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4-Field Galerkin/Least-Squares Method For Polymer Flows

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ABSTRACT

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In this thesis, a new finite element method, 4-field Galerkin/Least-Squares method, is presented to solve viscoelastic flow problems. The 4-field GLS naturally includes the SUPG and PSPG terms to stabilize the oscillations caused by advection-dominated terms. In addition, it introduces a new variable $L = \nabla \mathbf{v}$, so that the second order derivative of $\mathbf{v}$ is avoided, and the basis functions can be chosen as piecewise linear functions. This feature substantially enlarges the space of the basis and weighting functions. The Galerkin terms in this formulation guarantee that the traction term $\mathbf{n} \cdot \mathbf{T}$ appears naturally by integration by part, which serves as an important boundary condition for free surface flow. Moreover, the 4-field GLS successfully circumvents the LBB condition on velocity and conformation fields. The 4-field GLS is tested with a carefully defined set of benchmark problems for both Newtonian and non-Newtonian fluid. It is found to be robust, accurate and efficient.
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Chapter 1
Introduction

1.1 Introduction

Microstructured liquids, such as blood, colloidal suspensions, liquid crystals, and polymer solutions play a vital role in such diverse fields as biology, medicine, and chemical engineering. As an important branch of fluid dynamics, the research on flows of polymeric liquids began in the 1940s and continues to draw more and more attention. The processing of polymeric liquids requires both synthesis and physical processing. Because the physical properties of microscopic polymeric objects depend dramatically on the arrangement of the molecules, controlling molecular stretch and orientation is crucial for the quality of the final product. To better understand and control these properties, it is desirable to model polymer flows in specified geometries.

Before the advent of numerical simulation, the properties of polymer flows could only be obtained though experimentation, which required costly equipment and complicated operations. As an alternative, numerical simulation allows convenient manipulation of various parameters, and also can be used to simulate flows that are impossible to duplicate in laboratory. Recent advances in computer power have made possible computational modeling of polymer flows in increasingly complex two-dimensional domains, in the presence of free surfaces (Cairncross, Schunk, Baer, Rao and Sackinger 2000), and more recently in three dimensional domains (Xue, Phan-Thien and Tanner 1995).

In polymeric liquids, the stress at a point in space does not depend solely on the
velocity gradient at that point. It must be described by an additional differential
or integral equation. Alternatively, the conformation tensor can be introduced. The
conformation tensor is a coarse-grained representation of molecular properties such
as polymer stretch and orientation. Its evolution is described by a partial differential
equation (Beris and Edwards 1994). The stress at a point in space can then be
expressed in terms of conformation tensor $\mathbf{M}$ and velocity gradient.

Thus, in this approach, the complete set of differential equations required to char-
acterize the flow system now includes the conservation equations for mass, momen-
tum, and conformation. These equation sets are nonlinear and can be solved ana-
lytically only in very rare cases. A great deal of research concentrates on numerical
methods, especially the finite element method.

In contrast to the finite difference method, the finite element method is applied
easily to irregular domains even when free boundaries are present, and the size of
the elements can be controlled by placing finer tessellations in particular areas of the
domain, where high gradients are expected to appear. In addition, basis functions
of first or higher order can be selected to meet the precision requirement of the
simulation.

Like other numerical methods, the finite element method is often limited by sta-
bility issues. Instability is mainly caused by dominant advection terms and by the
violation of certain compatibility conditions, which restrict the allowable combina-
tions of the interpolation for the pressure, velocity and conformation fields. The
stability of the Galerkin form is weakened by the presence of large advective terms,
and the choice of basis functions, which is restricted by the occurrence of differential constraints such as the continuity equation in incompressible flows.

The 4-field Galerkin/Least-Squares formulation proposed in this thesis attempts to resolve these problems. This formulation introduces stabilization terms that counterbalance the effect of advection terms without compromising accuracy. Moreover, it circumvents the compatibility condition, so that velocity, conformation, velocity gradient and pressure interpolations can employ basis functions of the same order. This feature substantially enlarges the feasible space of basis functions and greatly simplifies the process of code parallelization on distributed memory architecture.

In the following sections of this chapter, the concept of constitutive equations is introduced, and then the methodology for modeling of polymer flow is presented.

1.2 Constitutive Equations for Polymeric Liquids

The salient microstructural features of polymer molecules are their length, stiffness, and degree of entanglement, which depend on molecular structure, polymer concentration, solvent quality, and temperature. Moreover, the conformation of the polymer chains and their degree of entanglement can be affected by the velocity gradient in a flow.

Two categories of theories model the microstructure of polymer flow, the fine-grained and the coarse-grained theories.

The fine-grained theories represent microstructure by means of many micromechanical elements obeying stochastic differential equations. For example, polymer molecules can be approximated by a bead-rod model such as that shown in figure 1.1.
Each bead is subjected to forces such as a drag force, a constraint force, and a random force. The drag force is generated by the relative motion between beads and the surrounding fluid; the constraint force is due to the rigidity of the connecting rods; the random force comes from the random collisions between parts of the polymer molecules (beads) and molecules in the fluid. The solvent is assumed to be a continuum, and the velocity of the liquid represents the mean velocity of the solvent. The random force accounts for the fluctuations of solvent velocity around such mean value. A balance of all these forces yields the momentum conservation equation of each bead. A large number of molecules are simulated to obtain statistically meaningful results.

![Diagram showing forces on a bead](image)

**Figure 1.1** Modeling of polymer using a fine-grained theory. Each bead is subject to a drag force, a random force, and a constraint force.

In contrast to the fine-grained models, the coarse-grained theories introduce field variables that are expectation values of microstructural features. The equations of change of the model describe how the microstructural features evolve and how they interact with other variables like velocity and temperature. Coarse-grained models introduce fewer variables and equations than the fine-grained model, and are therefore
computationally economical. The work described in this thesis is restricted to liquids described by coarse-grained model without an explicit entanglement variable.

The relationship between force and deformation is called a constitutive relation. For polymeric liquids, deformation is measured by conformation tensor $\mathbf{M}$, while force is measured by stress tensor $\mathbf{T}$. The definition and equation of change of $\mathbf{M}$, and examples of the relation between $\mathbf{M}$ and stress tensor $\mathbf{T}$, are given in section 1.2.3.

### 1.2.1 Polymer Conformation

At the simplest level of description, the conformation of a polymer molecule can be represented by its end-to-end vector $\mathbf{r}$ as shown in figure 1.2.

![Figure 1.2](image)

**Figure 1.2** Definition of end-to-end vector of a polymer molecule.

The conformation of a set of polymer molecules in a flow is characterized by the distribution function $\Psi(\mathbf{r}, \mathbf{x}, t)$, which is the number of chains per unit mass of liquid whose end-to-end vector falls between $\mathbf{r}$ and $\mathbf{r} + d\mathbf{r}$, and whose center of mass is between $\mathbf{x}$ and $\mathbf{x} + d\mathbf{x}$. The conformation tensor $\mathbf{M}$ is defined as

$$M(\mathbf{x}, t) = \int_{r \in \mathbb{R}^3} d\mathbf{r} \Psi(\mathbf{r}, \mathbf{x}, t) \mathbf{rr}$$ (1.1)
\[ M \] contains important, albeit crude, information about the conformation of the polymer. Being symmetric by definition, \( M \) has three orthogonal eigenvectors that denote the three principal directions along which the polymer is stretched or contracted. The three corresponding eigenvalues denote the magnitude with which the polymer segment is compressed or stretched. If the polymer undergoes no stretching or orientation, \( M = aI \) (Fig. 1.3).

**Figure 1.3** Molecular interpretation of the eigenvalues and eigenvectors of the conformation dyadic (reprinted from Pasquali (2000), with permission). If the polymer undergoes no stretching or orientation, \( M = aI \) as shown in the left figure. The direction and degree of stretching is denoted by the eigenvector and eigenvalues of \( M \).

As any extensive variable, \( M \) obeys a conservation equation:

\[
\frac{\partial}{\partial t} \rho M = -\nabla \cdot (\nu \rho M + J_M) + M_g
\]  

(1.2)

where \( J_M \) is the diffusive flux of conformation, and \( M_g \) is the generation term, which includes conformation changes induced by flow and molecular relaxation.

The generation term \( M_g \) includes the contributions of molecular stretching, molecular relative orientation, solid body rotation and molecular relaxation. Pasquali (2000) proposed the following transport equation for the flows of untangled polymer
solutions:

\[
\frac{\partial M}{\partial t} + \mathbf{v} \cdot \nabla M = \left( \frac{1}{(c_p N)^2} \right) M_g \quad = \quad 2\xi \frac{D : M}{I : M} \quad \text{molecular stretching}
\]

\[
+ \zeta (M \cdot D + D \cdot M - 2 \frac{D : M}{I : M} - M)
\quad \text{molecular orientation}
\]

\[
+ \mathbf{M} \cdot \mathbf{W} + \mathbf{W}^T \cdot \mathbf{M}
\quad \text{solid-body rotation}
\]

\[
- \frac{1}{\lambda} (g_0 I + g_1 M + g_2 M^2)
\quad \text{molecular relaxation}
\]

where \(D = \nabla \mathbf{v} + \nabla \mathbf{v}^T\) is the rate of strain, and \(\mathbf{W} = \nabla \mathbf{v} - \nabla \mathbf{v}^T\) is the vorticity. \(\xi(M)\) and \(\zeta(M)\) denote the polymer resistance to stretching and orientation respectively.

### 1.2.2 Constitutive Relations

A constitutive relation is the relation between stress and deformation. In polymer flow, the stress dyadic \(\mathbf{T}\) is split into isotropic, viscous, and elastic components as

\[
\mathbf{T} = -p \mathbf{I} + \tau + \sigma
\]

where \(\tau\) is the viscous stress, \(p\) is the pressure, and \(\sigma\) is the elastic stress.

The viscous stress \(\tau\) obeys Newton’s law of viscosity,

\[
\tau = 2\mu D
\]

By using an extension of continuum thermodynamics, Pasquali (2000) obtained the following constitutive relation of the elastic stress:

\[
\sigma_{\text{elastic}} = 2\rho \xi \frac{M}{I : M} \frac{\partial a}{\partial M}
\quad \text{stress by molecular stretching}
\]
\[ +2\rho \zeta \left( -\frac{M}{I:M} M : \frac{\partial a}{\partial M} + M : \frac{\partial a}{\partial M} \right) \]

where \( a(T, M) \) is the Helmholtz free energy. The same result was derived previously by Grmela and Carreau (1987) with other methods.

Equation 1.6 provides an important relationship between conformation, Helmholtz free energy, and elastic stress, which couples the conformation to the momentum equation, as discussed in detail in section 1.2.3.

1.2.3 Examples of Constitutive Equations

A constitutive model is a set of assumptions and idealizations about the molecular or structural forces and motions that produce stress. Constitutive equations can be used in numerical simulations to test the credibility of the corresponding constitutive model.

Most of the well-known constitutive equations can be expressed with different forms of the constitutive functions \( \xi(M) \), \( \zeta(M) \), \( g_0(M) \), \( g_1(M) \), \( g_2(M) \), and \( a(M) \) in equations 1.3 and 1.6. Three different models of polymer behavior are included in this section.

Oldroyd-B Model

The Oldroyd-B model represents the polymer as a dumbbell where the beads are connected by a linear (Hookean) spring (Macosko 1994). The following assumptions are made in the model: molecules follow large-scale deformations affinely; thus \( \zeta = 1, \xi = 1 \); the molecular relaxation rate depends linearly on the distance of the conformation tensor from its equilibrium value, i.e. \( g_0 = -1, g_1 = 1, g_2 = 0 \); the Oldroyd-B
model has the following equation of change of conformation from equation 1.3.

$$\frac{\partial \mathbf{M}}{\partial t} = -\mathbf{v} \cdot \nabla \mathbf{M} + \nabla \mathbf{v}^T \cdot \mathbf{M} + \mathbf{M} \cdot \nabla \mathbf{v} - \frac{1}{\lambda} (\mathbf{M} - \mathbf{I})$$  (1.7)

Introducing the Upper Convected Derivative:

$$\nabla \mathbf{M} = \frac{\partial \mathbf{M}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{M} - \nabla \mathbf{v}^T \cdot \mathbf{M} - \mathbf{M} \cdot \nabla \mathbf{v}$$  (1.8)

yields a more compact version of the Oldroyd-B,

$$\nabla \mathbf{M} = -\frac{1}{\lambda} (\mathbf{M} - \mathbf{I})$$  (1.9)

The elastic stress $\sigma$ is proportional to the conformation $\mathbf{M}$ as

$$\sigma = G \mathbf{M}$$  (1.10)

and the expression of the isothermal Helmholtz free energy is

$$a = \frac{G}{2\rho} [\text{tr} \mathbf{M} - 3]$$  (1.11)

Giesekus Model

Giesekus (1966) proposed a class of constitutive equations based on anisotropic drag. Derived from the simple dumbbell theory for dilute solutions, this theory added a direction-dependent friction coefficient.

