DISCONTINUOUS GALERKIN FINITE ELEMENT METHOD FOR
SIMULATION OF A TRANSCRIPTION PROCESS MODEL

by

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ABSTRACT

The classical traffic flow PDE from the 1950s is used to model the biological process of transcription; the process of transferring genetic information from DNA to mRNA, in an E. coli gene. Polymerase elongating along the DNA strand encounter frequent but short pauses which are incorporated into the transcription model as several traffic lights. These pauses result in a delay in the transcription time and a delay function is defined to quantify this effect. Numerical simulations of the PDE model are conducted using a discontinuous Galerkin finite element method (DG) formulation. The entropy satisfying weak solution of the PDE model with a single pause is derived using the method of characteristics. This weak solution is used to show convergence of the DG formulation even though the flux function is not smooth. Once convergence of the DG solution is established for one pause, the numerical simulation for multiple pauses is used to calculate the delay due to the pauses and determine their effect on the overall transcription time.

Preliminary parameter studies show a complex relationship between pause location and delay values. To determine the effect of pause clustering on protein production, an ongoing research goal is optimization of the delay function with respect to pause location. For preliminary work on this optimization problem, a DG formulation used to solve a sensitivity equation for a linear hyperbolic PDE with a spatial interface parameter is derived to gain insight for the more complicated nonlinear traffic flow PDE.
CHAPTER 1

INTRODUCTION

Protein synthesis consists of the two stages of transcription and translation. Transcription is the process of transferring genetic information from DNA to messenger RNA (mRNA). During transcription, an RNA polymerase (RNAp) initiates on one end of the DNA strand then translocates along the strand unwrapping the double helix and transcribing the genetic information into an mRNA molecule. Once termination is reached, the mRNA disconnects and becomes available for translation. Translation is then the process of ribosomes elongating along the mRNA strand to produce protein.

Transcription and translation consist of four essential processes: assembly of the machinery at the start of the strand, movement initiation, elongation and termination. Both of these bio-polymerization processes can be viewed as movement of a complex machine (either RNAp or ribosomes) along a one-dimensional strand (either DNA or mRNA). The current research focuses on a mathematical model which describes the elongation stage of transcription, along with pausing. That is, we study the process of polymerase translocating along the DNA strand to read in and copy the genetic information from the nucleotides. Through experimental observation, it is known that the motion of the RNAp is not uniform, but in fact, the polymerase
transcribes rapidly and frequently pauses. Single molecule observation using optical traps indicate that the duration of the pauses is roughly bi-modal [1] with mean $1.2 \pm 0.1$ seconds with amplitude 60% and $6 \pm 0.4$ seconds with amplitude 40%. It is believed that the existence of both transcriptional and translational pauses forms one component of a sophisticated cellular control mechanism that produces proteins at a rate that is optimal based on the environmental conditions that the cell is subject to at any given time [2]. Recent research has focused on the effect that these pauses have on transcription rates and the overall protein production rate of the cell. Several types of models have been studied; however, some of the common themes center around the estimation of polymerase density on the DNA strand, the estimation of transcription rates as well as the investigation of spatial location and time durations of transcriptional pauses and their effects on transcription (and thereby protein production). In particular, so-called “clusters” of bottleneck codons in ribosomal translation have been observed experimentally, and using stochastic models these bottlenecks have been determined to decrease the protein production rate by at least a factor of two [3].

The current research seeks to address similar issues for the transcription process. We use a partial differential equation (PDE) in nonlinear conservation law form in order to model the transcription process. In the 1950’s, this particular PDE was introduced as a basic continuum model for analyzing traffic flow. Although it was originally criticized as a traffic flow model because it neglected driver reaction times,
the PDE is shown to be useful for describing and analyzing the fundamental elements of the transcription process and the effects that the transcriptional pauses may have on average transcription time. The aforementioned experimental results related to pausing are incorporated into the mathematical model as traffic lights within the traffic flow model.

In order to give context to some of the ideas presented here, note that in a 2010 paper by Mier-y-Teran-Romero et al. [4], under simplifying assumptions providing a nearly constant elongation speed for ribosomes, the authors derive a linear conservation law to model the biological process of translation. The model has the form

\[ z_t + (\beta(x, t)z)_x = 0 \]

with appropriate boundary and initial conditions where \( z(x, t) \) is the density of ribosomes along the messenger RNA chain, and \( \beta(x, t) \) is a function representing the elongation speed in space and time that is assumed to be slowly varying about some constant equilibrium value. In [5], Davis et al. use ideas similar to that of [4] in order to develop a nonlinear conservation law model for the biological process of transcription where the primary difference is that the elongation speed is no longer assumed to be roughly constant. This assumption is changed in order to incorporate information about the experimentally observed pauses polymerase experience during the transcription process [1]. The resulting mathematical model is the classic traffic flow PDE [6, 7]

\[ z_t + (\beta(x, t)(1 - z))_x = 0 \]  \hspace{1cm} (1.1)
where $z(x,t)$ is the density of polymerase along the DNA chain and $\beta(x,t)$ is a piecewise constant function representing the elongation speed. The goal of this thesis work is to give a very brief overview of the different categories of transcription models, to describe some of the relevant biological questions that can be answered using the traffic flow model and to detail the use of a Discontinuous Galerkin finite element method (DG) as the main computational means for simulation of the PDE. This leads us to provide some qualitative answers to some of the questions posed.

Although the motivation for the work is the study of the biological mechanism of transcription, the discussion begins with a general description of the numerical techniques that are used for all simulations contained here. Chapter 2 provides an overview of the discontinuous Galerkin finite element method using an explicit Runge-Kutta time integration to solve a scalar nonlinear conservation law. DG was originally developed to solve hyperbolic partial differential equations and is a natural choice for approximating solutions with discontinuities due to the localized nature of the spatial discretization. The primary components of any DG formulation are discussed and the specific choices for simulations computed in Chapters 3 and 4 are detailed.

In Chapter 3, the classic traffic flow model (1.1) is introduced and a single pause is incorporated into the model as a discontinuous flux coefficient. The entropy satisfying weak solution is derived and verified to be an integral solution of the conservation law. The pause results in a discontinuous solution that can be numerically approximated using the DG method. Error analysis is conducted on the single pause model to test
the accuracy of the numerical scheme as well as to debug the numerical coding for future use with multiple pauses where the weak solution is not known.

In Chapter 4, the full biological model is studied where multiple pauses are incorporated into the PDE as discontinuities in the flux coefficient, $\beta(x, t)$. A delay function is defined to quantify the overall effect pauses have on the instantaneous transcription speed. Error analysis is conducted on the delay calculation using the one pause model and its weak solution showing first order convergence at the final time when a linear basis is used for the spatial discretization of the DG solution. Numerical simulations of the PDE model are conducted to determine an instantaneous transcription speed which produces the experimentally observed transcription time while also imposing the pause duration and frequency observed by Block et al. [1]. The results of this section indicate a large variability in the overall transcriptional time for various realizations of multiple pause configurations, and this naturally motivates a brief parameter study to illustrate the complex nature of the relationship between pause locations, pause durations and transcription time. This fuels our interest in applying sensitivity analysis techniques to quantify the effects of small changes in locations and durations of pauses on the transcription time.

In Chapter 5, preliminary analysis for developing a discontinuous Galerkin finite element method to compute sensitivities with respect to interface parameters within a scalar conservation law is conducted. The sensitivity equation derived from a linear conservation law with a piecewise continuous flux coefficient is analyzed with the
goal of extending the numerical scheme to the nonlinear model in Chapter 3. Using the proposed DG formulation, error analysis is conducted on two similar examples highlighting difficulties with using the proposed numerical flux function.
CHAPTER 2

DISCONTINUOUS GALERKIN FINITE ELEMENT FORMULATION

The discontinuous Galerkin finite element method (DG) is a numerical method designed to combine the ideas of numerical flux functions and slope limiters for stability of the finite volume method [8] with the geometric flexibility and high-order accuracy of solutions to the weak formulation of the finite element method as described in [9, 10, 11]. The method was first proposed by Reed and Hill in 1973 [12] to solve the steady-state neutron transport problem

\[ \sigma u + \nabla \cdot (a(x)u) = f \]

where \(\sigma\) is a real-valued constant and \(a(x)\) is piecewise constant. The method was then extended to nonlinear conservation laws in [13] by using a linear basis to discretize in space and a forward Euler scheme to step through time, but the scheme was shown to be unstable. The instability was resolved by introducing the use of slope limiters and a class of Runge-Kutta time integration schemes [14, 15].

The method is characterized by a discretization of the spatial domain of the PDE into elements and a local approximation of the weak solution to the PDE on each element resulting in a system of ODEs in time. This system is then solved by a high-order total variation diminishing Runge-Kutta (RK) method along with a slope limiter to guarantee stability of the scheme and ensure convergence to the entropy satisfying
weak solution [16]. Finally a numerical flux function is used to connect the local solutions on the boundary of the elements and build the global solution. In contrast to traditional finite elements, the weak form is solved locally on each element as opposed to the entire spatial domain. The local, and therefore, discontinuous nature of the approximation allows for a more natural capturing of potential discontinuities at interfaces, but it also requires the introduction of a numerical flux function to build the global solution.

In the following chapter, a discontinuous Galerkin finite element method is formulated for solving a scalar conservation law, as outlined by Hesthaven and Warburton in [11]. First a spatial discretization is chosen and the localized weak formulation of the PDE is derived. Then a numerical flux function is defined to approximate the true flux from the PDE and finalize the weak form. Finally a stable integration method is introduced to step through time.

Consider the scalar conservation law

\[ u_t + (f(u))_x = 0, \quad x \in (L, R), \quad t > 0 \]  
\[ u(x, 0) = u_0(x) \]

where \( f(u) \) is a flux function which may be linear or nonlinear, \( u_0(x) \) is a prescribed initial condition and a boundary condition is assigned at the inflow boundary.
To formulate the DG solution of the PDE, first discretize the spatial domain and develop the localized weak formulation on each element. The notation used in the following formulation comes from [11].

Divide $\Omega = [L, R]$ into $K$ elements, $D^k = [x^k_l, x^k_r]$, such that $x^k_r = x^{k+1}_l$. Since the method allows for discontinuities across the elements, all interior nodes are doubly labeled as shown in Figure 1.

![Figure 1: Spatial Discretization of the domain $[L, R]$](image)

Define the function space

$$V = \{v \in L^2(\Omega) : v|_{D^k} \in H^1(D^k) \text{ for } k = 1, 2, \cdots, K\}$$

where $L^2(\Omega)$ is the space of (Lebesgue) square integrable functions on $\Omega$

$$L^2(\Omega) = \{v : \Omega \to \mathbb{R} : ||v||_2 < \infty\}$$

with inner product and norm

$$< u, v > = \int_\Omega u(x)v(x)dx, \quad ||v||_2 = < v, v >^{1/2}.$$

The Sobolev space, $H^1(D^k)$, is the subspace of functions in $L^2(D^k)$ such that their
first generalized derivative is also in $L^2(D^k)$.

$$H^1(D^k) = \{v : D^k \to \mathbb{R} | v, v' \in L^2(D^k)\}$$

Let $V^k$ be a finite dimensional subspace of $H^1(D^k)$; typically a space of polynomials of some prescribed degree on the $k^{th}$ element. The DG method is a localized finite element scheme in the sense that a discontinuous approximate solution, $u_h$, to the PDE is found such that $u_h|_{D^k} = u_h^k \in V^k$. Therefore the local finite dimensional subspace, $V^k$, and an approximate solution to the weak formulation on $D^k$ found in $V^k$ is the focus of the spatial discretization rather than the global solution, $u_h$.

For the following formulation and simulations, the basis of Lagrange interpolating polynomials defined by the Legendre Gauss Lobatto interpolation points is used for the localized finite dimensional subspaces. As discussed in [11], this results in a well-conditioned mass matrix for the semi-discrete form. Let $\{x_j^k\}_{j=1}^{N_p}$ be the set of $N_p$ interpolation points on $D^k$ and define $V^k = \text{span}\{\ell_i^k(x)\}_{i=1}^{N_p}$ where for $x \in D^k$, the Lagrange polynomial is defined by

$$\ell_i^k(x) = \prod_{\substack{j = 1 \\ j \neq i}}^{N_p} \frac{x - x_j^k}{x_i^k - x_j^k}$$

For the local formulation, we use the traditional Galerkin finite element method approach, but on each element. In the PDE, we replace $u$ with a finite dimensional approximation, multiply by a test function, $v \in V^k$, and integrate by parts over the element $D^k$. We find $u_h^k \in V^k$ such that

$$\int_{D^k} \left( \frac{\partial u_h^k}{\partial t} + \frac{\partial f^k(u_h^k)}{\partial x} \right) v dx = 0 \quad \forall v \in V^k$$
Or equivalently, in weak form, find \( u_h^k \in V^k \) such that

\[
\int_{D^k} \frac{\partial u_h^k}{\partial t} v dx - \int_{D^k} f^k(u_h^k) \frac{dv}{dx} dx + f^k(u_h^k) v \bigg|_{x_i^k}^{x_r^k} = 0 \quad \forall v \in V^k
\]

where \( f^k \) is an approximation of the flux as defined in (2.4).

Since \( u_h^k \) is allowed to be discontinuous at the nodes of the spatial discretization, the evaluation of the flux on the boundary of the element is replaced with a numerical flux, \( f^*(u) \), which is a function of the local solutions at the interface. The numerical flux is an approximation to \( f(u) \) on the boundary of the element whose purpose is to connect the local finite element solutions for construction of the global solution on \( \Omega \) and impose any boundary or interface conditions from the PDE. More details are included in the section beginning on page 13.

Therefore, the local DG formulation is to find \( u_h^k \in V^k \) such that

\[
\int_{D^k} \frac{\partial u_h^k}{\partial t} v dx - \int_{D^k} f^k(u_h^k) \frac{dv}{dx} dx + f^*(u) v \bigg|_{x_i^k}^{x_r^k} = 0 \quad \forall v \in V^k \tag{2.3}
\]

To define the semi-discrete form, expand the local solution as a linear combination of the basis functions on \( V^k \),

\[
u_h^k(x, t) = \sum_{j=1}^{N_p} u_h^k(x_j^k, t) \ell_j^k(x).
\]

Also, approximate the local flux, \( f^k(u) \), in \( D^k \) as an interpolation at the points \( \{x_j^k\}_{j=1}^{N_p} \) as

\[
f^k(u_h^k(x, t)) = \sum_{j=1}^{N_p} f(u(x_j^k, t)) \ell_j^k(x). \tag{2.4}
\]
Then the local approximate solution within the finite dimensional subspace must satisfy (2.3) for each of the basis functions, \( v(x) = \ell^k_i(x) \).

\[
\int_{D^k} \sum_{j=1}^{N_p} \frac{d u^k_h(x^k_j, t)}{dt} \ell^k_j(x) \ell^k_i(x) dx - \int_{D^k} \sum_{j=1}^{N_p} f(x^k_j, t) \ell^k_j(x) \frac{d \ell^k_i(x)}{dx} dx
+ f^*(u^k_h \ell^k_i(x)|_{x^k_i}) = 0 \\
\sum_{j=1}^{N_p} \int_{D^k} \ell^k_j(x) \ell^k_i(x) dx \frac{d u^k_h(x^k_j, t)}{dt} - \sum_{j=1}^{N_p} \int_{D^k} \ell^k_j(x) \frac{d \ell^k_i(x)}{dx} dx f(x^k_j, t)
+ f^*(u^k_h \ell^k_i(x)|_{x^k_i}) = 0
\]

(2.5)

This can be done more succinctly if one defines the local mass and stiffness matrices as

\[
M^k_{ij} = \int_{D^k} \ell^k_i(x) \ell^k_j(x) dx \\
S^k_{ij} = \int_{D^k} \ell^k_i(x) \frac{d \ell^k_j(x)}{dx} dx
\]

and the vectors

\[
\vec{u}^k_h = [u^k_h(x^k_1, t), \ldots, u^k_h(x^k_{N_p}, t)]^T \\
\vec{f}^k = [f(x^k_1, t), \ldots, f(x^k_{N_p}, t)]^T \\
\vec{\ell}^k = [\ell^k_1, \ldots, \ell^k_{N_p}]^T
\]

Finally, the semi-discrete scheme is to find \( \vec{u}^k_h \) that satisfies

\[
M^k \frac{d \vec{u}^k_h}{dt} - S^k \vec{f}^k = -f^*(u^k_h \ell^k(x^k_r)) + f^*(u^k_h \ell^k(x^k_l)).
\]

(2.6)

The matrix-vector equation defines a system of \( N_p \) ODEs in time.

Two final notes about the formulation:

1. The initial condition is projected onto the finite dimensional subspace and then used during the first iteration of the time integration to solve (2.6).
2. The inflow boundary condition is imposed by the numerical flux function to determine the local solution on the appropriate element. At the outflow boundary, the numerical flux is defined to be consistent with the true flux function.

**Numerical Flux**

The numerical flux function, \( f^*(u) \), is defined on the boundary of the elements as an approximation to the true flux, \( f(u) \), from the conservation law. It depends on the local solutions at the boundary of the element and all neighboring elements. If \( u^- \) represents the local solution on the boundary internal to \( D^k \) and \( u^+ \) is the local solution on the boundary external to \( D^k \), then numerical fluxes have the form

\[
f^* = f^*(u^-, u^+)
\]

The DG method was devised so that if a degree zero basis is chosen, then (2.3) reduces to

\[
\int_{D^k} \frac{\partial u^h_k}{\partial t} \, dx + f^*(u) \bigg|_{x^k_l}^{x^k_r} = 0
\]

which when integrated over the time interval, \((t_n, t_{n+1})\),

\[
\int_{D^k} u^h_k(x, t_{n+1}) - u^h_k(x, t_n) \, dx + \int_{t_n}^{t_{n+1}} f^*(u(x^k_r, t)) - f^*(u(x^k_l, t)) \, dt = 0 \quad (2.7)
\]

then defines a finite volume method [8]. The numerical flux function is adopted from the finite volume theory and defined so that (2.7) is stable and consistent with the PDE.
One way to guarantee stability of a numerical method used to solve a nonlinear scalar conservation law is to ensure that the scheme is monotone, as given below and defined in [17]. These methods were developed to prevent artificial oscillations near the numerical approximation of discontinuities and ensure stability by preserving the monotonicity of the initial condition in the approximate solution at each time step.

In the following definition, let $\Omega$ represent the spatial domain of a scalar conservation law.

**Definition 1** *(Monotone Numerical Scheme)* A numerical scheme is monotone if

$$u_0(x) \geq v_0(x) \quad \forall x \in \Omega$$

holds for two initial conditions and the corresponding approximations to (2.1) are

$$U_n^m \approx u(x_m, t_n) \quad \text{and} \quad V_n^m \approx v(x_m, t_n),$$

then

$$U_n^m \geq V_n^m \quad \forall m \quad \Rightarrow \quad U_{n+1}^m \geq V_{n+1}^m \quad \forall m.$$

One of the severe limitations of the monotone schemes is that they are only first-order accurate [17, 10] and a proof of this result is included in [18]. A benefit of implementing a DG method is that by using a polynomial basis of arbitrary degree, higher-order accuracy can be achieved [10].

