerical methods could be improved further if larger simulations are to be performed with the model. All of the simulations with the model presented in this dissertation were performed with a constant time step and uniform spatial discretization. Adaptive mesh refinement could be implemented to refine features of the flow near the aggregate without having to use a finer mesh for all space and time. Many aspects of the computation could be done in parallel. This would allow for even longer simulations to be performed in a reasonable amount of time.

Before the development of the closure model, all previous simulations of the continuum model were performed in a periodic domain. No simulations had been performed that involved interaction with solid walls. With the addition of solid walls, we encountered an instability in the Navier-Stokes solver that was unexpected. In order to understand the instability, we analyzed a model problem that we believe captures the essence of the instability. This analysis showed that the method was extremely sensitive to the discretization near the boundary. We were able to obtain a stable scheme by carefully choosing the form of the discrete operators near the boundary.

Another numerical challenge arises in simulating a pressure driven flow for which the computational domain represents only a portion of the actual domain. For example, if one were to simulate the flow through a portion of an artery, the flow though the rest of the circulation system must be accounted for in the boundary conditions at the upstream and downstream edges of the domain. We introduce a simple model that couples the flux through the domain and the pressure drop across the domain. We propose numerical methods to account for the fluid outside the domain, and we analyze the stability of these methods for a simple flow and discuss their applicability for more complicated flows.

Putting all these numerical components together, we were able to perform simulations of aggregate growth on the wall of a parallel plate flow chamber. There is a problem with the model equations themselves in the presence of solid walls. The no slip condition...
for platelets is inappropriate because it implies that activated platelets at the wall are permanently attached to the wall, whereas real platelets only attach, via molecular bonds, to damaged portions of the wall. However, it is not clear what the proper boundary condition at the solid wall should be, so we impose the no slip condition and note its effect on the results. This inconsistency at the solid wall raises the question of how to simulate an injured wall. We model the injury by creating a region of the domain near the boundary where platelets flowing through this region become activated.

Simulations of parallel plate flow are intended to evaluate the model’s applicability to simulate platelet aggregation in a physiological setting. Many of the parameters are chosen to be comparable to values for flows in large arteries. The values of the stress formation rate, the stress breaking rate, and the activation rates are not known, and so these parameters are varied while exploring the model behavior. For some parameter sets, the aggregate covered the injury zone quickly and then grew more slowly. For some other parameter sets the aggregate showed uncontrolled growth, both upstream and downstream from the injury zone. Even when the growth seemed confined to the area near the injury zone, downstream growth eventually occurred when the simulation was run for a longer time.

The problem with the boundary conditions is partly responsible for the uncontrolled growth along the wall shown in some of these simulations. Platelets that get activated near the boundary because of activator flowing downstream, are forced to stay on the boundary. The simple activation chemistry must also be improved in future versions of the model to account for inhibitors that may limit growth away from the injury zone.

We demonstrated that the form of the breaking rate function affects the aggregates that result. When the links broke more readily, the platelets that became activated at the upstream edge of the aggregate were not able to attach to the growing aggregate because the fluid stresses were too high. These activated platelets flowed downstream until enough links could form to resist the flow. When the links were able to sustain more energy, they were able to attach at the upstream edge of the aggregate, causing the aggregate to grow vertically, rather than horizontally. These simulations show that the mechanical properties of the links may be important in controlling aggregate growth.

Performing these growth simulations demonstrated some deficiencies with the model’s ability to capture the behavior of real platelet aggregates. All of the aggregates that resulted in these simulations formed with the platelet concentration of the undisturbed
state, which accounts for only 0.3% of the volume. Therefore these aggregates cannot represent actual platelet aggregates, which are made up of densely packed platelets. This problem cannot be easily fixed without significant changes to the model. Nonactivated platelet transport is dominated by advection. In order for the platelet concentration to become significantly larger than the concentration present in the plasma, it must be possible for a low concentration to increase by platelets flowing to this location. Because activated platelets move with the fluid velocity, if the fluid is carrying new platelets to a location in space, the old platelets must be carried away.

Treating the material as a single phase is too restrictive, and our results suggest the need to investigate multiple phase models. In such a model, the fluid and the platelets could move with their own velocity fields, and there would be interaction between these two velocities which depends on the volume fractions of each phase. The fluid could be allowed to flow through small regions of aggregating platelets. This type of model also has the advantage that platelets would not be forced to satisfy the no slip boundary condition.