Like the Oldroyd model, the Giesekus model also assumes that the dumbbells follow large-scale deformations affinely, $\zeta = 1$, $\xi = 1$; and the rate of relaxation is a quadratic function of the distance of the conformation tensor from its equilibrium value, i.e. $g_0 = \alpha - 1$, $g_1 = 1 - 2\alpha$, $g_2 = \alpha$. The corresponding constitutive equation is

$$\nabla \mathbf{M} = -\frac{1}{\lambda} \left[ (\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2 \right]$$  (1.12)
The elastic stress $\sigma$ is also proportional to the conformation $M$

$$\sigma = GM$$  \hspace{1cm} (1.13)

and the expression of the isothermal Helmholtz free energy is

$$a = \frac{G}{2\rho} [\text{tr} M - 3]$$  \hspace{1cm} (1.14)

**Affinely deforming, finitely extensible molecules (FENE-P Model)**

The FENE-P model (Bird, Armstrong and Hassager 1987) represents a polymer as a dumbbell with a nonlinear spring connecting the beads. Besides affine deformation, the FENE-P model introduces the important assumptions that the molecules have finite maximum extension, and their rate of relaxation grows infinitely fast as the average molecular extension approaches its maximum value. Thus in the FENE-P Model, $\xi = 1$, $\zeta = 1$, $g_0 = -1$, $g_1 = 1$, $g_2 = \frac{b-1}{b-\frac{1}{3}}$, where $b$ is the ratio of the maximum length square of the polymer molecules to their equilibrium average length square, which controls the molecular extensibility. The FENE-P model neglects hydrodynamic interaction. It has the following constitutive equation:

$$\nabla M = -\frac{1}{\lambda} \left( \frac{b-1}{b-\frac{1}{3}} M - I \right)$$  \hspace{1cm} (1.15)

The elastic stress $\sigma$ and free energy $a$ have the following expressions:

$$\sigma = G \frac{b-1}{b-\frac{1}{3}} M$$  \hspace{1cm} (1.16)

$$a = -\frac{3G}{2\rho} (b-1) \ln \frac{b-\frac{1}{3}}{b-1}$$  \hspace{1cm} (1.17)

Hereafter, the Giesekus model and Oldroyd-B model are used as examples to illustrate different finite element formulations.
1.3 Modeling of Polymer Flows

1.3.1 Governing Equations

The equations that govern the flow of a polymer solution include the conservation of mass, momentum, and equation of change of conformation. Assuming that the liquid has constant density, and using the Giesekus model as an example, the governing equations for steady state can be written as:

\[ \nabla \cdot \mathbf{v} = 0 \quad (1.18) \]

\[ \rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \cdot \left[ -p \mathbf{I} + \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T) + GM \right] = 0 \quad (1.19) \]

\[ \mathbf{v} \cdot \nabla \mathbf{M} - \nabla \mathbf{v}^T \cdot \mathbf{M} - \mathbf{M} \cdot \nabla \mathbf{v} + \frac{1}{\lambda} \left[ (\alpha - 1) \mathbf{I} + (1 - 2\alpha)\mathbf{M} + \alpha \mathbf{M}^2 \right] = 0 \quad (1.20) \]

A new variable \( \mathbf{L} = \nabla \mathbf{v} \) is introduced to obtain the following set of first-order partial differential equations:

\[ \nabla \cdot \mathbf{v} = 0 \quad (1.21) \]

\[ \rho \mathbf{v} \cdot \mathbf{L} - \nabla \cdot \left( -p \mathbf{I} + \mu (\mathbf{L} + \mathbf{L}^T) + GM \right) = 0 \quad (1.22) \]

\[ \mathbf{v} \cdot \nabla \mathbf{M} - \mathbf{L}^T \cdot \mathbf{M} - \mathbf{M} \cdot \mathbf{L} + \frac{1}{\lambda} \left[ (\alpha - 1) \mathbf{I} + (1 - 2\alpha)\mathbf{M} + \alpha \mathbf{M}^2 \right] = 0 \quad (1.23) \]

\[ \mathbf{L} - \nabla \mathbf{v} + \frac{1}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} = 0 \quad (1.24) \]

1.3.2 Finite Element Formulation

Here a new Galerkin/Least-Squares (GLS) method is introduced to build the weak form for this problem. \( q, w, S, \) and \( E \) are sets of weighting functions for \( p, v, M \) and \( L \). Each independent variable is approximated by a linear combination of a finite number of basis functions as follows.

Pressure: \[ p = p^0 q^0 \]
Velocity: \( \mathbf{v} = \psi_\alpha^p \mathbf{w}_i^\alpha, \quad \mathbf{w}_i^\alpha = \psi_\alpha^v \mathbf{e}_i \)

Conformation: \( \mathbf{M} = M_{ij}^\alpha \mathbf{S}_{ij}^\alpha, \quad \mathbf{S}_{ij}^\alpha = \psi_\alpha^M \mathbf{e}_i \mathbf{e}_j \)

Velocity Gradient: \( \mathbf{L} = L_{ij}^\alpha \mathbf{E}_{ij}^\alpha, \quad \mathbf{E}_{ij}^\alpha = \psi_\alpha^L \mathbf{e}_i \mathbf{e}_j \) \( (1.25) \)

where \( \psi_\alpha^p, \psi_\alpha^v, \psi_\alpha^M, \psi_\alpha^L \) are sets of scalar basis functions for pressure, velocity, conformation tensor and velocity gradient and \( \mathbf{e}_i, \mathbf{e}_j \) are orthonormal basis vectors. Summation on the Greek and italic repeated indices is implied. The linear combination of scalar basis function with unit vectors or tensors forms the vector/tensor weighting functions \( \mathbf{w}_i^\alpha, \mathbf{S}_{ij}^\alpha \) and \( \mathbf{E}_{ij}^\alpha \). The dummy index \( \alpha \) represents the basis functions and their coefficients. Using these basis functions, the following Galerkin/Least-Squares formulation can be obtained:

\[
\int_\Omega \left( (q + \tau_{\text{cond}} \rho \nabla \cdot \mathbf{w}) (\nabla \cdot \mathbf{v}) \right) d\Omega \\
+ \int_\Omega \left\{ \mathbf{w} + \tau_{\text{trans}} \left[ \rho \mathbf{v} \cdot \nabla \mathbf{w} + \rho \mathbf{w} \cdot \nabla \mathbf{v} + \nabla q - \nabla \cdot \mathbf{u} (\mathbf{E} + \mathbf{E}^T) - \nabla \cdot \mathbf{S} \right] \right\} \\
\cdot \left[ \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p - \nabla \cdot \mu (\mathbf{L} + \mathbf{L}^T) - \nabla \cdot (\mathbf{G} \mathbf{M}) \right] d\Omega \\
+ \int_\Omega \frac{1}{\eta} \left\{ \mathbf{S} + \tau_{\text{const}} \left[ -\lambda (-\mathbf{w} \cdot \nabla \mathbf{M} - \mathbf{v} \cdot \nabla \mathbf{S} + \mathbf{E}^T \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{E} + \mathbf{L}^T \cdot \mathbf{S} + \mathbf{S} \cdot \mathbf{L}) \\
+ (1 - 2\alpha) \mathbf{S} + \alpha \mathbf{M} \cdot \mathbf{S} + \alpha \mathbf{S} \cdot \mathbf{M} \right] \right\} \\
\cdot \left[ -\lambda (-\mathbf{w} \cdot \nabla \mathbf{M} + \mathbf{L}^T \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{L}) + (\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2 \right] d\Omega \\
+ \int_\Omega \mu \left[ \mathbf{E} + \tau_{\text{gradv}} (\mathbf{E} - \nabla \mathbf{w} + \frac{1}{3} (\nabla \cdot \mathbf{w}) \mathbf{I}) \right] \\
\cdot \left[ \mathbf{L} - \nabla \mathbf{v} + \frac{1}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} \right] d\Omega = 0 \quad (1.26) \]

Note that \( \nabla \cdot \mathbf{S} \) is a variation of \( \nabla \cdot \mathbf{G} \mathbf{M} \). Equation 1.26 yields four weighted residual equations by setting three out of the four weighting functions to zero in
turn. The numerical solution to this equation set and stabilization techniques will be discussed in detail in chapter 3.

1.4 Thesis Organization

The main effort of this research is to assess the stability, accuracy, and efficiency of the proposed 4-field GLS formulation. Substantial effort has been devoted to the implementation of this formulation in a finite element program, which has a robust frontal solver with LU factorization with full pivoting. Extensive tests with a carefully designed set of benchmark problems demonstrate that the 4-field GLS method gives satisfactory performance for solving viscoelastic problems.

Chapter 2 reviews the development of finite element formulations for solving viscoelastic flow problems in the last two decades. The discussion focuses on the EVSS based methods and several weighted residual formulations with stabilization such as GLS and SUPG methods. Chapter 3 details the 4-field GLS method and the corresponding weighted residual equations and solution strategy. Chapter 4 presents the numerical simulations of the 4-field GLS with Newtonian benchmark problems: lid-driven-cavity, flow around a cylinder, 4-to-1 contraction and stick-slip problem. Chapter 5 examines the performance of the 4-field GLS method on viscoelastic flows, including flow around a cylinder, 4-to-1 contraction and stick-slip problem. Chapter 6 is a summary of the 4-field GLS method.
Chapter 2
Literature Review

2.1 Introduction

In the last decade, significant progress has been made in finite element methods for viscoelastic flow, especially regarding to the stabilization problem.

A major source of numerical instability is the dominant advection term in the constitutive equation. With the Galerkin formulation, numerical oscillation appears in computed stress. This problem can be resolved by using finer mesh, more accurate and smooth interpolation of velocity gradient, or adding Streamline-Upwind/Petrov-Galerkin (SUPG) or Discontinuous-Galerkin (DG) terms to the Galerkin formulation. Some methods not only provide stability in advection-diffusion problem, but also address other issues, such as the Babuska and Brezzi (LBB) condition.

The LBB condition is a compatibility requirement that restricts the feasible spaces of basis and weighting functions. It is also referred to as the inf-sup condition. Violation of this condition causes spatial oscillations in the computed pressure field. During the past two decades, extensive studies have been carried out to find combinations of basis functions that satisfy the LBB condition, or to formulate alternative weighted residual forms whose stability can be proved directly, without recourse to the LBB condition (Brezzi and Pitkaranta 1984). Many combinations of function spaces that satisfy the LBB condition in Newtonian flows have been reviewed by Stenberg (1990). Since the early 1990s, the idea of combining the traditional Galerkin formulation with a least-squares form started to gain attention. The Galerkin/Least-Squares formu-
lation can successfully circumvent the LBB condition; its application to compressible and incompressible flows, as well as other systems, further proves its flexibility (Hughes, Franca and Hulbert 1989).

From the mathematical point of view, these stabilization methods fall into two classes. The first one focuses on manipulating the strong form of the equation to make explicit the elliptic term; the EVSS, and DEVSS methods fall into this class. These methods are discussed in section 2.3. The second class focuses on formulating a stable weak form; this class includes the SUPG and GLS methods. These methods are introduced in section 2.4.

2.2 Governing Equations

The physical problem considered here is the steady state flow with no body force. For simplicity, the Giesekus model will be examined to demonstrate the mathematical formulation. The momentum equation, continuity equation, and the constitutive equation form the following set of governing equations:

\[ \nabla \cdot \mathbf{v} = 0 \quad (2.1) \]

\[ \rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \cdot \mathbf{T} = 0 \quad (2.2) \]

\[ \mathbf{v} \cdot \nabla \mathbf{M} - \nabla \mathbf{v}^T \cdot \mathbf{M} - \mathbf{M} \cdot \nabla \mathbf{v} + \frac{1}{\lambda} [(\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2] = 0 \quad (2.3) \]

where the total stress \( \mathbf{T} \) is composed of the following contributions:

\[ \mathbf{T} = -\rho \mathbf{I} + \tau + \sigma \quad (2.4) \]

where \( \tau \) is a general viscous stress with viscosity \( \mu \):

\[ \tau \equiv \mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T) \quad (2.5) \]
and $\sigma$ is the elastic contribution.

$\Omega$ is the computational domain, bounded by $\Gamma$. $\Gamma$ is composed of $\Gamma_v$ and $\Gamma_h$, where the following boundary conditions hold:

$$\mathbf{v} = \mathbf{v}_0 \text{ on } \Gamma_v \quad (2.6)$$

$$\mathbf{n} \cdot \mathbf{T} = t \text{ on } \Gamma_h \quad (2.7)$$

where $\mathbf{v}_0$ and $t$ are specified velocity and traction on boundaries.

### 2.3 Elastic Viscous Split Stress

The stability of a numerical solution obtained by applying the Galerkin method to the momentum equation is tied to the presence of the viscous term (Sun, Smith, Armstrong and Brown 1999). The EVSS method increases the viscous contribution by splitting the stress into viscous and elastic parts. The splitting is deemed to be legitimate because the additional stabilization term is zero in the strong form and becomes vanishingly small in the weak form when approaching the exact solution (Rajagopalan, Armstrong and Brown 1990).

#### 2.3.1 DEVSS Formulation

A Discrete Elastic Viscous Split Stress (DEVSS) method was introduced by Guenette and Fortin (1995). In this method, an elliptic stabilization term is added to the discrete version of the momentum equation.

Equation 2.3 becomes an algebraic equation relating $\mathbf{M}$ and $\nabla \mathbf{v}$ when the flow is in a stagnation region where $\mathbf{v} = 0$. Therefore, Szady, Salamon, Liu, Armstrong and Brown (1995) introduced a new variable $\mathbf{L} = \nabla \mathbf{v}$, which has the same basis function
as $M$, to satisfy the compatibility requirement of the momentum equation. Moreover, the introduction of $L$ makes it possible to approximate all the variables, except for $v$, with first order continuous basis functions.

