ABSTRACT

DeVAULT, KRISTEN J. Numerical Study of Two Problems in Fluid Flow: Cavitation and Cerebral Circulation. (Under the direction of Dr. Pierre A. Gremaud).

Two different computational models of fluid flow are considered. First, the possibility of cavitation is investigated numerically in two and three dimensions for the spherically symmetric, barotropic, Navier-Stokes equations. A splitting method is derived in order to allow the use of known solutions to the corresponding inviscid Euler equations. Results indicate cavitation is possible in the presence of high Mach numbers. This work is intended to be a stepping off point in the search for analytic solutions showing cavitation in multi-dimensional compressible flows.

Second, a blood flow model for circulation in the Circle of Willis (CoW) is derived. It is calibrated using ensemble Kalman filtering and validated against clinical data. The resulting model is then used to predict the effects of common anatomical variations within the CoW on blood perfusion in the brain, both under normal circumstances and in the event of a stroke.
Numerical Study of Two Problems in Fluid Flow: Cavitation and Cerebral Circulation

by

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DEDICATION

This work is dedicated to my parents for encouraging me to follow my dreams and to my sister for helping me to keep a sense of humor along the way.
Kristen Jean DeVault was born in Ludington, Michigan and grew up in Laurel, Maryland. She graduated from the University of Maryland with a Bachelor of Science degree in Mathematics in May of 2002. After graduating, she went on to work as a Mathematician for the Department of Defense at the Naval Surface Warfare Center in Dahlgren, Virginia. While there, she began taking graduate courses part-time through the University of Virginia.

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Chapter 1

Introduction

Computational models have vastly varied uses in the field of applied mathematics. On the more theoretical side, they can be used as a tool to gain insight into as yet unsolved theoretical problems giving other researchers a better idea of what to be looking for. In a more applied and interdisciplinary direction, they can be used to investigate biological variations within the human body. Not to mention the myriad of applications in between. In this work, two different computational models relating to fluid flow will be considered: cavitation in compressible flows and cerebral circulation in the Circle of Willis.

While not immediately apparent, there are a number of similarities between these two models. First, axisymmetric flows will be considered in both cases. In the vacuum formation problem, axisymmetric flows will be considered in order to take advantage of existing results for related equations. For the cerebral circulation model, axisymmetric flows will be considered to simplify the model to a point where it can be used to generate patient specific results in a reasonable amount of time. Another similarity between the two models is that viscous flows are considered in both cases. For the cavitation problem, this amounts to focusing on the Navier-Stokes equations rather than the inviscid Euler equations, for which theoretical results are already known (see section 3.7.2). In the blood flow model, there is no choice since blood is a viscous fluid. Finally, collocation methods (see section 2.2) are used in both models to ensure a high level of accuracy with a small number of spatial nodes, allowing us
to get accurate results in a reasonable amount of time.

There are also a number of differences between the two problems. In the cavitation problem, pockets of zero density within the solution are sought. Thus, the density must be allowed to change during the simulation requiring us to consider the equations for compressible fluid flow. For the cerebral blood flow problem, blood, which is essentially incompressible, is being modeled, so the incompressible fluid flow equations are used. Since there are known solutions to the inviscid equations corresponding to the viscous cavitation model, a splitting method (see section 3.8.3) will be used to allow the known inviscid solutions to be taken into account when solving the viscous equations. For the blood flow problem, there are no related solutions and therefore a simpler unsplit method is used. The final major difference in the two problems is the size of the Reynolds numbers considered. The Reynolds number is inversely proportional to the viscosity (see section 4.15). In the cavitation problem, fluid with low viscosity and therefore high Reynolds numbers will be considered. Conversely, in the cerebral circulation problem the flow of blood, which has a much lower Reynolds number, will be considered.

Chapter 2 will cover a number of fundamental ideas which apply to both of the problems. The cavitation problem will be discussed in detail in chapter 3 while the cerebral circulation problem will be discussed in chapter 4. Chapter 5 contains a few overall conclusions and final remarks.
Chapter 2

Numerical Considerations

In the applications considered in the following chapters, accuracy and speed will be important factors in choosing the numerical methods used to solve the given problems. One easy way to speed up a method is to reduce the number of nodes at which a solution is calculated. However, reducing the number of nodes often leads to decreases in the accuracy of the method. Thus, it is important to look for methods that achieve high levels of accuracy with a small number of nodes. One such class of methods are collocation methods.

2.1 Spatial Discretization

A common method for interpolating polynomials is through the use of trigonometric polynomials. This type of interpolation can be very useful when working with smooth periodic functions, however, it can lead to large amounts of error when dealing with discontinuous functions or extending nonperiodic functions in a periodic manner. This type of error is known as the Gibbs phenomenon and shows up as high frequency oscillations near jumps. A better option when dealing with nonperiodic functions is to use algebraic polynomial interpolation.
2.1.1 Lagrange Interpolation

One example of interpolation using algebraic polynomials is Lagrange interpolation. Given a set of \( n + 1 \) points in \( \mathbb{R} \), with

\[
x_0 < x_1 < \cdots < x_n,
\]

consider the Lagrange Polynomials

\[
L_i(x) = \prod_{k=0, k \neq i}^{n} \frac{x-x_k}{x_i-x_k},
\]

(2.1)

for \( i = 0, 1, \ldots, n \), which have the properties

\[
L_i(x) \in \mathcal{P}_n, \quad i = 0, 1, \ldots, n, \\
L_i(x_j) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases},
\]

where \( \mathcal{P}_n \) is the set of polynomials of degree less than or equal to \( n \).

**Theorem 2.1 (Lagrange Interpolation)** Given \( n + 1 \) data points \((x_i, f_i), i = 0, 1, \ldots, n\) with \( x_i \neq x_j \) for \( i \neq j \), the unique polynomial \( p(x) \in \mathcal{P}_n \) which interpolates the data points is

\[
p(x) = \sum_{i=0}^{n} f_i L_i(x) = \sum_{i=0}^{n} f_i \prod_{k=0, k \neq i}^{n} \frac{x-x_k}{x_i-x_k}.
\]

(2.2)

**Proof.** Suppose there exists \( \tilde{L}_i \) such that \( \tilde{L}_i \in \mathcal{P}_n \) and \( \tilde{L}_i(x_j) = \delta_{ij} \).

Then \( L_i - \tilde{L}_i \in \mathcal{P}_n \) and \( L_i - \tilde{L}_i \) has \( n + 1 \) distinct zeros, namely \( x_0, x_1, \ldots, x_n \). Thus, \( L_i - \tilde{L}_i = 0 \), or \( L_i \equiv \tilde{L}_i \). Therefore the \( L_i \)'s are unique making \( p(x) \) unique as well.

Finally, \( p(x_j) = \sum_{i=0}^{n} f_i L_i(x_j) = \sum_{i=0}^{n} f_i \delta_{ij} = f_j \Rightarrow p(x) \) interpolates the data.

Assuming the \( f_j \)'s were values of a function \( f(x) \) at the given \( x_j \)'s, a statement can be made about the relationship between \( f(x) \) and \( p(x) \).
\textbf{Theorem 2.2} Let \(x_0, x_1, \ldots, x_n\) be \(n + 1\) distinct points in \([a, b]\). Then if \(f \in C^{n+1}([a, b])\), for each \(x \in [a, b]\), there exists a \(\xi(x)\) in \((a, b)\) such that

\[ f(x) - p(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i) \tag{2.3} \]

where \(p(x)\) is the Lagrange interpolating polynomial defined above.

\textit{Proof.} For \(x = x_k\), \(f(x_k) = p(x_k)\) and \(\frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{i=0}^{n} (x - x_i) = 0\).

For \(x\) fixed with \(x \neq x_k\), \(k = 0, 1, \ldots, n\), define \(g(t)\) for \(t \in [a, b]\) as follows

\[ g(t) = f(t) - p(t) - (f(x) - p(x)) \prod_{i=0}^{n} \frac{t - x_i}{x - x_i}. \]

Then, if \(t = x_k\), \(g(x_k) = f(x_k) - p(x_k) - (f(x) - p(x)) \prod_{i=0}^{n} \frac{x_k - x_i}{x - x_i} = 0\). Similarly, if \(t = x\), \(g(x) = f(x) - p(x) - (f(x) - p(x)) \prod_{i=0}^{n} \frac{x - x_i}{t - x_i} = 0\). Therefore, \(g \in C^{n+1}([a, b])\) and vanishes at \(n + 2\) points. Thus, by the generalized Rolle’s Theorem, there exists \(\xi \in (a, b)\) such that \(g^{(n+1)}(\xi) = 0\). Which means

\[ 0 = g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - p^{(n+1)}(\xi) - (f(x) - p(x)) \frac{d^{n+1}}{dt^{n+1}} \left( \prod_{i=0}^{n} \frac{t - x_i}{x - x_i} \right)_{\xi}. \]

Since \(p \in P_n\), \(p^{(n+1)} = 0\). Also, \(\prod_{i=0}^{n} \frac{t - x_i}{x - x_i}\) is a polynomial of degree \(n + 1\) in \(t\), or more precisely

\[ \prod_{i=0}^{n} \frac{t - x_i}{x - x_i} = \frac{t^{n+1}}{\prod_{i=0}^{n} (x - x_i)} + q(t), \]

where \(q(x) \in P_n\). Thus,

\[ \frac{d^{n+1}}{dt^{n+1}} \left( \prod_{i=0}^{n} \frac{t - x_i}{x - x_i} \right) = \frac{(n+1)!}{\prod_{i=0}^{n} (x - x_i)}. \]

Substituting this into the relation above, gives

\[ 0 = f^{(n+1)}(\xi) - (f(x) - p(x)) \frac{(n+1)!}{\prod_{i=0}^{n} (x - x_i)}, \]

or,

\[ f(x) - p(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x - x_i). \]
Using Lagrange interpolation on equally spaced nodes can still lead to large amounts of error. However, if well chosen unevenly spaced nodes are used, the error can be reduced significantly. The next section will discuss a family of polynomials known as Chebyshev polynomials and show how they are related to choosing the best set of unevenly spaced nodes to get the smallest error between the function and its interpolant.

2.1.2 Chebyshev Polynomials

The Chebyshev polynomials are defined recursively as follows

\[ T_0(x) = 1, \]
\[ T_1(x) = x, \]
\[ T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x), \quad n \geq 2. \]

Figure 2.1 shows the first six Chebyshev polynomials on the interval \([-1, 1]\). Sometimes, an alternate form of the definition of Chebyshev polynomials is helpful. In the upcoming derivation, the definition stated in Proposition 2.1 will be needed in addition to the recursive definition.
Proposition 2.1 The Chebyshev polynomials $T_n(x)$, defined recursively above, are equivalent to $\cos(n \arccos x)$ on $[-1, 1]$.

Proof.

- $n = 0$ : $T_0(x) = 1 = \cos(0 \cdot \arccos x)$
- $n = 1$ : $T_1(x) = x = \cos(1 \cdot \arccos x)$
- $n > 1$ : assume $T_k(x) = \cos(k \arccos x)$ for $k = 0, 1, \ldots, n - 1$ and let $y = \arccos x$. Then

$$T_n(x) = T_n(\cos y) = 2 \cos(y)T_{n-1}(\cos(y)) - T_{n-2}(\cos(y)) = 2 \cos(y) \cos((n-1)y) - \cos((n-2)y)$$

$$= 2 \left[ \frac{1}{2} (\cos(ny) + \cos((n-2)y)) \right] - \cos((n-2)y)$$

$$= \cos(ny) + \cos((n-2)y) - \cos((n-2)y)$$

$$= \cos(ny)$$

$$= \cos(n \arccos x).$$

$\Rightarrow$ By induction, $T_n(x) = \cos(n \arccos x)$ for any $n \geq 0$.

□

In order to derive the optimal nodes to be used in the interpolation, the following result will be needed.

Proposition 2.2 (Optimality Property of Chebyshev Polynomials) Let $\tilde{\mathcal{P}}_n$ be the set of polynomials of degree $n$ with leading coefficient 1. Then

$$\max_{-1 \leq x \leq 1} \frac{|T_n(x)|}{2^{n-1}} \leq \max_{-1 \leq x \leq 1} |p(x)|$$

for any $p \in \tilde{\mathcal{P}}_n$.

Proof. Assume there exists $p(x) \in \tilde{\mathcal{P}}_n$ such that

$$\max_{-1 \leq x \leq 1} |p(x)| < \frac{1}{2^{n-1}}$$
and let

\[ r(x) = \frac{T_n(x)}{\frac{2^{n-1}}{2^n}} - p(x). \]

Since \( \frac{T_n(x)}{\frac{2^{n-1}}{2^n}} \) is in \( \tilde{\mathcal{P}}_n \) and \( p(x) \) is in \( \tilde{\mathcal{P}}_n \), \( r(x) \) is of degree less than or equal to \( n - 1 \).

Consider \( x'_k = \cos \left( \frac{k\pi}{n} \right) \), for \( k = 0, 1, \ldots, n \).

\[
T_n(x) = \cos (n \arccos x) \\
\Rightarrow T'_n(x) = \frac{n \sin (n \arccos(x))}{\sqrt{1 - x^2}} \\
\Rightarrow T'_n(x'_k) = T'_n \left( \cos \left( \frac{k\pi}{n} \right) \right) \\
= \frac{n \sin (n \arccos \cos \left( \frac{k\pi}{n} \right))}{\sqrt{1 - \cos^2 \left( \frac{k\pi}{n} \right)}} \\
= \frac{n \sin (k\pi)}{\sin \left( \frac{k\pi}{n} \right)} = 0 \text{ for } k = 0, 1, \ldots, n.
\]

Thus the \( x'_k \)'s are extreme points of \( T_n(x) \) and

\[
T_n(x'_k) = T_n \left( \cos \left( \frac{k\pi}{n} \right) \right) \\
= \cos \left( n \arccos \cos \left( \frac{k\pi}{n} \right) \right) \\
= \cos(k\pi) \\
= (-1)^k \\
\Rightarrow r(x'_k) = \frac{T_n(x'_k)}{\frac{2^{n-1}}{2^n}} - p(x'_k) = \frac{(-1)^k}{\frac{2^{n-1}}{2^n}} - p(x'_k).
\]

Also, by assumption, \( \max_{-1 \leq x \leq 1} |p(x)| \leq \frac{1}{2^{n-1}} \), so

\[
k \text{ even: } r(x'_k) = \frac{1}{2^{n-1}} - p(x'_k) \\
> \frac{1}{2^{n-1}} - \frac{1}{2^{n-1}} = 0 \\
k \text{ odd: } r(x'_k) = \frac{-1}{2^{n-1}} - p(x'_k) \\
< \frac{-1}{2^{n-1}} + \frac{1}{2^{n-1}} = 0.
\]

Therefore, \( r(x) \) changes sign at least \( n \) times on \([-1, 1]\). But \( r(x) \) is of degree less than or equal to \( n - 1 \), so \( r(x) \equiv 0 \) making \( p(x) = \frac{T_n(x)}{\frac{2^{n-1}}{2^n}} \). Thus,

\[ \max_{-1 \leq x \leq 1} |p(x)| = \frac{1}{2^{n-1}}. \] Contradiction!
\[ \Rightarrow \max_{-1 \leq x \leq 1} |p(x)| \geq \frac{1}{2^{n-1}} = \max_{-1 \leq x \leq 1} \left| \frac{T_n(x)}{2^{n-1}} \right|. \]

2.1.3 Optimal Node Placement

From the error formula (2.3), it is apparent that to reduce the error in the approximation, one must work with the location of the nodes since one has no control over \( \xi(x) \). Therefore, a polynomial of degree \( n + 1 \) with leading coefficient 1, which has the smallest maximum value is desired. By the optimality property just shown (Proposition 2.2), it is known that this polynomial is the (normalized) Chebyshev polynomial of degree \( n + 1 \). Since the desired Chebyshev polynomial is defined on the interval \([-1, 1]\), in order to use an arbitrary interval \([a, b] \), a change of variables that maps -1 to \( a \) and 1 to \( b \) must be used, \( i.e. \)

\[ \tilde{x} = \frac{1}{2} \left[ (b - a)x + a + b \right]. \]

Since the nodes used in the Lagrange interpolation are the roots of the polynomial in the error formula, the nodes are chosen to be the zeros of \( T_{n+1} \), namely

\[ x_k = \cos \left( \frac{(2k + 1)\pi}{2(n + 1)} \right), \]

for \( k = 0, 1, 2, \ldots, n \).

Notice that the nodes above do not contain the endpoints of the domain. Sometimes is it necessary to include one or both of the endpoints as nodes. The so-called Chebyshev-Gauss-Radau nodes (containing one endpoint) and Chebyshev-Gauss-Lobatto nodes (containing both endpoints) can be derived in a similar manner. In summary, the best choice of nodes on the interval \([-1, 1]\) is one of the following, depending on whether or not nodes at the endpoints are desired:

- Chebyshev-Gauss

\[ x_k = \cos \left( \frac{(2k + 1)\pi}{2(n + 1)} \right), \quad \text{for } k = 0, 1, \ldots, n, \]  

(2.4)
- Chebyshev-Gauss-Radau

\[ x_k = \cos \left( \frac{2\pi k}{2n-1} \right), \quad \text{for } k = 0, 1, \ldots, n - 1, \]  

(2.5)

- Chebyshev-Gauss-Lobatto

\[ x_k = \cos \left( \frac{k\pi}{n} \right), \quad \text{for } k = 0, 1, \ldots, n. \]  

(2.6)

### 2.2 Collocation Methods

Collocation methods are designed to approximate the solution to a given problem by a function that satisfies the equations exactly at a given set of points. By choosing the points in an intelligent way, a high level of accuracy can be achieved even with a very small number of points. Section 2.2.1 gives a detailed derivation of collocation methods and section 2.2.4 describes a study of the accuracy of such methods when applied to problems similar to those that will show up in later chapters.

#### 2.2.1 Derivation

First a collocation method for a scalar differential equation will be derived\(^1\) and then it will be extended to systems of differential equations.

Consider the following scalar ODE

\[ y' = f(t, y). \]  

(2.7)

Begin by choosing a set of \( s \) distinct collocation points,

\[ 0 \leq c_1 < c_2 < \cdots < c_s \leq 1, \]

and \( \phi(t) \), a polynomial of degree \( \leq s \), such that

\[ \phi(t_{n-1}) = y_{n-1} \]  

(2.8)

\[ \phi'(t_i) = f(t_i, \phi(t_i)) \quad i = 1, 2, \ldots, s, \]  

(2.9)

\(^1\)This derivation closely follows the explanation given in [3].
where \( h \) is the size of the time interval and \( t_i = t_{n-1} + c_i h \). Note that this uniquely defines the polynomial \( \phi(t) \).

This is an \( s \)-stage implicit Runge-Kutta method if \( y_n = \phi(t_n) \) [3].

**Extension to Systems of Differential Equations**

In the case of a system of differential equations

\[
y' = f(t, y),
\]

\( \phi(t) \) is simply replaced by a vector of polynomials \( \Phi(t) \).

### 2.2.2 Boundary Conditions

When Chebyshev-Gauss-Lobatto (CGL) nodes are used, there are nodes at each end and therefore the boundary conditions can be implemented directly. On the other hand, when Chebyshev-Gauss-Radau (CGR) nodes are used, there is no node at the origin or inner boundary, therefore any boundary conditions that are needed at the origin must be implemented indirectly. Luckily, in the cases considered later, there are no explicit boundary conditions at the origin when CGR nodes are used.

To enforce a boundary condition at a specific node, one of the differential equations related to that node is replaced by the equation for the boundary condition. Which equation is dropped depends on the form of the boundary condition being implemented. In the vacuum case, the boundary condition being implemented is related to the velocity, therefore the differential equation for the velocity is removed at the appropriate node. In the blood flow case, both flow and pressure conditions are implemented, thus which equation will be removed depends on the specific vessel.

