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METHODS FOR COMPUTATIONAL POPULATION DYNAMICS

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BRUCE P. AYATI

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In memory of my mother

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LIST OF ILLUSTRATIONS

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ABSTRACT

We consider two classes of numerical methods for approximating solutions to certain partial differential equations, motivated by the study of biological populations.

In Chapter 2, we propose a method for approximating solutions of a model of age-dependent population diffusion with random dispersal. This method, unlike previous methods, allows for variable time steps and independent age and time discretizations. We use a moving age discretization that transforms the problem to a system of parabolic equations. The system is then solved by backward differences in time and a Galerkin approximation in space; the equations that need to be solved at each step treat each age group separately. A priori L^2 error estimates are obtained by an energy analysis. These estimates are superconvergent in the age variable. We present a postprocessing technique which capitalizes on the superconvergence.

In Chapter 3, we analyze a single step method for solving second-order parabolic initial–boundary value problems. The method uses a step-doubling extrapolation scheme in time based on backward Euler and a Galerkin approximation in space. The technique is shown to be a second-order correct approximation in time. Since step-doubling can be used as a mechanism for step-size control, the analysis is done for variable time steps. The stability properties of step-doubling are contrasted with those of Crank-Nicolson, and more generally those of extrapolated theta-weighted schemes.

In Chapter 4, we combine and modify the methods developed in Chapters 2 and 3 to approximate solutions to models of swarm colony development of the bacteria *Proteus mirabilis*. These models consist of an age-dependent partial differential equation with nonlinear diffusion which describes the behavior of motile bacteria and is coupled at each point in space to an ordinary differential equation which describes the behavior of the immotile bacteria.

CHAPTER 1

INTRODUCTION

The theoretical and computational study of biological populations can be made more effective by the use of substantial amounts of mathematics. Numerical analysis has played a large role in the advancement of the physical sciences but has had much less impact on the biological sciences. It is the intent of this thesis to illustrate some of the roles numerical analysis can play in population dynamics.

In modeling how populations change over time, it might appear sufficient to know how the population is distributed in space. However, for many organisms, their behavior is dependent not only on their population density in space, but their age distribution as well. One would not expect a community of older organisms to behave the same as a younger community.

In his classic work of 1951, Skellam [39] considered the effects of diffusion on populations. Sharpe and Lotka in 1911 and McKendrick in 1926 considered population models with linear age structure [43]. More recently, Gurtin and MacCamy [17] considered models with nonlinear age structure. Rotenberg [38] and Gurtin [16] posed models dependent on both age and space. Gurtin and MacCamy [18] differentiated between two kinds of diffusion in these models: diffusion due to random dispersal, and diffusion towards an area of less crowding. Existence and uniqueness results can be found for various forms of these models in Busenberg and Iannelli [5], di Blasio [8], di Blasio and Lamberti [9], Langlais [26], and MacCamy [30]. Further analysis has been done by several authors [21, 24, 27, 31].

Continuous models that incorporate the age structure of a population contribute to the understanding of various systems in ecology, epidemiology, demography, population genetics, and cell growth. These models have an extensive literature (see [6, 10, 19, 36, 43] and references therein). Models that more accurately represent the system under study, by also taking into account the spatial structure of the population, will generally be more complicated; the literature in this field is correspondingly more sparse than the spatially homogeneous case (see [5, 8, 12, 24, 26, 31], among others). These models will often result in nonlinear partial differential equations that will not have analytic solutions and will need to be evaluated numerically. The dimensionality of the problem, age in addition to time and space, makes these problems more complicated numerically.

We thus have a class of mathematical and biological problems that are computationally expensive. There has been much investigation into numerical methods for solving models with just age structure [1, 11, 25, 29, 33]. For models with both age and space structure, methods have been developed for populations that diffuse to avoid crowding [32] and for random dispersal [22, 23, 28]. These methods all require uniform age and time discretizations with the age step chosen to equal the time step. In Chapter 2, we develop and analyze new numerical methods to efficiently and robustly solve the equations resulting from these models. These methods allow for nonuniform and independent age and time discretizations.

The methods for the age-dependent equations involve transforming these equations to systems of parabolic equations. Parabolic equations also can be effective models of populations when the behavior of the population being modeled is weakly dependent on age. In Chapter 3, we analyze a step-doubling Galerkin method for solving parabolic problems. Step-doubling [13] is an effective way of controlling the step-size in an adaptive simulation while providing second-order accuracy in time. We compute approximate solutions to an example system of parabolic equations.

Parabolic equations have applicability that go far beyond what is presented here and step-doubling is an effective way of approximating solutions to other time-dependent systems [20]. It is thus noted that Chapter 3 has value outside of the mathematical study of biological populations.

Reaction–diffusion equations have had much success in describing biological pattern formation [34]. Age-structured diffusion models are an alternative means to describe such phenomena. They are particularly suited for situations when the patterns are formed independently of the chemical structure of the system. This is the case in *Proteus mirabilis* swarm colony development. On typical laboratory media, *Proteus mirabilis* cells form colonies with radial symmetry and regularly spaced concentric terraces. These colonies are formed by a swarming–consolidation cycle, the timing of which is largely independent of the nature of the agar surface [37].

Much of the work in this thesis was motivated by the Esipov–Shapiro model of *Proteus mirabilis* swarm colony development [10]. In this model, there are two stages of bacteria. The motile stage is described by an age-dependent nonlinear diffusion equation, which is coupled to an ordinary differential equation at each point in space which describes the non-motile stage. The creation of motile bacteria is governed by these ordinary differential equations. In this problem, there are very rapid changes in space requiring very small time steps, although the age dependence is smooth. In Chapter 4, we combine and modify the age-dependent methods and step-doubling to compute approximate solutions to a modified Esipov–Shapiro model.

CHAPTER 2

A METHOD FOR AN AGE-DEPENDENT POPULATION MODEL WITH NONLINEAR DIFFUSION

In this chapter, we consider a numerical method for solving an age-dependent population model with spatial diffusion. There has been much investigation into numerical methods for solving models with just age structure [1, 7, 11, 25, 29, 33, 41]. For models with both age and space structure, Milner developed a method for populations that diffuse to avoid crowding [32]. Kim [22], Kim and Park [23], and Lopez and Trigiante [28] developed methods for random dispersal. All these methods involve uniform time and age discretizations with the age step chosen to equal the time step.

We use a moving age discretization that allows for a method with nonuniform age and time discretizations. The age step need not equal the time step. Instead, the positions of the age nodes are adjusted by the time step. The method posed preserves the important fact that age and time advance together. The age and time discretizations are linked only in the sense that each new cohort comes into existence at the beginning of a time step.

Having variable time steps gives us the ability to choose the time steps adaptively to assure robustness and efficiency. Advantages of independent age and time discretizations are fewer computations and less memory use when the dependence on age is weak relative to the dependence on time. In the previous methods, any incorporation of age into a model meant a dramatic increase in computational expense. With the methods posed in this chapter, dependence on age can be modeled with a moderate increase in computational cost. It is hoped that the existence of these methods will increase the use of age-structure when it plays some role in the behavior of a population but is not dominant.

The population is approximated by piecewise constant functions in age, which are generally only first-order correct. However, the computed solution is shown to be a second-order correct approximation of the average value on each subinterval. We present a postprocessing technique that utilizes this superconvergence property to obtain second-order correct approximations in age using continuous piecewise linear functions.

The organization of this chapter is as follows. In Section 2.1, we present the continuous model and our assumptions on that model. In Section 2.2, we present a model that is discrete in age and continuous in space and time. In Section 2.3, we present a fully discrete method for approximating solutions to the continuous model. In Section 2.4, we provide *a priori* error bounds for the approximate solution that are superconvergent in the age variable. In Section 2.5, we present and analyze a postprocessing technique to capitalize on the superconvergence. In Section 2.6, we bound the error that results from truncating the infinite age domain to a finite domain. In Section 2.7, we discuss the relationship between the methods posed in this paper and finite difference methods.

Much of this chapter is taken from another manuscript by the author [3].

2.1 The Continuous Model

We consider the age-dependent population model with nonlinear diffusion,

$$\partial_t u + \partial_a u = \nabla \cdot k(\mathbf{x}, p)\nabla u - \mu(\mathbf{x}, a, p)u, \qquad \mathbf{x} \in \Omega,\ a \geq 0,\ t \geq 0. \tag{2.2.1}$$

where ∇ and $\nabla\cdot$ denote the gradient and the divergence, respectively, in $\mathbf{x}$. The diffusion arises from the symmetric random motion of each individual (Fickian diffusion). Isotropic random motion results in diffusion of the form $\nabla^2(ku)$. The choice between the two diffusions is biological [35]. The function $u(\mathbf{x}, a, t)$ represents the distribution of individuals, $\Omega \subset \mathbb{R}^n$ represents the spatial domain, a represents age, and t represents time. The function $\mu \geq 0$ is the death rate. The total population density, p, is given by

$$p(\mathbf{x},t) = \int_0^\infty u(\mathbf{x},a,t)\,da, \qquad \mathbf{x} \in \Omega,\ t \geq 0. \tag{2.2.2}$$

We have a birth condition

$$u(\mathbf{x},0,t) = \mathcal{B}(\mathbf{x}, u(\mathbf{x},\cdot,t)), \qquad \mathbf{x} \in \Omega,\ t \geq 0, \tag{2.2.3}$$

that is dependent on the entire population distribution. We have a Neumann boundary condition, with ν denoting the outward normal to $\partial\Omega$,

$$k(\mathbf{x},p)\nabla u \cdot \nu = 0, \qquad x \in \partial\Omega,\ a \geq 0,\ t \geq 0, \tag{2.2.4}$$

that represents an isolated habitat. The initial condition is

$$u(\mathbf{x},a,0) = u^0(\mathbf{x},a), \qquad \mathbf{x} \in \Omega,\ a \geq 0. \tag{2.2.5}$$

Langlais [26] proved the existence of unique non-negative solutions for the case when k, μ, and β are independent of $\mathbf{x}$. A corresponding treatment for the system (2.2.1)–(2.2.5) is beyond the scope of this chapter; we will instead concentrate on the numerical aspects of the problem. Thus, we assume existence and uniqueness of smooth, non-negative solutions.

We make several assumptions:

Condition 2.1. *There exists constants C_0 and C_1 such that for $(\mathbf{x},p) \in \Omega \times \mathbb{R}$, k satisfies $0 < C_0 \leq k(\mathbf{x},p) \leq C_1$ and μ satisfies $0 < C_0 \leq \mu(\mathbf{x},a,p) \leq C_1$ for all a.*

Condition 2.2. *The functions $k(\mathbf{x},p)$ and $\mu(\mathbf{x},a,p)$ are uniformly Lipschitz continuous with respect to p with Lipschitz constant K. The derivative $\partial_p k(\mathbf{x},p)$ exists. The derivative $\partial_a \mu(\mathbf{x},a,p)$ exists and is bounded.*

Condition 2.3. *Let $\mathbb{R}^+$ denote the non-negative real numbers. The birth condition, $\mathcal{B} : L^1(\mathbb{R}^+) \cap L^2(\mathbb{R}^+) \to \mathbb{R}$, satisfies the Lipschitz condition*

$$|\mathcal{B}(\mathbf{x}, \varphi(\mathbf{x}, \cdot, t)) - \mathcal{B}(\mathbf{x}, \psi(\mathbf{x}, \cdot, t))| \leq \\ K\left(\left(1 + \|\varphi\|_{L^1(\mathbb{R}^+)}\right)\left|\int_0^\infty (\varphi - \psi)\, da\right| + \|\varphi - \psi\|_{H^{-1}(\mathbb{R}^+)}\right),$$

and is bounded. Here, $H^{-1}(\mathbb{R}^+)$ is the dual to $H^1(\mathbb{R}^+)$.

Condition 2.4. *The initial condition, $u^0(\mathbf{x}, a)$, is bounded and there exists $\tilde{a}_{max}$ such that $u^0(\mathbf{x}, a) = 0$ for $a > \tilde{a}_{max}$.*

An example of the birth condition is

$$\mathcal{B}(\mathbf{x}, \varphi(\mathbf{x}, \cdot, t)) = \int_0^\infty \beta(\mathbf{x}, a, \Phi)\varphi(\mathbf{x}, a, t)\, da,$$

where $\beta \geq 0$ is the birth rate and Φ is the integral of φ with respect to age. Condition 2.3 is satisfied if β is uniformly Lipschitz continuous as a function of Φ; if $\beta(\mathbf{x}, a, \Phi)$, considered as a function of a, is in $H^1(\mathbb{R}^+)$, with H^1-norm bounded independently of $\mathbf{x}$ and Φ; and $\varphi \in L^1(\mathbb{R}^+) \cap L^2(\mathbb{R}^+)$, as a function of age.

If we make a transformation to a moving reference frame in age, $w(\mathbf{x}, c, t) = u(\mathbf{x}, c + t, t)$, then the resulting system is

$$\partial_t w = \nabla \cdot k(\mathbf{x}, p)\nabla w - \mu(\mathbf{x}, c + t, p)w, \qquad \mathbf{x} \in \Omega,\ c \geq -t,\ t \geq 0, \tag{2.2.6}$$

$$w(\mathbf{x}, -t, t) = \mathcal{B}(\mathbf{x}, w(\mathbf{x}, \cdot, t)), \qquad \mathbf{x} \in \Omega,\ t \geq 0, \tag{2.2.7}$$

$$k(\mathbf{x}, p)\nabla w \cdot \nu = 0, \qquad \mathbf{x} \in \partial\Omega,\ c \geq -t,\ t \geq 0, \tag{2.2.8}$$

$$p(\mathbf{x}, t) = \int_{-t}^\infty w(\mathbf{x}, c, t)\, dc, \qquad \mathbf{x} \in \Omega,\ t \geq 0, \tag{2.2.9}$$

$$w(\mathbf{x}, c, 0) = u^0(\mathbf{x}, c), \qquad \mathbf{x} \in \Omega,\ c \geq -t. \tag{2.2.10}$$

2.2 The Age-Discrete Model

We discretize age for all time by using an infinite mesh, $c_{-\infty} < \cdots < c_{-1} < c_0 < c_1 < \cdots c_\infty$. Each age interval $[c_i, c_{i+1})$, $-\infty < i < \infty$, can be thought of as defining a *cohort*. The infinite mesh is a useful analytical tool; the actual c_i's may be determined adaptively as the calculation progresses. We denote the partition determined by the set of points $\{c_i\}$ by γ. If $c_{i+1} > -t$, we define the *active cohort* to be $\mathcal{C}_i(t) = [\max(c_i, -t), c_{i+1})$, with length $\Delta c_i(t)$. We denote by $\mathcal{A}(\gamma, t)$ the space of functions which are constant over each $\mathcal{C}_i$, extended to be zero for $c < -t$. We let W_i denote the age-discrete approximation to w on $\mathcal{C}_i$ and $W(x, t)$ denote the corresponding function in $\mathcal{A}(\gamma, t)$. As we will see in Section 2.6, $\lim_{a\to\infty} u = 0$, so in practice we need only consider W_i for c_{i+1} in the interval $[-t, a_{\max} - t]$, for a suitably large choice of $a_{\max}$. We define the age-averaging operator, $\mathsf{A} : L^1_{\text{loc}} \to \mathcal{A}$, by setting its value on $\mathcal{C}_i$ to

$$\mathsf{A}_i(\varphi) = \frac{1}{\Delta c_i} \int_{\mathcal{C}_i} \varphi(c)\ dc,$$

for every i such that $c_{i+1} > -t$. To motivate the choices in the definition of the age-discrete model, we apply the age-averaging operator to Equation (2.2.6). We note that if $-t \in \mathcal{C}_i(t)$,

$$\mathsf{A}_i(\partial_t w) = \partial_t \mathsf{A}_i(w) + \frac{1}{\Delta c_i} \left(\mathsf{A}_i(w) - \mathcal{B}\right).$$

For the death term, we have

$$\begin{aligned} \mathsf{A}_i(\mu w) &= \mathsf{A}_i(\mu)\mathsf{A}_i(w) + \mathsf{A}_i((\mu - \mathsf{A}_i(\mu))w) \\ &= \mathsf{A}_i(\mu)\mathsf{A}_i(w) + \mathsf{A}_i((\mu - \mathsf{A}_i(\mu))(w - \mathsf{A}_i(w))), \end{aligned}$$

Thus $\mathsf{A}_i(\mu)\mathsf{A}_i(w)$ is a 2nd-order correct approximation of $\mathsf{A}_i(\mu w)$, if μ and w are smooth. We will obtain a 2nd-order correct model in age by using a parabolic equation for the population density over each cohort,

$$\partial_t W_i(\mathsf{x}, t) = \nabla \cdot k(\mathsf{x}, P) \nabla W_i(\mathsf{x}, t) - \bar{\mu}_i(\mathsf{x}, t, P) W_i(\mathsf{x}, t) + B_i(\mathsf{x}, t, W), \tag{2.2.11}$$

for every i such that $c_{i+1} > -t$. If $c_{i+1} = -t$, then $W_i = \mathcal{B}(\mathsf{x}, W)$. The death modulus is

$$\bar{\mu}_i(\mathsf{x}, t, \varphi) = \frac{1}{\Delta c_i} \int_{\mathcal{C}_i} \mu(\mathsf{x}, c+t, \varphi)\, dc.$$

The birth term is

$$B_i(\mathsf{x}, t, \varphi) = \begin{cases} \frac{1}{\Delta c_i}\left(\mathcal{B}(\mathsf{x}, \varphi) - \mathsf{A}_i(\varphi)\right), & \text{if } -t \in \mathcal{C}_i(t), \\ 0, & \text{otherwise.} \end{cases}$$

We take $W_i = 0$ for $c_{i+1} < -t$. The term $\mathsf{A}_i(W_i)/\Delta c_i$ in $B_i(\mathsf{x}, t, W)$ accounts for the conservation of population as the length of the active birth interval increases. Notice that if we temporarily neglect the k and μ terms, then

$$\partial_t \left(\Delta c_i W_i\right) = \mathcal{B}(\mathsf{x}, W_i), \qquad -t \in \mathcal{C}_i(t).$$

The age-discrete total population density, P, is obtained by integrating W in the age variable. The equations are coupled only through B and P.

2.3 The Fully Discrete Method

We fully discretize the problem by using a backward difference method in time and a Galerkin method in space. Let $(\cdot, \cdot)$ denote the L^2 inner product on Ω. Over each cohort, a weak form of equation (2.2.11) is given by, for every $v \in H^1(\Omega)$,

$$(\partial_t W_i, v) + k(P; W_i, v) + (\bar{\mu}(\mathsf{x}, t, P) W_i, v) = (B_i, v). \qquad (2.2.12)$$

Here, we reuse the symbol k to denote the form

$$k(P; \varphi, v) = \int_\Omega k(\mathsf{x}, P) \nabla\varphi \cdot \nabla v \, d\mathsf{x};$$

the distinction between the form and $k(\mathsf{x}, P)$ should be clear from context.