After adding the term

$$\nabla \cdot \eta_a (\nabla v + \nabla v^T) - \nabla \cdot \eta_a (L + L^T)$$

to the momentum equation 2.2, the following DEVSS formulation is obtained:

$$-\rho v \cdot \nabla v + \nabla \cdot (pI + \sigma + \mu(\nabla v + \nabla v^T)) + \nabla \cdot \eta_a (\nabla v + \nabla v^T - L - L^T) = 0$$

Guenette and Fortin (1995) showed that the term $\nabla \cdot \eta_a (\nabla v + \nabla v^T) - \nabla \cdot \eta_a (L + L^T)$ stabilizes the numerical method, and $\eta_a$ is a stabilization coefficient which is constant in this formulation.

As proposed by Pasquali and Scriven (2002) and Pasquali (2000), this formulation can also be interpreted as a momentum equation, in which the viscous stress $\tau$ is defined as

$$\tau = \mu(L + L^T) + \eta_a(\nabla v + \nabla v^T - L - L^T)$$

(2.9)

In the DEVSS formulation, the additional term goes to zero if exact solution is achieved.

2.4 Weighted Residual Formulations

The Streamline-Upwind/Petrov-Galerkin (SUPG) method (Marchal and Crochet 1987) and the Discontinuous-Galerkin (DG) method (Fortin and Pierre 1987) can successfully overcome the difficulties associated with the advective term. EVSS-based
methods are always combined with DG or SUPG to achieve better performance. Liu, Bornside, Armstrong and Brown (1998) used the DEVSS-G/SUPG method on two-dimensional flow around a cylinder in a channel, while Sun et al. (1999) applied DAVSS/DG and DAVSS/SUPG methods to the same problem. In this section, several stabilization techniques are reviewed.

As a basis for all the stabilization formulation in this section, the Galerkin form will be reviewed for reference.

2.4.1 Galerkin Formulation

Choosing \(q, w, S\) as the weighting functions of pressure, velocity, and conformation tensor, the following weak form can be constructed:

\[
\begin{align*}
    r &= \int_{\Omega} q \nabla \cdot v d\Omega + \int_{\Omega} w \cdot (\rho v \cdot \nabla v - \nabla \cdot \mathbf{T}) d\Omega \\
    &+ \int_{\Omega} S : \left\{ \nabla M + \frac{1}{\lambda} \left[ (\alpha - 1)I + (1 - 2\alpha)M + \alpha M^2 \right] \right\} d\Omega \\
    &= 0
\end{align*}
\]  

(2.10)

where the upper convected derivative \(\nabla\) is defined in equation 1.8.

The traction term \(n \cdot T\) appears naturally by integrating by parts the Galerkin term in the momentum equation and using the divergence theorem:

\[
\begin{align*}
    \int_{\Omega} w \cdot \nabla \cdot T d\Omega \\
    &= \int_{\Omega} \nabla \cdot (w \cdot T^T) d\Omega - \int_{\Omega} T^T : (\nabla w) d\Omega \\
    &= \int_{\Gamma} n \cdot T \cdot w d\Gamma - \int_{\Omega} T : (\nabla w) d\Omega \\
    &= \int_{\Gamma} t \cdot w d\Gamma - \int_{\Omega} T : (\nabla w) d\Omega
\end{align*}
\]  

(2.11)
where \( t \) is the prescribed traction on the boundary \( \Gamma \) and \( T = T^T \). Then the Galerkin residual becomes:

\[
\tau = \int_\Omega q \nabla \cdot v d\Omega + \int_\Omega w \cdot (\rho v \cdot \nabla v) d\Omega \\
- \int_\Gamma t \cdot w d\Gamma + \int_\Omega T : (\nabla w) d\Omega \\
+ \int_\Omega \mathbf{S} : \left\{ \nabla \mathbf{M} + \frac{1}{\lambda} \left[ (\alpha - 1)I + (1 - 2\alpha)M + \alpha M^2 \right] \right\} d\Omega \\
= 0 \tag{2.12}
\]

### 2.4.2 SUPG Formulation

The SUPG formulation was proposed by Brooks and Hughes (1982) to stabilize flows at high Reynolds number. This formulation is achieved by introducing \( w + \tau_{SUPG} v \cdot \nabla w \) as the new momentum weighting function, where \( w \) is the original weighting function for the Galerkin form.

The SUPG formulation of the problem is:

\[
\tau = \int_\Omega q \nabla \cdot v d\Omega + \int_\Omega w \cdot (\rho v \cdot \nabla v) d\Omega \\
- \int_\Gamma t \cdot w d\Gamma + \int_\Omega T : (\nabla w) d\Omega \\
+ \int_\Omega \mathbf{S} : \left[ \nabla \mathbf{M} + \frac{1}{\lambda} \left( (\alpha - 1)I + (1 - 2\alpha)M + \alpha M^2 \right) \right] d\Omega \\
+ \sum_{e} \int_{\Omega_e} \delta \cdot (\rho v \cdot \nabla v - \nabla \cdot \mathbf{T}) d\Omega \\
= 0 \tag{2.13}
\]

where the SUPG function \( \delta \) is defined as

\[
\delta = \tau_{SUPG} v \cdot \nabla w \tag{2.14}
\]
The stabilization coefficient $\tau_{SUPG}$ is selected as

$$\tau_{SUPG} = \frac{h}{2 \|v\|_h} z(Re_v)$$  \hspace{1cm} (2.15)

as proposed by Franca and Muller (1992), where $Re_v$ is the element Reynolds number, based on the local velocity $v$ and element length $h$.

$$Re_v = \frac{\|v\|_h}{2\mu}$$  \hspace{1cm} (2.16)

The element length $h$ is defined to be equal to the diameter of the circle which is area-equivalent to the element formula. The function $z(Re)$ is defined as

$$z(Re) = \begin{cases} Re/3, & 0 \leq Re \leq 3, \\ 1, & 3 < Re. \end{cases}$$  \hspace{1cm} (2.17)

SUPG is a consistent weak form, i.e., the formulation is satisfied by the exact solution. This property ensures that oscillations are prevented without introducing excessive numerical diffusion or “over-stabilization”. SUPG has been successfully applied to both incompressible and compressible flows.

2.4.3 PSPG and GLS Formulation

The basis functions have to satisfy the compatibility conditions arising from the weighted residual form. However, different weak forms require different compatibility conditions. PSPG and GLS allow the use of basis functions with the same order of interpolation.

The LBB Condition

The governing equations 2.1–2.3 show that the pressure enters the system through the term $\nabla \cdot \mathbf{T} = -\nabla p + \nabla \cdot (\mathbf{\tau} + \mathbf{\sigma})$. The function of the LBB condition is to guar-
antee that the contribution from the pressure is properly represented in the weighted residual. In the weighted residual form, the pressure term is represented by the term \( \int_{\Omega} p \mathbf{I} : \nabla \mathbf{w} d\Omega \) in equations 2.10 and 2.13. If, e.g., the pressure basis function is symmetric with respect to the center of the element, and the velocity weighting function \( \mathbf{w} \) is linear, then

\[
\int_{\Omega} p \mathbf{I} : \nabla \mathbf{w} d\Omega = \int_{\Omega} p \nabla \cdot \mathbf{w} d\Omega = 0 \tag{2.18}
\]

In this case the contribution from pressure to the weighted residual form is totally eliminated.

Therefore, the feasible spaces of trial function need to satisfy some compatibility conditions. Brezzi and Babuska investigated the mathematical framework of this problem and developed the well-known LBB condition (Brezzi and Fortin 1991):

\[
\inf_{0 \neq q \in \mathcal{P}_h} \sup_{0 \neq \mathbf{w} \in \mathcal{V}_h} \frac{\langle \nabla \cdot \mathbf{w}, q \rangle}{\|\mathbf{w}\|_1 \|q\|_0} \geq C > 0 \tag{2.19}
\]

where \( \mathcal{P}_h \) and \( \mathcal{V}_h \) are the spaces of pressure and velocity basis functions. The LBB condition has the following equivalent form

\[
\sup_{0 \neq \mathbf{w} \in \mathcal{V}_h} \frac{\langle \nabla \cdot \mathbf{w}, q \rangle}{\|\mathbf{w}\|_1} \geq C \|q\|_0 \quad \forall q \in \mathcal{P}_h \tag{2.20}
\]

which guarantees that the contribution from each pressure basis function in at least one element is large enough to be represented in the weighted residual form, so that it can produce a good approximation to the exact solution of the original differential equation.

The basis functions of the conformation tensor also need to satisfy the compatibility condition, which requires the interpolation to be rich enough with respect to
the velocity interpolation.

Although numerous feasible combinations of velocity and pressure have been developed, the LBB condition is still a very inconvenient restriction from an implementational standpoint, particularly for three-dimensional problems. Both the PSPG and the GLS formulations can successfully circumvent the LBB condition.

**PSPG Formulation**

As a generalization of the Petrov-Galerkin formulation, the Pressure-Stabilized Petrov-Galerkin (PSPG) (Tezduyar and Shih 1992) adds to the Galerkin form a set of integrals over elements. Such integrals involve the product of the residual of the momentum equation and the gradient of the pressure weighting function, and introduces the term with the form \( \nabla q \cdot \nabla p \) to give "adequate" representation to pressure. The PSPG form of the governing equations can be written as:

\[
\begin{align*}
  r &= \int_\Omega q \nabla \cdot \mathbf{v} \, d\Omega + \int_\Omega \mathbf{w} \cdot (\rho \mathbf{v} \cdot \nabla \mathbf{v}) \, d\Omega \\
  &\quad - \int_\Gamma t \cdot \mathbf{w} \, d\Gamma + \int_\Omega \mathbf{T} : (\nabla \mathbf{w}) \, d\Omega \\
  &\quad + \int_\Omega \mathbf{S} : \left[ \nabla \mathbf{M} + \frac{1}{\lambda} ((\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2) \right] \, d\Omega \\
  &\quad + \sum_{e=1}^{n_e} \int_{\Omega_e} \tau_{PSPG} \nabla q \cdot (\rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \cdot \mathbf{T}) \, d\Omega \\
  &= 0
\end{align*}
\]  

(2.21)

where

\[
\tau_{PSPG} = \frac{h}{2 \| \mathbf{v} \| z(R_e^*)} 
\]  

(2.22)
and \( Re \) has been defined in equation 2.16. \( h \) and \( \tau(Re) \) have the same definition used in the SUPG formulation.

**Galerkin/Least-Squares Formulation**

The Galerkin/Least-Squares formulation for Newtonian flow of the momentum equation adds a least-squares term of the momentum equation to the traditional Galerkin weak form. The weak form of the governing equations is:

\[
\begin{align*}
  r & = \int_{\Omega} q \nabla \cdot \mathbf{v} d\Omega + \int_{\Omega} \mathbf{w} \cdot (\rho \mathbf{v} \cdot \nabla \mathbf{v}) d\Omega \\
  & - \int_{\Gamma} t \cdot \mathbf{w} d\Gamma + \int_{\Omega} \mathbf{T} : (\nabla \mathbf{w}) d\Omega \\
  & + \int_{\Omega} \mathbf{S} : \left[ \nabla \mathbf{M} + \frac{1}{\lambda} \left( (\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2 \right) \right] d\Omega \\
  & + \sum_{e=1}^{n_{el}} \int_{\Omega_e} \tau_{GLS} \left[ \rho \mathbf{v} \cdot \nabla \mathbf{w} + \rho \mathbf{w} \cdot \nabla \mathbf{v} - \nabla \cdot \mathbf{S} \right] \cdot [\rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla \cdot \mathbf{T}] d\Omega \\
  & = 0
\end{align*}
\]

(2.23)

\( \tau_{GLS} \) has the same expression as \( \tau_{SUPG} \) reported in equations 2.15 to 2.17. The first five integrals in equation 2.23 arise from the Galerkin form while the remaining set of integrals are the least-squares terms of the momentum equation, which are added to assure the numerical stability of the computations. The coefficient \( \tau_{GLS} \) determines the weight of the least squares term. This GLS formulation can be considered as a generalization of the stabilization based on the SUPG procedure employed for incompressible flows. Moreover, it successfully circumvents the LBB condition, so that equal-order interpolation functions can be used for velocity and pressure, which substantially enlarges the spaces of interpolation functions.
Chapter 3
4-field Galerkin/Least-Squares Method

3.1 4-field Galerkin/Least-Squares Formulation

Modeling of microstructured liquids is of great importance in many engineering applications. This thesis proposes a 4-field Galerkin/Least-Squares formulation for viscoelastic flow. Its accuracy, efficiency, and robustness are demonstrated through a set of benchmark problems.

3.1.1 Governing Equations

The Giesekus model is chosen as an example to demonstrate the formulation

\[
\nabla \mathbf{M} + \frac{1}{\lambda} \left[ (\alpha - 1)\mathbf{I} + (1 - 2\alpha)\mathbf{M} + \alpha \mathbf{M}^2 \right] \\
= \frac{\partial \mathbf{M}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{M} - \nabla \mathbf{v}^T \cdot \mathbf{M} - \mathbf{M} \cdot \nabla \mathbf{v} + \frac{1}{\lambda} \left[ (\alpha - 1)\mathbf{I} + (1 - 2\alpha)\mathbf{M} + \alpha \mathbf{M}^2 \right] \\
= 0
\]

(3.1)

The stress tensor \( \mathbf{T} \) is composed of pressure, viscous contribution \( \mathbf{T} \), and elastic contribution \( \mathbf{\sigma} \) as follows:

\[
\mathbf{T} = -p\mathbf{I} + \mathbf{T} + \mathbf{\sigma}
\]

(3.2)

where \( \mathbf{\sigma} = \mathbf{G}\mathbf{M} \) and \( \mathbf{T} \) is defined in equation 3.4 below. A new variable \( \mathbf{L} \), introduced by Pasquali and Scriven (2002) and Pasquali (2000), is used to approximate the velocity gradient

\[
\mathbf{L} - \nabla \mathbf{v} + \frac{1}{3}(\nabla \cdot \mathbf{v})\mathbf{I} = 0
\]

(3.3)
thus,

\[ \mathbf{\tau} = \mu (\mathbf{L} + \mathbf{L}^T) \]  \hspace{1cm} (3.4)

and the equations of motion become a set of first order partial differential equations.