### 2.2.3 Differentiation Matrices

Given a set of values of a function \( f \) at the Chebyshev nodes \( x_i \) where \( f_i = f(x_i) \), let \( p(x) \) be the Lagrange interpolating polynomial

\[
p(x) = \sum_{i=0}^{n} f_i \mathcal{L}_i(x),
\]

(2.10)
where
\[ \mathcal{L}_i(x) = \prod_{k=0, k \neq i}^{n} \frac{x - x_k}{x_i - x_k}. \]

Thus,
\[ p'(x) = \sum_{i=0}^{n} f_i \mathcal{L}_i'(x). \tag{2.11} \]

Letting \( q_j = p'(x_j) \), leads to
\[ q_j = p'(x_j) = \sum_{i=0}^{n} f_i \mathcal{L}_i'(x_j), \]

which can be written in matrix form as
\[ \vec{q} = D \vec{f}, \tag{2.12} \]

where \( D_{ij} = \mathcal{L}_i'(x_j) \). Plugging in the definition of \( \mathcal{L} \) (and lots of algebra) leads to the following expressions for the elements of \( D \) depending on the choice of Chebyshev nodes:

- **Chebyshev-Gauss-Radau nodes**

  \[
  D_{ij} = \begin{cases} 
  \frac{n(n-1)}{3}, & i = j = 0; \\
  \frac{N \cos \left( \frac{2Nj+1}{2N-1} \right) + (N-1) \cos \left( \frac{2(N-1)j+1}{2N-1} \right)}{c_0 \sin^2 \left( \frac{2\pi j}{2N} \right)}, & i = 1, \ldots, n - 1, j = 0; \\
  \frac{c_i}{2c_j(x_i-x_j)}, & i \neq j, i = 0, \ldots, n - 1, j = 1, \ldots, n - 1; \\
  -\sum_{k=0, k \neq 1}^{n-1} D_{ik}, & i = j = 1, \ldots, n - 1; \\
  \end{cases}
  \]

  where

  \[
  c_i = \begin{cases} 
  1 - 2n, & i = 0; \\
  -\frac{N \cos \left( \frac{2\pi i}{2N-1} \right) + (N-1) \cos \left( \frac{2\pi (N-1)j+i}{2N-1} \right)}{2x_i}, & i = 1, \ldots, n - 1; \\
  \end{cases}
  \]

- **Chebyshev-Gauss-Lobatto nodes**

  \[
  D_{ij} = \begin{cases} 
  \frac{2n^2+1}{6}, & i = j = 0; \\
  -\frac{2n^2+1}{6}, & i = j = n; \\
  \frac{c_i (-1)^{i+j}}{c_j (x_i-x_j)}, & i \neq j, i, j = 0, \ldots, n; \\
  -\sum_{k=0, k \neq 1}^{n-1} D_{ik}, & i = j = 1, \ldots, n - 1; \\
  \end{cases}
  \]
where 

\[ c_i = \begin{cases} 
2, & i = 0, n \smallskip 
1, & \text{otherwise}.
\end{cases} \]

Note that in the above definitions, the expressions for the diagonal elements have been replaced by the negative row sums of the off diagonal elements. This is done to reduce the error and ensure that the derivative of a constant is identically zero. While an explicit expression can be derived for the diagonal elements, in practice they are calculated as above.

In the applications discussed later, Chebyshev collocation in space will be used in solving partial differential equations (PDEs). For a general linear \( n \)th order PDE in one spatial dimension

\[
\sum_{i=0}^{n} \alpha_i \frac{\partial^i u}{\partial t^i} + \sum_{i=0}^{n} \beta_i \frac{\partial^i u}{\partial x^i} = f(x,t),
\]

this amounts to replacing the spatial derivatives by multiplication by \( D \), more precisely,

\[
\sum_{i=0}^{n} \alpha_i \frac{\partial^i U}{\partial t^i} + \sum_{i=0}^{n} \beta_i D^i U = F,
\]

where

\[
U_j = u(x_j,t),
\]

\[
F_j = f(x_j,t),
\]

and \( x_j \) is the \( j \)th spatial node. This leaves an ordinary differential equation (ODE) which can be solved using traditional numerical methods.

### 2.2.4 Accuracy

In this section the accuracy of Chebyshev collocation will be compared to that of a more common finite difference scheme. For this example Chebyshev-Gauss-Lobatto nodes will be used for the collocation scheme and equally spaced nodes will be used for the finite difference scheme. The accuracy of the Chebyshev derivative
Figure 2.2: Accuracy of Chebyshev differentiation versus finite difference differentiation as a function of the number of nodes. (top) The error in the Chebyshev method decreases much faster than that of the finite difference method until it reaches machine precision. (bottom) The finite difference scheme shows 2nd order convergence while the Chebyshev method shows spectral convergence.

versus a centered finite difference derivative will be considered as well as the use of Chebyshev collocation versus finite difference in the process of solving a simple advection equation.

**Spectral Accuracy of Chebyshev Differentiation Matrix**

To show the spectral accuracy of the Chebyshev Differentiation matrix versus the second order accuracy of centered finite differences, consider the following function

\[ f(x) = e^{-\frac{x^2}{2}}, \]

which has derivative

\[ f'(x) = -xe^{-\frac{x^2}{2}}. \]

To check the accuracy of a given approximation to the derivative, the following
definition of error will be used

\[ \text{error} = \max_j \left| F'_j - (DF)_j \right|, \]

where

\[ F_j = f(x_j), \]
\[ F'_j = f'(x_j), \]

\( x_j \) is the \( j \)th spatial node, and \( D \) is the differentiation matrix. Figure 2.2 (top) shows how the error drops much faster with respect to the number of nodes used in the case of the Chebyshev differentiation matrix than for the finite difference differentiation matrix. In fact, the Chebyshev differentiation has reached machine accuracy with only 20 nodes. This explains the change in the tail of the plot since adding more nodes cannot reduce the error below machine precision. Figure 2.2 (bottom) shows an estimate of the order of convergence of each of the methods. As expected, the finite difference method shows 2nd order convergence. On the other hand, the order of convergence of the Chebyshev method continues to increase until the error reaches near machine precision. This is called spectral accuracy. More precisely, spectral accuracy is when the error decreases faster than any negative power of the number of nodes.

**Application to Advection Equation**

As a test problem, consider the following advection initial-boundary value problem

\[
\begin{aligned}
  u_t + 2u_x &= 0, \\
  u_t(0, t) &= -12 \text{sech}^2 (3(2t + 1)) \tanh (3(2t + 1)), \\
  u(x, 0) &= \text{sech}^2 (3(x - 1)),
\end{aligned}
\]

which has solution

\[ u(x, t) = \text{sech}^2 (3(x - 2t - 1)). \]

In each case, the MATLAB solver `ode15s` is used for the time integration. Figure 2.3 shows a comparison of the accuracy obtained using the Chebyshev collocation
Figure 2.3: Comparison of the maximum error over space and time versus the number of nodes for the solution of the advection initial-boundary value problem (2.13) using MATLAB’s \texttt{ode15s} solver in time with Chebyshev collocation or finite difference derivatives in space. The solution using the Chebyshev collocation derivative achieves a smaller amount of error with 64 nodes than the centered finite difference method achieves with 512 nodes. The tolerances given are the relative and absolute tolerance parameters for the MATLAB solver. The fact that the two finite difference curves are almost identical indicates that the total error is dominated by the error in the finite difference approximation of the spatial derivative. The collocation curves, on the other hand, are quite different. This indicates that the overall error is dominated by the error from the timestepping scheme.
derivative in space versus the centered finite difference derivative in space. It is easy to see that the Chebyshev method achieves a smaller amount of error with 64 nodes than the finite difference method achieves with 512 nodes. It is also apparent from the figure that after a certain point no more accuracy is gained with the Chebyshev method by adding more nodes. This is related to the findings in the previous section that the Chebyshev derivative reaches machine precision with a very small number of nodes.

2.3 Time Integration

Consider again, the initial-boundary value problem (2.13). Using the Chebyshev differentiation matrix to approximate the spatial derivatives reduces the problem to an ODE in time. Thus, the next step is to determine an appropriate time integration method. There are two main considerations when choosing a time integration method: accuracy and stability. Generally, the more accuracy that is required, the more difficult the method is and the longer it will take to run. In addition, both accuracy and stability can lead to restrictions on the maximum allowable step size, which can also cause simulations to take a long time to run. For this reason, a simple method with sufficient accuracy and as much stability as possible is sought in order to keep the time required to run the simulation reasonable.

Two simple methods for solving ODEs are forward and backward Euler. Forward Euler (FE),

$$y_{n+1} = y_n + \Delta x f(x_n, y_n),$$

(2.14)

has the benefit of being explicit and therefore no knowledge of the desired solution is needed in order to find the solution. However, the explicit nature of this method causes it to have tight restrictions on the size of time steps in order to maintain stability as is seen in section 2.3.4. Backward Euler (BE),

$$y_{n+1} = y_n + \Delta x f(x_{n+1}, y_{n+1}),$$

(2.15)

on the other hand, is an implicit method which allows it to take into account the solution at the next time step when stepping forward in time. The implicit nature of
BE makes it more difficult to solve but removes the tight restriction on the size of the time step seen with FE. In fact, in section 2.3.4 it is shown that BE is an A-stable method which is a highly desirable property in a numerical solver. BE is a specific case of a family of methods known as Backward Difference Formulae (BDF). In the previous section, the MATLAB solver ode15s was used to do the time integration. This is another specific case of a BDF method.

2.3.1 Backward Difference Formulae

Some multi-step methods are efficient on stiff\(^2\) problems (like the ones encountered in the upcoming chapters). The most popular methods are based on Newton-Cotes quadratures\(^3\) and are known as the Backward Difference Formulae (BDF) [9]. BDF methods are implicit methods that are often very efficient for solving stiff ODEs. Given an ODE that is to be solved numerically, the decision of whether to use numerical integration or numerical differentiation must be made. Unlike most other multi-step methods, BDF methods rely on numerical differentiation.

Consider

\[
\begin{cases}
    y' = f(x, y) & x > x_0 \\
    y(x_0) = y_0
\end{cases}
\]

and let \( x_0 < x_1 < \cdots < x_k \) with \( x_k = x_0 + k\Delta x \). Also, let \( p(x) \) be the Lagrange interpolating polynomial of degree \( k \) through \( x_0, x_1, \ldots, x_k \),

\[ p(x_i) = y(x_i) \quad i = 0, 1, \ldots, k. \]

Next replace \( y'(x_k) \) by \( p'(x_k) \) in equation (2.16). By the Lagrange formula there exists \( \alpha_0, \alpha_1, \ldots, \alpha_k \), independent of \( y \) and \( \Delta x \) such that

\[ y'(x_k) \approx \frac{1}{\Delta x} (\alpha_k y(x_k) + \cdots + \alpha_0 y(x_0)). \]

BDF coefficients can be found for any \( k \). Consider the case \( k = 1 \) as an example. When \( k = 1 \),

\[ p(x) = \sum_{i=0}^{1} y_i \mathcal{L}_i(x). \]

\(^2\)For a definition of stiffness see, for example, [3].

\(^3\)For a definition of Newton-Cotes quadratures see, for example, [56].
In order to find the appropriate coefficients, \( \mathcal{L}_0, \mathcal{L}_1, \mathcal{L}_0', \) and \( \mathcal{L}_0' \), will be needed and can be found as follows:

\[
\mathcal{L}_0(x) = \frac{x-x_1}{x_0-x_1} = \frac{-1}{\Delta x} (x-x_1) \Rightarrow \mathcal{L}_0'(x) = \frac{-1}{\Delta x},
\]

\[
\mathcal{L}_1(x) = \frac{x-x_0}{x_1-x_0} = \frac{1}{\Delta x} (x-x_0) \Rightarrow \mathcal{L}_1'(x) = \frac{1}{\Delta x}.
\]

Thus,

\[
p'(x_1) = y_0 \mathcal{L}_0'(x) + y_1 \mathcal{L}_1'(x)
\]

\[
= y_0 \left( \frac{-1}{\Delta x} \right) + y_1 \left( \frac{1}{\Delta x} \right)
\]

\[
= \frac{1}{\Delta x} (y_1 - y_0).
\]

Replacing \( p'(x_1) \) with \( f(x_1, y_1) \) and solving for \( y_1 \) leads to the following iteration procedure:

\[
y_1 = y_0 + \Delta x f(x_1, y_1),
\]

which is exactly backward Euler (BE).

The same procedure can be followed to find the coefficients associated with \( k > 1 \). Coefficients for \( k = 1, 2, 3, 4 \) can be found in table (2.1).

<table>
<thead>
<tr>
<th>( k )</th>
<th>( \alpha_0 )</th>
<th>( \alpha_1 )</th>
<th>( \alpha_2 )</th>
<th>( \alpha_3 )</th>
<th>( \alpha_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-1</td>
<td>1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>\frac{1}{2}</td>
<td>-2</td>
<td>\frac{3}{2}</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>\frac{1}{3}</td>
<td>\frac{3}{2}</td>
<td>-3</td>
<td>\frac{11}{6}</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>\frac{1}{4}</td>
<td>\frac{3}{2}</td>
<td>3</td>
<td>-4</td>
<td>\frac{25}{12}</td>
</tr>
</tbody>
</table>

### 2.3.2 Analysis of Multistep Methods

In this section multi-step methods are considered and their order of accuracy is determined. Since BE is simply BDF with \( k = 1 \), as was shown in section 2.3.1, this discussion will apply to both BE and generic BDF methods.
Begin by considering a generic $k$-step multi-step method
\[
\alpha_k y_{k+n} + \alpha_{k-1} y_{k-1+n} + \cdots + \alpha_0 y_n = \Delta x \{ \beta_k f(x_{n+k}, y_{n+k}) + \cdots \\
+ \beta_0 f(x_n, y_n) \} \quad n = 0, 1, \ldots \quad (2.17)
\]

The local error of equation (2.17) is defined as
\[
\epsilon = y(x_k) - y_k,
\]
where $y(x)$ is the exact solution of
\[
\begin{cases}
  y' = f(x, y) \\
y(x_0) = y_0,
\end{cases}
\]
and $y_k$ is the numerical solution from equation (2.17) using the exact starting values $y_i = y(x_i)$, $i = 0, \ldots, k - 1$. Next, define the linear differential operator
\[
\mathcal{L}(y, x, \Delta x) = \sum_{i=0}^{k} (\alpha_i y(x + i\Delta x) - \Delta x \beta_i y'(x + i\Delta x)).
\]

It can be shown that
\[
\epsilon = y(x_k) - y_k = \left( \alpha_k I - \Delta x \beta_k \frac{\partial f}{\partial y}(x_k, \eta) \right)^{-1} \mathcal{L}(y, x, \Delta x),
\]
where $\eta$ is between $y(x_k)$ and $y_k$. The method defined by equation (2.17) is said to be of order $p$ if one of the following holds:

1. $\epsilon = O(\Delta x^{p+1})$,
2. $\mathcal{L}(y, x, \Delta x) = O(\Delta x^{p+1})$.

**Theorem 2.3** Equation (2.17) is of order $p$ iff
\[
\sum_{i=0}^{k} \alpha_i = 0 \quad \text{and} \quad \sum_{i=0}^{k} \alpha_i i^q = q \sum_{i=0}^{k} \beta_i i^{q-1} \quad \text{for} \quad q = 1, \ldots, p.
\]

**Proof.** See [56].
For example, consider BDF with $k = 2$. Here,

$$\begin{align*}
\alpha_2 &= \frac{3}{2}, & \alpha_1 &= -2, & \alpha_0 &= \frac{1}{2}, \\
\beta_2 &= 1, & \beta_1 &= 0, & \beta_0 &= 0,
\end{align*}$$

and thus,

$$\sum_{i=0}^{k} \alpha_i = \frac{1}{2} - 2 + \frac{3}{2} = 0,$$

which satisfies the first condition. Checking the second condition for $q = 1, 2, 3$ shows that BDF with $k = 2$ is of order 2. In fact, it can be shown that BDF with $k$ steps is of order $k$. In particular, this means that BE is first order.

### 2.3.3 Newton’s Method

Since implicit methods will be used to solve the problems presented in the upcoming chapters, an efficient way to solve a highly nonlinear system will be needed. For this work, a small number of steps of Newton’s method will be sufficient. Consider the system of equations $g(y) = 0$, where the solution $y$ is sought.

Let $y^0$ be the initial guess and let $y^n$ be the current iterate. Consider the first order Taylor expansion of $g$ about $y^n$ evaluated at $y^{n+1}$

$$0 = g(y^n) + \frac{\partial g}{\partial y}(y^n)(y^{n+1} - y^n). \tag{2.18}$$

Solving equation (2.18) for $y^{n+1}$ gives the Newton iteration scheme

$$y^{n+1} = y^n - \left(\frac{\partial g}{\partial y}(y^n)\right)^{-1}g(y^n), \quad n = 0, 1, \ldots \tag{2.19}$$

This iteration continues until $||g(y^n)|| \leq tol$ where $tol$ is a predetermined tolerance parameter.

Newton’s method is used to find the (approximate) solution to a system of equations of the form $g(y) = 0$. Thus, in order to use Newton’s method, the problems considered will need to be formulated in this way. The Backward Euler (BE) scheme found in section 2.3.1 is

$$y^n = y^{n-1} + h_n f(t_n, y^n),$$
or equivalently,
\[ g(y) \equiv y - y^{n-1} - h_n f(t_n, y) = 0, \]

which is in the proper form. From this one gets
\[ \frac{\partial g}{\partial y} = I - h_n \frac{\partial f}{\partial y}. \]

Thus, in the case of BE, the Newton iteration is
\[ y^n = y^{n-1} - \left( I - h_n \left( \frac{\partial f}{\partial y} \right)^{-1} \right) g(y^n), \quad n = 1, 2, 3, \ldots \quad (2.20) \]

A similar derivation can be followed to find the Newton iteration for BDF.

2.3.4 Stability

To analyze the stability of a numerical method applied to \( y' = f(x, y) \), consider the linearized problem
\[ \bar{y}'(x) = J(x)\bar{y}(x), \quad (2.21) \]

where \( f \) is linearized in the neighborhood of \( u \). More precisely, let \( y'(x) = f(x, u(x)) + \frac{\partial f}{\partial y}(x, u(x))(y(x) - u(x)) + \cdots \) and \( \bar{y}(x) = y(x) - u(x) \). Then
\[ \bar{y}'(x) = \frac{\partial f}{\partial y}(x, u(x))\bar{y}(x) + \cdots = J(x)\bar{y}(x) + \cdots, \]

where \( J(x) \) is the Jacobian of the system evaluated at \( u(x) \), i.e. \( (J(x))_{ij} = \frac{\partial f_i}{\partial y_j}(x, u(x)) \).

Looking at Backward Euler (BE) this leads to
\[ y^{n+1} = y^n + \Delta x J y^{n+1} \]
\[ \Rightarrow (I - \Delta x J) y^{n+1} = y^n \]
\[ \Rightarrow y^{n+1} = (I - \Delta x J)^{-1} y^n, \]

or \( y^{n+1} = R(\Delta x J) y^n \) with \( R(z) = I - z \). The function \( R(z) \) is called the stability function of the method. The set \( S = \{ x \in \mathbb{C} : |R(z)| \leq 1 \} \) is the stability domain of the method. A method with \( \mathbb{C}^{-} \subset S \) where \( \mathbb{C}^{-} = \{ x \in \mathbb{C} : \text{Re}(z) \leq 0 \} \) is called A-stable. For BE, \( S = \{ z \in \mathbb{C} : \frac{1}{1-z} \leq 1 \} \) is the exterior of the circle of radius 1, centered at \( z = 1 \). Thus, BE is an A-stable method.