It has been shown that the method (2.7) will be monotone and therefore stable if the numerical flux from the finite volume method (equivalently the discontinuous
finite element method with a degree zero spatial discretization) has the following properties \[10, 11\]:

1. \(f^*(u^-, u^+)\) is locally Lipschitz and consistent with the flux, \(f^*(u, u) = f(u)\),
2. nondecreasing in the first argument and
3. nonincreasing in the second argument.

Examples of well-known numerical fluxes, as stated in \[10\], that satisfy these properties are the following:

1. Godunov flux

\[
f^*(u^-, u^+) = \begin{cases} 
\min_{u^- \leq u \leq u^+} f(u) & u^- \leq u^+ \\
\max_{u^+ \leq u \leq u^-} f(u) & \text{otherwise}
\end{cases}
\]

2. Engquist-Osher flux

\[
f^*(u^-, u^+) = \int_0^{u^+} \min(f'(s), 0)ds + \int_0^{u^-} \max(f'(s), 0)ds + f(0)
\]

3. Lax-Friedrichs flux

\[
f^*(u^-, u^+) = \{\{f(u)\}\} + \frac{C}{2} [u], \quad C = \max_{\inf u_0(x) \leq u \leq \sup u_0(x)} |f'(u)|
\]

where \(\{\{f\}\} = \frac{f^- + f^+}{2}\) is the average across the interface and \([u] = \hat{n}^-u^- + \hat{n}^+u^+\) is the jump along the outward normal. For the one-dimensional problem, \(\hat{n} = \pm 1\).
4. Local Lax-Friedrichs flux

\[
f^*(u^-, u^+) = \{\{f(u)\}\} + \frac{C}{2}[u], \quad C = \max_{\min(u^-, u^+) \leq u \leq \max(u^-, u^+)} |f'(u)| \quad (2.8)
\]

For the model problem presented in Chapters 3 and 4, the Local Lax-Friedrichs flux is used in the implementation of the DG formulation.

Even though the numerical flux is chosen to provide monotonicity and stability of the basic finite volume scheme, this choice no longer guarantees stability when an arbitrary basis is used for a DG scheme [10]. In the next section, a class of Runge-Kutta time integration schemes is outlined to guarantee stability.

**Time Integration**

The final step for implementation of the DG formulation is solving the system of ODEs in time. In the semi-discrete scheme (2.6), invert the local mass matrix to rewrite the system in the form

\[
\frac{d\tilde{u}_h^k}{dt} = (M^k)^{-1} \left[ S^k \tilde{f}_h^k - f^*(u_h^k)\tilde{\ell}_h^k(\tilde{x}_r^k) + f^*(u_h^k)\tilde{\ell}_h^k(\tilde{x}_l^k) \right]
\]

or, more succinctly as

\[
\frac{d\tilde{u}_h^k}{dt} = L(\tilde{u}_h^k, t).
\]

If the conservation law has a smooth solution, then a standard high-order accurate Runge-Kutta method is appropriate; however for nonlinear problems or problems with discontinuous initial/boundary data which results in a discontinuous solution, more care needs to be taken.
Approximating a nonlinear flux, \( f(u) \), by an interpolation or attempting to capture discontinuities created by shocks causes the approximate solution to have artificial oscillations. These issues are dealt with by the introduction of a post processing technique known as slope limiting. Slope limiting is a way of removing oscillations over any element where they are detected by adjusting the slope of the approximate solution. In the development of finite volume methods, slope limiters were derived to guarantee that a first order forward Euler scheme was stable when applied to the semi-discrete system of ODEs in time for a nonlinear hyperbolic PDE. But to gain higher accuracy than first order in time, a class of Runge-Kutta methods were developed to be total variation diminishing (TVD) and therefore stable whenever an Euler method was also TVD as discussed in [19, 20, 21] and defined below. The total variation of a function is a quantity used to measure artificial oscillations within the function.

**Definition 2 (Total Variation Diminishing)** The total variation of a function defined at a discrete time, \( t_n \), for a set of grid nodes, \( \{x_j\}_{j=0}^M \), is

\[
TV(u(x, t_n)) = \sum_{j=0}^{M-1} |u(x_{j+1}, t_n) - u(x_j, t_n)|
\]

The function is total variation diminishing (TVD) if

\[
TV(u(x, t_{n+1})) \leq TV(u(x, t_n)) \quad \forall n
\]

By ensuring that the total variation of the approximate solution does not increase, oscillations in the neighborhood of discontinuities can be reduced or eliminated and
guarantee stability of the numerical scheme. Since slope limiters are needed for stability of a basic Euler method, they will then also be needed for stability of the higher order Runge-Kutta method.

Consider a standard Runge-Kutta method

\[
\begin{align*}
    u^{(0)} &= u^n \\
    u^{(i)} &= \sum_{m=0}^{i-1} \alpha_{im} u^{(m)} + \beta_{im} \Delta t L(u^{(m)}, t^n + \gamma_m \Delta t) & \text{for } i = 1, \ldots, s \\
    u^{n+1} &= u^{(s)}
\end{align*}
\]

where

\[
\Delta t \leq c \Delta t_{FE}, \quad c = \min_{i,k} \frac{\alpha_{i,k}}{\beta_{i,k}}
\]

and \(\Delta t_{FE}\) is the time step from the forward Euler scheme.

As shown in [19, 20, 21], if \(\alpha_{im} \geq 0 \quad \forall i, m\) and \(\sum_{m=0}^{i-1} \alpha_{im} = 1\) then the RK stages are convex combinations of forward Euler steps. Therefore if a forward Euler time integration is TVD, each stage of the RK integration will also be TVD and so will the resulting RK method.

One example of a basic slope limiter is the \texttt{minmod} function. It is based on a piecewise-linear reconstruction from finite volume methods. At some time step, suppose the local solution has the form

\[
u^k_h = \bar{u}^k_h + (x - x^k_0)(u^k_h)_x
\]

where \(x^k_0\) is the center of \(D^k\) and \(\bar{u}^k_h\) is the average value over the element.
Then the slope limited version of the local solution is

\[
\prod u_h^k(x) = \bar{u}_h^k + (x - x_0^k)m\left((u_h^k)_x, \frac{\bar{u}_{h}^{k+1} - \bar{u}_h^k}{h}, \frac{\bar{u}_h^k - \bar{u}_h^{k-1}}{h}\right)
\]

(2.9)

where the minmod function, \(m\), with \(n\) inputs is defined to be

\[
m(a_1, \ldots, a_n) = \begin{cases} 
    s \min_{1 \leq i \leq n} |a_i|, & |s| = 1 \\
    0, & |s| \neq 1
\end{cases}
\]

\[
s = \frac{1}{n} \sum_{i=1}^{n} \text{sign}(a_i)
\]

In (2.9), the minmod slope limiter compares an approximation to the spatial derivative over the element and the respective difference quotients using the two neighboring elements. If these slopes all have the same sign, then the slope of the local solution over the element is chosen to be the smallest in absolute value. But if the slopes do not have the same sign, then an oscillation is detected, the slope is set to be zero and the local solution is the average value over the element.

Figure 2 compares the DG approximation of a piecewise constant function with and without the use of the minmod slope limiter. In Figure 2a, artificial oscillations are detected in a neighborhood of the discontinuity which are removed with the use of a slope limiter, as shown in Figure 2b.

To maintain stability of the scheme, the explicit RK method is combined with a slope limiter that is applied after each stage of the RK function evaluations. Even though the slope limiter guarantees stability, it also has an adverse effect on accuracy. One issue with using a slope limiter is the smearing of discontinuities and local extrema, as seen by the smooth transition in Figure 2b. Since an artificial oscillation is determined by changes in the sign of slope, all local maxima and minima are
Figure 2: Comparison of an approximation of a piecewise constant with and without slope limiting. Without slope limiting, artificial oscillations are detected in a neighborhood of the discontinuity.

incorrectly identified as oscillations. Another issue with using a slope limiter is that regardless of the degree of the basis used on $V^k$, the slope limited version results in a linear approximation reducing the accuracy of the solution. Therefore a generalized slope limiter has been developed so that a standard slope limiter is applied to the approximate solution when oscillations are detected in the neighborhood of extremum or shocks as described above. But if no oscillation is detected, then the higher degree approximation is still attained on the corresponding element rather than using the minimum slope and building a linear approximation. There is still reduced accuracy in a neighborhood of shocks, but the overall performance is improved with a generalized slope limiter [11, 10].

An example of an optimal third order TVD RK scheme used in later simulations
is included below and found in [11]. The scheme is optimal in the sense that the time step can be taken to be as large as the time step used for the forward Euler scheme.

First, apply the slope limiter to the initial condition.

\[ u(x,0) = u_0(x) \Rightarrow u^0 = \prod u_0(x) \]

where \( \prod \) is the chosen slope limiter. For this work, the slope limiter is exclusively the \texttt{minmod} function. Then for \( n = 0, 1, 2, \cdots, m \)

\[
\begin{align*}
    u^{(1)} &= \prod [u^n + \Delta tL(u^n, t^n)] \\
    u^{(2)} &= \prod [\frac{3}{4}u^n + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta tL(u^{(1)}, t^n + \Delta t)] \\
    u^{n+1} &= \prod [\frac{1}{3}u^n + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta tL(u^{(2)}, t^n + \frac{1}{2}\Delta t)]
\end{align*}
\]

where the time step, \( \Delta t \), is chosen to satisfy the CFL condition

\[
\Delta t \leq \frac{\Delta x}{\max_k |f'(u(x_k, t))|}
\]

and the max is computed over all interpolation points chosen in the spatial domain.
CHAPTER 3

TRAFFIC FLOW MODEL

Consider the conservation law given by

\[ z_t + f(z)_x = 0, \quad -\infty < x < \infty, \quad t > 0 \]  
\[ z(x, 0) = z_0(x) \]

where \( z(x, t) \) is the traffic density and \( f \) is the flux function. As proposed by Lighthill and Whitham and also Richards [6, 7], assume that velocity is dependent only on density so that the flux is

\[ f(z) = v(z)z = v_m \left(1 - \frac{z}{z_m}\right) z \]

where \( v_m \) is the maximum velocity and \( z_m \) is the maximum density.

In this chapter, the weak solution to the traffic flow model with a single pause is derived and numerical results using a DG formulation are provided. The weak solution is derived following a discussion included in [22] although the incorporation of a discontinuous flux coefficient to model traffic lights is not included in that text.

**Integral Solution**

In general, a smooth solution of (3.1) cannot be found. Instead of searching for a classical solution to the PDE, a weak or integral solution of the PDE is sought. The
derivation of the weak form of the general conservation law is standard and can be found in a partial differential equation text book, see [23, 17], for example.

Define the set of test functions to be

\[ C^1_0(\mathbb{R} \times \mathbb{R}^+) = \{ \phi(x,t) : \mathbb{R} \times \mathbb{R}^+ \to \mathbb{R} | \phi \in C^1(R \times R^+), \text{Supp}(\phi) \subset [a,b] \times [c,d] \} \]

\( C^1_0 \) is the space of continuously differentiable functions with compact support; that is, \( \phi \) is identically zero outside a bounded subset of its domain.

In order to derive the integral solution, multiply the PDE in (3.1) by a test function, \( \phi \), and integrate over the domain.

\[
\int_0^\infty \int_{-\infty}^\infty [z_t + (f(z))_x] \phi \, dx \, dt = 0, \forall \phi \in C^1_0 \\
\int_{-\infty}^\infty \int_0^\infty z_t \phi \, dt \, dx + \int_0^\infty \int_{-\infty}^\infty (f(z))_x \phi \, dx \, dt = 0, \forall \phi \in C^1_0
\]

Applying integration by parts,

\[
\int_{-\infty}^\infty \left[ z\phi \right]_{t=0}^{\infty} \, dx + \int_0^\infty \left[ (f(z))_x \phi \right]_{x=\infty}^{\infty} \, dt = 0, \forall \phi \in C^1_0 \\
\int_{-\infty}^\infty \left[ -z(x,0)\phi(x,0) \right] \, dx - \int_0^\infty \int_{-\infty}^\infty f(z)\phi_x \, dx \, dt = 0, \forall \phi \in C^1_0 \\
\int_0^\infty \int_{-\infty}^\infty z\phi_t + f(z)\phi_x \, dx \, dt + \int_{-\infty}^\infty z_0(x)\phi(x,0) \, dx = 0, \forall \phi \in C^1_0
\]

where the compact support of the test functions implies that

\[ \lim_{x \to \pm \infty} \phi(x,t) = \lim_{t \to \infty} \phi(x,t) = 0. \]

Since the derivatives have been moved onto the test function, the weak solution requires less smoothness than a classical solution of the PDE.
For the following model problems, the weak solution is derived using the method of characteristics and the integral form is verified. In addition to finding the characteristic curves, shock curves are found by imposing the Rankine-Hugoniot condition. Any curve of discontinuity or “shock curve” must satisfy the Rankine-Hugoniot condition in order for the weak solution to satisfy the integral form.

The following definitions are standard and can be found, for example, in [23, 17].

**Definition 3** (Rankine-Hugoniot Condition) The shock curve propagates with speed, $\sigma$, given by

$$\sigma = \frac{[f]}{[z]} = \frac{f(z(x^-, t)) - f(z(x^+, t))}{z(x^-, t) - z(x^+, t)}$$

$[f]$ and $[z]$ measure the jump in the flux and density at the location of the discontinuity.

In general, weak solutions of a nonlinear PDE are not unique. In order to determine the physically relevant solution, weak solutions must satisfy an entropy condition in a neighborhood of discontinuities. The basic entropy condition which is sufficient for the model problems considered in this chapter is defined below.

**Definition 4** (Entropy Condition) A discontinuity propagating with speed $\sigma$ satisfies the entropy condition if

$$f'(z_l) > \sigma > f'(z_r)$$

where $z_l$ is the limiting solution to the left of the shock and $z_r$ is the limiting solution to the right of the shock.
Since the flux function (3.3) is concave, the entropy condition is equivalent to

\[ z_l < z_r \]

i.e., the entropy solution is increasing across a curve of discontinuity at any given time.

**Traffic After a Red Light Turns Green**

First, the simple case of modeling the density of traffic after the light turns green is considered. The initial condition in (3.5) is used to model this behavior using a piecewise constant function. To the left of the light located at \( x = 0 \), the stopped traffic is backed up to the maximum density of \( z = z_m \). To the right of the light, it is assumed that enough time has passed that the density is at the minimum, \( z = 0 \), as shown in Figure 3.

![Figure 3: Plot of the initial condition in (3.5).](image-url)
26

\[ z_t + \left( v_m \left( 1 - \frac{z}{z_m} \right) z \right)_x = 0, \quad x \in \mathbb{R}, \quad t > 0 \quad (3.4) \]

\[ z(x, 0) = \begin{cases} z_m & x < 0 \\ 0 & x \geq 0 \end{cases} \quad (3.5) \]

**Weak Solution**

The weak solution of (3.4) - (3.5) is found using the method of characteristics. Let \( x = x(t) \) be a characteristic curve and examine how the solution, \( z(x, t) = z(x(t), t) \), changes along the characteristic. Using the chain rule, the total derivative with respect to \( t \) is

\[ \frac{d}{dt} z(x(t), t) = \frac{\partial z}{\partial t} + \frac{\partial z}{\partial x} \frac{dx}{dt} \]

From the conservation law (3.1),

\[ \frac{\partial z}{\partial t} + \frac{df}{dz} \frac{\partial z}{\partial x} = 0 \]

Therefore, if \( \frac{dx}{dt} = \frac{df}{dz} \) for all \((x, t)\), then

\[ \frac{d}{dt} z(x(t), t) = \frac{\partial z}{\partial t} + \frac{\partial z}{\partial x} \frac{dx}{dt} = \frac{\partial z}{\partial t} + \frac{df}{dz} \frac{\partial z}{\partial x} = 0 \]

Combining these observations, the characteristic curves are defined by the system

\[ x'(t) = f'(z) \quad (3.6) \]

\[ \frac{d}{dt} z(x(t), t) = 0 \quad (3.7) \]

Equation (3.7) implies that the solution is constant along the characteristics. Therefore if \( x(0) = x_0 \) and \( z(x(0), 0) = z(x_0, 0) \) is known from the initial condition,
then \(z(x(t), t) = z(x_0, 0)\) for all \(t > 0\). To find the characteristic equations, one solves the ODE

\[
x'(t) = f'(z(x_0, 0)), \quad x(0) = x_0
\]

where \(x(t)\) satisfies (3.6) to determine that the characteristics are

\[
x(t) = f'(z(x_0, 0)) t + x_0
\]

For the given flux function (3.3) and initial condition (3.5), the solution can be found explicitly. Figure 4 includes a graph of the characteristics derived below.

1. If the characteristic through \((x, t)\) intersects the \(x\)-axis at \(x_0 < 0\), the solution is \(z = z_m\) and the characteristic has slope \(f'(z_m) = -v_m\). The characteristic is

\[
x = -v_m t + x_0 \tag{3.8}
\]

2. If the characteristic through \((x, t)\) intersects the \(x\)-axis at \(x_0 > 0\), the solution is \(z = 0\) and the characteristic has slope \(f'(0) = v_m\). The characteristic is

\[
x = v_m t + x_0 \tag{3.9}
\]

To determine the solution in the region of the \(xt\)-plane not included by the above characteristics, consider the initial value problem

\[
\frac{dx}{dt} = \frac{df}{dz}, \quad x(0) = 0, \quad \text{for } -v_m t < x < v_m t
\]

Since the solution is constant along the characteristics, \(\frac{df}{dz}\) is also a constant along each characteristic. Therefore the solution of the differential equation is

\[
x = \frac{df}{dz} t
\]
Figure 4: Plot of characteristics in $xt$-plane with slope either $-\frac{1}{v_m}$ or $\frac{1}{v_m}$. Along the characteristics with slope $-\frac{1}{v_m}$, the solution is $z = z_m$ while the solution along the characteristics with slope $\frac{1}{v_m}$ is $z = 0$.

which, after computing the derivative of the flux, is found to be

$$\frac{x}{t} = \frac{df}{dz} = v_m \left(1 - \frac{2z}{z_m}\right).$$

Solving this equation for $z$ gives

$$z = \frac{z_m}{2} - \frac{z_m x}{2v_m t},$$

which is called the rarefaction wave.

Then the expression for the solution to (3.4) - (3.5) is

$$z = \begin{cases} 
\frac{z_m}{2} - \frac{z_m x}{2v_m t} & x \leq -v_m t \\
0 & -v_m t < x < v_m t \\
2v_m t & v_m t \leq x
\end{cases}$$

(3.11)

This solution is continuous, yet not differentiable everywhere, and defines the density of traffic for $t > 0$ as flow begins after the light turns green. The rarefaction wave expression defines the density of traffic as it increases ahead of the light and
decreases behind the light. Figure 5 includes a time snapshot of the solution and depicts the corners and therefore nondifferentiability at $x = -v_m t$ and $x = v_m t$.

