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ABSTRACT

Derivation and Numerical Simulation of Oxygen Transport in Blood Vessels

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Modeling and simulating the transport of oxygen in blood provides critical insight on the planning of cardiovascular surgeries. Mathematical simulation provides a quantitative angle on the understanding of changes in hemodynamics. Due to the complexity of the cardiovascular circulation, this is a computationally challenging task. Further, oxygen transport is coupled to the velocity field of blood. Thus, the numerical solution of the transport equation requires either the specification or the computation of the velocity field of blood. The latter approach is expensive when the three-dimensional Navier Stokes equations are considered, and the a-priori specification of the velocity does not account for changes in the velocity field. To counteract these difficulties, we propose a model reduction of the convection diffusion equation of oxygen in a compliant vessel with varying radius. We obtain a one-dimensional equation coupled to the reduced model of blood flow. We employ discontinuous Galerkin methods to efficiently solve the resulting system in one vessel. We show stability of the proposed numerical scheme for a general nonlinear convection diffusion equation. We verify the model using the method of manufactured solutions. We extend the numerical method to a bifurcation of vessels, and we simulate oxygen transport in a three vessel network.
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Chapter 1

Introduction and Literature Review

This chapter illustrates the approaches to simulate the dynamics of blood flow and oxygen transport. First, I discuss the formulation of a mathematical model in Section 1.1. In Section 1.2, I survey the methods used to numerically solve this model.

1.1 Modeling Blood Flow and Oxygen Transport

Oxygen is transported with the velocity field of blood. Thus, modeling oxygen transport necessitates the use of a blood flow model. Accordingly, I first review the blood flow model in Section 1.1.1. Then, I discuss the oxygen transport equation and the way it couples to the reduced blood flow model in Section 1.1.2.

1.1.1 Modeling Blood Flow

The dynamics of blood flow are described by the incompressible Navier-Stokes equations, a three dimensional non-linear system of partial differential equations. This system of equations is numerically difficult to simulate and requires the specification of boundary conditions which are not well known [8, 7]. Thus, a computationally efficient simulation demands the use of approximate models.

Barnard et al. propose an approximation for the incompressible Navier-Stokes equations [7]. They perform an asymptotic model reduction of the equations. In order to conduct this reduction, they assume that the vessel radius is much smaller than its length. Then, the authors write the equations in non-dimensional form and neglect all the terms of lower
order. Next, the authors integrate the equations to arrive at a one dimensional system. This system describes the dynamics of the cross-sectional area of the vessel and of the averaged blood velocity or momentum. This reduced model has been tested against measured physiological data and has resulted in similar qualitative and quantitative characteristics [18]. Because of this validation and its inexpensive implementation, this system is popular in the hemodynamics literature [21].

Integral to this model derivation is the specification of an axial velocity profile which provides closure to the system [9, 21]. Different choices have been discussed in the literature. For example, Womersley theory was employed to iteratively construct a time dependent velocity profile rather than a priori determining it [5]. This method provides a framework for modeling the shear stress on the wall and for calculating velocity profiles [4, 5]. Another approach is to specify a steady state velocity profile. A common choice is the no-slip and the flat velocity profile. The latter choice yields multiple simplifications. First, it leads to a system written in conservative form where its Riemann invariants can be derived [21]. Second, it simplifies the theoretical analysis for the existence and uniqueness of solutions [9]. Puelz et al. perform a comparison for different shapes of the no-slip velocity profile which is determined by the Coriolis coefficient $\alpha$ [21]. The authors conclude that $\alpha = 1.1$ is a sound choice when the quantities of interest are area and momentum.

1.1.2 Modeling Oxygen Transport

Now that I have discussed the blood flow model, I will survey the different approaches to model oxygen transport. Oxygen is transported in blood either as bound to hemoglobin or as free oxygen dissolved in plasma [17]. The two phenomena can be modeled using a three dimensional nonlinear convection diffusion equation. The nonlinearity arises from the non-linear dependence of the saturation of oxygen, ratio of hemoglobin bound to oxygen to total hemoglobin, on the partial pressure of oxygen in plasma [17]. This dependence can
be linearized altering the diffusion coefficient and the hemoglobin carrying capacity from variable quantities to constants [17]. The effect of this linearization is more prominent in local variations of the concentration rather than in averaged quantities [17].

The numerical solution of the transport equation requires either the specification [6] or the computation of the velocity field of blood [17]. The latter approach is computationally expensive if the three dimensional Navier Stokes equations are considered. The a priori specification does not account for changes in the velocity field. To counteract these difficulties, we propose a model reduction of the convection diffusion equation of oxygen. The result is a one dimensional equation coupled to the reduced model of blood flow.

This one dimensional equation describes the transport of the radially averaged concentration of oxygen. The derivation of this equation requires the identification of the radial variation of concentration. The problem of determining this variation was first studied by Taylor in 1953 [26]. The author considers a pipe of constant radius and a steady state no slip velocity profile.

To determine the radial variation of the concentration, Taylor presents two different sets of assumptions on the nature of convection and diffusion of a solute in a tube. The first states that convection has the dominant effect on the solute where it is longitudinally transported in a short period of time. In contrast, the second declares that diffusion renders the concentration of the solute radially uniform faster than convection transports it [26]. Taylor derives conditions on the diffusion coefficient, length and radius of the tube by which the second set of assumptions holds [26, 27]. These assumptions allow for the explicit computation of approximate solutions to the concentration of the solute; thus, they provide a way to quantify its radial variations. We will employ this second assumption to provide a closure relation to the reduced oxygen transport equation.

Several mathematicians worked on providing a theoretical basis for the seminal paper by
Taylor [26]. The first was the work by Aris [2]. He calculated the moments of the concentration using Fourier-Bessel analysis. Aris concluded that the dynamics of dispersion can be captured by the first two moments [2]. Another mathematical formulation was obtained by Mercer and Roberts [16]. The authors employed the centre manifold theory to derive the same equation. The use of this theory provides a systemic way to examine dispersion in pipes of varying radius [16]. This will be particularly useful in future research directions since blood vessels have a compliant wall. More recent work by Azer generalized the result by Taylor to time dependent flow [4]. This generalization provides a framework to deal with more general velocity profiles.

1.2 Numerical Methods

The blood flow model used in this work can be viewed as a hyperbolic system of conservation laws [21]. The numerical methods devised for such systems are vast. In Section 1.2.1, I discuss these methods with particular emphasis on their application to the blood flow model. In Section 1.2.2, I survey the numerical methods for convection diffusion equations, which describe oxygen transport.

1.2.1 Numerical Methods for Conservation Laws

A large class of finite difference methods exists for systems of conservation laws. However, such methods have several limitations. Monotone methods preserve important properties of the solution, such as the total variation diminishing property, and they converge to the entropy solution; but, these methods can at most be first order accurate [22]. The other difficulty lies in the highly oscillatory behavior of higher order methods around discontinuities [22]. To resolve these difficulties, a class of methods called “high resolution methods” was devised. These methods are obtained by applying modifications, such as flux and slope limiter methods, to the higher order methods [22].
These high resolution methods are used for numerically solving the reduced blood flow model. For example, a high order finite difference method, the two step Lax-Wendroff method, is used in [9] to numerically solve the reduced blood flow model. The authors perform numerical studies for shock formulation using this method. While these methods are relatively easy to code and capture shocks in the solution, they are not easily extended to complex geometries and boundary conditions. Thus, properties from finite element methods must be sought to resolve these difficulties.

A generalization of the Lax-Wendroff method to incorporate finite element schemes is called the Taylor-Galerkin method. Formaggia et al. have applied this method to the blood flow model [14]. This idea of using finite element method is further extended by Cockburn and Shu. They propose a method which combines properties of the high resolution methods and the discontinuous Galerkin methods [12]. The authors apply it to a system of conservation laws [12]. They use a discontinuous Galerkin discretization in space and a total variational diminishing Runge Kutta discretization in time (RKDG). This method combines the use of numerical fluxes, used in high resolution schemes, with finite element discretizations. Thus, the authors obtain a method that has the elegant properties of both schemes. Most importantly, it is both a high order and a stable method [11].

This RKDG method has been applied to the reduced blood flow model by Puelz et al. [21]. The authors compare the upwind and Lax-Friedrichs numerical fluxes as incorporated in the RKDG scheme. They conclude that the convergence rates for the two different fluxes are the same when using the method of manufactured solutions.

A numerical scheme that is different from the RKDG method and the finite difference schemes is the numerical method of characteristics. Acosta et al. propose its use for the reduced blood flow model. The authors derive and prove a priori estimates to guarantee stability and an asymptotic linear rate of convergence [1]. Further, they utilize the theory of
Riemann invariants, projections onto a piece-wise linear space and quadrature rules to build up the algorithm [1]. This method provides a less computationally expensive alternative with less restrictions on the time step to the RKDG scheme at the price of lower accuracy [1].

1.2.2 Numerical Schemes for the Oxygen Transport Equation

The oxygen transport equation is a convection diffusion equation. The literature on the numerical schemes for this set of equations is vast. In this section, I pay particular emphasis on the discontinuous Galerkin methods.

The Runge Kutta discontinuous Galerkin (RKDG) method for conservation laws was extended for convection-diffusion equations by Cockburn and Shu [12]. The main idea is to write this second order equation as a system of first order equations. Then, the RKDG method is applied to this system. This family of methods, named the local discontinuous Galerkin method (LDG), is proven to be $L^2$ stable for scalar equations. The authors also show that the method for the linear case is $k$-th order accurate when polynomials of degree $k$ is used [11]. However, this numerical scheme introduces auxiliary variables, which increase the computational cost of the numerical method [10].

To avoid the introduction of auxiliary variables, Cheng and Shu propose a method which relies on repeated integration by parts and a careful selection of the numerical fluxes at the interfaces [10]. While this class of methods does not introduce auxiliary variables, repeated integration by parts deals with integrals of the flux [10]. Hence, the authors propose a method which is derived from performing integration by parts only once. However, the authors do not justify the choice of left traces when treating the diffusion.

Another class of methods which uses both left and right traces is called the interior penalty discontinuous Galerkin. This method, discussed and studied in [24], is used to treat the
diffusion term. It uses penalty and jump terms to spatially discretize the problem and attain stability.

The aforementioned numerical methods for problems with elliptic terms were surveyed and studied by Arnold et al. [3]. The authors clarify links between the interior penalty methods and the careful choice of numerical fluxes. In this thesis, I combine the interior penalty method to treat diffusion with the Lax Friedrichs flux to discretize the nonlinear convection term.

1.2.3 Outline

The outline of this thesis is as follows. Chapter 2 introduces the blood flow model and the numerical method used to solve it. The three dimensional equation modeling oxygen transport is reduced to one dimension in Section 3.1, which is an important contribution of this thesis. After obtaining the one dimensional equation, a numerical method is developed and studied for a general nonlinear convection diffusion equation in Chapter 4. Further, Section 4.2 proves a stability result for this numerical scheme. In Chapter 5, we present the fully discretized numerical scheme for the transport equation with Dirichlet boundary conditions in Section 5.1 and for Dirichlet and Neumann conditions in Section 5.2. We perform numerical experiments on one vessel using the method of manufactured solutions in Section 5.3. Subsequently, Section 5.4 extends this numerical method to a network of vessels with junction nodes where the model is tested for a three vessel bifurcation. Finally, we present a conclusion and future research directions in Chapter 6.
Chapter 2

Reduced Blood Flow Model

The one dimensional oxygen transport equation will be coupled to the reduced blood flow model. For sake of completeness, a short discussion of this blood flow model is presented. In the first section, I briefly introduce this model and write it as a system of conservation laws. Subsequently, the second section presents the Runge Kutta discontinuous Galerkin method for such systems. The material presented in this chapter is from [21, 9].

2.1 Mathematical Model

The \((A,Q)\) system is obtained from the asymptotic reduction of the axisymmetric incompressible Navier Stokes equations. The resulting model is one dimensional describing the averaged quantities. For the derivation of this model, see [9]. The \((A,Q)\) model is the following:

\[
\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0 \tag{2.1.1}
\]
\[
\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \alpha \frac{Q^2}{A} \right) + \frac{A}{\rho} \frac{\partial p}{\partial x} = 2\pi \nu R \left[ \frac{\partial V_x}{\partial r} \right]_{r=R} \tag{2.1.2}
\]

where \(R\) is the inner vessel radius, \(A\) is the scaled cross sectional area, \(Q\) is the momentum:

\[
Q = AU \tag{2.1.3}
\]
and \( U \) is the radial average of the velocity in the axial direction \( V_x \):

\[
U = \frac{2}{R^2} \int_0^R V_x r \, dr
\]  

(2.1.4)

The parameters, \( \rho \) and \( \nu \), are the density and the kinematic viscosity respectively. The state equation for the pressure \( p \) that closes the system is:

\[
p = p_0 + \psi(A; A_0, \kappa)
\]  

(2.1.5)

where

\[
\psi(A, A_0, \kappa) = \kappa (A^{1/2} - A_0^{1/2})
\]  

(2.1.6)

where \( A_0 \) is the area of the vessel at reference pressure \( p_0 \) and \( \kappa \) is positive constant.