Figure 2.4 shows the stability domains for BDF with \( k = 1, 2, 3, 4, 5 \).
Figure 2.4: Stability regions for BDF methods with $k = 1, 2, 3, 4, 5$. In each case, the stability region is the area outside the curve.
2.4 Basic Statistical Concepts

There are a few statistical concepts which will aide in the understanding of upcoming sections. A brief description of relevant topics is contained in this section. For a more thorough background, see any introductory statistics book, e.g. [16].

A random variable is any rule that associates a number with each possible outcome of an experiment. In later chapters, blood flow velocity will be considered as a random variable from which a number of samples have been collected. From these samples, the sample mean, which is simply the average value of the samples, can be calculated. The variability of the samples, which is measured as the average squared deviation from the mean and is called the variance, will also be of interest. The standard deviation, which is the square root of the variance, is another measure of the variability. The standard deviation is more useful for direct comparison because it has units that are the same as that of the samples. When looking at multiple random variables which have some dependancy on each other, their covariance, which is a measure of how strongly the random variables are correlated, can be considered. Finally, in certain instances, a given set of data will need to be perturbed according to a given probability distribution which is known as stochastic perturbation.

2.5 Kalman Filtering

Kalman filtering is a recursive algorithm that can be used to optimize parameters in a linear model. It uses model results and data values at each time step to adjust the parameters until the optimal parameters have been found. Central to all types of Kalman filtering is the matrix known as the “Kalman gain”. The Kalman gain is used to create the a posteriori state estimates as weighted averages of the a priori state estimates and the discrepancies between the predicted measurements and the actual measurements [65]. It is chosen to minimize the a posteriori estimate error covariance and is built from the a priori estimate error covariance matrix.
2.5.1 Derivation

The Kalman filter is a sequential filtering method which involves advancing the model forward in time until there are measurements available and then reinitializing the model to take the data into account. The model is used to create the model forecast, $x^f$, and then updated based on available data, $d$, to create the model analysis, $x^a$. The analysis update is based on the forecast covariance, $P^f$, the analysis covariance, $P^a$, the measurement error, $\epsilon$, the measurement covariance, $R$, and the measurement operator, $H$. Specifically, $x^a$ is a weighted linear combination of the state predicted by the model, $x^f$, and the covariances related to the measurements [18]. This linear combination is determined by the Kalman gain, $K$.

The matrix $K$, is chosen to minimize the a posteriori error estimate

$$x - x^a,$$

where $x$ is the true state. This is equivalent to minimizing the trace of the analysis error covariance,

$$P^a = \text{cov}(x - x^a).$$

Substituting in the definition of $x^a$, namely,

$$x^a = x^f + KH(x - x^f) + K\epsilon,$$

and using the properties of covariance leads to

$$P^a = \text{cov}((I - KH)(x - x^f) - K\epsilon)$$

$$= (I - KH)\text{cov}(x - x^f)(I - KH)^T + K\text{cov}(\epsilon)K^T$$

$$= (I - KH)P^f(I - KH)^T + KRK^T.$$

Expanding this equation gives the following expression for the analysis error covariance

$$P^a = P^f - KH P^f - P^f H^T K^T + K\left(HP^fH^T + R\right)K^T.$$ 

Since trace is a linear operator and $P^f$ is symmetric, the trace of the analysis error covariance can be expressed as

$$\text{tr}(P^a) = \text{tr}(P^f) - 2\text{tr}(KH P^f) + \text{tr}\left(K\left(HP^fH^T + R\right)K^T\right).$$
Thus, the Kalman gain will satisfy

\[
0 = \frac{d\text{tr}(P^a)}{dK} = -2(HP^f)^T + K(HP^f H^T + R)^T + K(HP^f H^T + R)
\]

\[
= -2(HP^f)^T + 2K(HP^f H^T + R),
\]

where the symmetry of $P^f$ and $R$ and the following properties of the trace

\[
\frac{d\text{tr}(AXB)}{dX} = A^TB^T,
\]

\[
\frac{d\text{tr}(XBX^T)}{dX} = XB^T + XB,
\]

have been used to simplify the expression.

Therefore, to minimize the a posteriori estimate error, $K$ is chosen such that

\[
(HP^f)^T = K(HP^f H^T + R)
\]

or

\[
K = P^f H^T (HP^f H^T + R)^{-1}.
\]

When dealing with a nonlinear problem, one can use the Extended Kalman filter, which requires the direct calculation of an error covariance matrix at each timestep, or the Ensemble Kalman filter (EnKF), which approximates the error covariance matrix using an ensemble of states. The EnKF has been used in this work to avoid the costly direct calculation of the error covariance matrix.

### 2.5.2 Ensemble Kalman Filtering

In the EnKF, the observations are treated as random variables with mean equal to the actual measurement and covariance defined by $R$. Since the EnKF uses estimates based on the ensemble members to create the Kalman gain, the larger the ensemble size the better the results will be [18]. In fact, to avoid singular matrices in the analysis step, the number of ensemble members, $N$, needs to be greater than the number of measurement locations\(^4\). There are multiple statistically consistent ways

\(^4\)For the cerebral blood flow project discussed later, this amounts to needing an ensemble size greater than six since there are six outflow vessels at which measurements are taken.
to advance the individual ensemble members at each time step, however, to ensure that the ensemble maintains the correct error statistics, it is best to update each ensemble member using the perturbed observations.

The filtering scheme is as follows:

1. Perturb the initial conditions in a statistically consistent way to create the matrix of ensemble members $A$, where each column is an ensemble state, i.e. $A_{sj} = x_j$.

2. Calculate the matrix of ensemble means $\bar{A} = A\mathbf{1}_N$, where $\mathbf{1}$ is an $N \times N$ matrix with elements $(\mathbf{1}_N)_{i,j} = \frac{1}{N}$.

3. Calculate the ensemble perturbation matrix $A' = A - \bar{A} = A(\mathbb{I} - \mathbf{1}_N)$.

4. Create a measurement perturbation matrix $E$ based on the prescribed covariances of the measurements where the columns are the individual perturbations, i.e. $E_{sj} = \epsilon_j$.

5. Create the perturbed measurement matrix $D$ where $D_{sj} = d_j = d + \epsilon_j$ and $d$ is the current measurement.

6. Create the ensemble of innovation vectors $D' = D - HA$, where $H$ is the measurement operator.

7. Calculate the analysis $A^a$ using the formula

   $$A^a = A + A'A'^T H^T \left( H A'A'^T H^T + E E^T \right)^{-1} D'$$

   where the following substitutions have been made

   - $P_e = \frac{A'A'^T}{N-1}$,
   - $R_e = \frac{E E^T}{N-1}$.

8. Set $A = A^a$.

9. Repeat steps 2 through 8 until the final time has been reached.
Handling Nonlinear Observation Functions

In the previous discussion, the matrix $H$ was used to calculate the measurement value predicted by the model. Often the function defining the measurements that will be taken is nonlinear and therefore cannot be described by a matrix, as is the case with the Circle of Willis model described in Chapter 4. In order to get around this restriction, the predicted measurements can be appended to the end of the state vector at each step. Then the measurement operator $H$ is simply a sparse matrix which “picks-off” the appended values.

Using EnKF for Parameter Estimation

The EnKF can also be used for parameter estimation. By appending the parameters to be optimized to the end of the state vector and allowing them to vary with some predetermined variance the EnKF will determine the values which best fit the data. This idea will be used in section 4.8 to estimate the resistance and compliance parameters related to the boundary conditions in the Circle of Willis model.
Chapter 3

Cavitation in Compressible Flows

3.1 Introduction

Although fluid mechanics has been an active field of research for many years, there are still many unanswered questions when it comes to solutions of both the Euler equations of gas dynamics and the Navier-Stokes equations. When solutions are known, they are often known for a specific subset of cases and the results are difficult (if not impossible) to extend to a more general case. For example, it can easily be shown (see Section 3.7.1) that given the proper initial conditions, cavitation will occur in a one-dimensional inviscid flow, modeled by the Euler equations. However, when trying to extend this up to multi-dimensional flow, the result becomes much more difficult to achieve. In fact, when considering multi-dimensional viscous flows, the question of cavitation is still open. This chapter details a careful numerical study of cavitation in multi-dimensional compressible flows. Specifically, the spherically symmetric, compressible Navier-Stokes equations in 2- and 3-dimensions (2- and 3-D) are considered. The focus will mainly be on the barotropic case but some preliminary results related to the full Navier-Stokes equations will also be mentioned.

Cavitation in compressible flows is an important question because the Navier-Stokes equations are derived from first principles based on the underlying assumption that the fluid is non-dilute and can therefore be described as a continuum. However, if cavitation occurs, this assumption no longer holds. Thus, if cavitation is a possibility,
one must be careful to watch for it and handle it properly.

### 3.1.1 Review of Previous Work

Much more is known in the case of 1-D flow\(^1\) than is known for multi-D flow. In the case of a 1-D viscous gas, it has been shown [38] that bounding the density, \(\rho\), strictly away from zero at time \(t = 0\) ensures a unique solution with positive density at all future times. No such results seem to be currently known for the standard Navier-Stokes equations in multi-D with constant transport coefficients. Searching for similar results in the multi-D case is a highly active area of research. One technical reason that seems to prevent this type of \textit{a priori} bound on the density (as well as the bound used by Hoff in [24]) in multi-D is that the integral bounds themselves are stronger in 1-D than they are in multi-D due to the geometrical factor of \(r^{n-1}\) in spatial integrals (\textit{i.e.} \(dx = \text{const} \ast r^{n-1} dr\)).

A similar result, without uniqueness, has been shown specifically for large and discontinuous data [26]. In the case of isentropic\(^2\) or isothermal\(^3\) flows with small restrictions on the initial conditions, there exists a global weak solution with density bounded above and below by zero. Thus, there is at least one solution of the Navier-Stokes equations without cavitation even for Riemann-type data with arbitrarily large jumps. An extension of this result for some flows, for the full Navier-Stokes system can be found in [33]. In contrast, it is well known that vacuum formation can occur for the 1-D inviscid Euler equations (see section 3.7.1 for details).

Further results for the 1-D case include those of Hoff and Smoller [30] who showed that any, everywhere defined, weak solution of the Navier-Stokes equations which satisfies some natural weak integrability assumptions cannot contain a vacuum in a nonempty set unless the initial data do so. A refinement of this solution is available in [17].

Corresponding analysis for the 2- and 3-D spherically symmetric (essentially 1-D) solutions was done by Xin and Yuan in [66]. Here they provide sufficient conditions to

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\(^1\)1-D flow is equivalent to multi-D flow with planar symmetry.

\(^2\)Isentropic means having constant entropy.

\(^3\) Isothermal means occurring at constant temperature.
rule out vacuum formation and give detailed information on the behavior of a vacuum region should one exist.

It is important to note that the results shown here do not contradict the above results as vacuum formation in 1-D has not been observed and there is no uniqueness result in higher dimensions where the results clearly suggest vacuum formation.

Currently, much less is known about compressible flows in higher dimensions. In fact, known results roughly fall into one of two categories: (1) large and rough data that possibly contains vacuum states; and (2) small\(^4\), possibly rough data with density bounded away from zero.

For case (1), the existence of weak solutions was established by Lions [39] for compressible barotropic flow. Recent extensions of this work include [19, 20] and references therein. More is known for case (2). In fact, it has been shown in [34, 35, 44] that sufficiently smooth data generates a globally smooth solution without cavitation for the full Navier-Stokes equations. See chapter 9 of [46] for a representative result in the case of barotropic flow.

There are a number of results in multi-D that pertain only to very specific cases. Global existence and uniqueness of compressible flows in multi-D for solutions in so-called critical spaces was established by Danchin in [12, 13, 14]. For flows with less regularity, Hoff has shown [25] that given data which is sufficiently close to a constant state, in a suitable norm, with density and temperature bounded away from zero, there exists a global weak solution with the same properties at all later times in 1-D. No corresponding result seems to be known for large data in several spatial dimensions. For isothermal flow with spherical symmetry, there exists a global weak solution for large symmetric data [24]. This solution is obtained as the limit of solutions in shells \( \{0 < a \leq r \leq b\} \) as \( a \downarrow 0 \). To find this solution, the equations are expressed in Lagrangian coordinates and combined with an energy estimate to find a priori bounds on the density which do not depend on \( a \). This result guarantees the existence of a weak solution but the a priori bounds are not strong enough to determine whether the solution contains a vacuum at the center. This result was

\(^4\)Small data refers to data that is close to a constant state in a suitable norm.
extended to the full Navier-Stokes system in [28].

Cavitation and Uniqueness

The issues of cavitation, uniqueness, and definition of solution are closely related. For example, consider the 1-D Navier-Stokes system with Riemann-type data

$$\rho_0(x) \equiv \bar{\rho} > 0 \quad u_0(x) = \begin{cases} -\bar{u} & \text{for } x < 0 \\ \bar{u} & \text{for } x > 0 \end{cases} \quad \text{with } \bar{u} > 0. \quad (3.1)$$

One weak solution was provided by Hoff in [26]. This solution did not contain vacuum. Alternatively, one could piece together the solutions of two disjoint flows in surrounding vacuum

$$\rho^-_0(x) = \begin{cases} \bar{\rho} & \text{for } x < 0 \\ 0 & \text{for } x > 0 \end{cases} \quad u^-_0(x) = \begin{cases} -\bar{u} & \text{for } x < 0 \\ \emptyset & \text{for } x > 0 \end{cases} \quad (3.2)$$

$$\rho^+_0(x) = \begin{cases} 0 & \text{for } x < 0 \\ \bar{\rho} & \text{for } x > 0 \end{cases} \quad u^+_0(x) = \begin{cases} \emptyset & \text{for } x < 0 \\ \bar{u} & \text{for } x > 0 \end{cases} \quad (3.3)$$

where $\emptyset$ implies that there is no velocity where there is no matter. Solutions $(\rho^-, u^-)$ and $(\rho^+, u^+)$ can be constructed which satisfy a physical no-traction boundary condition along the vacuum-fluid interface. For details, see [10, 11, 36, 37]. Then, a solution to the original problem can be constructed by concatenating these solutions. Thus, an open vacuum region exists at time $t = 0^+$. An important point to note is that Hoff’s solution is defined everywhere on $\mathbb{R} \times \mathbb{R}^+$ whereas the second solution is only defined on the support of its density.

The issue of non-uniqueness for 1-D compressible Navier-Stokes flows related to vacuum formation was considered in detail in [29]. In multi-D the existence of a solution without vacuum is unknown as is the uniqueness of general weak solutions. Known uniqueness results pertain to sufficiently smooth and small solutions [44] and flows in critical spaces [12, 13, 14]. The only uniqueness result for flows with possible discontinuities in density fields is due to Hoff [27].

The Navier-Stokes equations were derived based on a continuum assumption, therefore non-uniqueness issues in the presence of vacuum are not surprising (see
[19] for a discussion of this point). Related to this assumption is the issue of a physical boundary condition at a vacuum-fluid interface. The appropriate condition would be one of vanishing traction, i.e. the vacuum should not exert a force on the fluid. In the present work, only the onset of cavitation is considered and no attempt is made to track the evolution of the vacuum region after formation. This eliminates the need to impose such a boundary condition.

**Well-posedness**

For a discussion of well-posedness in the presence of vacuum see [10, 11, 36] for the full 1-D case and [19] for the full multi-D case. One might ask whether more accurate models would lead to stronger results. One specific example would be the case of non-constant transport coefficients which is considered in [6, 45]. In fact, it has been shown that the non-uniqueness encountered in [29] can be attributed to the assumption of constant transport coefficients [41, 42, 64, 67, 68, 69].

**Additional Remarks**

It is important to note that in higher spatial dimensions it should be easier to generate a vacuum since the fluid has more directions in which to move. Thus, proving the non-existence of cavitation in 1-D does not rule out the possibility of cavitation in higher dimensions. This idea can be quantified in the corresponding inviscid system. Consider the Euler equations with spherically symmetric Riemann-type data. More precisely, let \(|u_0| \equiv \bar{u}\) with \(u_0\) pointed radially away from the origin. Then there exists a threshold value \(\hat{u}(n)\) of \(\bar{u}\), where \(n\) is the spatial dimension, such that \(\bar{u} > \hat{u}(n)\) implies immediate vacuum formation [70]. It can be shown that \(\hat{u}(1) > \hat{u}(2) > \hat{u}(3)\). In 1-D, Hoff showed [24] that there exists a weak solution without vacuum, i.e. \(\hat{u}(1) = \infty\). This does not rule out solutions with cavitation in higher dimensions since \(\hat{u}(n) < \infty\) for \(n = 2, 3\) does not cause a contradiction to the result above. In fact, since there is no uniqueness result in the general 1-D case, there may also be a solution with cavitation in 1-D (see notes on uniqueness above).
3.1.2 Overview of Model

To begin, the equations are nondimensionalized leaving a set of dimensionless parameters over which a parameter space study can be done. The corresponding Euler equations (for which there are known solutions) are used as a test of the numerical method used in the study. One of the biggest challenges in this study is numerical stability. When the Euler equations are solved in 1-D with initial conditions that include large jumps, cavitation occurs (see Section 3.7.1). However, given the same set of initial conditions, an inviscid flow, modeled by the Navier-Stokes equations, does not show cavitation. Thus, it is important to control the amount of numerical diffusion, as it could lead to incorrect results. For this reason, a splitting algorithm is used to maintain the lack of diffusion in the convective part of the problem. See Section 3.8.3 for more details on this splitting algorithm.

To ensure a highly accurate solution with as few spatial nodes as possible, a pseudo-spectral spatial discretization involving Chebyshev-Gauss-Radau/Lobatto nodes (see Section 2.1) is used. This gives a high level of accuracy with very few spatial nodes allowing the model to run quickly and still produce reliable results.

Cavitation occurs when the density $\rho$ goes to zero. As $\rho$ approaches 0, the system becomes increasingly stiff due to the fact that the time derivative of the velocity is multiplied by $\rho$ (see equation (3.16)). When $\rho = 0$, the system becomes “infinitely stiff” and becomes differential algebraic instead of strictly differential. Thus, the method used to integrate in time must be able to handle a differential algebraic system should it occur. For this study, the BDF style time discretization offered by Matlab’s $\texttt{ode15s}$ is used. For more information on BDF see Section 2.3.1. For information on the specific implementation used in $\texttt{ode15s}$ see [43].

Since computers use finite precision arithmetic, it is highly unlikely that the method will calculate an exact density of 0, even in the case of cavitation. Thus, a cutoff at which cavitation is considered to have occurred must be determined. In this study, a density below $10^{-14}$ is considered to signify vacuum formation. In addition, the behavior of the solution in phase space is considered and required to indicate vacuum formation as well. See Section 3.7.2 for more information on the expected
behavior in phase space. It is important to note that there is no attempt to track the vacuum region past formation. Since the occurrence of cavitation is the main question in this study, the simulation is stopped when the presence of vacuum is detected.

An important thing to note is that the uniqueness of general weak solutions is unknown. Thus, even if a solution with cavitation is determined to exist, this does not mean that a solution without cavitation is not possible as well. Also, one must be careful not to read too much into the physicality of solutions found which include cavitation. As mentioned above, the equations were derived based on a continuum assumption and therefore do not apply to the case when vacuum regions are present.

A precise formulation of the problem follows.