Together with the conservation equations of mass and momentum, the following set of governing equations is obtained:

\[ \nabla \cdot \mathbf{v} = 0 \]  \hspace{1cm} (3.5)

\[ -\rho \mathbf{v} \cdot \mathbf{L} + \nabla \cdot (-p \mathbf{I} + \mu (\mathbf{L} + \mathbf{L}^T) + GM) = 0 \]  \hspace{1cm} (3.6)

\[ \mathbf{v} \cdot \nabla \mathbf{M} - \mathbf{L}^T \cdot \mathbf{M} - \mathbf{M} \cdot \mathbf{L} + \frac{1}{\chi} \left[ (\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2 \right] = 0 \]  \hspace{1cm} (3.7)

\[ \mathbf{L} - \nabla \mathbf{v} + \frac{1}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} = 0 \]  \hspace{1cm} (3.8)

Equations 3.5 – 3.8 form a set of first-order partial differential equations in the variables \( \mathbf{v}, p, \mathbf{L}, \) and \( \mathbf{M} \).

### 3.1.2 4-field Galerkin/Least-Squares Formulation

Multiplying each of the equations in the strong form (equation 3.5-3.8) by a linear combination of the basis function of the associated variable (pressure for the continuity equation, velocity for the momentum equation, conformation for the constitutive equation, and velocity gradient for the interpolation equation) and the derivative of the equation with respect to the field variables, and adding the results yields the 4-field Galerkin/Least-Squares weighted residual form:

\[
\int_\Omega (q + \tau_{\text{cont}} \rho \nabla \cdot \mathbf{w})(\nabla \cdot \mathbf{v})d\Omega \\
+ \int_\Omega \left\{ \mathbf{w} + \tau_{\text{mom}} \rho \left[ \rho \mathbf{v} \cdot \nabla \mathbf{w} + \rho \mathbf{w} \cdot \nabla \mathbf{v} + \nabla q - \nabla \cdot \mu (\mathbf{E} + \mathbf{E}^T) - \nabla \cdot \mathbf{GS} \right] \right\}
\]
\[
\begin{align*}
\cdot \left[ \rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p - \nabla \cdot \mu (\mathbf{L} + \mathbf{L}^T) - \nabla \cdot (\mathbf{GM}) \right] \, d\Omega \\
+ \int_{\Omega} \frac{1}{\eta} \left\{ \mathbf{S} + \tau_{\text{cons}} \left[ -\lambda (-\mathbf{w} \cdot \nabla \mathbf{M} - \mathbf{v} \cdot \nabla \mathbf{S} + \mathbf{E}^T \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{E} + \mathbf{L}^T \cdot \mathbf{S} + \mathbf{S} \cdot \mathbf{L} \right] \\
+ (1 - 2\alpha) \mathbf{S} + \alpha \mathbf{M} \cdot \mathbf{S} + \alpha \mathbf{S} \cdot \mathbf{M} \right\} \\
\cdot \left[ -\lambda (-\mathbf{v} \cdot \nabla \mathbf{M} + \mathbf{L}^T \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{L}) + (\alpha - 1) \mathbf{I} + (1 - 2\alpha) \mathbf{M} + \alpha \mathbf{M}^2 \right] \, d\Omega \\
+ \int_{\Omega} \mu \left[ \mathbf{E} + \tau_{\text{gradv}} (\mathbf{E} - \nabla \mathbf{w} + \frac{1}{3} (\nabla \cdot \mathbf{w}) \mathbf{I}) \right] \\
\cdot \left[ \mathbf{L} - \nabla \mathbf{v} + \frac{1}{3} (\nabla \cdot \mathbf{v}) \mathbf{I} \right] \, d\Omega = 0 \\
\end{align*}
\] (3.9)

In equation 3.9, \( \Omega \) is the flow domain, \( p, \mathbf{w}, \mathbf{S}, \) and \( \mathbf{E} \) are sets of weighting functions. Each independent variable is approximated with linear combination of finite number of basis functions as

**Pressure:** \( p = p^\alpha q^\alpha \)

**Velocity:** \( \mathbf{v} = \psi_\mathbf{v}^\alpha \mathbf{w}_\mathbf{v}^\alpha, \quad \mathbf{w}_\mathbf{v}^\alpha = \psi_\mathbf{v}^\alpha \mathbf{e}_i \)

**Conformation:** \( \mathbf{M} = M^\alpha \mathbf{S}^\alpha, \quad \mathbf{S}^\alpha_{ij} = \psi_M^\alpha \mathbf{e}_i \mathbf{e}_j \)

**Velocity Gradient:** \( \mathbf{L} = L^\alpha \mathbf{E}^\alpha, \quad \mathbf{E}^\alpha_{ij} = \psi_L^\alpha \mathbf{e}_i \mathbf{e}_j \)

where \( \psi_p^\alpha, \psi_\mathbf{v}^\alpha, \psi_M^\alpha, \) and \( \psi_L^\alpha \) are sets of scalar weighting functions for pressure, velocity, conformation tensor, and velocity gradient. \( \mathbf{e}_i, \mathbf{e}_j \) are orthonormal basis vectors. The linear combination of scalar weighting function with unit vector or tensor forms the vector/tensor weighting function \( \mathbf{w}_\mathbf{v}^\alpha, \mathbf{S}^\alpha_{ij}, \) and \( \mathbf{E}^\alpha_{ij} \). The dummy index \( \alpha \) ranges from 1 to the number of basis functions.

After integration by parts, the momentum residual term naturally introduces the
traction boundary condition

\[
\int_{\Omega} \left\{ w + \tau_{\text{mom}} \frac{\lambda}{\rho} \left[ \rho v \cdot \nabla w + \rho w \cdot \nabla v + \nabla q - \nabla \cdot \mu (E + E^T) - \nabla \cdot G S \right] \right\} \\
\cdot \left[ \rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM) \right] d\Omega
\]

\[= \int_{\Omega} w \cdot \rho v \cdot \nabla v d\Omega - \int_{\Omega} w \cdot \nabla T d\Omega \\
+ \int_{\Omega} \left\{ \frac{\lambda}{\rho} \tau_{\text{mom}} \left[ \rho v \cdot \nabla w + \rho w \cdot \nabla v + \nabla q - \nabla \cdot \mu (E + E^T) - \nabla \cdot G S \right] \right\} \\
\cdot \left[ \rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM) \right] d\Omega
\]

\[= \int_{\Omega} w \cdot \rho v \cdot \nabla v d\Omega - \int_{\Gamma} t \cdot w d\Gamma + \int_{\Omega} T : (\nabla w) d\Omega \\
+ \int_{\Omega} \left\{ \frac{\lambda}{\rho} \tau_{\text{mom}} \left[ \rho v \cdot \nabla w + \rho w \cdot \nabla v + \nabla q - \nabla \cdot \mu (E + E^T) - \nabla \cdot G S \right] \right\} \\
\cdot \left[ \rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM) \right] d\Omega
\]

(3.10)

Combining equation 3.10 with equation 3.9 yields the following Galerkin/Least-Squares formulation where traction boundary conditions appear explicitly.

\[
\int_{\Omega} (q + \tau_{\text{cont}} \rho \nabla \cdot w) (\nabla \cdot v) d\Omega \\
+ \int_{\Omega} w \cdot \rho v \cdot \nabla v d\Omega - \int_{\Gamma} t \cdot w d\Gamma + \int_{\Omega} T : (\nabla w) d\Omega \\
+ \int_{\Omega} \left\{ \frac{\lambda}{\rho} \tau_{\text{mom}} \left[ \rho v \cdot \nabla w + \rho w \cdot \nabla v + \nabla q - \nabla \cdot \mu (E + E^T) - \nabla \cdot S \right] \right\} \\
\cdot \left[ \rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM) \right] d\Omega
\]

\[
\int_{\Omega} \frac{1}{\eta} \left\{ S + \tau_{\text{cons}} \left[ -\lambda (-w \cdot \nabla M - v \cdot \nabla S + E^T \cdot M + M \cdot E + L^T \cdot S + S \cdot L) \\
+ (1 - 2\alpha) S + \alpha M \cdot S + \alpha S \cdot M \right] \right\} \\
+ \int_{\Omega} \mu \left[ E + \tau_{\text{grad}} (E - \nabla w + \frac{1}{3} (\nabla \cdot w) I) \right]
\]
\[ L - \nabla v + \frac{1}{3} (\nabla \cdot v) I \right] d\Omega = 0 \quad (3.11) \]

### 3.1.3 Features of 4-field GLS formulation

The 4-field GLS formulation has the following features.

- The Galerkin/Least-Squares formulation is a combination of Galerkin residual and Least-Squares residual. If we set

\[ \tau_{\text{cont}} = \tau_{\text{mom}} = \tau_{\text{cons}} = \tau_{\text{gradv}} = 0 \quad (3.12) \]

then equation 3.9 becomes the Galerkin formulation. Because of the Galerkin term, the traction term \( n \cdot T \) appears naturally by integration by part. The traction term serves as an important boundary condition for free surface flows, particularly in small scale problem where capillarity effects are strong.

- The 4-field GLS formulation introduces a new variable \( L = \nabla v \) so that the second order derivative of \( v \) is avoided. Therefore, this formulation is compatible with interpolation functions that are piecewise linear.

- The 4 field GLS form is consistent, i.e., the exact solution of the strong form in equation 3.8 satisfies equation 3.11. The weighted residual vanishes if the exact solution is inserted into the formulation.

- The 4-field GLS naturally includes the SUPG and PSPG stabilizing terms, thus it can stabilizes spatial oscillations caused by advective terms. The contribution
from the momentum residual can be written as:

\[
\int_{\Omega} \left\{ w + \tau_{\text{mom}} \frac{\lambda}{\rho} \left[ \rho v \cdot \nabla w + \rho w \cdot \nabla v + \nabla q - \nabla \cdot \mu (E + E^T) - \nabla \cdot G S \right] \right\} \\
\cdot \left[ \rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM) \right] d\Omega
\]

= \int_{\Omega} \left\{ w + \tau_{\text{mom}} \frac{\lambda}{\rho} \rho v \cdot \nabla w \right\} \cdot \text{[MOMENTUM RESIDUAL]} d\Omega

+ \int_{\Omega} \left\{ \tau_{\text{mom}} \frac{\lambda}{\rho} \nabla q \right\} \cdot \text{[MOMENTUM RESIDUAL]} d\Omega

+ ... \quad (3.13)

In equation 3.13, the first term is the SUPG stabilization term from equation 2.13, and the second term is the PSPG stabilization term from equation 2.21.

- 4-field GLS successfully circumvents the LBB condition. Equal order interpolation functions for velocity, pressure, stress, and velocity gradient can be employed in the weak form.

3.2 Weighted Residual Equations and Solutions Strategy

3.2.1 Weighted Residual Equations

The weighted residual form of the equation set can be obtained by setting to zero in turn three of the four weighting functions in equation 3.11:

\[
r^\alpha_q = \int_{\Omega} q^\alpha \nabla \cdot \mathbf{v} d\Omega
\]

\[
+ \int_{\Omega} \frac{\lambda}{\rho} \tau_{\text{mom}} \nabla q^\alpha \cdot \left[ \rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM) \right] d\Omega
\]

\[
(3.14)
\]
\[ r_{w_{i}}^{\alpha} = \int_{\Omega} (\tau_{\text{cont}} \rho \nabla \cdot w_{i}^{\alpha}) \cdot (\nabla \cdot v) \, d\Omega \]
\[ + \int_{\Omega} w_{i}^{\alpha} \cdot \rho v \cdot \nabla v d\Omega - \int_{\Gamma} t \cdot w_{i}^{\alpha} d\Gamma + \int_{\Omega} T : (\nabla w_{i}^{\alpha}) d\Omega \]
\[ + \int_{\Omega} \left\{ \frac{\lambda}{\rho} \tau_{\text{mom}} [\rho v \cdot \nabla w_{i}^{\alpha} + \rho w_{i}^{\alpha} \cdot \nabla v] \right\} \cdot [\rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu(L + L^{T}) - \nabla \cdot (GM)] \, d\Omega \]
\[ + \int_{\Omega} \frac{1}{\eta} \tau_{\text{cons}} \lambda(-w_{i}^{\alpha} \cdot \nabla M) \]
\[ : [\lambda(-v \cdot \nabla M + L^{T} \cdot M + M \cdot L) - (\alpha - 1)I - (1 - 2\alpha)M - \alpha M^{2}] \, d\Omega \]
\[ + \int_{\Omega} \mu \tau_{\text{gradev}} \left[ -\nabla w_{i}^{\alpha} + \frac{1}{3} (\nabla \cdot w_{i}^{\alpha}) I \right] : \left[ L - \nabla v + \frac{1}{3} (\nabla \cdot v) I \right] \, d\Omega \]