The parameter \( \alpha \) is the Coriolis coefficient given by [9]:

\[
\alpha = \frac{1}{U^2} \frac{2}{R^2} \int_0^R r V_x^2 \, dr
\]  

(2.1.7)

The Coriolis coefficient is a correction parameter resulting from the averaging of the Navier-Stokes equations. Note that its value reduces to \( \alpha = 1 \) when a steady state velocity profile is considered \( V_x = U \).

A relation between \( V_x \) and \( r \) must also be determined. One particular choice for the velocity profile \( V_x \) is the no-slip velocity profile [20, 9]:

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

(2.1.8)

where \( \gamma \) is a parameter. Using the definition (2.1.7), a relation between \( \gamma \) and \( \alpha \) can be
determined:

\[
\gamma = \frac{2 - \alpha}{\alpha - 1} \tag{2.1.9}
\]

This velocity profile and the following definition allows the system to be written in a conservative form [21].

\[
\Psi = \int_{A_0}^{A} \psi(\zeta; A_0, \kappa) d\zeta \tag{2.1.10}
\]

Then, we have

\[
\frac{\partial}{\partial x}(A\psi - \Psi) = \frac{\partial A}{\partial x}\psi + A \frac{\partial \psi}{\partial x} - \frac{\partial}{\partial x}\Psi \\
= \frac{\partial A}{\partial x}\psi + A \frac{\partial \psi}{\partial x} - \psi(A; A_0, \kappa) \frac{\partial A}{\partial x} \\
= A \frac{\partial \psi}{\partial x} = A \frac{\partial \rho}{\partial x}
\]

This allows us to write \((2.1.2)\) in conservative form as such:

\[
\frac{\partial}{\partial t} \begin{bmatrix} A \\ Q \end{bmatrix} + \frac{\partial}{\partial x} \begin{bmatrix} \alpha Q^2 + \frac{1}{\rho} (A\psi - \Psi) \\ -2\pi \nu \frac{\alpha}{\alpha - 1} \frac{Q}{A} \end{bmatrix} = \begin{bmatrix} 0 \\ -2\pi \nu \frac{\alpha}{\alpha - 1} \frac{Q}{A} \end{bmatrix} \tag{2.1.11}
\]

For the particular choice of \(\psi\) in \((2.1.6)\), we have

\[
\frac{1}{\rho}(A\psi - \Psi) = \frac{\kappa}{\rho} \left( A(A^{1/2} - A_0^{1/2}) - \int_{A_0}^{A} (\zeta^{1/2} - A_0^{1/2}) d\zeta \right) \\
= \frac{\kappa}{3\rho} \left( A^{3/2} - A_0^{3/2} \right)
\]

Therefore the system can be written in the following way:

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial}{\partial x} \mathbf{F}(\mathbf{U}) = \mathbf{S}(\mathbf{U}) \tag{2.1.12}
\]
where

\[
U = \begin{bmatrix} A \\ Q \end{bmatrix}
\] (2.1.13)

\[
F(U) = \begin{bmatrix} Q \\ \alpha \frac{Q^2}{A} + \frac{\kappa}{3\rho} (A^{3/2} - A_0^{3/2}) \end{bmatrix}
\] (2.1.14)

\[
S(U) = \begin{bmatrix} 0 \\ -2\pi \nu \frac{\alpha}{\alpha - 1} \frac{Q}{A} \end{bmatrix}
\] (2.1.15)

This system, in addition to the oxygen transport equation derived, will be numerically solved in Chapter 4.

### 2.2 Runge Kutta Discontinuous Galerkin Method

The reduced model of blood flow was written in conservative form (2.1.12) in the previous section. This section considers the numerical solution of a general system in conservative form:

\[
\frac{\partial U}{\partial t} + \frac{\partial}{\partial x} F(U) = S(U), \quad \text{in } [0, L] \times (0, T]
\] (2.2.1)

\[
U(\cdot, 0) = U_0(\cdot) \quad \text{in } [0, L]
\] (2.2.2)

Consider a uniform partition of the interval [0, L] given by:

\[
\bigcup_{\epsilon=0}^{N} I_\epsilon = [0, L], \quad I_\epsilon = [x_\epsilon, x_{\epsilon+1}], \quad \text{and} \quad h = x_{\epsilon+1} - x_\epsilon
\] (2.2.3)

We use a discontinuous Galerkin finite element method. The space of the trial function \( U_h^k \)
is the same as the space of the test functions $V_h^k$ given by:

$$U_h^k = \{ \phi : [0, L] \to \mathbb{R} \text{ st. } \phi |_{I_e} \in P^k(I_e), \ \forall e = 0, ..., N \}$$  \hspace{1cm} (2.2.4)

Functions in $V_h$ are allowed to have discontinuities at the interfaces $x_e$. We now derive the scheme. First we multiply (2.2.1) by a vector test function $\Phi_h \in V_h^k \times V_h^k$ and we integrate over one interval $I_e$:

$$\int_{I_e} \frac{\partial U}{\partial t} \cdot \Phi_h + \int_{I_e} \frac{\partial}{\partial x} F(U) \cdot \Phi_h = \int_{I_e} S(U) \cdot \Phi_h, \quad \forall \Phi_h \in V_h^k \times V_h^k$$  \hspace{1cm} (2.2.5)

Integrating by parts, we obtain

$$\int_{I_e} \frac{\partial U}{\partial t} \cdot \Phi_h = \int_{I_e} S(U) \cdot \Phi_h + \int_{I_e} F(U) \cdot \frac{\partial \Phi_h}{\partial x} - (F(U) \cdot \Phi_h) |_{\partial I_e}, \quad \forall \Phi_h \in V_h^k \times V_h^k$$  \hspace{1cm} (2.2.6)

Note the ambiguity in the term $(F(U) \cdot \Phi_h) |_{\partial I_e}$. If the function $U$ is allowed to be discontinuous on the interfaces, $x_e$ and $x_{e+1}$, then $F(U(x_e))$ and $F(U(x_{e+1}))$ are not well defined. Hence, a definition for the traces of a function, $\phi_h \in V_h^k$, at these interfaces is needed.

$$\phi^\pm(x_e) = \lim_{\epsilon \to 0, \epsilon > 0} \phi(x_e \pm \epsilon), \quad e = 1, ..., N$$  \hspace{1cm} (2.2.7)

$$\phi^+(x_0) = \lim_{\epsilon \to 0, \epsilon > 0} \phi(x_0 + \epsilon)$$  \hspace{1cm} (2.2.8)

$$\phi^-(x_{N+1}) = \lim_{\epsilon \to 0, \epsilon < 0} \phi(x_{N+1} - \epsilon)$$  \hspace{1cm} (2.2.9)

We will use a numerical flux $F^{nf}(\cdot, \cdot)$. The requirements, as given in [11], are:
- **Consistency:**

\[
F^{nf}(U, U) = F(U) \tag{2.2.10}
\]

This requirement guarantees that in the case of constant flow, the numerical flux is the same as the true flux.

- **Lipschitz continuity:** \(F^{nf}(\cdot, \cdot)\) is Lipschitz continuous at \((U, U)\) if there exists \(K \geq 0\) and \(\epsilon > 0\) such that for all \(V, W\) in a ball centered around \(U\) with radius \(\epsilon\),

\[
\|F^{nf}(V, W) - F(U)\| \leq K \max(\|V - U\|, \|W - U\|) \tag{2.2.11}
\]

This requirement establishes consistency since as the two arguments converge to a constant value \(U\), the numerical flux converges to the true flux smoothly.

- **Monotonicity:** \(F^{nf}(\cdot, \cdot)\) is non-decreasing in the first argument and non-increasing in the second. The motivation for this is to make the scheme a monotone finite volume scheme when the approximate solution \(U_h\) is piece-wise constant [13].

The most commonly used flux is the Lax-Friedrichs flux. To define it, we need definitions for the jumps and averages.

The averages of the flux function are:

\[
\{F(U_h)\} \big|_{x_e} := \frac{1}{2}(F(U_h^+(x_e)) + F(U_h^-(x_e))), \quad \forall \ e = 1, \ldots, N \tag{2.2.12}
\]

\[
\{F(U_h)\} \big|_{x_0} := \frac{1}{2}(F(U_h^+(x_0)) + F(U_{inlet})) \tag{2.2.13}
\]

\[
\{F(U_h)\} \big|_{x_{N+1}} := \frac{1}{2}(F(U_{outlet}) + F(U_h^-(x_{N+1}))) \tag{2.2.14}
\]

where \(U_{inlet}\) and \(U_{outlet}\) are the boundary data at the inlet \(x = 0\) and at the outlet \(x = L\) respectively.
The jump of $U_h$ at the nodes $x_e$ is defined by:

$$[U_h]_{x_e} := U_h^+(x_e) - U_h^-(x_e) \quad e = 1, ..., N \quad (2.2.15)$$

$$[U_h]_{x_0} := U_h^+(x_0) - U_{\text{inlet}} \quad (2.2.16)$$

$$[U_h]_{x_{N+1}} := U_{\text{outlet}} - U_h^-(x_{N+1}) \quad (2.2.17)$$

The local Lax Friedrichs flux is now given by [21]:

$$F^{nf}(U_h)_{x_e} = \{F(U_h)\}_{x_e} - \frac{1}{2} \max(|\lambda_1^\pm|, |\lambda_2^\pm|)[U_h]_{x_e} \quad (2.2.18)$$

where $\lambda_1^+, \lambda_2^+ \text{ and } \lambda_1^-, \lambda_2^-$ are the eigenvalues of the Jacobian of $F$ evaluated at $U_h^+$ and $U_h^-$ respectively.

Thus, the semi-discrete DG formulation is given by:

$$\int_{L_e} \frac{\partial U_h}{\partial t} \cdot \Phi_h = \int_{L_e} S(U_h) \cdot \Phi_h + \int_{L_e} F(U_h) \cdot \frac{\partial \Phi_h}{\partial x} - F^{nf}(U_h)_{|x_{e+1}} \cdot \Phi_h^-(x_{e+1}) + F^{nf}(U_h)_{|x_{e}} \cdot \Phi_h^+(x_{e})$$

(2.2.19)

for all $e = 0, ..., N$

Defining $L_e(\cdot, \cdot)$ as

$$L_e(U_h, \Phi_h) := \int_{L_e} S(U_h) \cdot \Phi_h + \int_{L_e} F(U_h) \cdot \frac{\partial \Phi_h}{\partial x} - F^{nf}(U_h)_{|x_{e+1}} \cdot \Phi_h^-(x_{e+1}) + F^{nf}(U_h)_{|x_{e}} \cdot \Phi_h^+(x_{e})$$

(2.2.20)

we obtain the semi-discrete formulation as in [21]:

$$\int_{L_e} \frac{\partial U_h}{\partial t} \cdot \Phi_h = L_e(U_h, \Phi_h) \quad \forall \Phi_h \in V_h^k \times V_h^k, \quad \forall e = 0, ..., N \quad (2.2.21)$$

$$U_h(0) = P_h U_0 \quad (2.2.22)$$
where $P_h$ is the $L_2$ projection operator on the space $V_h^k \times V_h^k$.

In this thesis, we use a two stage Runge Kutta method. Thus, the fully discrete system is the following [20, 13].

Given $U^n_h$, compute $V^n_h$ and $U^{n+1}_h$ in $V_h^k \times V_h^k$ such that

\begin{align}
\int_{I_e} V^n_h \cdot \Phi_h &= \int_{I_e} U^n_h \cdot \Phi_h + \Delta t L_e(U^n_h, \Phi_h) \\
\int_{I_e} U^{n+1}_h \cdot \Phi_h &= \frac{1}{2} \int_{I_e} V^n_h \cdot \Phi_h + \frac{1}{2} \int_{I_e} U^n_h \cdot \Phi_h + \frac{\Delta t}{2} L_e(V^n_h, \Phi_h)
\end{align}

(2.2.23) (2.2.24)

for all $\Phi_h \in V_h^k \times V_h^k$ and $e = 0, ..., N$.

The resulting scheme is the Runge Kutta discontinuous Galerkin method applied to systems of conservation laws. It was developed in [11]. For more details on implementation of this method and the specification of inlet and outlet data for the blood flow model, see [21].
Chapter 3

Oxygen Transport Equation

This chapter contains one important contribution of this work, the reduced oxygen transport model and its coupling to the reduced blood flow model.