### 3.2 Compressible Navier-Stokes Equations

Begin with the invariant form of the compressible Navier-Stokes equations (see [46] for a derivation) which is as follows

\[
\begin{align*}
\rho_t + \nabla \cdot (\rho \bar{u}) &= 0 \\
(\rho \bar{u})_t + \nabla \cdot (\rho \bar{u} \otimes \bar{u}) &= \nabla (-p + \lambda \nabla \cdot \bar{u}) + \nabla \cdot (2\mu D) \\
E_t + \nabla \cdot ((E + p) \bar{u}) &= \nabla \cdot (\lambda (\nabla \cdot \bar{u}) \bar{u} + 2\mu D \cdot \bar{u} - \bar{q})
\end{align*}
\]  

(3.4) \hspace{2cm} (3.5) \hspace{2cm} (3.6)

where \( \rho \) is the density, \( \bar{u} = (u_1, \ldots, u_n)^T \) is the fluid velocity, \( n \) is the spatial dimension, \( p \) is the pressure, \( E \) is the total energy, \( D \) is the deformation tensor, \( \bar{q} \) is the heat flux vector, and \( \lambda \) and \( \mu \) are the viscosity coefficients. Also,

\[
E = \rho \left( e + \frac{1}{2} \bar{u}^2 \right), \quad D_{ij} = (\partial_i u_j + \partial_j u_i)/2, \quad \bar{q} = -\kappa \nabla \theta,
\]

where \( e \) is the internal energy, \( \kappa \) is the coefficient of heat conductivity, and \( \theta \) is the temperature. Then, restrict the model to the ideal and polytropic (perfect) gases where

\[
p = \mathcal{R} \rho \theta, \quad e = c_v \theta,
\]

where \( \mathcal{R} \) is the gas constant and \( c_v \) is the specific heat at constant volume. The local sound speed is

\[
c = \sqrt{\frac{\gamma p}{\rho}}.
\]
where $\gamma = 1 + \mathcal{R}/c_v$ is the adiabatic exponent. In addition, all transport coefficients are assumed to be constant ($c_v$, $\lambda$, $\mu$, $\kappa$).

### 3.3 Symmetric Flow

As stated above, the simplest possible case will be considered, symmetric flow. In this case, the velocity is directed away from the origin and all quantities are functions of the distance to the origin and time only. Let $x$ denote a point in space and set $r = |x|$. Then $\rho(r,t) = \rho(x,t)$ and $\vec{u}(x,t) = u(r,t)\hat{r}$. This leads to the symmetric form of the Navier-Stokes equations

\begin{align}
\rho_t + (\rho u)_{\xi} &= 0 \\
\rho(u_t + uu_r) + p_r &= \nu u_{\xi r} \\
c_v\rho(\theta_t + u\theta_r) + p\theta_{\xi} &= \kappa\theta_{\xi r} + \nu(u_{\xi})^2 - \frac{2m\mu}{r^m}(r^{m-1}u^2)_r
\end{align}

where $m = n - 1$, $\xi = \partial_r + \frac{m}{r}$, and $\nu = \mu + \lambda$. It is important to note that $\partial_{\xi r} \neq \partial_r\xi$ when $n \neq 1$. The domain consists of the interior of the ball $B_b$ of radius $b$ centered at the origin and the initial conditions are

\begin{align}
\rho(r,0) &= \rho_0 \\
u(r,0) &= u_0(r) \quad r \leq b, \\
\theta(r,0) &= \theta_0
\end{align}

where $u_0$ is a non-negative function in 2- and 3-D and is odd with positive values for $r > 0$ in 1-D and $\rho_0$ and $\theta_0$ are large positive constants. Specific initial and boundary conditions will be discussed in Section 3.6.

### 3.4 Non-dimensional Form of the Symmetric Equations

In order to identify the fundamental parameters of the problem, it is common to nondimensionalize the variables. Nondimensionalization introduces physically meaningful dimensionless parameters which help in correctly interpreting the results. For
example, the Reynolds number, $\mathcal{R}e$, which is the ratio of the inertial forces to the speed of sound in the fluid, enables us to refer to the viscosity of the fluid in a physically meaningful way by relating the viscosity coefficient to the scale of the problem. The viscosity of a fluid is related to its resistance to movement or flow. The viscosity coefficient of a fluid alone says nothing about the fluid but the Reynolds number can be used to describe how gas-like the fluid behaves. Nondimensionalization starts with the choice of a characteristic length, velocity, density, and temperature,

\[
\bar{r} := b, \\
\bar{u} := \max_{0 \leq r \leq b} |u_0(r)|, \\
\bar{\rho} := \max_{0 \leq r \leq b} \rho_0(r), \\
\bar{\theta} := \max_{0 \leq r \leq b} \theta_0(r),
\]

respectively. From these, the characteristic time and pressure are defined as

\[
\bar{t} := \frac{\bar{r}}{\bar{u}} \quad \text{and} \quad \bar{p} := p(\bar{\rho}, \bar{\theta}).
\]

This leads to the nondimensionalized independent variables

\[
R := \frac{r}{\bar{r}} \quad \text{and} \quad T := \frac{t}{\bar{t}},
\]

and the nondimensionalized dependent variables

\[
D := \frac{\rho}{\bar{\rho}}, \quad U := \frac{u}{\bar{u}}, \quad \Theta := \frac{\theta}{\bar{\theta}}, \quad \text{and} \quad P := \frac{p}{\bar{p}},
\]

which are functions of $R$ and $T$. Reverting back to the original symbols, the nondimensionalized system is

\[
\rho_t + (\rho u)_{\xi} = 0, \quad (3.11)
\]

\[
\rho (u_t + uu_r) + \frac{1}{\gamma M^2} (\rho \theta)_r = \frac{1}{\mathcal{R}e} u_{\xi r}, \quad (3.12)
\]

\[
\rho (\theta_t + u \theta_r) + (\gamma - 1) \rho \theta u_{\xi} = \frac{1}{\Pr \mathcal{R}e} \theta_{\xi r}, \quad (3.13)
\]

\[
+ \gamma (\gamma - 1) \frac{M^2}{\mathcal{R}e} \left( \frac{(u_{\xi})^2}{\nu} \frac{2m \mu (r^{m-1} u^2)_r}{r^m} \right), \quad (3.14)
\]
where the following dimensionless parameters have been introduced:

\[ M := \left| \frac{\bar{u}}{\bar{c}} \right| = \text{Mach number}, \quad \bar{c} = \text{sound speed} = \sqrt{\frac{\gamma \bar{p}}{\bar{\rho}}}, \]

\[ \text{Re} := \frac{\bar{r} \bar{\rho} \bar{u}}{\nu} = \text{Reynolds number}, \quad \text{and} \]

\[ \text{Pr} := \frac{\nu c_v}{\kappa} = \text{Prandtl number}. \]

### 3.5 Barotropic Flow

In order to simplify the problem even further, first consider the barotropic case. This involves making the assumption that the pressure is a function of the density alone (and not a function of the temperature) and includes the isentropic and isothermal cases. The pressure function is of the form

\[ p(\rho) = a\rho^\gamma \]

where \( a > 0 \) is a constant. This has the benefit of decoupling the third equation and reducing the problem to a system of two equations instead of three. The nondimensionalized form of the barotropic equations can be derived in a manner similar to that of section 3.4 with \( \bar{p} = p(\bar{\rho}) = a\bar{\rho}^\gamma \). The nondimensionalized system for barotropic flow is therefore

\[ \rho_t + (\rho u)_\xi = 0, \quad (3.15) \]

\[ \rho (u_t + uu_r) + \frac{1}{\gamma M^2} (\rho^\gamma)_r = \frac{1}{\text{Re}} u_{\xi r} \quad (3.16) \]

where the Mach number is now

\[ M := \left| \frac{\bar{u}}{\bar{c}} \right| = \frac{|\bar{u}|}{\sqrt{a\gamma \bar{\rho}^{\gamma-1}}}. \]

### 3.6 Initial and Boundary Conditions

The initial conditions for the nondimensionalized vacuum formation problem are as follows

\[ \rho(r, 0) = 1 \text{ for } 0 \leq r \leq 1, \quad u(r, 0) = u_0(r) = \begin{cases} 1 & \text{if } r > 0, \\ 0 & \text{if } r = 0, \end{cases} \quad (3.17) \]
where $r = 1$ is the outer boundary of the nondimensionalized computational domain. This corresponds to constant initial density and a strong force in the outward direction everywhere except at the origin at which the initial velocity is 0 to maintain the symmetry of the system.

Although one would expect to need two boundary conditions, one at each end of the computational domain, one boundary condition comes for free from the symmetry of the system, namely

$$u(0,1) = 0, \quad t > 0.$$  

In addition, the following boundary condition is imposed at the outer boundary of the computational domain

$$u(1,t) = 1, \quad t > 0. \quad (3.18)$$

An alternate boundary condition that was considered was $u(1,t) = 0$ corresponding to a reflective/no-flow boundary. However, this condition leads to steep gradients and unwanted numerical boundary layer effects in the numerical solution. Since vacuum formation is expected at the origin after a very short period of time this boundary condition will actually have little or no effect on whether vacuum formation occurs.

### 3.7 Euler Equations

The Euler equations of gas dynamics are the formal limit of the Navier-Stokes equations as the viscosity tends towards zero. While there are numerous resources available to show that this is true in the case of incompressible fluids, the body of literature that is available related to compressible fluids is limited. It also takes some work in order to show that the solution to the Euler equations is indeed the limit of the solutions to the Navier-Stokes equations as the viscosity tends towards zero. A proof of this fact is given in [60].

#### 3.7.1 One-dimensional Case

As was stated above, the Euler equations are the formal limit of the Navier-Stokes equations as the viscosity tends to zero (equivalently, $Re \to \infty$). Specifically,
consider the isentropic Euler equations, i.e. the limit of equations (3.15) and (3.16) as \( Re \to \infty \),

\[
\rho_t + (\rho u)_x = 0,
\]
\[
\rho (u_t + uu_x) + \frac{1}{\gamma M^2} (\rho^\gamma)_x = 0,
\]

along with the Riemann initial conditions

\[
\rho(r, 0) = 1 \quad \forall r, \quad u(r, 0) = \begin{cases} 
-1 & \text{if } r < 0, \\
1 & \text{if } r > 0.
\end{cases}
\]

It turns out that the isothermal case (\( \gamma = 1 \)) behaves quite differently from the general isentropic case (\( \gamma > 1 \)).

**The Isothermal Case**

In the isothermal case, the solution consists of two rarefaction waves

\[
\begin{bmatrix}
\rho \\
u
\end{bmatrix}(r, t) = \begin{cases}
\begin{bmatrix}1 \\ -1\end{bmatrix} & \text{if } \frac{r}{t} < -1 - \frac{1}{M}, \\
\begin{bmatrix}e^{-(M^2+M+1)} \\ \frac{1}{M} \end{bmatrix} & \text{if } -1 - \frac{1}{M} < \frac{r}{t} < -\frac{1}{M}, \\
\begin{bmatrix}e^{-M} \\ 0\end{bmatrix} & \text{if } -\frac{1}{M} < \frac{r}{t} < \frac{1}{M}, \\
\begin{bmatrix}e^{M(1-M-1)} \\ \frac{1}{M} \end{bmatrix} & \text{if } \frac{1}{M} < \frac{r}{t} < 1 + \frac{1}{M}, \\
\begin{bmatrix}1 \\ 1\end{bmatrix} & \text{if } 1 + \frac{1}{M} < \frac{r}{t}.
\end{cases}
\]

(3.19)

Of specific importance is the fact that no matter how large the Mach number \( M \) is, no cavitation occurs.
The General Isentropic Case

For the general isentropic case, the solution again consists of two rarefaction waves. However, in this case, the size of the Mach number determines whether or not cavitation occurs. Specifically, for \( M > \frac{2}{\gamma - 1} \), the solution \( \begin{bmatrix} \rho \\ u \end{bmatrix}(r, t) = \)

\[
\begin{cases}
\begin{bmatrix} 1 \\ -1 \end{bmatrix} & \text{if } \frac{r}{t} < -1 - \frac{1}{M}, \\
\begin{bmatrix} \left( \frac{2}{\gamma + 1} - M \frac{\gamma - 1}{\gamma + 1} (1 + \frac{r}{t}) \right)^{2/(\gamma - 1)} \\ \frac{1}{M(\gamma + 1)} (2 + (1 - \gamma) M + 2M^2 \frac{r}{t}) \end{bmatrix} & \text{if } -1 - \frac{1}{M} < \frac{r}{t} < -1 + \frac{2}{\gamma - 1} \frac{1}{M}, \\
\begin{bmatrix} 0 \\ \emptyset \end{bmatrix} & \text{if } -1 + \frac{2}{\gamma - 1} \frac{1}{M} < \frac{r}{t} < 1 - \frac{2}{\gamma - 1} \frac{1}{M}, \\
\begin{bmatrix} \left( \frac{2}{\gamma + 1} + M \frac{\gamma - 1}{\gamma + 1} (-1 + \frac{r}{t}) \right)^{2/(\gamma - 1)} \\ \frac{1}{M(\gamma + 1)} (-2 + (-1 + \gamma) M + 2M^2 \frac{r}{t}) \end{bmatrix} & \text{if } 1 - \frac{2}{\gamma - 1} \frac{1}{M} < \frac{r}{t} < 1 + \frac{1}{M}, \\
\begin{bmatrix} 1 \\ 1 \end{bmatrix} & \text{if } 1 + \frac{1}{M} < \frac{r}{t},
\end{cases}
\]
contains a vacuum region. On the other hand, when 0 < \mathcal{M} < \frac{2}{\gamma-1}, no cavitation occurs, and the solution is

\[
\begin{bmatrix}
\rho \\
u
\end{bmatrix}(r, t) =
\begin{cases}
1 & \text{if } \frac{r}{t} < -1 - \frac{1}{\mathcal{M}}, \\
\begin{bmatrix}
\left(\frac{2}{\gamma+1} - \mathcal{M} \frac{\gamma-1}{\gamma+1} \left(1 + \frac{r}{t}\right)\right)^{2/(\gamma-1)} \\
\frac{1}{\mathcal{M}(\gamma+1)} \left(2 + (1 - \gamma) \mathcal{M} + 2 \mathcal{M} \frac{r}{t}\right)
\end{bmatrix} & \text{if } -1 - \frac{1}{\mathcal{M}} < \frac{r}{t} < -\frac{1}{\mathcal{M}} + \frac{2-1}{2}, \\
\begin{bmatrix}
(1 - \frac{\mathcal{M}}{2} (\gamma - 1))^{\frac{2}{\gamma-1}} \\
0
\end{bmatrix} & \text{if } -\frac{1}{\mathcal{M}} + \frac{2-1}{2} < \frac{r}{t} < \frac{1}{\mathcal{M}} - \frac{2-1}{2}, \\
\begin{bmatrix}
\left(\frac{2}{\gamma+1} + \mathcal{M} \frac{\gamma-1}{\gamma+1} (-1 + \frac{r}{t})\right)^{2/(\gamma-1)} \\
\frac{1}{\mathcal{M}(\gamma+1)} (-2 + (-1 + \gamma) \mathcal{M} + 2 \mathcal{M} \frac{r}{t})
\end{bmatrix} & \text{if } \frac{1}{\mathcal{M}} - \frac{\gamma-1}{2} < \frac{r}{t} < 1 + \frac{1}{\mathcal{M}}, \\
\begin{bmatrix}
1 \\
1
\end{bmatrix} & \text{if } 1 + \frac{1}{\mathcal{M}} < \frac{r}{t}.
\end{cases}
\]

3.7.2 Multi-dimensional Axisymmetric Case

Similarity solutions have been considered for the 2- and 3-D axisymmetric problems. It has been shown that no closed form solutions can be found. However, analysis shows that solutions without swirls may contain cavitation if \(\gamma > 1\) but not if \(\gamma = 1\), see [70], §7.4.

Consider the case where \(\gamma > 1\) following [70]. Self-similar solutions to

\[
\begin{aligned}
\rho_t + (\rho u)_\xi &= 0, \\
\rho (u_t + uu_r) + \frac{1}{\gamma \mathcal{M}^2} (\rho^\gamma)_r &= 0,
\end{aligned}
\]

are sought in the form

\[
\rho = \rho(s), \quad u = u(s), \quad \text{where } s = \frac{t}{r}.
\]
Figure 3.1: Solutions to the axisymmetric Euler Equations in 2 spatial dimensions with $\gamma = 1.4$. Note the difference in behavior of the density as $r$ approaches 0. Cavitation occurs for $M = 3.1$ (dashed line), but not for $M = 2.9$ (solid line). This is in agreement with the critical Mach number shown in Figure 3.2(b).

This leads to the system of ordinary differential equations

$$\rho_s = \frac{m \rho u (1 - su)}{s^2 c^2 - (1 - su)^2},$$ \hspace{1cm} (3.23)

$$u_s = \frac{sc^2 u}{s^2 c^2 - (1 - su)^2},$$ \hspace{1cm} (3.24)

$$\rho(0) = 1, \quad u(0) = 1,$$ \hspace{1cm} (3.25)

where $c = \frac{1}{M} \rho^{\gamma-1}$. Figure 3.1 shows results for different Mach numbers when $\gamma = 1.4$.

The extension of these 2-D results to 3-D is as follows. Begin by introducing
\[ I = su \text{ and } K = sc \text{ and rewriting (3.23) and (3.24) as} \]
\[ \frac{dI}{d\tau} = I \left( (1 - I)^2 - (1 + m) K^2 \right) \equiv I \mathcal{F}(I, K), \quad (3.26) \]
\[ \frac{dK}{d\tau} = K \left( (1 - I)^2 - K^2 - \frac{m}{2} (\gamma - 1) I (1 - I) \right) \equiv K \mathcal{G}(I, K), \quad (3.27) \]
\[ \frac{ds}{d\tau} = s \left( (1 - I)^2 - K^2 \right), \quad (3.28) \]

where \( \mathcal{F} \) and \( \mathcal{G} \) have the obvious definitions and a new independent variable \( \tau \) has been introduced by (3.28) in order to make (3.26,3.27) an autonomous system.

In the \((I, K)\) phase plane, the stationary points of (3.26,3.27) are \((0, 0), (1, 0), (0, 1), \) and \(Q = \left( \frac{2}{\gamma(1+m)+1-m}, \frac{1}{\gamma(1+m)+1-m} \right) \). If the region \( \Omega \subset \mathbb{R}^2 \) is defined by
\[ \Omega = \left\{\left( I, K \right); I > 0, K > 0, \mathcal{G} > 0 \text{ for } 0 < I \leq \frac{2}{\gamma(1+m)+1-m}, \mathcal{F} > 0 \text{ for } \frac{2}{\gamma(1+m)+1-m} \leq I < 1 \right\}, \]

and a simple sign study is done along \( \partial \Omega \), \( \Omega \) is found to be invariant under (3.26,3.27) and therefore the system (3.26,3.27,3.28) has solution curves from \((0, 0) \) to \((0, 1), (1, 0), \) or \(Q\). It can be shown that there exists a critical value of the Mach number, \( M^* \), such that the solution \((\rho, u)\) of (3.23,3.24,3.25) is defined for \(0 < s < \infty \) and converges to \((I, K) = Q\) as \( s \to \infty \). While there does not seem to be an explicit formula for \( M^* \), one can solve (3.23,3.24,3.25) numerically and find an approximate value of \( M^* \). Figure 3.2(a) shows the numerically calculated integral curves mentioned above and Figure 3.2(b) shows the approximated critical Mach number in 2- and 3-D.

### 3.8 Discretization and Numerical Analysis

The numerical approach used to investigate this problem is based on a splitting algorithm between the Euler equations and a diffusive equation. This splitting algorithm allows the similarity solutions described in Section 3.7 to be used. These solutions can be found to a high degree of accuracy using the Matlab ODE solver.
ode15s which is a variation of BDF (see Section 2.3.1). Here the splitting algorithm is illustrated for the barotropic case.