(3.15)

\[ r_{S_{ij}}^{\alpha} = \int_{\Omega} \left[ -\frac{\lambda}{\rho} \tau_{\text{mom}} \nabla \cdot GS_{ij}^{\alpha} \right] \]
\[ \cdot [\rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu(L + L^{T}) - \nabla \cdot (GM)] \, d\Omega \]
\[ + \int_{\Omega} \frac{1}{\eta} \left\{ S_{ij}^{\alpha} + \tau_{\text{cons}} \left[ \lambda(-v \cdot \nabla S_{ij}^{\alpha} + L^{T} \cdot S_{ij}^{\alpha} + S_{ij}^{\alpha} \cdot L) \right. \right. \\
\[ - (1 - 2\alpha)S_{ij}^{\alpha} - \alpha M \cdot S_{ij}^{\alpha} - \alpha S_{ij}^{\alpha} \cdot M \right\} \]
\[ : [\lambda(-v \cdot \nabla M + L^{T} \cdot M + M \cdot L) - (\alpha - 1)I - (1 - 2\alpha)M - \alpha M^{2}] \, d\Omega \]

(3.16)

\[ r_{E_{ij}}^{\alpha} = \int_{\Omega} \frac{\lambda}{\rho} \tau_{\text{mom}} \left[ -\nabla \cdot \mu(E + E^{T}) \right] \]
\[ \cdot [\rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu(L + L^{T}) - \nabla \cdot (GM)] \, d\Omega \]
\[ + \int_{\Omega} \frac{1}{\eta} \tau_{\text{cons}} \lambda(E_{ij}^{\alpha T} \cdot M + M \cdot E_{ij}^{\alpha}) \]
\[ : [\lambda(-v \cdot \nabla M + L^{T} \cdot M + M \cdot L) - (\alpha - 1)I - (1 - 2\alpha)M - \alpha M^{2}] \, d\Omega \]
\[ + \int_{\Omega} \mu [E_{ij}^{\alpha} + \tau_{\text{gradev}} E_{ij}^{\alpha}] : \left[ L - \nabla v + \frac{1}{3} (\nabla \cdot v) I \right] \, d\Omega \]
where $r_q^\alpha$, $r_{w_i}^\alpha$, $r_{S_{ij}}^\alpha$, and $r_{E_{ij}}^\alpha$ are the weighted residuals of the equations. The subscript on the residual identifies the type of residual equation, the superscript labels the residual equation in the set. In this work, bilinear basis functions are used for all the independent variables: $\psi_p$, $\psi_v$, $\psi_L$, and $\psi_M$.

Combining the expression of the weighting functions and equations 3.14 to 3.17 yields a set of nonlinear algebraic equations which can be solved by Newton’s method. The algorithm and derivation of the analytical Jacobian are discussed in the following section.

### 3.2.2 Newton's method with analytical Jacobian

In order to simplify the procedure of Newtonian iteration, equation set 3.14 to 3.17 is denoted as:

\[
\begin{align*}
    r_q^\alpha(p^\beta, v_k^\beta, M_{kl}^\beta, L_{kl}^\beta) & = 0 \\
    r_{w_i}^\alpha(p^\beta, v_k^\beta, M_{kl}^\beta, L_{kl}^\beta) & = 0 \\
    r_{S_{ij}}^\alpha(p^\beta, v_k^\beta, M_{kl}^\beta, L_{kl}^\beta) & = 0 \\
    r_{E_{ij}}^\alpha(p^\beta, v_k^\beta, M_{kl}^\beta, L_{kl}^\beta) & = 0
\end{align*}
\]

where $\alpha$ and $\beta$ change from 1 to the number of basis functions; $i$, $j$, $k$, and $l$ range from 1 to the number of spatial dimensions. The 4-field GLS developed in this thesis is general, while the calculation is restricted to 2-D problems. Each element has 4 basis functions. Conformation $\mathbf{M}$ is symmetric by definition, so only the diagonal and super-diagonal components are taken as unknowns. In all there are $10 \times$ (number of
basis functions) unknowns, and the same number of equations associated with each element.

Newton's method is one of the most powerful methods to solve non-linear systems of the form $f(x) = 0$. In $n$-dimensional non-linear system, it has the form

$$x_{k+1} = x_k - J_f(x_k)^{-1}f(x_k)$$  \hspace{1cm} (3.22)

where $x_k$ is the approximation to the exact solution at $k - 1$th iteration. $J_f(x)$ is the Jacobian matrix of the nonlinear function $f$.

$$\{J_f(x)\}_{ij} = \frac{\partial f_i(x)}{\partial x_j}\hspace{1cm} (3.23)$$

Instead of inverting the Jacobian matrix, we solve the linear system

$$J_f(x_k)s_k = -f(x_k)\hspace{1cm} (3.24)$$

then take the next iteration

$$x_{k+1} = x_k + s_k$$  \hspace{1cm} (3.25)

The process is repeated until the approximate solution meets the convergence criterion.

For equation system 3.18 to 3.21, the corresponding Jacobian matrix has the following form:

$$J = \begin{bmatrix}
\frac{\partial r_{ij}^a}{\partial p^a} & \frac{\partial r_{ij}^a}{\partial q^a} & \frac{\partial r_{ij}^a}{\partial \dot{q}_k} & \frac{\partial r_{ij}^a}{\partial \dot{x}_{kl}} \\
\frac{\partial r_{ij}^a}{\partial \dot{p}^a} & \frac{\partial r_{ij}^a}{\partial \dot{q}_k} & \frac{\partial r_{ij}^a}{\partial \ddot{q}_k} & \frac{\partial r_{ij}^a}{\partial \ddot{x}_{kl}} \\
\frac{\partial r_{ij}^a}{\partial \dot{v}_{ij}} & \frac{\partial r_{ij}^a}{\partial \dot{v}_{ij}} & \frac{\partial r_{ij}^a}{\partial \ddot{v}_{ij}} & \frac{\partial r_{ij}^a}{\partial \ddot{v}_{ij}} \\
\frac{\partial \phi_{ij}}{\partial \dot{p}^a} & \frac{\partial \phi_{ij}}{\partial \dot{q}_k} & \frac{\partial \phi_{ij}}{\partial \ddot{q}_k} & \frac{\partial \phi_{ij}}{\partial \ddot{x}_{kl}} \\
\frac{\partial \phi_{ij}}{\partial \dot{v}_{ij}} & \frac{\partial \phi_{ij}}{\partial \dot{v}_{ij}} & \frac{\partial \phi_{ij}}{\partial \ddot{v}_{ij}} & \frac{\partial \phi_{ij}}{\partial \ddot{v}_{ij}} \\
\frac{\partial \phi_{ij}}{\partial p^a} & \frac{\partial \phi_{ij}}{\partial q^a} & \frac{\partial \phi_{ij}}{\partial \dot{q}_k} & \frac{\partial \phi_{ij}}{\partial \dot{x}_{kl}}
\end{bmatrix}$$
where each entry in this Jacobian, such as \( \frac{\partial r^\alpha_{pq}}{\partial p^q} \), is a matrix whose size is determined by the number of basis functions and nodes. For example:

\[
\frac{\partial r^\alpha_q}{\partial p^\beta} = \\
\begin{bmatrix}
\frac{\partial r^1_1}{\partial p^1} & \frac{\partial r^1_2}{\partial p^2} & \frac{\partial r^1_3}{\partial p^3} & \frac{\partial r^1_4}{\partial p^4} \\
\frac{\partial r^2_1}{\partial p^1} & \frac{\partial r^2_2}{\partial p^2} & \frac{\partial r^2_3}{\partial p^3} & \frac{\partial r^2_4}{\partial p^4} \\
\frac{\partial r^3_1}{\partial p^1} & \frac{\partial r^3_2}{\partial p^2} & \frac{\partial r^3_3}{\partial p^3} & \frac{\partial r^3_4}{\partial p^4} \\
\frac{\partial r^4_1}{\partial p^1} & \frac{\partial r^4_2}{\partial p^2} & \frac{\partial r^4_3}{\partial p^3} & \frac{\partial r^4_4}{\partial p^4}
\end{bmatrix}
\]

If each non-zero entry of the tensor is treated as an independent scalar variable, as is commonly done, the equation set becomes a set of 10 equations and 10 unknowns at each node in a 2-dimensional flow. That means approximately 100 derivatives are needed to obtain the Jacobian. On the other hand, if the unknowns are kept in their tensor/vector form, there are only 4 equations and 16 derivatives needed (Pasquali 2000). The second approach is adopted here. The derivatives of momentum residual are listed here as an example. Note that the derivative of the stabilization coefficients \( \tau_{cont} \), \( \tau_{mom} \), \( \tau_{conf} \), and \( \tau_{cons} \) with respect to \( p \), \( v \), \( M \), and \( L \) are neglected.

Derivative with respect to pressure basis function coefficients:

\[
\frac{\partial r^\alpha_{wi}}{\partial p^\beta} = \int_{\Omega} \left[ \frac{\lambda_{\text{mom}}}{\rho} (\rho v \cdot \nabla w^\alpha_i + \rho w^\alpha_i \cdot \nabla v) \right] \cdot \nabla q^\beta d\Omega \tag{3.26}
\]

Derivative with respect to velocity basis functions coefficients:

\[
\frac{\partial r^\alpha_{wi}}{\partial v^\beta_j} = \int_{\Omega} (\tau_{cont} \rho \nabla \cdot w^\alpha_i) (\nabla \cdot w^\beta_j) d\Omega \\
+ \int_{\Omega} w^\alpha_i \cdot \rho w^\beta_j \cdot \nabla v d\Omega + \int_{\Omega} w^\alpha_i \cdot \rho v \cdot \nabla w^\beta_j d\Omega \\
+ \int_{\Omega} \frac{\lambda_{\text{mom}}}{\rho} (\rho w^\beta_j \cdot \nabla w^\alpha_i + \rho w^\alpha_i \cdot \nabla w^\beta_j)
\]
\[
\begin{aligned}
&\cdot \left[\rho \mathbf{v} \cdot \nabla \mathbf{v} + \nabla p - \nabla \cdot \mu (\mathbf{L} + \mathbf{L}^T) - \nabla \cdot (GM)\right] d\Omega \\
+ \int_\Omega \frac{\lambda \tau_{\text{mom}}}{\rho} (\rho \mathbf{v} \cdot \nabla \mathbf{w}_i^\alpha + \rho \mathbf{w}_i^\alpha \cdot \nabla \mathbf{v}) \\
\cdot (\rho \mathbf{w}_j^\beta \cdot \nabla \mathbf{v} + \rho \mathbf{v} \cdot \nabla \mathbf{w}_j^\beta) d\Omega \\
+ \int_\Omega \frac{1}{\eta} \tau_{\text{cons}} \lambda (-\mathbf{w}_i^\alpha \cdot \nabla \mathbf{M}) : \left[\lambda (-\mathbf{w}_j^\beta \cdot \nabla \mathbf{M})\right] d\Omega \\
+ \int_\Omega \mu \tau_{\text{gradv}} \left[\nabla \mathbf{w}_i^\alpha + \frac{1}{3} (\nabla \cdot \mathbf{w}_i^\alpha) \mathbf{I}\right] : \left[-\nabla \mathbf{w}_j^\beta + \frac{1}{3} (\nabla \cdot \mathbf{w}_j^\beta) \mathbf{I}\right] d\Omega
\end{aligned}
\]

(3.27)

Derivative with respect to conformation basis functions coefficients:

\[
\frac{\partial \tau_{\mathbf{w}_i^\alpha}}{\partial M_{kl}^\beta} = \int_\Omega \left[\frac{\lambda \tau_{\text{mom}}}{\rho} (\rho \mathbf{v} \cdot \nabla \mathbf{w}_i^\alpha + \rho \mathbf{w}_i^\alpha \cdot \nabla \mathbf{v})\right] : \left[-\nabla \cdot (GS_{kl}^\beta)\right] d\Omega \\
+ \int_\Omega \tau_{\text{cons}} \frac{\lambda}{\eta} (-\mathbf{w}_i^\alpha \cdot \nabla S_{kl}^\beta) \\
: \left[\lambda (\mathbf{v} \cdot \nabla \mathbf{M} + \mathbf{L}^T \cdot \mathbf{M} + \mathbf{M} \cdot \mathbf{L}) - (\alpha - 1) \mathbf{I} - (1 - 2\alpha) \mathbf{M} - \alpha \mathbf{M}^2\right] d\Omega \\
+ \int_\Omega \tau_{\text{cons}} \frac{\lambda}{\eta} (-\mathbf{w}_i^\alpha \cdot \nabla \mathbf{M}) \\
: \left[\lambda (\mathbf{v} \cdot \nabla S_{kl}^\beta + \mathbf{L}^T \cdot S_{kl}^\beta + S_{kl}^\beta \cdot \mathbf{L}) - (1 - 2\alpha) S_{kl}^\beta - \alpha \cdot S_{kl}^\beta \cdot \mathbf{M} - \alpha \cdot S_{kl}^\beta\right] d\Omega
\]

(3.28)

Derivative with respect to velocity gradient basis functions coefficients:

\[
\frac{\partial \tau_{\mathbf{w}_i^\alpha}}{\partial L_{kl}^\beta} = \int_\Omega \left[\frac{\lambda \tau_{\text{mom}}}{\rho} (\rho \mathbf{v} \cdot \nabla \mathbf{w}_i^\alpha + \rho \mathbf{w}_i^\alpha \cdot \nabla \mathbf{v})\right] \\
\cdot \left[-\nabla \cdot \mu (E_{kl}^\beta + E_{kl}^{\beta T})\right] d\Omega \\
+ \int_\Omega \tau_{\text{cons}} \frac{\lambda}{\eta} [\lambda (-\mathbf{w}_i^\alpha \cdot \nabla \mathbf{M})] : \left[\lambda (E_{kl}^{\beta T} \cdot \mathbf{M} + \mathbf{M} \cdot E_{kl}^{\beta T})\right] d\Omega \\
+ \int_\Omega \mu \tau_{\text{gradv}} \left[\nabla \mathbf{w}_i^\alpha + \frac{1}{3} (\nabla \cdot \mathbf{w}_i^\alpha) \mathbf{I}\right] : E_{kl}^\beta d\Omega
\]

(3.29)
3.2.3 Parameter Design

The choice of stabilization parameters can strongly affect the numerical solution. The stabilization coefficients used here for the continuity and momentum are originated by Tezduyar and Shih (1992).