Oxygen is transported as free oxygen dissolved in plasma and as oxygen bound to hemoglobin. For sake of the model reduction analysis, which is the main focus of this chapter, we consider the following general equation,

\[
\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = D \Delta c
\]

(3.0.1)

where \( \mathbf{u} \) is the velocity field of blood. One can think of \( c \) as either the concentration of free oxygen or the concentration of oxygen bound to hemoglobin with \( D \) being the respective diffusion coefficient. Alternatively, a convection diffusion equation can be derived by adding the equations of the two separate forms and assuming certain relations between them [17, 6].

The model reduction analysis for (3.0.1) is carried in Section 3.1. The chapter ends with the calculations for the commonly used no-slip velocity profile in Section 3.2.

3.1 Model Reduction

This section performs the model reduction on equation (3.0.1). Numerically solving (3.0.1) requires the computation of the velocity field of blood which is described by the Navier Stokes equations. This is a computationally challenging task especially when a simulation of blood flow and oxygen transport in the vessel network of the human body is sought. The importance of the reduced blood flow model lies in its inexpensive implementation and its
validation against physiological data. This section’s goal is to utilize this model with a one
dimensional oxygen transport equation. To understand how the transport of oxygen can be
coupled to the reduced blood flow model (2.1.2), we perform an asymptotic reduction on the
convection diffusion equation (3.0.1). In the first part of the derivation, we employ the same
assumptions needed to arrive at the reduced blood flow model from the incompressible Navier
Stokes equations [9]. These assumptions will be clarified throughout the derivation.

Consider the cylindrical coordinates \((x, r, \theta)\) and the velocity components \((V_x, V_r, V_\theta)\) where
\(V_\theta\) is assumed to be zero. Equation (3.0.1) in cylindrical coordinates reads

\[
\frac{\partial c}{\partial t} + V_x \frac{\partial c}{\partial x} + V_r \frac{\partial c}{\partial r} = D \left( \frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} + \frac{\partial^2 c}{\partial x^2} \right)
\] (3.1.1)

where \(D\) is a constant diffusion coefficient.

The first step is to write the equation in non-dimensional form and apply scaling arguments.
Thus, we define the non-dimensional variables [9]:

\[
r = R_0 \tilde{r}, \quad x = \lambda \tilde{x}, \quad t = \frac{\lambda}{V_0} \tilde{t}, \quad c = c_0 \tilde{c}, \quad V_x = V_0 \tilde{V}_x, \quad V_r = U_0 \tilde{V}_r
\] (3.1.2)

where the following holds

\[
\frac{U_0}{V_0} = \frac{R_0}{\lambda} = \epsilon_0
\] (3.1.3)

Since the vessel’s length is assumed to be much larger than its radius, we have \(\epsilon_0 \ll 1\).
This is the same assumption needed in the derivation of the reduced blood flow from the
incompressible Navier Stokes equations in [9].

Substituting (3.1.2) in (3.1.1), the non-dimensional transport equation for the concentration
\[ V_0 \frac{\partial (c_0 \tilde{c})}{\partial t} + \frac{V_0 \partial (c_0 \tilde{c})}{\partial x} + \tilde{V} \frac{U_0}{R_0} \frac{\partial (c_0 \tilde{c})}{\partial r} = D \left( \frac{1}{R_0^2} \frac{\partial^2 (c_0 \tilde{c})}{\partial r^2} + \frac{1}{R_0^2} \frac{1}{\tilde{r}} \frac{\partial (c_0 \tilde{c})}{\partial \tilde{r}} + \frac{1}{\lambda^2} \frac{\partial^2 (c_0 \tilde{c})}{\partial \tilde{x}^2} \right) \]  

(3.1.4)

Multiplying (3.1.4) by $\lambda/V_0$, we obtain:

\[ \frac{\partial (c_0 \tilde{c})}{\partial t} + \tilde{V}_x \frac{\partial (c_0 \tilde{c})}{\partial x} + \tilde{V}_r \frac{U_0 \lambda}{V_0 R_0} \frac{\partial (c_0 \tilde{c})}{\partial r} = D \left( \frac{\lambda}{V_0 R_0^2} \frac{\partial^2 (c_0 \tilde{c})}{\partial r^2} + \frac{\lambda}{V_0 R_0^2} \frac{1}{\tilde{r}} \frac{\partial (c_0 \tilde{c})}{\partial \tilde{r}} + \frac{1}{\lambda V_0} \frac{\partial^2 (c_0 \tilde{c})}{\partial \tilde{x}^2} \right) \]

(3.1.5)

We note from (3.1.3) that $U_0 \lambda = V_0 R_0$. Then (3.1.5) reads,

\[ \frac{\partial (c_0 \tilde{c})}{\partial t} + \tilde{V}_x \frac{\partial (c_0 \tilde{c})}{\partial x} + \tilde{V}_r \frac{\partial (c_0 \tilde{c})}{\partial r} = D \frac{\lambda}{V_0 R_0^2} \left( \frac{\partial^2 (c_0 \tilde{c})}{\partial r^2} + \frac{1}{\tilde{r}} \frac{\partial (c_0 \tilde{c})}{\partial \tilde{r}} + \frac{R_0^2}{\lambda^2} \frac{\partial^2 (c_0 \tilde{c})}{\partial \tilde{x}^2} \right) \]

(3.1.6)

We note that the term

\[ \frac{R_0^2}{\lambda^2} = \epsilon_0^2, \quad \epsilon_0 \ll 1 \]

(3.1.7)

Neglecting $O(\epsilon_0^2)$ terms, equation (3.1.6) in non-dimensional form becomes:

\[ \frac{\partial (c_0 \tilde{c})}{\partial t} + \frac{\partial (c_0 \tilde{c})}{\partial x} + \tilde{V}_r \frac{\partial (c_0 \tilde{c})}{\partial r} = D \frac{\lambda}{V_0 R_0^2} \left( \frac{\partial^2 (c_0 \tilde{c})}{\partial r^2} + \frac{1}{\tilde{r}} \frac{\partial (c_0 \tilde{c})}{\partial \tilde{r}} \right) \]

(3.1.8)

Multiplying equation (3.1.8) by $\tilde{r}$, we obtain:

\[ \tilde{r} \frac{\partial \tilde{c}}{\partial t} + \tilde{r} \tilde{V}_x \frac{\partial \tilde{c}}{\partial x} + \tilde{r} \tilde{V}_r \frac{\partial \tilde{c}}{\partial r} = \tilde{r} D_1 \left( \frac{\partial^2 \tilde{c}}{\partial \tilde{r}^2} + \frac{1}{\tilde{r}} \frac{\partial \tilde{c}}{\partial \tilde{r}} \right) \]

(3.1.9)

where

\[ D_1 = D \frac{\lambda}{V_0 R_0^2} = \frac{D}{U_0 R_0} \]

(3.1.10)

which is the inverse of the Peclet number [23].
Blood is an incompressible fluid and the incompressibility condition in spherical coordinates reads [9]:

\[
\frac{1}{r} \frac{\partial (rV_r)}{\partial r} + \frac{\partial V_x}{\partial x} = 0 \tag{3.1.11}
\]

We multiply equation (3.1.11) by \(r\),

\[
\frac{\partial (rV_r)}{\partial r} + r \frac{\partial V_x}{\partial x} = 0 \tag{3.1.12}
\]

Writing (3.1.12) in non-dimensional form, we obtain

\[
\frac{1}{R_0} \frac{\partial (U_0 R_0 \tilde{r} \tilde{V}_r)}{\partial \tilde{r}} + \frac{1}{\lambda} \frac{\partial (R_0 \tilde{r} \tilde{V}_x)}{\partial \tilde{x}} = 0 \tag{3.1.13}
\]

Multiplying (3.1.13) by \(1/U_0\) and noting from (3.1.3) that \(V_0 R_0 = U_0 \lambda\), the incompressibility condition in non-dimensional variables reads:

\[
\frac{\partial (\tilde{r} \tilde{V}_r)}{\partial \tilde{x}} + \frac{\partial (\tilde{r} \tilde{V}_x)}{\partial \tilde{r}} = 0 \tag{3.1.14}
\]

We use the product rule on the following terms

\[
\frac{\partial (\tilde{r} \tilde{c} \tilde{V}_x)}{\partial \tilde{x}} = \tilde{r} \tilde{V}_x \frac{\partial \tilde{c}}{\partial \tilde{x}} + \tilde{c} \frac{\partial (\tilde{r} \tilde{V}_x)}{\partial \tilde{x}} \tag{3.1.15}
\]
\[
\frac{\partial (\tilde{r} \tilde{c} \tilde{V}_r)}{\partial \tilde{r}} = \tilde{r} \tilde{V}_r \frac{\partial \tilde{c}}{\partial \tilde{r}} + \tilde{c} \frac{\partial (\tilde{r} \tilde{V}_r)}{\partial \tilde{r}} \tag{3.1.16}
\]

We add equations (3.1.15) and (3.1.16). Then, we use the incompressibility condition in non-dimensional form (3.1.14) to obtain

\[
\frac{\partial (\tilde{r} \tilde{c} \tilde{V}_x)}{\partial \tilde{x}} + \frac{\partial (\tilde{r} \tilde{c} \tilde{V}_r)}{\partial \tilde{r}} = \tilde{r} \tilde{V}_x \frac{\partial \tilde{c}}{\partial \tilde{x}} + \tilde{r} \tilde{V}_r \frac{\partial \tilde{c}}{\partial \tilde{r}} \tag{3.1.17}
\]
Thus, we can write (3.1.9) in conservative form as such

$$\tilde{r} \frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial (\tilde{r}\tilde{c} \tilde{V}_x)}{\partial \tilde{x}} + \frac{\partial (\tilde{r}\tilde{c} \tilde{V}_r)}{\partial \tilde{r}} = D_1 \left( \tilde{r} \frac{\partial^2 \tilde{c}}{\partial \tilde{r}^2} + \frac{\partial \tilde{c}}{\partial \tilde{r}} \right)$$

(3.1.18)

Note that

$$\frac{\partial}{\partial \tilde{r}} \left( \tilde{r} \frac{\partial \tilde{c}}{\partial \tilde{r}} \right) = \tilde{r} \frac{\partial^2 \tilde{c}}{\partial \tilde{r}^2} + \frac{\partial \tilde{c}}{\partial \tilde{r}}$$

(3.1.19)

We substitute (3.1.19) in (3.1.18), to obtain

$$\tilde{r} \frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{\partial (\tilde{r}\tilde{c} \tilde{V}_x)}{\partial \tilde{x}} + \frac{\partial (\tilde{r}\tilde{c} \tilde{V}_r)}{\partial \tilde{r}} = D_1 \frac{\partial}{\partial \tilde{r}} \left( \tilde{r} \frac{\partial \tilde{c}}{\partial \tilde{r}} \right)$$

(3.1.20)

We assume that the vessel has a thin wall and define $R$ to be the inner vessel radius, which depends on $\tilde{x}$ and $\tilde{t}$. We define $\tilde{R}$ to be the non-dimensional inner vessel radius.

$$R = R_0 \tilde{R}$$

(3.1.21)

We integrate (3.1.20) with respect to $\tilde{r}$ from $\tilde{r} = 0$ to $\tilde{r} = \tilde{R}$ and we use Leibniz rule.

$$\frac{\partial}{\partial \tilde{t}} \int_0^{\tilde{R}} \tilde{r} \tilde{c} d\tilde{r} - \tilde{R} [\tilde{c}]_{\tilde{R}} \frac{\partial \tilde{R}}{\partial \tilde{t}} + \frac{\partial}{\partial \tilde{x}} \int_0^{\tilde{R}} \tilde{r} \tilde{c} \tilde{V}_x d\tilde{r} - \tilde{R} [\tilde{c} \tilde{V}_x]_{\tilde{R}} \frac{\partial \tilde{R}}{\partial \tilde{x}} + \tilde{R} [\tilde{c} \tilde{V}_r]_{\tilde{R}} = D_1 \frac{\partial}{\partial \tilde{r}} \left[ \tilde{r} \frac{\partial \tilde{c}}{\partial \tilde{r}} \right]_{\tilde{r} = \tilde{R}}$$

(3.1.22)

We consider the streamline boundary condition specified in [9]:

$$\frac{\partial \tilde{R}}{\partial \tilde{t}} + [\tilde{V}_x]_{\tilde{R}} \frac{\partial \tilde{R}}{\partial \tilde{x}} = [\tilde{V}_r]_{\tilde{R}}$$

(3.1.23)

We assume that the wall of the vessel is impermeable [26].

$$\frac{\partial c}{\partial r} \bigg|_{r=R} = c_0 \frac{\partial \tilde{c}}{\partial \tilde{r}} \bigg|_{\tilde{r}=\tilde{R}} = 0$$

(3.1.24)
We substitute (3.1.24) and (3.1.23) in (3.1.22). Then, equation (3.1.22) reads

\[
\frac{\partial}{\partial \tilde{t}} \int_{0}^{\tilde{R}} \tilde{r} \tilde{c} d\tilde{r} + \frac{\partial}{\partial \tilde{x}} \int_{0}^{\tilde{R}} \tilde{r} \tilde{c} \tilde{V}_{x} d\tilde{r} = 0 \tag{3.1.25}
\]