![Figure 5: Plot of the solution (3.11) at time $t = 0.5$.](image)

**Verification of Solution**

On the domain $D = \{(x, t) \mid -v_m t < x < v_m t, \ t > 0\}$, the rarefaction wave (3.10) satisfies the conservation law.

$$z_t + (f(z))_x = \frac{\partial}{\partial t} \left( \frac{z_m}{2} - \frac{z_m x}{2v_m t} \right) + \frac{\partial}{\partial x} \left( \frac{v_m z_m}{4} \left( 1 - \left( \frac{x}{v_m t} \right)^2 \right) \right) = \frac{z_m x}{2v_m t^2} = 0$$

To verify that (3.11) is a weak solution to (3.4) - (3.5), one must show that

$$\int_0^\infty \int_{-\infty}^\infty z \phi_t + f(z) \phi_x \, dx \, dt = -\int_{-\infty}^\infty z_0(x) \phi(x, 0) \, dx \quad \forall \phi \in C^1_0$$

For ease of notation, denote the rarefaction wave in (3.10) by $\tilde{z} = \tilde{z}(x, t)$. 
\[
\int_{0}^{\infty} \int_{-\infty}^{\infty} z\phi_t + f(z)\phi_x dx dt \\
= \int_{0}^{\infty} \int_{-\infty}^{-v_m t} z_m \phi_t dx + \int_{-v_m t}^{v_m t} z\phi_t + f(\bar{z})\phi_x dx dt \\
= \int_{-\infty}^{\infty} \int_{0}^{\infty} z_m \phi_t dt dx + \int_{0}^{\infty} \int_{-v_m t}^{v_m t} z\phi_t dt dx \\
+ \int_{0}^{\infty} \int_{-v_m t}^{-v_m t} \bar{z}\phi_t dt dx \\
+ \int_{-\infty}^{\infty} \int_{x/v_m}^{\infty} f(\bar{z})\phi_x dx dt \\
= \int_{-\infty}^{0} z_m \phi \left[ \int_{-x/v_m}^{x/v_m} dx + \int_{x/v_m}^{\infty} \bar{z} \phi \right] \left[ \int_{t=x/v_m}^{\infty} \bar{z} \phi dt \right] \left[ \int_{t=-x/v_m}^{-x/v_m} \bar{z} \phi dt \right] \right] dx \\
+ \int_{0}^{\infty} \int_{x/v_m}^{\infty} f(\bar{z})\phi_x dx dt \\
= \int_{-\infty}^{0} z_m \phi (x, 0) dx - \int_{0}^{\infty} \int_{-v_m t}^{v_m t} \bar{z}_t \phi dx dt \\
+ \int_{-\infty}^{\infty} \int_{-v_m t}^{v_m t} \bar{z}_t \phi dx dt - \int_{0}^{\infty} \int_{-v_m t}^{v_m t} (f(\bar{z}))_x \phi dx dt \\
= -\int_{-\infty}^{\infty} z_0 (x) \phi (x, 0) dx, \ \forall \phi \in C^1_0
\]

where \( \bar{z}(x, -x/v_m) = z_m \) and \( \int_{0}^{\infty} \int_{-v_m t}^{v_m t} \left[ \bar{z}_t + (f(\bar{z}))_x \right] \phi dx dt = 0 \) since \( \bar{z} \) solves the conservation law and is continuously differentiable on \(-v_m t < x < v_m t\).

**DG Performance**

This section contains a DG simulation of (3.4) - (3.5) using the formulation described in Chapter 2. Error analysis is performed using the weak solution (3.11).

For the numerical simulation, the maximum density and velocity are normalized to a value of one. (In Chapter 4, dimensionless variables for the full biological model are introduced rescaling the traffic flow model resulting in this choice of density and
velocity parameters.) Therefore the PDE model simplifies to

\[ z_t + [(1 - z)z]_x = 0 \quad x \in (-0.5, 0.5), \quad t > 0 \quad (3.12) \]

\[ z(x, 0) = \begin{cases} 
1 & x < 0 \\
0 & x > 0 
\end{cases} \quad (3.13) \]

\[ z(-0.5, t) = \begin{cases} 
1 - \frac{x}{2t} & t \leq 1/2 \\
1/2 - \frac{x}{2t} & t > 1/2 
\end{cases} \quad (3.14) \]

where the true solution (3.11) is used to define the boundary condition at the inflow boundary, \( x = -0.5 \). Even though a boundary condition is not needed for derivation of the weak solution, one is necessary for the definition and implementation of the numerical flux function on the first element of the spatial discretization.

Define the \( L^2 \) error over the spatial domain as

\[ L^2(-0.5, 0.5) = \left( \int_{-0.5}^{0.5} (z(x, T) - z_h(x, T))^2 dx \right)^{1/2} \]

where \( z(x, T) \) is the true solution and \( z_h(x, T) \) is the DG solution at the final time \( T \).

Using the interpolation points on each element, the integral is approximated using the Composite Trapezoid Rule.

Using a linear basis, the \( L^2 \) error at the final time \( T \) is computed for a range of spatial discretizations from \( \mathcal{K} = 40 \) to \( \mathcal{K} = 1280 \) elements. In Table 1, the error is computed over the spatial domain \( x \in (-0.5, 0.5) \) at the final time \( T = 0.7 \), and note that the convergence rate is first order. In Figure 6 the contour plot of the numerical solution is graphed depicting the rarefaction wave in the region \( -t < x < t \).

Using the solution of (3.4) - (3.5), the weak solution of the full model problem including a traffic light or pause occurring during a parameterized interval of time can
Table 1: Table of error calculations for traffic flow model in (3.4) - (3.5) with $z_m = v_m = 1$. $L^2$-error is calculated at final time $T = 0.7$ showing that the convergence is first order.

<table>
<thead>
<tr>
<th>$K$</th>
<th>$L^2(-0.5, 0.5)$</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>0.0093003</td>
<td>1.0096169</td>
</tr>
<tr>
<td>80</td>
<td>0.0046193</td>
<td>1.0047441</td>
</tr>
<tr>
<td>160</td>
<td>0.0023021</td>
<td>1.0022017</td>
</tr>
<tr>
<td>320</td>
<td>0.0011493</td>
<td>1.0009151</td>
</tr>
<tr>
<td>640</td>
<td>0.0005743</td>
<td>1.0009151</td>
</tr>
<tr>
<td>1280</td>
<td>0.0002841</td>
<td>1.0151167</td>
</tr>
</tbody>
</table>

Figure 6: Contour plot of DG solution using 320 elements. The contour plot depicts the rarefaction wave in the region $-t < x < t$.

be derived. First, the weak solution will be derived with the stop beginning at time $t = 0$. Then using a shift in time, the temporal location of the pause is parameterized and the weak solution is derived.
Traffic with One Red Light

Traffic with one red light at $x = 0$ beginning at $t = 0$ and lasting for a duration of $\tau$ can be modeled by the conservation law

$$z_t + \left( v_m(x, t) \left( 1 - \frac{z}{z_m} \right) z \right)_x = 0 \quad x \in (-L/2, L/2), \quad t > 0 \quad (3.15)$$

$$z(x, 0) = z_0 \quad (3.16)$$

$$z(-L/2, t) = z_0 \quad (3.17)$$

where

$$v_m(x, t) = \begin{cases} 0 & x = 0; \quad t \leq \tau \\ v_m & \text{otherwise} \end{cases}$$

The flux coefficient, $v_m(x, t)$, is a piecewise constant function representing the maximum velocity. It replaces the constant maximum velocity coefficient in (3.3) and represents a maximum velocity of $v_m$ except at the location of the red light $x = 0$ where it assumes the value of 0 for a duration of time given by $\tau$.

The constant initial density and boundary condition are used to model a constant flow of traffic except for when the red light is active. Assume that the initial density satisfies $z_0 < \frac{z_m}{2}$ so that the initial density is low to moderate and the corresponding flux is increasing with density.

Once again, the method of characteristics is used to find the weak solution and the characteristic curves satisfy (3.6) - (3.7). But unlike the previous case, the occurrence of the red light produces discontinuities in the solution which can be found by examining the shocks.
Shocks

When characteristic curves intersect, indicating the solution is multi-valued, shock curves are created defining regions of discontinuity in the solution. The Rankine-Hugoniot condition is used to determine the shock speed and the shocks are verified to obey an entropy condition.

For \( 0 < t < \tau \), there are three shocks emanating from \( x = 0 \).

1. To the left of the light, the density jumps from its initial value of \( z_0 \) to its maximum value of \( z_m \) due to the traffic backing up behind the light. The shock speed is

\[
\frac{dx_1}{dt} = -v_m \left( \frac{1 - \frac{z_0}{z_m}}{z_m - z_0} \right) z_0 = -\frac{v_m z_0}{z_m}, \quad x_1(0) = 0
\]

resulting in the shock

\[
x_1(t) = -\frac{v_m z_0}{z_m} t \tag{3.18}
\]

Since the limiting solution to the left of \( x_1(t) \) is \( z_l = z_0 \) and the limiting solution to the right of \( x_1(t) \) is \( z_r = z_m \), \( x_1(t) \) satisfies the entropy condition, \( z_l < z_r \).

2. At \( x = 0 \), the density jumps from \( z_m \) to 0 due to the clearing out of the traffic ahead of the light. The shock speed is

\[
\frac{dx_2}{dt} = 0, \quad x_2(0) = 0
\]

resulting in the shock

\[
x_2(t) = 0
\]
3. To the right of the light, the density jumps from 0 to $z_0$ due to the constant initial density to the right of the light being unaffected by the traffic stop. The shock speed is

$$\frac{dx_3}{dt} = -v_m \left(1 - \frac{z_0}{z_m}\right) \frac{z_0}{-z_0} = \frac{v_m(z_m - z_0)}{z_m}, \quad x_3(0) = 0$$

resulting in the shock

$$x_3(t) = \frac{v_m(z_m - z_0)}{z_m} t \quad (3.19)$$

Since the limiting solution to the left of $x_3(t)$ is $z_l = 0$ and the limiting solution to the right of $x_3(t)$ is $z_r = z_0$, $x_3(t)$ satisfies the entropy condition, $z_l < z_r$.

Using the shocks to determine the domain, the expression for the solution during the time of the red light, $0 \leq t < \tau$, is

$$z = \begin{cases} 
z_0 & x < \frac{-v_m z_0}{z_m} t \\
z_m & \frac{-v_m z_0}{z_m} t < x < 0 \\
0 & 0 < x < \frac{v_m(z_m - z_0)}{z_m} t \\
z_0 & \frac{v_m(z_m - z_0)}{z_m} t < x
\end{cases} \quad (3.20)$$

At $t = \tau$, the light turns green resulting in a problem similar to (3.4) - (3.5). As traffic begins to flow at $x = 0$, a rarefaction wave is created from the maximum density of $z_m$ to the minimum density of 0. Using (3.10) and shifting time by $\tau$, the expression for the density in this region is

$$z_w(x, t) = \frac{z_m}{2} - \frac{z_m x}{2v_m(t - \tau)} \quad (3.21)$$
Outside of this rarefaction wave is the region unaffected by the traffic light. In this region, the solution maintains the constant initial density of $z_0$ resulting in two shock curves bordering the rarefaction wave. The density jumps from $z_0$ to $z_w$ (or similarly from $z_w$ to $z_0$) and therefore there is a shock speed of

$$\frac{dx_s}{dt} = \frac{f(z_w) - f(z_0)}{z_w - z_0} = v_m \left[ 1 - \frac{z_w + z_0}{z_m} \right]$$

Substituting the expression for the rarefaction wave into the shock speed results in the first order linear ODE

$$\frac{dx_s}{dt} = v_m \left[ \frac{1}{2} + \frac{x_s}{2v_m(t - \tau)} - \frac{z_0}{z_m} \right]$$

Using the integrating factor

$$\mu = e^{\int \frac{1}{t - \tau} dt} = (t - \tau)^{-1/2}$$

the general solution is

$$x_s(t) = 2v_m \left[ \frac{1}{2} - \frac{z_0}{z_m} \right] (t - \tau) + c(t - \tau)^{1/2} \quad (3.22)$$

1. To find the appropriate initial condition for the left shock, let $t_1$ be the time at which the shock (3.18) emanating to the left from $(0,0)$ intersects the characteristic (3.8) to the left of the rarefaction wave (shifted in time by $\tau$). This is the time such that

$$-\frac{z_0v_m t_1}{z_m} = -v_m(t_1 - \tau)$$

This intersection is the creation of a shock bounding the rarefaction wave on the left, as depicted in Figure 7.
Figure 7: Plot of two shocks and a characteristic. The solid curve and curve marked with an x are shocks emanating from $x = 0$ at $t = 0$. The curve marked with an * is a characteristic bordering the rarefaction wave defined by $x_{cl} = -v_m(t - \tau)$. The intersection of the characteristic and shock creates the shock, $x_{sl}$, at the time, $t_1$.

Therefore

$$t_1 = \frac{z_m \tau}{z_m - z_0}$$

To find the left shock after the light turns green, solve the IVP

$$\frac{dx_{sl}}{dt} = v_m \left[ \frac{1}{2} + \frac{x_{sl}}{2v_m(t - \tau)} - \frac{z_0}{z_m} \right], \quad x_{sl}(t_1) = \frac{-z_0v_m t_1}{z_m} = \frac{-z_0v_m \tau}{z_m - z_0}$$

Imposing the initial condition in the general solution (3.22), yields the constant

$$\frac{-z_0v_m \tau}{z_{\text{max}} - z_0} = v_m \left[ 1 - \frac{2z_0}{z_{\text{max}}} \right] \left( \frac{z_{\text{max}} \tau}{z_{\text{max}} - z_0} - \tau \right) + c \left( \frac{z_{\text{max}} \tau}{z_{\text{max}} - z_0} - \tau \right)^{1/2}$$

$$-v_m z_0 \tau = v_m \tau \left[ 1 - \frac{2z_0}{z_m} \right] z_0 + c \tau^{1/2}(z_m - z_0)^{1/2} z_0^{1/2}$$

$$c = \frac{-v_m z_0^{1/2} \tau^{1/2}}{z_m - z_0^{1/2}} = -2v_m \left[ \frac{z_0 \tau}{z_m - z_0} \right]^{1/2} \left( 1 - \frac{z_0}{z_m} \right).$$

The left shock is

$$x_{sl}(t) = v_m \left[ 1 - \frac{2z_0}{z_m} \right] (t - \tau) - 2v_m \left[ \frac{z_0 \tau(t - \tau)}{z_m - z_0} \right]^{1/2} \left( 1 - \frac{z_0}{z_m} \right), \quad t \geq t_1 \ (3.23)$$
To verify the entropy condition, consider the limiting solutions on each side of the shock. To the left of the shock, the limiting solution is determined by the constant initial condition; \( z_l = z_0 \). To the right of the shock, the limiting solution is determined by the rarefaction wave.

\[
z_r(t) = \lim_{x \to x_{r,l}(t)} \frac{z_m}{2} - \frac{z_m x}{2 v_m (t - \tau)} \\
= \frac{z_m}{2} \left[ 1 - \left( 1 - \frac{2z_0}{z_m} \right) + 2 \left( \frac{z_0 \tau}{(z_m - z_0)(t - \tau)} \right)^{1/2} \left( 1 - \frac{z_0}{z_m} \right) \right] \\
= z_0 + \left[ \frac{z_0 \tau}{(z_m - z_0)(t - \tau)} \right]^{1/2} (z_m - z_0)
\]

Note that:

- \( z_r(t_1) = z_m \)
- \( z_r(t) > z_0 \) for all \( t \geq t_1 \)
- \( \lim_{t \to \infty} z_r(t) = z_0 \)

Therefore the entropy condition, \( z_l < z_r \), is satisfied for all \( t \geq t_1 \).

2. Similarly, to find the appropriate initial condition for the right shock, let \( t_2 \) be the time at which the shock (3.19) emanating to the right from \((0, 0)\) intersects the characteristic (3.9) to the right of the rarefaction wave (shifted in time by \( \tau \)). This is the time such that

\[
\frac{v_m (z_m - z_0)}{z_m} t_2 = v_m (t_2 - \tau)
\]

This intersection is the creation of a shock bounding the rarefaction wave on the right, as depicted in Figure 8.
Figure 8: Plot of two shocks and a characteristic. The solid curve and the curve marked by an x are shocks emanating from \( x = 0 \) at \( t = 0 \). The curve marked by an * is a characteristic bordering the rarefaction wave defined by \( x_{cr} = v_m(t - \tau) \). The intersection of the characteristic and shock creates the shock, \( x_{sr} \), at the time, \( t_2 \).

Therefore

\[ t_2 = \frac{z_m \tau}{z_0} \]

To find the right shock after the light turns green, solve the IVP

\[
\frac{dx_{sr}}{dt} = v_m \left[ \frac{1}{2} + \frac{x_{sr}}{2v_m(t - \tau)} - \frac{z_0}{z_m} \right], \quad x_{sr}(t_2) = v_m(t_2 - \tau) = v_m \left( \frac{z_m}{z_0} - 1 \right) \tau
\]

Imposing the initial condition in the general solution (3.22), yields the constant

\[
v_m \left( \frac{z_m}{z_0} - 1 \right) \tau = v_m \left[ 1 - \frac{2z_0}{z_m} \right] \tau \left( \frac{z_m}{z_0} - 1 \right) + c \tau^{1/2} \left( \frac{z_m}{z_0} - 1 \right)^{1/2}
\]

\[
v_m \left( \frac{z_m}{z_0} - 1 \right)^{1/2} \tau^{1/2} = v_m \left[ 1 - \frac{2z_0}{z_m} \right] \tau^{1/2} \left( \frac{z_m}{z_0} - 1 \right)^{1/2} + c
\]

\[
c = \frac{2z_0v_m}{z_m} \left( \frac{z_m}{z_0} - 1 \right)^{1/2} \tau^{1/2}.
\]

The right shock is

\[
x_{sr}(t) = v_m \left[ 1 - \frac{2z_0}{z_m} \right] (t - \tau) + \frac{2z_0v_m}{z_m} \left( \frac{z_m}{z_0} - 1 \right) \left( t(t - \tau) \right)^{1/2}, \quad t \geq t_2 \quad (3.24)
\]
To verify the entropy condition, consider the limiting solutions on each side of the shock. To the left of the shock, the limiting solution is determined by the rarefaction wave. To the right of the shock, the limiting solution is determined by the constant initial condition; $z_r = z_0$.

$$z_l(t) = \lim_{x \to x_{sr}(t)} \frac{z_m x}{2} - \frac{z_m}{2v_m(t - \tau)}$$

$$= \frac{z_m}{2} \left[ 1 - \left( 1 - \frac{2z_0}{z_m} \right) - \frac{2z_0}{z_m} \left[ \left( \frac{z_m}{z_0} - 1 \right) \frac{\tau}{t - \tau} \right]^{1/2} \right]$$

$$= z_0 \left[ 1 - \left[ \left( \frac{z_m}{z_0} - 1 \right) \frac{\tau}{t - \tau} \right]^{1/2} \right]$$

Note that:

- $z_l(t_2) = 0$
- $z_l(t) < z_0$ for all $t \geq t_2$
- $\lim_{t \to \infty} z_l(t) = z_0$

Therefore the entropy condition, $z_l < z_r$, is satisfied for all $t \geq t_2$.