The expression of the stabilization coefficients for momentum is

$$
\tau_{mom} = \left[ \left( \frac{2|u^h|_2}{h_e} \right)^2 + \left( \frac{4\nu}{h_e^2} \right)^2 \right]^{-1/2}
$$

(3.30)

where $|u^h|_p = \left( \sum_{d=1}^{n} |u^h_d|^p \right)^{\frac{1}{p}}$ is the pointwise velocity norm, $h_e$ is the element length and $\nu = \mu/\rho$ is the kinematic viscosity. The coefficient $\tau_{cont}$ is defined as

$$
\tau_{cont} = |u^h|_2 h_e \xi(Re_e)
$$

(3.31)

where the element Reynolds number $Re_e$ and $\xi(Re_e)$ are defined as

$$
Re_e = \frac{|u^h| h_e}{2\nu}
$$

(3.32)

$$
\xi(Re_e) = \begin{cases} 
Re/3, & 0 \leq Re < 3, \\
1, & 3 \leq Re.
\end{cases}
$$

(3.33)

The stabilization coefficient for conformation was proposed by Behr (1991).

$$
\tau_{cons} = \begin{cases} 
\max(1, \frac{h^e}{2|u^h|_2}), & \lambda |u^h|_2 > 1 \\
\max(1, h^e), & \lambda |u^h|_2 \leq 1
\end{cases}
$$

(3.34)

Finally,

$$
\tau_{gradv} = \tau_{cons}
$$

(3.35)

The stabilization coefficient for the velocity gradient can also be taken simply as

$$
\tau_{gradv} = 1.
$$
Chapter 4
Numerical Examples – Newtonian Cases

Here the 4-field GLS method (GLS4 method) is restricted to the 3-field Newtonian case (velocity, pressure, and velocity gradient). 3-field GLS retains all the features of GLS4 (see section 3.1.3) and it successfully circumvents the LBB condition. Numerical tests are carried out on a set of Newtonian benchmark problems: lid-driven-cavity, flow around a cylinder, 4-to-1 contraction, and stick-slip problem.

For each test case, bilinear basis functions are used for all the variables. The weighted residuals are evaluated with 3-point Gaussian integration in each direction. Stabilization coefficients are chosen according to section 3.2.3. At \( \text{Re} > 0 \), the set of algebraic equations is non-linear. Analytical Jacobian is employed and the criteria for convergence are based on both the norm of the residual and the norm of the Newton’s update in the terminal iteration. Quadratic convergence was observed as expected. The initial guesses of all the variables are set to zero.

First-order arc-length continuation was used to obtain results at increasing \( \text{Re} \). If the new step converged within three iterations, the size of the next continuation step was doubled, and if it converged in more than six iterations, the size of the next continuation step was reduced by 75%.

4.1 Lid-driven-cavity

In order to assess the performance of 4-field GLS at high Reynolds number, the flow in a square lid-driven cavity with unit side length is computed at \( \text{Re} = 0, 400, \) and 5000. The simulation is carried out on meshes with different tessellations such
as $20 \times 20$, $40 \times 40$, $60 \times 60$, and $80 \times 80$. The results are compared to the solution from $20 \times 20$ and $40 \times 40$ mesh with a Galerkin code from Pasquali (2000). The Galerkin code uses biquadratic basis functions; thus, a $n \times n$ Galerkin mesh has the same number of velocity degree of freedom as a $2n \times 2n$ GLS mesh.

No-slip conditions are imposed on all the boundaries. The vertical and horizontal velocities are set to zero at the bottom and side walls. The vertical velocity is set to zero and the horizontal velocity is set to 1 at the top and two corners shared by the top and side walls.

4.1.1 $Re = 0$

Reynolds number $Re = 0$ is the simplest case for Newtonian flow, which eliminates the influence of convection. The horizontal velocity at the midline $x = 0.5$ and vertical velocity at the centerline $y = 0.5$ are often chosen as characteristic velocities to examine the correctness of the solution.

The velocity at the centerline and midline from 4-field GLS and Galerkin formulations is presented in figures 4.1(a) and 4.1(b) respectively. The figures shows that at low Reynolds number the simulation converges on a relatively coarse mesh.

The streamlines and pressure contours in a lid-driven-cavity at $Re = 0$ with GLS4 formulations are presented in figures 4.2(a) and 4.2(b).

4.1.2 $Re = 400$

The horizontal velocity at the centerline $x = 0.5$ and the vertical velocity at the centerline $y = 0.5$ calculated with the 4-field GLS formulation (on $40 \times 40$, $60 \times 60$, and $80 \times 80$ meshes) and Galerkin formulation (on $20 \times 20$ and $40 \times 40$ meshes) are
Figure 4.1  (a) Vertical velocity at $y = 0.5$ with Galerkin and the 4-field GLS at $Re = 0$. (b) Horizontal velocity at $x = 0.5$ with Galerkin and the 4-field GLS method at $Re = 0$. The result from the 40 x 40 mesh with the 4-field GLS coincides with that from 20 x 20 mesh with the Galerkin method.

Franca and Muller (1992) obtained the numerical solution for lid-driven-cavity with the GLS method with quadratic basis functions. Figure 4.4(a) shows that the horizontal velocity at the centerline computed with the 4-field GLS and with the method of Franca are very close to each other.

We can also see that the velocity curves are still shifting slightly as the mesh becomes denser. To ensure that the Galerkin and the 4-field GLS method converges towards the same value, Richardson extrapolation is used to assess the convergence. For the Galerkin method with quadratic velocity basis functions, velocity has 3rd order convergence rate; and the 4-field GLS method with all linear basis function can converge quadratically (Behr 1994). From the extrapolation curves for the Galerkin and the 4-field GLS methods in figure 4.4(b), we can see that the numerical solutions
Figure 4.2  (a) Streamlines of lid-driven-cavity with the 4-field GLS formulation with 40 × 40 mesh at Re = 0. 29 equally spaced contours lines are plotted. The maximum is 1.05 × 10\(^{-2}\) and the minimum is \(-9.14 \times 10^{-2}\). (b) Pressure contours of lid-driven-cavity with the 4-field GLS formulation with 40 × 40 mesh at Re = 0.29 equally spaced contour lines are plotted. The maximum is 66.9 and the minimum is −66.3.

from these two formulations converge towards the same result.

The streamlines and pressure contours of lid-driven-cavity at Re = 400 are presented in figures 4.5(a) and 4.5(b).

4.1.3 Re = 5000

At high Reynolds number, the 4-field GLS formulation also gives satisfactory performance. The stabilization terms successfully control the possible oscillation caused by the convection term. The horizontal velocity at the centerline \(x = 0.5\) and vertical velocity at the centerline \(y = 0.5\) calculated with the 4-field GLS formulation (on 40 × 40, 60 × 60 and 80 × 80 meshes) and Galerkin formulation (on 20 × 20 and
$40 \times 40$ meshes) is presented in figure 4.7(a) and figure 4.6(b). Extrapolation curves in figure 4.7(b) show that the numerical solutions from these two formulations converge towards the same result.
Figure 4.3  (a) Horizontal velocity at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh for the Galerkin method and $40 \times 40$, $60 \times 60$ mesh for the 4-field GLS method at $Re=400$. (b) Vertical velocity at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh for the Galerkin method and $40 \times 40$, $60 \times 60$ mesh for the 4-field GLS method at $Re=400$. (c) Pressure at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh for the Galerkin and $40 \times 40$, $60 \times 60$ mesh for the 4-field GLS method at $Re=400$. (d) Pressure at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh using the Galerkin method and $40 \times 40$, $60 \times 60$ mesh using the 4-field GLS at $Re=400$. 
Figure 4.4  (a) Vertical velocity at \( y=0.5 \) with \( 30 \times 30 \) mesh for the 4-field GLS method and Frances's \( 16 \times 16 \) Q2S/Q2S-serendipity mesh at \( \text{Re}=400 \). (b) Vertical velocity at \( y = 0.5 \) \( x=0.9 \) at \( \text{Re} = 400 \) at different mesh sizes. Richardson extrapolation is applied here, which shows that the vertical velocity at \( y = 0.5 \) \( x = 0.9 \) at \( \text{Re} = 5000 \) from Galerkin method and 4-field GLS method converge towards the same value as element size becomes smaller (mesh becomes finer). For the Galerkin method with quadratic velocity basis functions, velocity has 3rd order convergence rate; and the 4-field GLS method with all linear basis function can converge quadratically.
Figure 4.5  (a) Streamlines of lid-driven-cavity with the 4-field GLS method with $40 \times 40$ mesh at $Re = 400$. 29 equally spaced contour lines are plotted. The maximum is 0.016 and the minimum is $-0.091$. (b) Pressure contours of lid-driven-cavity with the 4-field GLS formulation with $40 \times 40$ mesh at $Re = 400$. 29 equally spaced contour lines are plotted. The maximum is 167.1 and the minimum is $-45.5$. 
Figure 4.6  (a) Horizontal velocity at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh using the Galerkin method and $40 \times 40$, $60 \times 60$ mesh using the 4-field GLS method at $Re=5000$. (b) Vertical velocity at $y = 0.5$ with $20 \times 20$, $40 \times 40$ mesh for the Galerkin method and $40 \times 40$, $60 \times 60$ mesh using the 4-field GLS method at $Re=5000$. (c) Pressure at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh using the Galerkin method and $40 \times 40$, $60 \times 60$ mesh using the 4-field GLS method at $Re=5000$. (d) Pressure at $y = 0.5$ with $20 \times 20$, $40 \times 40$ mesh using the Galerkin method and $40 \times 40$, $60 \times 60$ mesh using the 4-field GLS method at $Re=5000$. 
Figure 4.7  (a) Horizontal velocity at $x = 0.5$ with $20 \times 20$, $40 \times 40$ mesh using the Galerkin method and $40 \times 40$, $60 \times 60$ mesh using the 4-field GLS method at $Re=5000$. (b) Richardson extrapolation is applied here, which shows that the vertical velocity at $y = 0.5$ $x = 0.9$ at $Re = 400$ from Galerkin method and GLS4 method converge towards the same value as element size becomes smaller (mesh becomes finer). For the Galerkin method with quadratic velocity basis functions, velocity has 3rd order convergence rate; and the 4-field GLS method with all linear basis function can converge quadratically.
4.2 Flow Around a Cylinder in a Channel

The flow around a cylinder between two parallel plates, as shown in figure 4.8, is a classical benchmark problem. To make easy comparison with other literature results, the ratio of the cylinder diameter to the width of the channel is set to 1:8.

![Diagram of flow around a cylinder](image)

**Figure 4.8** Physical problem of flow around a cylinder.

This geometry is symmetric about the centerline, so only half of the flow field is calculated. The cylinder is centered at the origin, the calculation domain is extended from $-10R$ to $12R$, where $R=1$ is the radius of the cylinder.

The mesh for the calculation is shown in figure 4.9. It contains 2056 elements, 8451 nodes, and total number of degrees of freedom is 15190.

Parabolic velocity profile is imposed at inflow; no-slip boundary condition is applied at the top wall, and a symmetric boundary condition at the center line. On the symmetry boundary, liquid cannot go across the symmetry line, that is $\mathbf{n} \cdot \mathbf{v} = 0$; the shear stress is zero along the symmetry line.

To assess the solution, we examine the horizontal velocity and velocity gradient component $L_{yy}$ along the symmetry line. Figure 4.10 shows that the 4-field GLS
Figure 4.9  Mesh for flow around a cylinder. This mesh contains 2056 elements, 8451 nodes.

method result is in excellent agreement with the solution from the Galerkin method.

Another quantity of interest is the drag force exerted by the fluid on the cylinder.

Faxén (1946) derived an approximate formula for the drag exerted by flow on the surface of cylinder at \(\text{Re} = 0\), which is

\[
f_d = -4\pi\mu \frac{u_0}{U_0 - (1 + \sum_i W_i A_i) \ln \Lambda + \sum_i V_i A_i}
\]

(4.1)

where \(u_0\) is the maximum horizontal velocity in a cross section of the slot far away from the cylinder, \(\Lambda \equiv R/h\) is the ratio of cylinder radius \(R\) to slot half-width \(h\), \(U_0 = -0.9156892732\). The coefficients are reported by Faxén (1946) and Pasquali (2000).

As the 4-field GLS method solution of flow around a cylinder is achieved, the drag force can be computed as

\[
f_d \equiv -2 \int_S e_1 \cdot n : T dS
\]

(4.2)

where \(S\) is the surface of the half-cylinder, \(e_1\) is a horizontal unit vector, and \(n\) is the
Figure 4.10 Graphs of the velocity gradient component $L_{yy}$ and horizontal velocity $v_x$ along the axis of symmetry at Re=0, where $x = -1$ and $x = 1$ are the front and rear stagnation points, respectively.
unit normal pointing from the liquid into the cylinder. The integral was computed with 3-point Gaussian quadrature.