We write (3.1.25) in dimensional variables

\[
\lambda \frac{V_{0}}{\lambda} \frac{\partial}{\partial t} \int_{0}^{R} R_{0}^{2} c_{0} r c d r + \lambda \frac{V_{0}}{\lambda} \frac{\partial}{\partial x} \int_{0}^{R} R_{0}^{2} c_{0} r c V_{x} d r = 0 \tag{3.1.26}
\]

This leads to the following equation in dimensional form:

\[
\frac{\partial}{\partial t} \int_{0}^{R} r c d r + \frac{\partial}{\partial x} \int_{0}^{R} r c V_{x} d r = 0 \tag{3.1.27}
\]

The terms in (3.1.27) are radial averages. To declutter notation, we define

\[
\langle f \rangle = 2 \frac{R^{2}}{R^{2}} \int_{0}^{R} r f d r \tag{3.1.28}
\]

We write (3.1.27) in terms of (3.1.28)

\[
\frac{\partial}{\partial t} \left( \frac{R^{2}}{2} \langle c \rangle \right) + \frac{\partial}{\partial x} \left( \frac{R^{2}}{2} \langle c V_{x} \rangle \right) = 0 \tag{3.1.29}
\]

The second term in (3.1.29) is the average of the product. Next, we write this term as the product of the averages and a diffusive term. We consider the following definitions, known as Gray’s decomposition [15].

\[
\hat{C} = c - \langle c \rangle \tag{3.1.30}
\]

\[
\hat{U} = V_{x} - \langle V_{x} \rangle \tag{3.1.31}
\]
These definitions are important because of the following identity

$$\langle \hat{C} \hat{U} \rangle = \langle (c - \langle c \rangle)(V_x - \langle V_x \rangle) \rangle$$

$$= \langle cV_x \rangle - \langle c \rangle \langle V_x \rangle - \langle V_x \rangle \langle c \rangle + \langle c \rangle \langle V_x \rangle$$

$$= \langle cV_x \rangle - \langle c \rangle \langle V_x \rangle \quad (3.1.32)$$

Substituting (3.1.32) in the second term of (3.1.29), we get

$$\frac{\partial}{\partial x} \left( \frac{R^2}{2} \langle cV_x \rangle \right) = \frac{\partial}{\partial x} \left( \frac{R^2}{2} \left( \langle V_x \rangle \langle c \rangle + \langle \hat{C} \hat{U} \rangle \right) \right) \quad (3.1.33)$$

Then, equation (3.1.29) reads:

$$\frac{\partial R^2 \langle c \rangle}{\partial t} + \frac{\partial (R^2 \langle V_x \rangle \langle c \rangle)}{\partial x} + \frac{\partial}{\partial x} \langle R^2 \hat{C} \hat{U} \rangle = 0 \quad (3.1.34)$$

**Remark 1.** If a flat velocity profile is considered, then $$\hat{U} = 0$$. Thus, equation (3.1.34) becomes a pure convection equation regardless of the concentration profile $$c(r)$$:

$$\frac{\partial R^2 \langle c \rangle}{\partial t} + \frac{\partial (R^2 \langle V_x \rangle \langle c \rangle)}{\partial x} = 0 \quad (3.1.35)$$

What remains to specify is a relation between $$\hat{C}$$ and $$\hat{U}$$, which must be determined to provide closure to the system. We note that $$\hat{U}$$ is specified by the choice of the axial velocity profile $$V_x$$, which is also needed to provide closure to the reduced blood flow model (2.1.2).

To study the radial variation of $$c$$, we assume that $$V_r \ll V_x$$. We have the following equation from (3.1.1):

$$\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} = \frac{1}{D} \frac{\partial c}{\partial t} + \frac{1}{D} V_x \frac{\partial c}{\partial x} \quad (3.1.36)$$
Based on the discussion from [26], it is assumed that the time necessary for the radial variation in \( c \) to become negligible is very short with respect to the time needed for a change in \( c \) to happen due to convection along the longitudinal axis.

Let \( \epsilon \) be such that \( 0 < \epsilon \ll 1 \). We assume the solute will move with mean velocity, \( \langle V_x \rangle \) over a short period of time \( \tau = \epsilon t \) [26, 4]. We introduce the following change of variable

\[
g(r, \tau, x) = c(r, \frac{\tau}{\epsilon}, x + \langle V_x \rangle \frac{\tau}{\epsilon})
\]

(3.1.37)

We have the following

\[
\frac{\partial g}{\partial x} = \frac{\partial c}{\partial x}
\]

(3.1.38)

\[
\frac{\partial g}{\partial r} = \frac{\partial c}{\partial r}
\]

(3.1.39)

\[
\frac{\partial g}{\partial \tau} = \frac{1}{\epsilon} \frac{\partial c}{\partial t} + \frac{\langle V_x \rangle}{\epsilon} \frac{\partial c}{\partial x}
\]

(3.1.40)

Substituting (3.1.40) in (3.1.36) yields

\[
\frac{\partial^2 g}{\partial r^2} + \frac{1}{r} \frac{\partial g}{\partial r} = \frac{1}{D} \left( \epsilon \frac{\partial g}{\partial \tau} + \langle V_x \rangle \frac{\partial g}{\partial x} \right)
\]

(3.1.41)

Since \( \epsilon \ll 1 \), we consider the \( \mathcal{O}(1) \) terms:

\[
\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} = \frac{\dot{U}(r)}{D} \frac{\partial c}{\partial x}
\]

(3.1.42)

Because the time period is very short \( \mathcal{O}(\epsilon) \), it is reasonable to assume that the flux of the concentration is the same as the flux of the mean concentration:

\[
\frac{\partial c}{\partial x} \approx \frac{\partial \langle c \rangle}{\partial x}
\]

(3.1.43)
Thus, (3.1.42) reads
\[
\frac{\partial^2 c}{\partial r^2} + \frac{1}{r} \frac{\partial c}{\partial r} = \frac{\hat{U}(r)}{D} \frac{\partial \langle c \rangle}{\partial x}
\] (3.1.44)

We also enforce the impermeability condition, which was essential in the derivation of (3.1.18)
\[
\left. \frac{\partial c}{\partial r} \right|_{r=R} = 0
\] (3.1.45)

To solve (3.1.44) with condition (3.1.45), we multiply (3.1.44) by \(r\):
\[
\frac{\partial}{\partial r} \left( r \frac{\partial c}{\partial r} \right) = \frac{\hat{U}(r)}{D} \frac{\partial \langle c \rangle}{\partial x}
\] (3.1.46)

We integrate and obtain
\[
\frac{\partial c}{\partial r} \bigg|_{r=R} = \frac{1}{D} \frac{\partial \langle c \rangle}{\partial x} \int_0^r \hat{U}(s) ds + \ell
\] (3.1.47)

where \(\ell\) is a constant. By the definition of \(\hat{U}\)
\[
\frac{\partial c}{\partial r} \bigg|_{r=R} = \frac{1}{RD} \frac{\partial \langle c \rangle}{\partial x} \int_0^R \hat{U}(r) r dr + \ell = \ell
\] (3.1.48)

To satisfy the impermeability condition (3.1.45), we obtain
\[
\ell = 0
\]

Integrating again, we obtain
\[
c = \frac{1}{D} \frac{\partial \langle c \rangle}{\partial x} \int_0^r \frac{1}{z} \int_0^z \hat{U}(s) s ds dz + \eta
\] (3.1.49)

where \(\eta\) is a constant. We write \(\eta = \langle c \rangle + \zeta\) where \(\zeta\) is to be determined such that consistency is ensured in the sense that:
\[
\frac{2}{R^2} \int_0^R cr dr = \langle c \rangle
\] (3.1.50)
Thus,

\[ c = \langle c \rangle + \frac{1}{D} \frac{\partial \langle c \rangle}{\partial x} \int_0^r \frac{1}{z} \int_0^z \hat{U}(s)sdsdz + \zeta \]  

(3.1.51)

We now have an expression for \( \hat{C} \).

\[ \hat{C} = c - \langle c \rangle = \frac{1}{D} \frac{\partial \langle c \rangle}{\partial x} \int_0^r \frac{1}{z} \int_0^z \hat{U}(s)sdsdz + \zeta \]  

(3.1.52)

Thus, we can evaluate \( \langle \hat{U}\hat{C} \rangle \):

\[ \langle \hat{U}\hat{C} \rangle = \frac{2}{R^2D^2} \frac{\partial \langle c \rangle}{\partial x} \int_0^R r\hat{U}(r) \left( \int_0^r \frac{1}{z} \int_0^z \hat{U}(s)sdsdz + \zeta \right) dr \]  

(3.1.53)

Substituting (3.1.53) in equation (3.1.34), we obtain:

\[ \frac{\partial}{\partial t}(R^2\langle c \rangle) + \frac{\partial}{\partial x}(R^2\langle V_x \rangle \langle c \rangle) + \frac{2}{D} \frac{\partial}{\partial x} \left( \frac{\partial \langle c \rangle}{\partial x} \int_0^R \hat{U}r \left( \int_0^r \frac{1}{z} \int_0^z \hat{U}(s)sdsdz + \zeta \right) dr \right) = 0 \]  

(3.1.54)

Note that by the definition of \( \hat{U} \),

\[ \int_0^R \hat{U}(r)r\zeta dr = 0 \]  

(3.1.55)

For readability, we switch to the following notation

\[ C = \langle c \rangle \]  

(3.1.56)

\[ U = \langle V_x \rangle \]  

(3.1.57)

Using this notation and equation (3.1.55), equation (3.1.54) reads

\[ \frac{\partial}{\partial t}(R^2C) + \frac{\partial}{\partial x}(R^2UC) + \frac{2}{D} \frac{\partial}{\partial x} \left( \frac{\partial C}{\partial x} \int_0^R \hat{U}r \left( \int_0^r \frac{1}{z} \int_0^z \hat{U}(s)sdsdz \right) dr \right) = 0 \]  

(3.1.58)
Using the definitions of the reduced blood flow model, \( A = R^2 \) and \( Q = UA \), we obtain the following equation:

\[
\frac{\partial}{\partial t}(AC) + \frac{\partial}{\partial x}(QC) + \frac{2}{D} \frac{\partial}{\partial x} \left( \frac{\partial C}{\partial x} \int_0^R \hat{U} r \left( \int_0^r \int_0^z \hat{U}(s) ds dz \right) dz \right) \bigg|_{x=0} = 0 \tag{3.1.59}
\]

We couple this equation to the blood flow model where we solve for \( Q \) and \( A \) at each time step. We use these computed quantities in the transport equation.

This equation is in agreement with the \( \mathcal{O}(\epsilon) \) terms derived in [4]. Note that this equation depends on \( \hat{U} \) which is determined by the choice of the velocity profile. A common choice in the blood flow model is the no-slip velocity profile. Thus, I perform the calculations for this particular choice in the next section.

### 3.2 Calculations for the No-Slip Velocity Profile

Consider a specific velocity profile, no slip velocity profile, as the one in [21]:

\[
V_x(r) = \frac{\gamma + 2}{\gamma} U \left( 1 - \left( \frac{r}{R} \right)^\gamma \right) \tag{3.2.1}
\]

We have the following specific expression for \( \hat{U} \),

\[
\hat{U}(r) = V_x(r) - U = \frac{2}{\gamma} U - \frac{\gamma + 2}{\gamma} U \left( \frac{r}{R} \right)^\gamma \tag{3.2.2}
\]

We substitute (3.2.2) in (3.1.51) and evaluate the expression. We obtain the following

\[
c = C + \zeta + K \left( \frac{R^\gamma}{2\gamma} r^2 - \frac{r^{\gamma+2}}{(\gamma+2)\gamma} \right) \tag{3.2.3}
\]
where

\[ K = \frac{U}{DR^\gamma} \frac{\partial C}{\partial x} \] (3.2.4)

and \( \zeta \) is such that the consistency constraint (3.1.50) is satisfied. We conclude that

\[ \zeta = KR^{\gamma+2}\omega(\gamma) \] (3.2.5)

where

\[ \omega(\gamma) = \frac{2}{\gamma(\gamma + 2)(\gamma + 4)} - \frac{1}{4\gamma} \] (3.2.6)

Thus the final form of the radial variation of \( c \) is:

\[ \hat{C} = c - C = K \left( \frac{R^\gamma}{2\gamma} r^2 - \frac{r^{\gamma+2}}{(\gamma + 2)\gamma} + R^{\gamma+2}\omega(\gamma) \right) \] (3.2.7)

We substitute (3.2.7) an (3.2.2) in (3.1.53) and (3.1.59) to obtain

\[ \frac{\partial (R^2C)}{\partial t} + \frac{\partial}{\partial x} (R^2UC) - \frac{\beta}{D} \frac{\partial}{\partial x} \left( (R^2U)^2 \frac{\partial C}{\partial x} \right) = 0 \] (3.2.8)