And finally for $\frac{-v_m z_0}{z_m} t < x < 0$ and $\tau \leq t < t_1$ or $0 < x < \frac{v_m(z_m - z_0)}{z_m} t$ and $\tau \leq t < t_2$ the solution to (3.4) - (3.5) applies with time shifted by $\tau$. Using (3.11),
the expression for the solution in this region is

$$z = \begin{cases} 
  z_0 & x < \frac{-v_m z_0}{z_m} t; \quad \tau \leq t < t_1 \\
  \frac{z_m x}{2} - \frac{z_m}{2v_m (t - \tau)} & -\frac{v_m z_0}{z_m} t < x < -v_m (t - \tau); \quad \tau \leq t < t_1 \\
  -v_m (t - \tau) < x < 0; \quad \tau \leq t < t_1 \\
  \frac{z_m x}{2} - \frac{z_m}{2v_m (t - \tau)} & 0 < x < v_m (t - \tau); \quad \tau \leq t < t_2 \\
  v_m (t - \tau) < x < \frac{v_m (z_m - z_0)}{z_m} t; \quad \tau \leq t < t_2 \\
  v_m (z_m - z_0) & v_m (z_m - z_0) t < x; \quad \tau \leq t < t_2 \\
  z_0 & 
\end{cases}$$

(3.25)

Figure 9 includes a plot of all derived shock curves and bordering characteristics. The plot also includes a labeling of the solution values, whether constant or defined by the rarefaction wave, in each of the corresponding regions of the domain. This is used as an outline for building the weak solution.

Figure 9: Plot of all shocks and bordering characteristics. The values of the solution are labeled in each region including the constant values 0, $z_0$ and $z_m$ and the rarefaction wave defined by $z_w$ (3.21).
Weak Solution

Using (3.20), (3.21), (3.23), (3.24) and (3.25), the weak solution to (3.15) - (3.17) is

\[
\begin{align*}
\begin{cases}
z_0 & \text{if } x < -v_m z_0 t; \quad t < t_1 \\
z_m & \text{if } -v_m z_0 t < x < 0; \quad t < \tau \\
z_m & \text{if } -v_m z_0 t < x < -v_m(t - \tau); \quad \tau \leq t < t_1 \\
\frac{z_m}{2} - \frac{z_m x}{2v_m(t - \tau)} & \text{if } -v_m(t - \tau) < x < 0; \quad \tau \leq t < t_1 \\
0 & \text{if } x < x_{sl}; \quad t \geq t_1 \\
\frac{z_m}{2} - \frac{z_m x}{2v_m(t - \tau)} & \text{if } 0 < x < \frac{v_m(z_m - z_0)}{z_m} t; \quad t < \tau \\
z_m & \text{if } 0 < x < v_m(t - \tau); \quad \tau \leq t < t_2 \\
v_m(t - \tau) < x < \frac{v_m(z_m - z_0)}{z_m} t; \quad \tau \leq t < t_2 \\
z_0 & \text{if } \frac{v_m(z_m - z_0)}{z_m} t < x; \quad t < t_2 \\
0 & \text{if } x < x_{sr}; \quad t \geq t_2 \\
\frac{z_m}{2} - \frac{z_m x}{2v_m(t - \tau)} & \text{if } 0 < x < x_{sr}; \quad t \geq t_2 \\
z_0 & \text{if } x_{sr} < x; \quad t \geq t_2 
\end{cases}
\end{align*}
\]

Verification of Solution

To verify that (3.26) is a weak solution of (3.15) - (3.16), one must show that

\[
\int_0^\infty \int_{-\infty}^\infty z \phi_t + f(z) \phi_x dx dt = -\int_{-\infty}^\infty z_0(x) \phi(x, 0) dx, \quad \forall \phi \in C^1_0
\]

As verified on page 29, the rarefaction wave is a solution of the conservation law.

In order to verify that (3.26) is a weak solution, \( \mathbb{R} \times \mathbb{R}^+ \) will be broken into five domains based on the definition of the solution within each domain.

The functions \( x_1(t) \) from (3.18) on the interval \( 0 \leq t \leq t_1 \), \( x_3(t) \) from (3.19) on the interval \( 0 \leq t \leq t_2 \), \( x_{sl}(t) \) from (3.23) on the interval \( t \geq t_1 \) and \( x_{sr}(t) \) from (3.24)
on the interval \( t \geq t_2 \) are the shocks determined by the Rankine-Hugoniot condition. The expressions

\[
x_{cl}(t) = -v_m(t - \tau) \quad \text{and} \quad x_{cr}(t) = v_m(t - \tau)
\]

are the characteristic curves that intersect \( x_1(t) \) and \( x_3(t) \) creating the shocks \( x_{sl}(t) \) and \( x_{sr}(t) \), respectively.

Define the five domains as

\[
D_1 = \{(x, t) \mid x_1(t_1) < x < 0, \ (x_1)^{-1} < t < (x_{cl})^{-1}\}
\]
\[
D_2 = \{(x, t) \mid x < x_1(t), \ 0 < t < t_1\} \cup \{(x, t) \mid x < x_{sl}(t), \ t_1 < t\}
\]
\[
D_3 = X_1 \cup X_2 \cup X_3
\]
\[
D_4 = \{(x, t) \mid x_3(t) < x, \ 0 < t < t_2\} \cup \{(x, t) \mid x_{sr}(t) < x, \ t_2 < t\}
\]
\[
D_5 = \{(x, t) \mid 0 < x < x_3(t_2), \ (x_3)^{-1} < t < (x_{cr})^{-1}\}
\]

where

\[
X_1 = \{(x, t) \mid x_{cl}(t) < x < x_{cr}(t), \ \tau < t < t_1\}
\]
\[
X_2 = \{(x, t) \mid x_{sl}(t) < x < x_{cr}(t), \ t_1 < t < t_2\}
\]
\[
X_3 = \{(x, t) \mid x_{sl}(t) < x < x_{sr}(t), \ t_2 < t\}
\]

Figure 10 is a duplication of Figure 9 where rather than labeling the solution values within the domain, the five domain subsets, \( D_1 - D_5 \), are labeled for clarification of their definition relative to the characteristics and shocks.
Figure 10: Plot of all shocks and bordering characteristics. The five subsets of the domain used for verification of the weak solution are labeled within the graph.

On $D_1$, the solution is given by the maximum density, $z = z_m$ and the double integral over $D_1$ is

$$\iint_{D_1} z\phi_t + f(z)\phi_x dA = \int_{x_1(t_1)}^{0} \int_{(x_1)^{-1}}^{(x_{cl})^{-1}} z_m \phi_t dt dx$$

$$= \int_{x_1(t_1)}^{0} z_m (\phi(x, (x_{cl})^{-1}) - \phi(x, (x_1)^{-1})) dx$$

$$= \int_{x_1(t_1)}^{0} z_m \phi(x, (x_{cl})^{-1}) dx + \int_{0}^{t_1} z_m \phi(x(t, t)) x'(t) dt$$

The left shock, $x_{sl}(t)$, is not monotone and is therefore not invertible. In fact, by using the first derivative test, $x_{sl}(t)$ is initially decreasing, has a unique local minimum and then increases for the rest of time. Let $x_m = \min x_{sl}(t)$ and then $(x_m, t_m)$ is the location of the unique minimum. Define $(x_{sl})_L^{-1}$ to be the inverse on $t_1 \leq t \leq t_m$ and $(x_{sl})_U^{-1}$ to be the inverse on $t > t_m$.

On $D_2$, the solution is given by the constant initial condition, $z = z_0$ and the double integral over $D_2$ is
\[
\iint_{D_2} z_\phi + f(z) \phi z dA = \int_{-\infty}^{x_m} \int_0^\infty z_0 \phi t dt dx + \int_{x_m}^{x_{sl}(t_1)} \int_0^{(x_{sl}(t_1))^{-1}} z_0 \phi t dt dx \\
+ \int_{x_{sl}(t_1)}^{x_1(t)} \int_0^{x_1(t)} z_0 \phi t dt dx + \int_{x_m}^{\infty} \int_0^{(x_{sl}(t_1))^{-1}} z_0 \phi t dt dx \\
+ \int_{0}^{t_1} \int_{-\infty}^{x_{sl}(t)} f(z_0) \phi x dt dx + \int_{t_1}^{\infty} \int_{-\infty}^{(x_{sl}(t))^{-1}} f(z_0) \phi x dt dx \\
= - \int_{-\infty}^{x_m} z_0 \phi (x, 0) dx + \int_{x_m}^{x_{sl}(t_1)} z_0 (\phi(x, (x_{sl})^{-1}) - \phi(x, 0)) dx \\
+ \int_{x_{sl}(t_1)}^{t_1} z_0 (\phi(x, (x_{sl})^{-1}) - \phi(x, 0)) dx - \int_{x_m}^{\infty} z_0 \phi(x, (x_{sl})^{-1}) dx \\
+ \int_{0}^{t_1} f(z_0) \phi(x_1(t), t) dt + \int_{t_1}^{\infty} f(z_0) \phi(x_{sl}(t), t) dt \\
= - \int_{-\infty}^{x_m} z_0 \phi(x, 0) dx + \int_{t_1}^{t_1} z_0 \phi(x_{sl}(t), t) x'_{sl}(t) dt \\
+ \int_{x_{sl}(t_1)}^{t_1} z_0 \phi(x_1(t), t) x'_{sl}(t) dt - \int_{t_1}^{\infty} z_0 \phi(x_{sl}(t), t) x'_{sl}(t) dt \\
+ \int_{0}^{t_1} f(z_0) \phi(x_1(t), t) dt + \int_{t_1}^{\infty} f(z_0) \phi(x_{sl}(t), t) dt \\
= - \int_{-\infty}^{x_{sl}(t_1)} z_0 \phi(x, 0) dx + \int_{t_1}^{\infty} (f(z_0) - z_0 x'_{sl}(t)) \phi(x_{sl}(t), t) dt \\
+ \int_{0}^{t_1} (f(z_0) - z_0 x'_{sl}(t)) \phi(x_1(t), t) dt
\]

On \( D_3 \), the solution is given by the rarefaction wave, \( z = z_w \). On this domain, the rarefaction wave is continuously differentiable and has been shown to satisfy the conservation law.

Let \( t^* > t_m \) be the time such that \( x_{sl}(t^*) = x_{sl}(t_1) \) and \( T \) be the time such that \( x_{sl}(T) = 0 \).

The double integral over \( D_3 \) is
\[
\int_\Omega z \phi_t + f(z) \phi_x dA = \int_{x_{sl}(t_1)}^{x_{sl}(t_2)} z_{w} \phi_t dt + \int_0^T \int_{x_{sl}(t_1)}^{x_{sl}(t_2)} z_{w} \phi_t dt dx
\]
\[
\int\int_{D_4} z\phi_t + f(z)\phi_x dA = \int_0^{x_3(t_2)} \int_0^{(x_3)^{-1}} z_0\phi_t dt dx + \int_{x_3(t_2)}^{\infty} \int_0^{(x_{sr})^{-1}} z_0\phi_t dt dx \\
+ \int_0^{t_2} \int_{x_3(t)}^{\infty} f(z_0)\phi_x dx dt + \int_{t_2}^{\infty} \int_{x_{sr}(t)}^{\infty} f(z_0)\phi_x dx dt \\
= \int_0^{x_3(t_2)} z_0(\phi(x, (x_3)^{-1}) - \phi(x, 0)) dx + \int_{x_3(t_2)}^{\infty} z_0(\phi(x, (x_{sr})^{-1}) - \phi(x, 0)) dx \\
- \int_0^{t_2} f(z_0)\phi(x_3(t), t) dt - \int_{t_2}^{\infty} f(z_0)\phi(x_{sr}(t), t) dt \\
= - \int_0^{t_2} z_0\phi(x, 0) dx + \int_0^{t_2} (z_0x_3'(t) - f(z_0))\phi(x_3(t), t) dt \\
+ \int_{t_2}^{\infty} (z_0x_{sr}'(t) - f(z_0))\phi(x_{sr}(t), t) dt \\
= - \int_0^{t_2} z_0\phi(x, 0) dx + \int_{t_2}^{\infty} (z_0x_{sr}'(t) - f(z_0))\phi(x_{sr}(t), t) dt \\
\text{since} \\
\quad x_3'(t) = \frac{f(z_0)}{z_0}
\]

On \(D_5\), the solution is given by \(z = 0\) and therefore \(\int\int_{D_5} z\phi_t + f(z)\phi_x dA = 0\).

Let

\[U = D_1 \cup D_2 \cup D_3 \cup D_4 \cup D_5\]
then combining the previous five integrals verifies the weak solution.

\[
\int_U z\phi_t + f(z)\phi_x dA = \int_0^\infty \int_{-\infty}^\infty z\phi_t + f(z)\phi_x dt dx
\]

\[
= \int_{x_1(t_1)}^0 z_m \phi(x, (x_{cl})^{-1}) dx + \int_0^{t_1} z_m \phi(x_1(t), t)x'_1(t) dt
\]

\[+ - \int_{x_1(t_1)}^0 z_0 \phi(x, 0) dx + \int_{t_1}^\infty (f(z_0) - z_0 x'_1(t)) \phi(x_{sl}(t), t) dt\]

\[+ \int_0^\infty (f(z_0) - z_0 x'_1(t)) \phi(x_1(t), t) dt\]

\[+ \int_{t_1}^\infty (z_w(x_{sl}(t), t)x'_1(t) - f(z_w(x_{sl}(t), t))) \phi(x_{sl}(t), t) dt\]

\[\]

\[+ \int_{t_1}^\infty z_m \phi(x, (x_{cl})^{-1}) dx\]

\[+ \int_{x_{cl}(t_1)}^\infty (f(z_w(x_{sr}(t), t)) - z_w(x_{sr}(t), t)x'_1(t)) \phi(x_{sr}(t), t) dt\]

\[\]

\[\]

\[= - \int_{x_{cl}(t_1)}^\infty z_0 \phi(x, 0) dx + \int_0^{t_1} [(z_m - z_0)x'_1(t) + f(z_0)] \phi(x_1(t), t) dt\]

\[+ \int_{t_1}^\infty [f(z_0) - f(z_w(x_{sl}(t), t)) - (z_0 - z_w(x_{sl}(t), t)x'_1(t))] \phi(x_{sl}(t), t) dt\]

\[+ \int_{t_1}^\infty [f(z_w(x_{sr}(t), t)) - f(z_0) - (z_w(x_{sr}(t), t) - z_0)x'_1(t)] \phi(x_{sr}(t), t) dt\]

\[= - \int_{x_{cl}(t_1)}^\infty z_0 \phi(x, 0) dx \quad \forall \phi \in C_0^1\]

since

\[x'_1(t) = \frac{f(z_0) - f(z_m)}{z_0 - z_m} = \frac{f(z_0)}{z_0 - z_m}\]

and

\[x'_1(t) = \frac{f(z_0) - f(z_w)}{z_0 - z_w}\]
Parameterized Time

Traffic with one red light at $x = 0$ with parameterized starting time and duration can be modeled by the conservation law

$$ z_t + \left(v_m(x,t) \left(1 - \frac{z}{z_m}\right) z\right)_x = 0 \quad x \in (-L/2, L/2), \quad t > 0 \quad (3.27) $$

$$ z(x,0) = z_0 \quad (3.28) $$

$$ z(-L/2,t) = z_0 \quad (3.29) $$

where

$$ v_m(x,t) = \begin{cases} 0 & x = 0; \quad \xi \leq t \leq \zeta \\ v_m & \text{otherwise} \end{cases} \quad (3.30) $$

$v_m(x,t)$ represents a maximum velocity of $v_m$ except at the location of the red light $x = 0$ where it assumes the value of 0 during the time $\xi \leq t \leq \zeta$

The weak solution can be found by shifting (3.26) in time by $\xi$ and replacing the duration $\tau$ with $\Delta t = \zeta - \xi$. Also, recall $t_1 = \frac{z_m \Delta t}{z_m - z_0}$ and $t_2 = \frac{z_m \Delta t}{z_0}$.

The shifted location of the shocks after the light turns green are

$$ x_l = x_{sl}(t-\xi) = v_m \left[1 - \frac{2z_0}{z_m}\right] (t-\zeta) - 2v_m \left[\frac{z_0 \Delta t (t - \zeta)}{z_m - z_0}\right]^{1/2} \left(1 - \frac{z_0}{z_m}\right) $$

$$ x_r = x_{sr}(t-\xi) = v_m \left[1 - \frac{2z_0}{z_m}\right] (t-\zeta) + 2z_0v_m \left[\frac{z_m}{z_0} - 1\right] (t - \zeta) \Delta t^{1/2} $$
Therefore the weak solution is

\[
\begin{align*}
z &= \begin{cases}
z_0 & \quad t < \xi \\
z_0 & \quad x < \frac{-v_m z_0}{z_m} (t - \xi); \quad t < t_1 + \xi \\
z_m & \quad -v_m z_0 (t - \xi) < x < 0; \quad t < \zeta \\
z_m & \quad \frac{-v_m z_0}{z_m} (t - \xi) < x < -v_m (t - \xi); \\
\frac{z_m}{2} - \frac{z_m x}{2v_m (t - \xi)} & \quad \xi \leq t < t_1 + \xi \\
z_0 & \quad -v_m (t - \xi) < x < 0; \quad \zeta \leq t < t_1 + \xi \\
z_m & \quad x < x_l; \quad t \geq t_1 + \xi \\
0 & \quad x_l < x < 0; \quad t \geq t_1 + \xi \\
z_m & \quad 0 < x < \frac{v_m (z_m - z_0)}{z_m} (t - \xi); \quad t < \zeta \\
0 & \quad 0 < x < v_m (t - \xi); \quad \zeta \leq t < t_2 + \xi \\
v_m (t - \xi) & \quad < x < \frac{v_m (z_m - z_0)}{z_m} (t - \xi); \quad \zeta \leq t < t_2 + \xi \\
\frac{z_m}{2} - \frac{z_m x}{2v_m (t - \xi)} & \quad 0 < x < x_r; \quad t \geq t_2 + \xi \\
z_0 & \quad x < x_l; \quad t \geq t_2 + \xi \\
z_m & \quad x_l < x < 0; \quad t \geq t_2 + \xi \\
z_0 & \quad 0 < x < x_r; \quad t \geq t_2 + \xi \\
z_m & \quad x < x_l; \quad t \geq t_2 + \xi
\end{cases}
\end{align*}
\]

\[(3.31)\]

**DG Performance**

In this section, we give the results of a sample of computations using the DG formulation described in Chapter 2. For the numerical simulation, the maximum density and velocity are normalized to a value of one. Using \(z_0 = 0.31\), \(\xi = 0.2\) and \(\zeta = 0.3\), Figure 11 includes a contour plot of the DG simulation of the solution to (3.27) - (3.29) depicting the expected behavior as in Figure 9. Due to the smoothing of discontinuities and extrema in the solution caused by the use of a slope limiter, error analysis is done in a neighborhood away from the shocks at the final time, as outlined in [10]. Using a linear basis, the minmod slope limiter and \(K = 160\)
elements, Figure 12a includes a graph of the true solution and the DG solution at
the final time $T = 0.7$. There is an excellent agreement between the two solutions
except in a neighborhood of the shocks, as shown by the pointwise error in Figure
12b. In Table 2 the $L^2$ error at the final time $T = 0.7$ is computed for a range of
spatial discretizations from $K = 40$ to $K = 1280$. The error is computed over the
subset of the spatial domain $(-0.5, 0.5)$ satisfying $|x - x_s| \geq 0.01$ where $x_s$ is the
location of a shock at $T$. Note that the convergence is at least first order. In [11],
for a sufficiently smooth flux and monotone numerical flux, the order of convergence
should be $N + 1/2$ where $N$ is the degree of the basis functions used to span the finite
dimensional subspace. Due to the discontinuous nature of the flux function in (3.27),
we do not expect nor do we observe that order of convergence. For some refinements
of the mesh, the order is larger than 1.5 ($N = 1$ for the error calculations), but it is
more commonly less than the expected order if a smooth flux had been used.