The work presented in this dissertation is a significant contribution to the modeling of platelet aggregation. The closure model proposed and analyzed appears to capture the behavior of the full model but with a system that closes on the fluid scale. The elimination of the small scale dependence has made exploring the system computationally possible. The results from these computational experiments highlighted areas of the model that must be improved in the future in order to capture the behavior of real platelet aggregates.
APPENDIX A

MODEL DERIVATIONS

A.1 Derivation of equation (2.36)

Begin by multiplying equation (2.31) through by $1/2 S(|y|)yy^T$, and then integrate over all $y$ to get

\[
\mathbf{a} + \mathbf{u} \cdot \nabla \mathbf{a} + \frac{1}{2} \int (y \cdot \nabla \mathbf{u}) \cdot \nabla_y E S(|y|) yy^T dy = \frac{1}{2} \int \left( \alpha(|y|) \phi^2 - \beta(|y|) E \right) S(|y|) yy^T dy.
\]

(A.1)

In order to show that this equation is equivalent to (2.36), we show that

\[
\frac{1}{2} \int (y \cdot \nabla \mathbf{u}) \cdot \nabla_y E S(|y|) yy^T dy = -\mathbb{E} \nabla \mathbf{u} - \left( \mathbb{E} \nabla \mathbf{u} \right)^T
\]

\[
- \frac{1}{2} \int (y^T \nabla u) |y|^{-1} S'(|y|) E(x, y, t) yy^T dy,
\]

and

\[
\frac{1}{2} \int \alpha(|y|) \phi^2 S(|y|) yy^T dy = a_2 \phi^2 \mathbb{E},
\]

(A.2)

with $a_2$ given by

\[
a_2 = \frac{2\pi}{3} \int_0^\infty \alpha(r) S(r) r^4 dr.
\]

(A.3)

We first verify (A.2). Consider the $ij^{th}$ element of the left side of equation (A.2):

\[
\frac{1}{2} \int (y \cdot \nabla \mathbf{u}) \cdot \nabla_y E S(|y|) y_i y_j dy = \frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} \frac{\partial E}{\partial y_n} S(|y|) y_i y_j dy
\]

(A.5)

where we use the convention that summation over repeated indices is assumed. Integrating by parts with respect to $y_n$ gives

\[
\frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} \frac{\partial E}{\partial y_n} S(|y|) y_i y_j dy = \frac{1}{2} \int \frac{\partial y_m}{\partial y_n} \frac{\partial u_n}{\partial x_m} ES(|y|) y_i y_j dy
\]

\[
\quad - \frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} E \frac{\partial}{\partial y_n} \left( S(|y|) \right) y_i y_j dy
\]

(A.6)
The first of the three terms on the right side is zero because
\[ \frac{\partial y_m}{\partial y_n} \frac{\partial u_n}{\partial x_m} = \delta_{mn} \frac{\partial u_n}{\partial x_m} = \frac{\partial u_m}{\partial x_m} = \nabla \cdot \mathbf{u} = 0, \] (A.7)
which follows from the incompressibility of the fluid. Using the product rule to expand
the derivative, the second term on the right side of (A.6) becomes
\[ \frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} E \frac{\partial}{\partial y_n} \left( S (|y|) \right) y_i y_j \, d\mathbf{y} = \frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} E y_n |y|^{-1} S' (|y|) y_i y_j \, d\mathbf{y}, \] (A.8)
which corresponds to the integral on the right side of (A.2). Finally, consider the third
integral on the right side of (A.6). Expanding the derivative using the chain rule gives
\[ \frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} ES (|y|) \frac{\partial}{\partial y_n} (y_i y_j) \, d\mathbf{y} = \frac{1}{2} \int y_m \frac{\partial u_n}{\partial x_m} ES (|y|) \left( \delta_{in} y_j + \delta_{jn} y_i \right) \, d\mathbf{y} \]
\[ = \frac{\partial u_i}{\partial x_m} \sigma_{mj} + \frac{\partial u_m}{\partial x_j} \sigma_{mi} \]
\[ = \sigma \nabla \mathbf{u} + \left( \sigma \nabla \mathbf{u} \right)^T. \] (A.9)

Using (A.7), (A.8), and (A.9) with (A.6) gives (A.2).