We define \( A = R^2 \) the momentum \( Q = AU \) as in [9]. The equation now reads,

\[ \frac{\partial (AC)}{\partial t} + \frac{\partial}{\partial x} (QC) - \frac{\beta}{D} \frac{\partial}{\partial x} \left( Q^2 \frac{\partial C}{\partial x} \right) = 0 \] (3.2.9)

where

\[ \beta = \frac{2(\gamma + 2)}{\gamma} \left( \frac{1}{2\gamma(\gamma + 4)} - \frac{1}{2\gamma(\gamma + 2)^2} + \frac{\omega(\gamma)}{\gamma + 2} \right) \] (3.2.10)

**Remark 2.** If \( \gamma = 2 \), we have that \( \beta = 1/48 \) which is the diffusive coefficient found by Taylor [27].
Note that the value of $\gamma$ determines the Coriolis coefficient $\alpha$ which given in (2.1.7):

$$\alpha = \frac{1}{U^2 R^2} \frac{2}{R} \int_0^R rV_x^2 dr \quad (3.2.11)$$

Substituting the no slip velocity profile $V_x$ in equation (3.2.1)

$$\alpha = \frac{2 + \gamma}{\gamma + 1} \quad (3.2.12)$$

or equivalently,

$$\gamma = \frac{2 - \alpha}{\alpha - 1} \quad (3.2.13)$$

Thus, $\beta$ can be represented as a function of the Coriolis coefficient $\alpha$ in the following way:

$$\beta = \frac{\alpha}{2 - \alpha} \left( \frac{(\alpha - 1)^2}{(3\alpha - 2)(2 - \alpha)} + \frac{(\alpha - 1)^3}{\alpha^2(2 - \alpha)} - \frac{2\alpha - 2}{\alpha} \omega \left( \frac{2 - \alpha}{\alpha - 1} \right) \right) \quad (3.2.14)$$

We note that $\alpha = 1$ corresponds to a flat velocity profile [21] and

$$\beta(\alpha = 1) = 0 \quad (3.2.15)$$

This is consistent with the Remark 1 in the sense that the resulting equation is a pure convection equation. Figure 3.1 shows the diffusion coefficient $\beta$ as a function of the Coriolis coefficient $\alpha$. 

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Equations (3.2.9) describe the radially averaged quantities of a solute’s concentration in blood with the no slip velocity profile. It is coupled to the equations governing the cross section area of the vessel and the radially averaged velocity $U = Q/A$.

The resulting coupled system of partial differential equations is:

$$\frac{\partial A}{\partial t} + \frac{\partial Q}{\partial x} = 0$$

(3.2.16)

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x} \left( \alpha \frac{Q^2}{A} \right) + \frac{A}{\rho} \frac{\partial p}{\partial x} = -2\pi\nu \frac{\alpha}{\alpha - 1} \frac{Q}{A}$$

(3.2.17)

$$\frac{\partial (AC)}{\partial t} + \frac{\partial}{\partial x} (QC) - \frac{\beta}{D} \frac{\partial}{\partial x} \left( Q^2 \frac{\partial C}{\partial x} \right) = 0$$

(3.2.18)

System (3.2.18) is the set of equations that I will numerically solve in Chapter 5.
Chapter 4

Stability Analysis of the Semi-Discrete Scheme

The previous chapter reduced the convection diffusion equation from three dimensions to one dimension. In this chapter, we formulate and study a numerical method for a general one dimensional nonlinear convection-diffusion equation. This method incorporates the Lax-Friedrichs numerical flux and the interior penalty discontinuous Galerkin terms. The main result of this chapter is the numerical stability of the scheme established in Theorem 2.

4.1 Model Problem and Semi-Discrete Formulation

We consider the one dimensional equation.

\[
\begin{align*}
\partial_t u + \partial_x (f(u)) - \partial_x (a(u) \partial_x u) &= s(t), \quad x \in [0, L], t \in (0, T] \\
u(x, 0) &= u_0(x), \quad x \in [0, L] \\
u(0,t) &= 0, \quad t \in (0, T] \\
u(L,t) &= 0, \quad t \in (0, T]
\end{align*}
\] (4.1.1)

where \(a(u)\) is bounded below by a positive constant and \(s : (0, T] \rightarrow L^2[0, L]\) is such that:

\[
\int_0^T ||s(t)||^2_{L^2[0,L]} < \infty
\]
We consider a uniform partition of the interval $[0, L]$ given by

$$
\bigcup_{e=0}^{N} I_e = [0, L], \quad I_e = [x_e, x_{e+1}], \quad \text{and} \quad h = x_{e+1} - x_e
$$

(4.1.5)

The space of test functions is the following

$$\mathbb{V}^k_h = \{ \phi : [0, L] \rightarrow \mathbb{R} \text{ st. } \phi |_{I_e} \in \mathbb{P}^k(I_e), \quad \forall e = 0, ..., N \}$$

(4.1.6)

To present the discontinuous Galerkin scheme, we need definitions for the left and right traces, the jump terms and the average terms.

The traces of a function $\phi \in \mathbb{V}^k_h$ at the interfaces of an element are given in the following way:

$$u_h(x_e^+) = \lim_{\epsilon \to 0, \epsilon > 0} u_h(x_e + \epsilon), \quad e = 0, ..., N$$

(4.1.7)

$$u_h(x_e^-) = \lim_{\epsilon \to 0, \epsilon > 0} u_h(x_e - \epsilon), \quad e = 1, ..., N + 1$$

(4.1.8)

We define the jump terms as

$$[u_h]|_{x_e} = u_h(x_e^+) - u_h(x_e^-), \quad e = 1, ..., N - 1$$

(4.1.9)

$$[u_h]|_{x_0} = u_h(x_0^+)$$

(4.1.10)

$$[u_h]|_{x_{N+1}} = -u_h(x_{N+1}^-)$$

(4.1.11)
The average terms are the following:

\[
\{ f(u_h) \}|_{x_e} = \frac{1}{2} \left( f(u_h(x_e^+)) + f(u_h(x_e^-)), \quad e = 1, ..., N - 1 \right) \quad (4.1.12)
\]

\[
\{ f(u_h) \}|_{x_0} = \frac{1}{2} \left( f(u_h(x_0^+)) + f(0) \right) \quad (4.1.13)
\]

\[
\{ f(u_h) \}|_{x_{N+1}} = \frac{1}{2} \left( f(0) + f(u_h(x_{N+1}^-)) \right) \quad (4.1.14)
\]

This method utilizes the interior penalty discontinuous Galerkin (IPDG) method in [24] and the Lax Friedrichs flux [13]. We will use the Lax-Friedrichs numerical flux for the convection term and the IPDG method for the diffusion term. We multiply (4.1.1) by a test function \( v \in V^k_h \) and integrate by parts.

The resulting scheme is the following: find \( u_h \in V^k_h \) such that:

\[
\int_{I_e} (\partial_t u_h)v_h dx - \int_{I_e} f(u_h)\partial_x v_h dx
\]

\[
+ \hat{f}(u_h^+, u_h^-)|_{x_{e+1}} v_h(x_{e+1}^-) - \hat{f}(u_h^+, u_h^-)|_{x_e} v_h(x_e^+) + H_e(u_h, v_h) = \int_{I_e} s(t)v_h dx
\]

(4.1.15)

for all \( v_h \in V^k_h \) and for all \( e \in \{0, ..., N\} \), where the numerical flux \( \hat{f} \) is the Lax Friedrichs flux. For readability, we use the following shorthand notation in the text:

\[
u_h^- = u_h(x_e^-) \quad (4.1.16)\]

\[
u_h^+ = u_h(x_e^+) \quad (4.1.17)\]

Then, the definition of the Lax Friedrichs flux is given by

\[
\hat{f}(u_h^+, u_h^-)|_{x_e} = \frac{1}{2} \{ f(u_h) \}|_{x_e} = \frac{1}{2} \max_{\min(u_h^-, u_h^+) \leq w \leq \max(u_h^-, u_h^+)} |f'(w)| [u_h]|_{x_e}, \quad \forall \ e = 0, ..., N
\]

(4.1.18)

The term \( H_e(u_h, v_h) \) is the sum of the fluxes attained from applying the interior penalty
discontinuous Galerkin method on one element. For interior elements, \( e \in \{1, \ldots, N-1\} \), we have

\[
\mathcal{H}_e(u_h, v_h) = \int_{I_e} a(u_h)(\partial_x u_h)(\partial_x v_h)dx \\
+ \{a(u_h)(\partial_x u_h)\}|_{v_1} v_h(x^+) - \{a(u_h)(\partial_x u_h)\}|_{x_{e+1}} v_h(x_{e+1}^-) \\
- \frac{\epsilon}{2} (a(u_h)(\partial_x u_h))|_{x_{e+1}} [u_h]\|_{x_e} + a(u_h)(\partial_x u_h))|_{x_{e+1}} [u_h]\|_{x_e} \\
+ \frac{\sigma}{h} (v_h(x^+_e)[u_h]\|_{x_e} - v_h(x^-_{e+1})[u_h]\|_{x_{e+1}}) \\
\]

(4.1.19)

For the first element, \( e = 0 \), we have

\[
\mathcal{H}_0(u_h, v_h) = \int_{I_0} a(u_h)(\partial_x u_h)(\partial_x v_h)dx \\
+ a(u_h)(\partial_x u_h)\|_{x_0} v_h(x^-_0) - \{a(u_h)(\partial_x u_h)\}|_{x_1} v_h(x^-_1) \\
- \frac{\epsilon}{2} (2a(u_h)(\partial_x v_h)\|_{x_0} [u_h]\|_{x_1} + a(u_h)(\partial_x v_h)\|_{x_1} [u_h]\|_{x_1}) \\
+ \frac{\sigma}{h} ([u_h]\|_{x_0} v_h(x^-_0) - [u_h]\|_{x_1} v_h(x^-_1)) \\
\]

(4.1.20)

For the last element, \( e = N \), we have:

\[
\mathcal{H}_N(u_h, v_h) = \int_{I_N} a(u_h)(\partial_x u_h)(\partial_x v_h)dx \\
+ \{a(u_h)(\partial_x u_h)\}|_{x_N} v_h(x^-_N) - \{a(u_h)(\partial_x u_h)\}|_{x_{N+1}} v_h(x^-_{N+1}) \\
- \frac{\epsilon}{2} (a(u_h)(\partial_x v_h)\|_{x_N} [u_h]\|_{x_{N+1}} + 2a(u_h)(\partial_x v_h)\|_{x_{N+1}} [u_h]\|_{x_{N+1}}) \\
+ \frac{\sigma}{h} ([u_h]\|_{x_N} v_h(x^-_N) - [u_h]\|_{x_{N+1}} v_h(x^-_{N+1})) \\
\]

(4.1.21)

where \( \sigma \) is a penalty parameter and \( \epsilon \in \{-1, 0, 1\} \). The terms involving \( \epsilon \) and \( \sigma \) are zero when \( \mathcal{H}(u, v_h) \) is evaluated at the exact solution \( u \), ensuring consistency of the method. The penalty term is important for the stability of the scheme.
4.2 Stability of the Semi-Discrete Scheme

Certain properties of the numerical flux are integral to the scheme’s stability. In particular, the Lax Friedrichs numerical flux is a monotone flux, non-decreasing in the first argument and non-increasing in the second argument. Because the following result is important in the stability analysis, I restate it and present its proof from [10] below:

**Theorem 1.** Let \( u_h \in V^k_h \) and define

\[
F(u_h(x^e_e)) = \int_0^{u_h(x^e_e)} f(u) du
\]

(4.2.1)

The following inequality holds

\[
[F(u_h)]|_{x_e} - \hat{f}(u^-_h, u^+_h)|_{x_e} [u_h]|_{x_e} \geq 0 \quad \forall e = 0, \ldots, N
\]

(4.2.2)

Note that \([F(u_h)]|_{x_e}\) is given by the following:

\[
[F(u_h)]|_{x_e} = F(u_h(x^+_{e})) - F(u_h(x^-_{e})) \quad e = 1, \ldots, N
\]

(4.2.3)

\[
[F(u_h)]|_{x_0} = F(u_h(x^+_{0})) - F(0)
\]

(4.2.4)

\[
[F(u_h)]|_{x_{N+1}} = F(0) - F(u_h(x^-_{N+1}))
\]

(4.2.5)

and \(\hat{f}(\cdot, \cdot)\) is the Lax Friedrichs flux given in (4.1.18).