![Figure 11: A contour plot of solution $z(x, t)$ with $z_0 = 0.2$ where $v_m(x, t)$ incorporates
a pause at $x = 0$, $\xi = 0.2$ and $\zeta = 0.3$ from equation (3.30). The DG solution was
simulated using a linear basis and 640 elements.](image-url)
(a) The dashed curve is the graph of the DG simulation of the PDE model in (3.27). The solid curve represents the true solution as given in (3.31).

(b) Pointwise error depicting loss of accuracy in a neighborhood of the shocks.

Figure 12: Solution and Pointwise Error at $T = 0.7$ using 160 elements.

<table>
<thead>
<tr>
<th>$K$</th>
<th>$L^2(D)$</th>
<th>order</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td>0.0261613</td>
<td>1.298247</td>
</tr>
<tr>
<td>80</td>
<td>0.01063770</td>
<td>2.562706</td>
</tr>
<tr>
<td>160</td>
<td>0.0018005</td>
<td>3.030085</td>
</tr>
<tr>
<td>320</td>
<td>0.0002204</td>
<td>3.030085</td>
</tr>
<tr>
<td>640</td>
<td>0.0001165</td>
<td>0.9203823</td>
</tr>
<tr>
<td>1280</td>
<td>0.0000428</td>
<td>1.4429830</td>
</tr>
</tbody>
</table>

Table 2: Error calculations at the final time $T = 0.7$ with one pause located at $x = 0$ during the time interval $0.2 < t < 0.3$. $D$ is a subset of the domain defined by $D = \{ x \in (-0.5, 0.5) : |x - x_s| \geq 0.01 \}$ where $x_s$ is the location of a shock at $T$.

Now that convergence of the DG formulation from Chapter 2 for the one pause model has been established, multiple pauses are incorporated into the traffic flow model as parameterized discontinuities in the flux coefficient. Then the model is used to represent the biological process of transcription and numerical simulations of the PDE model are used to study the effect of pauses on the overall transcription time.
CHAPTER 4

BIOLOGICAL MODEL

This chapter begins with a brief summary of the most commonly used models for the study of transcription and translation that led to the use of the traffic flow model used in this work. Models for the elongation stage of transcription and translation fall into three broad categories. The most detailed treat the polymerase motion as a stochastic ratchet with detailed energy balance at each step along the DNA [24, 25, 26]. A simplified class of models have a long tradition in the physics community under the TASEP label (Totally Asymmetric Simple Elongation Process) [27, 28, 29, 30, 31, 32]. It was first proposed by Spitzer in 1970, and in the last 15 years this model has been applied to biological systems including the translation process [33, 34, 32, 3]. The TASEP model consists of particles that stochastically advance along a one-dimensional collection of discrete sites, in a preferred direction and under the exclusion constraint that no two particles can occupy the same position.

The second class of elongation models are ordinary differential equation (ODE) models. A classical model of MacDonald, Gibbs and Pipkin [35, 36] considers a group of identical DNA strands and characterizes the mean occupancy at each position of the strand. The model uses a system of $k$ ordinary differential equations where $k$ is the length of the template strand (see also [37]). The state variables $z_j$ are the
probabilities that the \( j^{th} \) position is occupied by the front of the elongating machine. The state of \( z_j \) is determined by the balance of the rate of elongation \( v_j \) of the front from position \( j \) to \( j + 1 \) and the rate of elongation \( v_{j-1} \) from \( j - 1 \) forward to \( j \)

\[
\frac{dz_j}{dt} = v_{j-1} - v_j. \tag{4.1}
\]

The elongation rate for the interior nucleotides (the ones that are not at the initiation or termination sites) takes the form of a nonlinear expression that accounts for conditional probability that the \( j + 1^{st} \) nucleotide is empty given that the \( j^{th} \) nucleotide is occupied. Assuming that the polymerase occupies exactly one nucleotide along the strand, MacDonald et al. [35] approximate this conditional probability by \( z_j(1 - z_{j+1}) \). The elongation rate, \( v_j \), then takes the form

\[
v_j := \beta_j z_j(1 - z_{j+1}). \tag{4.2}
\]

Here \( \beta_j \) is the rate at which a polymerase moves between the position \( j \) and \( j + 1 \), \( z_j \) is the probability that the position \( j \) is occupied and \((1 - z_{j+1})\) is the probability that the position \( j + 1 \) is empty. Note that the simplicity of (4.2) is predicated on the assumption that the length of a single RNAP is equal to one nucleotide. This assumption does not reflect biological reality. For example, in [38], the length of an RNAP is estimated to be 32 nucleotides.

The third class of models are those where both time and the template strand are assumed to be continuous resulting in a PDE model. Under simplifying assumptions of a constant elongation speed and a termination speed equal to that of elongation
speed, Heinrich and Rapoport [37] consider the process of ribosomal translation. A 2010 paper by Mier-y-Teran-Romero et al. [4] revisits and improves the Heinrich and Rapoport model by starting with the same system of ODEs for occupancy probabilities to explicitly derive a linear hyperbolic partial differential equation model. Their PDE model has the form

$$z_t + (\beta(x,t)z)_x = 0, \quad 0 < x < L, \quad t > 0$$

where $\beta(x,t)$ is the elongation speed as a ribosome passes position $x$ at time $t$. The main assumption needed to derive the linear PDE model in [4] is that the elongation rates, identified with $\beta(x,t)$, change very little in both time and space.

In [5], the approximately constant elongation rate assumption was abandoned and it was shown that the classical nonlinear traffic flow model introduced in the 1950’s by Lighthill and Whitham and separately by Richards [6, 7] can be rigorously linked to the ordinary differential equation model (4.1) for the motion of the polymerase on DNA. Following a similar approach to that of [4], it is shown that the difference equation formed by a time discretization of the ODE model is equivalent to the finite volume formulation of a basic Godunov scheme applied to the traffic flow PDE. Then it can be concluded that a discrete (forward Euler) solution of the system of ODEs converges to a weak solution of the PDE, under an appropriate definition of correspondence between the elongation rate $\beta_j$ in (4.2) and the function $\beta(x,t)$ in the
nonlinear traffic flow model

\[ z_t + (\beta(x,t)(1 - z)z)_x = 0, \quad 0 < x < L, \quad t > 0. \]

A benefit of the nonlinear model over the previously studied linear model [4] is that it can be used to investigate the effect of “crowding” or high density of polymerases.

**Nonlinear Model**

In [5], Davis et al. propose the classic traffic flow PDE as a continuum model to quantify the effect of ubiquitous pauses on the rate of RNAp transcription. We begin by making the simplifying assumption that the length of the polymerase consists of one nucleotide. Since one nucleotide is occupied by a single polymerase during the transcription process, the maximum density parameter from (3.3) is \( z_m = 1 \). The nonlinear model has the form

\[
\begin{align*}
    z_T + [\bar{\beta}(X,T)(1 - z)z]_X &= 0, \quad X \in (-L/2, L/2), \quad T > 0 \quad (4.3) \\
    z(X,0) &= z_0 \quad (4.4) \\
    z(-L/2,T) &= z_0 \quad (4.5)
\end{align*}
\]

where \( T \) is time measured in seconds, \( X \) is a continuum version of the length of a DNA strand that would be measured in units of the number of nucleotides in a discrete setting, and \( L \) is the length of the DNA strand in terms of those units. The function \( z(X,T) \) represents the density of RNAp on the DNA strand as a function of space and time. The location and time duration of the transcriptional pauses are
specified through the definition of the coefficient \( \bar{\beta}(X, T) \), within the flux function, in a piecewise manner described formally at first as

\[
\bar{\beta}(X, T) = \begin{cases} 
0 & \text{pause} \\
v_m & \text{no pause}
\end{cases} = v_m \begin{cases} 
0 & \text{pause} \\
1 & \text{no pause}
\end{cases} = v_m \beta(X, T) \quad (4.6)
\]

where \( v_m \) is the (constant) maximum velocity. The definition of the flux coefficient specifying the location of the pauses will be made more precise after a rescaling of time and space to nondimensional variables.

**Nondimensional Model**

The flux function of the nonlinear model is differentiable except on a set of measure zero due to the discontinuity in the flux coefficient. For the numerical simulations, time and space are rescaled to

\[
t = \frac{v_m T}{L} \quad \text{and} \quad x = \frac{X}{L}
\]

Therefore if \( g(X, T) = g(X(x), T(t)) \) is a differentiable function almost everywhere, then by the multivariable chain rule

\[
\frac{\partial g}{\partial T} = \frac{\partial g}{\partial t} \frac{dt}{dT} = \frac{v_m}{L} g_t \\
\frac{\partial g}{\partial X} = \frac{\partial g}{\partial x} \frac{dx}{dX} = \frac{1}{L} g_x
\]

Using the dimensionless variables, (4.3) is equivalent to

\[
\frac{v_m}{L} z_t + \frac{1}{L} (v_m \beta(x, t)(1 - z) z)_x = 0, \quad x \in (-0.5, 0.5), \quad t > 0
\]
which simplifies to

\[ \frac{\partial z}{\partial t} + (\beta(x,t)(1-z))_x = 0, \quad x \in (-0.5, 0.5), \quad t > 0 \]

Combining the rescaled PDE with the initial and boundary data, one arrives at

the nondimensional traffic flow model considered for the remainder of this work is

\[ \frac{\partial z}{\partial t} + (\beta(x,t)(1-z))_x = 0, \quad x \in (-0.5, 0.5), \quad t > 0 \quad (4.7) \]

\[ z(x, 0) = z_0 \quad (4.8) \]

\[ z(-0.5, t) = z_0 \quad (4.9) \]

Now we briefly describe the choices for \( z_0 \) and \( \beta(x,t) \) that are based on the

biological literature available for rrn operon or other genes. According to [39], there

are on average 53.4 RNAp on the rrn operon. Since the length of the RNAp is 32

nucleotides [38] and the length of the rrn operon is 5450 nucleotides, an estimate of

the amount of the DNA strand that is covered is approximately \( \frac{53.4(32)}{5450} = 0.31 \);

that is, on average 31% of the DNA strand is occupied by polymerase. This is

incorporated into the PDE model as constant initial and boundary conditions (4.8) -

(4.9); \( z_0 = 0.31 \).

The piecewise constant flux coefficient is determined by the experimental results

in [1] reporting the duration of the transcriptional pauses and is defined in terms of

the location in space and time and the length of the pause. For \( i = 1, 2, \ldots M \), \( x_i \) is

the (spatial) nucleotide location of the \( i \)th pause, \( t_i \) is the time at which the pause

begins and \( d_i \) is the time duration of the pause. Here, both \( t_i \) and \( d_i \) are assumed to
be measured in dimensionless time (using the conversion factor $v_m/L$).

$$\beta(x,t) = \begin{cases} 
0 & x = x_i \text{ and } t_i \leq t \leq t_i + d_i, \text{ for } i = 1, 2, \ldots M \\
1 & \text{otherwise}
\end{cases}$$

(4.10)

The pauses are uniformly distributed in both time and space using Matlab’s random number generator. Using the experimentally observed pause duration mean times of $1.2 \pm 0.1$ seconds with amplitude 60% and $6 \pm 0.4$ seconds with amplitude 40% [1], the pause durations are determined using the exponential probability distribution function

$$p(t) = \frac{0.6L}{v_m\mu_1}e^{-\frac{vt}{vm\mu_1}} + \frac{0.4L}{v_m\mu_2}e^{-\frac{vt}{vm\mu_2}}$$

where $\mu_1 = 1.2$ and $\mu_2 = 6$.

To summarize the approach, for a given initial and background density of $z_0$ and for a given realization of a set of pauses generated in the manner described above, equations (4.7) - (4.9) are used to determine the RNAp density over a chosen time interval $[0, T]$. One is then able to compute the total transcription time and assess the effect that a given set of pauses has on the average transcription time experienced by an average RNAp. The following section describes the computation of the average time delay experienced by each RNAp and how that computation leads to an initial assessment of the effects of transcriptional pauses.

**Delay Due to Pauses**

In Escherichia coli, an rrn operon of length 5450 nucleotides has been studied and estimated to transcribe on average in 60 seconds, [40]. If one assumes that the
elongation rate of the RNAp is constant and that the transcribing polymerase does not experience any pausing, then using a basic \( d = rt \) relationship, an estimate of the average transcription speed is 91 nt/sec. However, it is known from experimental results that polymerase pause frequently during the transcription process causing a delay in the overall transcription time and affecting the instantaneous transcription speed, [1, 41, 5, 42]. Due to the delay in the transcription time, the transcription speed is expected to be faster than the previous basic estimate. Using the numerical simulations of the traffic flow model, the effect of the pauses on the transcription time is quantified and the average experienced delay is used to estimate the instantaneous transcription speed.

**Quantifying the Delay**

In order to determine the effect the pauses have on RNAp transcription, the solution of (4.7) - (4.9) with flux coefficient (4.10) is compared to the solution of the same PDE (4.7) - (4.9) using a constant maximum velocity flux coefficient, \( \beta(x, t) = 1 \) for all \((x, t)\).

The flux function from (4.7) is given by

\[
f(z(x, t)) = \beta(x, t)(1 - z)z .
\]

For any \( t > t_0 \), the number of polymerase that has reached the termination site, \( x = 0.5 \), in the time \([t_0, t]\) is given by

\[
F(t) = \int_{t_0}^{t} f(z(0.5, u))du .
\]
Given constant initial and boundary conditions, if $\beta(x, t) = 1$ for all $(x, t)$, then the solution to the model problem is also constant, $z(x, t) = z_0$ for all $(x, t)$. Using this solution, the flux at the termination site, referred to as the reference flux, is constant,

$$f_R = z_0(1 - z_0).$$

Therefore, if the polymerase does not pause during the transcription process and if the initial density is a constant, $z_0$, then the total number of polymerase to reach the termination site of the DNA strand during the $[t_0, t]$ is given by

$$N(t) = \int_{t_0}^{t} f_R du = z_0(1 - z_0)(t - t_0).$$

To determine the delay, the amount of additional time required for an $N(t)$ amount of polymerase that has encountered pauses to reach the termination site must be computed. For any $t > t_0$, the goal is to calculate the amount of time required for the polymerases that have been stopped by pauses to reach the right boundary and compare that time with the amount of time that is required for the same number of polymerases that have not encountered pauses to arrive at the termination site. To find this comparable time, define $q(t)$ to be the instant of time such that

$$\int_{t_0}^{q(t)} f(z(0.5, u)) du = N(t) = f_R(t - t_0).$$

(4.11)

The time, $q(t) - t$, is the delay experienced by flux of polymerase. The estimated
average delay per polymerase over the interval \([t_0, t_1]\) is then calculated by

\[
d(t_0, t_1) = \frac{1}{\int_{t_0}^{t_1} f(z(0.5, t))dt} \int_{t_0}^{t_1} f(z(0.5, t))(q(t) - t)dt
\]

(4.12)

where \(t_0\) is an arbitrary time before the first of the delayed polymerases reached the right boundary and \(t_1\) is an arbitrary time after the last of the polymerases affected by the pause has reached the termination site.

**Computation of \(q(t)\)**

To compute the flux at the termination site, the model problem (4.7) - (4.9) is solved using a DG formulation with a linear basis and the local Lax-Friedrichs numerical flux, as described in Chapter 2. In order to compute \(q(t)\), the integral of the flux at the termination site must be approximated. Since the flux is known at the time values used to solve the system of ODEs (2.6) from the semi-discrete form of the PDE, \(q(t)\) is initialized as this set of discrete time values, \(\{q_0, q_1, \cdots, q_m\}\) with \(q_0 = t_0\) and then \(t\) is left to be determined using (4.11). The integral of the flux is approximated using the Composite Trapezoid Rule with the set of time values from the ODE solve and the new set of discrete time values is computed as

\[
t_i = t_0 + \frac{1}{f_R} \int_{t_0}^{q_i} f(z(0.5, u))du, \quad i = 0, 1, \cdots, m.
\]

(4.13)

The Composite Trapezoid Rule provides the approximation

\[
t_i = t_0 + \frac{1}{f_R} \sum_{j=1}^{i} \frac{1}{2} [f(z(0.5, q_j)) + f(z(0.5, q_{j-1}))](q_j - q_{j-1}), \quad i = 1, 2, \cdots, m.
\]
The Composite Trapezoid Rule is used to approximate the integral of the flux because it uses a low order approximation to the integrand. Once multiple pauses are introduced to the system as discontinuities in the flux coefficient (4.10), as is the case in the biologically relevant model, the flux function at the termination site becomes highly oscillatory. For the oscillatory and non-differentiable integrand, less error is introduced by using a lower order approximation to the integral. Therefore in order to compute the average delay over a subset of the time interval (4.13), the numerically approximated flux from the DG solution is interpolated at these time values using Matlab’s linear interpolation function and the Trapezoid rule is used to approximate the integrals within the delay formula (4.12).

The delay calculation is first applied to the one pause model. Using the weak solution derived in Chapter 3, error analysis is conducted showing convergence as the spatial mesh size is refined.

**Error Calculations for the Delay**

Consider the model problem (4.7) - (4.9) with $z_0 = 0.31$ and flux coefficient given by

$$\beta(x,t) = \begin{cases} 
0 & x = 0; \ 0.2 \leq t \leq 0.3 \\
1 & \text{otherwise}
\end{cases} \quad (4.14)$$

Figure 13 includes graphs of the true and numerically approximated density and the corresponding computed flux at the termination site. The DG solution is simulated using 160 elements, a linear basis and the local Lax-Friedrichs numerical flux.
The weak solution is provided on page 50 in Chapter 3. For the true delay calculation, the parameter values used in (3.31) are \( \xi = 0.2, \, \zeta = 0.3 \) and \( z_m = v_m = 1 \).

There is a similar loss of accuracy in the density at the termination site, \( z(0.5, t) \), in a neighborhood of the traveling shock as observed in the density at the final time, \( z(x, T) \), in Figure 12a of Chapter 3 due to the use of a slope limiter.

Figure 13: DG and true solution of the nonlinear PDE at \( x = 0.5 \) where a pause is located at \( x = 0 \) during times \( 0.2 \leq t \leq 0.3 \) using 160 elements. The solid curve is the true solution and the dashed curve is the solution using a DG simulation.

Using the true solution (3.31) at \( x = 0.5 \) to compute the flux function and \( q(t) \) from (4.11), the true value of the delay over the interval \( (0, 2.84) \) is estimated to be \( D = 0.0422086 \) in dimensionless time. The right end point of time 2.84 was chosen so that all polymerases affected by the pause have reached the termination site and the density at \( x = 0.5 \) has returned to the constant density of \( z_0 = 0.31 \). Table 3 includes the delay, \( d \), computed using the DG simulation to evaluate the flux at
\( x = 0.5 \) for a range of spatial discretizations. The DG simulation was computed using \( \Delta t = 0.0001 \) so that the CFL condition of the TVD RK method was satisfied for each of the considered mesh sizes. The table compares the average delay using the true solution and the DG solution showing first order convergence.

| \( K \) | \( d \)  | \( |D - d|\)  | order     |
|-------|--------|--------|-----------|
| 40    | 0.0316603 | 0.0105483 |            |
| 80    | 0.0374607 | 0.0047480 | 1.1516275  |
| 160   | 0.0399146 | 0.0022940 | 1.0494425  |
| 320   | 0.0410612 | 0.0011474 | 0.9994793  |
| 640   | 0.0416378 | 0.0005709 | 1.0071947  |
| 1280  | 0.0419272 | 0.0002814 | 1.0203922  |

Table 3: The average delay for the model in (4.7)–(4.9) with (4.14) computed using the DG solution with a variety of spatial grids. The error in the third column is computed using the average delay computed using the true solution.