The drag force calculated from the 4-field GLS code is 15.814, from Galerkin code is 15.741, from Faxen's formula is 15.713, and from Sun is 15.712. The difference is within 1%. The streamline, velocity and pressure contours obtained using the 4-field GLS and Galerkin at Re = 0 are presented in figure 4.11(a) to 4.12(b). All of the figures exhibit symmetry about the cylinder as expected, except for minor details due to the asymmetry of the mesh, which is finer downstream of the cylinder.
Figure 4.11  (a) Streamlines for flow around a cylinder with the 4-field GLS method at Re=0. 11 equally spaced contour lines are plotted, the maximum is 8.00 and the minimum is $-3.13 \times 10^{-3}$.  (b) Pressure contours for flow around a cylinder with the 4-field GLS method at Re=0. 30 equally spaced contour lines are plotted. The maximum is $2.57 \times 10^{-2}$ and the minimum is $-5.23$. 
Figure 4.12  (a) Horizontal velocity contour for flow around a cylinder with the 4-field GLS method at $Re=0$. 11 equally spaced contour lines are plotted. The maximum is 1.63 and the minimum is $-8.58 \times 10^{-4}$. (b) Vertical velocity contour for flow around a cylinder with the 4-field GLS method at $Re=0$. 12 equally spaced contour lines are plotted. The maximum is 0.462 and the minimum is $-0.453$. 
4.3 4-to-1 Contraction

The physical problem corresponding to 4-to-1 contraction is depicted in figure 4.13. The computational domain covers the upper half of the geometry. A parabolic velocity profile with unit flow rate is imposed at the inflow and outflow. The no-slip boundary condition is applied on the upper boundary, and a symmetry boundary condition is applied on the lower boundary (symmetry plane).

![Figure 4.13 4-1 contraction](image)

In this geometry, a singularity is present at the re-entrant corner; this causes very high stress in its vicinity. Using the mesh in figure 4.14, the Galerkin formulation exhibits oscillation around the corner. Although the 4-field GLS also produces oscillating solutions in the vicinity of the singular point, it can obtain a relatively smooth profile as shown in figure 4.15.

Horizontal velocities from Galerkin and GLS at the inflow and outflow of the contraction section are also quantities of interest; they are compared in figure 4.16.

The streamline, velocity, pressure contour and velocity at inflow and outflow of the contraction obtained from the mesh in figure 4.14 are presented in figures 4.17(a)
Figure 4.14  Mesh of 4-1 contraction. This mesh has 320 elements and 1365 nodes.

through 4.18(b).
Figure 4.15  Velocity gradient component $L_{yy}$ along the horizontal line $y = 1$ with the 4-field GLS (top) and the Galerkin (bottom) methods at $Re = 0$. 
Figure 4.16  Comparison of horizontal velocity at the inflow and outflow of the contraction section from the Galerkin and 4-field GLS method at Re = 0.

(a)

(b)

Figure 4.17  (a) Streamline of 4-to-1 contraction with the 4-field GLS method at Re=0. 11 equally spaced contour lines are plotted. The maximum is 1 and the minimum is 0. (b) Pressure contour for 4-to-1 contraction with the 4-field GLS method at Re=0. 21 equally spaced contour lines are plotted. The maximum is 55.2 and the minimum is 0.
Figure 4.18  (a) Vertical velocity contour of 4-to-1 contraction with the 4-field GLS method at Re=0. 11 equally spaced contour lines are plotted. The maximum is 1.49 and the minimum is $-2.34 \times 10^{-3}$. (b) Horizontal velocity contour of 4-to-1 contraction with the 4-field GLS method at Re=0. 11 equally spaced contour lines are plotted. The maximum is 0.024 and the minimum is $-3.1$. 
4.4 Stick-Slip Problem

Stick-slip flow is the first step of approximation to free surface problems. The corresponding physical problem is shown in figure 4.19; the no-slip condition is imposed on the left half of the upper and lower boundaries, whereas perfect slip is imposed on the boundaries of the other half. A parabolic velocity profile with unit flowrate is imposed at the inflow and pressure is specified at the outflow.

![Figure 4.19 Stick slip problem. The left half of the upper and lower boundaries are no-slip and the boundaries of the other half are full slip. The width of the geometry is 1, the length is 4, where the stick and the slip part have the same length.](image)

In this problem, a difficulty arises at the transition from stick boundary (Dirichlet boundary condition) to slip boundary (Neumann boundary condition). The transition point is singular for both Newtonian and non-Newtonian flow. A relatively coarse mesh (figure 4.20) and a finer mesh (figure 4.21) are used in the simulation.

The velocity gradient component $L_{yx}$ along the upper boundary is presented in figure 4.22. The solution obtained with the Galerkin method exhibits oscillations in the vicinity of the transition point. As the mesh grows denser, the oscillation is squeezed to close vicinity but the amplitude increases. On the other hand, 4-field GLS presents a much smoother approximation, and the result exhibits better behavior as
Figure 4.20  Coarse mesh for stick-slip problem. This is a 50x10 mesh with 500 elements and 2121 nodes.

Figure 4.21  Fine mesh for stick-slip problem. This is a 100x20 mesh with 2000 elements and 8241 nodes.

the mesh becomes finer.

The velocity and pressure profiles along the upper boundary and symmetry line (center line) are also characteristic quantities for comparison. The solutions from the 4-field GLS and the Galerkin methods are presented in figure 4.23. Richardson (1970) obtained an analytical solution for this problem. A comparison of 4-field GLS result with the analytical solution is shown in figure 4.24. The coarse mesh does a reasonable job of approximating the velocity and pressure fields, although close to the abrupt change in velocity near the transition point, the velocity has some variation.
Figure 4.22 Velocity gradient component \( L_{yx} \) along upper boundary from coarse mesh (50 x 10) and fine mesh (100 x 20) with the Galerkin and 4-field GLS method.

The streamline, velocity and pressure contour obtained with the GLS formulation at \( Re = 0 \) are presented in figures 4.25(a) to 4.26(b).

4.5 Conclusion

In this chapter, the performance of the 4-field GLS formulation is assessed with the following Newtonian benchmark problems: lid-driven-cavity, flow around cylinder, 4-to-1 contraction, and stick-slip flow. For all the cases, the formulation gives satisfactory results.

The most significant feature of the 4-field GLS is its compatibility with equal
Figure 4.23 Velocity, pressure at centerline and upper boundary. The first figure depicts the velocity along the center line; the second figure depicts the velocity along the upper boundary; the third figure depicts the pressure profile along the center line.

order basis function. The numerical tests in this chapter confirm the feasibility of this method for Newtonian cases. Tests on lid-driven-cavity prove that the method is robust even at high Reynolds number. For flow around a cylinder, the drag force calculated from the 4-field GLS is in excellent agreement with other independently obtained results, which confirms the accuracy of the formulation. The 4-to-1 contraction and stick-slip problem further demonstrate the ability of the 4-field GLS to simulate geometries with singularities.
Figure 4.24  Comparison of analytical solution and the 4-field GLS result of velocity and pressure profile at centerline and upper boundary.

Because linear basis functions are used for all the variables of 4-field GLS, with the same mesh, the 4-field GLS spends less time in every Newton iteration than the Galerkin method as expected. As a trade off, the result is less accurate than the Galerkin method with the same mesh.
Figure 4.25  (a) Streamlines of stick-slip problem with GLS formulation at Re=0. 11 equally spaced contour lines are plotted. The maximum is 0.99 and the minimum is 0. (b) Pressure contour of stick-slip problem with GLS formulation at Re=0. 20 equally spaced contour lines are plotted. The maximum is 6.5 and the minimum is -15.
Figure 4.26  (a) Vertical velocity contour of stick-slip problem with GLS formulation at Re=0. 10 equally spaced contour lines are plotted. The maximum is 0.197 and the minimum is 0. (b) Horizontal velocity contour of stick-slip problem with GLS formulation at Re=0. 10 equally spaced contour lines are plotted. The maximum is 1.4 and the minimum is 0.
Chapter 5
Numerical Examples – Viscoelastic Cases

The 4-field GLS formulation is tested in viscoelastic flow around a cylinder in a channel. In this test case, bilinear basis functions are used for all the variables. Initially, stabilization coefficients are chosen according to the expressions in section 3.2.3, then an alternate set is selected, as discussed in detail in section 5.3.

All the results were computed with the analytical Jacobian, as described in section 3.2.2. The weighted residuals are evaluated with 3-point Gaussian integration in each direction. Quadratic convergence of Newton’s method was observed at low to moderate Weissenberg number up to 2. Here, the Weissenberg number is defined as the ratio of the material characteristic relaxation time $\lambda$ to the characteristic flow time $t$. For flow around a cylinder, $Ws=Q\lambda/hR$, where $h$ is the height of the channel, $R$ is the radius of the cylinder, and $Q$ is the flowrate. The criteria for convergence are based on both the norm of the residual and the norm of the Newton’s update in the terminal iteration. The velocity, pressure, and velocity gradient obtained at a low Weissenberg number are chosen as the initial guess for the viscoelastic problems. The initial guess of conformation is set to identity.

First-order arc-length continuation was used to obtain the result for increasing Weissenberg number. If the new step converged within three iterations, the size of the next continuation step was doubled; if it converged in more than six iterations, the size of the next continuation step was reduced by 75%.
5.1 Problem setup and Mesh Generation

The physical problem of flow around a cylinder is shown in figure 4.8. The computational domain covers the upper half of the geometry.

The ratio of solvent viscosity to total viscosity is set to

\[ \beta = \frac{\mu}{\mu + \eta_p} = 0.59 \]  

(5.1)

where \( \eta_p \) and \( \mu \) are the viscosity of the polymer and the solvent, respectively.

The calculations are carried out on two meshes. The first mesh is shown in figure 5.1(a) (Mesh1); it contains 4504 elements and 18353 nodes. The second mesh, 5.1(b) (Mesh2) has a finer tessellation, which contains 9696 elements and 39285 nodes. Both of the meshes cover the physical domain ranging from \(-60R\) to \(120R\).

As the Weissenberg number increases, the polymer in the flow needs a longer downstream length to relax. Sun et al. (1999) showed that the flow is insensitive to further displacement of the open boundaries in the range of Weissenberg number examined.

A parabolic velocity profile is imposed at the inflow and pressure is imposed at the outflow; the no-slip boundary condition is applied at the top. Symmetry boundary conditions are applied on the lower boundary, that is, liquid can not cross the symmetry line, \( \mathbf{n} \cdot \mathbf{v} = 0 \); the shear stress is zero along the symmetry line \( \mathbf{t} \mathbf{n} : \mathbf{T} = 0 \). No-slip boundary condition is imposed at the cylinder's surface. A fully developed conformation profile is applied at the inflow.

The Oldroyd-B model is chosen as a test case. This model assumes that the molecular relaxation rate depends linearly on the distance of the conformation tensor from its equilibrium value, which means the constitutive parameter \( \alpha \) in equation 3.1
is set to 0.

Mesh1 and Mesh2 are employed to compute the Oldroyd-B flow. The velocity, pressure, and velocity gradient are taken from the Newtonian solution and used as initial guess for the solution at $Ws = 0.01$. The initial guess of conformation is set to $M = I$.

5.2 Simulation results

Using Mesh1 and Mesh2 physically meaningful results can be obtained up to $Ws = 1.9$. When the Weissenberg number exceeds this limit, the conformation tensor $M$ exhibits a negative eigenvalue in a small region of the mesh. The conformation components at the outflow remain constant along the stream-wise direction, thus the length of the flow domain is long enough for the polymer to relax at high Weissenberg number.

The convergence of the results with respect to the refinement of mesh is examined by comparing the solutions obtained with Mesh1 and Mesh2. As shown in table 5.1, at $Ws = 1.6$, the maximum values of the velocity and velocity gradient components computed on Mesh1 and Mesh2 agreed to within 0.5%. The maximum values of the conformation components agreed to within 1.6%.

To ensure the correctness of the 4-field GLS method, the results are compared with those computed with the Galerkin method. The resulting conformation component along the centerline from the two methods are presented in figure 5.2, and they are in excellent agreement with each other.

Further comparison with the results reported by Sun et al. (1999) and Pasquali
<table>
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<tr>
<th></th>
<th>$v_2$</th>
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<th>$L_{21}$</th>
<th>$L_{11}$</th>
<th>$M_{22}$</th>
<th>$M_{12}$</th>
<th>$M_{11}$</th>
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<td>2.1964</td>
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<td>2.2033</td>
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<td>difference</td>
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<td>0%</td>
<td>0.16%</td>
<td>0.46%</td>
<td>0.34%</td>
<td>1.6%</td>
<td>0.25%</td>
<td>0.19%</td>
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</table>

**Table 5.1** Maximum values of the velocity components, the velocity gradient components and the conformation components computed on Mesh1 and Mesh2 at $Ws = 1.6$.

(2000) between the maximum value of pressure and velocity and the Cartesian components of elastic stress conformation components are listed in tables 5.2 and 5.3. The elastic stress is defined as $\sigma_{ij} \equiv (\eta_p/\lambda)(M_{ij} - \delta_{ij})$.

The results from the 4-field GLS method are in excellent agreement with the results reported by Pasquali (2000); the results obtained here also agree with those of Sun et al. (1999) very well except for the maximum value of the streamwise normal elastic stress $\sigma_{11}$ in the wake of the cylinder — the difference is 64%.