We now verify (A.3) and (A.4). Because of symmetry and the fact that the off diagonal
terms are odd functions of at least one component of \( \mathbf{y} \), all the off diagonal terms in (A.3)
must be zero, and so this integral defines a diagonal tensor. Also because of symmetry,
the elements on the diagonal must be the same. Therefore the integral in (A.3) is a
multiple of the identity tensor. To compute this multiple we write the integral as
\[ \frac{1}{2} \int \alpha (|y|) \phi^2 S (|y|) \mathbf{y} \mathbf{y}^T \, d\mathbf{y} = \frac{\alpha \phi^2}{6} \int \alpha (|y|) S (|y|) |y|^2 \, d\mathbf{y}. \] (A.10)
The integrand is only a function of \( |\mathbf{y}| \), and so we change into spherical coordinates to get
\[ \frac{\alpha \phi^2}{6} \int \alpha (|y|) S (|y|) |y|^2 \, d\mathbf{y} = \frac{4\pi \phi^2}{6} \int_0^\infty \alpha (r) S (r) r^4 \, dr. \] (A.11)
From this last equation, (A.3) follows with \( a_2 \) defined by (A.4).
MULTIGRID ON CELL-CENTERED GRIDS

In this appendix we discuss implementing multigrid on a cell-centered grid. This discussion is not intended to be a complete description of multigrid. The problem solved is

\[-\Delta u = f, \tag{B.1}\]

or more generally

\[au - b\Delta u = f, \tag{B.2}\]

on a rectangular domain with either Dirichlet or Neumann conditions on each of the four boundaries. The discretization near the boundary using a cell-centered grid is significantly different from the discretization using a vertex-centered grid, regardless of the solution technique. For a vertex-centered grid, grid points exist on the physical boundary, but for a cell-centered grid, the closest grid point is \(h/2\) away, where \(h\) represents the spacing between mesh points. This is demonstrated in Figure B.1. Not having points on the boundary makes discretizing Dirichlet boundary conditions slightly more difficult, but discretizing Neumann boundary conditions is straightforward. The alignment of the coarse grids is another difference between the two democratizations. For vertex-centered grids, the coarse grid points form a subset of the fine grid points. For cell-centered grids, coarse grid points do not correspond to fine grid points, as is demonstrated in Figure B.2.

B.1 Transfer Operators

The simplest method of obtaining coarse grid data from fine grid data is to average the four fine grid values inside the cell of the coarse grid.

\[u_{i,j}^{2h} = \frac{1}{4} \left( u_{2i,2j}^h + u_{2i-1,2j}^h + u_{2i,2j-1}^h + u_{2i-1,2j-1}^h \right). \tag{B.3}\]
Figure B.1: For a vertex-centered grid (a), the boundary data are given at grid points. For a cell-centered grid (b), the boundary location does not correspond with the boundary points.

Figure B.2: For a vertex-centered grid (a), coarse grid points from a subset of fine grid points. For a cell-centered grid (b), the coarse and fine grids are distinct sets of points.
Note that the prolongation operator obtained from the adjoint of this restriction is just constant interpolation. For vertex-centered grids the prolongation operator which corresponds to the adjoint of the full weighting operator is bilinear interpolation.

For prolongation, one option is to set fine grid values to be equal to the closest coarse grid value, which corresponds to adjoint of the restriction operator (B.3). This interpolation is only first order accurate. To interpolate to second order, the three nearest points can be used, or the four nearest points. The stencils of these operators are given below, using the notation of [40].

\[
\begin{array}{c}
\text{Using the three nearest points:} \\
\frac{1}{4} \\
\begin{pmatrix}
1 & 1 \\
1 & 2 & 2 & 1 \\
1 & 2 & 2 & 1 \\
1 & 1
\end{pmatrix}
\end{array}
\] \quad \text{(B.4)}

\[
\begin{array}{c}
\text{Using the four nearest points:} \\
\frac{1}{16} \\
\begin{pmatrix}
1 & 3 & 3 & 1 \\
3 & 9 & 9 & 3 \\
3 & 9 & 9 & 3 \\
1 & 3 & 3 & 1
\end{pmatrix}
\end{array}
\] \quad \text{(B.5)}

Both of these operators provide second order interpolants. Restriction operators could be defined using the adjoints of these operators, but simple averaging provides a second order accurate restriction with fewer points.