In the previous paragraphs, convergence of the delay calculation for the single pause model using a DG formulation has been established. Expanding on this result by incorporating several pauses into the model, so as to be consistent with experimental results, the delay calculation can be used to improve on the estimate for the instantaneous transcription speed to recover the transcription time of 60 seconds.

**Multiple Pause Model**

In order to determine the effect of pausing, the PDE model (4.7) - (4.9) is simulated with several pauses incorporated into the flux coefficient, (4.10). The number of pauses has not been measured for ribosomal RNA transcription, but it is assumed
that polymerase on the rrn operon encounter pauses in amount that is consistent with
other genes. In [43, 42], it has been observed that polymerase encounter six pauses
per minute of elongation. If \( \tau \) is the mean duration of a pause and a polymerase
initiates on the DNA strand at time, \( t \), where \( t \in [0, T] \) for a final time \( T \) in seconds,
then the polymerase will encounter six pauses if there are

\[
n = \frac{6T}{\tau}
\]  

(4.15)

pauses uniformly distributed in time and space. The location and duration of the
pauses are defined by the flux coefficient, \( \beta(x, t) \). Using the bi-modal mean duration
times observed in [1], the weighted mean duration time is

\[
\tau = 0.6(1.2) + 0.4(6) = 3.12 
\]

seconds where forty percent of the pauses are chosen to be long pauses with mean
duration 6 seconds and the other sixty percent are short pauses with mean duration
1.2 seconds.

Since the instantaneous transcription speed that allows for pausing is expected
to be faster than 91 nt/sec, the PDE model is simulated for a range of elongation
velocities, \( v_m \), beginning at 90 nt/sec and ending with 220 nt/sec. Using the computed
delay value, the transcription time is then calculated to see if the experimentally
observed time of 60 seconds is achieved.

In Figure 14, the PDE model was simulated using a DG formulation with 1000
elements and a linear basis for the spatial discretization and the local Lax-Friedrichs
numerical flux. For each choice of the elongation speed and each realization of pauses,
the PDE solution is simulated using a final time sufficient for computing the delay
over five minutes of transcription time. Then using average delay per polymerase, the average crossing time, or time needed for the polymerase to transcribe the DNA, is computed as

\[ CT = \frac{L}{v_m} (1 + d) \]  

(4.16)

where \( L = 5450 \) is the length of the rrn operon, \( v_m \) is the elongation speed in nt/sec and \( d \) is the average delay as defined in (4.12). The delay is computed over the time interval \( \left( 1, 1 + \frac{300L}{v_m} \right) \) of length equivalent to five minutes where the left endpoint of 1 is chosen since that is the amount of dimensionless time required to travel from initiation to termination without any pausing. In Figure 14a, for each elongation speed, ten simulations were run using a randomization of \( n \) (4.15) pauses and the corresponding crossing times were indicated with an x. The circle indicates the average of the ten crossing times. Note that the average crossing times are all within the range of 200 - 350 seconds, significantly higher than the desired 60 second transcription time. One theory to explain this is that the assumption that the rrn operon experiences the same number of pauses as other genes is incorrect. To test this theory, in Figure 14b, similar calculations were performed, but the number of pauses was decreased. For each simulation, the number of pauses was chosen to be \( n = \frac{T}{\tau} \), one-sixth the number proposed originally. The resulting crossing time values were in the much more reasonable range of 40 - 140 seconds, but in both sets of simulations, the variability in the average crossing time for a fixed elongation speed is high.

Figures 15a and 15b include the realizations of uniformly distributed (in space and
(a) The number of pauses were chosen using (4.15).

(b) The number of pauses were chosen using one-sixth the amount defined by (4.15).

Figure 14: Crossing times calculated for a range of elongation speeds, \( v_m \). Ten simulations were run for each of the selected speeds using pauses uniformly distributed in time and space.

time) pauses for the two simulations corresponding to the minimum and maximum crossing times for elongation speed \( v_m = 150 \text{ nt/sec} \) in Figure 14b. The blue indicates points in the \( xt \)-plane for which \( \beta(x, t) = 0 \) and defines the spatial (nucleotide) location and duration of the pauses. Using the solution to the PDE model with this flux coefficient, the flux, \( f(z(x, t)) = z(1 - z) \), is computed at the termination site \( x = 0.5 \) as a function of time, \( t \), and graphed in Figures 15c and 15d. The incorporation of several pauses into the PDE model produces a highly oscillatory flux function that must be integrated when defining \( q(t) \) and computing the average delay value. Figures 15e and 15f show how these pause distributions produce \( q(t) \) functions with differing behavior. For this elongation speed and ten randomizations of pauses, the minimum crossing time is 69 seconds and the maximum is 132 seconds.
(a) Set of pauses that produces the minimum crossing time value.

(b) Set of pauses that produces the maximum crossing time value.

(c) Using the pauses in Figure 15a, plot of the flux at the termination site.

(d) Using the pauses in Figure 15b, plot of the flux at the termination site.

(e) Plot of $t$ and $q(t)$ defined by the flux in Figure 15c used to compute the delay.

(f) Plot of $t$ and $q(t)$ defined by the flux in Figure 15d used to compute the delay.

Figure 15: Comparison of the pause distributions and the resulting flux and $q(t)$ functions for the minimum (69 sec) and the maximum (132 sec) crossing time values for $v_m = 150$ nt/sec in Figure 14b.
Parameter Studies

The calculations in the previous section indicate that there is a high variability in the delay function due to the randomization of the pause locations and durations. For preliminary analysis of the interaction among pauses, a first study is done showing monotonicity in the delay with respect to spatial location and then two parameter studies are considered showing a complex interaction between two pauses. In the first case, two pauses have a fixed duration and spatial location and the average delay is calculated as a function of the time between the pauses. In the second case, two pauses have a fixed duration and time between pauses and the average delay is calculated as a function of the spatial location of the later pause.

Parameterized Location of One Pause

For this analysis, one pause with a fixed starting time and duration is considered. The flux coefficient function is defined by

\[
\beta(x, t) = \begin{cases} 
0 & x = -0.4 + \frac{i}{200}; \quad 0.2 \leq t \leq 0.3 \\
1 & \text{otherwise}
\end{cases}
\]

for \(i = 0, 1, 2, \cdots, 160\) so that the spatial location of the pause varies from \(x = -0.4\) to \(x = 0.4\) within the overall spatial domain \([-0.5, 0.5]\).

In Figure 16, using \(\beta = 132\) nt/sec, the average delay per polymerase is computed over the dimensionless time interval \((0, 4.2)\) and plotted as a function of the spatial location of the pause. Over a fixed time interval, the delay function is monotonically decreasing as a function of the spatial location of the pause. This study suggests
that pauses that occur closer to the initiation site cause a larger delay value and therefore polymerase have a larger transcription time than pauses that occur near the termination site.

Figure 16: Results of the first parameter study showing monotonicity of the delay function.

Parameterized Time Between Pauses

For this analysis, two nonoverlapping pauses are fixed at the same spatial location and have the same fixed duration. The flux coefficient function constructing the pauses is defined by

$$
\beta(x, t) = \begin{cases} 
0 & x = 0; \quad 0.2 \leq t \leq 0.3 \quad \text{or} \quad 0.4 + i(0.1) \leq t \leq 0.5 + i(0.1) \\
1 & \text{otherwise}
\end{cases}
$$

where $i = 1, 2, \ldots, 58$. The parameter, $i$, is used to define the time between the end of the first pause and the beginning of the second pause. The average delay per polymerase is calculated for each parameter $i$ over the time interval $(0, 12.585)$. The initial density as defined in (4.8) is also varied to determine if the interaction between
the two pauses is enhanced by the background density value.

(a) Surface plot of the average delay for a range of initial density values \((4.8)\) and time between the two pauses. 

(b) Cross sections of the average delay plot for several initial density values \(z_0\) in \((4.8)\) and time between the two pauses.

Figure 17: Results of parameter study beginning on page 71.

Figure 17a shows that for each choice of background density \(z_0\), there is a minimum delay value (Figure 17b), as the parameter \(i\) determining the time between the two pauses is varied from 0.2 to 5.9 in small increments. And as the initial/background density increases, the minimum delay value is achieved using a larger time between the pauses.

**Parameterized Location of a Second Pause**

For this analysis, one pause is fixed at \(x = 0\) during the times \(0.1 \leq t \leq 0.15\) and the spatial location of the second pause is varied but its time duration is also fixed at 0.05. The interaction of these two pauses produces an average delay function that attains both local minimum and local maximum values. For the simulations,
the second pause is spatially located at $x = -0.4 + i/200$ for $i = 0, 1, 2, \cdots, 160$ during the times $0.6 \leq t \leq 0.65$. This includes locations that are effectively located at nucleotide locations that are behind the fixed pause on the DNA as well as some which are located ahead of it on the strand.

Figure 18: Results of parameter study beginning on page 72.

A local maximum and two local minima in the delay are observed in Figure 18a. This indicates that the interaction of the backup caused by these pauses can affect
the overall average crossing times of the RNAP in complex ways, thereby affecting the total number of mRNAs that are produced in a given time period. Figures 18c and 18d include the contour plots of the simulations corresponding to the local minimum delay values indicating that the minima occur when the starting time and location of the second pause intersects the shock emanating from the release of the first pause. Figure 18b includes the contour plot of the simulation corresponding to the maximum delay value indicating that it occurs when the characteristic created by the release of the second pause intersects the shock emanating from the first pause.
Based on over 20 years of molecular studies, biologists assert that in *E. coli* there exists a complex control mechanism that aligns the cell’s rRNA production rate with its protein requirements, [2]. The results in the section entitled Parameter Studies on page 70 clearly indicate that when multiple pauses are incorporated into the transcription model, the average transcription time of an RNA polymerase is increased (when compared with an average transcription time when no pauses are introduced into the model), thereby the rate of protein production is also affected. Indeed, Figure 18 indicates that the spatial locations of the pauses affect the average delay experienced per RNAp in complicated ways. Certain configurations of two pauses are shown to minimize the average delay; while another configuration is show to result in a maximum delay value. Similar phenomena has been studied in the related mechanism of mRNA translation by Chou and Lakatos [3]. Using a TASEP model with inhomogeneous hopping rates, the work in that paper demonstrates that the existence of one so-called “defect” or “bottleneck” codon can significantly decrease the elongation speed and thereby decrease protein production. This defect codon is the translational process equivalent of our RNAp pause located at a specific nucleotide. Moreover, Chou and Lakatos show that a carefully chosen cluster of a small number
of these defect codons can reduce protein production by at least a factor of two. They also assert that configurations where multiple defect codons are spaced more than a certain number of codons away from each other have little affect on the total protein production. One goal of the current research is to apply sensitivity analysis techniques to the traffic flow model developed in Chapter 4 in order to investigate a similar clustering phenomena in the context of transcription. In the following paragraphs, we pose a very basic model optimization problem related to the idea of the clustering of transcriptional pauses. This serves to motivate the discussion of the main topic of sensitivity computation in this chapter.

Consider the delay function given in equation (4.12) defined over a fixed time interval and dependent on a spatial parameter, \( \tau \), defining pause location. We seek to find the value \( \tau^* \) that minimizes the cost function

\[
J(\tau) = \frac{1}{\int_{t_0}^{t_1} f(z(0.5, t; \tau)) dt} \int_{t_0}^{t_1} f(z(0.5, t; \tau))(q(t) - t) dt
\]

subject to the constraint that \( z(x, t; \tau) \) satisfies

\[
z_t + (\beta(x, t)(1 - z))_x = 0, \quad x \in (-0.5, 0.5), \quad t > 0
\]

\[
z(x, 0) = 0.31
\]

\[
z(-0.5, t) = 0.31
\]

where

\[
\beta(x, t) = \begin{cases} 
0 & x = 0; \ t_1 \leq t \leq t_1 + d \\
& \text{or } x = \tau; \ t_2 \leq t \leq t_2 + d \\
1 & \text{otherwise}
\end{cases}
\]
and the parameter $\tau$ is restricted to belong to the set $\tau \in (-0.5, 0) \cup (0, 0.5)$. To quantify the affect of pause clustering, we optimize the delay function subject to $z(x, t; \tau)$ satisfying the traffic flow model for transcription. If one uses a gradient approach to solving this optimization problem, then one seeks to find $\tau^* \in (-0.5, 0) \cup (0, 0.5)$ such that

$$\frac{d}{d\tau} J(\tau^*) = 0.$$ 

Foregoing a lengthy discussion, we note that the computation of this derivative also requires the computation of the sensitivity, $s(x, t; \tau) = \frac{d}{d\tau} z(x, t; \tau)$. The focus of this chapter is two-fold. The first covers a portion of the mathematical process required to derive a sensitivity equation for a problem of this type. A sensitivity equation is one for which the sensitivity function $s(x, t; \tau)$ is a solution. These equations are particularly tricky when the parameter of interest is one that determines spatial locations of discontinuities in the data within a PDE. The second focus of this chapter is the construction of appropriate numerical methods for computing these types of sensitivities. We begin with a general discussion of sensitivity analysis and then move to a basic linear conservation law problem that illustrates some of the basic ideas as well as the subtle issues that must be considered to obtain accurate sensitivity calculations.

Sensitivity analysis is the study of how small changes in parameters of a mathematical model affect the state variables of the model. When considering spatial
parameters that define an interface or the location of discontinuities within the coefficients of a differential equation, solutions of the state equation and sensitivity equation typically do not belong to the same function space because of differing smoothness properties of the solutions. Hence, one must take care when posing numerical methods for finding the weak solutions to both the state and sensitivity equations simultaneously. In [44], Davis et al. demonstrated for an elliptic problem that complications can arise when attempting to implement a traditional finite element method to solve coupled state and sensitivity equations with interface conditions unless the sensitivity equation is posed correctly and appropriate basis functions for each finite element space are used. In order to avoid the issues encountered when using a standard finite element method, a discontinuous Galerkin finite element method is used to study sensitivities with respect to interface parameters. The DG method is considered primarily for the assumed piecewise continuous nature of the approximate solution. Since smoothness is imposed only on the local solution on each element, a convenient and computationally efficient result of implementing a DG formulation for solving the coupled state and sensitivity equations is that the basis functions and resulting mass and stiffness matrices are used for both approximations reducing the cost of the numerical method.

Computations of sensitivities fall into two broad categories: “discretize-then-differentiate” methods or “differentiate-then-discretize” methods. In the first class of methods, a numerical scheme is used to approximate the state function and then
at the discrete level, an approximation, most commonly a finite difference, of the derivative of the state with respect to a parameter is computed to find the sensitivity. From the notation used in our previous discussion, the expression for the sensitivity takes the form
\[
s(x, t; \tau) = \frac{d}{d\tau} z(x, t; \tau) \approx \frac{z(x, t; \tau + \Delta \tau) - z(x, t; \tau - \Delta \tau)}{2\Delta \tau}.
\]
In the second class of methods known as Continuous Sensitivity Equation Methods (CSEMs), the sensitivity equation is derived by formally differentiating the PDE and initial/boundary data for the state function with respect to the studied parameter. Then the sensitivity PDE is discretized, and a numerical method is imposed to calculate the sensitivity. For the work presented in this chapter, the CSEM is imposed to compute sensitivities with respect to a spatial parameter.

In the following section, the sensitivity with respect to a spatial parameter for a linear conservation law is derived and a discontinuous Galerkin finite element method formulation to solve the coupled state and sensitivity equations is proposed. This is preliminary work done in order to develop the appropriate numerical flux functions for the sensitivity equation resulting from the interface conditions and to illustrate the difficulties that arise even with a basic linear problem. The goal of ongoing research is to apply these results to the nonlinear traffic flow model and to demonstrate that one can use sensitivity analysis to pose some basic optimization problems that address issues related to spatial clustering of transcriptional pauses. We begin with a basic linear PDE and systematically develop the weak solutions and interface conditions
required to carefully derive the appropriate sensitivity PDE.

**Linear Conservation Law**

Initially, the basic advection equation is considered

\[ \frac{\partial z}{\partial t} + a \frac{\partial z}{\partial x} = 0, \quad x \in (L, R), \quad t > 0 \] (5.1)

\[ z(x, 0) = z_0(x) \] (5.2)

\[ z(L, t) = g(t) \] (5.3)

where the advection speed, \( a \), is assumed to be a positive constant so that \( x = L \) is the inflow boundary and it is appropriate to assign a boundary condition at this endpoint of the spatial domain. The functions \( z_0(x) \) and \( g(t) \) denote the initial and boundary conditions, respectively. Assume that the initial and boundary conditions are defined so that \( z_0(L) = g(0) \) and \( az_0'(L) = -g'(0) \). This assumption ensures that (5.1) - (5.3) has a smooth solution for every point in its domain, \( D = \{(x, t) : x \in [L, R], t > 0\} \).

Once the exact solution is derived, the advection speed is replaced with a piecewise constant coefficient function introducing an interface into the basic model problem. The exact solution of the advection equation can then be used to derive a weak solution of the linear conservation law with a discontinuous flux function.

**Exact Solution**

The exact solution of (5.1) - (5.3) can be found using the method of characteristics. This is a standard example and can be found in most PDE text books, see [8] for
example. Let \( x = x(t) \) be a characteristic curve and examine how the solution, \( z = z(x(t), t) \), changes along the characteristic. Using the chain rule, the total derivative with respect to \( t \) is

\[
\frac{d}{dt} z(x(t), t) = z_x(x(t), t)x'(t) + z_t(x(t), t)
\]

From the conservation law (5.1),

\[
z_x(x(t), t)a + z_t(x(t), t) = 0
\]

Combining these results, the characteristic curves are defined by the system

\[
x'(t) = a \tag{5.4}
\]

\[
\frac{d}{dt} z(x(t), t) = 0 \tag{5.5}
\]

The second equation (5.5) of the system states that \( z(x, t) \) is constant along the characteristic curve, \( x(t) \). If \( x(0) = x_0 \) and \( z(x(0), 0) = z(x_0, 0) \) is known using the initial condition, then \( z(x(t), t) = z(x_0, 0) \) for all \( t > 0 \). To determine the characteristic equations, solve the IVP

\[
x'(t) = a, \quad x(0) = x_0
\]

to find

\[
x(t) = at + x_0
\]

In the \( xt \)-plane, the characteristics are lines with slope \( m = \frac{1}{a} \) as defined by

\[
t = \frac{1}{a} (x - x_0)
\]
and plotted in Figure 19.