Let \((\rho_n, u_n)\) be the solution at time \(t_n = n\Delta t\) where \(\Delta t\) is the time step and begin by taking an “Euler step”. This involves solving equations (3.15) and (3.16) from \(t_n\) to \(t_{n+1}\) with the initial conditions

\[
\rho(\cdot, t_n) = \rho_n \quad \text{and} \quad u(\cdot, t_n) = u_n,
\]

and denoting the solution \((\rho^*, u^*)\). Next, take a “diffusive step”, or more precisely, solve

\[
\rho^* u_t = \frac{1}{Re} u_{\xi r}
\]

from \(t_n\) to \(t_{n+1}\), with initial condition

\[
u(\cdot, t_n) = u^*.
\]

### 3.8.1 Discretization for Euler Step

Let \((\rho_n(r_j), u_n(r_j))\) be given values at time \(t^n\) and node \(r_j\). A family of similarity solutions is defined as in Section 3.7.2. Let \(s^n_j = \frac{u^n}{\rho^n}\) be the slopes corresponding to
the above points and $s_j^{n+1} = \frac{t_j^{n+1}}{r_j}$ be the slopes at the next time step, see Figure 3.3. Then solve equations (3.23, 3.24) from $s = s_j^n$ to $s = s_j^{n+1}$ with initial conditions

$$\rho(s_j^n) = \rho_n(r_j) \text{ and } u(s_j^n) = u_n(r_j).$$

(3.31)

### 3.8.2 Discretization for Diffusive Step

For the diffusive step, Chebyshev collocation in space is used. This gives us a high level of accuracy with a low number of nodes for the smooth solutions expected here. To avoid the coordinate singularity at $r = 0$ in 2- and 3-D that arises when switching to spherical coordinates, Chebyshev-Gauss-Radau (CGR) nodes are used,

$$r_j = \frac{1}{2} \left( 1 + \cos \left( \frac{2\pi j}{2N-1} \right) \right), \quad j = 0, 1, \ldots, N - 1,$$

(3.32)

where $N$ is the number of nodes. In 1-D, the coordinate singularity does not occur so the standard Chebyshev-Gauss-Lobatto (CGL) nodes are used.
For $r \in (0,1)$ and $t > 0$, an approximation $u_N$ of $u$ of the form

$$u_N(r,t) = \sum_{i=0}^{N-1} U_i(t) \psi_i(r),$$  \hspace{1cm} (3.33)

is desired, where $\{\psi_i\}_{i=0}^{N-1}$ are the Lagrange interpolating polynomials at the CGR/CGL nodes on $[0,1]$, i.e. $\psi_i(x_j) = \delta_{ij}$. Thus, interpolation over the CGR/CGL nodes of the function $u = u(r,t)$ takes the form

$$I_N u(r,t) = \sum_{j=0}^{N-1} u(r_j,t) \psi_j r$$  \hspace{1cm} (3.34)

Then, by definition, the Chebyshev collocation derivative of $u$ with respect to $r$ at the given nodes is

$$\frac{\partial}{\partial r} (I_N u)(r_l, t) = \sum_{j=0}^{N-1} u(r_j,t) \psi_j j'(r_l) = \sum_{j=0}^{N-1} D_{lj} u(r_j,t),$$  \hspace{1cm} (3.35)

where $D_{lj} = \psi'_j(r_l)$, see Section 2.2.3 for details.

If $\rho = 0$ (or very close to it), the differential equation for $u$ degenerates into an algebraic equation leaving a Differential Algebraic Equation (DAE). The level of difficulty this causes depends on the index of the system. The index is determined by the number of times all or part of the system must be differentiated in order to return the system to a system of ODEs. In this case, the index is found to be 1. At the continuous level this corresponds to checking that the only nonsingular solution to $\partial_r \dot{u} + \frac{m_r}{r} \partial_r \dot{u} - \frac{m_r}{r^2} \dot{u} = 0$ with $\dot{u}(1) = 0$, is the trivial solution $\dot{u} = 0$. This can also be shown on the discrete level as was shown in [15]. Thus, a solver that can handle a semi-explicit DAE of index 1 is needed. Matlab’s `ode15s`, which implements a variation of BDF, is one such solver.

### 3.8.3 Splitting Algorithm

The splitting algorithm works as follows. First, a specific Mach number $M$, Reynolds number $Re$, number of nodes $N$, step size $\Delta t$, and number of time steps $N_t$ are chosen. Next, $\rho_0$ and $u_0$ are initialized according to the given initial conditions.
(see equations 3.17). Then, the spatial nodes are cycled through and an Euler step is taken at each. This involves solving (3.23) and (3.24), with the initial conditions (3.6) and setting
\[ \rho^*(r_j) = \rho(s_j^{n+1}) = \rho_{n+1}(r_j) \] and \[ u^*(r_j) = u(s_j^{n+1}). \]
Finally, (3.29, 3.30) is solved and
\[ u_{n+1}(r_j) = u(r_j, t_{n+1}), \quad j = 0, ..., N - 1. \]
This process, is repeated for each time step until a solution at the final time is found.

### 3.9 Numerical Results

Equations (3.15) and (3.16) were solved using the method described above (see section 3.8.3). A grid of Mach and Reynolds numbers for different values of the adiabatic exponent, \( \gamma \), were considered. The initial and boundary conditions used are given by (3.17) and (3.18), respectively.

For this study, the number of mesh points used was fixed at \( N = 32 \) after determining that an increase to higher \( N \) does not change the solution significantly. Since the numerical density is always an increasing function of \( r \) based on the way the system is setup, one only needs to look at the node closest to \( r = 0 \) to check for vacuum formation because if it occurs, it will show up here first. Also, if vacuum formation occurs, it is expected to happen very rapidly. This expectation comes from the fact that in the 1-D Euler case, vacuum formation occurs instantaneously at \( r = 0 \). In 2- and 3-D there is no node at \( r = 0 \) so it will take a small amount of time for any vacuum region that forms to reach the “first” node.

Here a calculation is considered to show vacuum formation if both of the following apply

1. for some time \( t \), with \( 0 < t < .005 \) seconds, \( \rho_N(r_{N-1}, t) < tol = 10^{-14} \),
2. the solution at the node closest to \( r = 0 \) shows the “proper” time evolution in phase space (see Figure 3.4).

The second condition follows from the results found in Section 3.7.2.
Figure 3.4: Phase diagrams for the Euler and Navier-Stokes solutions at the node closest to the origin in 3-D with $M = 1.2$ (no vacuum) and $M = 2.7$ (vacuum). For the Navier-Stokes solution, the Reynolds number is $Re = 10^6$.

### 3.9.1 The 1-Dimensional Case

The above method cannot be used directly in 1-D. However, using an adapted method, no vacuum formation was observed for the 1-D Navier-Stokes system (see Figure 3.5). It is important to note that the absence of vacuum formation in this case is consistent with the solutions found by Hoff [26], who considers a similar setup.

### 3.9.2 The Multi-Dimensional Barotropic Case

In the multi-D barotropic case, vacuum formation was observed for “large enough” values of the Mach number. Figure 3.6 shows the regions where vacuum formation occurs. The regions marked *inconclusive* refer to places where the method could not resolve the solution long enough in time or when one of the two criteria mentioned above held but not the other. The results were found to be relatively insensitive to the discretization parameters leading to the belief that vacuum formation is indeed a property of the analytic solution and not an artifact of the numerics used to solve the problem.

Since the fluid has more directions in which to move in higher dimensions, one would expect that vacuum formation would be easier, i.e. possible at a lower Mach
Figure 3.5: One-dimensional Navier-Stokes and Euler solutions for $\gamma = 1.4, M = 10$. Left: solutions at time $t = 0.5$ with $Re = 10^4$; Right: solutions at time $t = 0.002$ with $Re = 10^6$. For these values, both the one-dimensional Euler solution and the multi-dimensional Navier-Stokes solution show vacuum formation, while the 1-D Navier-Stokes solution does not.

number, in 3-D than in 2-D. As expected, vacuum forms more readily in 3-D than in 2-D as can be seen in Figure 3.6. In addition, increasing the adiabatic exponent, $\gamma$, also makes it easier for vacuum to form.

3.9.3 The Full System

Construction of self-similar solutions to the nonisentropic Euler equations is still an open question and therefore there is no basis for the above splitting algorithm in this case. However, preliminary results based on an unsplit algorithm indicate that vacuum formation is possible for the full system as well.

3.10 Conclusions

As shown in Section 3.9 the numerical results indicate that vacuum formation is possible in solutions of multi-dimensional compressible Navier-Stokes flows. This was shown for the case where the initial velocity was discontinuous and sufficiently large with initial density bounded away from zero. One-dimensional results that are consistent with currently available analytic results and multi-dimensional results that do
Figure 3.6: Vacuum formation regions for 2- and 3-D barotropic flows with $\gamma = 1.4$. Left: 2-D; Right: 3-D.

not contradict current analytic results were given. It is important to note that in this study no attempt was made to follow the vacuum region past its formation. Determination of whether the vacuum formation is instantaneous as in the corresponding Euler equations was also not considered at this time.
Chapter 4

Circle of Willis

4.1 Introduction

The brain receives approximately 15-20% of the total cardiac output. Maintenance of proper blood supply to the brain is important in maintaining proper brain function. Reduced blood flow to the brain can cause loss of brain cells and can lead to permanent disabilities. As a natural safeguard, the brain is equipped with a network of vessels known as the Circle of Willis (CoW) which allows redundancies in blood supply. A reduction of blood flow to the brain can be caused by conditions such as blood clots, stroke, or hardening of the vessels in or leading to the brain. In fact, according to the National Stroke Association, stroke is the third leading cause of death in America and the leading cause of adult disability. An important aspect of the CoW is its geometry. More than 50% of the population have one or more missing or underdeveloped vessels within the CoW [40]. These differences can affect how a patient recovers after a stroke or how they respond to medical treatment or surgery. Computed waveforms based on patient-specific data may help in diagnosing certain diseases such as diabetes, vascular disease, and stiffening of the arteries, which all cause changes in the pulse waveform. This information may be helpful in determining how to treat diabetics and others known to have a higher rate of anatomical variation within the CoW.

A complete CoW has three inflow vessels, the basilar artery and the left and right internal carotid arteries, and six outflow vessels, the left and right anterior, middle,
and posterior cerebral arteries, see Figure 4.1. As is suggested by their names, the anterior cerebral arteries supply the front of the brain, the middle cerebral arteries supply the center of the brain, and the posterior cerebral arteries supply the back of the brain. In addition, the CoW contains three communicating arteries, the anterior communicating artery and the left and right posterior communicating arteries. The anterior communicating artery allows blood to flow between the left and right sides of the brain while the posterior communicating arteries allow blood to flow between the front and back of the brain. Figure 4.1 shows a mockup of the section of the arterial system that will be modeled in the following sections. During the derivation and analysis of the model, the focus will be on the complete CoW. In section 4.10.3 the effects of common anatomical variations on blood perfusion will be considered.

Correctly modeling the CoW is also interesting from a modeling or numerical standpoint. There are a number of important considerations one must make when determining how to appropriately model cerebral blood flow. One decision is how to model the vessel walls. Two choices for vessel wall models are elastic and visco-
elastic models. The most common choice is elastic vessel walls. This choice determines how the vessel walls will interact with the blood and directly affects the number of equations which will need to be solved. Another consideration is whether blood flow is Newtonian or non-Newtonian. Finally, one must choose how to link the vessels together to form the network. This is an important consideration as the CoW is one of the few arterial structures in the body that do not branch in a repeating bifurcating pattern making it harder to model properly.

4.2 Background

4.2.1 Review of Previous Work

The following is a brief discussion of previous work related to blood flow modeling and specifically to the circle of Willis. This review is separated into four sections to highlight the specific issues of vessel wall properties, fluid properties, 1-D vs. multi-D models, and boundary conditions. There is also a section devoted specifically to the review of a paper by Alastruey, et. al. in 2006 [1] that looked at many of the same questions as will be considered in section 4.10.3.

Elastic vs. Visco-elastic Vessel Walls

Most studies model the vessel walls as elastic rather than viscoelastic, see for example [1, 31, 49, 53, 55, 58, 63]. Elastic walls reduce the number of equations that need to be solved allowing higher dimensional models to become more feasible, however, elastic vessels can produce shock-like flow patterns which are physically unrealistic [2]. Even the visco-elastic model is not complete since vessel walls are made up of multiple layers each of which is anisotropic and is made up of different amounts of elastic fibers and smooth muscle [55]. For an example of a vessel wall model with multiple layers, see [32].
Newtonian vs. non-Newtonian Fluid

Researchers disagree as to the importance of the non-Newtonian properties of the blood. Some say that for the medium and large vessels, treating the blood as a Newtonian fluid gives a good approximation ([54] as cited in [55]). Others point to recent studies that suggest that the non-Newtonian effects are important [5, 7]. For this reason, many researchers stick to the simpler Newtonian model [1, 51, 55, 63] while others have considered a non-Newtonian model [7, 53].

One-D vs. Multi-D Models

Most 2- and 3-D blood flow models include only a single vessel or bifurcation [53, 55] or use a rigid model for the vessel walls [7, 21]. The model considered here includes sixteen vessel segments and multiple bi- and tri-furcations. Thus, 2- and 3-D models are impractical for this problem since real-time results are desired. A 1-D model limits the details within the flow but the overall effect of differing geometries is interesting in and of itself without attention to the specific details. Even a 1-D model is not trivial because there are bifurcations and trifurcations as well as multiple inflows and outflows to the system to deal with.

Boundary Conditions

The inflow boundary conditions are what drives the system. They correspond in some way to the beating of the heart. While transparent outflow boundary conditions may seem like an appropriate choice at first, they are actually a very poor imitation of what is happening in the rest of the arterial system. Since the vessels in the rest of the arterial system provide time dependent resistance to flow, the boundary conditions at the outflows must appropriately model this resistance. Commonly used boundary conditions include the pure resistance condition [57], the windkessel condition [1, 47, 50, 55, 58], and the structured tree condition [49, 51]. It is important to choose the appropriate boundary conditions because different boundary conditions lead to changes in the relative importance of the individual vessels [21].
Common Geometric Variations

The anatomical variations study in Section 4.10.3 is similar to a study done by Alastrauey, et. al. [1]. This section provides a review of the major findings of this paper in order to allow for easy comparison between results.

The model they consider is a one-dimensional, non-linear model with elastic vessel walls. Their initial conditions are

\[ A = A_0 \quad \text{and} \quad U = 0. \]

Instead of modeling the Circle of Willis (CoW) by itself, they model all vessels in the arterial network between the ascending aorta and the CoW outflow vessels. To drive the system they use a periodic inflow function made up of a half sine wave with duration .3 seconds followed by zero velocity with duration .7 seconds. For external boundary conditions they use a three-element windkessel condition which takes into account the resistance and compliance of the peripheral network of vessels through its three parameters. These parameters are determined based on previously published physiological data and the desire to minimize the total impedance of the windkessel model itself. At the vessel junctions, conservation of mass and continuity of total pressure conditions are imposed. In their model, total occlusions are modeled by setting the velocity to zero at the appropriate location. Partial occlusions are modeled by reducing the calibre of the vessel. They used a discontinuous Galerkin scheme with a spectral/hp spatial discretization and second order Adams-Bashforth time integration scheme to advance the solution in time. During each simulation the model was run until the results were periodic which usually took about ten periods.

The cases that were studied include:

- whether the communicating arteries and the collateral pathways they create are necessary in a healthy brain,

- the effects of common anatomical variations of the CoW in the presence of an occluded ICA or VA,

- the effects of occlusions of afferent (inflow) vessels,
the effects of partial occlusions of communicating arteries in the presence of an occluded ICA.

Through these studies they determined that the system does not require the collateral pathways in healthy subjects. In fact, removal of the communicating arteries from an otherwise complete CoW causes less than a 1% change in the mean outflow at the efferent vessels. However, the communicating arteries become necessary if the subject has a missing ACA or PCA along with an occluded ICA or VA. Specifically, when an ICA is occluded, the ACoA becomes a critical collateral pathway, whereas when a VA is occluded the PCoAs become the critical collateral pathways. Throughout this study they determined that the worst possible scenario (of those studied) is a missing ACA along with a complete occlusion of the contralateral ICA.

An important point to note is that this study looks at the compensatory ability of the CoW itself to reduce the effects of pathological alterations and does not take into account the ability of the rest of the circulatory system to respond to the alterations.

### 4.3 Model

The current model of the Circle of Willis (CoW) consists of sixteen vessel segments connected through intersection conditions. In order to build the model, a model for a single vessel segment is derived first and then the segments are linked together appropriately to form the CoW.

#### 4.3.1 Single Vessel Model

To begin with, a number of somewhat standard assumptions in hemodynamic modeling are made:

- blood density is constant,
- blood flow is axisymmetric with no swirls,
- vessels are tethered in the longitudinal direction (i.e. they have fixed lengths),
-
variables are averaged across cross-sections.

The flow is assumed to obey the incompressible Navier-Stokes equations:

\[
\begin{align*}
\rho (\partial_t u + u \cdot \nabla u) - \nabla \cdot \sigma &= \rho g, \quad (4.1) \\
\nabla \cdot u &= 0,
\end{align*}
\]

where \(\rho\) is the density, \(u\) is the velocity, \(\sigma = -pI + 2\mu \epsilon\) is the stress tensor, \(g\) is the acceleration due to gravity, \(p\) is the pressure, \(\epsilon = \frac{1}{2} (\nabla u + \nabla u^T)\) is the strain-rate tensor, and \(\mu\) is the dynamic viscosity. If \(\mu\) is allowed to depend on \(\epsilon\) one can account for the non-Newtonian behavior of the blood. The incompressible Navier-Stokes equations (4.1, 4.2) are obtained from the compressible Navier-Stokes equations (3.4-3.6) by making the assumption that the density is constant (see [8] for details).

Since each vessel is considered to be an axisymmetric tube of variable diameter, the shape of each vessel can be described by a function \(R\) such that \(R(x,t)\) is the radius of the vessel at the point \(x\) along the longitudinal axis of the vessel at time \(t\). Using cylindrical coordinates along with the above assumptions the velocity is \(u = \langle v, 0, u \rangle\) and the strain rate tensor is

\[
\epsilon = \begin{bmatrix}
\partial_r u & 0 & \frac{1}{2} (\partial_r v + \partial_x u) \\
0 & \frac{v}{r} & 0 \\
\frac{1}{2} (\partial_r v + \partial_x u) & 0 & \partial_x u
\end{bmatrix}.
\]

The Navier-Stokes equations (4.1, 4.2) can then be rewritten as

\[
\begin{align*}
\rho (\partial_t v + v \partial_r v + u \partial_x v) &= \quad -\partial_r p + \partial_r (\mu \partial_r v) + \mu \partial_r \left(\frac{v}{r}\right) + \partial_x (\mu \partial_x v) \\
&+ \partial_r \mu \partial_r v + \partial_x \mu \partial_r u + \rho g_r, \quad (4.3) \\
\rho (\partial_t u + v \partial_r u + u \partial_x u) &= \quad -\partial_x p + \partial_r (\mu \partial_r u) + \mu \partial_r \left(\frac{u}{r}\right) + \partial_x (\mu \partial_x u) \\
&+ \partial_r \mu \partial_x v + \partial_x \mu \partial_x u + \rho g_x, \quad (4.4) \\
\frac{1}{r} \partial_r (rv) + \partial_x u &= 0,
\end{align*}
\]

where (4.3) is the radial momentum equation, (4.4) is the axial momentum equation, (4.5) is the continuity equation, and \(g_r\) and \(g_x\) are the radial and axial components of gravity respectively.
In order to model the viscoelasticity of the vessel walls, the Kelvin model (see [23]) is used which states

\[ p - p_0 + \tau_\sigma \partial_t p = \frac{Eh}{r_0} (s + \tau_\epsilon \partial_t s), \]  

(4.6)

where \( s = 1 - \sqrt{\frac{A_0}{A}} \), \( A = \pi R^2 \) and \( \tau_\sigma \) and \( \tau_\epsilon \) are the pressure and strain relaxation times, respectively.

In order to nondimensionalize the problem the following characteristic quantities are chosen

- flow: \( q_0 \),
- radius: \( r_0 \),
- radial velocity: \( v_0 \).

From these the following additional characteristic quantities can be derived

- surface area: \( A_0 = \pi r_0^2 \),
- axial velocity: \( u_0 = \frac{q_0}{A_0} \),
- length: \( x_0 = \frac{r_0}{v_0} \),
- time: \( t_0 = \frac{r_0}{v_0} = \frac{x_0}{u_0} \),
- pressure: \( p_0 = \rho u_0^2 \),
- dynamic viscosity: \( \mu_0 \).