### B.2 Ghost Cells

If the restriction operator used is simple averaging, no modifications are needed near the boundary. The form of the interpolation and Laplacian operators must be modified at points adjacent to the boundary. By placing extra cells called ghost cells around the boundary, the standard operators can be applied at points near the boundary. The value of the function in a ghost cell has no physical meaning. The value is set to whatever it needs to be so that the same form of the operator can be applied at interior points and at points near the boundary. Therefore the value of the ghost cells depends on what operator is being applied. The method for setting them is not only different for different boundary conditions, but it is also different for relaxation, interpolation, and computing the residual. Additionally, the use of ghost cells separates the multigrid routines from the boundary conditions, making the multigrid code more general.
B.2.1 Dirichlet Boundary Conditions

For Dirichlet boundary conditions, the difference equation corresponding to the discretization of (B.1) at points adjacent to the left boundary (but not corner points) is

\[
-\frac{8}{3}u_{1/2,j} - \frac{4}{3}u_{2,j} + 6u_{1,j} - u_{1,j+1} - u_{1,j-1} = h^2 f_{1,j},
\]

where \( u_{1/2,j} \) represents the known Dirichlet data at the boundary. Due to the irregular spacing near the boundary, this is only a first order accurate approximation. The form of this difference equation can be derived in several ways. By computing the gradient using center differencing, the location of this gradient is at cell edges, except at points where the boundary data are involved. The gradient involving a boundary point is midway between the cell center and the cell edge, as shown in Figure B.3. The Laplacian at the cell center is the divergence of this gradient. Following this reasoning gives difference equations of the same form as (B.6).

B.2.1.1 Residuals

Consider a layer of ghost cells surrounding the domain. Equation (B.6) can be replaced with the standard approximation to the Laplacian,

\[
-u_{0,j} - u_{2,j} + 4u_{1,j} - u_{1,j+1} - u_{1,j-1} = h^2 f_{1,j}.
\]

The value of \( u_{0,j} \) has no physical meaning, so it can be assigned any value which gives an at least \( \mathcal{O}(h) \) approximation to the Laplacian. The value which is consistent with

![Figure B.3: The Laplacian is computed near the boundary, by first computing the gradient at the black squares, and then taking the divergence of this gradient.](image)
equation (B.6), is
\[ u_{0,j} = \frac{8}{3} u_{1/2,j} - 2 u_{1,j} + \frac{1}{3} u_{2,j}. \]  
\( (B.8) \)

Equation (B.8), can also be viewed as quadratic extrapolation to the ghost cell. This is the value that must be set before computing the residual.

**B.2.1.2 Point Relaxation**

For Dirichlet boundaries, equation (B.8) seems like a natural choice for setting the ghost cells. Computational experiments show that this method converges for smoothing alone, but when used in a multigrid algorithm, the observed convergence is much slower than for vertex-centered grids.

The form of the relaxation scheme, motivates another way of setting ghost cells. If ghost cells were not used, a point relaxation at a point adjacent to the left boundary would take the form
\[ v_{1,j} = \frac{1}{6} \left( h^2 f_{1,j} + \frac{8}{3} u_{1/2,j} + \frac{4}{3} u_{2,j} + u_{1,j+1} + u_{1,j-1} \right). \]  
\( (B.9) \)

With the use of a ghost cell, equation (B.9) takes the same form as on the interior
\[ v_{1,j} = \frac{1}{4} \left( h^2 f_{1,j} + u_{0,j} + u_{2,j} + u_{1,j+1} + u_{1,j-1} \right). \]  
\( (B.10) \)

The value of the ghost cells can be chosen so that performing a relaxation using (B.10) is equivalent to using (B.9). The ghost cell must have the value
\[ u_{0,j} = \frac{1}{3} h^2 f_{1,j} + \frac{16}{9} u_{1/2,j} - \frac{1}{5} u_{2,j} - \frac{1}{3} u_{1,j+1} - \frac{1}{3} u_{1,j-1}. \]  
\( (B.11) \)

Note that this formula is quite different in character than (B.8).