If \((x, t)\) lies on the characteristic \(x(t)\) and \(x_0 > L\) and therefore \(x > at + L\), then \(x(t)\) intersects \(t = 0\) before it intersects \(x = L\) in the \(xt\)-plane and the solution of the PDE is given by the initial condition.

\[
z(x, t) = z(at + x_0, t) = z_0(x_0) = z_0(x - at), \quad x > at + L
\]

If \((x, t)\) lies on the characteristic \(x(t)\) and \(x_0 < L\) and therefore \(x < at + L\), then \(x(t)\) intersects \(x = L\) before it intersects \(t = 0\) in the \(xt\)-plane and the solution of the PDE is given by the boundary condition. The line through \((L, t_0)\) with slope \(m = \frac{1}{a}\) is

\[
t - t_0 = \frac{1}{a} (x - L)
\]

Therefore if the characteristic through \((x, t)\) also passes through \((L, t_0)\) where \(t_0 > 0\), the solution of the PDE is

\[
z(x, t) = z(at + x_0, t) = g(t_0) = g \left( t - \frac{x - L}{a} \right), \quad x < at + L
\]
The exact solution of the scalar advection equation is

\[
z(x, t) = \begin{cases} 
g(t - \frac{x-L}{a}), & L \leq x \leq at + L 
z_0(x - at), & at + L < x \leq R \end{cases}
\] (5.6)

Note: Since \( z_0(L) = g(0) \), then the solution is defined to be \( z(x, t) = z_0(x - at) = g(t - \frac{x-L}{a}) \) on the characteristic line \( x = L + at \).

**Piecewise Continuous Flux Function**

In order to develop a DG formulation to analyze sensitivities with respect to spatial interface parameters, a piecewise constant flux coefficient is introduced into the advection equation, and the weak solution of the state and sensitivity with respect to the parameterized spatial location of the discontinuity are studied. Although quite basic, this example provides us with insight into the appropriate numerical flux function for the DG calculations. Consider the PDE

\[
z_t + (a(x; \tau)z)_x = 0, \quad x \in (L, R), \quad t > 0
\] (5.7)

\[
z(x, 0) = z_0(x)
\] (5.8)

\[
z(L, t) = g(t)
\] (5.9)

where

\[
a(x; \tau) = \begin{cases} 
a_1, & L \leq x \leq \tau 
a_2, & \tau < x \leq R \end{cases}
\]

and \( a_1 \) and \( a_2 \) are assumed to be positive to remain consistent with \( x = L \) being an inflow boundary. As in the previous section, assume that the initial and boundary conditions are defined so that \( z_0(L) = g(0) \) and \( a_1z'_0(L) = -g'(0) \).
Restricting the spatial domain to $[L, \tau]$, the flux coefficient is single valued, $a(x; \tau) = a_1$, and the PDE (5.7) reduces to the advection equation. Using (5.6), the weak solution on $[L, \tau]$ is

$$z(x, t) = \begin{cases} 
  g \left( t - \frac{x-L}{a_1} \right) & L \leq x \leq a_1 t + L \leq \tau \\
  z_0(x - a_1 t) & a_1 t + L < x \leq \tau 
\end{cases}$$

To find the weak solution for $x \in (\tau, R]$, consider the advection equation

$$z_t + (a_2 z)_x = 0, \quad x \in (\tau, R), \quad t > 0$$

$$z(x, 0) = z_0(x)$$

$$z(\tau, t) = \begin{cases} 
  g \left( t - \frac{\tau-L}{a_1} \right) & \tau \leq a_1 t + L \\
  z_0(\tau - a_1 t) & \tau > a_1 t + L
\end{cases}$$

where the boundary condition at $x = \tau$ is defined by evaluating the solution in (5.10) at $x = \tau$ to enforce continuity of the weak solution on the entire spatial domain, $[L, R]$. This results in the interface condition

$$\lim_{x \to \tau^-} z(x, t) = \lim_{x \to \tau^+} z(x, t) \quad \text{for all } t$$

for the state function.

Then, once again using (5.6), the weak solution to the advection equation with piecewise continuous advection speed is

$$z(x, t) = \begin{cases} 
  g \left( t - \frac{x-L}{a_1} \right) & L \leq x < a_1 t + L \leq \tau \\
  z_0(x - a_1 t) & a_1 t + L < x \leq \tau \\
  g \left( t - \frac{x-\tau}{a_2} - \frac{\tau-L}{a_1} \right) & \tau \leq x < a_2 t + \frac{a_1}{a_2}(L - \tau) \\
  z_0(\tau - a_1 t + \frac{a_1}{a_2}(x - \tau)) & \tau < x < a_2 t + \tau, \ x \geq \tau + a_2 t + \frac{a_2}{a_1}(L - \tau) \\
  z_0(x - a_2 t) & a_2 t + \tau < x \leq R
\end{cases}$$

(5.12)
Figure 20 provides a graph of the characteristic curves for the advection equation with piecewise constant advection speed. The highlighted characteristics are $x = a_1 t + L$, $x = \tau + a_2 t + \frac{a_2}{a_1} (L - \tau)$ and $x = a_2 t + \tau$.

![Figure 20: Characteristic Curves for the Scalar Advection Equation with Piecewise Constant Speed](image)

**Interface Conditions**

The parameter $\tau$ introduces an interface at $x = \tau$ into the advection equation where the advection speed discontinuously changes at this spatial location. In the following section, the sensitivity equation will be derived by differentiating with respect to $\tau$. (This is similar to the spatial parameter $x_i$ in the piecewise continuous flux coefficient (4.10) of the transcription model on page 58.) The smoothness of the state function, $z(x,t)$, is examined in order to determine the interface conditions for the equation. This will be important for the sensitivity equation considered in the following section.

For smooth initial and boundary conditions where $z_0(L) = g(0)$, we verify that the
solution of the state equation, \( z(x,t) \), is continuous. Given the well-defined boundary and initial conditions at the point \((0,0)\) in the \(xt\)-plane, the only potential region of discontinuity is the line \( x = \tau \).

Define \( \bar{t} \) to be the time such that

\[
\bar{t} = \lim_{x \to \tau} \frac{x - L}{a_1} = \frac{\tau - L}{a_1} = \lim_{x \to \tau} \frac{x - \tau - \frac{a_2}{a_1}(L - \tau)}{a_2}.
\]

This is the time for which the solution switches between the initial and boundary condition at the spatial value \( x = \tau \).

1. For \( t \leq \bar{t} \)

\[
\lim_{x \to \tau^-} z(x,t) = \lim_{x \to \tau^-} z_0(x - a_1 t) = z_0(\tau - a_1 t)
\]

\[
\lim_{x \to \tau^+} z(x,t) = \lim_{x \to \tau^+} z_0(\tau - a_1 t + \frac{a_1}{a_2}(x - \tau)) = z_0(\tau - a_1 t)
\]

2. For \( t > \bar{t} \)

\[
\lim_{x \to \tau^-} z(x,t) = \lim_{x \to \tau^-} g\left( t - \frac{x - L}{a_1} \right) = g\left( t - \frac{\tau - L}{a_1} \right)
\]

\[
\lim_{x \to \tau^+} z(x,t) = \lim_{x \to \tau^+} g\left( t - \frac{x - \tau - L}{a_2} - \frac{\tau - L}{a_1} \right) = g\left( t - \frac{\tau - L}{a_1} \right)
\]

Since

\[
\lim_{x \to \tau^-} z(x,t) = \lim_{x \to \tau^+} z(x,t) \quad \forall t,
\]

the state function, \( z(x,t) \), is continuous; however, it is not smooth. The assumption that \( a_1 z'_0(L) = -g'(0) \) ensures that the spatial derivative is continuous along the characteristics \( x = a_1 t + L \) and \( x = \tau + a_2 t + \frac{a_2}{a_1}(L - \tau) \), but the spatial derivative,
$z(x,t)$, does not exist in the classical sense at $x = \tau$ for $t > 0$ due to the change in the advection speed at the interface, i.e. $a_1 \neq a_2$. In addition, the discontinuity in the spatial derivative advects along the characteristic $x = a_2 t + \tau$. This can be seen by considering the weak solution and computing its spatial derivative on the intervals $[L, \tau)$ and $(\tau, \tau + a_2 (L - \tau)]$. This can be seen by considering the weak solution and computing its spatial derivative on the intervals $[L, \tau)$ and $(\tau, \tau + a_2 (L - \tau)]$.

\[
\begin{aligned}
z_x(x,t) &= \begin{cases} 
-\frac{1}{a_1} g' \left( t - \frac{x - L}{a_1} \right) & L \leq x < a_1 t + L < \tau \\
-\frac{1}{a_2} g' \left( t - \frac{x - \tau - L}{a_2} \right) & a_1 t + L \leq x < \tau \\
\frac{a_1}{a_2} z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) & \tau < x \leq a_2 t + \tau, \\
z_0'(x - a_2 t) & a_2 t + \tau < x \leq R 
\end{cases}
\end{aligned}
\]

1. For $t \leq \bar{t}$

\[
\begin{aligned}
\lim_{x \to \tau^-} z_x(x,t) &= \lim_{x \to \tau^-} z_0'(x - a_1 t) = z_0'(\tau - a_1 t) \\
\lim_{x \to \tau^+} z_x(x,t) &= \lim_{x \to \tau^+} \frac{a_1}{a_2} z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) = \frac{a_1}{a_2} z_0'(\tau - a_1 t)
\end{aligned}
\]

2. For $t > \bar{t}$

\[
\begin{aligned}
\lim_{x \to \tau^-} z_x(x,t) &= \lim_{x \to \tau^-} -\frac{1}{a_1} g' \left( t - \frac{x - L}{a_1} \right) = -\frac{1}{a_1} g' \left( t - \frac{\tau - L}{a_1} \right) \\
\lim_{x \to \tau^+} z_x(x,t) &= \lim_{x \to \tau^+} -\frac{1}{a_2} g' \left( t - \frac{x - \tau - L}{a_2} \right) = -\frac{1}{a_2} g' \left( t - \frac{\tau - L}{a_1} \right)
\end{aligned}
\]

3. For $t \geq 0$

\[
\begin{aligned}
\lim_{x \to (a_2 t + \tau)^-} z_x(x,t) &= \lim_{x \to (a_2 t + \tau)^-} \frac{a_1}{a_2} z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) = \frac{a_1}{a_2} z_0'(\tau) \\
\lim_{x \to (a_2 t + \tau)^+} z_x(x,t) &= \lim_{x \to (a_2 t + \tau)^+} z_0'(x - a_2 t) = z_0'(\tau)
\end{aligned}
\]

(5.13)
The smoothness of the spatial derivative of the flux, \((a(x; \tau)z(x, t))_x\), is examined as the function is needed for the sensitivity computation. Unlike the spatial derivative of the state function, the spatial derivative of the flux has removable discontinuities along \(x = \tau\) for all \(t > 0\). Also, because of the discontinuity of \(a\), it is discontinuous at \((\tau, 0)\) and this discontinuity then advects along the characteristic \(x = a_2 t + \tau\). The spatial derivative of the flux is continuous for all other points in the \(xt\)-plane given the piecewise constant definition for \(a(x; \tau)\) and the smoothness of \(z(x, t)\) away from the interface \(x = \tau\).

\[
(a(x; \tau)z(x, t))_x = \begin{cases} 
-g'(t - \frac{x - L}{a_1}) & L \leq x \leq a_1 t + L < \tau \\
 a_1 z_0'(x - a_1 t) & a_1 t + L < x < \tau \\
 -g'(t - \frac{x - \tau}{a_2} - \frac{\tau - L}{a_1}) & \tau < x \leq \tau + a_2 t + \frac{a_2}{a_1} (L - \tau) \\
 a_1 z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) & \tau < x < a_2 t + \tau, \\
 a_2 z_0'(x - a_2 t) & x > \tau + a_2 t + \frac{a_2}{a_1} (L - \tau) \leq a_2 t + \tau < x \leq R.
\end{cases}
\]

1. At \(t = 0\)

\[
\lim_{x \to \tau^-} (a(x; \tau)z(x, 0))_x = \lim_{x \to \tau^-} a_1 z_0'(x) = a_1 z_0'(\tau) \\
\lim_{x \to \tau^+} (a(x; \tau)z(x, 0))_x = \lim_{x \to \tau^+} a_2 z_0'(x) = a_2 z_0'(\tau)
\]

2. For \(0 < t \leq \bar{t}\)

\[
\lim_{x \to \tau^-} (a(x; \tau)z(x, t))_x = \lim_{x \to \tau^-} a_1 z_0'(x - a_1 t) = a_1 z_0'(\tau - a_1 t) \\
\lim_{x \to \tau^+} (a(x; \tau)z(x, t))_x = \lim_{x \to \tau^+} a_1 z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) = a_1 z_0'(\tau - a_1 t)
\]
3. For $t > \bar{t}$

\[
\lim_{x \to \tau^-} (a(x; \tau)z(x, t))_x = \lim_{x \to \tau^-} -g' \left( t - \frac{x - L}{a_1} \right) = -g' \left( t - \frac{\tau - L}{a_1} \right)
\]

\[
\lim_{x \to \tau^+} (a(x; \tau)z(x, t))_x = \lim_{x \to \tau^+} -g' \left( t - \frac{x - \tau - L}{a_2} - \frac{\tau - L}{a_1} \right) = -g' \left( t - \frac{\tau - L}{a_1} \right)
\]

4. For $t > 0$

\[
\lim_{x \to (a_2 t + \tau)^-} (a(x; \tau)z(x, t))_x = \lim_{x \to (a_2 t + \tau)^-} a_1 z_0' (\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) = a_1 z_0' (\tau)
\]

\[
\lim_{x \to (a_2 t + \tau)^+} (a(x; \tau)z(x, t))_x = \lim_{x \to (a_2 t + \tau)^+} a_2 z_0' (x - a_2 t) = a_2 z_0' (\tau)
\]

Therefore the state and spatial derivative of the flux satisfy the following interface conditions

\[
\lim_{x \to \tau^-} z(x, t) = \lim_{x \to \tau^+} z(x, t) \text{ for all } t \geq 0 \quad (5.14)
\]

\[
\lim_{x \to \tau^-} (a(x; \tau)z(x, t))_x = \lim_{x \to \tau^+} (a(x; \tau)z(x, t))_x \text{ for all } t > 0
\]

**Sensitivity Equation**

To gain insight into the DG formulation for the nonlinear conservation law with an interface parameter, the simpler linear problem is studied. Define

\[
s(x, t; \tau) = \frac{d}{d\tau} z(x, t; \tau)
\]

to be the sensitivity with respect to $\tau$, the parameter that determines the spatial location of the change in the advection speed.
By considering the advection equation (5.7) - (5.9) on the two spatial domains 
\[ [L, \tau] \text{ and } (\tau, R] \] separately, differentiating with respect to \( \tau \) and assuming there is 
enough smoothness in the solution in order to interchange the order of differentiation, 
the sensitivity equation is 
\[
\frac{ds}{dt} + \left( a(x; \tau)s \right)_x = 0, \quad x \in (L, R), \quad t > 0
\] 
(5.15)
\[
s(x, 0) = 0 \quad (5.16)
\]
\[
s(L, t) = 0 \quad (5.17)
\]

In addition to the PDE, boundary and initial conditions, interface conditions 
resulting from the discontinuous coefficient in the flux function must be enforced 
by the numerical scheme in order to accurately simulate the sensitivity. Since \( \tau \) 
defines the spatial location of the discontinuity in the advection speed, then for a 
fixed parameter value, the spatial variable depends on \( \tau \). Then by computing the 
total derivative of (5.14) with respect to \( \tau \) and interchanging the limits, the interface 
condition for the sensitivity is determined.

\[
\frac{d}{d\tau} \lim_{x \to \tau^+} z(x, t; \tau) = \frac{d}{d\tau} \lim_{x \to \tau^-} z(x, t; \tau)
\]

\[
\lim_{x \to \tau^+} z_x(x, t; \tau) + s(x, t; \tau) = \lim_{x \to \tau^-} z_x(x, t; \tau) + s(x, t; \tau)
\]

\[
\lim_{x \to \tau^+} s(x, t; \tau) = \lim_{x \to \tau^-} s(x, t; \tau) + \lim_{x \to \tau^-} z_x(x, t; \tau)
\]

\[
- \lim_{x \to \tau^+} z_x(x, t; \tau)
\] 
(5.18)

Note: For ease of notation, the dependence of \( z \) and \( s \) on the parameter, \( \tau \), will be 
suppressed in further calculations and expressions.
By differentiating (5.12) with respect to \( \tau \), the weak solution of the sensitivity equation (5.15) - (5.17) that satisfies (5.18) is

\[
s(x, t) = \begin{cases} 
0 & \text{if } L \leq x \leq \tau \\
\left( \frac{1}{a_2} - \frac{1}{a_1} \right) g' \left( t - \frac{x-\tau}{a_2} - \frac{\tau-L}{a_1} \right) & \text{if } \tau < x \leq \tau + a_2 t + \frac{a_2}{a_1}(L - \tau) \\
\left( 1 - \frac{a_1}{a_2} \right) z_0' \left( \tau - a_1 t + \frac{a_1}{a_2} (x - \tau) \right) & \text{if } \tau < x < a_2 t + \tau, \\
0 & \text{if } a_2 t + \tau \leq x \leq R
\end{cases}
\]  
(5.19)

**Interface Conditions**

Using the weak solution of the sensitivity equation and the spatial derivative of the state function, the derived interface condition is verified and an additional condition due to the behavior of the advection equation is described. The sensitivity is discontinuous at \( x = \tau \) and along the characteristic \( x = a_2 t + \tau \). Due to the assumption \( a_1 z_0'(L) = g'(0) \) on the state function, the sensitivity is continuous along the characteristic \( x = \tau + a_2 t + \frac{a_2}{a_1}(L - \tau) \).

1. For \( t \leq \bar{t} \)

\[
\lim_{x \to \tau^-} s(x, t) = 0 \\
\lim_{x \to \tau^+} s(x, t) = \lim_{x \to \tau^+} \left( 1 - \frac{a_1}{a_2} \right) z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) \\
= \left( 1 - \frac{a_1}{a_2} \right) z_0'(\tau - a_1 t)
\]
2. For $t > \bar{t}$

\[
\lim_{x \to \tau^-} s(x, t) = 0
\]

\[
\lim_{x \to \tau^+} s(x, t) = \lim_{x \to \tau^+} \left( \frac{1}{a_2} - \frac{1}{a_1} \right) g' \left( t - \frac{x - \tau}{a_2} - \frac{\tau - L}{a_1} \right) = \left( \frac{1}{a_2} - \frac{1}{a_1} \right) g' \left( t - \frac{\tau - L}{a_1} \right)
\]

3. For a fixed $t > 0$

\[
\lim_{x \to (a_2 t + \tau)^-} s(x, t) = \lim_{x \to (a_2 t + \tau)^-} \left( 1 - \frac{a_1}{a_2} \right) z_0' (\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) = \left( 1 - \frac{a_1}{a_2} \right) z_0' (\tau)
\]

\[
\lim_{x \to (a_2 t + \tau)^+} s(x, t) = 0
\]

The flux function, $a(x; \tau)s(x, t)$, has similar discontinuities as seen in $s(x, t)$ due to the piecewise constant nature of the flux coefficient.

\[
a(x; \tau)s(x, t) = \begin{cases} 
0 & L \leq x \leq \tau \\
\left(1 - \frac{a_2}{a_1}\right) g'(t - \frac{x - \tau}{a_2} - \frac{\tau - L}{a_1}) & \tau < x \leq \tau + a_2 t + \frac{a_2}{a_1} (L - \tau) \\
(a_2 - a_1) z_0'(\tau - a_1 t + \frac{a_1}{a_2} (x - \tau)) & \tau < x < a_2 t + \tau, \\
0 & x > a_2 t + \tau + \frac{a_2}{a_1} (L - \tau) \\
\end{cases}
\]

Therefore, in addition to the interface condition (5.18), the flux function of the sensitivity equation has a similar condition that travels along the characteristic $x = a_2 t + \tau$ for $t > 0$.

\[
\lim_{x \to (a_2 t + \tau)^+} a(x; \tau)s(x, t) = \lim_{x \to (a_2 t + \tau)^-} a(x; \tau)s(x, t) + \lim_{x \to (a_2 t + \tau)^-} a(x; \tau)z_x(x, t) \\
- \lim_{x \to (a_2 t + \tau)^+} a(x; \tau)z_x(x, t) \quad (5.20)
\]
The interface condition for the flux function of the sensitivity equation at $x = \tau$ with $t = 0$, in particular the jump in the spatial derivative of the flux function of the state equation, travels along the characteristic

$$x = a_2t + \tau.$$

This is due to the behavior of the advection equation causing a discontinuity in the sensitivity flux at all points $(x, t)$ along this characteristic. In the following section, the interface conditions are incorporated into the numerical flux function to define a DG formulation for solving the state and sensitivity equations.