The computation of drag exerted on the cylinder was discussed in chapter 4. For viscoelastic flow, as the Weissenberg number grows, the drag drops slightly as $0 < Ws < 1$, then it starts to increase. The drag coefficient was computed on Mesh1 and Mesh2 with $\eta_a = 0.59$. The results are in excellent agreement with the drag force reported by Pasquali (2000) and Sun et al. (1999), as displayed in figure 5.3.
<table>
<thead>
<tr>
<th>Field</th>
<th>Sun et al. (1999) max</th>
<th>Sun et al. (1999) min</th>
<th>4-field GLS max</th>
<th>4-field GLS min</th>
<th>difference max</th>
<th>difference min</th>
<th>$\Delta_{\text{max}}%$</th>
<th>$\Delta_{\text{min}}%$</th>
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<td>0.5460</td>
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<td>0.3835</td>
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<td>16.2726</td>
<td>-0.1501</td>
<td>6.3732</td>
<td>-0.0197</td>
<td>64.3800</td>
<td>15.1427</td>
</tr>
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<td>-0.0617</td>
<td>0.0225</td>
<td>-2.0492</td>
<td>-1.0319</td>
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<td>5.9809</td>
<td>-0.1321</td>
<td>0.2379</td>
<td>0.0005</td>
<td>4.1416</td>
<td>-0.3756</td>
</tr>
</tbody>
</table>

Table 5.2  Comparison between the maximum value of the components of velocity, of pressure, and of the Cartesian components of elastic stress at $Ws = 2$ reported by Sun et al. (1999).

Streamlines, contour plots of pressure, velocity, and conformation components calculated with Mesh2 at $Ws = 1.9$ are presented in figures 5.4 to 5.10.

The molecular stretch and orientation of the polymer can be obtained from the conformation tensor. The normalized eigenvectors of the conformation tensor represent the three mutually perpendicular directions along which the polymer is oriented. The corresponding eigenvalues represent the square of the principal stretch ratios of a flowing ensemble of polymer segments; when the polymer is at equilibrium, the eigenvalues are unity.

The classical coordinate-based definition of shear and extension is not a direct indication of conformation change. The stretch and orientation of polymer are deter-
Table 5.3  Comparison between the maximum value of the components of velocity, of pressure, and of the Cartesian components of elastic stress at $W_s = 2$ reported by Pasquali (2000).

mined by the shear and extension caused by the surrounding flow. Extension implies stretching the molecules along their preferred orientation; shear implies rotating the polymer with respect to the principal axes of the rate of strain, so each molecule is alternatively elongated and contracted by the rate of strain.

The following definitions of molecular extension and shear rate were introduced by Pasquali (2000) to represent the tendency to elongate and orient the polymer:

\[
\dot{\epsilon}_M = m_2 m_2 : D
\]

(5.2)

\[
\dot{\gamma}_M = |m_1 m_2 : D|
\]

(5.3)

where $m_1$ and $m_2$ are the normalized eigenvectors of $M$ corresponding respectively to the smallest and to the largest eigenvalues of $M$. 
Figures 5.11 and 5.12 show the shear and extension rate contours. The largest extension rate appears in the neighborhood of the upstream stagnation point on the cylinder and in the wake of the cylinder by the downstream stagnation point. The region of highest shear rate is at the waist of the cylinder.

The contours of largest and smallest molecular size are shown in figures 5.13 and 5.14. In the upstream section, the molecules are compressed in the streamline direction and stretched in the cross-stream direction. As the flow passes around the cylinder, the molecules are compressed in the cross-stream direction and elongated in the streamline-direction.

First-order arc-length continuation was used to obtain results for increasing Weissenberg number. Physically meaningful solutions could not be obtained for $Ws > 2.0$, because the conformation tensor could not remain positive definite in the whole computational domain. Figure 5.15 shows that as the Weissenberg number increases, $M_{11}$ experiences a steeper and higher peak in at the rear stagnation point, until it is no longer captured by the mesh.

5.3 Stabilization

The stabilization coefficients defined in section 3.2.3 were adopted in the simulation reported in section 5.2, however, strange behaviors were observed. As shown in figure 5.16, if the conformation stabilization coefficient defined in equation 3.35 was used, the drag matches the literature value only at low Weissenberg number, $Ws < 0.5$. Therefore, an adjustable coefficient $a < 1$ was introduced to control the effect of stabilization. The conformation stabilization coefficient $\tau_{conf-new} =$
$a \times \tau_{conj/old}$. As $a$ decreases, the drag is accurate over a wider range. When $a = 0$, the drag coefficient computed by 4-field GLS is in excellent agreement with literature value in the whole range of Weissenberg number examined.

Another point, which is worthy of further discussion, is the weak form. If the complete 4-field GLS weak form is adopted, as shown in equation 1.26, the simulation fails to converge at very low Weissenberg number. An incomplete least square form was introduced by removing the terms $-\nabla \cdot \mu (E + E^T) - \nabla \cdot S$ in the momentum contribution to the weak form, which changes the formulation to equation 5.4; this formulation gives satisfactory results.

$$
\int_{\Omega} (q + \tau_{cont} \rho \nabla \cdot w)(\nabla \cdot v) d\Omega
+ \int_{\Omega} \left\{ w + \tau_{mom} [\rho v \cdot \nabla w + \rho w \cdot \nabla v + \nabla q] \right\}
\cdot [\rho v \cdot \nabla v + \nabla p - \nabla \cdot \mu (L + L^T) - \nabla \cdot (GM)] d\Omega
+ \int_{\Omega} \frac{1}{\eta} \left\{ S + \tau_{cons} \left[ -\lambda (-w \cdot \nabla M - v \cdot \nabla S + E^T \cdot M + M \cdot E + L^T \cdot S + S \cdot L) + (1 - 2\alpha)S + \alpha M \cdot S + \alpha S \cdot M \right] \right\}
\cdot \left[ -\lambda (-v \cdot \nabla M + L^T \cdot M + M \cdot L) + (\alpha - 1)I + (1 - 2\alpha)M + \alpha M^2 \right] d\Omega
+ \int_{\Omega} \mu \left[ E + \tau_{gradu}(E - \nabla w + \frac{1}{3} (\nabla \cdot w)I) \right]
\cdot \left[ L - \nabla v + \frac{1}{3} (\nabla \cdot v)I \right] d\Omega = 0

(5.4)

Using Mesh1 and Mesh2, physically meaningful results can be obtained up to roughly $Ws = 1.9$.

Because linear basis functions are used for all the variables of the 4-field GLS, with the same mesh, the 4-field GLS spends less time in every iteration than the Galcrkin
method as expected. A comparison of the computational speed of the 4-field GLS method and Galerkin method is listed in Table 5.4.

In addition, the compatibility with equal order basis function can greatly simplify the future parallelization of the code.

<table>
<thead>
<tr>
<th></th>
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</table>

Table 5.4 Comparison of the computational speed of the 4-field GLS method and Galerkin method.

5.4 Conclusion

In this chapter, the performance of the 4-field GLS formulation with flow around a cylinder is evaluated.

For all the test cases, the solution from the 4-field GLS and Galerkin method are
in excellent agreement with each other at low and moderate Weissenberg number.

Nevertheless, there are still some unusual behaviors whose origins remain un-
known. The full least-squares formulation fails to converge at low Weissenberg num-
ber, and the terms arising from the velocity gradient and conformation basis func-
tions in the least-squares form of the momentum equation must be dropped. More-
over, using the least-squares stabilization in the weighting terms of the conformation
transport equation ($\tau_{\text{cons}} \neq 0$) yields incorrect results for the drag coefficient on the
cylinder. In summary, the best computational results reported here were obtained
with a weak form which has the least-square stabilization of the continuity equation
(to handle incompressibility) and of the Newtonian momentum equation (to handle
high Reynolds number and incompressibility). The weighting of the conformation
and velocity gradient equation adopted here eventually reduces to plain Galerkin.
Nonetheless, the appropriate choice of weak form and stabilization coefficient is an
interesting topic for further research.
Figure 5.1  (a) Mesh for the flow around a cylinder. This mesh has 4504 elements and 18353 nodes. (b) Mesh for the flow around a cylinder. This mesh has 9696 elements and 39285 nodes.
Figure 5.2  Component of conformation tensor $M_{11}$ along the centerline at $Ws = 1.6$, $\beta = 0.59$ with the 4-field GLS and the Galerkin method.

Figure 5.3  Drag coefficient at different Weissenberg number at $\beta = 0.59$ with the 4-field GLS and the Galerkin method.
Figure 5.4  Streamlines of the flow around a cylinder at $W_s = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced streamlines are plotted. The maximum is 8 and the minimum is 0.

Figure 5.5  Contours of the horizontal velocity $v_1$ of the flow around cylinder at $W_s = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 1.64 and the minimum is 0.
Figure 5.6  Contours of the vertical velocity $v_2$ of the flow around cylinder at $W_s = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 0.45 and the minimum is $-0.44$.

Figure 5.7  Contours of pressure of the flow around a cylinder at $W_s = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 10 and the minimum is 0.
Figure 5.8  Contours of conformation $M_{22}$ of the flow around a cylinder at $W_s = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 24.9 and the minimum is 0.37.

Figure 5.9  Contours of Conformation $M_{12}$ of the flow around a cylinder at $W_s = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 13.6 and the minimum is $-9.6$.

Figure 5.10  Contours of the conformation $M_{11}$ of the flow around a cylinder at $W_s = 1.9$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 63.2 and the minimum is 0.12.
Figure 5.11  Contours of extension rate of the flow around a cylinder at $Ws = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 1.03 and the minimum is 0.

Figure 5.12  Contours of shear rate of the flow around a cylinder at $Ws = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 0.45 and the minimum is $-0.17$. 
Figure 5.13  Contours of the smallest molecule size of the flow around cylinder at $Ws = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 1.14 and the minimum is 0.26.

Figure 5.14  Contours of largest molecule size of the flow around cylinder at $Ws = 1.9$, $\beta = 0.59$, with the 4-field GLS methods. 11 equally spaced contour lines are plotted. The maximum is 80.4 and the minimum is 0.96.
Figure 5.15  Conformation component $M_{11}$ along the outflow symmetry line of the flow around a cylinder at $\beta = 0.59$, with the 4-field GLS method. As the Weissenberg number increases, $M_{11}$ experiences a steeper and higher peak in at the rear stagnation point, until it is no longer captured by the numerical approximation.
Figure 5.16  Drag coefficient of the flow around a cylinder at $\beta = 0.59$, with the 4-field GLS methods at different adjustable factor $a$. 
Chapter 6
Summary

In this thesis, a new finite element method, based on a restricted verification of a 4-field Galerkin/Least Squares method, is presented to solve viscoelastic problems. As a combination of Galerkin and Least-Squares weighted-residual methods, it benefits from the features of both of these methods.

Firstly, the 4-field GLS naturally includes the SUPG and PSPG stabilization terms, so it can stabilize the oscillations caused by advection-dominated terms, or spurious pressure modes.

Secondly, the 4-field GLS formulation introduces a new variable $L = \nabla v$, so that the second order derivative of $v$ is avoided, and the test function can be chosen as piecewise linear functions with piecewise constant derivatives. This feature substantially enlarges the space of the trial and weighting functions.

Thirdly, the Galerkin terms in this formulation guarantee that the traction term $n \cdot T$ appears naturally by integration by part, which serves as an important boundary condition for free surface flow, particularly in small scale problem where capillary has strong effects.

In addition, the 4-field GLS successfully circumvents the LBB condition on velocity and conformation fields. Equal order interpolation functions for velocity, pressure, stress, and velocity gradient can be employed in the weak form.

The 4-field GLS is tested with a carefully defined set of benchmark problems for both Newtonian (3-field GLS) and non-Newtonian flow. For Newtonian cases,
tests on lid-driven-cavity prove that the method is robust, and stabilization terms successfully avoid the oscillation that may appear at high Reynolds number. For flow around a cylinder, the drag force calculated from the Newtonian 3-field GLS is in excellent agreement with other independently developed methods, which confirms the accuracy of the formulation. The 4-to-1 contraction and stick-slip problems further demonstrate the ability of the Newtonian 3-field GLS to simulate geometries with singularities.

For viscoelastic cases, two things are noticed: terms connected with the velocity gradient and conformation basis function must be removed from the weighting factors in the momentum equation; and the least-squares term in the conformation evolution equation must be removed. After the modification, the solutions from the 4-field GLS and Galerkin method are in excellent agreement with each other at moderate Weissenberg number up to $W_s=1.9$. The drag exerted on the cylinder changes as Weissenberg number increases; the drag coefficient curve from 4-field GLS is in excellent agreement with those from the Galerkin method and other literature values.

Because linear basis functions are used for all the variables of 4-field GLS, with the same mesh, the 4-field GLS spends less time in every iteration than the Galerkin method as expected. As a trade off, the result is less accurate than the Galerkin method with the same mesh. However, the compatibility with equal order basis function can greatly simplify code parallelization.

As a combination of the Galerkin and Least-Squares method, the 4-field GLS still has a lot of potential for improvement. Experience from the previous tests shows that
an appropriate choice of weak form and stabilization coefficients can greatly improve the performance of the method. Some of the terms that were dropped in this study may be reintroduced provided that optimal stabilization coefficients can be developed.
References


HUGHES, J. R., FRANCA, L. P. AND HULBERT, G. M. 1989 A New Finite Element