Let $\mathcal{M}$ denote a finite dimensional subspace of $H^1(\Omega)$. Let $\tilde{W}_i^j \in \mathcal{M}$ denote the approximate solution to (2.2.12) at the j-th time step, t^j. Define $\Delta t^j = t^j - t^{j-1}$ and $\Delta c_i^j = \Delta c_i(t^j)$. We assume that the time discretization is a refinement of the age discretization. Specifically, we require that $[-t^j, -t^{j-1}] \subseteq [c_i, c_{i+1}]$ for some i, and we denote this i by $\mathsf{b}(j)$. We use the notation $\bar{\mu}_i^j(\varphi) = \bar{\mu}_i(\mathsf{x}, t^j, \varphi)$. The fully discrete method is defined by the system

$$\left(\frac{\tilde{W}_i^j - \tilde{W}_i^{j-1}}{\Delta t^j}, v\right) + k(\tilde{P}^{j-1}; \tilde{W}_i^j, v) + (\bar{\mu}_i^j(\tilde{P}^{j-1})\tilde{W}_i^j, v) = (B_i^j(\tilde{W}^{j-1}), v), \tag{2.2.13}$$

for every $v \in \mathcal{M}$. If $-t^{j-1} = c_{i+1}$, then $\tilde{W}_i^{j-1}$ is initialized to the elliptic projection into $\mathcal{M}$ of $\mathcal{B}(\mathsf{x}, \tilde{W}^{j-1})$. Let $\tilde{W}^j = \{\tilde{W}_i^j : \text{ all } i\}$. The term $\tilde{P}^j$ is obtained by integrating $\tilde{W}_i^j$. The birth function is $B_i^j(\varphi) = B_i(\mathsf{x}, t^j, \varphi)$, if $i = \mathsf{b}(j)$, or $B_i^j(\varphi) = 0$, otherwise. By lagging $\tilde{P}$ and b at each time step, the discrete equations are coupled to each other only by values which are known before the step is taken. Thus, for each i, we only need to solve an independent linear system.

2.4 Error Analysis

The analysis follows that of Wheeler [44] for parabolic equations. For discrete time and age, the value of $\varphi(\cdot, t^j)$ will be denoted by φ^j, and the average value of φ on $\mathcal{C}_i$ at time t^j will be denoted by φ_i^j. It is convenient to use $H^{-1}(\Omega)$ to denote the dual of $H^1(\Omega)$. Let $\|\cdot\|$, $\|\cdot\|_{L^\infty}$, $\|\cdot\|_{H^1}$, and $\|\cdot\|_{H^{-1}}$ denote the L^2, L^∞, H^1 and H^{-1} norms over Ω, respectively. Suppose that χ is a normed space with norm $\|\cdot\|_\chi$. Then, for any sufficiently nice function φ, such that $\varphi(c) \in \chi$, let

$$|||\varphi|||_\chi^2 = \int_{-\infty}^{\infty} \|\varphi(c)\|_\chi^2 \, dc.$$

A lack of a subscript indicates $\chi = L^2(\Omega)$.

We show that the approximate solution $\tilde{W}$ is close to a function X, which is the elliptic projection in space and the L^2-projection in age of the true solution w. For each (c,t), we take $\tilde{X}(c,t) \in \mathcal{M}$ such that $k(p; w - \tilde{X}, v) = 0$ for all $v \in \mathcal{M}$ and such that $(w - \tilde{X}, 1) = 0$. Similarly, for each t, we take $Y(t) \in \mathcal{M}$ to satisfy

$k(p; p-Y, v) = 0$ for all $v \in \mathcal{M}$ and $(p - Y, 1) = 0$. We choose $X(t) \in \mathcal{M} \otimes \mathcal{A}$ such that $X(t) = \mathsf{A}(\tilde{X}(c,t))$. We set

$$\vartheta = \tilde{W} - X, \;\; \eta = \mathsf{A}(w) - X, \;\; \varpi = \tilde{P} - Y, \text{ and } \sigma = p - Y.$$

Theorem 2.1. *Assume Conditions 2.1 – 2.3 hold. Let h denote the length of the longest cohort. Set $Q^j = \Omega \times [t^{j-1}, t^j]$, and define $\Lambda^j = \|\!|\partial_t w\|\!|^2_{L^2(Q^j)} + \|\partial_t p\|^2_{L^2(Q^j)} + \|\partial_t w_{\mathsf{b}(j)}\|^2_{L^2(Q^j)} + \|\!|\partial_{tt} w\|\!|^2_{L^2(Q^j)} + \|\partial_{tt} p\|^2_{L^2(Q^j)}$. There exists positive constants δ and C^*, dependent only on K, C_0, C_1, $\|\!|w\|\!|_{L^\infty}$, $\|w\|_{L^\infty(\mathbb{R}\times\Omega)}$, $\|w\|^2_{L^1(\mathbb{R})\otimes L^2(\Omega)}$, $\|\!|\nabla X\|\!|_{L^\infty}$, $\|p\|_{L^\infty}$, $\|\nabla Y\|_{L^\infty}$, and $\|\partial_a \mu\|^2_{L^\infty(\mathbb{R}^+\times\Omega)}$, such that, provided $\Delta t^j < \delta$ for $1 \le j \le m$,*

$$\begin{aligned}\|\!|\vartheta^m\|\!|^2 + \|\varpi^m\|^2 \le C^*\left(\|\!|\vartheta^0\|\!|^2 + \|\varpi^0\|^2\right) + \\ C^* \sum_{j=1}^{m} \Bigg(\Lambda^j \Delta t^j + h^4 \left(\|\!|\partial_c w^j\|\!|^2 + \|\!|\partial_c w^{j-1}\|\!|^2\right) + \left\|\frac{\eta^j - \eta^{j-1}}{\Delta t^j}\right\|^2_{H^{-1}} \\ + \|\!|\eta^j\|\!|^2 + \|\!|\eta^{j-1}\|\!|^2 + \|\eta^{j-1}_{\mathsf{b}(j)}\|^2 \\ + \left\|\frac{\sigma^j - \sigma^{j-1}}{\Delta t^j}\right\|^2_{H^{-1}} + \|\sigma^j\|^2 + \|\sigma^{j-1}\|^2 \Bigg) \Delta t^j.\end{aligned} \tag{2.2.14}$$

Remark. By this result, the approximation is superconvergent in age. Although a piecewise constant approximation is normally only first-order correct, we have ϑ and ϖ of second-order in age.

Proof. Applying the age-averaging operator, A, to Equation (2.2.6) gives

$$\begin{aligned}\partial_t \mathsf{A}_i(w) &= \nabla \cdot k \nabla \mathsf{A}_i(w) + B_i(\mathsf{x}, t, w) \\ &\quad - \left(\bar{\mu}_i(\mathsf{x}, t, p)\mathsf{A}_i(w) + \mathsf{A}_i(\,[\mu - \mathsf{A}_i(\mu)][w - \mathsf{A}_i(w)]\,)\right),\end{aligned}$$

for every i such that $c_{i+1} > -t$. If $-t^{j-1} < c_{i+1}$, set $w_i^{j-1} = \mathsf{A}_i(w^{j-1})$. If $-t^{j-1} = c_{i+1}$, set $w_i^{j-1} = w(\mathsf{x}, -t^{j-1}, t^{j-1})$. Lagging p and $\mathcal{B}$, we get, at time t^j,

$$\begin{aligned}&\left(\frac{w_i^j - w_i^{j-1}}{\Delta t^j}, v\right) + k(p^{j-1}; w_i^j, v) + (\bar{\mu}_i^j(p^{j-1}) w_i^j, v) \\ &\quad = (B_i^j(w^{j-1}), v) + \left(B_i^j(w^j) - B_i^j(w^{j-1}), v\right) + (\rho_i^j, v) - (g_i^j, v) \\ &\qquad + k(p^{j-1} - p^j; w_i^j, v) + \left(\left(\bar{\mu}_i^j(p^{j-1}) - \bar{\mu}_i^j(p^j)\right) w_i^j, v\right),\end{aligned} \tag{2.2.15}$$

where

$$\rho_i^j = \frac{w_i^j - w_i^{j-1}}{\Delta t^j} - \partial_t w_i^j,$$
$$g_i^j = \mathsf{A}_i(\,[\mu(\mathsf{x}, c+t^j, p^j) - \mathsf{A}_i(\mu(\mathsf{x}, c+t^j, p^j))][w^j - \mathsf{A}_i(w^j)]\,).$$

Let $v = \Delta c_i^j \vartheta_i^j$ and subtract (2.2.15) from (2.2.13) to get

$$\begin{aligned}
&\frac{1}{\Delta t^j}(\vartheta_i^j - \vartheta_i^{j-1}, \Delta c_i^j \vartheta_i^j) + k(\tilde{P}^{j-1}; \tilde{W}_i^j, \Delta c_i^j \vartheta_i^j) \\
&- k(p^{j-1}; w_i^j, \Delta c_i^j \vartheta_i^j) + (\bar{\mu}_i^j(\tilde{P}^{j-1})\tilde{W}_i^j - \bar{\mu}_i^j(p^{j-1})w_i^j, \Delta c_i^j \vartheta_i^j) \\
&\quad = (B_i^j(\tilde{W}^{j-1}) - B_i^j(w^{j-1}), \Delta c_i^j \vartheta_i^j) \\
&\qquad + \left(B_i^j(w^{j-1}) - B_i^j(w^j), \Delta c_i^j \vartheta_i^j\right) + (g_i^j - \rho_i^j, \Delta c_i^j \vartheta_i^j) \\
&\qquad + \left(\frac{\eta_i^j - \eta_i^{j-1}}{\Delta t^j}, \Delta c_i^j \vartheta_i^j\right) + k(p^{j-1} - p^j; w_i^j, \Delta c_i^j \vartheta_i^j) \\
&\qquad + \left(\left(\bar{\mu}_i^j(p^{j-1}) - \bar{\mu}_i^j(p^j)\right) w_i^j, \Delta c_i^j \vartheta_i^j\right).
\end{aligned} \tag{2.2.16}$$

Equation (2.2.16) makes sense for $-t^{j-1} = c_{i+1}$, since in this case, $w_i^{j-1} = \mathcal{B}(\mathsf{x}, w^{j-1})$ and $\tilde{W}_i^{j-1}$ is the elliptic projection in space of $\mathcal{B}(\mathsf{x}, \tilde{W}^{j-1})$. Rearranging terms, we get

$$\begin{aligned}
&\frac{1}{\Delta t^j}(\vartheta_i^j - \vartheta_i^{j-1}, \Delta c_i^j \vartheta_i^j) \\
&+ k(\tilde{P}^{j-1}; \vartheta_i^j, \Delta c_i^j \vartheta_i^j) + (\bar{\mu}_i^j(\tilde{P}^{j-1})\vartheta_i^j, \Delta c_i^j \vartheta_i^j) \\
&\quad = \left\{\Delta c_i^j (k(\mathsf{x}, Y^{j-1}) - k(\mathsf{x}, \tilde{P}^{j-1}), \nabla X_i^j \cdot \nabla \vartheta_i^j)\right\}_1 \\
&\qquad + \left\{\Delta c_i^j (k(\mathsf{x}, p^{j-1}) - k(\mathsf{x}, Y^{j-1}), \nabla X_i^j \cdot \nabla \vartheta_i^j)\right\}_2 \\
&\qquad + \left\{\Delta c_i^j (k(\mathsf{x}, p^j) - k(\mathsf{x}, p^{j-1}), \nabla X_i^j \cdot \nabla \vartheta_i^j)\right\}_3 \\
&\qquad + \left\{((\bar{\mu}_i^j(p^{j-1}) - \bar{\mu}_i^j(\tilde{P}^{j-1}))w_i^j, \Delta c_i^j \vartheta_i^j)\right\}_4 \\
&\qquad + \left\{((\bar{\mu}_i^j(p^{j-1}) - \bar{\mu}_i^j(p^j))w_i^j, \Delta c_i^j \vartheta_i^j)\right\}_5 \\
&\qquad + \left\{\left(\frac{\eta_i^j - \eta_i^{j-1}}{\Delta t^j} + \bar{\mu}_i^j(\tilde{P}^{j-1})\eta_i^j, \Delta c_i^j \vartheta_i^j\right)\right\}_6 \\
&\qquad - \left\{(\rho_i^j, \Delta c_i^j \vartheta_i^j)\right\}_7 \\
&\qquad + \left\{(g_i^j, \Delta c_i^j \vartheta_i^j)\right\}_8 \\
&\qquad + \left\{(B_i^j(\tilde{W}^{j-1}) - B_i^j(w^{j-1}), \Delta c_i^j \vartheta_i^j)\right\}_9 \\
&\qquad + \left\{(B_i^j(w^{j-1}) - B_i^j(w^j), \Delta c_i^j \vartheta_i^j)\right\}_{10} \\
&\quad = I_1 + I_2 + I_3 + I_4 + I_5 + I_6 + I_7 + I_8 + I_9 + I_{10},
\end{aligned} \tag{2.2.17}$$

where I_1 – I_{10} refer to the corresponding bracketed expressions. Using Conditions 2.1 – 2.2, Hölder's inequality, and the arithmetic-geometric inequality, $yz \leq \frac{1}{2}(\varepsilon y^2 + (1/\varepsilon)z^2)$, we get the following bounds:

$$\begin{aligned}
|I_1| &\leq \Delta c_i^j (K|\varpi^{j-1}|, |\nabla X_i^j \cdot \nabla \vartheta_i^j|) \\
&\leq \Delta c_i^j \left(\frac{K^2}{C_0} \|\nabla X_i^j\|_{L^\infty}^2 \|\varpi^{j-1}\|^2 + \frac{C_0}{4} \|\vartheta_i^j\|_{H^1}^2 \right); \\
|I_2| &\leq \Delta c_i^j \left(\frac{K^2}{C_0} \|\nabla X_i^j\|_{L^\infty}^2 \|\sigma^{j-1}\|^2 + \frac{C_0}{4} \|\vartheta_i^j\|_{H^1}^2 \right); \\
|I_3| &\leq \Delta c_i^j \left(\frac{K^2}{C_0} \|\nabla X_i^j\|_{L^\infty}^2 \|p^j - p^{j-1}\|^2 + \frac{C_0}{4} \|\vartheta_i^j\|_{H^1}^2 \right); \\
|I_4| &\leq \Delta c_i^j (K|\tilde{P}^{j-1} - p^{j-1}|, |w_i^j \vartheta_i^j|) \leq \Delta c_i^j \left(\frac{K}{2} \|w_i^j\|_{L^\infty} \left(\|\tilde{P}^{j-1} - p^{j-1}\|^2 + \|\vartheta_i^j\|^2 \right) \right); \\
|I_5| &\leq \frac{\Delta c_i^j K}{2} \|w_i^j\|_{L^\infty} \left(\|p^j - p^{j-1}\|^2 + \|\vartheta_i^j\|^2 \right); \\
|I_6| &\leq \Delta c_i^j \left(\frac{1}{C_0} \left\| \frac{\eta_i^j - \eta_i^{j-1}}{\Delta t^j} \right\|_{H^{-1}}^2 + \frac{C_0}{4} \|\vartheta_i^j\|_{H^1}^2 + \frac{C_1}{2} \left(\|\eta_i^j\|^2 + \|\vartheta_i^j\|^2 \right) \right); \\
|I_7| &\leq \frac{\Delta c_i^j}{2} \left(\frac{1}{4} \|\partial_{tt} w\|_{L^2(Q^j)}^2 \Delta t^j + \|\vartheta_i^j\|^2 \right); \\
|I_8| &\leq \frac{\Delta c_i^j}{2} \left(\|g_i^j\|^2 + \|\vartheta_i^j\|^2 \right).
\end{aligned}$$

Collecting the terms I_1 – I_8 and using the bounds $k(\tilde{P}^{j-1}; \vartheta_i^j, \vartheta_i^j) \geq C_0 \|\vartheta_i^j\|_{H^1}^2$ and $(\bar{\mu}_i^j(\tilde{P})\vartheta_i^j, \vartheta_i^j) \geq C_0 \|\vartheta_i^j\|^2$, and the fact that $(y+z)^2 \leq 2(y^2 + z^2)$, we get

$$\begin{aligned}
\frac{\Delta c_i^j}{\Delta t^j} (\vartheta_i^j - \vartheta_i^{j-1}, \vartheta_i^j) \leq& \qquad (2.2.18) \\
& \Delta c_i^j C_2 \left(\|\varpi^{j-1}\|^2 + \|\sigma^{j-1}\|^2 + \|p^j - p^{j-1}\|^2 \right) \\
& + \frac{\Delta c_i^j}{2C_0} \left\| \frac{\eta_i^j - \eta_i^{j-1}}{\Delta t^j} \right\|_{H^{-1}}^2 + \frac{\Delta c_i^j C_1}{2} \|\eta_i^j\|^2 + \frac{\Delta c_i^j}{2} \|g_i^j\|^2 \\
& + \frac{\Delta c_i^j}{8} \|\partial_{tt} w\|_{L^2(Q^j)}^2 \Delta t^j + \Delta c_i^j C_3 \|\vartheta_i^j\|^2 + I_9 + I_{10},
\end{aligned}$$

where

$$\begin{aligned}
C_2 &= \frac{K^2}{C_0} \|\nabla X_i^j\|_{L^\infty}^2 + K \|w_i^j\|_{L^\infty}, \\
C_3 &= K \|w_i^j\|_{L^\infty} + \frac{C_1}{2} - C_0 + 1.
\end{aligned}$$

Recall that $\mathsf{b}(j)$ denotes the index of the birth interval at time t^j. If $i \neq \mathsf{b}(j)$, then $I_9 = I_{10} = 0$ and $\Delta c_i^j = \Delta c_i^{j-1}$. For the left hand side of (2.2.18), we make the estimate

$$\begin{aligned}
\frac{\Delta c_i^j}{\Delta t^j}(\vartheta_i^j - \vartheta_i^{j-1}, \vartheta_i^j) &= \frac{\Delta c_i^j}{2\Delta t^j}\left(\|\vartheta_i^j\|^2 - \|\vartheta_i^{j-1}\|^2 + \|\vartheta_i^j - \vartheta_i^{j-1}\|^2\right) \\
&\geq \frac{1}{2\Delta t^j}\left(\Delta c_i^j \|\vartheta_i^j\|^2 - \Delta c_i^{j-1}\|\vartheta_i^{j-1}\|^2\right).
\end{aligned}$$