With these characteristic quantities each of the given quantities can be nondimensionalized by letting \( \bar{\alpha} = \frac{\alpha}{\alpha_0} \) where \( \alpha \) refers to one of the quantities listed above. In terms of the nondimensionalized variables (with the bars dropped for notational
convenience), equations (4.3, 4.4, and 4.6) take the form

\[
\partial_r p = \left( \frac{v_0}{u_0} \right)^2 \left( -\partial_t v - v \partial_r v - u \partial_x v \right)
+ \frac{v_0}{u_0} \frac{\mu_0}{\rho r_0 u_0} \left( 2 \partial_r r v + \partial_r \left( \frac{v}{r} \right) + \partial_x u_x \right)
+ \left( \frac{v_0}{u_0} \right)^3 \frac{\mu_0}{\rho r_0 u_0} \partial_{xx} v - \frac{r_0 g}{u_0^2} e_r \cdot k,
\]

(4.7)

\[
\partial_t u + v \partial_r u + u \partial_x u = -\partial_x p + \frac{\mu_0}{\rho r_0 v_0} \left( \partial_{xx} u + \frac{1}{r} \partial_r u \right)
+ \frac{v_0}{u_0} \frac{\mu_0}{\rho r_0 u_0} (2 \partial_{xx} u + \partial_{xx} v)
- \frac{g}{u_0 v_0} e_x \cdot k,
\]

(4.8)

\[
\partial_t p - \frac{1}{2} \frac{\tau_e}{\tau_\sigma} \frac{Eh}{r_0 p_0} A^{-3/2} \partial_t A = \frac{t_0}{\tau_\sigma} (1 - p) + \frac{t_0}{\tau_\sigma} \frac{Eh}{r_0 p_0} (1 - A^{-1/2}),
\]

(4.9)

where \(e_r\) and \(e_x\) are unit vectors in the coordinate directions \(r\) and \(x\) respectively and \(k\) is the unit vertical vector. The continuity equation (4.5) does not change during nondimensionalization because \(\frac{v_0}{r_0} = \frac{u_0}{x_0}\). The equations can be simplified a bit more by taking into account the fact that the axial velocity, \(u_0\), is much larger than the radial velocity, \(v_0\), i.e. \(u_0 \gg v_0\), and therefore equations (4.7, 4.8) simplify to

\[
\partial_r p = \frac{r_0 g}{u_0^2} e_r \cdot k,
\]

(4.10)

\[
\partial_t u + v \partial_r u + v \partial_a = = \partial_x p + \frac{\mu_0}{\rho r_0 v_0} \left( \partial_{xx} u + \frac{1}{r} \partial_r u \right) - \frac{g}{u_0 v_0} e_x \cdot k.
\]

(4.11)

The final equations are obtained through averaging across cross-sections. The following derivation follows [51]. Assume that the fluid moves with the vessel at the wall. This corresponds to the no-slip boundary condition commonly used in fluid mechanics. Mathematically this means

\[
r(t) = R(x(t), t).
\]

This relation can be used as a boundary condition by taking the time derivative to get

\[
\dot{r} = R' \dot{x} + \dot{R} \Leftrightarrow v(R(x,t), t) = R'(x,t)u(R(x,t), t) + \dot{R}(x,t).
\]

(4.12)
Integrating the continuity equation (4.5) over a cross-section and using this boundary condition gives

$$2\pi R \dot{R} + \partial_x \left( 2\pi \int_0^R u r \, dr \right) = 0,$$

which is equivalent to

$$\partial_t A + \partial_x q = 0,$$

where $q = 2\pi \int_0^R u r \, dr$ is the dimensionless flux. Integrating the simplified radial momentum equation (4.10) leads to the following relation

$$\int_0^R \partial_r pr \, dr = 0 \iff p(R, x, t) = \frac{1}{R} \int_0^R p(r, x, t) \, dr \equiv P(x, t). \quad (4.13)$$

Assuming the pressure is independent of $r$, means $p(r, x, t) = P(x, t)$. Integrating (4.11) and using the boundary condition (4.12) gives

$$\partial_t q + \partial_x \left( 2\pi \int_0^R u^2 r \, dr \right) + A \partial_x p = \frac{1}{Re} R \partial_r u(R, x, t) - \frac{e_x \cdot k}{F} A, \quad (4.14)$$

where the following nondimensional parameters have been introduced

\begin{align*}
\text{Reynolds number } & Re = \frac{\rho r_0 v_0}{2\pi \mu_0}, \quad (4.15) \\
\text{Froude number } & F = \frac{u_0 v_0}{\sqrt{g r_0}}. \quad (4.16)
\end{align*}

An additional assumption is still needed to relate the axial velocity, $u$, to the averaged quantities $A$, $Q$, and $P$. Letting $U = Q/A$ be the average axial velocity, leads to

$$U = \frac{2}{R^2} \int_0^R ur \, dr.$$

An axial velocity is sought with the following profile

$$u(r, x, t) = \frac{\gamma + 2}{\gamma} U(x, t) \left( 1 - \left( \frac{r}{R(x, t)} \right)^\gamma \right),$$

where $\gamma$ determines the flow profile (with $\gamma = 2$ corresponding to Poiseuille flow) and the factor $\frac{\gamma + 2}{\gamma}$ ensures that the average of $u$ is $U$. Re-expressing the axial momentum equation (4.14) in terms of the averaged variables gives

$$\partial_t Q + \frac{\gamma + 2}{\gamma} \partial_x \left( \frac{Q^2}{A} \right) + A \partial_x P = -\frac{\gamma + 2}{Re} \frac{Q}{A} - \frac{e_x \cdot k}{F} A.$$
Averaging the Kelvin relation (4.6) amounts to replacing \( p \) by \( P \). This along with the continuity equation leads to

\[
\partial_t P + \frac{\tau_e}{\tau_\sigma} \frac{1}{\mathcal{M}^2} A^{-3/2} \partial_x Q = \frac{1}{\mathcal{W}} (1 - P) + \frac{2}{\mathcal{W} \mathcal{M}^2} (1 - A^{-1/2}),
\]

where the following nondimensional parameters have been introduced

\[
\begin{align*}
\text{Weissenberg number } &\mathcal{W} = \frac{\tau_e v_0}{r_0}, \quad (4.17) \\
\text{Mach number } &\mathcal{M} = \frac{u_0}{c_0}, \quad (4.18)
\end{align*}
\]

where \( c_0 = \sqrt{\frac{E_h}{2 \rho_0}} \) is the Moens-Korteweg speed.

The model can now be written in matrix form as

\[
(\partial_t + B \partial_x) \begin{bmatrix} A \\ Q \\ P \end{bmatrix} = G,
\]

where

\[
B = \begin{bmatrix}
0 & \frac{\gamma + 2}{\gamma + 1} \left( \frac{Q}{A} \right)^2 & 0 \\
-\frac{\gamma + 2}{\gamma + 1} \left( \frac{Q}{A} \right)^2 & \frac{2 \gamma + 2}{\gamma + 1} \frac{Q}{A} & A \\
0 & \frac{\tau_e}{\tau_\sigma} \frac{1}{\mathcal{M}^2} A^{-3/2} & 0
\end{bmatrix}
\quad \text{and} \quad
G = \begin{bmatrix}
0 \\
-\frac{2 + 2 Q}{\mathcal{W} \mathcal{M}^2} - \frac{\tau_e}{\tau_\sigma} (1 - A^{-1/2}) \\
\frac{1}{\mathcal{W}} (1 - P) + \frac{2}{\mathcal{W} \mathcal{M}^2} (1 - A^{-1/2})
\end{bmatrix}.
\]

The number of boundary conditions needed can be found by looking at the eigenvalues of \( B \) which are found to be

\[
\lambda_{1,3} = \frac{\gamma + 2 Q}{\gamma + 1 \ A} \mp \sqrt{\frac{\gamma + 2}{(\gamma + 1)^2} \left( \frac{Q}{A} \right)^2 + \frac{\tau_e}{\tau_\sigma} \frac{1}{\mathcal{M}^2 A^{1/2}}}, \quad \lambda_2 = 0.
\]

Assuming that \( A > 0 \), all three eigenvalues are real, ensuring that the system is hyperbolic. Unfortunately, without further assumptions, the sign of \( \lambda_{1,3} \) and the strict hyperbolicity of the system cannot be established. However, in all attempted simulations with realistic parameters \( \lambda_1 < 0, \lambda_3 > 0 \), and smooth solutions have been observed.
Table 4.1: Parameters in single vessel model after nondimensionalization.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Name</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{M}$</td>
<td>Mach Number</td>
<td>$\mathcal{M} = \frac{u_0}{c_0}$, where $c_0 = \sqrt{\frac{Eh}{2\rho r_0}}$</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynold Number</td>
<td>$Re = \frac{\rho r_0 u_0^2}{2\pi \mu_0}$</td>
</tr>
<tr>
<td>$\mathcal{F}$</td>
<td>Froude Number</td>
<td>$\mathcal{F} = \frac{q r_0^2}{2 \pi \rho r_0}$</td>
</tr>
<tr>
<td>$\mathcal{W}$</td>
<td>Weissenberg Number</td>
<td>$\mathcal{W} = \frac{q r_0^2}{2 \pi \rho r_0}$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic Viscosity of the Blood</td>
<td>$\mu = 1$</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Incline Angle of the Vessel</td>
<td>$\phi = 0$</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Vessel Wall Relaxation Ratio</td>
<td>$\tau = \frac{\tau_\sigma}{r_0}$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Flow Profile of the Blood</td>
<td>$\gamma = 2$</td>
</tr>
</tbody>
</table>

4.3.2 Choice of Model Parameters

As is apparent from the previous section, there are a number of parameters that show up in the nondimensionalized model. Table 4.1 lists these parameters and their definitions.

The first three parameters can be derived directly from the characteristic quantities given in the previous section. The fourth also requires knowledge of the relaxation time used in the viscoelastic constitutive equation. In this case, the value used for $\tau_\sigma$ was .125. The dynamic viscosity is set to one because the blood is currently being modeled as a Newtonian fluid. At this time, the CoW is considered to lie in a plane and thus the incline angle is set to zero.

The final two parameters are a little trickier as they are difficult to actually measure. For this study, values of $\tau = 1$ and $\gamma = 2$ have been used. Setting $\tau$ to one is essentially removing the viscoelasticity from the problem. It has been suggested that a value of $\tau = 4$, which was measured in-vitro in sheep would be a better approximation [61]. The choice of $\gamma = 2$ corresponds to a Poiseuille flow. Some researchers have suggested that a higher value of $\gamma$ might be a better model of what is actually happening [22, 62]. During this study, simple tests were run to test the effects of changing $\tau$ and $\gamma$ on the calculated perfusions and how well they fit the data.\(^1\) Figure 4.2 shows the calculated velocities over two periods in the LMCA. In all four cases,

\(^1\)In each case, the boundary condition parameters were optimized for the specific values of $\tau$ and $\gamma$ used. See Section 4.8 for details.
Figure 4.2: Comparison of calculated velocities in the LMCA using different values of $\tau$ and $\gamma$. Based on this preliminary test, there does not seem to be evidence that the alternate values give a better fit to the data.

there was no evidence to suggest that changing these values from the ones given above would provide a better fit to the data.

### 4.3.3 Multiple Vessel (Network) Model

This model for flow in the individual vessel segments now needs to be linked together to form the network of collateral vessels known as the CoW. Figure 4.1 shows the part of the arterial network to be modeled. The dotted lines mark where vessels are broken into segments to allow the implementation of internal boundary conditions. Internal boundary conditions are discussed in detail in Section 4.4.4. The specific geometry of the network is based on patient specific data. The values used in this study can be found in Table 4.3 and a discussion of the data collection related to this study can be found in Section 4.7.

The single vessel model has three equations in three unknowns which must be solved at each node at each time step. For this study four nodes in each vessel and time steps of .02 seconds are used. Thus, there are 600 unknowns per vessel segment per second or 9600 unknowns in the system per second.
4.4 Boundary Conditions

There are two types of boundary conditions that are used in this model which will be referred to as external boundary conditions and intersection conditions. External boundary conditions refer to those that link the model of the CoW to the peripheral arteries while intersection conditions will refer to those that link together the vessels of the CoW itself. Each type of condition will be discussed separately.

4.4.1 Resistance and Windkessel Boundary Conditions

As mentioned above, external boundary conditions are those that link the CoW to the periphery. Two commonly used external boundary conditions that will be considered in this work are a pure resistance condition and a windkessel condition. The windkessel boundary condition is more difficult to implement but leads to better results in the end.

The Pure Resistance Condition

The pure resistance condition says that the pressure and flow at the end of the vessel obey the following relation

$$\frac{p}{q} = R,$$

(4.20)

where \( p \) is the pressure, \( q \) is the flow, and \( R \) is a resistance parameter that is constant in time. This boundary condition has been shown to produce flow and pressure curves that are in phase which is generally not the case physiologically [52].

The Windkessel Condition

The windkessel condition is a model that imitates an electrical circuit with two resistors in sequence with a capacitor. Each resistor has its own resistance parameter, \( R^s \) and \( R^p \), and the capacitor is modeled by a compliance parameter \( C \). The windkessel condition says that the pressure and flow at the end of the vessel obey the following relation

$$R^s \partial_t q + \frac{R^s + R^p}{R^p C} q = \partial_t p + \frac{1}{R^p C} p,$$

(4.21)
where, again, $p$ is the pressure and $q$ is the flow.

### 4.4.2 Structured Tree Boundary Condition

In an attempt to better model the peripheral blood flow, a structured tree boundary condition was implemented. It is based on the fact that beyond the CoW the arterial network is essentially a bifurcating tree. This tree can be approximated by an asymmetric binary tree where the length and radius of the daughter vessels are scaled by parameters $\alpha$ and $\beta$ at each bifurcation. The equations that are satisfied within the tree are similar to those satisfied in the CoW except that the vessels in the tree are considered to be elastic instead of viscoelastic. This amounts to changing the constitutive equation (4.6) to

$$p - p_0 = \frac{4Eh}{3r_0} \left(1 - \sqrt{\frac{A_0}{A}}\right).$$  \hspace{1cm} (4.22)

The structured tree condition was first introduced by Mette Olufsen in 1998 [48] as part of her Ph.D. thesis. A detailed description the original derivation is given in chapter 5 of [52]. It has been used in many different models since, see e. g. [51, 59]. Recently, a simpler derivation of this boundary condition which maintains the diffusive term in the momentum equation was published by Azer and Peskin [4]. The derivation below is similar to their derivation but follows the notation used above.

Begin with the incompressible Navier-Stokes equations along with an elastic constitutive equation,

$$A_t = -Q_x$$  \hspace{1cm} (4.23)

$$Q_t = -2\frac{\gamma + 2}{\gamma + 1} \left(\frac{Q}{A}\right) Q_x + \frac{\gamma + 2}{\gamma + 1} \left(\frac{Q}{A}\right)^2 A_x - \frac{1}{\rho} \rho P_x - 2\frac{\pi \mu (\gamma + 2)}{\rho} \frac{Q}{A}$$  \hspace{1cm} (4.24)

$$P = p_0 + \frac{Eh}{r_0} \left(1 - \sqrt{\frac{A_0}{A}}\right).$$  \hspace{1cm} (4.25)

In this case, the choice of elastic vessel walls is a first step in simplifying the system to something with a known solution. Since the boundary condition is essentially a zero dimensional model of the periphery, the error introduced by assuming the vessel
walls are elastic should not be the dominating source of error. Note that the equations within the tree are not nondimensionalized. This is due to the change in scale at each generation of the tree. Nondimensionalizing everything to the scale of the root vessel defeats the purpose and nondimensionalizing each generation individually leads to an algebraic mess when trying to keep track of the different scales.

**Eliminating $A$**

Later, the impedance, which requires values for $P$ and $Q$, will be calculated. Thus, $A$ will be eliminated from the equations using the constitutive equation, (4.25). Solving (4.25) for $A$ leads to

$$A = \frac{\pi r_0^2}{1 - \frac{3r_0}{4Eh} (P - p_0)}$$

(4.26)

and thus,

$$A_\xi = \frac{3\pi r_0^3}{2Eh} \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^{-3} \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right] - \frac{3}{P_\xi}$$

(4.27)

where $\xi = r, t$. Plugging this into the continuity equation (4.23) and rearranging,

$$\frac{3\pi r_0^3}{2Eh} \frac{P_t}{P_x} + \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^3 Q_x = 0.$$  

(4.28)

Similarly, plugging (4.26) and (4.27) into (4.24) leads to

$$Q_t = -\frac{2(\gamma + 2)}{\pi r_0^2(\gamma + 1)} Q \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^2 Q_x$$

$$+ \frac{3r_0(\gamma + 2)}{2Eh(\gamma + 1)} Q^2 \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right] P_x$$

$$- \frac{\pi r_0^3}{\rho} \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^{-2} P - x$$

$$- \frac{2\mu(\gamma + 2)}{r_0^2} Q \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^2.$$
Thus, the system in $P$ and $Q$ is

\[
\frac{3\pi r_0^3}{2Eh} P_t = - \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^3 Q_x
\]

\[
\left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^2 Q_t = - \frac{2(\gamma + 2)}{\pi r_0^2(\gamma + 1)} Q \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^4 Q_x
\]

\[
+ \frac{3r_0(\gamma + 2)}{4Eh(\gamma + 1)} Q^2 \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^3 P_x
\]

\[
- \frac{\pi r_0^2}{\rho} P_x - \frac{2\mu(\gamma + 2)}{\rho r_0^2} Q \left[ 1 - \frac{3r_0}{4Eh} (P - p_0) \right]^4
\]

\[
(4.31)
\]

**Linearization**

Next, linearize $P$ and $Q$ about $P = p_0$ and $Q = 0$, i.e.

\[
P = p_0 + \epsilon p_1 + \epsilon^2 p_2 + \cdots \approx p_0 + \epsilon p_1,
\]

\[
Q = 0 + \epsilon q_1 + \epsilon^2 q_2 + \cdots \approx \epsilon q_1.
\]

In doing so, the continuity equation becomes

\[
\frac{3\pi r_0^3}{2Eh} \epsilon \partial_t p_1 = - \left[ 1 - \frac{3r_0}{4Eh} \epsilon p_1 \right]^3 \epsilon \partial_x q_1,
\]

which is equivalent to

\[
\frac{3\pi r_0^3}{2Eh} \epsilon \partial_t p_1 = - \epsilon \partial_x q_1,
\]

to first order in $\epsilon$. Thus, the linearized form of the continuity equation is

\[
p_t + \frac{2Eh}{3\pi r_0^3} q_x = 0,
\]

where the subscript 1’s have been dropped for ease of notation.