**Proof.** Let \( e \in \{0, \ldots, N\} \). By the mean value theorem, there exists \( \xi \) between \( u_h(x^+_{e}) \) and \( u_h(x^-_{e}) \) such that

\[
[F(u_h)]|_{x_e} = F(u_h(x^+_{e})) - F(u_h(x^-_{e})) = f(\xi)[u_h]|_{x_e}
\]

(4.2.6)
Note that
\[ \hat{f}(\xi, \xi) = f(\xi) \]  

(4.2.7)

Thus, (4.2.6) becomes
\[ [F(u_h)]|_{x_e} = \hat{f}(\xi, \xi)[u_h]|_{x_e} \]  

(4.2.8)

Case 1: If \( u_h(x_e^+) \geq u_h(x_e^-) \), then \( [u_h]|_{x_e} \geq 0 \). This implies, \( \xi \in (u_h(x_e^-), u_h(x_e^+)) \). Because the flux is monotone,
\[ \hat{f}(\xi, \xi) \geq \hat{f}(u_h^-, u_h^+)|_{x_e} \]  

(4.2.9)

Case 2: If \( u_h(x_e^+) < u_h(x_e^-) \), then \( [u_h]|_{x_e} < 0 \). Therefore, \( \xi \in (u_h(x_e^+), u_h(x_e^-)) \). Because the flux is monotone,
\[ \hat{f}(\xi, \xi) \leq \hat{f}(u_h^-, u_h^+)|_{x_e} \]  

(4.2.10)

From case 1 (4.2.9) and case 2 (4.2.10), we conclude that
\[ \left( \hat{f}(\xi, \xi) - \hat{f}(u_h^-, u_h^+)|_{x_e} \right) [u_h]|_{x_e} \geq 0 \]  

(4.2.11)

Substituting (4.2.8) in (4.2.11), we obtain the result
\[ [F(u_h)]|_{x_e} - \hat{f}(u_h^-, u_h^+)|_{x_e} [u_h]|_{x_e} \geq 0 \]  

(4.2.12)

We note that the same arguments apply for \( e = 0 \) and \( e = N \), the only difference is that we set \( u_h(x_{N+1}^+) = 0 \) and \( u_h(x_0^-) = 0 \).

The following theorem is a stability result for the numerical method 4.1.15.

**Theorem 2.** If \( a(u) \) is bounded below and above uniformly
\[ 0 < C_0 \leq a(u) \leq C_1 \]  

(4.2.13)
If $\epsilon = -1$ or $\epsilon = 0$, we assume $\sigma$ is a large enough number. If $\epsilon = 1$, we can choose $\sigma = 1$.

Then, the discontinuous Galerkin scheme (4.1.15) is $L^2$ stable:

$$\|u_h(t)\|^2_{L^2[0,L]} \leq C \left( \|u_0\|^2_{L^2[0,L]} + \int_0^t \|s(\tau)\|^2_{L^2[0,L]} d\tau \right) \quad (4.2.14)$$

where $u_0$ is the initial condition and $C$ is a constant independent of $h$.

Proof. Let $v_h = u_h$ in (4.1.15), then

$$\int_{I_e} (\partial_t u_h) u_h dx - \int_{I_e} f(u_h) \partial_x u_h dx$$

$$+ \hat{f}(u_h^+, u_h^-)|_{x_{e+1}} u_h(x_{e+1}) - \hat{f}(u_h^+, u_h^-)|_{x_e} u_h(x_e^+) + \mathcal{H}_e(u_h, u_h) = \int_{I_e} s(t) u_h dx$$

(4.2.15)

Applying a change of variables,

$$du = \partial_x(u_h) dx$$

(4.2.16)

we rewrite the second term as

$$\int_{x_e}^{x_{e+1}} f(u_h) \partial_x u_h dx = \int_{u_h(x_e^+)}^{u_h(x_{e+1})} f(u) du$$

(4.2.17)

Using definition (4.2.1) and equation (4.2.17), we obtain the following:

$$\int_{x_e}^{x_{e+1}} f(u_h) \partial_x u_h dx = F(u_h(x_e^-)) - F(u_h(x_e^+))$$

(4.2.18)

Substituting (4.2.18) in (4.2.15) and noting that

$$\int_{I_e} (\partial_t u_h) u_h dx = \frac{1}{2} \frac{d}{dt} \int_{I_e} u_h^2 dx$$

(4.2.19)
we obtain the following:

\[
\frac{1}{2} \frac{d}{dt} \int_{I_e} u_h^2 dx - F(u_h(x_{e+1}^-)) + F(u_h(x_e^+)) + \hat{f}(u_h^+, u_h^-)|_{x_{e+1}} u_h(x_{e+1}^-) - \hat{f}(u_h^+, u_h^-)|_{x_e} u_h(x_e^+) + \mathcal{H}_e(u_h, u_h) = \int_{I_e} s(t) u_h dx
\]

(4.2.20)

We sum equation (4.2.20) over all the elements, from \(e = 0, \ldots, N\)

\[
\frac{1}{2} \frac{d}{dt} \int_0^L u_h^2 dx + \sum_{e=0}^{N+1} \left( [F(u_h)]|_{x_e} - \hat{f}(u_h^+, u_h^-)[u_h]|_{x_e} \right) + \sum_{e=0}^N \mathcal{H}_e(u_h, u_h) = \int_0^L s(t) u_h dx
\]

(4.2.21)

By Theorem 1, we have

\[
[F(u_h)]|_{x_e} - \hat{f}(u_h^+, u_h^-)[u_h]|_{x_e} \geq 0
\]

(4.2.22)

Then,

\[
\frac{1}{2} \frac{d}{dt} \int_0^L u_h^2 dx + \sum_{e=0}^N \mathcal{H}_e(u_h, u_h) \leq \int_0^L s(t) u_h dx
\]

(4.2.23)

Next, we investigate the term \(\mathcal{H}_e(u_h, u_h)\) defined for \(e = 1, \ldots, N - 1\) in (4.1.19), for \(e = 0\) in (4.1.20) and for \(e = N\) in (4.1.21). Summing \(\mathcal{H}_e(u_h, u_h)\) from \(e = 0, \ldots, N\), we obtain

\[
\sum_{e=0}^N \mathcal{H}_e(u_h, u_h) = \sum_{e=0}^N \int_{I_e} a(u_h)(\partial_x u_h)^2 dx + (1 - \epsilon) \sum_{e=1}^N \left( (a(u_h)\partial_x u_h)[u_h]|_{x_e} \right)^2 + \sum_{e=0}^{N+1} \sigma_h [u_h]^2|_{x_e} + (1 - \epsilon) a(u_h(x_{e+1}^-))\partial_x u_h(x_{e+1}^-)[u_h]|_{x_{e+1}} + (1 - \epsilon) a(u_h(x_0^+))\partial_x u_h(x_0^+)[u_h]|_{x_0} + (1 - \epsilon) a(u_h(x_{N+1}^-))\partial_x u_h(x_{N+1}^-)[u_h]|_{x_{N+1}}
\]

(4.2.24)
Substituting (4.2.24) in (4.2.23) yields

\[
\frac{1}{2} \frac{d}{dt} \int_0^L u_h^2 dx + \sum_{e=0}^N \int_{I_e} a(u_h)(\partial_x u_h)^2 dx + \sum_{e=0}^{N+1} \frac{\sigma}{h} [u_h]_{x_e}^2 \leq \int_0^L s(t) u_h dx \\
+ |1 - \epsilon| \sum_{e=1}^N \{|a(u_h)(\partial_x u_h)| |x_e| [u_h]|_{x_e}| \\
+ |(1 - \epsilon)a(u_h(x_0^+))\partial_x u_h(x_0^+)[u_h]|_{x_0}| \\
+ |(1 - \epsilon)a(u_h(x_{N+1}^-))\partial_x u_h(x_{N+1}^-)[u_h]|_{x_{N+1}|} \\
(4.2.25)
\]

Note that if \( \epsilon = 1 \), then the result follows by Gronwall’s inequality. This is explicitly explained in the inequalities following (4.2.37). We now assume that \( \epsilon \neq 1 \).

By the triangle inequality, for \( e = 1, \ldots, N \)

\[
\{|a(u_h)(\partial_x u_h)| |x_e| [u_h]|_{x_e}| \leq \frac{1}{2} \left( |a(u_h(x_e^+))\partial_x u_h(x_e^+)| + |a(u_h(x_e^-))\partial_x u_h(x_e^-)| \right) |[u_h]|_{x_e} \\
(4.2.26)
\]

By the upper bound on \( a(u) \) (4.2.13) and the trace inequality, there exists a constant \( C \) independent of \( h \) such that

\[
|a(u_h(x_e^+))\partial_x u_h(x_e^+)| \leq C h^{-\frac{1}{2}} ||\partial_x u_h||_{L^2(I_e)} \\
|a(u_h(x_e^-))\partial_x u_h(x_e^-)| \leq C h^{-\frac{1}{2}} ||\partial_x u_h||_{L^2(I_{e-1})} \\
(4.2.27, 4.2.28)
\]

By Young’s inequality, bounds (4.2.27) and (4.2.28), for any \( \kappa^2 \in \mathbb{R} \) we have

\[
|a(u_h(x_e^+))\partial_x u_h(x_e^+)||[u_h]|_{x_e}| \leq \frac{C}{\kappa^2} |a(u_h(x_e^+))\partial_x u_h(x_e^+)|^2 + \frac{\kappa^2}{2h} |[u_h]|_{x_e}^2 \\
(4.2.29)
\]

\[
|a(u_h(x_e^-))\partial_x u_h(x_e^-)||[u_h]|_{x_e}| \leq \frac{C}{\kappa^2} |a(u_h(x_e^-))\partial_x u_h(x_e^-)|^2 + \frac{\kappa^2}{2h} |[u_h]|_{x_e}^2 \\
(4.2.30)
\]

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We use bounds (4.2.29) and (4.2.30) in the triangle inequality (4.2.26) to obtain
\[
|\{a(\partial_x u_h)\}|_{x_e} [u_h]_{x_e} \leq \frac{1}{2} \left( \frac{1}{\kappa^2} C \left( ||\partial_x (u_h)||^2_{L^2(I_e)} + ||\partial_x (u_h)||^2_{L^2(I_{e-1})} \right) + \frac{\kappa^2}{2h} [u_h]^2_{x_e} \right) \tag{4.2.31}
\]

for some \( C \) independent of \( h \) and for all \( e \in \{1, \ldots, N\} \).

We use the same arguments to bound the last two terms
\[
|a(u_h(x_0^+))\partial_x (u_h(x_0^+))[u_h]|_{x_0} \leq \frac{1}{\kappa^2} C ||\partial_x (u_h)||^2_{L^2(I_0)} + \frac{\kappa^2}{4h} [u_h]^2_{x_0} \tag{4.2.32}
\]
\[
|a(u_h(x_{N+1}^-))\partial_x (u_h(x_{N+1}^-))[u_h]|_{x_{N+1}} \leq \frac{1}{\kappa^2} C ||\partial_x (u_h)||^2_{L^2(I_N)} + \frac{\kappa^2}{4h} [u_h]^2_{x_{N+1}} \tag{4.2.33}
\]

for some constant \( C \) independent of \( h \).

Inequalities (4.2.31), (4.2.32) and (4.2.33) result in the following bound:
\[
|1 - \epsilon| \sum_{e=1}^{N} |\{a(u_h)(\partial_x u_h)\}|_{x_e} [u_h]_{x_e} \\
+ |(1 - \epsilon)a(u_h(x_0^+))\partial_x u_h(x_0^+)[u_h]|_{x_0} | + |(1 - \epsilon)a(u_h(x_{N+1}^-))\partial_x u_h(x_{N+1}^-)[u_h]|_{x_{N+1}} |
\leq \frac{C}{\kappa^2} \sum_{e=0}^{N} ||\partial_x u_h||^2_{L^2(I_e)} + \sum_{e=0}^{N} \frac{\kappa^2}{4h} [u_h]^2_{x_e} \tag{4.2.34}
\]

We use the bound (4.2.34) and the lower bound on \( a(u_h) \) (4.2.13) to obtain the following
\[
\frac{1}{2} \frac{d}{dt} \int_0^L u_h^2 dx + (C_0 - \frac{C}{\kappa^2}) \sum_{e=0}^{N} ||\partial_x (u_h)||^2_{L^2(I_e)} + h^{-1}(\sigma - \frac{\kappa^2}{4}) \sum_{e=0}^{N+1} |u|^2_{x_e} \leq \int_0^L s(t) u_h dx \tag{4.2.35}
\]

We choose
\[
\kappa^2 = \frac{C}{C_0} \tag{4.2.36}
\]

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If $\sigma$ is large enough, we have

$$\frac{1}{2} \frac{d}{dt} \int_0^L u_h^2 dx \leq \int_0^L s(t) u_h dx \quad (4.2.37)$$

By Cauchy-Schwarz’s and Young’s inequalities,

$$\frac{1}{2} \frac{d}{dt} ||u_h(t)||^2_{L^2[0,L]} \leq \frac{1}{2} \left( ||s(t)||^2_{L^2[0,L]} + ||u_h(t)||^2_{L^2[0,L]} \right) \quad (4.2.38)$$

We integrate from $t = 0$ to $t$,

$$||u_h(t)||^2_{L^2(0,L)} \leq ||u_h(0)||^2_{L^2[0,L]} + \int_0^t ||s(\tau)||^2_{L^2[0,L]} d\tau + \int_0^t ||u_h(\tau)||^2_{L^2[0,L]} d\tau \quad (4.2.39)$$

By Gronwall’s inequality, there exists a constant $C$, independent of $h$ such that

$$||u_h(t)||^2_{L^2[0,L]} \leq C \left( ||u_h(0)||^2_{L^2[0,L]} + \int_0^t ||s(\tau)||^2_{L^2[0,L]} d\tau \right) \quad (4.2.40)$$

$\Box$
Chapter 5

Fully Discrete Scheme and Numerical Experiments

This chapter develops the fully discrete discontinuous Galerkin scheme as applied to the concentration equation derived in Chapter 3. The method for Dirichlet boundary conditions is presented in Section 5.1 and for Dirichlet and Neumann boundary conditions in Section 5.2. Numerical experiments using the method of manufactured solutions are included in Section 5.3. Section 5.4 extends the numerical method to a network of vessels and shows numerical experiments on a three vessel network.