If $i = \mathsf{b}(j)$, then $\Delta c_i^j = \Delta c_i^{j-1} + \Delta t^j$. For the left hand side of (2.2.18), we make the estimate

$$\begin{aligned}
\frac{\Delta c_i^j}{\Delta t^j}(\vartheta_i^j - \vartheta_i^{j-1}, \vartheta_i^j) &= \frac{\left(\Delta c_i^j\|\vartheta_i^j\|^2 - \Delta c_i^{j-1}\|\vartheta_i^{j-1}\|^2\right)}{2\Delta t^j} + \|\vartheta_i^j\|^2 - (\vartheta_i^{j-1}, \vartheta_i^j) \\
&\quad + \frac{\Delta c_i^{j-1}}{2\Delta t^j}\|\vartheta_i^j - \vartheta_i^{j-1}\|^2 \\
&\geq \frac{\left(\Delta c_i^j\|\vartheta_i^j\|^2 - \Delta c_i^{j-1}\|\vartheta_i^{j-1}\|^2\right)}{2\Delta t^j} + \|\vartheta_i^j\|^2 - (\vartheta_i^{j-1}, \vartheta_i^j).
\end{aligned}$$

We note that the H^{-1}-norm is bounded by the L^2-norm. For the birth terms we make the estimates

$$\begin{aligned}
I_9 &= \left(\mathcal{B}(\mathsf{x}, \tilde{W}^{j-1}) - \mathcal{B}(\mathsf{x}, w^{j-1}), \vartheta_i^j\right) - (\mathsf{A}_i(\tilde{W}^{j-1} - w^{j-1}), \vartheta_i^j) \\
&\leq 2K^2\left(\|w^{j-1}\|^2_{L^1(\mathbb{R})\otimes L^2(\Omega)}\|\tilde{P}^{j-1} - p^{j-1}\|^2 + \|\tilde{W}^{j-1} - w^{j-1}\|^2_{H^{-1}(\mathbb{R})\otimes L^2(\Omega)}\right) \\
&\quad + \frac{1}{2}\|\vartheta_i^j\|^2 - (\vartheta_i^{j-1}, \vartheta_i^j) + \|\eta_i^{j-1}\|^2 \\
&\leq 2K^2\left(\|w^{j-1}\|^2_{L^1(\mathbb{R})\otimes L^2(\Omega)}\|\tilde{P}^{j-1} - p^{j-1}\|^2 + 3\left(|||\vartheta^{j-1}|||^2 + |||\eta^{j-1}|||^2\right.\right. \\
&\quad \left.\left. + \ \|\mathsf{A}(w^{j-1}) - w^{j-1}\|^2_{H^{-1}(\mathbb{R})\otimes L^2(\Omega)}\right)\right) + \frac{1}{2}\|\vartheta_i^j\|^2 - (\vartheta_i^{j-1}, \vartheta_i^j) + \|\eta_i^{j-1}\|^2, \\
I_{10} &= \left(\mathcal{B}(\mathsf{x}, w^j) - \mathcal{B}(\mathsf{x}, w^{j-1}), \vartheta_i^j\right) - (\mathsf{A}_i(w^j - w^{j-1}), \vartheta_i^j) \\
&\leq 2K^2\left(\|w^{j-1}\|^2_{L^1(\mathbb{R})\otimes L^2(\Omega)}\|p^j - p^{j-1}\|^2 + |||w^j - w^{j-1}|||\right) \\
&\quad + \frac{1}{2}\|\vartheta_i^j\|^2 + \|w_i^j - w_i^{j-1}\|^2.
\end{aligned}$$

We make the appropriate bounds, for each i, of the left hand side of (2.2.18), of I_9, and of I_{10}. We then sum over i to get

$$\begin{aligned}\frac{1}{2\Delta t^j}\left(|||\vartheta^j|||^2 - |||\vartheta^{j-1}|||^2\right) \leq& \qquad (2.2.19)\\ & C_4\left(\|\varpi^{j-1}\|^2 + \|\sigma^{j-1}\|^2 + \|p^j - p^{j-1}\|^2\right)\\ &+ 6K^2\left(|||\vartheta^{j-1}|||^2 + |||\eta^{j-1}|||^2 + \|\mathsf{A}(w^{j-1}) - w^{j-1}\|^2_{H^{-1}(\mathbb{R})\otimes L^2(\Omega)}\right)\\ &+ \|w^j_{\mathsf{b}(j)} - w^{j-1}_{\mathsf{b}(j)}\|^2 + \|\eta^{j-1}_{\mathsf{b}(j)}\|^2 + 2K^2|||w^j - w^{j-1}|||^2\\ &+ \frac{1}{C_0}\left\|\frac{\eta^j - \eta^{j-1}}{\Delta t^j}\right\|^2_{H^{-1}} + \frac{C_1}{2}|||\eta^j|||^2 + \frac{1}{2}|||g^j|||^2\\ &+ \frac{1}{8}|||\partial_{tt}w|||^2_{L^2(Q^j)}\Delta t^j + C_5|||\vartheta^j|||^2,\end{aligned}$$

where

$$\begin{aligned} C_4 &= \frac{K^2}{C_0}|||\nabla X^j|||^2_{L^\infty} + K|||w^j|||_{L^\infty} + 4K^2\|w^{j-1}\|^2_{L^1(\mathbb{R})\otimes L^2(\Omega)},\\ C_5 &= K\|w^j\|_{L^\infty(\Omega\times\mathbb{R})} + \frac{C_1}{2} - C_0 + 1.\end{aligned}$$

Before we can use the above evolution inequality to get bounds on the error, we need corresponding relationships for the total population density. We integrate equation (2.2.6) over c and take the inner product with a test function $v \in \mathcal{M}$ to obtain

$$(\partial_t p, v) - (\mathcal{B}, v) + k(p; p, v) + \left(\int_{-t}^{\infty} \mu(\mathsf{x}, c+t, p)w\, dc\,, v\right) = 0.$$

Then

$$\begin{aligned}\left(\frac{p^j - p^{j-1}}{\Delta t^j}, v\right) - k(p^j; p^j, v) + \left(\int_{-t^j}^{\infty} \mu(\mathsf{x}, c+t^j, p^{j-1})w^j\ dc,\ v\right)&\\ = (\mathcal{B}(\mathsf{x}, w^{j-1}), v) + (\mathcal{B}(\mathsf{x}, w^{j-1}) - \mathcal{B}(\mathsf{x}, w^j), v) + (\varrho^j, v)&\\ + \left(\int_{-t^j}^{\infty}(\mu(\mathsf{x}, c+t^j, p^{j-1}) - \mu(\mathsf{x}, c+t^j, p^j))w^j\, dc,\ v\right).& \qquad (2.2.20)\end{aligned}$$

where

$$\varrho^j = \frac{p^j - p^{j-1}}{\Delta t^j} - \partial_t p^j$$

From equation (2.2.13) we obtain

$$\left(\frac{\tilde{P}^j - \tilde{P}^{j-1}}{\Delta t^j}, v\right) + k(\tilde{P}^{j-1}; \tilde{P}^j, v) + \left(\int_{-t^j}^{\infty} \bar{\mu}_i^j(\tilde{P}^{j-1})\tilde{W}^j \, dc, \, v\right)$$
$$= (\mathcal{B}(\mathsf{x}, \tilde{W}^{j-1}), v). \quad (2.2.21)$$

Let $v = \varpi^j$ and subtract (2.2.20) from (2.2.21) to get

$$\begin{aligned}
&\frac{1}{\Delta t^j}(\varpi^j - \varpi_i^{j-1}, \varpi^j) + k(\tilde{P}^{j-1}; \tilde{P}^j, \varpi^j) - k(p^{j-1}; p^j, \varpi^j) \\
&+ \left(\sum_i \bar{\mu}_i^j(\tilde{P}^{j-1})\tilde{W}_i^j - \bar{\mu}_i^j(p^{j-1}) w_i^j \Delta c_i^j, \, \varpi^j\right) \\
&\quad = (\mathcal{B}(\mathsf{x}, \tilde{W}^{j-1}) - \mathcal{B}(\mathsf{x}, w^{j-1}), \varpi^j) + (\mathcal{B}(\mathsf{x}, w^{j-1}) - \mathcal{B}(\mathsf{x}, w^j), \varpi^j) \\
&\qquad + \left(\frac{\sigma_i^j - \sigma_i^{j-1}}{\Delta t^j}, \varpi^j\right) + k(p^{j-1} - p^j; p^j, \varpi^j) + \left(\|g^j\|_{L^2(\mathbb{R})} - \varrho^j, \varpi^j\right) \\
&\qquad + \left(\int_{-t}^{\infty} (\mu(\mathsf{x}, c + t^j, p^{j-1}) - \mu(\mathsf{x}, c + t^j, p^j)) w^j \; dc, \, \varpi^j\right).
\end{aligned}$$

This has a form similar to (2.2.16). We handle the non-birth terms as before. For the birth terms, we directly apply Condition 2.3. Then

$$\begin{aligned}
&\frac{1}{2\Delta t^j}\left(\|\varpi^j\|^2 - \|\varpi^{j-1}\|^2\right) \leq \qquad (2.2.22) \\
&\qquad C_6\left(\|\varpi^{j-1}\|^2 + \|\sigma^{j-1}\|^2 + \|p^j - p^{j-1}\|^2\right) \\
&\qquad + 6K^2\left(|\!|\!|\vartheta^{j-1}|\!|\!|^2 + |\!|\!|\eta^{j-1}|\!|\!|^2 + \|\mathsf{A}(w^{j-1}) - w^{j-1}\|^2_{H^{-1}(\mathbb{R})\otimes L^2(\Omega)}\right) \\
&\qquad + 2K^2 |\!|\!|w^j - w^{j-1}|\!|\!|^2 + \frac{1}{C_0}\left\|\frac{\sigma^j - \sigma^{j-1}}{\Delta t^j}\right\|^2_{H^{-1}} + \frac{C_1}{2}\|\sigma^j\|^2 \\
&\qquad + \frac{1}{8}\|\partial_{tt} p\|^2_{L^2(Q^j)} \Delta t^j + C_7\|\varpi^j\|^2 + \frac{1}{2}|\!|\!|g^j|\!|\!|^2,
\end{aligned}$$

where

$$\begin{aligned}
C_6 &= \frac{K^2}{C_0}\|\nabla Y^j\|^2_{L^\infty} + K\|p^j\|_{L^\infty} + 4K^2\|w^{j-1}\|^2_{L^1(\mathbb{R})\otimes L^2(\Omega)}. \\
C_7 &= K\left(\|p^j\|_{L^\infty} + 2\right) + \frac{C_1}{2} - C_0 + 2.
\end{aligned}$$

We make the estimates (see Appendix A),

$$\begin{aligned}
\|p^j - p^{j-1}\|^2 &\leq \Delta t^j \|\partial_t p\|^2_{L^2(Q^j)}, \\
\|\!|w^j - w^{j-1}|\!\|^2 &\leq \Delta t^j \|\!|\partial_t w|\!\|^2_{L^2(Q^j)}, \\
\|w^j_{\mathsf{b}(j)} - w^{j-1}_{\mathsf{b}(j)}\|^2 &\leq \Delta t^j \|\partial_t w_{\mathsf{b}(j)}\|^2_{L^2(Q^j)}, \\
\|\mathsf{A}(w^{j-1}) - w^{j-1}\|^2_{H^{-1}(\mathbb{R})\otimes L^2(\Omega)} &\leq \left(\frac{h}{\pi}\right)^4 \|\!|\partial_c w^{j-1}|\!\|^2, \\
\|\!|g^j|\!\|^2 &\leq \|\mu - \mathsf{A}(\mu)\|^2_{L^\infty(\mathbb{R}^+\times\Omega)} \|\!|w^j - \mathsf{A}(w^j)|\!\|^2 \\
&\leq \left(\frac{h^4}{4\pi^2}\right) \|\partial_a \mu\|^2_{L^\infty(\mathbb{R}^+\times\Omega)} \|\!|\partial_c w^j|\!\|^2.
\end{aligned}$$

Then, adding 2.2.19 and 2.2.22 and assuming Δt^j is sufficiently small, we apply a discrete Gronwall's inequality (see Appendix B) to get the stated result. □

2.5 Postprocessing the Computational Results

In this section, we present a postprocessing result which capitalizes on the superconvergence shown in Theorem 2.1. In this postprocessing method, we apply a transformation that takes the first-order correct piecewise constant approximation in age to a second-order correct continuous piecewise linear approximation. We define the transformation $\mathsf{T} : \mathcal{A}(\gamma) \to \tilde{\mathcal{A}}(\gamma)$, where $\tilde{\mathcal{A}}(\gamma)$ is the space of functions which are continuous and are linear over each $\mathcal{C}_i$, so that for $\varphi \in \mathcal{A}(\gamma)$ and $\psi \in \tilde{\mathcal{A}}(\gamma)$, $\psi = \mathsf{T}(\varphi)$ has values at the nodes given by

$$\begin{aligned}
\psi(c_i) &= \frac{\Delta c^j_{i-1}\varphi_i + \Delta c^j_i \varphi_{i-1}}{\Delta c^j_{i-1} + \Delta c^j_i}, && \text{if } i > \mathsf{b}(j), \\
\psi(-t^j) &= \max\left(\psi(c_{i+1}) - \Delta c^j_i F\ ,\ 0\right), && \text{if } i = \mathsf{b}(j),
\end{aligned}$$

where F is any first-order correct approximation to the first derivative in age on the cohort $\mathcal{C}_{\mathsf{b}(j)}$, such as $(\psi(c_{\mathsf{b}(j)+2}) - \psi(c_{\mathsf{b}(j)+1}))/\Delta c^j_{\mathsf{b}(j)+1}$. We note that T preserves non-negativity. If φ is the midpoint values or average values on the cohorts of a smooth, non-negative function ω, then ψ will be a second-order correct approximation to ω.

We restrict attention to the case when $\mathcal{M}$ is the space of continuous piecewise linear functions. Such functions are non-negative if and only if the nodal values are non-negative. Let $\mathcal{W}^j$ denote the result of applying T to $\tilde{W}^j$ at each spatial node. Then $\mathcal{W}^j$ is in $\mathcal{M} \otimes \tilde{\mathcal{A}}$. Observe that $\mathcal{W}^j$ is a second-order correct approximation to the true solution w, provided w is sufficiently smooth.

2.6 Truncating the Age Domain

In order to approximate solutions to (2.2.1)–(2.2.5) in practice, we need to truncate the age domain to a finite domain, $[0, a_{\max}]$. We can bound the error that results from such a truncation because of the exponential decay of the solution as a tends towards infinity. At any point in time, we can consider the population density for any particular age group, u, to be the solution to a linear problem with continuous time-dependent coefficients. We look along the age-time characteristics, $da/dt = 1$, so that $a = t + \tau$ for some constant τ. We then have

$$\partial_t u(\mathsf{x}, t) = \nabla \cdot k(\mathsf{x}, t) \nabla u(x, t) - \mu(\mathsf{x}, t) u(\mathsf{x}, t),$$

with boundary condition

$$k(\mathsf{x}, t) \nabla u(\mathsf{x}, t) \cdot \nu = 0.$$

The new meanings of u, k and μ should be clear from context. Define

$$\hat{\mu}(a) = \inf_{x \in \Omega,\ p \geq 0} \mu(\mathsf{x}, a, p), \text{ and let } z(\mathsf{x}, t) = \exp\left(\int_0^{t+\tau} \hat{\mu}(s)\ ds \right) u(\mathsf{x}, t).$$

Then

$$\partial_t z(\mathsf{x}, t) = \nabla \cdot k(\mathsf{x}, t) \nabla z + (\hat{\mu} - \mu) z.$$

By a comparison theorem [40], assuming $u \in C^2(\Omega) \times C^1([0, T])$, we have

$$\max_{0 \leq t \leq T,\ \mathsf{x} \in \Omega} z(\mathsf{x}, t) \leq \max_{\mathsf{x} \in \Omega} z(\mathsf{x}, 0) = \max_{\mathsf{x} \in \Omega} u(\mathsf{x}, 0).$$

Thus

$$\max_{0\le t\le T,\ \mathsf{x}\in\Omega} u(\mathsf{x},t) \le \max_{\mathsf{x}\in\Omega} \exp\left(-\int_0^{t+\tau} \hat{\mu}(s)\ ds\right) u(\mathsf{x},0).$$

We assume Conditions 2.3 and 2.4 hold. Then, for all characteristic lines, $u(\mathsf{x},0) \le M$, for some constant M. The solution to (2.2.1)–(2.2.5) satisfies

$$u(\mathsf{x},a,t) \le M \exp\left(-\int_0^{a} \hat{\mu}(s)\ ds\right).$$

We thus require the integral of μ with respect to a to increase at least linearly.

