A SPECTRAL GALERKIN APPROXIMATION OF THE POROUS MEDIUM EQUATION

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We present new numerical methods for the porous media equation (PME), a non-linear parabolic PDE used to model a variety of diffusive processes. It is well-known that, unlike the archetypal linear parabolic heat equation, the PME evolves compactly supported initial data to compactly supported solutions for all time. Compactness of solutions gives rise to the "free boundary" of the support set, which itself exposes computational concerns. Additionally, it is well-known that solutions of the PME tend to a self-similar Barenblatt-Pattle solution as time tends to infinity.

We introduce new spectral Galerkin (sG) methods for this problem: solutions that are the result of forcing truncated series expansions in bases of functions to satisfy a finite-dimensional, weak formulation of the PDE. We prove that by carefully tracking the free boundary and adding the Barenblatt-Pattle solution to our bases of functions our numerical solutions preserve the correct asymptotic behavior as time tends to infinity. Our method is preferable for long-time numerical simulations because it preserves this useful property whereas previous methods do not. Numerical experiments suggest convergence to the true solution for all time as the number of basis functions tends to infinity. Next, we investigate sG methods for an equation of unsteady filtration (EUF), of which the PME is a special case. We show that the asymptotic computational cost of our approach is better than that exhibited by prior methods based on finite-difference discretizations.

BIOGRAPHICAL SKETCH

The author was born in San Antonio, TX, in March of 1976. He was raised there and studied mathematics at Texas A&M University. After graduation he began a doctoral program in biometrics at Cornell University. He soon found his taste for statistics waning, so he transferred into the Center for Applied Mathematics where he picked up the subject of this dissertation.

I dedicate this research to my family who supported me throughout its production.

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CHAPTER 1

INTRODUCTION

We will construct spectral Galerkin (sG) solutions to the following partial differential equation (PDE) initial value problem (IVP):

Find u such that

$$u_t = (u^m)_{xx} \text{ in } \mathbb{R} \times (0, T], \, m > 1, \tag{1.1}$$

$$u(\,\cdot\,, 0) = u_0, \text{ in } \mathbb{R}. \tag{1.2}$$

Equation (1.1) is known as the porous medium equation (PME).

The PME can be used to describe the flow of a fluid or gas in a porous medium. For $m > 1$ we get a model for interstellar diffusion of galactic populations [27], for $m = 2$ we get the equation of thin saturated regions in porous media [32], for $m \geq 2$ we get models for spatial spread of biological populations [16], for $m = 4$ we get the equation for thin liquid films spreading under gravity [7], while for $m = 7$ we get a zeroth order approximation from the study of radiative heat transfer by Marshak waves [24]. Lacey et al. [23] give more examples and references.

Let $(f, g) = \int_{\mathbb{R}} f(x)\, g(x)\, dx$, then $(\,\cdot\,,\cdot\,)$ is an inner product if we identify functions differing only on sets of measure zero. Consider the weak formulation of the PME:

Find u such that

$$(u_t, \psi) = ((u^m)_{xx}, \psi), \tag{1.3}$$

for all smooth ψ with compact support. A sG solution of the PME is a function of the form $U = \sum_{j=0}^{N} \beta_j(t)\, \phi_j(x)$, where $\{\phi_j\}_{j=0}^{N}$ is a set of linearly independent functions known as the set of trial functions and where $\{\beta_j(t)\}_{j=0}^{N}$ have been determined by forcing a discrete version of (1.3) to hold:

Find $\{\beta_j(t)\}_{j=0}^{N}$ in the expression for U such that

$$(U_t, \psi_i) = ((U^m)_{xx}, \psi_i), \tag{1.4}$$

for $i = 0, \ldots, N$, where $\{\psi_i\}_{i=0}^{N}$ is a set of linearly independent functions known as the set of test functions. Equation (1.4) can be rewritten in a way that shows that the residuals, $U_t - (U^m)_{xx}$, are orthogonal to the subspace spanned by $\{\psi_i\}_{i=0}^{N}$: U satisfies (1.4) if and only if U satisfies

$$(U_t - (U^m)_{xx}, \psi_i) = 0, \tag{1.5}$$

for $i = 0, \ldots, N$.

For sG methods the space of trial functions and the space of test functions are polynomials or trigonometric polynomials of degree at most N. Strictly speaking, Galerkin methods are those where $\{\phi_i\}_{i=0}^{N} = \{\psi_i\}_{i=0}^{N}$ is an orthonormal set. While we use the same set for the trial and test functions, we briefly entertain the use of a non-orthogonal set.

In this dissertation we cite original authors, though [1, 31, 20] survey many results about PME problems and are excellent sources at which to begin studying this PDE. Good starting points to study sG methods, and, more generally, spectral methods are [5, 13, 17, 37, 36, 8]. In the remainder of this introduction we give preliminary results that will be useful throughout this dissertation and use these results to define our problem more clearly.