**B.2.1.3 Interpolation**

The method for setting ghost cells before interpolating depends on the type of interpolation being used (three-point or four-point). In either case, for points adjacent to the boundary a modified interpolation stencil can be worked out using grid points and the boundary data. Only the results for four-point linear interpolation are presented here.
In this case, the ghost cell is set by linearly interpolating in one dimension. On the left edge

\[ u_{0,j} = u_{1/2,j}^b - u_{1,j}. \]  

(B.12)

Unlike relaxation, the corner ghost cell must be set as well. The corner should be set by the formula

\[ u_{0,0} = u_{1/2,1}^b + u_{1,1/2}^b + u_{1,1}. \]  

(B.13)

### B.2.2 Neumann Boundaries

To derive the form of the discrete Laplacian adjacent to the boundary, begin by discretizing the boundary condition

\[ \frac{\partial u}{\partial n} = g. \]  

(B.14)

This boundary condition applies at the physical boundary. A second order discretization at the left boundary is

\[ \frac{u_{1,j} - u_{0,j}}{h} = g_j. \]  

(B.15)

Of course, the value \( u_{0,j} \) is outside the domain, meaning this is the formula for the ghost cell for the residual operator, but not the relaxation formula.

Without the ghost cell, the form of the difference equation at a point adjacent to the left boundary is

\[ -u_{2,j} + 3u_{1,j} - u_{1,j+1} - u_{1,j-1} = h^2 f_{1,j} - hg_j. \]  

(B.16)

A point relaxation at the left boundary would take the form

\[ v_{1,j} = \frac{1}{3} \left( h^2 f_{1,j} - hg_j + u_{2,j} + u_{1,j+1} + u_{1,j-1} \right). \]  

(B.17)

The value of the ghost cell must be set using the same idea used in the Dirichlet case. That is, set the cell so that relaxation near the boundary is equivalent relaxation with a modified stencil. The values used for setting these points are given in the summary.

Before interpolation, the ghost cells are set by linearly interpolating using the boundary data for the slope of the interpolant. The results for the homogeneous case are given in the summary.

### B.2.3 Helmholtz Problem

When solving time dependent problems using a Crank-Nicholson type of scheme, the operator \( aI - b\Delta \) must be inverted at each time step, where \( a \) and \( b \) are positive constants.
The values used for setting ghost cells for the interpolation and the computation of the residual are identical to the previous case. The values used for relaxation are set using the same idea as before (set them so that the relaxation is equivalent to the eliminated case). All the values for different boundary conditions are given in the summary section. The values used for the standard Laplacian can be recovered by setting $a = 0, b = 1$.

\section*{B.3 Summary}

Tables B.1, B.2, and B.3 give the method used for setting the ghost cells for a cell-centered grid. These are appropriate for the problem

\[(aI - b\Delta)u = f,\]  \hfill (B.18)

where $a$ and $b$ are nonnegative constants. In the formulas below it is assumed that $A = h^2a$ and $F = h^2f$. Also, it is assumed that Neumann boundary data has been multiplied by a factor of $h$. The weights used for the interpolation ghost cells are only appropriate for homogeneous boundary conditions. All of these formulas are presented for the left boundary and the bottom left corner. The same weights should be used at other locations with suitable rearrangement.
### Table B.1: Ghost cells weights for relaxation

<table>
<thead>
<tr>
<th></th>
<th>D. Edge</th>
<th>N. Edge</th>
<th>D. Corner</th>
<th>N. Corner</th>
<th>N. Left - D. Bot.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$u_N$</td>
<td>$-2b$</td>
<td>$b$</td>
<td>$(A-8b)/3$</td>
<td>$2b$</td>
<td>$(A+b)/3$</td>
</tr>
<tr>
<td>$u_S$</td>
<td>$-2b$</td>
<td>$b$</td>
<td>–</td>
<td>–</td>
<td>–</td>
</tr>
<tr>
<td>$u_E$</td>
<td>$(A-2b)/3$</td>
<td>$b$</td>
<td>$(A-8b)/3$</td>
<td>$2b$</td>
<td>$-b$</td>
</tr>
<tr>
<td>$F$</td>
<td>$-2$</td>
<td>$1$</td>
<td>$-4$</td>
<td>$2$</td>
<td>$-1$</td>
</tr>
<tr>
<td>data (W)</td>
<td>$(8A+32b)/3$</td>
<td>$-(A+4b)$</td>
<td>$(8A+32b)/3$</td>
<td>$-(A+4b)$</td>
<td>$-(A+4b)$</td>
</tr>
<tr>
<td>data (S)</td>
<td>$-$</td>
<td>$-$</td>
<td>$(A+4b)/3$</td>
<td>$-(A+4b)/3$</td>
<td>$(8A+32b)/3$</td>
</tr>
<tr>
<td>$\delta$</td>
<td>$(A+6b)^{-1}$</td>
<td>$(A+3b)^{-1}$</td>
<td>$(A+8b)^{-1}$</td>
<td>$(A+2b)^{-1}$</td>
<td>$(A+5b)^{-1}$</td>
</tr>
</tbody>
</table>