The error bound on $a > a_{\max}$ is given by the exponential decay. For the region $[0, a_{\max}]$, we use an energy analysis to bound the error caused by truncating the age domain. We use tildes to denote solutions and coefficients of the age-truncated problem on $[0, a_{\max}]$. Define $\epsilon_u = u - \tilde{u}$. Then, along characteristics,

$$\partial_t \|\epsilon_u\|^2 = \left((k-\tilde{k})\nabla u, \nabla\epsilon_u\right) + ((\mu-\tilde{\mu})u, \epsilon_u) - \left(\tilde{k}\nabla\epsilon_u, \nabla\epsilon_u\right) + (\tilde{\mu}\epsilon_u, \epsilon_u).$$

Let $\epsilon_p = p - \tilde{p}$. Then bounds similar to those in Section 2.4 give

$$\frac{1}{2}\partial_t\|\epsilon_u\|^2 \le \left(\frac{K^2}{4C_0}\|\nabla u\|^2_{L^\infty} + \frac{K}{2}\|u\|^2_{L^\infty}\right)\|\epsilon_p\|^2 + \left(C_1 + \frac{K}{2}\|u\|^2_{L^\infty}\right)\|\epsilon_u\|^2.$$

We redefine $\||\cdot\||$ so that the integration over a only goes from 0 to $a_{\max}$. Integrating and applying Condition 2.3, we get

$$\begin{aligned}\frac{1}{2}\partial_t\||\epsilon_u\||^2 \le \frac{K}{2}\|u(\mathsf{x},a_{\max},t)\|^2 &+ \left(\frac{K^2}{4C_0}\||\nabla u\||^2_{L^\infty} + \frac{K}{2}\left(\||u\||^2_{L^\infty}+1\right)\right)\|\epsilon_p\|^2 \\ &+ \left(C_1 + \frac{K}{2}\left(\|u\|^2_{L^\infty(\Omega\times[0,a_{\max}])}+1\right)\right)\||\epsilon_u\||^2. \quad (2.2.23)\end{aligned}$$

For the error in the total population density, we similarly get

$$\frac{1}{2}\partial_t\|\epsilon_p\|^2 \le C_8\|\epsilon_p\|^2 + \frac{K}{2}\||\epsilon_u\||^2, \quad (2.2.24)$$

where

$$C_8 = \frac{K^2}{4C_0}\|\nabla p\|^2_{L^\infty} + K\left(\|p\|^2_{L^\infty} + \frac{1}{2}\right) + C_1.$$

Let $C^{**}(t)$ be the maximum of the relevant coefficients at a time t. Then, adding equations (2.2.23) and (2.2.24), we get

$$\partial_t\left(\||\epsilon_u\||^2 + \|\epsilon_p\|^2\right) \le K\|u(\mathsf{x},a_{\max},t)\|^2 + C^{**}(t)\left(\||\epsilon_u\||^2 + \|\epsilon_p\|^2\right).$$

We assume $a_{\max} > \tilde{a}_{\max}$, from Condition 2.4, so that $u(\mathsf{x}, a_{\max}, 0) = 0$. Applying a Gronwall's inequality [15], we get the following result:

Theorem 2.2. *Assume Conditions 2.1 – 2.4 hold. There exists $C^{**}(t)$, dependent only on K, C_0, C_1, $|||u|||_{L^\infty}$, $\|u\|_{L^\infty(\Omega\times\mathbb{R})}$, $|||\nabla u|||_{L^\infty}$, $\|p\|_{L^\infty}$, and $\|\nabla p\|_{L^\infty}$, such that*

$$\left(|||\epsilon_u|||^2 + \|\epsilon_p\|^2\right)(t) \leq K \int_0^t \|u(\mathsf{x}, a_{max}, s)\|^2 \ exp\left[\int_s^t C^{**}(r)dr\right] ds.$$

2.7 Relationship to Finite Difference Methods

In one or two space dimensions, the simplest space–time discretization of Equation (2.2.11) would be a backward Euler method in time and finite differences in space; in two-space we use a regular rectangular mesh. In the context of the methods posed in this paper, this spatial discretization corresponds to the use of continuous piecewise linear finite elements with mass lumping as the quadrature rule. In two dimensions, we use a regular rectangular mesh where each rectangle is subdivided into two triangles. In this context, the mass lumping replaces the integral over a triangle by the product of the area and the average of the integrand at the vertices. By using this discretization of Equation (2.2.11), and a postprocessing technique, we get convergence that is first-order correct in time, and second-order correct in age and space. By using mass lumping as the quadrature rule, we guarantee non-negativity of the computed solution [42].

CHAPTER 3

A STEP-DOUBLING GALERKIN METHOD FOR PARABOLIC PROBLEMS

In this chapter we consider a numerical method for solving second-order parabolic initial–boundary value problems. This single-step method consists of taking two half-steps of backward Euler over a time interval to obtain one approximate solution and then a single step over that same interval to obtain another [13]. This gives us two things: the two approximations can be compared to get an estimate of the size of the error; and the two first-order correct approximations can be extrapolated to obtain a second-order correct approximate solution. We use a Galerkin method for the spatial discretization.

The analysis is done using an energy method. Since one of the reasons to use step-doubling is step-size control, the analysis is done for variable time steps. The method also can be viewed as a rational approximation to the exponential (but not a Padé approximation [14]). Bramble and Sammon [4] showed convergence in the case of fixed time steps for a class of single step methods, including this method, that can be represented as rational approximations to the exponential.

The stability properties are contrasted with those of Crank-Nicolson for the case of a first-order linear ordinary differential equation, and more generally those of extrapolated theta-weighted schemes.

We apply step-doubling to an example system. This system can be viewed as a prototype model for negative chemotaxis.

3.1 The Linear Equation

We consider a second order linear parabolic partial differential equation with initial condition and homogeneous Dirichlet boundary condition on a bounded spatial domain Ω and a time interval $J = [t_0, t_f]$:

$$\partial_t y - \nabla \cdot a(x)\nabla y + b(x,t)\cdot \nabla y = f(x,t), \qquad x \in \Omega,\ t \in J, \tag{3.3.1}$$

$$y(x,t) = 0, \qquad x \in \partial\Omega,\ t \in J, \tag{3.3.2}$$

$$y(x,t_0) = y_0(x), \qquad x \in \Omega, \tag{3.3.3}$$

where ∇ and $\nabla\cdot$ denote the gradient and divergence, respectively, in x. In variational form, for every $v \in H_0^1(\Omega)$, we get,

$$(\partial_t y, v) + a(y,v) + b(y,v) = (f,v). \tag{3.3.4}$$

We let $(\cdot,\cdot)$ denote the L^2 inner product. We reuse the symbols a and b to denote the forms

$$\begin{aligned} a(\varphi,\psi) &= \int_\Omega a(x)\nabla\varphi \cdot \nabla\psi \; dx, \\ b(\varphi,\psi) &= \int_\Omega (b(x,t)\cdot\nabla\varphi)\,\psi \; dx. \end{aligned}$$

The distinction between the forms and the functions should be clear from context.

3.2 The Method

To approximate solutions to (3.3.1)-(3.3.3), we use a step-doubling method based on backward Euler with local in time extrapolation. We consider a nonuniform time discretization, $t_0 < t_1 < \cdots < t_m = t_f$. We set $\Delta t_n = t_n - t_{n-1}$, for $n = 1 \ldots m$. Let φ_n denote the value of φ at time t_n and $\varphi_{n-1/2}$ denote the value of φ at time

$(t_n + t_{n-1})/2$. We let $\mathcal{M}$ denote a finite dimensional subspace of $H^1_0(\Omega)$. We take $\tilde{D}_{n-1/2}$, D_n, S_n, Y_{n-1} to be in $\mathcal{M}$. We solve the system:

$$\left(\frac{\tilde{D}_{n-1/2} - Y_{n-1}}{\Delta t_n/2}, v\right) + a(\tilde{D}_{n-1/2}, v) + b(\tilde{D}_{n-1/2}, v) = (f_{n-1/2}, v), \quad (3.3.5)$$

$$\left(\frac{D_n - \tilde{D}_{n-1/2}}{\Delta t_n/2}, v\right) + a(D_n, v) + b(D_n, v) = (f_n, v), \quad (3.3.6)$$

$$\left(\frac{S_n - Y_{n-1}}{\Delta t_n}, v\right) + a(S_n, v) + b(S_n, v) = (f_n, v). \quad (3.3.7)$$

The computed solution at time t_n is set to $Y_n = 2D_n - S_n$.

3.3 Convergence

We show second-order convergence in time by an energy analysis [42]. Let $\|\cdot\|$ denote the L^2 norm and $\|\cdot\|_A$ the norm induced by $a(\cdot,\cdot)$.

3.3.1 Some Basic Relationships

Define

$$\begin{aligned}
\tilde{d}_{n-1/2} &= y_{n-1/2} + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2}, \\
d_n &= y_n + \frac{(\Delta t_n)^2}{4}\partial_t^2 y_n, \\
s_n &= y_n + \frac{(\Delta t_n)^2}{2}\partial_t^2 y_n.
\end{aligned}$$

Then

$$\left(\frac{\tilde{d}_{n-1/2} - y_{n-1}}{\Delta t_n/2}, v\right) + a(\tilde{d}_{n-1/2}, v) + b(\tilde{d}_{n-1/2}, v)$$
$$= (f_{n-1/2}, v) + (\mu_{n-1/2}, v) + \frac{(\Delta t_n)^2}{8}\left(a(\partial_t^2 y_{n-1/2}, v) + b(\partial_t^2 y_{n-1/2}, v)\right), \quad (3.3.8)$$

$$\left(\frac{d_n - \tilde{d}_{n-1/2}}{\Delta t_n/2}, v\right) + a(d_n, v) + b(d_n, v)$$
$$= (f_n, v) + (\mu_n, v) + \frac{(\Delta t_n)^2}{4}\left(a(\partial_t^2 y_n, v) + b(\partial_t^2 y_n, v)\right), \quad (3.3.9)$$

$$\left(\frac{s_n - y_{n-1}}{\Delta t_n}, v\right) + a(s_n, v) + b(s_n, v)$$
$$= (f_n, v) + (\nu_n, v) + \frac{(\Delta t_n)^2}{2}\left(a(\partial_t^2 y_n, v) + b(\partial_t^2 y_n, v)\right), \quad (3.3.10)$$

where

$$\begin{aligned}
\mu_{n-1/2} &= \frac{\tilde{d}_{n-1/2} - y_{n-1}}{\Delta t_n/2} - \partial_t y_{n-1/2} \\
\mu_n &= \frac{d_n - \tilde{d}_{n-1/2}}{\Delta t_n/2} - \partial_t y_n, \\
\nu_n &= \frac{s_n - y_{n-1}}{\Delta t_n} - \partial_t y_n.
\end{aligned}$$

Adding Equations (3.3.5) and (3.3.6) gives

$$\left(\frac{D_n - Y_{n-1}}{\Delta t_n}, v\right) + a\left(\frac{\tilde{D}_{n-1/2} + D_n}{2}, v\right) + b\left(\frac{\tilde{D}_{n-1/2} + D_n}{2}, v\right)$$
$$= \frac{1}{2}(f_n + f_{n-1/2}, v). \quad (3.3.11)$$

Subtracting Equation (3.3.7) from twice (3.3.11) gives

$$\left(\frac{Y_n - Y_{n-1}}{\Delta t_n}, v\right) + a(Y_n, v) + b(Y_n, v) + a(\tilde{D}_{n-1/2} - D_n, v)$$
$$+ b(\tilde{D}_{n-1/2} - D_n, v) = (f_{n-1/2}, v). \quad (3.3.12)$$

For the true solution, we apply the variational form (3.3.4) to $y_{n-1/2}$ to get

$$\left(\frac{y_n - y_{n-1}}{\Delta t_n}, v\right) + a(y_n, v) + b(y_n, v) + a(y_{n-1/2} - y_n, v)$$
$$+ b(y_{n-1/2} - y_n, v) = (f_{n-1/2}, v) + (\rho_n, v), \quad (3.3.13)$$

where

$$\rho_n = \frac{y_n - y_{n-1}}{\Delta t_n} - \partial_t y_{n-1/2}.$$

3.3.2 Projections

We use elliptic projections in constructing our argument [44]. We choose $W_n, X_n, \tilde{X}_{n-1/2}, Z_n \in \mathcal{M}$ such that for every $v \in \mathcal{M}$,

$$\begin{aligned} a(y_n - W_n, v) + b(y_n - W_n, v) &= 0, \\ a(d_n - X_n, v) + b(d_n - X_n, v) &= 0, \\ a(\tilde{d}_{n-1/2} - \tilde{X}_{n-1/2}, v) + b(\tilde{d}_{n-1/2} - \tilde{X}_{n-1/2}, v) &= 0, \\ a(s_n - Z_n, v) + b(s_n - Z_n, v) &= 0. \end{aligned}$$

Set

$$\begin{aligned} \eta_n &= y_n - W_n, & \vartheta_{n-1} &= Y_n - W_n, \\ \chi_n &= d_n - X_n, & \delta_n &= D_n - X_n, \\ \tilde{\chi}_{n-1/2} &= \tilde{d}_{n-1/2} - \tilde{X}_{n-1/2}, & \tilde{\delta}_{n-1/2} &= \tilde{D}_{n-1/2} - \tilde{X}_{n-1/2}, \\ \zeta_n &= s_n - Z_n, & \sigma_n &= S_n - Z_n. \end{aligned}$$

3.3.3 Relationships Satisfied by the Two Half-steps

Subtracting Equation (3.3.8) from (3.3.5) and Equation (3.3.9) from (3.3.6) gives

$$\begin{aligned} &\left(\frac{\tilde{\delta}_{n-1/2} - \vartheta_{n-1}}{\Delta t_n/2}, v\right) + a(\tilde{\delta}_{n-1/2}, v) + b(\tilde{\delta}_{n-1/2}, v) \\ &\qquad = (q_{n-1/2}, v) - \frac{(\Delta t_n)^2}{8}\left(a(\partial_t^2 y_{n-1/2}, v) + b(\partial_t^2 y_{n-1/2}, v)\right), \end{aligned} \tag{3.3.14}$$

$$\begin{aligned} &\left(\frac{\delta_n - \tilde{\delta}_{n-1/2}}{\Delta t_n/2}, v\right) + a(\delta_n, v) + b(\delta_n, v) \\ &\qquad = (q_n, v) - \frac{(\Delta t_n)^2}{4}\left(a(\partial_t^2 y_n, v) + b(\partial_t^2 y_n, v)\right), \end{aligned} \tag{3.3.15}$$

where

$$q_{n-1/2} = \frac{\tilde{\chi}_{n-1/2} - \chi_{n-1}}{\Delta t_n/2} - \mu_{n-1/2},$$
$$q_n = \frac{\chi_n - \tilde{\chi}_{n-1/2}}{\Delta t_n/2} - \mu_n.$$

In Equation (3.3.14), take $v = \tilde{\delta}_{n-1/2} - \vartheta_{n-1}$. Then

$$\frac{2}{\Delta t_n}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2 + a(\tilde{\delta}_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) + b(\tilde{\delta}_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1})$$
$$+ \frac{(\Delta t_n)^2}{8}\Big(a(\partial_t^2 y_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) + b(\partial_t^2 y_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1})\Big)$$
$$= (q_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}).$$

Using the fact that $w(w-z) = ((w^2 - z^2) + (w-z)^2)/2$ and Schwarz' Inequality, we get

$$\frac{2}{\Delta t_n}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2 + \frac{1}{2}\Big(\|\tilde{\delta}_{n-1/2}\|_A^2 - \|\vartheta_{n-1}\|_A^2 + \|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|_A^2\Big)$$
$$+ \frac{(\Delta t_n)^2}{8}\Big(a(\partial_t^2 y_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) + b(\partial_t^2 y_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1})\Big)$$
$$\leq (q_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) + \overline{b}\|\nabla\tilde{\delta}_{n-1/2}\|\,\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|.$$

Set $K = (\overline{b}/\underline{a})^2$. The arithmetic–geometric mean inequality, $wz \leq \frac{\varepsilon}{2}w^2 + \frac{1}{2\varepsilon}z^2$, gives

$$(q_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) \leq 2\Delta t_n\|q_{n-1/2}\|^2 + \frac{1}{8\Delta t_n}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2,$$
$$\overline{b}\|\nabla\tilde{\delta}_{n-1/2}\|\,\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\| \leq K\Delta t_n\|\tilde{\delta}_{n-1/2}\|_A^2 + \frac{1}{4\Delta t_n}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2,$$
$$\frac{(\Delta t_n)^2}{8}\,a(\partial_t^2 y_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) \leq \frac{(\Delta t_n)^4}{16}\|\partial_t^2 y_{n-1/2}\|_A^2 + \frac{1}{16}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|_A^2,$$
$$\frac{(\Delta t_n)^2}{8}\,b(\partial_t^2 y_{n-1/2}, \tilde{\delta}_{n-1/2} - \vartheta_{n-1}) \leq \frac{K(\Delta t_n)^5}{32}\|\partial_t^2 y_{n-1/2}\|_A^2 + \frac{1}{8\Delta t_n}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2.$$

Then

$$\begin{aligned}\frac{3}{2\Delta t_n}&\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|^2\\&+\frac{1}{2}\left((1-2K\Delta t_n)\|\tilde{\delta}_{n-1/2}\|_A^2-\|\vartheta_{n-1}\|_A^2\right)+\frac{7}{16}\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|_A^2\\&\le 2\Delta t_n\|q_{n-1/2}\|^2+\frac{2(\Delta t_n)^4+K(\Delta t_n)^5}{32}\|\partial_t^2 y_{n-1/2}\|_A^2.\end{aligned}\tag{3.3.16}$$

In Equation (3.3.15) take $v=\delta_n-\tilde{\delta}_{n-1/2}$. Then similarly,

$$\begin{aligned}\frac{3}{2\Delta t_n}&\|\delta_n-\tilde{\delta}_{n-1/2}\|^2\\&+\frac{1}{2}\left((1-2K\Delta t_n)\|\delta_n\|_A^2-\|\tilde{\delta}_{n-1/2}\|_A^2\right)+\frac{7}{16}\|\delta_n-\tilde{\delta}_{n-1/2}\|_A^2\\&\le 2\Delta t_n\|q_n\|^2+\frac{2(\Delta t_n)^4+K(\Delta t_n)^5}{32}\|\partial_t^2 y_n\|_A^2.\end{aligned}\tag{3.3.17}$$

Assume $\Delta t_n<\frac{1}{2K}$. Adding $(1-2K\Delta t_n)$ times Equation (3.3.17) to (3.3.16) to get rid of the $\|\tilde{\delta}_{n-1/2}\|_A^2$ terms gives

$$\begin{aligned}\frac{3}{2\Delta t_n}&\left(\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|^2+(1-2K\Delta t_n)\|\delta_n-\tilde{\delta}_{n-1/2}\|^2\right)\\&+\frac{1}{2}\left((1-2K\Delta t_n)^2\|\delta_n\|_A^2-\|\vartheta_{n-1}\|_A^2\right)\\&+\frac{7}{16}\left((1-2K\Delta t_n)\|\delta_n-\tilde{\delta}_{n-1/2}\|_A^2+\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|_A^2\right)\\&\le 2\Delta t_n\left(\|q_{n-1/2}\|^2+(1-2K\Delta t_n)\|q_n\|^2\right)\\&\quad+\frac{3(\Delta t_n)^4}{64}\left(\|\partial_t^2 y_{n-1/2}\|_A^2+\|\partial_t^2 y_n\|_A^2\right).\end{aligned}\tag{3.3.18}$$

3.3.4 Relationships Satisfied by the Single Step

Subtracting Equation (3.3.7) from (3.3.6) gives

$$\left(\frac{D_n-\tilde{D}_{n-1/2}}{\Delta t_n/2}-\frac{S_n-Y_{n-1}}{\Delta t_n},v\right)+a(D_n-S_n,v)+b(D_n-S_n,v)=0.\tag{3.3.19}$$