Oleĭnik, Kalashnikov and Yui-Lin [29] show that (1.1)-(1.2) has a weak solution if u_0 is a continuous non-negative function with $(u_0^m)_x$ bounded. One by-product of their construction is the *comparison principle*: if $u(x,t) \leq w(x,t)$, $\forall x \in \mathbb{R}$, are two solutions of the PME, then $u(x,t') \leq w(x,t')$, $\forall x \in \mathbb{R}$, if $t' > t$. Their analysis shows that the PME preserves mass, so that $\int_{\mathbb{R}} u(x,t)\, dx$ is independent of time, if u is a solution to (1.1). Suppose that, in addition to the above conditions on u_0 for the existence of weak solutions, u_0 is compactly supported. In this case, Oleĭnik, et al. also show that solutions will have compact support for all time. This anomaly defies the characteristic flavor of the paragon linear parabolic PDE, the heat equation $u_t = u_{xx}$: no solution to the linear heat equation has compact support for any positive time [11]. The compact support of solutions of the PME defines at least two free boundaries such that $u > 0$ between the two free boundaries and $u = 0$ otherwise. We restrict our study to the case when u_0 is compactly supported and such that only two free boundaries occur. This can be done by restricting u_0 to be of a certain class as will be demonstrated below. Denote by ξ_ℓ the smallest (leftmost) free boundary, by ξ_r the largest (rightmost), and by ξ some free boundary, when either the context is clear or irrelevant. As solutions to (1.1)-(1.2) are translation invariant, we locate the spatial origin so that $\xi_\ell(0)+\xi_r(0) = 0$; that is, we translate u_0 such that its support lies equally on both sides of the origin. We denote the support of $u(x,t)$ by $\Xi(t) = (\xi_\ell(t), \xi_r(t))$ and $\Xi = \{(x,t) : x \in \Xi(t)\}$. Our approximate solutions to (1.1)-(1.2) will ultimately be constructed in approximations of Ξ.

A central player to our method is a self-similar solution due to Barenblatt [2] and Pattle [30]. We will refer to this solution as the Barenblatt-Pattle solution and denote it by B. It is given by

$$B(x, t) = t^{-\alpha}\left[A - C\frac{x^2}{t^{2\beta}}\right]_+^{1/(m-1)}, \tag{1.6}$$

where $[z]_+ = \max(0, z)$. The parameters α, β, and C depend on m: $\alpha = \beta = 1/(m+1)$, $C = \beta(m-1)/(2m)$. Note that $B(x,t) > 0$ for $x \in \Xi(t)$ and $B(x,t) = 0$ otherwise, where $\xi_\ell(t) = -\xi_r(t) = -t^\beta (A/C)^{1/2}$. The parameter A determines the mass of $B(x,t)$, $\int_{\mathbb{R}} B(x,t)\, dx$. For a derivation of this solution see [1]. Figure 1.1 shows the Barenblatt-Pattle solution for various values of m.

Knerr [22] showed that if $u_0^{m-1}(x) \in \mathcal{O}\left((x-\xi(0))^2\right)$, as $|x-\xi(0)| \to 0$, then