The first two equations of (3.2.18) are numerically solved using the Runge Kutta discontinuous Galerkin method described in Section 2.2. The concern of this chapter is the numerical solution of the convection diffusion equation (3.2.9).

5.1 Numerical Scheme for Dirichlet Boundary Conditions

The reduced oxygen transport equation (3.2.9) derived in Section 3.1 is repeated below with Dirichlet boundary conditions

\[
\frac{\partial (AC)}{\partial t} + \frac{\partial (QC)}{\partial x} - \frac{\beta}{D} \frac{\partial}{\partial x} \left( Q^2 \frac{\partial C}{\partial x} \right) = 0, \quad x \in [0, L]
\]

\[C(x, 0) = C_0(x), \quad x \in [0, L]\]  \hspace{1cm} (5.1.2)

\[C(0, t) = C_{\text{inlet}}\]  \hspace{1cm} (5.1.3)

\[C(L, t) = C_{\text{outlet}}\]  \hspace{1cm} (5.1.4)
Let $\mathbb{V}_h^k$ be the test function space:

$$
\mathbb{V}_h^k := \{ \phi : [0, L] \rightarrow \mathbb{R} \text{ st. } \phi |_{I_e} \in P^k(I_e), \quad \forall e = 0, ..., N \} \quad (5.1.5)
$$

where $I_e$ and $h$ are given by

$$
I_e = [x_e, x_{e+1}], \quad h = x_{e+1} - x_e, \quad e = 0, ..., N \quad (5.1.6)
$$

The traces of $C_h$ are defined on the interfaces of the elements in the following way

$$
C_h(x_e^+) = \lim_{\epsilon > 0, \epsilon \to 0} C_h(x_e + \epsilon) \quad e = 0, ..., N \quad (5.1.7)
$$

$$
C_h(x_e^-) = \lim_{\epsilon < 0, \epsilon \to 0} C_h(x_e + \epsilon) \quad e = 1, ..., N + 1 \quad (5.1.8)
$$

We define the jump of $C_h \in \mathbb{V}_h^k$ as:

$$
[C_h]|_{x_e} = C_h(x_e^+) - C_h(x_e^-) \quad e = 1, ..., N \quad (5.1.9)
$$

$$
[C_h]|_{x_0} = C_h(x_0) - C_{\text{inlet}} \quad (5.1.10)
$$

$$
[C_h]|_{x_{N+1}} = C_{\text{outlet}} - C_h(x_{N+1}^-) \quad (5.1.11)
$$

We define the average of a function $f(C_h)$ as:

$$
\{f(C_h)\}|_{x_e} = \frac{1}{2} (f(C_h(x_e^+)) + f(C_h(x_e^-)) \quad e = 1, ..., N \quad (5.1.12)
$$

$$
\{f(C_h)\}|_{x_0} = \frac{1}{2} (f(C_h(x_0^+)) + f(C_{\text{inlet}})) \quad (5.1.13)
$$

$$
\{f(C_h)\}|_{x_{N+1}} = \frac{1}{2} (f(C_{\text{outlet}}) + f(C_h(x_{N+1}^-))) \quad (5.1.14)
$$

Let $A_h$ and $Q_h$ be the discontinuous Galerkin approximations to $A$ and $Q$ respectively.
We multiply equation (5.1.2) by $\phi_h \in V_h^k$ and integrate on every element

$$
\int_{I_e} \frac{\partial (A_h C_h)}{\partial t} \phi_h + \int_{I_e} \frac{\partial}{\partial x} (Q_h C_h) \phi_h dx - \int_{I_e} \frac{\beta}{D} \frac{\partial^2 C_h}{\partial x^2} \phi_h dx = 0
$$

(5.1.15)

for all $e = 0, ..., N$

We integrate by parts the second and third terms in (5.1.15):

$$
\int_{I_e} \frac{\partial}{\partial x} (Q_h C_h) \phi_h dx = - \int_{I_e} Q_h C_h \frac{\partial \phi_h}{\partial x} dx + \hat{f}_{e+1} (C_h, Q_h) \phi_h(x_e^-) - \hat{f}_e (C_h, Q_h) \phi_h(x_e^+)
$$

(5.1.16)

$$
- \int_{I_e} \frac{\beta}{D} \frac{\partial}{\partial x} \left( Q_h^2 \frac{\partial C_h}{\partial x} \right) \phi_h dx = \frac{\beta}{D} \int_{I_e} Q_h^2 \frac{\partial C_h}{\partial x} \frac{\partial \phi_h}{\partial x} dx + \frac{\beta}{D} \mathcal{H}_e(C_h, \phi_h)
$$

(5.1.17)

where $\hat{f}_e(\cdot, \cdot)$ is the Lax Friedrichs flux given by,

$$
\hat{f}_e(C_h, Q_h) = \frac{1}{2} \left[ Q_h C_h \right]_{x_e} - \max(|Q_h(x_e^+)|, |Q_h(x_e^-)|)|C_h|_{x_e}, \quad \forall \ e = 0, ..., N
$$

(5.1.18)

and $\mathcal{H}_e(C_h, \phi_h)$ is the sum of the fluxes obtained from applying the interior penalty discontinuous Galerkin method on one element only.

For $e = 1, ..., N - 1$, we have:

$$
\mathcal{H}_e(C_h, \phi_h) = \left( Q_h^2 \frac{\partial C_h}{\partial x} \right)_{x_e} \phi_h(x_e^+) - \left( Q_h^2 \frac{\partial C_h}{\partial x} \right)_{x_{e+1}} \phi_h(x_{e+1})
$$

$$
- \frac{\epsilon}{2} \left( \left( Q_h(x_e^+) \right)^2 \frac{\partial \phi_h}{\partial x}(x_e^+)|C_h|_{x_e} + \left( Q_h(x_{e+1}) \right)^2 \frac{\partial \phi_h}{\partial x}(x_{e+1})|C_h|_{x_{e+1}} \right)
$$

$$
+ \frac{\sigma}{h} \left( |C_h|_{x_e} \phi_h(x_e^+) - |C_h|_{x_{e+1}} \phi_h(x_{e+1}) \right)
$$

(5.1.19)
For $e = 0$, we have

$$
\mathcal{H}_0(C_h, \phi_h) = (Q_h(x_0^+))^2 \frac{\partial C_h}{\partial x}(x_0^+) \phi_h(x_0^+) - (Q_h(x_0^-))^2 \frac{\partial C_h}{\partial x}(x_0^-) \phi_h(x_0^-)
$$

$$
- \epsilon \left( (Q_h(x_0^+))^2 \frac{\partial \phi_h}{\partial x}(x_0^+) |_{x_0^+} + (Q_h(x_1^-))^2 \frac{\partial \phi_h}{\partial x}(x_1^-) |_{x_1^-} \right)
$$

$$
+ \frac{\sigma}{h} \left( [C_h]_{x_0} \phi_h(x_0^+) - [C_h]_{x_1} \phi_h(x_1^-) \right)
$$

(5.1.20)

For $e = N$, we have:

$$
\mathcal{H}_N(C_h, \phi_h) = (Q_h(x_N^+))^2 \frac{\partial C_h}{\partial x}(x_N^+) \phi_h(x_N^+) - (Q_h(x_N^-))^2 \frac{\partial C_h}{\partial x}(x_N^-) \phi_h(x_N^-)
$$

$$
- \epsilon \left( (Q_h(x_N^-))^2 \frac{\partial \phi_h}{\partial x}(x_N^-) |_{x_N^-} + 2(Q_h(x_{N+1}^-))^2 \frac{\partial \phi_h}{\partial x}(x_{N+1}^-) |_{x_{N+1}^-} \right)
$$

$$
+ \frac{\sigma}{h} \left( [C_h]_{x_N} \phi_h(x_N^+) - [C_h]_{x_{N+1}} \phi_h(x_{N+1}^-) \right)
$$

(5.1.21)

where $\sigma$ is a penalty parameter for the jump terms and $\epsilon \in \{-1, 0, 1\}$. If $\epsilon = -1$ and $\sigma$ is bounded below by a sufficiently large constant, the method is the symmetric interior interior penalty DG method introduced by Wheeler and Arnold [24]. For $\epsilon = \sigma = 1$ the method is the nonsymmetric interior penalty DG method introduced by Riviere, Wheeler and Girault [24].

We define, for $e = 0, ..., N$:

$$
\mathcal{J}_e(C_h, \phi_h) = \int_{I_e} Q_h C_h \frac{\partial \phi_h}{\partial x} dx - \int_{I_e} (\phi(x_e^-) - \phi(x_{e+1}^-)) + \int_{I_e} (\phi(x_{e+1}^+ - \phi(x_e^+))
$$

$$
- \beta D \int_{I_e} Q_h \frac{\partial C_h}{\partial x} \frac{\partial \phi_h}{\partial x} dx - \frac{\beta}{D} \mathcal{H}_e(C_h, \phi_h)
$$

(5.1.22)

It follows that the weak formulation is given by:

$$
\int_{I_e} \frac{\partial (A_h C_h)}{\partial t} \phi_h = \mathcal{J}_e(C_h, \phi_h)
$$

(5.1.23)
for all $e = 0, ..., N$.

We use a two stage Runge Kutta method in time. Let $\Delta t$ denote the timestep. We obtain the following fully discretized scheme:

Given $A^n_{h}, Q^n_{h},$ computed using the RKDG method described in Section 2.2, and $C^n_{h}$, compute $W^{n+1}_{h}, C^{n+1}_{h}$ such that:

\[
\int_{I_e} A^{n+1}_{h} W^{n+1}_{h} \phi_{h} dx = \int_{I_e} A^{n+1}_{h} C^{n}_{h} \phi_{h} dx + \Delta t J_e(C^n_{h}, \phi_{h}) \tag{5.1.24}
\]

\[
\int_{I_e} A^{n+1}_{h} C^{n+1}_{h} \phi_{h} dx = \frac{1}{2} \int_{I_e} A^{n+1}_{h} C^{n}_{h} \phi_{h} dx + \frac{1}{2} \int_{I_e} A^{n+1}_{h} W^{n+1}_{h} \phi_{h} dx + \frac{\Delta t}{2} J_e(W^{n+1}_{h}, \phi_{h}) \tag{5.1.25}
\]

\[\forall \phi_{h} \in V_h, \; \forall e \in \{0, ..., N\}\]

5.2 Numerical Scheme for Neumann and Dirichlet Boundary Conditions

![Figure 5.1: A three vessel network with a junction point](image)
Equation (5.2.2) is solved on each vessel in the network described in Section 5.1 with Neumann boundary conditions at the outlet:

\[
\frac{\partial (AC)}{\partial t} + \frac{\partial}{\partial x} (QC) - \frac{\beta}{D} \frac{\partial}{\partial x} \left( Q^2 \frac{\partial C}{\partial x} \right) = 0, \quad x \in (0, L) \tag{5.2.1}
\]

\[
C(x, 0) = C_0(x), \quad x \in (0, 1) \tag{5.2.2}
\]

\[
C(0, t) = C_{inlet} \tag{5.2.3}
\]

\[
\frac{\partial C}{\partial x}(L, t) = 0 \tag{5.2.4}
\]

The same expressions for \(\hat{f}_e\) and \(H_e\), defined in Section 5.1, are used for \(e = 0, ..., N - 1\). But, the fluxes on the last interval are modified to take into account the Neumann boundary conditions.

\[
H_N(C_h, \phi_h) = \left\{ Q_h^2 \frac{\partial C}{\partial x} \right\}_{x_N} \phi_h(x_N^+) - \frac{\epsilon}{2} \left( Q_h(x_N^+)^2 \frac{\partial \phi_h}{\partial x}(x_N^+) [C_h]_{x_N} \right) + \frac{\sigma}{h}[C_h]_{x_N} \phi_h(x_N^+) \tag{5.2.5}
\]

and we take the left trace for \(\hat{f}_{N+1}(\cdot, \cdot)\)

\[
\hat{f}_{N+1}(C_h, Q_h) = Q_h(x_{N+1}^-) C_h(x_{N+1}^-) \tag{5.2.6}
\]

The scheme given by (5.1.24) and (5.1.25) is then used to solve the equations on the vessel network 5.1 in Section 5.4.
5.3 Numerical Experiment with Smooth Solutions

We use the method of manufactured solutions to verify the numerical scheme in one vessel of length $L = 1$. We use the following exact solutions

\begin{align*}
A(x, t) &= \cos(2\pi x) \cos(t) + 2 \\
Q(x, t) &= \cos(t) \sin(2\pi x) \\
C(x, t) &= e^{-x-t}
\end{align*}

and we apply the fully discrete scheme given in (5.1.24) and (5.1.25).