Subtracting Equation (3.3.10) from (3.3.9) gives

$$\left(\frac{d_n - \tilde{d}_{n-1/2}}{\Delta t_n/2} - \frac{s_n - y_{n-1}}{\Delta t_n}, v\right) + a(d_n - s_n, v) + b(d_n - s_n, v)$$
$$= (\gamma_n, v) - \frac{(\Delta t_n)^2}{4}\left(a(\partial_t^2 y_n, v) + b(\partial_t^2 y_n, v)\right), \quad (3.3.20)$$

where

$$\gamma_n = \mu_n - \nu_n = \frac{y_n - 2\tilde{d}_{n-1/2} + y_{n-1}}{\Delta t_n}.$$

Subtracting Equation (3.3.20) from (3.3.19) gives

$$\left(\frac{\delta_n - \tilde{\delta}_{n-1/2}}{\Delta t_n/2} - \frac{\sigma_n - \vartheta_{n-1}}{\Delta t_n}, v\right) + a(\delta_n - \sigma_n, v) + b(\delta_n - \sigma_n, v)$$
$$= (l_n, v) + \frac{(\Delta t_n)^2}{4}\left(a(\partial_t^2 y_n, v) + b(\partial_t^2 y_n, v)\right),$$

where

$$l_n = \left(\frac{\chi_n - \tilde{\chi}_{n-1/2}}{\Delta t_n/2} - \frac{\zeta_n - \eta_{n-1}}{\Delta t_n}\right) - \gamma_n.$$

Set $v = \delta_n - \sigma_n$ to get

$$\frac{1}{\Delta t_n}(2\delta_n - 2\tilde{\delta}_{n-1/2} - \sigma_n + \vartheta_{n-1}, \delta_n - \sigma_n) + \|\delta_n - \sigma_n\|_A^2 + b(\delta_n - \sigma_n, \delta_n - \sigma_n)$$
$$= (l_n, \delta_n - \sigma_n) + \frac{(\Delta t_n)^2}{4}\left(a(\partial_t^2 y_n, \delta_n - \sigma_n) + b(\partial_t^2 y_n, \delta_n - \sigma_n)\right),$$

or

$$\|\delta_n - \sigma_n\|_A^2 + b(\delta_n - \sigma_n, \delta_n - \sigma_n) + \frac{1}{\Delta t_n}\|\delta_n - \sigma_n\|^2$$
$$+ \frac{1}{\Delta t_n}\left((\delta_n - \tilde{\delta}_{n-1/2}, \delta_n - \sigma_n) + (\vartheta_{n-1} - \tilde{\delta}_{n-1/2}, \delta_n - \sigma_n)\right)$$
$$= (l_n, \delta_n - \sigma_n) + \frac{(\Delta t_n)^2}{4}\left(a(\partial_t^2 y_n, \delta_n - \sigma_n) + b(\partial_t^2 y_n, \delta_n - \sigma_n)\right).$$

Since

$$(l_n, \delta_n - \sigma_n) \le 2\Delta t_n \|l_n\|^2 + \frac{1}{8\Delta t_n}\|\delta_n - \sigma_n\|^2,$$
$$|b(\delta_n - \sigma_n, \delta_n - \sigma_n)| \le 2K\Delta t_n \|\delta_n - \sigma_n\|_A^2 + \frac{1}{8\Delta t_n}\|\delta_n - \sigma_n\|^2,$$
$$\frac{(\Delta t_n)^2}{4}\, a(\partial_t^2 y_n, \delta_n - \sigma_n) \le \frac{(\Delta t_n)^4}{16}\|\partial_t^2 y_n\|_A^2 + \frac{1}{4}\|\delta_n - \sigma_n\|_A^2,$$
$$\frac{(\Delta t_n)^2}{4}\, b(\partial_t^2 y_n, \delta_n - \sigma_n) \le \frac{K(\Delta t_n)^5}{8}\|\partial_t^2 y_n\|_A^2 + \frac{1}{8\Delta t_n}\|\delta_n - \sigma_n\|^2.$$

we get

$$\left(\frac{3}{4} - 2K\Delta t_n\right) \|\delta_n - \sigma_n\|_A^2 + \frac{5}{8\Delta t_n}\|\delta_n - \sigma_n\|^2$$
$$+ \frac{1}{\Delta t_n}\Big((\delta_n - \tilde{\delta}_{n-1/2}, \delta_n - \sigma_n) + (\vartheta_{n-1} - \tilde{\delta}_{n-1/2}, \delta_n - \sigma_n)\Big)$$
$$\leq \Delta t_n \|l_n\|^2 + \frac{(\Delta t_n)^4 + 2K(\Delta t_n^5)}{16}\|\partial_t^2 y_n\|_A^2.$$

Assume $\Delta t_n \leq \frac{1}{6K}\left(\leq \frac{1}{2K}\right)$. Using the arithmetic–geometric mean inequality, we get

$$\begin{aligned}
|(\vartheta_{n-1} - \tilde{\delta}_{n-1/2}, \delta_n - \sigma_n)| &\leq \|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2 + \frac{1}{4}\|\delta_n - \sigma_n\|^2, \\
|(\delta_n - \tilde{\delta}_{n-1/2}, \delta_n - \sigma_n)| &\leq (1 - 2K\Delta t_n)\|\delta_n - \tilde{\delta}_{n-1/2}\|^2 \\
&\quad + \frac{1}{4(1 - 2K\Delta t_n)}\|\delta_n - \sigma_n\|^2 \\
&\leq (1 - 2K\Delta t_n)\|\delta_n - \tilde{\delta}_{n-1/2}\|^2 \\
&\quad + \frac{3}{8}\|\delta_n - \sigma_n\|^2.
\end{aligned}$$

Then

$$\left(\frac{3}{4} - 2K\Delta t_n\right) \|\delta_n - \sigma_n\|_A^2$$
$$- \frac{1}{\Delta t_n}\Big((1 - 2K\Delta t_n)\|\delta_n - \tilde{\delta}_{n-1/2}\|^2 + \|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|^2\Big)$$
$$\leq \Delta t_n \|l_n\|^2 + \frac{(\Delta t_n)^4}{12}\|\partial_t^2 y_n\|_A^2. \quad (3.3.21)$$

3.3.5 Relationships Satisfied by the Full Extrapolated Step

Subtracting Equation (3.3.13) from (3.3.12) gives

$$\left(\frac{\vartheta_n - \vartheta_{n-1}}{\Delta t_n}, v\right) + a(\vartheta_n, v) + b(\vartheta_n, v)$$
$$+ a(\tilde{\delta}_{n-1/2} - \delta_n, v) + b(\tilde{\delta}_{n-1/2} - \delta_n, v) = (g_n, v),$$

where

$$g_n = \frac{\eta_n - \eta_{n-1}}{\Delta t_n} - \rho_n.$$

Take $v = \vartheta_n$ to get

$$\frac{1}{2\Delta t_n}\left(\|\vartheta_n\|^2 - \|\vartheta_{n-1}\|^2 + \|\vartheta_n - \vartheta_{n-1}\|^2\right) + \|\vartheta_n\|_A^2 - b(\vartheta_n, \vartheta_n)$$
$$+ a(\tilde{\delta}_{n-1/2} - \delta_n, \vartheta_n) + b(\tilde{\delta}_{n-1/2} - \delta_n, \vartheta_n) = (g_n, \vartheta_n).$$

Using the arithmetic–geometric mean inequality we get

$$\begin{aligned}
|a(\tilde{\delta}_{n-1/2} - \delta_n, \vartheta_n)| &\leq \frac{16}{27}\|\vartheta_n\|_A^2 + \frac{27}{64}\|\tilde{\delta}_{n-1/2} - \delta_n\|_A^2, \\
|b(\vartheta_n, \vartheta_n)| &\leq \frac{41}{432}\|\vartheta_n\|_A^2 + \frac{108K}{41}\|\vartheta_n\|^2, \\
|b(\tilde{\delta}_{n-1/2} - \delta_n, \vartheta_n)| &\leq \frac{1}{64}\|\tilde{\delta}_{n-1/2} - \delta_n\|_A^2 + 16K\|\vartheta_n\|^2, \\
|(g_n, \vartheta_n)| &\leq \frac{1}{2}\left(\|g_n\|^2 + \|\vartheta_n\|^2\right).
\end{aligned}$$

Then

$$\frac{1}{2\Delta t_n}\left(\|\vartheta_n\|^2 - \|\vartheta_{n-1}\|^2 + \|\vartheta_n - \vartheta_{n-1}\|^2\right) + \frac{5}{16}\|\vartheta_n\|_A^2 - \frac{7}{16}\|\tilde{\delta}_{n-1/2} - \delta_n\|_A^2$$
$$\leq \frac{1}{2}\|g_n\|^2 + C_1\|\vartheta_n\|^2, \quad (3.3.22)$$

where

$$C_1 = \frac{108K}{41} + 16K + \frac{1}{2}.$$

3.3.6 Combining the Relationships

Adding Equation (3.3.18) to $(1-2K\Delta t_n)$ times (3.3.22) to get rid of the $\|\tilde{\delta}_{n-1/2}-\delta_n\|_A^2$ term gives

$$\begin{aligned}
&\frac{(1-2K\Delta t_n)}{2\Delta t_n}\left(\|\vartheta_n\|^2-\|\vartheta_{n-1}\|^2+\|\vartheta_n-\vartheta_{n-1}\|^2\right)\\
&\quad+\frac{3}{2\Delta t_n}\left((1-2K\Delta t_n)\|\delta_n-\tilde{\delta}_{n-1/2}\|^2+\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|^2\right)\\
&\quad+\frac{5}{16}(1-2K\Delta t_n)\|\vartheta_n\|_A^2-\frac{1}{2}\|\vartheta_{n-1}\|_A^2\\
&\quad+\frac{1}{2}(1-2K\Delta t_n)^2\|\delta_n\|_A^2+\frac{7}{16}\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|_A^2\\
&\qquad\le\frac{3(\Delta t_n)^4}{64}\left(\|\partial_t^2 y_{n-1/2}\|_A^2+\|\partial_t^2 y_n\|_A^2\right)+2\Delta t_n\|q_{n-1/2}\|^2\\
&\qquad\quad+(1-2K\Delta t_n)\left(2\Delta t_n\|q_n\|^2+\frac{1}{2}\|g_n\|^2+C_1\|\vartheta_n\|^2\right)\\
&\qquad\le 2\Delta t_n\left(\|q_{n-1/2}\|^2+\|q_n\|^2\right)+\frac{1}{2}\|g_n\|^2+C_1\|\vartheta_n\|^2\\
&\qquad\quad+\frac{3(\Delta t_n)^4}{64}\left(\|\partial_t^2 y_{n-1/2}\|_A^2+\|\partial_t^2 y_n\|_A^2\right).
\end{aligned}\tag{3.3.23}$$

Taking 3/2 times Equation (3.3.21) plus Equation (3.3.23) to get rid of the $\|\delta_n-\tilde{\delta}_{n-1/2}\|^2$ and $\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|^2$ terms gives

$$\begin{aligned}
&\frac{1-2K\Delta t_n}{2\Delta t_n}\left(\|\vartheta_n\|^2-\|\vartheta_{n-1}\|^2+\|\vartheta_n-\vartheta_{n-1}\|^2\right)\\
&\quad+\frac{3}{2}(\frac{3}{4}-2K\Delta t_n)\|\delta_n-\sigma_n\|_A^2\\
&\quad+\frac{5}{16}(1-2K\Delta t_n)\|\vartheta_n\|_A^2-\frac{1}{2}\|\vartheta_{n-1}\|_A^2\\
&\quad+\frac{1}{2}(1-2K\Delta t_n)^2\|\delta_n\|_A^2+\frac{7}{16}\|\tilde{\delta}_{n-1/2}-\vartheta_{n-1}\|_A^2\\
&\qquad\le 2\Delta t_n\left(\|q_{n-1/2}\|^2+\|q_n\|^2+3\|l_n\|^2\right)+\frac{1}{2}\|g_n\|^2+C_1\|\vartheta_n\|^2\\
&\qquad\quad+\frac{3(\Delta t_n)^4}{64}\|\partial_t^2 y_{n-1/2}\|_A^2+\frac{11(\Delta t_n)^4}{64}\|\partial_t^2 y_n\|_A^2.
\end{aligned}\tag{3.3.24}$$

We now want more of $\|\vartheta_n\|_A^2$. Since $\vartheta_n = 2\delta_n - \sigma_n = \delta_n + (\delta_n - \sigma_n)$, we get by the arithmetic–geometric mean inequality,

$$\begin{aligned} \|\vartheta_n\|_A^2 &= \|\delta_n\|_A^2 + 2a(\delta_n, \delta_n - \sigma_n) + \|\delta_n - \sigma_n\|_A^2 \\ &\leq (1+\varepsilon)\left(\|\delta_n\|_A^2 + \frac{1}{\varepsilon}\|\delta_n - \sigma_n\|_A^2\right). \end{aligned}$$

Setting $\varepsilon = 16/37$ and multiplying by $9/32$ gives

$$\frac{9}{32}\|\vartheta_n\|_A^2 - \frac{477}{1184}\|\delta_n\|_A^2 - \frac{477}{512}\|\delta_n - \sigma_n\|_A^2 \leq 0. \tag{3.3.25}$$

Assume $\Delta t_n \leq \frac{1}{20K}\left(\leq \frac{1}{6K}\right)$. Then

$$\begin{aligned} \frac{5}{16}(1 - 2K\Delta t_n)\|\vartheta_n\|_A^2 &\geq \frac{9}{32}\|\vartheta_n\|_A^2, \\ \frac{3}{2}(1 - 2K\Delta t_n)\|\delta_n - \sigma_n\|_A^2 &\geq \frac{477}{512}\|\delta_n - \sigma_n\|_A^2, \\ \frac{1}{2}(1 - 2K\Delta t_n)^2\|\delta_n\|_A^2 &\geq \frac{477}{1184}\|\delta_n\|_A^2. \end{aligned}$$

Adding Equations (3.3.24) and (3.3.25) gives

$$\begin{aligned} &\frac{1}{3\Delta t_n}\left(\|\vartheta_n\|^2 - \|\vartheta_{n-1}\|^2\right) + \frac{1}{2}\left(\|\vartheta_n\|_A^2 - \|\vartheta_{n-1}\|_A^2\right) \\ &\quad + \frac{1}{3\Delta t_n}\|\vartheta_n - \vartheta_{n-1}\|^2 + \frac{7}{16}\|\tilde{\delta}_{n-1/2} - \vartheta_{n-1}\|_A^2 + \frac{1}{16}\|\vartheta_n\|_A^2 \\ &\qquad \leq 2\Delta t_n\left(\|q_{n-1/2}\|^2 + \|q_n\|^2 + 3\|l_n\|^2\right) + \frac{1}{2}\|g_n\|^2 + C_1\|\vartheta_n\|^2 \\ &\qquad\quad + \frac{3(\Delta t_n)^4}{64}\|\partial_t^2 y_{n-1/2}\|_A^2 + \frac{11(\Delta t_n)^4}{64}\|\partial_t^2 y_n\|_A^2. \end{aligned} \tag{3.3.26}$$

3.3.7 Bounds on the Time Truncation Error

We now need bounds on the L^2-norms of g_n, $q_{n-1/2}$, q_n, and l_n. For the part of g_n due to the error in approximating the time derivative we get

$$\begin{aligned} \rho_n &= \frac{y_n - y_{n-1}}{\Delta t_n} - \partial_t y_{n-1/2} \\ &= \frac{1}{\Delta t_n}\left(\int_{t_{n-1}}^{t_{n-1/2}} \frac{(t_{n-1} - t)^2}{2}\partial_t^3 y(x,t)\,dt + \int_{t_{n-1/2}}^{t_n} \frac{(t_n - t)^2}{2}\partial_t^3 y(x,t)\,dt\right); \end{aligned}$$

for that part of $q_{n-1/2}$ we get

$$\begin{aligned}
\mu_{n-1/2} &= \frac{\tilde{d}_{n-1/2} - y_{n-1}}{\Delta t_n/2} - \partial_t y_{n-1/2} \\
&= \frac{\left(y_{n-1/2} + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2}\right)}{\Delta t_n/2} \\
&\quad - \frac{\left(y_{n-1/2} - \frac{\Delta t_n}{2}\partial_t y_{n-1/2} + \Delta t(\Delta t_n)^2 8\partial_t^2 y_{n-1/2}\right)}{\Delta t_n/2} \\
&\quad - \frac{2}{\Delta t_n}\int_{t_{n-1/2}}^{t_{n-1}} \frac{(t_{n-1/2} - t)^2}{2}\partial_t^3 y(x,t)\ dt - \partial_t y_{n-1/2} \\
&= \frac{1}{\Delta t_n}\int_{t_{n-1}}^{t_{n-1/2}} (t_{n-1/2} - t)^2 \partial_t^3 y(x,t)\ dt;
\end{aligned}$$

for that part of q_n we get

$$\begin{aligned}
\mu_n &= \frac{d_n - \tilde{d}_{n-1/2}}{\Delta t_n/2} - \partial_t y_n \\
&= \frac{2}{\Delta t_n}\left[y_n + \frac{(\Delta t_n)^2}{4}\partial_t^2 y_n \right. \\
&\quad - \left(y_n - \frac{\Delta t_n}{2}\partial_t y_n + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_n + \int_{t_n}^{t_{n-1/2}} \frac{(t_{n-1/2} - t)^2}{2}\partial_t^3 y(x,t)\ dt\right) \\
&\quad \left. + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2}\right] - \partial_t y_n \\
&= \frac{\Delta t_n}{4}\left(\partial_t^2 y_n - \partial_t^2 y_{n-1/2}\right) + \frac{\Delta t_n}{4}\int_{t_n}^{t_{n-1/2}} \partial_t^3 y(x,t)\ dt;
\end{aligned}$$

and for the part of l_n due to the error in approximating the time derivative we get

$$\begin{aligned}
\gamma_n &= \frac{y_n - 2\tilde{d}_{n-1/2} + y_{n-1}}{\Delta t_n} \\
&= \frac{y_n - 2\left(y_{n-1/2} + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2}\right) + y_{n-1}}{\Delta t_n} \\
&= \frac{1}{\Delta t_n}\left(y_{n-1/2} + \frac{\Delta t_n}{2}\partial_t y_{n-1/2} + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2} + \int_{t_{n-1/2}}^{t_n} \frac{(t_n - t)^2}{2}\partial_t^3 y(x,t)\; dt\right) \\
&- \frac{2}{\Delta t_n}\left(y_{n-1/2} + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2}\right) \\
&+ \frac{1}{\Delta t_n}\left(y_{n-1/2} - \frac{\Delta t_n}{2}\partial_t y_{n-1/2} + \frac{(\Delta t_n)^2}{8}\partial_t^2 y_{n-1/2}\right. \\
&\left. + \int_{t_{n-1/2}}^{t_{n-1}} \frac{(t_{n-1} - t)^2}{2}\partial_t^3 y(x,t)\; dt\right) \\
&= \frac{1}{\Delta t_n}\left(\int_{t_{n-1/2}}^{t_{n-1}} \frac{(t_{n-1} - t)^2}{2}\partial_t^3 y(x,t)\; dt + \int_{t_{n-1/2}}^{t_n} \frac{(t_n - t)^2}{2}\partial_t^3 y(x,t)\; dt\right).
\end{aligned}$$