**DG Solution**

The state function satisfies the PDE

$$z_t + (a(x; \tau)z)_x = 0$$

along with the continuity interface condition at $x = \tau$

$$\lim_{x \to \tau^-} z(x, t) = \lim_{x \to \tau^+} z(x, t) \quad \text{for all } t.$$ 

The sensitivity satisfies the PDE

$$s_t + (a(x; \tau)s)_x = 0$$
along with the interface conditions

\[
\lim_{x \to \tau^+} s(x, t; \tau) = \lim_{x \to \tau^-} s(x, t; \tau) + \lim_{x \to \tau^-} z_x(x, t; \tau)
\]

\[
- \lim_{x \to \tau^+} z_x(x, t; \tau)
\]

\[
\lim_{x \to (a_2 t + \tau)^+} a(x; \tau) s(x, t) = \lim_{x \to (a_2 t + \tau)^-} a(x; \tau) s(x, t) + \lim_{x \to (a_2 t + \tau)^-} a(x; \tau) z_x(x, t)
\]

\[
- \lim_{x \to (a_2 t + \tau)^+} a(x; \tau) z_x(x, t)
\]

Using the variational form (2.3) derived for a scalar conservation law in Chapter 2, the state and sensitivity equations have similar semi-discrete forms for a DG solution.

Find \( z, s \in V^k \) that satisfy

\[
\int_{D^k} \frac{\partial z}{\partial t} \ell^k_j(x) dx - \int_{D^k} (a(x; \tau) z) \frac{d\ell^k_j}{dx} dx + (a(x; \tau) z)^* \ell^k_j(x) \bigg|_{x^k_i}^{x^k_r} = 0
\]

\[
\int_{D^k} \frac{\partial s}{\partial t} \ell^k_j(x) dx - \int_{D^k} (a(x; \tau) s) \frac{d\ell^k_j}{dx} dx + (a(x; \tau) s)^* \ell^k_j(x) \bigg|_{x^k_i}^{x^k_r} = 0
\]

for each of the basis functions, \( \ell^k_j(x) \), on the element \( D^k = [x^k_i, x^k_r] \) where \( f(u) = a(x; \tau) u \) is the linear flux function, where \( u \) represents either \( z \) or \( s \) depending on the context. The only difference between these two DG formulations is the choice of numerical flux function. Given the behavior of the advection equation, an upwinding numerical flux is appropriate for the state equation. The Local Lax-Friedrichs numerical flux (2.8) is upwinding if the true flux of the conservation law is of the form \( f(z) = az \) for a constant \( a \). This is used for the state equation.
For the sensitivity equation, the interface conditions are used to define the numerical flux since one of the primary purposes of the numerical flux is to weakly enforce all interface conditions. The sensitivity equation is also an advection equation with positive advection speeds, so the upwinding Lax-Friedrichs numerical flux may seem appropriate, but using it would find a zero solution given the zero initial and boundary conditions. Since the interface condition contains a jump in the spatial derivative of the state solution, the upwinding Lax-Friedrichs numerical flux must be modified to contain this jump information.

The numerical fluxes for the state and sensitivity equations are defined as

\[
(a(x)z)^* = a\{z\} + \frac{a}{2}[z]
\]

\[
(a(x)s)^* = a\{s\} + \frac{a}{2}[s] + a[z_x]
\]  

(5.21)

where the average and jump along the normal are defined as

\[
\{z\} = \frac{z^- + z^+}{2}
\]

\[
[z] = \hat{n}^- z^- + \hat{n}^+ z^+
\]

With these numerical fluxes, one solves the coupled system of ODEs (2.6) in time simultaneously using a total variation diminishing Runge-Kutta integration to find the state solution and sensitivity.

\[
M_k \frac{dz_k}{dt} - aS_k z_k = -(a(x)z)^* \ell^k(x^k_i) + (a(x)z)^* \ell^k(x^k_i)
\]

\[
M_k \frac{ds_k}{dt} - aS_k s_k = -(a(x)s)^* \ell^k(x^k_i) + (a(x)s)^* \ell^k(x^k_i)
\]
where $a$ is either $a_1$ or $a_2$ depending on whether $x < \tau$ or $x > \tau$, respectively, and the one-sided limits, \( \lim_{x \to \tau^-} a(x; \tau) = a_1 \) and \( \lim_{x \to \tau^+} a(x; \tau) = a_2 \), are observed in the local solution at the node corresponding to $x = \tau$.

**Notes on the Numerical Implementation**

A few remarks about implementation of the DG formulation from Chapter 2 for the system of state and sensitivity equations.

- The average calculation within the Local Lax-Friedrichs flux is altered so that the flux coefficient is treated as a constant on each element mimicking how the weak solution (5.12) was derived. This choice affects the numerical flux on the $k^{th}$ element where $x_k^l = \tau$. At this node, the numerical flux is \((a(x)z)^*(x_k^l) = a_2 z(x_{r}^{k-1}, t)\) reflecting the upwinding behavior of the Lax-Friedrichs flux but also enforcing the one-sided limit, \( \lim_{x \to \tau^+} a(x; \tau) = a_2 \).

- The numerical flux (5.21) for the sensitivity equation requires an approximation to the spatial derivative, $z_x(x, t)$, of the state function at the nodes. There are two reasonable options for approximating the spatial derivative at each time step: either computing the finite element derivative by differentiating the basis functions or using a finite difference approximation. For the finite element derivative, using the approximate local solution

\[
z(x, t) = \sum_{j=1}^{N_p} z_h^j(x_j^k, t) \ell_j^k(x),
\]
the approximate spatial derivative is then

\[ z_x(x, t) = \sum_{j=1}^{N_p} z^k_{x_j}(x^k_{x_j}, t) \frac{d\ell^k_{x_j}}{dx} \]

In the following examples, a finite difference approximation of the spatial derivative was used [45] and is detailed below. Given the local nature of the DG method, a forward difference is used at the left endpoint, \(x^k_l\), and a backward difference is used at the right endpoint, \(x^k_r\), for each of the elements \(k = 1, 2, \ldots, K\). Let \(\{x^k_j\}_{j=1}^{N_p}\) be the set of \(N_p = N + 1\) set of interpolation points defining the \(N^{th}\) degree Lagrange polynomials on the \(k^{th}\) element. The nodes of the spatial mesh are interpolation points for the basis functions on each element. Note that the choice of Legendre Gauss Lobatto interpolation points produces a set that are not equidistant and \(x^k_l = x^k_{1}\) and \(x^k_r = x^k_{N_p}\). Define the spatial differences

\[ p_1 = x^k_2 - x^k_1, \quad p_2 = x^k_3 - x^k_1, \quad q_1 = x^k_{N_p} - x^k_{N_p-1}, \quad q_2 = x^k_{N_p} - x^k_{N_p-2} \]

Then the forward difference approximation to the spatial derivative at \(x^k_l\) is

\[ z_x(x^k_l, t) \approx Az(x^k_l, t) + Bz(x^k_l + p_1, t) + Cz(x^k_l + p_2, t) \]

where

\[ A = \frac{-p_1 + p_2}{p_1 p_2}, \quad B = \frac{-p_2}{p_1(p_1 - p_2)}, \quad C = \frac{p_1}{p_2(p_1 - p_2)}. \]

The backward difference approximation to the spatial derivative at \(x^k_r\) is

\[ z_x(x^k_r, t) \approx Az(x^k_r, t) + Bz(x^k_r - q_1, t) + Cz(x^k_r - q_2, t) \]
where
\[ A = \frac{q_1 + q_2}{q_1 q_2}, \quad B = \frac{q_2}{q_1(q_1 - q_2)}, \quad C = -\frac{q_1}{q_2(q_1 - q_2)}. \]

- Since the state solution is continuous, a slope limiter is not needed to accurately approximate \( z(x, t) \). But given the discontinuities in the sensitivity solution at \( x = \tau \) and along the characteristic \( x = a_2 t + \tau \), a slope limiter is applied after each stage of the Runge-Kutta method when solving \( s(x, t) \). In fact, if the slope limiter is applied to the state approximation, the expected loss of accuracy in the neighborhood of extrema is observed and results in an unstable and inaccurate sensitivity calculation due to the presence of the spatial derivative of \( z(x, t) \) in the numerical flux for \( s(x, t) \).

In the following subsections, two examples are considered. In the first example, the initial condition is chosen so that the sensitivity is continuous at \( x = \tau \) when \( t = 0 \) reducing the error along the characteristic \( x = a_2 t + \tau \). In the second example, this condition is not met and more error is observed along the characteristic.

**Example 1**

Consider the scalar linear advection equation

\[ z_t + (a(x; \tau)z)_x = 0, \quad x \in (0, \pi), \quad t > 0 \quad (5.22) \]

\[ z(x, 0) = \sin(3x) \quad (5.23) \]

\[ z(0, t) = -\sin(3a_1 t) \quad (5.24) \]
along with the interface condition (5.11) where

$$a(x; \tau) = \begin{cases} \frac{a_1}{a_2} & 0 \leq x \leq \tau \\ \frac{a_1}{a_2} & \tau < x \leq \pi \end{cases}$$

(5.25)

and $\tau \in (0, \pi)$.

Using (5.12), a weak solution is

$$z(x, t) = \begin{cases} \sin(3(x - a_1 t)) & x \leq \tau \\ \sin(3(\tau - a_1 t + \frac{a_1}{a_2}(x - \tau))) & \tau < x < a_2 t + \tau \\ \sin(3(x - a_2 t)) & x \geq a_2 t + \tau \end{cases}$$

(5.26)

The sensitivity with respect to $\tau$, $s(x, t; \tau)$, satisfies the PDE

$$s_t + (a(x; \tau)s)_x = 0$$  

(5.27)

$$s(x, 0) = 0$$  

(5.28)

$$s(0, t) = 0$$  

(5.29)

along with the interface conditions (5.18) and (5.20).

Its weak solution is

$$s(x, t) = \begin{cases} 0 & x \leq \tau \\ 3 \left(1 - \frac{a_1}{a_2}\right) \cos(3(\tau - a_1 t + \frac{a_1}{a_2}(x - \tau))) & x < a_2 t + \tau \\ 0 & x \geq a_2 t + \tau \end{cases}$$

(5.30)

Note that if the interface conditions are not enforced, then a numerically simulated weak solution is the zero function, $s(x, t) = 0$.

Using the DG formulation outlined in Chapter 2 with $K = 80$ elements and an $N = 3$ degree basis of Lagrange interpolating polynomials, the coupled system for the state and sensitivity equations are simulated for the case of $a_1 = \frac{1}{4}$, $a_2 = \frac{1}{2}$ and $\tau = \frac{\pi}{2}$. Figures 21a and 21b include plots of the solutions at the final time,
$T = 2.55$. Figures 21c and 21d include plots of the pointwise error of the weak and DG solutions. In Table 4, the $L^2$ error over the domain $D = \{x \in [0, \pi] : |x - \pi/2| \geq 0.01$ and $|x - x_c| \geq 0.1\}$ with $x_c = a_2 T + \frac{\pi}{2}$ of the state and sensitivity is computed for a range of spatial discretizations.

(a) Exact (5.26) and DG simulation of the PDE model for the state equation in (5.22). The graphs of the functions are visually indistinguishable.

(b) The dashed curve is the graph of the DG simulation of the PDE model for the sensitivity in (5.27). The solid curve is the true solution as given in (5.30).

(c) Pointwise error between exact and DG solution of the state equation.

(d) Pointwise error between exact and DG solution of the sensitivity equation.

Figure 21: Solution and pointwise error at the final time, $T = 2.55$, using cubic basis function, $K = 80$ elements, $a_1 = \frac{1}{4}$, $a_2 = \frac{1}{2}$ and $\tau = \frac{\pi}{2}$.
Consider the scalar linear advection equation

\[ z_t + (a(x; \tau) z)_{xx} = 0, \quad x \in (0, \pi), \quad t > 0 \]  \hspace{1cm} (5.31)

\[ z(x, 0) = \cos(3x) \]  \hspace{1cm} (5.32)

\[ z(0, t) = \cos(3a_1 t) \]  \hspace{1cm} (5.33)

along with the interface condition (5.11) where \( a(x; \tau) \) is defined as in (5.25).

Using (5.12), a weak solution is

\[ z(x, t) = \begin{cases} 
\cos(3(x - a_1 t)) & x \leq \tau \\
\cos(3(\tau - a_1 t + a_1 a_2(x - \tau))) & \tau < x < a_2 t + \tau \\
\cos(3(x - a_2 t)) & x \geq a_2 t + \tau 
\end{cases} \]  \hspace{1cm} (5.34)

The sensitivity with respect to \( \tau \), \( s(x, t; \tau) \), also satisfies (5.27) - (5.29) with interface conditions (5.18) and (5.20). Its weak solution is

\[ s(x, t) = \begin{cases} 
0 & x \leq \tau \\
-3 \left(1 - \frac{a_1}{a_2}\right) \sin(3(\tau - a_1 t + a_1 a_2(x - \tau))) & x < a_2 t + \tau \\
0 & x \geq a_2 t + \tau 
\end{cases} \]  \hspace{1cm} (5.35)

Using a DG formulation outlined in Chapter 2 with \( K = 80 \) elements and an

\( N = 3 \) degree basis of Lagrange interpolating polynomials, the coupled system for

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<th>order</th>
<th>Error in ( s(x, t) )</th>
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<td>0.0000130</td>
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Table 4: \( L^2(D) \) error for the state (5.26) and sensitivity (5.30) where \( D = \{ x \in [0, \pi] : |x - \pi/2| \geq 0.01 \) and \( |x - x_c| \geq 0.1 \) and \( x_c = a_2 T + \frac{\pi}{2} \) is the spatial location along the characteristic at the final time \( T = 2.55 \).
the state and sensitivity equations are simulated. Figures 22a and 22b include plots of the solutions at the final time, $T = 2.55$. Figures 22c and 22d include plots of the pointwise error of the weak and DG solutions. Due to the lack of continuity in the sensitivity at $x = \tau$ and $t = 0$, there is a significant increase in the error along the characteristic $x = a_2 t + \tau$ at the final time, in comparison to the previous example.

For comparison, Figure 23 includes plots of the sensitivity and the pointwise error of the weak and DG solutions showing improvement along the characteristic when $\mathcal{K} = 640$ elements are used. Table 5 includes the $L^2$ error over the domain $D$, as defined in the previous example, of the state and sensitivity at the final time. The sensitivity appears to converge faster than in the previous example, but that is due to the exaggerated error along the characteristic $x = a_2 t + \tau$. Roughly, it takes between 160 and 320 elements to achieve the accuracy on $D$ seen in the previous example using 80 elements even though the solutions differ by a phase shift.

<table>
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<th>$\mathcal{K}$</th>
<th>Error in $z(x, t)$</th>
<th>Error in $s(x, t)$</th>
<th>order</th>
<th>order</th>
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</table>

Table 5: $L^2(D)$ error for the state (5.34) and sensitivity (5.35) where $D = \{ x \in [0, \pi] : |x - \pi/2| \geq 0.01 \text{ and } |x - x_c| \geq 0.1 \}$ and $x_c = a_2 T + \frac{\pi}{2}$ is the spatial location along the characteristic at the final time $T = 2.55$.

As shown in the previous two examples, the basic DG formulation using the
(a) Exact (5.34) and DG simulation of the PDE model for the state equation in (5.31). The graphs of the functions are visually indistinguishable.

(b) The dashed curve is the graph of the DG simulation of the PDE model for the sensitivity in (5.27). The solid curve is the true solution as given in (5.35).

(c) Pointwise error between exact and DG solution of the state equation.

(d) Pointwise error between exact and DG solution of the sensitivity equation.

Figure 22: Solution and pointwise error at the final time, $T = 2.55$, using cubic basis function, $K = 80$ elements, $a_1 = \frac{1}{4}$, $a_2 = \frac{1}{2}$ and $\tau = \frac{\pi}{2}$.

Numerical flux (5.21) converges to the desired sensitivity satisfying (5.15) - (5.17) along with the interface conditions (5.18) and (5.20). Both the state and sensitivity functions satisfied the same localized weak DG formulation, but were implemented using different numerical flux functions resulting in an inexpensive computation of the coupled system. Now that this DG formulation has been shown convergent for the
(a) The dashed curve is the graph of the DG simulation of the PDE model for the sensitivity in (5.27). The solid curve is the true solution as given in (5.35).

(b) Pointwise error between exact and DG solution of the sensitivity equation.

Figure 23: Solution and pointwise error at the final time, $T = 2.55$, using cubic basis function, $K = 640$ elements, $a_1 = \frac{1}{4}$, $a_2 = \frac{1}{2}$ and $\tau = \frac{\pi}{2}$.

linear problem, ongoing work includes extending the method to the nonlinear traffic flow model to compute sensitivities with respect to pause location and optimize the delay function.
CHAPTER 6

CONCLUSION AND FUTURE WORK

The classic traffic flow model along with a discontinuous flux coefficient defining multiple pauses is used to model the biological process of transcription. Numerical simulations of the PDE model were used to determine the effect pauses have on the transcription speed as an indirect effect on the cell’s protein production capabilities. The realization of random pauses distributed uniformly in space and time produces highly variable transcription times computed from the defined delay function dependent on the numerical simulation of the flux at the termination site of the DNA strand. The large range of transcription times results from differing behavior of the $q(t)$ function within the delay function. Parameter choices defining the number of pauses in addition to the transcription speed which is used to rescale the temporal variable are being considered to determine if an equilibrium can be reached in $q(t) - t$ eliminating the variability in the transcription time calculations.

Parameter studies conducted on the biological model demonstrate the effect parameterization of the location of one or two pauses has on the delay function. Full analysis of the sensitivity with respect to duration of pauses and the sensitivity with respect to location of pauses and how small changes in these parameters affect polymerase density and overall protein production is desired. The nonlinear PDE model is
simulated using a DG formulation and it is of interest to extend this numerical scheme to investigate these sensitivities. A DG formulation to numerically simulate the coupled state and sensitivity equation of a linear conservation law with a discontinuous flux coefficient introducing an interface parameter has been proposed and studied. Convergence of the DG formulation using the proposed numerical flux function to solve for the sensitivity has been established. Even though the weak solution of the nonlinear problem derived in Chapter 3 does not have the continuity of the model linear problem studied in Chapter 5, an ongoing research interest is the investigation of the use of the spatial derivative of the state within the numerical flux of the DG simulation of the sensitivity equation for the nonlinear problem when investigating the spatial interface parameter. And then once a convergent DG formulation is derived, the sensitivity can then be used to optimize the delay function to investigate the effect of pauses on protein production.
REFERENCES CITED


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