We let

\begin{align*}
\beta &= 1, \ D = 1, \ \sigma = 1, \ \epsilon = 1
\end{align*}

and consider the following physiological parameters as in [19]:

\begin{align*}
\alpha &= 1.1, \ \rho = 1.06, \ \kappa = 1, \ \mu = 3.302E-2, \ A_0 = 1, \ p_0 = 0
\end{align*}

Because of the explicit time stepping scheme and to study the spatial discretization, we take a small enough time step to keep the temporal error from polluting the result. We let $\Delta t = 10^{-7}$ and evolve the scheme for ten time steps for each polynomial degree, $k$. Table 5.1 shows the $L^2$ error and rates for $h = 1/2^i$ for $i = 1, \ldots, 5$. We recover a convergence rate of $k + 1$ when a polynomial of degree $k$ is used.
Table 5.1: L2 error and rates for the Concentration when using the IPDG method (5.1.24) and (5.1.25) with diffusion $\beta/D = 1$

We repeat the experiment with the same parameters but without diffusion $\beta/D = 0$. Table 5.2 shows the results. We recover the convergence rate of $k + 1$ when a polynomial of degree $k$ is used.

Table 5.2: L2 error and rates for the Concentration when using the IPDG method (5.1.24) and (5.1.25) without diffusion $\beta/D = 0$

5.4 Numerical Experiment on a Vessel Network

The inlet data for the two outgoing vessels needs to be prescribed. Section 5.4.1 presents the two conditions used to specify this data and shows results from numerical experiments on the three vessel network 5.1.
5.4.1 Conditions at the Junction Point

Consider the network of three vessels shown in Figure 5.1. The incoming vessel branches at a junction point into two outgoing vessels.

Let \( x^* \) denote the junction point, \( Q \) denote the flow in the incoming vessel and \( \hat{Q} \) denote the flow in the outgoing vessel.

An incoming vessel is considered to have flow into the junction if \( Q(x^*) \geq 0 \). An outgoing vessel is considered to have flow out of the junction if \( \hat{Q}(x^*) \geq 0 \). Conversely, if \( Q(x^*) < 0 \) and \( \hat{Q}(x^*) < 0 \) then the outgoing vessel is considered to have flow into the junction, but the incoming vessels has flow out of the junction. This labeling is summarized in the table below.

<table>
<thead>
<tr>
<th>Status</th>
<th>incoming</th>
<th>outgoing</th>
</tr>
</thead>
<tbody>
<tr>
<td>( Q \geq 0 ) ( \hat{Q} \geq 0 )</td>
<td>into junction</td>
<td>out of junction</td>
</tr>
<tr>
<td>( Q &lt; 0 ) ( \hat{Q} &lt; 0 )</td>
<td>out of junction</td>
<td>into junction</td>
</tr>
</tbody>
</table>

Table 5.3 : Labeling of the flow of vessels connecting to a junction point

At the junction point, let \( C_{in}^i \) denote the concentration of vessel \( i \) with flow into the junction. Let \( C_{out}^j \) be the concentration of vessel \( j \) with flow out of the junction. Note that this notation is at the level of the junction point. The computed value of \( C_{out}^j \) will be the inlet data prescribed for vessels with flow out of the junction.

The values for \( C_{in}^i \) are determined in the same way for all the vessels with flow into the junction. To declutter notation, I drop the superscript \( i \) and write the concentration at the inflow as \( C_{in} \). The value of \( C_{in} \) at time step \( t_{n+1} \), denoted by \( C_{in}^{n+1} \), is determined by using a new equation which approximates the original equation (3.2.9). This approximation is given by:

\[
\frac{\partial C}{\partial t} + \frac{Q_{in}}{A_{in}} \frac{\partial C}{\partial x} = 0
\]  

(5.4.1)
This approximation essentially means that we neglect diffusion at the junction point. Then, by the characteristics of equation (5.4.1), we obtain

\[ C^{n+1}_{in}(x^*) = C^n_{in}(x^* - \frac{Q_{in}}{A_{in}} \Delta t) \]  

(5.4.2)

where \( \Delta t \) is the time step. To determine \( C^j_{out} \), we assume the following:

1. Instantaneous mixing:
   \[ C^j_{out} = C_{out} \quad \forall j \]  
   (5.4.3)

2. Conservation of mass:
   \[ \sum_i Q^i_{in} C^i_{in} = \sum_j Q^j_{out} C^j_{out} \]  
   (5.4.4)

Substituting the first condition in the second, we solve for \( C_{out} \):

\[ C_{out} = \frac{\sum_i Q^i_{in} C^i_{in}}{\sum_j Q^j_{out}} \]  

(5.4.5)

By conservation of momentum, we have that

\[ \sum_i Q^i_{in} = \sum_j Q^j_{out} \]  

(5.4.6)

Thus, \( C_{out} \) is an averaged sum of \( \{ C^1_{in}, \ldots, C^N_{in} \} \) where \( N \) is the number of vessels with flow into the junction.

\[ C^j_{out} = \frac{\sum_i Q^i_{in} C^i_{in}}{\sum_i Q^i_{in}} \]  

(5.4.7)

5.4.2 Numerical Results

To test this labeling of flow in Table 5.3 and the junction conditions, (5.4.7), we solve the transport equation in the vessel network given in Figure 5.1. The first numerical experiment
we consider is when $A$ and $Q$ are fixed, $A = 1$ and $Q = 10$. We solve equation (3.2.9) on the three vessels, with
\[
\frac{\beta}{D} = 0.02
\] (5.4.8)
and use the same physiological parameters (5.3.5). We take polynomials of degree $k = 2$, a mesh size $h = 0.125$ and $\Delta t = 10^{-5}$. We solve the scheme till final time $T = 1$.

The initial concentration profile for all three vessels and the boundary conditions for $C$ in the incoming vessel are the following:

\[
C_i(x, 0) = 1.0 \quad i = 1, 2, 3
\] (5.4.9)
\[
C_1(0, t) = \begin{cases} 
2t + 1 & t \leq 0.5 \\
2 & t > 0.5 
\end{cases}
\] (5.4.10)

Figures 5.2 and 5.3 show the concentration profile as a function of time in the three vessels.

![Plot of the concentration evaluated at the midpoint of the first vessel as a function of time](image)

**Figure 5.2**: Plot of the concentration evaluated at the midpoint of the first vessel as a function of time.
A snapshot of the concentration in the three vessels with time is shown in Figure 5.4.

We kept the same parameters (5.3.5) and ran the simulation without the diffusion term $\beta/D = 0$. Figure 5.5 and Figure 5.6 show the evolution of the concentration evaluated at the midpoint of each vessel as a function of time.
Figure 5.5: Plot of the concentration evaluated at the midpoint of the first vessel as a function of time, $\beta/D = 0$.

Figure 5.6: Plot of the concentration evaluated at the midpoint of each of the two bifurcating vessels as a function of time, $\beta/D = 0$.

The evolution of the concentration at time $t = 0.38$ is given in Figure 5.4.
Figure 5.7: Plot of the concentration as a function of space in the three vessels at time $t = 0.38$, $\beta/D = 0$

We tested the numerical method with the junction conditions with varying $A$ and $Q$ where we impose a sinusoidal pressure waveform at the inlet of the network:

$$p(0, t) = 2664 \sin(\omega \pi t) \quad (5.4.11)$$

The inlet data for the area $A$ is determined from the following relation given in [21].

$$A(0, t) = \frac{1}{\kappa} \left( p(0, t) - p_0 + \kappa A_0^{\frac{1}{2}} \right)^2 \quad (5.4.12)$$

where $\beta/D = 0.02$ and the parameters $\kappa, p_0$ and $A_0$ are given in [25]. The inlet data for $Q$ is attained by extrapolating the Riemann invariants of the system (2.1.2). For details on how $Q$ at the inlet node is obtained, see [21]. We use the same initial conditions for $C$ given in (5.4.10) and we let the length of each vessel $L = 1$.

We vary $\omega$ and report the results. First, we set $\omega = 0.5$ in (5.4.11) to consider an increasing
positive pressure waveform at the inlet over the time domain \([0,1]\). Area and momentum as a function of time in the three vessels are plotted in Figure 5.8.

![Figure 5.8: Plot of the Area and Momentum calculated at the midpoint of the vessel with respect to time when \(\omega = 0.5\)](image)

The concentration profiles in the three vessels for \(\omega = 0.5\) as a function of time are given in Figures 5.9 and 5.10.

![Figure 5.9: Plot of the concentration evaluated at the midpoint of the first vessel as a function of time, \(\omega = 0.5\)](image)
Figure 5.10: Plot of the concentration evaluated at the midpoint of each of the two bifurcating vessels as a function of time, $\omega = 0.5$

A snapshot of the evolution of the concentration in the three vessels as a function of space is given in Figure 5.11.

Figure 5.11: Plot of the concentration as a function of space in the three vessels at time $t = 0.38$ with $\omega = 0.5$

Then, we consider an increasing and then decreasing positive pressure waveform at the inlet,
$\omega = 1$. Area and momentum as a function of time in the three vessels are plotted in Figure 5.12.

Figure 5.12: Plot of the Area and Momentum calculated at the midpoint of the vessel with respect to time when $\omega = 1$

The concentration profiles in the three vessels for $\omega = 1$ as a function of time are given in Figures 5.13 and 5.14.

Figure 5.13: Plot of the concentration evaluated at the midpoint of the first vessel as a function of time, $\omega = 1$
A snapshot of the evolution of the concentration in the three vessels as a function of space is given in Figure 5.15.

Next, we consider a full sin curve as the pressure waveform. This waveform is considered
to test the algorithm against negative values of momentum. We set $\omega = 2$ and repeat the experiment. Area and momentum as a function of time in the three vessels are plotted in Figure 5.16.

![Figure 5.16](image1.png)  
**Figure 5.16**: Plot of the Area and Momentum calculated at the midpoint of the vessel with respect to time when $\omega = 2$

The concentration profiles in the three vessels for $\omega = 2$ as a function of time are given in Figures 5.17 and 5.18.

![Figure 5.17](image2.png)  
**Figure 5.17**: Plot of the concentration evaluated at the midpoint of the first vessel as a function of time, $\omega = 2$
A snapshot of the evolution of the concentration in the three vessels as a function of space is given in Figure 5.19.

Figure 5.18: Plot of the concentration evaluated at the midpoint of each of the two bifurcating vessels as a function of time, $\omega = 2$.

Figure 5.19: Plot of the concentration as a function of space in the three vessels at time $t = 0.68$ with $\omega = 2$. 
Chapter 6

Conclusion and Future Work

The cardiovascular system has very complex and intricate dynamics. Simulating blood flow and oxygen transport in this system requires the numerical computation of partial differential equations in multiple vessels. This quickly yields a computationally expensive model. To gain critical insight into this dynamics without exhausting time and resources, approximate models must be formulated. Based on the success of the reduced blood flow model, we have derived a reduced model for the transport of oxygen. Further, we developed and proposed numerical methods for solving the oxygen transport equation effectively in one vessel and in a bifurcation of vessels. We proved the $L_2$ stability of this method as applied to a general nonlinear convection diffusion equation, and we validated it against manufactured solutions. We extended this numerical method to a vessel network and tested the model for a network of three vessels with varying pressure waveforms at the inlet.

Future research directions include verifying the reduced model against data and adding several vessels and organ beds to the model with the transport equation. This will allow us to study the impact of several cardiovascular surgeries. For example, a palliative treatment of severe pulmonary hypertension includes the connection of an oxygenation machine to the pulmonary circulation. Thus, an efficient simulation for oxygen transport would provide critical information on hemodynamic changes in such patients. The work presented in this thesis has several applications that extend farther from simulating the transport of oxygen. For instance, knowing the concentration of a drug at a certain region is significant for Magnetic Resonance Imaging (MRI) with contrast.
On the theoretical aspect, studying the convergence of the proposed method is ongoing research. Further research directions include the extension of the stability and convergence analysis for general boundary conditions and the generalization of the analysis to system of nonlinear conservation laws.
Bibliography


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