We then get the following bounds:

$$|\rho_n| \leq \frac{(\Delta t_n)^{3/2}}{4}\|\partial_t^3 y\|_{L^2([t_{n-1},t_n])}, \tag{3.3.27}$$

$$|\mu_{n-1/2}| \leq \frac{(\Delta t_n)^{3/2}}{4}\|\partial_t^3 y\|_{L^2([t_{n-1},t_n])}, \tag{3.3.28}$$

$$|\mu_n| \leq \frac{(\Delta t_n)^{3/2}}{2}\|\partial_t^3 y\|_{L^2([t_{n-1},t_n])}, \tag{3.3.29}$$

$$|\gamma_n| \leq \frac{(\Delta t_n)^{3/2}}{4}\|\partial_t^3 y\|_{L^2([t_{n-1},t_n])}. \tag{3.3.30}$$

3.3.8 Error Bound

Using the bounds (3.3.28)-(3.3.30), the fact that $(w+z)^2 \leq 2(w^2+z^2)$, and applying a discrete Gronwall's Inequality to Equation (3.3.26) gives the following result:

Theorem 3.1. *There exists positive constants ϵ and C dependent only on $\overline{b}/\underline{a}$ such that for $\Delta t_n < \epsilon$ for $1 \leq n \leq m$,*

$$\|\vartheta_m\|^2 + \|\vartheta_m\|_A^2 \le C\left(\|\vartheta_0\|^2 + \|\vartheta_0\|_A^2\right) +$$
$$C\sum_{n=1}^{m}\left[\Delta t_n\left(\left\|\frac{\zeta_n - \eta_{n-1}}{\Delta t_n}\right\|^2 + \left\|\frac{\tilde{\chi}_{n-1/2} - \chi_{n-1}}{\Delta t_n/2}\right\|^2 + \left\|\frac{\chi_n - \tilde{\chi}_{n-1/2}}{\Delta t_n/2}\right\|^2\right)\right.$$
$$+ (\Delta t_n)^4\left(\|\partial_t^2 y_{n-1/2}\|_A^2 + \|\partial_t^2 y_n\|_A^2\right) + (\Delta t_n)^3\|\partial_t^3 y\|_{L^2(\Omega\times[t_{n-1},t_n])}^2$$
$$\left. + \left\|\frac{\eta_n - \eta_{n-1}}{\Delta t_n}\right\|^2\right]\Delta t_n.$$

3.4 A Comparison with Crank-Nicolson and Extrapolated Theta-weighted Methods

We consider the problem $y' = Ay$ where A is a diagonalizable matrix. If $-a$ is an eigenvalue of A, we solve $y' = -ay$ over a time step Δt_n by step-doubling extrapolation to get

$$Y_n = \left[2\left(\frac{1}{1+\frac{a\Delta t_n}{2}}\right)^2 - \frac{1}{1+a\Delta t_n}\right]Y_{n-1},$$

and by Crank-Nicolson to get

$$Y_n = \left(\frac{2 - a\Delta t_n}{2 + a\Delta t_n}\right)Y_{n-1}.$$

It should be noted that step-doubling involves three times the work of Crank-Nicolson. These rational approximations to $\exp(-a\Delta t_n)$ are compared in Figure 1 for $a\Delta t_n \in \mathbb{R}^+$.

We consider a theta-weighted scheme for the problem $y' = -ay$. A single step of a theta-weighted scheme gives

$$\frac{S_n - Y_{n-1}}{\Delta t_n} = -\theta a S_n + (\theta - 1)aY_n, \qquad 0 \le \theta \le 1.$$

If we take two half steps over this time interval to get an approximate solution D_n and then extrapolate $Y_n = 2D_n - S_n$, we get a second-order correct approximation

$$Y_n = \left[2\left(\frac{1 + (\theta - 1)\frac{a\Delta t_n}{2}}{1 + \theta\frac{a\Delta t_n}{2}}\right)^2 - \frac{1 + (\theta - 1)a\Delta t_n}{1 + \theta a\Delta t_n}\right]Y_{n-1}.$$

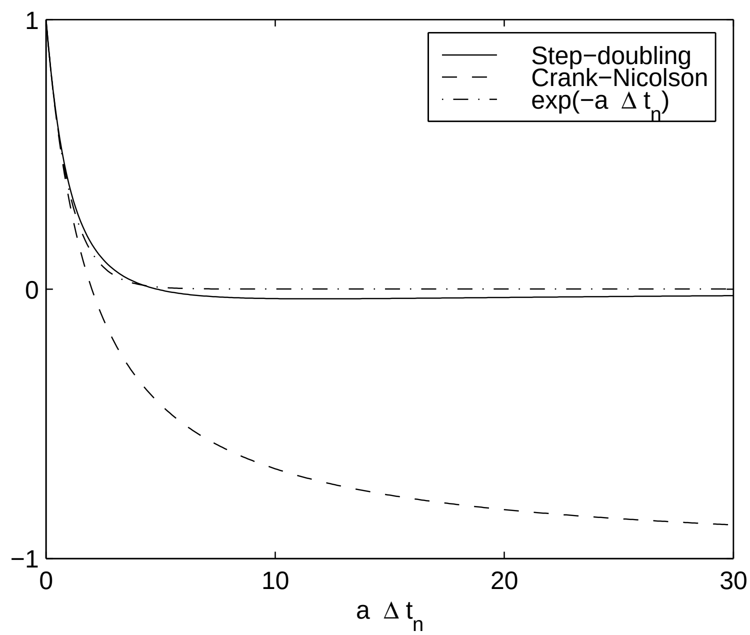

Figure 1: Amplification factors of step-doubling and Crank-Nicolson for the problem $y' = -ay$.

For large values of $a\Delta t_n$, the amplification factor is close to

$$2\left(\frac{\theta-1}{\theta}\right)^2 - \left(\frac{\theta-1}{\theta}\right)$$

and this is larger that one for $0 < \theta < \frac{2}{3}$. For such values of θ, step-doubling is only conditionally stable. In particular, by taking $\theta = \frac{1}{2}$, step-doubling takes Crank-Nicolson, a stable second-order correct method, and yields only a conditionally stable second-order correct method. Figure 2 shows the amplification factors for various values of θ.

3.5 An Example System

The approximate solutions computed in this section were obtained using the software toolkit BuGS [2]. BuGS is a toolkit for solving single space dimensional,

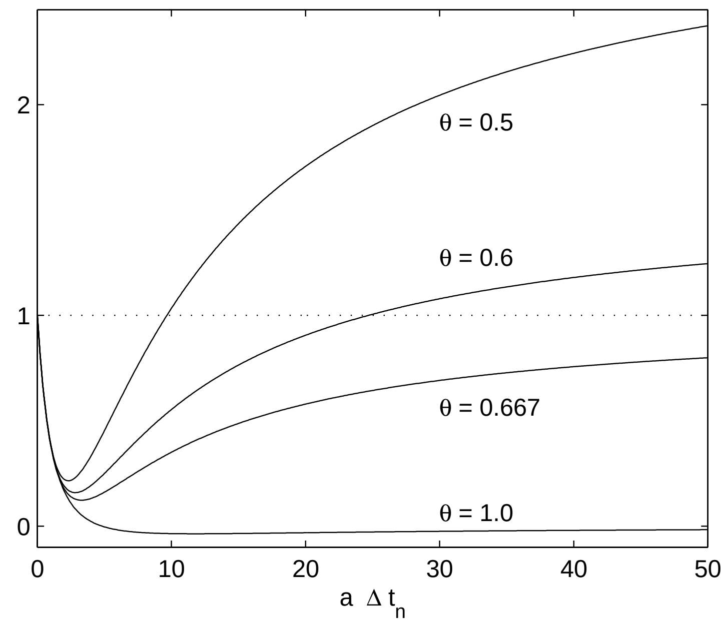

Figure 2: Amplification factors of step-doubling for various values of θ for a theta-weighted method.

nonlinear systems of partial differential equations which are at most order one in time and order two in space. The user defines the spatial discretization of the equations by writing a residual function based on first order backward differences in time. BuGS then uses the step-doubling method posed in this chapter to get a second-order accurate in time implicit finite difference scheme. BuGS also features step control for the convergence of Newton's method and automatic approximation of the Jacobi matrix.

For the spatial discretization, we used finite differences in space which correspond to continuous piecewise linear finite elements with mass lumping as the quadrature rule [42].

3.5.1 Problem

We consider the system, for $\beta(x,t)$, $\rho(x,t)$ and $\alpha(x,t)$:

$$\begin{aligned}
\beta_t - (\beta\beta_x)_x - K(\beta\rho_x)_x &= 0, \qquad x \in [0,a],\ t \in [0,T_f], && (3.3.31)\\
\rho_t - \beta - K(\beta\rho_x)_x + \text{rate}(\rho,\alpha) &= 0, \qquad x \in [0,a],\ t \in [0,T_f], && (3.3.32)\\
\alpha_t - \text{rate}(\rho,\alpha) &= 0, \qquad x \in [0,a],\ t \in [0,T_f], && (3.3.33)
\end{aligned}$$

where

$$\text{rate}(\rho,\alpha) = \max\{C\rho(\alpha_{\max} - \alpha), 0\}, \tag{3.3.34}$$

We take the boundary conditions

$$\beta_x = \rho_x = 0 \text{ on } \{0,a\} \tag{3.3.35}$$

and the initial conditions

$$\begin{aligned}
\beta(x,0) &= \max\{b - x^2, 0\}, \qquad x \in [0,a],\\
\rho(x,0) &= 0, \qquad x \in [0,a],\\
\alpha(x,0) &= 0, \qquad x \in [0,a].
\end{aligned} \tag{3.3.36}$$

This system models the movement of bacteria on a petri dish. The bacteria are moving away from their own waste. β is the bacterial population density, ρ is the concentration of waste or repellent, and α is the amount of repellent absorbed by the laboratory medium.

3.5.2 Results

We consider the system (3.3.31)- (3.3.36) with constants $K = 100$, $C = 100$, $\alpha_{\max} = 0.06$, $a = 25$, $b = 0.5$, $T_f = 16$, and with $N = 501$ uniform spatial nodes. BuGS gives Figures 3-8 as sample output. The profiles are $\Delta t = 2$ apart. If s is the solution from the single step and d the solution from the two half-steps, then we required $\|d - s\|_\infty < 0.001$ as the criterion for accepting a step. For other computational details, see the BuGS User Guide [2].

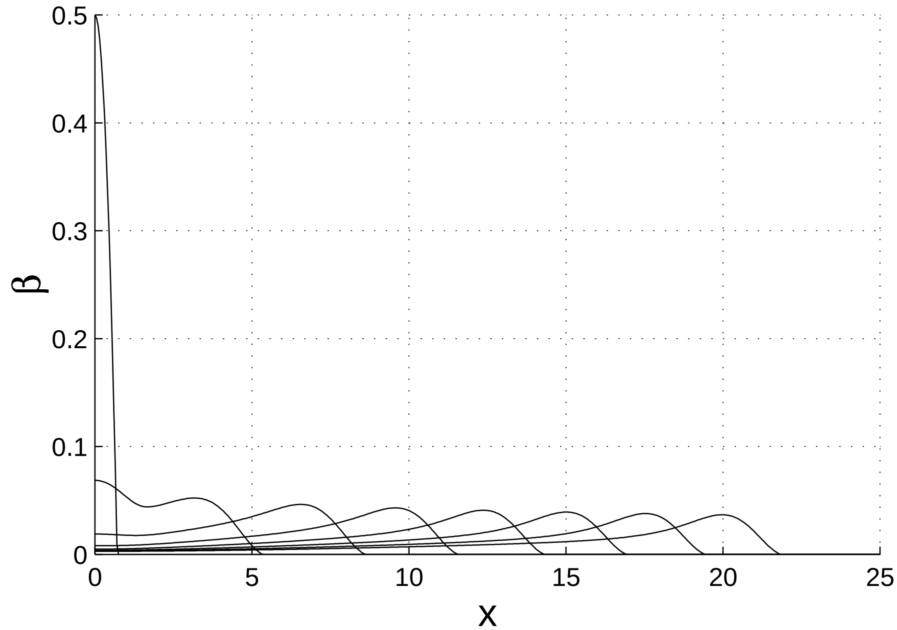

Figure 3: Bacterial population density profiles. Profiles are $t = 2$ apart.

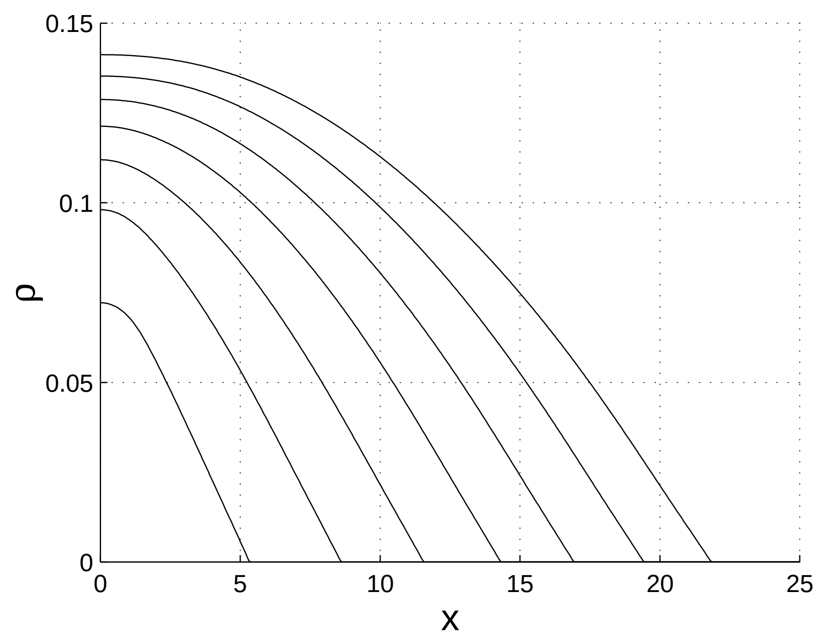

Figure 4: Repellent concentration profiles. Profiles are $t = 2$ apart.

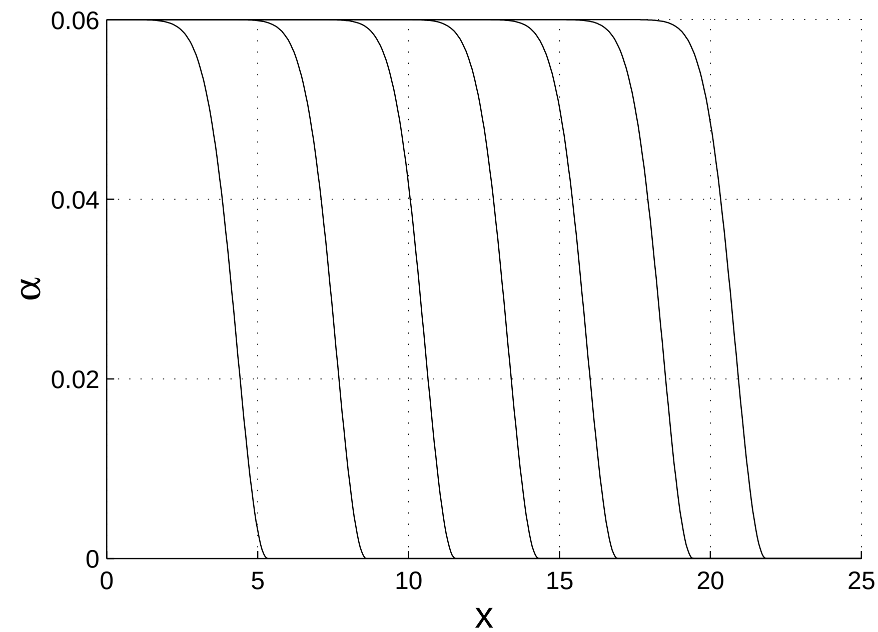

Figure 5: Absorbed repellent concentration profiles. Profiles are $t = 2$ apart.

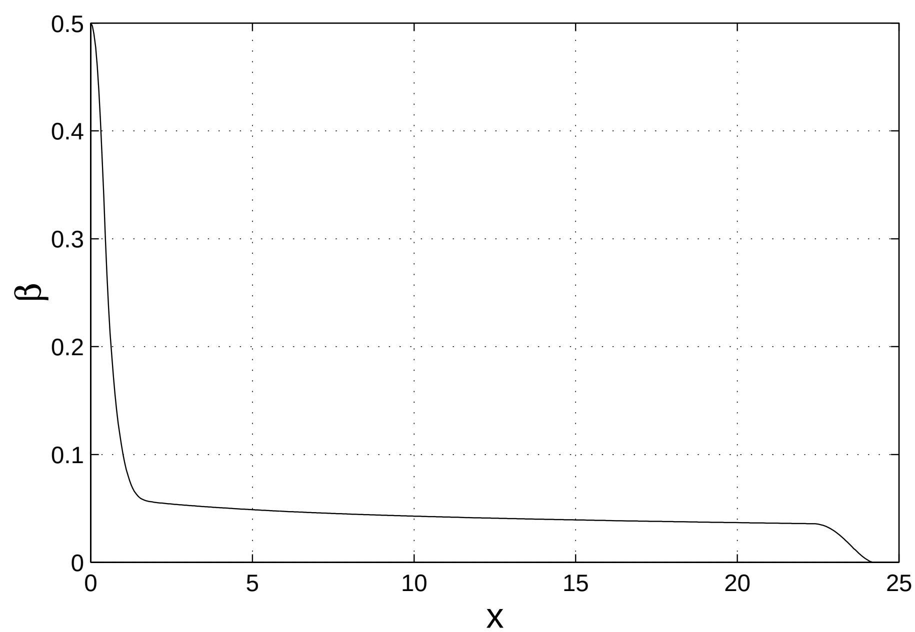

Figure 6: Maximum population profiles.