$\delta$ multiplies all weights

### Table B.2: Ghost cells weights for interpolation

<table>
<thead>
<tr>
<th>Type</th>
<th>Ghost Cell</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dirichlet Edge</td>
<td>$u_{0,j} = -u_{1,j}$</td>
</tr>
<tr>
<td>Neumann Edge</td>
<td>$u_{0,j} = u_{1,j}$</td>
</tr>
<tr>
<td>Dirichlet Corner</td>
<td>$u_{0,0} = u_{1,1}$</td>
</tr>
<tr>
<td>Neumann Corner</td>
<td>$u_{0,0} = u_{1,1}$</td>
</tr>
<tr>
<td>Neumann – Dirichlet Corner</td>
<td>$u_{0,0} = -u_{1,1}$</td>
</tr>
</tbody>
</table>

### Table B.3: Ghost cells weights for computing residuals

<table>
<thead>
<tr>
<th>Type</th>
<th>$u_C$</th>
<th>$u_E$</th>
<th>data (W)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Dirichlet</td>
<td>-2</td>
<td>1/3</td>
<td>8/3</td>
</tr>
<tr>
<td>Neumann</td>
<td>1</td>
<td>-</td>
<td>-1</td>
</tr>
</tbody>
</table>
APPENDIX C

BREAKING RATE FOR GRAB AND PULL EXPERIMENT

The scale factor that is used to convert the derivative of the breaking rate in the closure model to that in the full model for the grab and pull experiments, given in equation (5.12), is derived in this appendix. As was done in Chapter 3, the closure breaking rate can be obtained by replacing squared length with average squared length. The grab and pull experiments presented in this dissertation were first performed with the breaking rates defined for the closure model, and so we must back-engineer the corresponding breaking rate for the full model. To accomplish this task we first move back to dimensional variables. For clarity, dimensionless variables are presented with a hat above them.

Consider the linear breaking rate function (dimensionless) for the closure model

\[ \widehat{\beta}(w) = 1 + b (\hat{w}/w^* - 1), \]  

(C.1)

where \( w^* \) is the average link energy at which links form, defined by

\[ w^* = \frac{2C_4}{C_5}. \]  

(C.2)

Note that the numerator of this expression is \( 2C_4 \) rather than \( 3C_4 \), as in Chapter 4. This difference is because the code used for the full model only accounts for links in two dimensions, not three. Using the definitions of these dimensionless constants, \( w^* \) can be expressed as

\[ w^* = \frac{2C_4}{C_5} = \frac{2a_2Z}{a_0\Sigma}, \]  

(C.3)

where \( Z \) and \( \Sigma \) represent the variable scales for the aggregation intensity and stress.

The breaking rate function (C.1) can be expressed in terms of the dimensional values of the trace of the stress, denoted by \( T \), and the aggregation intensity as

\[ \widehat{\beta}(w) = 1 + b \left( \frac{a_0}{2a_2} \frac{T}{z} - 1 \right). \]  

(C.4)
The ratio \( T/z \) can be expressed in terms of the average square link length as

\[
\frac{T}{z} = \frac{S_0}{2} \left\langle |y|^2 \right\rangle, \tag{C.5}
\]

and (C.4) becomes

\[
\tilde{\beta}(w) = 1 + b \left( \frac{a_0 S_0}{4a_2} \left\langle |y|^2 \right\rangle - 1 \right). \tag{C.6}
\]

By nondimensionalizing \( y \) by the length scale \( L \), we see that the \( b_f \) should be defined by

\[
b_f = \frac{a_0 S_0 L^2}{4a_2} b. \tag{C.7}
\]

Using the definitions of the constants \( a_0 \) and \( a_2 \),

\[
b_f = \frac{\int_0^\infty \alpha(r) \, dr L^2}{\int_0^\infty r^2 \alpha(r) \, dr} \tag{C.8}
\]

Let the length scale \( L \) be defined by the support of the formation function. Expressing the integrals in (C.8) in terms the dimensionless length gives

\[
b_f = \frac{\int_0^1 \alpha(\tilde{r}) \, d\tilde{r}}{\int_0^1 \tilde{r}^2 \alpha(\tilde{r}) \, d\tilde{r}} b, \tag{C.9}
\]

which corresponds to equation (5.12).
REFERENCES


167