Similarly, the linearized form of the momentum equation is

\[
q_t + \frac{\pi r_0^2}{\rho} p_x + \frac{2\mu(\gamma + 2)}{\rho r_0^2} q = 0.
\]

\[
(4.33)
\]

Thus, the linearized, elastic, incompressible Navier-Stokes equations are

\[
p_t + \alpha q_x = 0,
\]

\[
q_t + \beta p_x + \delta q = 0,
\]

\[
(4.35)
\]
where,
\[
\alpha = \frac{2Eh}{3\pi r_0^3}, \\
\beta = \frac{\pi r_0^2}{\rho}, \\
\delta = \frac{2\mu(\gamma + 2)}{\rho r_0^2}.
\]

**Solution of Linearized Problem**

The next step is to solve the linearized system \((4.34, 4.35)\). To do so, take the Fourier Transform (in time) of the system to get
\[
i\omega \hat{p} + \alpha \hat{q}_x = 0, \\
i\omega \hat{q} + \beta \hat{p}_x + \delta \hat{q} = 0,
\]
where
\[
\hat{p} = \hat{p}(x, \omega) = \mathcal{F}[p](x, \omega) = \int_{-\infty}^{\infty} p(x, t) e^{i\omega t} dt.
\]

For now assume that \(\omega \neq 0\). The case when \(\omega = 0\) will be considered separately. Taking the derivative with respect to \(x\) of \((4.36)\) and plugging it into \((4.37)\) leads to
\[
\hat{q}_{xx} = \frac{\omega(i\delta - \omega)}{\alpha\beta} \hat{q}, 
\]
which has the solution
\[
\hat{q}(x, \omega) = ae^{\lambda(\omega)x} + be^{-\lambda(\omega)x},
\]
where
\[
\lambda(\omega) = \sqrt{\frac{\omega(i\delta - \omega)}{\alpha\beta}}.
\]
Plugging this back into equation \((4.36)\), gives the solution for \(\hat{p}\), namely,
\[
\hat{p}(x, \omega) = \frac{i\alpha}{\omega} \lambda(\omega) \left(ae^{\lambda(\omega)x} - be^{-\lambda(\omega)x}\right).
\]
Evaluating the solutions at $x = 0$ and $x = L$, gives

\[
\hat{q}(0, \omega) = a + b,
\]
\[
\hat{q}(L, \omega) = ae^{\lambda L} + be^{-\lambda L},
\]
\[
\hat{p}(0, \omega) = \frac{i\alpha \lambda}{\omega} (a - b),
\]
\[
\hat{p}(L, \omega) = \frac{i\alpha \lambda}{\omega} \left( ae^{\lambda L} - be^{-\lambda L} \right).
\]

Adding and subtracting the appropriate multiples of $\hat{q}(L, \omega)$ and $\hat{p}(L, \omega)$, leads to the following expressions for $a$ and $b$

\[
a = \frac{e^{-\lambda L}}{2} \left[ \hat{q}(L, \omega) - \frac{i\omega}{\alpha \lambda} \hat{p}(L, \omega) \right],
\]
\[
b = \frac{e^{\lambda L}}{2} \left[ \hat{q}(L, \omega) + \frac{i\omega}{\alpha \lambda} \hat{p}(L, \omega) \right],
\]

which can be plugged into the expressions for $\hat{q}(0, \omega)$ and $\hat{p}(0, \omega)$ to get

\[
\hat{p}(0, \omega) = \hat{p}(L, \omega) \cosh(\lambda L) - \frac{i\alpha \lambda}{\omega} \hat{q}(L, \omega) \sinh(\lambda L),
\]
\[
\hat{q}(0, \omega) = \hat{q}(L, \omega) \cosh(\lambda L) + \frac{i\omega}{\alpha \lambda} \hat{p}(L, \omega) \sinh(\lambda L).
\]

Next, define the quantity $\hat{z}$, which is often called the impedance, by $\hat{z} = \hat{p}/\hat{q}$.

From this definition and the relationships above, one can derive

\[
\hat{z}(0, \omega) = \frac{\hat{p}(0, \omega)}{\hat{q}(0, \omega)}
\]
\[
= \frac{\hat{p}(L, \omega) \cosh(\lambda L) - \frac{i\alpha \lambda}{\omega} \hat{q}(L, \omega) \sinh(\lambda L)}{\hat{q}(L, \omega) \cosh(\lambda L) + \frac{i\omega}{\alpha \lambda} \hat{p}(L, \omega) \sinh(\lambda L)}
\]
\[
= \frac{\hat{z}(L, \omega) \cosh(\lambda L) - \frac{i\alpha \lambda}{\omega} \sinh(\lambda L)}{\cosh(\lambda L) + \frac{i\omega}{\alpha \lambda} \hat{z}(L, \omega) \sinh(\lambda L)}.
\]

Thus, if the impedance at the terminal end of a vessel is known, the impedance at the proximal end can be calculated.

A similar relationship can be derived when $\omega = 0$. Consider (4.36) and (4.37) when $\omega = 0$. In this case, the system becomes

\[
\hat{q}_x = 0,
\]
\[
\hat{p}_x = \frac{\delta}{\beta} \hat{q}.
\]
The first equation tells us that \( \hat{q}(x, 0) = \) constant \( \equiv c \). Thus,
\[
\hat{q}(0, 0) = \hat{q}(L, 0) = c.
\]
Plugging this solution into the second equation and solving, gives
\[
\hat{p}(x, 0) = -\frac{\delta c}{\beta} x + d.
\]
Thus,
\[
\hat{p}(L, 0) = -\frac{\delta c L}{\beta} + d,
\]
\[
\hat{p}(0, 0) = d = \hat{p}(L, 0) + \frac{\delta c L}{\beta}.
\]
Finally,
\[
\hat{z}(0, 0) = \frac{\hat{p}(0, 0)}{\hat{q}(0, 0)}
= \frac{\hat{p}(L, 0) + \frac{\delta c L}{\beta}}{\hat{q}(L, 0)}
= \frac{\hat{p}(L, 0)}{\hat{q}(L, 0)} + \frac{\delta L}{\beta}
= \hat{z}(L, 0) + \frac{\delta L}{\beta}.
\]

**Calculating the Root Impedance**

In order to solve for the impedance at the root of the tree, the impedance at the terminal ends must be set and a way to cross a bifurcation must be determined. The following conditions should be satisfied at all bifurcations
\[
\hat{q}_L^p = \hat{q}_0^{d_1} + \hat{q}_0^{d_2},
\]
\[
\hat{p}_L^p = \hat{p}_0^{d_1} = \hat{p}_0^{d_2},
\]
where the superscript \( p \) denotes the parents vessel, the superscripts \( d_1 \) and \( d_2 \) refer to the daughter vessels, the subscript \( L \) refers to the terminal end of the given vessel, and the subscript \( 0 \) refers to the proximal end of the given vessel.
These conditions can be used to derive an equivalent condition to impose on \( \hat{z} \), namely,

\[
\frac{1}{\hat{z}_p} = \frac{\hat{q}_L^p}{p_L^p} = \frac{\hat{q}_0^d + \hat{q}_0^d}{p_L^p} = \frac{\hat{q}_0^d}{p_L^p} + \frac{\hat{q}_0^d}{p_L^p} = \frac{1}{\hat{z}_0^d} + \frac{1}{\hat{z}_0^d}.
\]

Thus, the appropriate condition to impose at a bifurcation is

\[
\frac{1}{\hat{z}_p} = \frac{1}{\hat{z}_0^d} + \frac{1}{\hat{z}_0^d}.
\]

(4.45)

The impedance (in Fourier space) can now be calculated at the root of the tree. Given an impedance to be imposed at the terminal ends of the tree, commonly \( \hat{z} = 0 \), one can calculate the impedances at the proximal ends of these vessels using (4.44). Then the bifurcation condition (4.45) can be used to “jump” the bifurcation. Continuing this process all the way up the tree, leads to an impedance at the root of the tree for each frequency \( \omega \).

**Transforming Back to Time Domain**

There are two ways to calculate and implement the pressure to be used as the boundary condition in time domain: (1) use the convolution theorem or (2) calculate \( \hat{p} \) directly and then transform it back. Using the convolution theorem,

\[
\hat{p} = \hat{z}\hat{q} \quad \Leftrightarrow \quad p = z \ast q.
\]

Thus, the impedances are transformed back to time domain and convolved with the flows at the boundary to get the pressure. Alternatively, the flow at the boundary can be Fourier transformed to get \( \hat{q} \) which can be multiplied by \( \hat{z} \) to find \( \hat{p} \), which can then be transformed back to find \( p(t) \) at the boundary.
4.4.3 Comparison of Total Variation for Windkessel and Structured Tree Boundary Conditions

While the structured tree condition does indeed capture more of the high frequency aspects of the flow, it also leads to a restriction on the size of the timestep. This comes from the fact that the timestep must be small enough to resolve these high frequency components. One way to see how this restriction comes about is to look at the total variation of the solution. For this test, consider a single vessel with a velocity imposed at the inflow. The model is run twice, once with the windkessel outflow boundary condition and once with the structured tree boundary condition. The discrete total variation,

\[ TV(u) = \sum_{i=0}^{N-1} |u(1,t_{i+1}) - u(1,t_i)|, \]  

(4.46)

of the solution at the outflow is then calculated, where \( u(x = 1, t) \) is the velocity at the efferent end of the vessel, \( t_i \) is the \( i \)th timestep, and \( N \) is the total number of timesteps taken.

Figure 4.3 shows a plot of the total variation in each case. In the case of the structured tree model, initially, as the size of the timestep decreases, the total variation increases rapidly. This is because with each reduction in the timestep, higher frequency components are being included in the solution, thus causing the solution to oscillate more rapidly. Eventually, the timestep becomes small enough that more than one timestep occurs between oscillations causing the total variation to drop.

On the other hand, since the windkessel model is not trying to resolve the high frequency components of the flow, it does not have trouble with large total variation. Also, since the most important aspect of the solution is the perfusions calculated from the end solutions, these high frequency effects are not important in this study. For this reason, the structured tree conditions will not be used in the model.

4.4.4 Intersection Conditions

In addition to external boundary conditions, a one-dimensional model of a network also requires internal boundary conditions or intersection conditions. These
Figure 4.3: Comparison of total variation in solution for windkessel outflow versus structured tree outflow in a single vessel. The total variation increases rapidly in the structured tree case due to the added high frequency components which are not fully resolved. Once all high frequency components have been resolved, the total variation drops. This limitation on the timestep makes the structured tree boundary condition less than ideal for our purposes.
conditions are used to link the individual vessels together to form the CoW network. These conditions determine what happens at the vessel bifurcations and trifurcations. Based on a study of the characteristics associated with the system, it can be shown that the number of internal boundary conditions needed is equal to the number of vessels at the intersection. This means that three conditions will be needed at a bifurcation and four conditions will be needed at a trifurcation. One of the conditions must ensure that mass is conserved. The easiest way to do this is to make sure that all the flows sum to zero, where flow towards the intersection in considered to be positive and flow away from the intersection is considered to be negative. The remaining conditions may include continuity of pressure or something more involved, such as continuity of total pressure. In [4] it was shown that both option (continuity of pressure and continuity of total pressure) lead to excellent results. For this study, conservation of flow and continuity of pressure are used. More precisely,

$$
\sum_{i=1}^{N_J} q_i = 0, \\
p_1 = p_2 = \cdots = p_{N_J},
$$

where $N_J$ is the number of vessels at intersection $J$ and flow is considered to be positive if it is flowing towards the intersection, as mentioned above.

### 4.5 Initial Conditions

The initial conditions used in this study are based on the specific geometry of the subject from which the data was collected. Each vessel starts with an initial cross-sectional area based on the measurements taken from an MRA image of the subject’s brain. The initial flow is constant within each vessel segment. The inflow vessels start with a uniform flow equal to the initial cross-sectional area times the initial velocity from the data. At major bifurcations (those which do not include a communicating artery) the initial flow is split evenly between the daughter vessels. The communicating arteries have an initial flow of zero. This ensures that the internal flow boundary conditions are satisfied at time $t = 0$. The internal pressure boundary conditions should also be satisfied at time $t = 0$. The simplest way to do this is to
set the initial pressure to a uniform value throughout the system. For this study, an initial pressure of 100 mmHg was chosen since normal blood pressure levels are thought to be between 80 and 120 mmHg.

4.6 Numerics

4.6.1 Spatial Discretization

Within each vessel the spatial discretization is done using Chebyshev collocation methods (see Section 2.2). As stated previously, this allows for a high level of accuracy using a small number of nodes. In fact, in this study it has been determined that the solutions within a given vessel are smooth enough that four nodes per vessel is plenty to achieve the desired level of accuracy (see below for details).

4.6.2 Temporal Discretization

Since the model should be able to run quickly with different patient specific geometries, as simple a method as possible is desired to perform the integration in time. Here backward Euler (BE) will be used. While BE is only a first order method, it is accurate enough to catch the major flow features very quickly which makes it a good choice in this case. Not only does BE run quickly because it is a simple method, it also allows us to take larger time steps because it is an A-stable method (see Section 2.3.4). Since BE is an implicit method, a nonlinear algebraic system of equations will need to be solved at each time step. Newton’s method (see Section 2.3.3) will be used with a small number of iterations to keep the model as fast as possible.

4.6.3 Verification of Discretization Resolution

It is important to verify that the number of spatial nodes is large enough and the size of the timesteps is small enough to ensure that an accurate solution is found. To do this, one can calculate what will be considered the “exact” solution by using a large number of spatial nodes and very small timesteps. A solution is then calculated
Table 4.2: Relative error statistics for the spatial and temporal resolution tests.

<table>
<thead>
<tr>
<th></th>
<th>Error Velocity Spatial Test</th>
<th>Error Pressure Spatial Test</th>
<th>Error Velocity Temporal Test</th>
<th>Error Pressure Temporal Test</th>
<th>Max</th>
</tr>
</thead>
<tbody>
<tr>
<td>LACA</td>
<td>0.0151</td>
<td>0.0483</td>
<td>0.0333</td>
<td>0.0361</td>
<td>0.0483</td>
</tr>
<tr>
<td>RACA</td>
<td>0.0067</td>
<td>0.0743</td>
<td>0.0377</td>
<td>0.0401</td>
<td>0.0743</td>
</tr>
<tr>
<td>LMCA</td>
<td>0.0059</td>
<td>0.0424</td>
<td>0.0298</td>
<td>0.0325</td>
<td>0.0424</td>
</tr>
<tr>
<td>RMCA</td>
<td>0.0045</td>
<td>0.0388</td>
<td>0.0369</td>
<td>0.0395</td>
<td>0.0395</td>
</tr>
<tr>
<td>LPCA</td>
<td>0.0349</td>
<td>0.0264</td>
<td>0.0326</td>
<td>0.0348</td>
<td>0.0349</td>
</tr>
<tr>
<td>RPCA</td>
<td>0.0260</td>
<td>0.0254</td>
<td>0.0347</td>
<td>0.0344</td>
<td>0.0347</td>
</tr>
<tr>
<td>Max</td>
<td>0.0349</td>
<td>0.0743</td>
<td>0.0377</td>
<td>0.0401</td>
<td>0.0743</td>
</tr>
</tbody>
</table>

with the desired number of spatial nodes (in this case, 4) and very small timesteps to verify that sufficient resolution is achieved in space. Finally, a solution is calculated with timesteps of the desired size (in this case, .02 s) and a large number of spatial nodes to verify that the resolution in time is sufficient. Table 4.2 shows the maximum relative error in the velocity and pressure in the six efferent vessels for both the spatial resolution test and the temporal resolution test.

### 4.6.4 Implementation of Boundary Conditions

Each vessel will have three equations to be solved at each of four nodes for a total of twelve equations in twelve unknowns per vessel. In order to implement the appropriate boundary conditions, two of these twelve equations will be replaced with boundary condition equations. Depending on the location of the individual vessel within the Circle of Willis these boundary conditions may take the form of a prescribed flow or a prescribed pressure. If the end of the vessel in question is connected to another vessel within the circle of willis, then the boundary condition corresponds to conservation of flow or continuity of pressure. If the end of the vessel is connected to the periphery, then the boundary condition corresponds to an inflow determined by experimental data or an outflow calculated using the resistance, windkessel, or structured tree boundary condition. See Section 4.4 for more information on specific boundary conditions.
4.7 Data

4.7.1 Collection and Details

The data used for the calibration and validation of this model was collected\(^2\) at Harvard Medical School by Drs. Vera Novak and Peng Zhao using digital doppler technology, magnetic resonance imaging (MRI), and a non-invasive, continuous, finger arterial blood pressure monitor at locations corresponding to the three inflow and six outflow locations. Figure 4.4 shows an example of the data.

Using digital doppler technology to measure blood flow in the brain involves placing a non-invasive probe over the eye, over the temple, under the chin, or at the base of the skull depending on which vessel data is being collected from. Because it is

\(^2\)This study was supported by an American Diabetes Association Grant, American Diabetes Association Clinical Scientist Award (1-06-CR-25), Cerebral perfusion and cognitive decline in type 2 diabetes to V. Novak, an NIH Older American Independence Center Grant 2P60 AG08812, NIH Program projects AG004390 and R01-NS045745.

Figure 4.4: Example of data collected in the right internal carotid artery (RICA).
a non-invasive procedure, the data is inherently noisy. In addition, data in different vessels has to be collected at different times due to limitations on availability of probes. Thus, some post-processing of the data must be done to ensure consistency across data sets.

The inflow data has been used as boundary conditions to drive the system and the outflow data has been used to test the accuracy of the model.

### 4.7.2 Geometry

The MRI data was used to determine the specific geometry of the Circle of Willis in the subject from which the flow data was collected. Figure 4.5 shows a mock-up of the Circle of Willis which, along with the information in Table 4.3, defines the specific geometry used in this study.
Table 4.3: Specific geometry of the Circle of Willis used for the calibration and validation of the model. The values in *italics* were missing from the data and had to be estimated.

<table>
<thead>
<tr>
<th>Vessel #</th>
<th>Name</th>
<th>Diameter (mm)</th>
<th>Length (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Basilar</td>
<td>3.00</td>
<td>8.25</td>
</tr>
<tr>
<td>2</td>
<td>R. PCA 1</td>
<td><em>2.2</em></td>
<td><em>3.33</em></td>
</tr>
<tr>
<td>3</td>
<td>L. PCA 1</td>
<td><em>2.2</em></td>
<td><em>3.33</em></td>
</tr>
<tr>
<td>4</td>
<td>R. PCA 2</td>
<td>2.20</td>
<td>7.56</td>
</tr>
<tr>
<td>5</td>
<td>L. PCA 2</td>
<td>2.20</td>
<td>7.56</td>
</tr>
<tr>
<td>6</td>
<td>R. PCoA</td>
<td><em>1.9</em></td>
<td><em>10.0</em></td>
</tr>
<tr>
<td>7</td>
<td>L. PCoA</td>
<td><em>1.9</em></td>
<td><em>10.0</em></td>
</tr>
<tr>
<td>8</td>
<td>R. Carotid</td>
<td>4.20</td>
<td>48.1</td>
</tr>
<tr>
<td>9</td>
<td>L. Carotid</td>
<td>4.20</td>
<td>48.1</td>
</tr>
<tr>
<td>10</td>
<td>R. MCA</td>
<td>2.68</td>
<td>21.1</td>
</tr>
<tr>
<td>11</td>
<td>L. MCA</td>
<td>2.68</td>
<td>21.1</td>
</tr>
<tr>
<td>12</td>
<td>R. ACA 1</td>
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<td>L. ACA 1</td>
<td>2.21</td>
<td>10.7</td>
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<tr>
<td>14</td>
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<td>2.00</td>
</tr>
<tr>
<td>15</td>
<td>R. ACA 2</td>
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<tr>
<td>16</td>
<td>L. ACA 2</td>
<td>2.30</td>
<td>23.0</td>
</tr>
</tbody>
</table>
4.7.3 Post-processing

Velocity Data

Since the data was collected at different times, post-processing is required to make sure that the data from different vessels is consistent. There are different ways the data could be processed to make it more consistent. The two options considered were scaling the overall length of eight periods in each dataset and scaling each period individually to be the same length. Figure 4.6 shows the effects of scaling the overall time only (top) and scaling each period individually (bottom). As can be seen from the figure, stretching each period individually makes the ECG output more consistent across periods. Thus, each heartbeat is stretched to have a length of one second. This stretching removes any differences in heart rate from one collection to the next. Then the ECG spikes for the heartbeats are lined up to maintain any phase differences between the vessels.
Pressure Data

The pressure data was scaled appropriately in time to correspond to the velocity data. Then a single profile was chosen to be used as the data.

4.8 Parameter Fitting

The EnKF has been used to optimize the parameters for both the resistance outflow boundary conditions and the windkessel outflow boundary conditions. In each case, an ensemble size of 100 was used. After processing a subset of the available data, the final parameter values are considered to be the optimal values based on the data. The model is then run using the original initial conditions and the optimized parameters and the results are compared to the data.