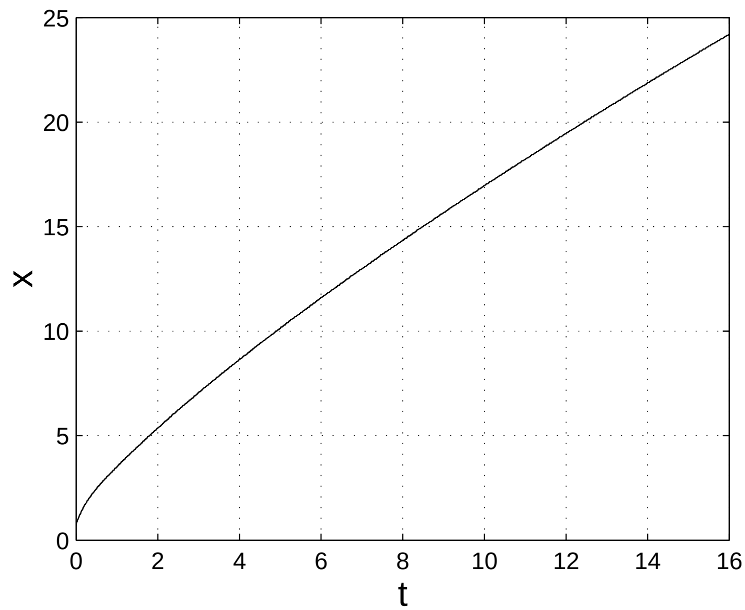

Figure 7: Position of bacterial front, β.

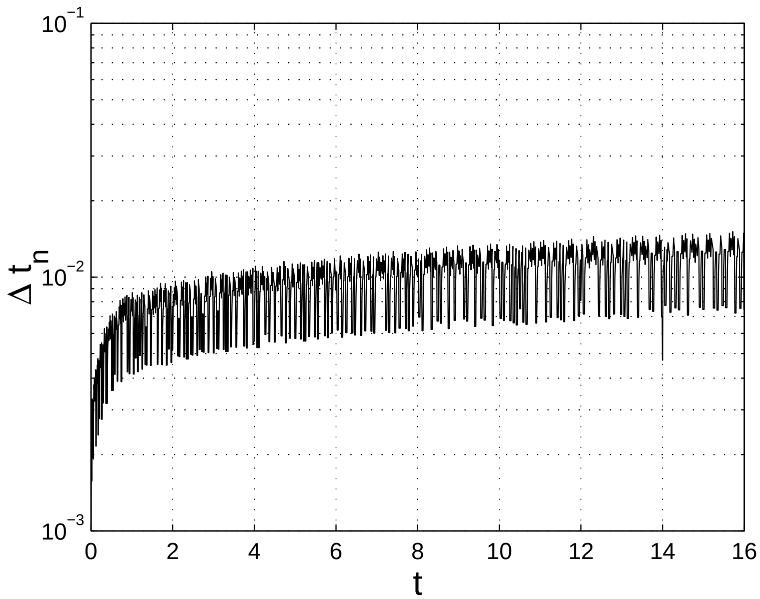

Figure 8: Step-size for the calculation, measured $\log_{10}$. The oscillations are due to degeneracies in the parabolic system. When a new space interval is breached by the bacterial front, the error as measured by step-doubling increases.

CHAPTER 4

NUMERICAL SIMULATIONS OF *PROTEUS MIRABILIS* SWARM COLONY DEVELOPMENT

A population where both age and space play vital roles is the *Proteus mirabilis* swarm colony. On typical laboratory media, *Proteus mirabilis* cells form colonies with radial symmetry and regularly spaced concentric terraces. These colonies are formed by a swarming-consolidation cycle, the timing of which is largely independent of the nature of the agar surface. After the formation of the first terrace, the velocity of the colony radius becomes periodic (see Figures 9 and 10) [37].

Esipov and Shapiro have formulated a model of this phenomenon with dependence on both age and space [10]. The bacteria follow a differentiation – dedifferentiation cycle between motile swarmer and immotile swimmer cells. An age-dependent nonlinear diffusion equation models the swarmer population, which is coupled to an ordinary differential equation at each point in space that models the swimmer population.

4.1 A Modified Esipov-Shapiro Model

We consider a radially symmetric, modified Esipov-Shapiro model. The variable r represents space in radially symmetric coordinates, the variable a represents age, and the variable t represents time. The function $u(r,a,t)$ represents the swarmer population density at radius r, age a and time t. The functions $p(r,t)$ and $v(r,t)$ represent the biomass density of swarmers and swimmer population density, respectively, at radius r and time t. The swimmer population density is measured in population density units (pdu) with pdu $= \frac{\text{ind}}{\text{cm}^2}$, where ind is some multiple of the

Figure 9: *Proteus mirabilis* swarm colonies. This photograph shows four inoculations on one petri dish that eventually merge. Photograph courtesy of James Shapiro and Oliver Rauprich.

number of individuals. The swarmer population density is measured in $\frac{\text{pdu}}{\text{hr}}$. The swarmer biomass density is measured in $\frac{\text{mg}}{\text{cm}^2}$.

We make several modifications. We use a radially symmetric geometry with no-flux boundary conditions, as would be the case on a petri dish. We use the biomass of swarmers, not the number of swarmers of all ages, as the measure of the total population density of swarmers.[1] We take the lower integration limit to be zero instead of some minimal age; the exponential weighting means that younger swarmers do not contribute as much as older swarmers. We use a diffusion which arises from isotropic random motion instead of Fickian diffusion [35]. In addition, we use different forms of the diffusivity, D, and the differentiation rate, ξ.

[1]The models written in [10] use the number of swarmers and not their biomass. However, per personal communication with Sergei Esipov, the biomass was used in the numerical computations. With the form of diffusivity in [10], using the number of swarmers will result in the diffusivity remaining zero.

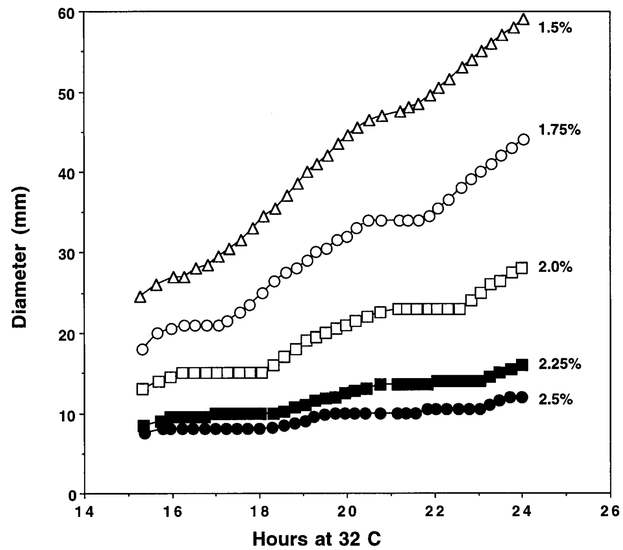

Figure 10: *Proteus mirabilis* swarm colony radius. The time it takes to form and consolidate a terrace is largely independent of the nature of the agar surface. The front velocity is periodic as a function of time with period independent of agar or glucose concentrations. The percentages indicated in this figure are for different agar concentrations. Figure courtesy of James Shapiro and Oliver Rauprich [37].

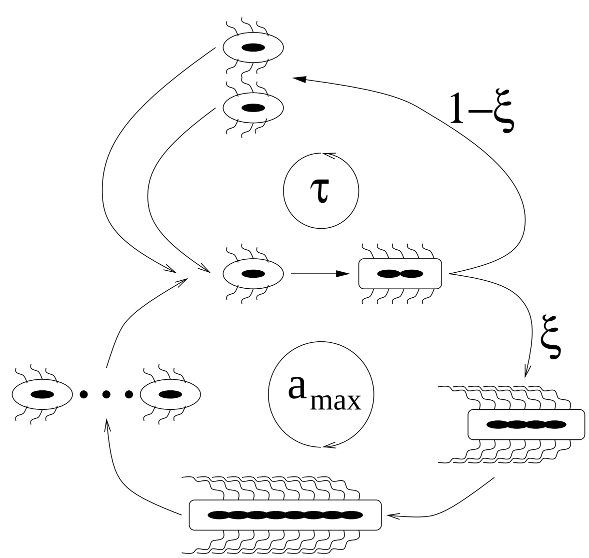

Figure 11: Differentiation-dedifferentiation cycle of *Proteus mirabilis*. Swimmers give rise to multicell swarmers with probability ξ. Swarmers continue to lengthen until they reach a maximum age, $a_{\max}$, at which point they rapidly breakdown into unicellular swimmers [10].

For the swarmers we have the system:

$$\partial_t u + \partial_a u = \frac{1}{r}\partial_r \left(r\partial_r (D(p)u) \right), \qquad r \in [0, r_m],\ a \in [0, a_{\max}],\ t \geq 0, \tag{4.4.1}$$

$$u(r, 0, t) = \frac{\xi(v)}{\tau} v(r, t), \qquad r \in [0, r_m],\ t \geq 0, \tag{4.4.2}$$

$$\partial_r \left(D(p(r_m, t)) u(r_m, a, t) \right) = 0, \qquad a \in [0, a_{\max}],\ t \geq 0, \tag{4.4.3}$$

$$u(r, a, 0) = 0, \qquad r \in [0, r_m],\ a \in [0, a_{\max}]. \tag{4.4.4}$$

The parameter τ is the time it takes a cell to subdivide. The total biomass is given by

$$p(r, t) = m_0 \int_0^{a_{\max}} u(r, a, t) e^{a/\tau}\, da, \qquad r \in [0, r_m],\ t \geq 0, \tag{4.4.5}$$

where $m_0 = \frac{\text{mg}}{\text{ind}}$ at age $a = 0$. We choose ind such that $m_0 = 1$. At each r the system for the swarmers is coupled to a growth equation for the swimmers:

$$\partial_t v = \frac{1 - \xi(v)}{\tau} v + u(r, a_{\max}, t), \qquad r \in [0, r_m],\ t \geq 0, \tag{4.4.6}$$

$$v(r, 0) = v_0(r), \qquad r \in [0, r_m]. \tag{4.4.7}$$

For the simulations in this chapter, we take the diffusivity to be

$$D(r, t) = D_0 p(r, t), \tag{4.4.8}$$

and the differentiation function to be

$$\xi(v) = \xi_0 \exp(-K(v - C)^2). \tag{4.4.9}$$

The initial condition has the form

$$v_0(r) = \begin{cases} H\left(2\left(\frac{r}{L}\right)^3 - 3\left(\frac{r}{L}\right)^2 + 1\right), & 0 \leq r \leq L, \\ 0, & r > L. \end{cases} \tag{4.4.10}$$

4.2 Mollifying the Birth Term

For the step control mechanisms of step-doubling to work more smoothly in conjunction with the age methods of Chapter 2, we find that we need to smooth out the birth term over several intervals. If all the birthing is done in the first cohort, the introduction of a new first cohort results in a sudden increase in the difficulty of the problem. The second derivative in the previous first cohort was limited by the opposing forces of birth and diffusion. With the sudden removal of birth, the second derivative becomes larger and step-doubling will indicate the need for smaller time steps. The time discretization becomes dependent upon the age discretization in an undesirable manner. To remove this dependence in the combination of the two numerical techniques, we use a mollified birth term. We use the moving reference frame and notation of Section 2.2. We take a bounded, measurable function $b(a)$ with support $[-s, s]$ that is symmetric about $a = 0$ and satisfies

$$\int_{-s}^{s} b(a)\ da = 1.$$

We choose Υ so that $\Upsilon'' = b$.

We now define a cohort by $[\max(c_i, -(t+s)), c_{i+1})$ to account for earlier birth. In a fully discrete context, neglecting diffusion and death, we take in the first age interval

$$\Delta c_i^j W_i^j = \mathcal{B}(\mathsf{x}, P^{j-1}) \int_{t^{j-1}}^{t^j} \int_{-(t+s)}^{c_{i+1}} b(c+s)\ dc\ dt + \Delta c_i^{j-1} W_i^{j-1}.$$

Using the fact that $\Delta c_i^j - \Delta c_i^{j-1} = \Delta t^j$ and dividing by $\Delta c_i^j \Delta t^j$, we get

$$\frac{W_i^j - W_i^{j-1}}{\Delta t^j} = \frac{\mathcal{B}(\mathsf{x}, P^{j-1})}{\Delta c_i^j \Delta t^j} \int_{t^{j-1}}^{t^j} \int_{-(t+s)}^{c_{i+1}} b(c+s)\ dc\ dt - \frac{W_i^{j-1}}{\Delta c_i^j}.$$

For the remaining cohorts, since $\Delta c_i^j = \Delta c_i^{j-1}$, we have

$$\frac{W_i^j - W_i^{j-1}}{\Delta t^j} = \frac{\mathcal{B}(\mathsf{x}, P^{j-1})}{\Delta c_i^j \Delta t^j} \int_{t^{j-1}}^{t^j} \int_{c_i}^{c_{i+1}} b(c+s)\ dc\ dt.$$

Thus motivated, we twice integrate to set our discrete birth term to

$$B_i^j(\mathsf{x}) = \frac{\mathcal{B}(\mathsf{x}, P^{j-1})}{\Delta c_i^j \Delta t^j} \left(\Upsilon(\Delta c_i^j) - \Upsilon(\Delta c_i^{j-1}) - \Upsilon'(-s)\Delta t^j \right) - \frac{W_i^{j-1}}{\Delta c_i^j},$$

in the first age interval and

$$B_i^j(\mathsf{x}) = \frac{\mathcal{B}(\mathsf{x}, P^{j-1})}{\Delta c_i^j \Delta t^j} \left[\Upsilon(c_{i+1} + t^j) - \Upsilon(c_{i+1} + t^{j-1}) - \left(\Upsilon(c_i + t^j) - \Upsilon(c_i + t^{j-1}) \right) \right],$$

in the other age intervals.

A particular form of b for which we have a closed form of Υ is

$$b(a) = \frac{1}{s} \left(2 \left(\frac{|a|}{s} \right)^3 - 3 \left(\frac{|a|}{s} \right)^2 + 1 \right), \qquad -s \leq a \leq s. \tag{4.4.11}$$

4.3 Numerical Computations

We apply the methods of Chapters 2 and 3 and Section 4.2 to approximate solutions to the System (4.4.1)-(4.4.7) with diffusivity given by Equation (4.4.8), differentiation parameter given by Equation (4.4.9) and initial condition given by Equation (4.4.10). We use radial piecewise linear basis functions in space with mass lumping as the quadrature rule. This corresponds to the finite differences of Appendix C.

We choose the parameters $D_0 = 10^{-2} \frac{\mathrm{cm}^2}{\mathrm{hr(mg/cm^2)}}$, $\tau = 1.5$ hours, $K = 5\mathrm{pdu}^{-2}$, $C = 6$ pdu, $\xi_0 = 0.5$, $H = 0.5$ pdu and $L = 0.1$ cm. For the space, age and time domains we take $r_m = 2.5$ cm, $a_{\max} = 4$ hours and $t \in [0, 40]$ hours.

For the age discretization we set $\Delta a = 0.1$ hours, where Δa is the uniform length of all but the first and last age intervals. In the moving reference frame of Section 2.2, this corresponds to evenly spaced c_i's. We use the mollifier of Equation (4.4.11) with $s = \Delta a$. We use a uniform discretization in space with $\Delta r = 0.0125$ cm. The time discretization is done adaptively using step-doubling. We use as a measure of the time-truncation error, e, the weighted max-norm of the relative difference,

$$e = \max_{i,j} \frac{\Delta a(j)}{\Delta a} \frac{|u_d(r(i), a(j)) - u_s(r(i), a(j))|}{|u_d(r(i), a(j))| + \varepsilon / \Delta a(j)}$$

where u_s and u_d are the approximations in age and space obtained by taking one time step and two time steps of the swarmer population, respectively, and $\Delta a(j)$ is the width of the j-th age interval. We similarly measure the time-truncation error in the swimmers by a relative error (without weighting by Δa).

We adjust the time step by the following: If $e \geq \text{tol}$, then we reject the step, and try again with a step size $\frac{\Delta t}{2}$. If $e < \text{tol}$, then we accept the step and adjust the next step according to the following:

- If $e < \frac{\text{tol}}{16}$, then $\Delta t_{\text{new}} = 2\Delta t_{\text{old}}$
- If $e < \frac{\text{tol}}{4}$, then $\Delta t_{\text{new}} = \sqrt{2}\Delta t_{\text{old}}$
- If $e < \frac{\text{tol}}{2}$, then $\Delta t_{\text{new}} = \sqrt[4]{2}\Delta t_{\text{old}}$
- If $e > \frac{3\,\text{tol}}{4}$, then $\Delta t_{\text{new}} = \frac{9}{10}\Delta t_{\text{old}}$

For the simulations presented here, tol$=10^{-3}$ and $\varepsilon = 10^{-6}$.

We present the results of a simulation using the above parameters. Figures 12 and 13 show the simulated *Proteus mirabilis* swarm colony at time $t = 40$ hours. Figures 14 and 15 show the distribution in both age and space of swarmer cells. Figure 16 shows the movement of the bacterial front over time. The velocity of the front becomes periodic with period approximately 6.8 hours. Figure 17 shows the time steps taken during the simulation. The difficulty of the problem is linked to the movement of the bacterial front.

We present a convergence study which shows second-order convergence in age of the simulation (see Figure 18). We parameterize a particular age discretization by Δa, which is the length of all but the first and last age intervals. We measure the error for this age discretization by the L^2-norm of the difference between it and the approximation obtained by using its refinement, the age discretization parameterized by $\Delta a/2$. We approximate solutions to the same problem as in Figures 12-17, but the simulation is only run up to time $t = 6$ hours instead of 40 hours. We use a non-adaptive time discretization to better compare different age discretizations.

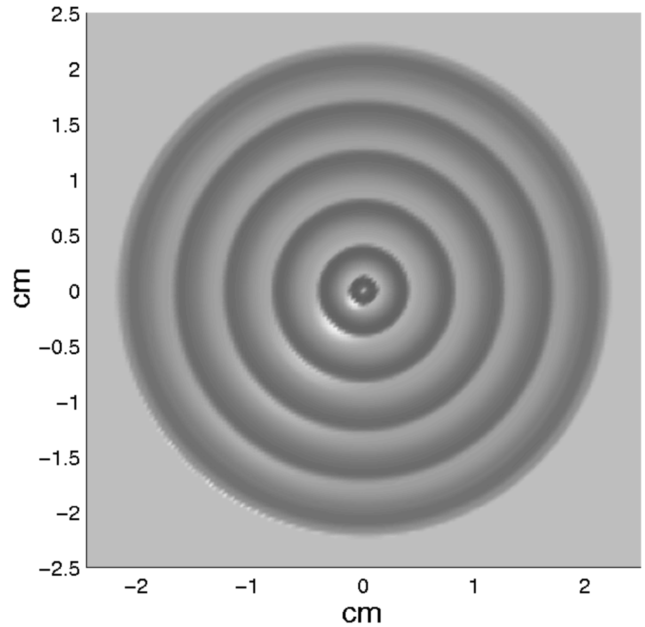

Figure 12: Simulated *Proteus mirabilis* swarm colony showing evenly spaced concentric terraces. The height is taken to be the inverse hyperbolic sine of the total biomass (swarmer biomass plus swimmer biomass, $p + m_0 v$).

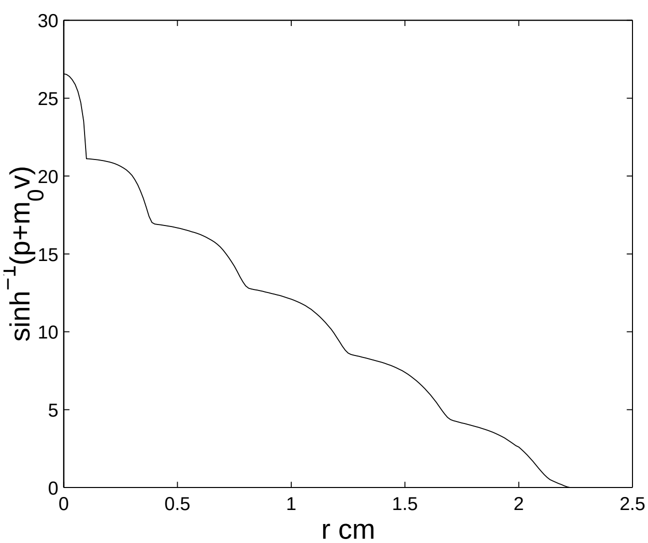

Figure 13: Profile of a simulated *Proteus mirabilis* swarm colony. This is the same colony as in Figure 12.

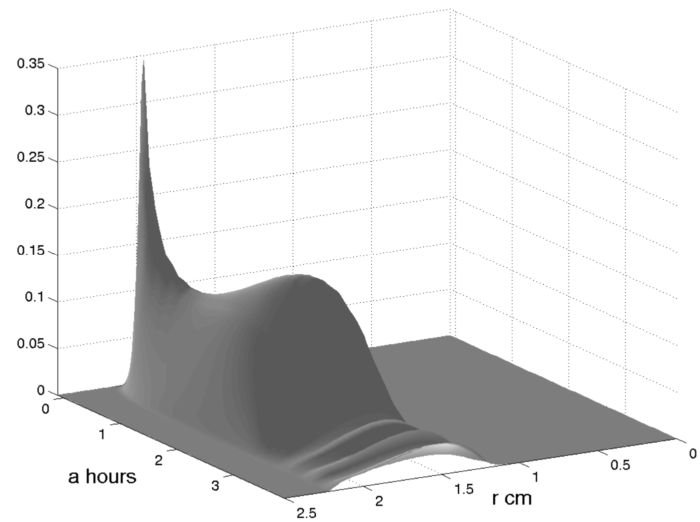

Figure 14: Surface plot of the swarmer population density, u, in age and space at time $t = 40$ hours.

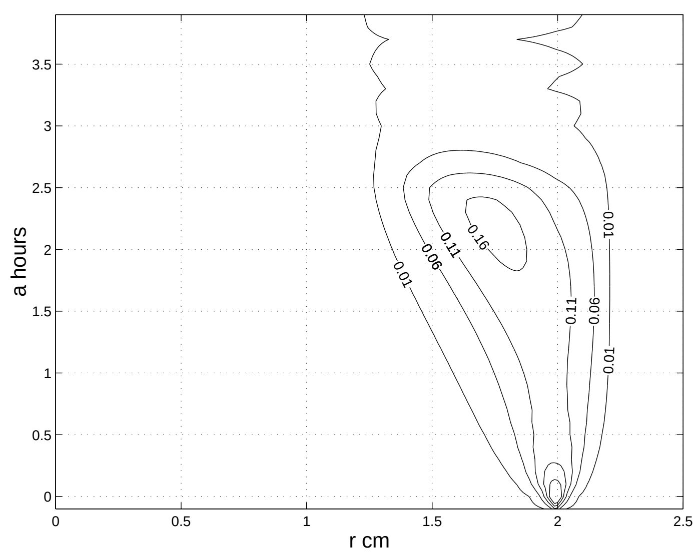

Figure 15: Contour plot of the swarmer population density, u, in age and space at time $t = 40$ hours.

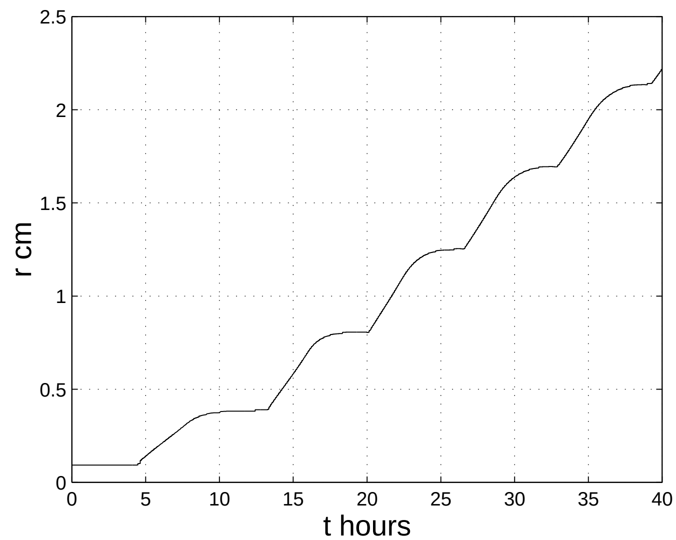

Figure 16: Time plot of the radius of the simulated *Proteus mirabilis* swarm colony. After the formation of the first terrace, the velocity of the front becomes periodic with period approximately 6.8 hours.

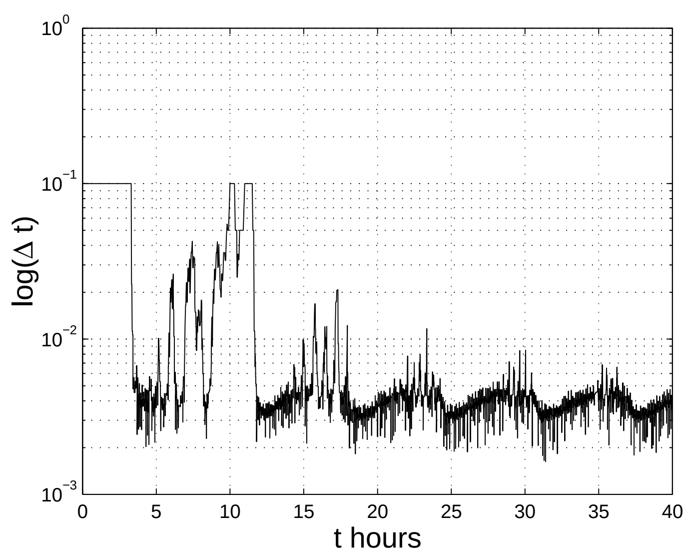

Figure 17: Time steps taken during the simulation of the *Proteus mirabilis* swarm colony. The difficulty of the problem is linked to the movement of the bacterial front.

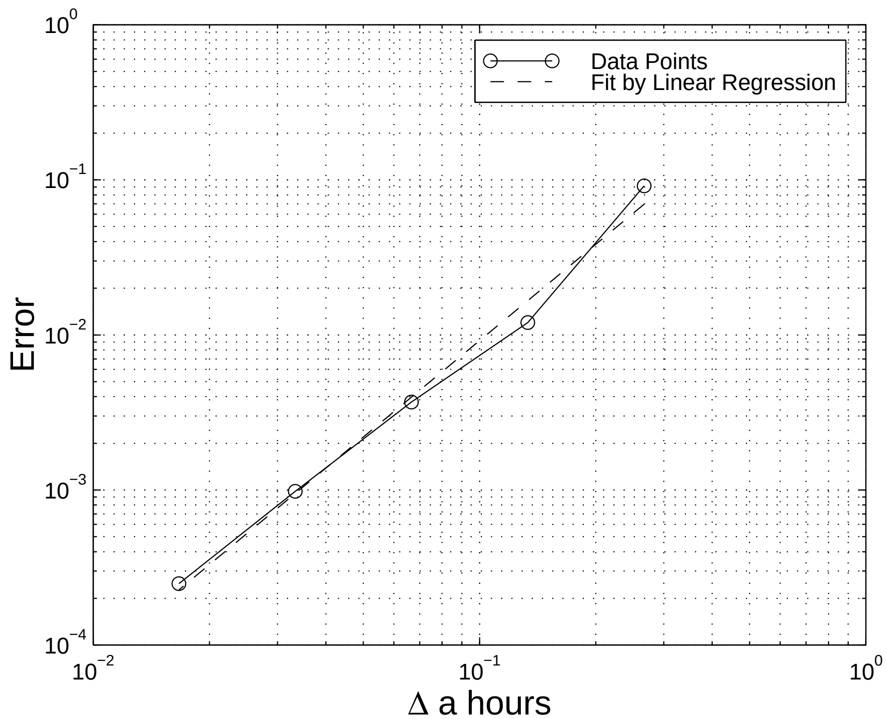

Figure 18: Convergence study in age showing second-order convergence. The slope of the linear fit is approximately 2.07. Error(Δa) is the L^2-norm at time $t = 6$ hours of the difference between the approximated swarmer population densities with Δa and $\Delta a/2$. By Δa we mean the uniform length of all but the first and last age intervals. The time step was maintained at $\Delta t = 10^{-3}$ hours, with occasional minor reductions made for alignment with the age discretization. We used a uniform spatial discretization with $\Delta r = 0.025$ cm.

CHAPTER 5

CONCLUSIONS

We have presented two classes of numerical methods. These were used in conjunction with each other to simulate efficiently and robustly a biological population whose dynamics have dependence on both age and space. The class of methods for approximating age-dependent populations undergoing diffusion were shown to be second-order correct approximations, after postprocessing, in the age variable. An empirical study further illustrated this property. These methods involved transforming the population model to a system of parabolic equations. The step-doubling Galerkin methods were shown to be second-order correct approximations in time for parabolic equations.

In the *Proteus mirabilis* swarm colony simulations, we see that the use of a simpler method of characteristics in age and time, where $\Delta t = \Delta a$ is constant (for example [22, 23, 32], would result in a much less efficient or accurate approximation. For example (see Figure 17), a comparably accurate approximation to the one presented could be obtained by using $\Delta t = \Delta a = 0.0025$. However, this would increase the size of the problem at each time step by a factor of 40, as well as increase the number of time steps.

With the simpler methods of characteristics, incorporating age into a population model is hampered by the enormous increase in computational cost. With the methods presented in this thesis, age-structure can be incorporated into a model at a level congruent with its importance in determining the behavior of the population.

It is hoped that the methods and analysis discussed in this thesis have illustrated the role computational science and numerical analysis can play in the study of actual populations. It is the opinion of the author that numerical methods will be of most value when they are motivated by an attempt to understand the behavior of real populations. In addition to elucidating the mathematics, it is with this research compass that generalizations and expansions of this work should be made.

One possible generalization of this work is the formulation and analysis of methods that use higher-order finite dimensional subspaces in age. This should include the development of notation and nomenclature that gives a solid framework for working on methods for the dynamics of structured populations in space.

Other useful work includes extending the analysis to deal with some of the more complicated features of the *Proteus mirabilis* swarm colony simulations, since it is likely these wrinkles will appear in other situations. An analysis of the use of birth mollifiers, at least in the case of piecewise constant approximations in age, is a worthwhile area of investigation. An analytical treatment of degenerate diffusions will also be of great value.

Possibly the most important and difficult generalizations will be to the models themselves. Models incorporating size structure instead of age structure will have characteristic curves that are no longer just lines with slope one, in fact these characteristics may change as the population changes. The formulation and analysis of these models can be expected to be more difficult. Examples of actual size-structured populations can provide the essential motivations for the simplifying assumptions made in the analysis, in particular with respect to the characteristic curves.

APPENDIX A

CALCULATION OF SOME COEFFICIENTS

In this appendix, we provide justification for some of the explicit constants used in our estimates. Without loss of generality, we consider the interval $[0,1]$ in obtaining these constants.

We first consider quantities which are bounded by an L^2-norm over an interval, such as our estimates of time differences. Take $f(s)$ such that $f \in H^1(0,1)$ and $\int_0^1 f\ ds = 0$. We wish to find C such that $\|f\|_{L^2} \leq C\|f'\|_{L^2}$. The operator $Lf = f''$, $L \geq 0$, has eigenvalues $\lambda_0 = 0 < \lambda_1 < \ldots$, where

$$\lambda_1 = \min_{f \perp 1} \frac{(Lf, f)}{(f, f)} = \pi^2 = \frac{\|f'\|_{L^2}^2}{\|f\|_{L^2}^2}.$$

Thus, $C = 1/\pi$. We note that $f(x) - f(y) = \int_y^x 1 \cdot f'(s)\ ds \leq \sqrt{|x-y|}\,\|f'\|_{L^2([y,x])}$, by Schwarz' Inequality.

We now consider $f : [0,1] \to \mathbb{R}$. We wish to find C such that $\|f - \bar{f}\|_{L^\infty} \leq C\|f'\|_{L^\infty}$. We have $f(x) - f(y) = \int_y^x f'(s)\ ds$. Then $|f(x) - \bar{f}| = |\int_0^1 \int_y^x f'(s)\ ds\ dy| \leq \|f'\|_{L^\infty} \int_0^1 |\int_x^y 1\ ds|\ dy| = \frac{1}{2}\|f'\|_{L^\infty}$. Thus, $C = \frac{1}{2}$.

APPENDIX B

A DISCRETE GRONWALL'S INEQUALITY

This appendix was provided by Todd Dupont. Some version of the following result is frequently used in analyzing numerical methods for time-dependent problems. This version is somewhat more flexible than many and is stated in such a way that it is natural to use for implicit methods.

Lemma B.1. *(Discrete Gronwall's Inequality) Take m positive and v^0 nonnegative. Suppose that for $1 \leq j \leq m$, Δt^j is positive, v^j, α^j, γ^j, and β^j are nonnegative, and $\Delta t^j \beta^j \leq \frac{1}{2}$. Let $C^m = exp(2.2 \sum_{j=1}^{m} \beta^j \Delta t^j)$. If, for each j,*

$$\frac{v^j - v^{j-1}}{\Delta t^j} + \gamma^j \leq \alpha^j + \beta^j (v^j + v^{j-1}),$$

then

$$v^m + \sum_{j=1}^{m} \gamma^j \Delta t^j \leq C^m \{v^0 + \sum_{j=1}^{m} \alpha^j \Delta t^j\}.$$

Proof. We have the condition

$$v^l + \gamma^l \Delta t^l \leq v^l + \frac{\gamma^l \Delta t^l}{1 - \beta^l \Delta t^l} \leq \left(\frac{1 + \beta^l \Delta t^l}{1 - \beta^l \Delta t^l}\right) v^{l-1} + \frac{\alpha^l \Delta t^l}{1 - \beta^l \Delta t^l}.$$

With $V^l = v^l + \sum_{j=1}^{l} \gamma^j \Delta t^j$, we get, for $1 \leq l \leq m$,

$$\begin{aligned} V^l &\leq \left(\frac{1 + \beta^l \Delta t^l}{1 - \beta^l \Delta t^l}\right) v^{l-1} + \frac{\alpha^l \Delta t^l}{1 - \beta^l \Delta t^l} + \sum_{j=1}^{l-1} \gamma^j \Delta t^j \\ &\leq \left(\frac{1 + \beta^l \Delta t^l}{1 - \beta^l \Delta t^l}\right) (\alpha^l \Delta t^l + V^{l-1}) \\ &\leq \exp(2.2 \beta^l \Delta t^l)(\alpha^l \Delta t^l + V^{l-1}), \end{aligned} \tag{B.B.1}$$

where we used the fact that, for $s \in [0, \frac{1}{2}]$, $(1+s)/(1-s) \leq \exp(2.2s)$. Divide the relation (B.B.1) by C^l to get

$$\frac{V^l}{C^l} \leq \alpha^l \Delta t^l + \frac{V^{l-1}}{C^{l-1}}.$$

Add these relations to get

$$\frac{V^m}{C^m} \leq v^0 + \sum_{j=1}^{m} \alpha^j \Delta t^j.$$

Multiply by C^m to get the stated result. □

APPENDIX C

RADIALLY SYMMETRIC FINITE DIFFERENCES

Consider a diffusion equation in radially symmetric form:

$$\partial_t u(r,t) = \frac{1}{r}\partial_r(rJ), \tag{C.C.1}$$

where J is either the Fickian flux, $D\partial_r u$, or an isotropic flux, $\partial_r(Du)$. Partition by annuli of radii r_i, $i = 0 \ldots n$. Use, for $i \neq 0$, the conservative discretization

$$\pi(r_{i+1/2}^2 - r_{i-1/2}^2)u_t(r_i,t) = 2\pi r_{i+1/2}J_{i+1/2} - 2\pi r_{i-1/2}J_{i-1/2},$$

where $J_{i\pm 1/2}$ is the flux at $r_{i\pm 1/2} = (r_i + r_{i\pm 1})/2$. This gives the equation

$$u_t(r_i,t) = \frac{r_{i+1/2}J_{i+1/2} - r_{i-1/2}J_{i-1/2}}{\frac{1}{2}(r_{i+1/2}^2 - r_{i-1/2}^2)}.$$

Note that the denominator is equal to $\frac{1}{2}(r_{i+1/2} + r_{i-1/2})(r_{i+1/2} - r_{i-1/2})$. Thus this discretization corresponds to a direct differencing of Equation (C.C.1) with r_i replaced by $\frac{1}{2}(r_{i+1/2} + r_{i-1/2})$, for $i \neq 0$.

For the case when $i = 0$, $r_0 = 0$ and a direct differencing does not make sense. Instead, do as above to get

$$\pi r_{1/2}^2 u_t(0,t) = 2\pi r_{1/2}J_{1/2},$$

which gives

$$u_t(0,t) = \frac{2J_{1/2}}{r_{1/2}}.$$

For a no-flux boundary condition, the conservative discretization is

$$\pi(r_n^2 - r_{n-1}^2)u_t(r_n,t) = -2\pi r_{n-1}J_{n-1},$$

which gives

$$u_t(r_i,t) = \frac{-r_{n-1}J_{n-1}}{\frac{1}{2}(r_n^2 - r_{n-1}^2)}.$$

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