4.8.1 EnKF Results

Figure 4.7(a) shows a comparison of the experimental data and the model output using the pure resistance boundary condition in the RMCA over one cardiac cycle. The results using the parameters obtained from the EnKF clearly provide a better fit to the data. Figure 4.7(b) shows a similar comparison, this time with the model results obtained using the windkessel boundary condition. In this case, the original parameters were chosen based on available literature and therefore the switch to the EnKF optimized parameters provides less of an improvement.

Although the velocity results look promising, the associated pressures calculated by the model are problematic. Figure 4.8(a) shows the pressures associated with the velocities from Figure 4.7(b). Since the pressure data is from the finger, the model results are not expected to match the pressure wave forms exactly but should be in roughly the same range. The overall lack of fit of the predicted pressures is not surprising since the EnKF optimized the parameters based solely on the velocity data without any knowledge of the associated pressure data. It is possible to scale the parameters determined by the EnKF in such a way that the predicted pressures fall in a more realistic range without significantly changing the predicted velocities.
Figure 4.7: Comparison of model velocity results to velocity data in the RMCA using (a) the resistance outflow boundary condition and (b) the windkessel outflow boundary condition. The EnKF optimization makes a marked improvement in the pure resistance case but only a slight change in the windkessel case. This is due to the fact that the original windkessel parameters were chosen based on available literature.

4.8.2 Rescaling of EnKF Results

The following relation is used to calculate the mean pressure $\hat{p}$

$$R_T = \frac{\hat{p}}{\hat{q}},$$

(4.47)

where $\hat{q}$ is the mean flow (calculated from the inflow data used to drive the system) and

$$R_T = \left( \sum_{ves} \frac{1}{R_{ves}} \right)^{-1}, \quad R_{ves} = R^s_{ves} + R^p_{ves},$$

(4.48)

is the total resistance. This gives a mean pressure of $\hat{p} \approx 134$ mmHg. Ideally, a mean pressure of approximately 94 mmHg is expected. To adjust the mean pressure of the system, each of the resistance parameters is multiplied by $94/134 \approx .7$. Figure 4.8(b) shows the results of running the simulation with the reduced resistances. As desired, the predicted velocities show little change while the predicted pressures now fall in a much more realistic range.
Figure 4.8: (a) Comparison of model blood pressure results in the RMCA to blood pressure data in the finger using the original and EnKF parameters. (b) Comparison of model velocities (top) and model blood pressures (bottom) to data after scaling the EnKF resistance parameters by .7.

4.9 Simple Sensitivity Analysis

A simple way to test the sensitivity of the solution within the CoW to the boundary condition parameters is to change the parameters in turn and see what effect this has on the solution. In order to determine the sensitivity of the solution to the value of a given parameter, solutions are calculated with the original parameter value and with a ten percent increase in the parameter value. The sensitivity is then the maximum over time of the difference between the two solutions, scaled by the size of the original solution. Thus, the sensitivity is a measure of the relative change in the solution caused by a ten percent change in the specified parameter.

Table 4.4 shows the rankings of how the outflow in each efferent vessel depends on the windkessel boundary condition parameters and Figure 4.9 shows the values that go along with these rankings. The curves in the figure show a clear cutoff after the first two parameters and again after the next ten parameters. These correspond to the sectioning in the table. As expected, the solution in a given outflow vessel is highly sensitive to its own resistance parameters, moderately sensitive to the resistance parameters of the other outflow vessels, and insensitive to the compliances.
Table 4.4: Results of a simple sensitivity analysis. As expected, the solution in a given outflow vessel is highly sensitive to its own resistance parameters, moderately sensitive to the resistance parameters of the other outflow vessels, and insensitive to the compliances.

<table>
<thead>
<tr>
<th></th>
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<th>RACA</th>
<th>LMCA</th>
<th>RMCA</th>
<th>LPCA</th>
<th>RPCA</th>
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<tr>
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</table>
4.10 Results

Validation of many blood flow models is limited by the lack of available data, and is therefore usually qualitative in nature. Access to clinical data allows this model to be validated in a more quantitative manner.

Since the cardiac cycle varies over time, even in a single subject, a given set of outflow data is not expected to be matched exactly using a given set of inflow data collected at a different time. To get around this, all of the available data is processed and a mean velocity profile is calculated for each inflow and outflow vessel, along with the associated variances. The simulation is then run with 20 different stochastically perturbed inflow velocity profiles. The mean predicted velocity in each outflow vessel is then compared to the corresponding mean velocity profile from the data. The mean inflow velocities are shown in Figure 4.10 and the mean outflow velocities are shown in Figure 4.11.

As was mentioned in section 4.7, the original data given to us by Dr. Novak and
Figure 4.10: Mean inflow velocities with associated standard deviation bars from data.
Figure 4.11: Mean outflow velocities with associated standard deviation bars from data.
the researchers at Harvard Medical School indicated that the patient had a symmetric CoW. During the testing and validation of the model it became apparent that the geometry data and the blood flow data were not in agreement. After bringing this to the attention of Dr. Novak, the geometry was remeasured and it was determined that the patient did not have a symmetric CoW after all. In Section 4.10.1 findings related to the original (symmetric) CoW geometry and the issues that lead to questioning these measurements will be discussed. Then, in Section 4.10.2, the fact that when the correct geometry is used, the model results match the data more consistently, will be shown. Finally, in Section 4.10.3 the effects of common anatomical variations within the CoW on blood perfusion throughout the brain will be discussed.

4.10.1 Complete CoW - Symmetric Geometry

First the model was run using the symmetric geometry. Table 4.5 shows a breakdown of how well the model results match the data. As is evident from the table, the model is doing an excellent job in the PCAs and the MCAs but doesn’t do as well in the ACAs. Looking at the mean velocity profiles in the left vessels versus their right counterparts shows a much larger discrepancy in the ACAs than in the PCAs and MCAs (see Figure 4.12). Since the model is setup in a geometrically symmetric manner, it is not surprising that the model results are roughly symmetric as well.\(^3\) Thus, fitting the data well in both the LACA and RACA is unlikely.

4.10.2 Complete CoW - Asymmetric Geometry

When the geometry was remeasured, it was discovered that the internal segments of the left and right ACAs (vessels 12 and 13 in Figure 4.5 and Table 4.3) actually have different radii. Table 4.6 shows a comparison of the old and new values of the radius in these two vessels. All other geometry values remained the same.

When the model was run with the updated geometry, the results looked much better. Table 4.7 and Figure 4.14 show the updated results.

\(^3\)Different inflows from the ICAs breaks the strict symmetry that would otherwise be expected based on a completely symmetric geometry.
Table 4.5: Complete CoW - Symmetric Geometry: After the stochastic version of the model has been run to create 20 realizations, the mean velocity profile is calculated in each vessel. These curves are then compared to the means calculated from the data. The table above shows the percentage of time the model mean is within one or two standard deviations (σ) of the data mean (μ) in each of the six outflow vessels.

<table>
<thead>
<tr>
<th></th>
<th>% within (μ − σ, μ + σ)</th>
<th>% within (μ − 2σ, μ + 2σ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>RPCA</td>
<td>44</td>
<td>90</td>
</tr>
<tr>
<td>LPCA</td>
<td>86</td>
<td>100</td>
</tr>
<tr>
<td>RMCA</td>
<td>90</td>
<td>100</td>
</tr>
<tr>
<td>LMCA</td>
<td>92</td>
<td>100</td>
</tr>
<tr>
<td>RACA</td>
<td>0</td>
<td>18</td>
</tr>
<tr>
<td>LACA</td>
<td>12</td>
<td>32</td>
</tr>
</tbody>
</table>

Figure 4.12: Comparison of left and right mean outflows.

Table 4.6: Updated geometry data for asymmetric CoW.

<table>
<thead>
<tr>
<th>Vessel #</th>
<th>Name</th>
<th>Old Diameter (mm)</th>
<th>New Diameter (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>R. ACA 1</td>
<td>2.21</td>
<td>3.40</td>
</tr>
<tr>
<td>13</td>
<td>L. ACA 1</td>
<td>2.21</td>
<td>2.00</td>
</tr>
</tbody>
</table>
Figure 4.13: Comparison of model results to data in the LMCA over multiple cardiac cycles.

Table 4.7: Complete CoW - Asymmetric Geometry: The table above shows the percentage of time the model mean is within one or two standard deviations ($\sigma$) of the data mean ($\mu$) in each of the six outflow vessels.

<table>
<thead>
<tr>
<th></th>
<th>% within $(\mu - \sigma, \mu + \sigma)$</th>
<th>% within $(\mu - 2\sigma, \mu + 2\sigma)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>RPCA</td>
<td>66</td>
<td>90</td>
</tr>
<tr>
<td>LPCA</td>
<td>48</td>
<td>100</td>
</tr>
<tr>
<td>RMCA</td>
<td>16</td>
<td>100</td>
</tr>
<tr>
<td>LMCA</td>
<td>54</td>
<td>100</td>
</tr>
<tr>
<td>RACA</td>
<td>32</td>
<td>98</td>
</tr>
<tr>
<td>LACA</td>
<td>40</td>
<td>84</td>
</tr>
</tbody>
</table>
Figure 4.14: Mean outflow velocities resulting from running the stochastic version of the model over 20 realizations.
Table 4.8: List of common anatomical variations within the Circle of Willis and the frequency at which they occur. *The frequency of missing all communicating arteries could not be found in the literature but was tested for completeness.

<table>
<thead>
<tr>
<th>Variation</th>
<th>Frequency</th>
</tr>
</thead>
<tbody>
<tr>
<td>Complete CoW</td>
<td>49%</td>
</tr>
<tr>
<td>Extra ACoA</td>
<td>10%</td>
</tr>
<tr>
<td>Missing ACA, seg 1</td>
<td>6%</td>
</tr>
<tr>
<td>Missing ACoA</td>
<td>1%</td>
</tr>
<tr>
<td>Missing One PCoA</td>
<td>9%</td>
</tr>
<tr>
<td>Missing Both PCoAs</td>
<td>9%</td>
</tr>
<tr>
<td>Missing All CoAs</td>
<td>*</td>
</tr>
<tr>
<td>Missing PCA, seg 1</td>
<td>9%</td>
</tr>
</tbody>
</table>

4.10.3 Common Incomplete Geometries

Now that the model has been calibrated and validated it can be used to determine the effects of common anatomical variations in the geometry of the Circle of Willis on the perfusion of the brain. Perfusion is a measure of the amount of blood supplied to a given area over one heartbeat. It is used as the method of comparison in this case because it is of interest to clinicians interested in the effects of differing geometries on blood supply to the brain. The geometries considered were chosen based on a study by Lippert and Pabst [40] and are listed in Table 4.8.

In order to investigate the effects of these anatomical variations, the model is run with each of the different geometries and the perfusions are calculated at each outflow point of the Circle of Willis. To ensure that any variations observed come from the variations in geometry and are not artifacts of some type of asymmetry, the variations will be completely symmetric except for the specified variation. This includes the inflow velocities and outflow parameters as well.

Figures 4.15 and 4.16 show two different representations of the resulting data. As expected, the changes in the geometry have little affect on the total perfusions (the lengths of the overall bars in Figure 4.16) but do affect the distribution of flow among the six outflow vessels. The most pronounced change occurs when both PCoAs are missing. This is due to the fact that for the full circle, roughly one third of the blood
flow through the PCAs comes from the ICAs and thus must travel through the PCoAs to get there. When the PCoAs are absent, this exchange of blood flow from the front to the back of the brain can not occur and therefore the amount of blood flowing out of the PCAs is reduced significantly.

Once baseline perfusions have been calculated for each anatomical variation under normal conditions, the effects of different types of strokes on the perfusions can be considered. Four types of strokes will be considered, a vertebral stroke, a basilar stroke, an ipsilateral\textsuperscript{4} carotid stroke, and a contralateral carotid stroke\textsuperscript{5}. In order to impose a stroke in a given inflow vessel, the inflow velocity is set to zero after one period. Since the vertebral arteries are not included in the model, a vertebral stroke is implemented by reducing the basilar inflow by one half.

Figure 4.17 shows an example in the case of an ipsilateral carotid stroke. It is interesting to note that even though the change in inflow velocity is abrupt, the CoW is able to compensate for the change very quickly and the flow returns to a periodic state within a single heartbeat (see Figure 4.18).

Once simulations have been run for each type of stroke in each anatomical variation, perfusions are calculated at each outflow in each case. Figures 4.19 and 4.20 show the results in the case of a complete CoW. As expected, the total perfusion is reduced in each case due to the reduction in blood flowing into the circle. Interestingly, the distribution of the total flow remains roughly the same in all cases. This indicates that the collateral pathways within the CoW are able to compensate for the change in inflow and disperse the available blood to maintain the individual perfusions as best as possible.

For the second variation, an extra ACoA, similar results are observed, in fact the presence of an extra anterior communicating artery seems to have almost no effect. The results for this case are shown in Figures 4.21 and 4.22.

A more noticeable change takes place in variation three, a missing LACA, segment

\textsuperscript{4}Since all anatomical variations are modeled on the left side of the CoW, an ipsilateral stroke will occur on the left side while a contralateral stroke will occur on the right side.

\textsuperscript{5}Note that in the case of a symmetric anatomical variation, the ipsilateral carotid and contralateral carotid strokes are simply mirror images of each other and therefore the figures will only show data for one of them.
Figure 4.15: Comparison of perfusions for different geometries in the absence of a stroke.
Figure 4.16: Comparison of perfusions for different geometries in the absence of a stroke. (Alternative Representation)

Figure 4.17: Inflow velocity over time in the event of a stroke.
Figure 4.18: Even though the change in inflow is abrupt in the event of a stroke, the blood flow velocity returns to a periodic state very quickly.

1, see Figures 4.23 and 4.24. In this case, the vertebral and basilar strokes affect the total inflow but not the way in which the flow is distributed amongst the vessels. However, in the case of the ipsilateral stroke (LICA), the perfusion is weighted more heavily toward the contralateral MCA and both ACAs. This is consistent with the geometry of the circle in that the location of the inflows favor the RMCA and the ACAs. For a contralateral stroke (RICA), the perfusion is weighted more towards the ipsilateral MCA and the PCAs. Again, this is consistent with the overall geometry of the circle.

For variation four, a missing ACoA, the results for the vertebral and basilar strokes are almost identical to those of the full circle. This makes sense since the system is still symmetric and therefore has no reason to favor one side over the other. However, in the event of a carotid stroke, a bias in perfusion is shown towards the contralateral side. This is consistent with the fact that the blood must travel much farther to perfuse the ipsilateral side since their is no direct pathway between the left and right sides when the ACoA is missing. Figures 4.25 and 4.26 show the results for this case.
(a) No Stroke

(b) Vertebral Stroke

(c) Basilar Stroke

(d) Left Internal Carotid Stroke

Figure 4.19: Comparison of perfusions in subject with complete CoW after different types of strokes.

Figure 4.20: Comparison of perfusions in subject with complete CoW after different types of strokes. (Alternative Representation)
Figure 4.21: Comparison of perfusions in subject with an extra ACoA after different types of strokes.

Figure 4.22: Comparison of perfusions in subject with extra ACoA after different types of strokes. (Alternative Representation)
Figure 4.23: Comparison of perfusions in subject with missing LACA, segment 1 after different types of strokes.
Figure 4.24: Comparison of perfusions in subject with missing LACA, segment 1 after different types of strokes. (Alternative Representation)

(a) No Stroke
(b) Vertebral Stroke
(c) Basilar Stroke
(d) Left Internal Carotid Stroke

Figure 4.25: Comparison of perfusions in subject with missing ACoA after different types of strokes.
In the case of a missing PCoA, the results are surprisingly consistent across each of the different types of strokes. In particular, the similarity of the perfusions calculated in the event of ipsilateral and contralateral carotid strokes (see Figures 4.27 and 4.28) seems unexpected. However, after considering the geometry further, the similarity is not too surprising since most of the compensation for the occluded vessel will come from the other carotid artery in both cases.

When both PCoAs are missing, major changes in blood perfusion can occur, see Figures 4.29 and 4.30. Specifically, in the case of a vertebral stroke, the perfusions to the back of the brain are reduced significantly and in the case of a basilar stroke, the back of the brain does not receive any blood at all. This is expected since there is no way for blood to get to the PCAs except from the basilar artery when both PCoAs are missing.

Similarly, when all the communicating arteries are missing, the effects of a vertebral or basilar stroke can be severe. In addition, due to the lack of communication between the left and right sides of the brain due to the lack of the ACoA, the middle and front portions of the ipsilateral side of the brain will receive no perfusion in the event of a carotid stroke. Results from this variation are shown in Figures 4.31 and 4.32.
Figure 4.27: Comparison of perfusions in subject with missing LPCoA after different types of strokes.
Figure 4.28: Comparison of perfusions in subject with missing LPCoA after different types of strokes. (Alternative Representation)

Figure 4.29: Comparison of perfusions in subject with missing L&R PCoAs after different types of strokes.
Figure 4.30: Comparison of perfusions in subject missing both PCoAs after different types of strokes. (Alternative Representation)

Figure 4.31: Comparison of perfusions in subject missing all communicating arteries after different types of strokes.
Finally, in the case of a missing LPCA, segment 1, the distribution of the total perfusion remains roughly the same in the event of a vertebral or basilar stroke. In the case of an ipsilateral carotid stroke (LICA), the perfusions are weighted towards the RMCA and RPCA while in the case of a contralateral stroke (RICA), the perfusions are weighted towards the LMCA. Again, these results are consistent with what is expected based on the new geometry. See Figures 4.33 and 4.34 for details.

Overall, it is obvious that the collateral pathways through the CoW play an important role in maintaining proper blood supply to the brain.
Figure 4.33: Comparison of perfusions in subject with missing LPCA, segment 1 after different types of strokes.
Figure 4.34: Comparison of perfusions in subject with missing LPCA, segment 1 after different types of strokes. (Alternative Representation)
Chapter 5

Final Remarks

The numerical results obtained from simulations run using the models described in this work have provided new insight into their respective problems.

Through a splitting method that incorporates known solutions to the corresponding inviscid Euler equations the multi-dimensional, compressible, barotropic, Navier-Stokes equations have been shown to indicate vacuum formation in the presence of large Mach numbers. This result was based on the presence of extremely low densities as well as the behavior of the solution over time in phase space. These numerical results can be seen as a launching point for further analytic investigation into the problem and may help in understanding the circumstances under which vacuums form, possibly leading towards an analytic solution to a previously unsolved problem.

In addition, a one dimensional model of blood flow in the Circle of Willis (CoW) has been calibrated and validated against clinical data. It has been shown that this one dimensional model with windkessel outflow boundary conditions provides excellent results. A structured tree boundary condition was also implemented but was shown to be inappropriate for the given application due to its tight restriction on the size of the timestep. A preliminary study of the importance of the viscoelasticity of the vessel walls showed that viscoelasticity may not be essential for good agreement with clinical data.

Once validated, the model was used to investigate the effects of common anatomical variations within the CoW on blood perfusion in the brain both under normal
conditions and in the event of different types of strokes. It was shown that the presence of collateral pathways through the CoW are an important aspect in the maintenance of proper blood supply to the brain, especially in the event of a stroke. It was also noted that in the cases where similar perfusion distributions can be reached after a stroke, the change in flow is balanced out almost immediately, reducing the potential for long-term damage due to lack of perfusion throughout the brain.

This model still has many aspects that need to be investigated. These include, but are not limited to, a more in-depth look at the importance of viscoelasticity versus elasticity in modeling the vessel walls, determining the effects of treating blood as a Newtonian fluid instead of a non-Newtonian fluid, and investigating the possibility of using stochastic partial differential equations in order to incorporate the uncertainties of the model parameters into the model. I hope to have the opportunity to continue to work on this project in the future.
Bibliography