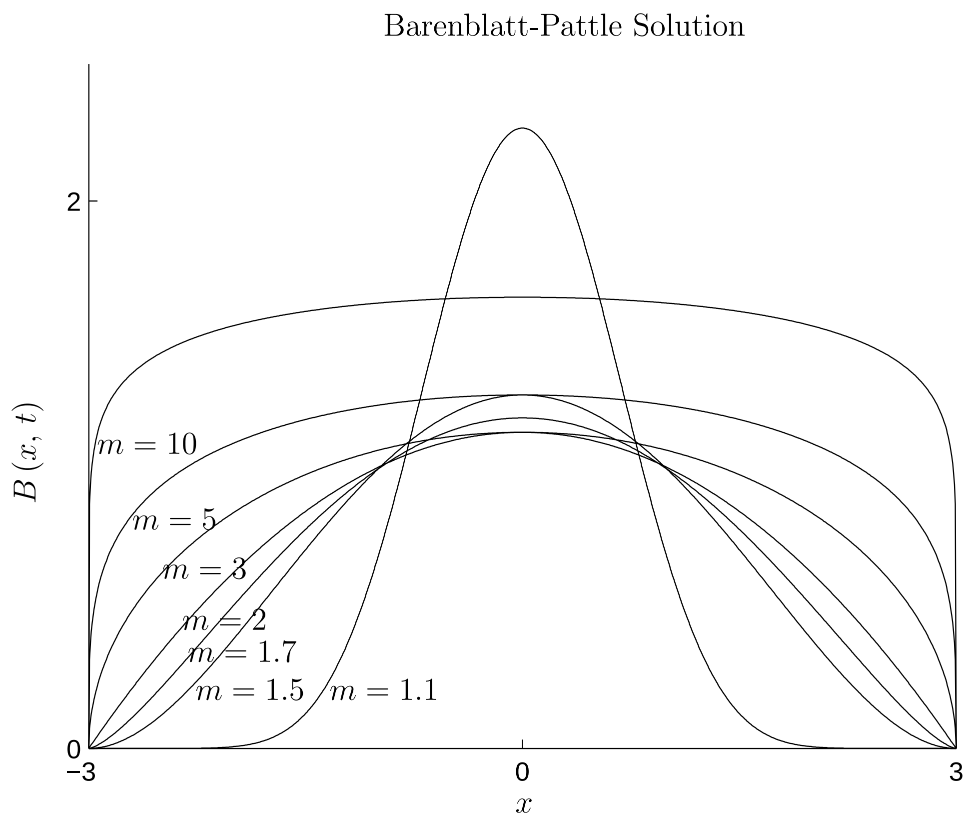

Figure 1.1: The Barenblatt-Pattle solution for various values of m (the upper-left corner of the character m touches the curves to which it corresponds.). Note that for $1 < m < 2$ the slope at the free boundary is zero, while for $m > 2$ the slope at the free boundary is infinite.

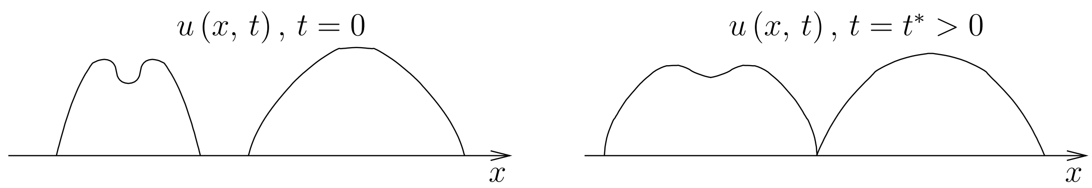

Figure 1.2: Two positive densities initially separated by interval of zero density eventually coalesce.

there is a $\tau > 0$ such that $\xi(t) = \xi(0)$, for all $t \in [0, \tau]$. This time, τ, is called a *waiting time*. In this thesis we do not consider u_0 that give rise to such waiting times.

Since one can always find a Barenblatt-Pattle solution that is everywhere dominated by the initial profile u_0, one can easily see that $-\xi_\ell$ and ξ_r are non-decreasing functions of t by appealing to the comparison principle. This also shows that, aside from u_0 that exhibit waiting times, the support must be ever-expanding. Suppose that the support of u_0 is not connected. Suppose that the support is two non-intersecting connected intervals, as in the example depicted in the schematic in Figure 1.2. Note that the supports of the two positive densities will join for some value of $t = t^* < \infty$ (see Figure 1.2). So, if we initially do not have disjoint positive densities, i.e. if the support of u_0 is connected, then u will never develop a disconnected support. Our study does not address u_0 with disconnected support.

We will construct approximations to (1.1)-(1.2) where we restrict u_0 to be bounded, compactly supported, and such that joining densities and waiting times are precluded.

The pressure equation (PE)

$$v_t = (m-1)\, v v_{xx} + v_x^2 \tag{1.7}$$

was useful in the development of our sG solutions. Letting $v = \frac{m}{m-1} u^{m-1}$, where u is a solution to (1.1), gives the PE. Note that the PE solution corresponding to a Barenblatt solution is quadratic in x. Authors use various multiples of the scaled pressure, v, to study solutions and free boundaries of the PME and associated problems. In essence, we will see that solving the PE gives insight to a much better numerical solution methodology that can be more widely applicable.

Along with the Barenblatt-Pattle solution (1.6) and the PE (1.7), Kamenomostskaya's asymptotic result has influenced our sG solutions. In [21] she proved that solutions of (1.1)-(1.2), where u_0 is continuous, non-negative, and compactly supported, tend to particular Barenblatt-Pattle solutions as $t \to \infty$.

This thesis is an exploration for a method to solve (1.1)-(1.2) accurately and quickly. Some of the directions initially taken resulted in experiments whose results pointed us towards better methods. Such experiments are referenced in this thesis though not always presented.

For purposes of error analysis in chapter 4 we will need the following PDE IVP:

Find u such that

$$u_t = \varphi(u)_{xx}, \text{ in } \mathbb{R} \times (0, T], \tag{1.8}$$

$$u(\cdot, 0) = u_0, \text{ in } \mathbb{R}, \tag{1.9}$$

where $\varphi(s)$ is defined for $s \geq 0$, $\varphi(s) > 0$ and $\varphi'(s) > 0$ for $s > 0$, and $\varphi(0) = \varphi'(0) = 0$. Equation (1.8) is a generalization of the PME, known as the equation of unsteady filtration (EUF). Oleĭnik, et al. [29] proved that this problem has solutions if u_0 is a continuous non-negative bounded function such that $\varphi(u_0)_x$ is bounded.

The rest of this thesis is structured as follows. In chapter 2 we describe two sG solutions and some of their features, consider the implications of the choice of basis for $\{\phi_j\}_{j=0}^{N}$, and discuss some details of computing with these methods. In chapter 3 we show how the Barenblatt-Pattle solution is an attractor for one of the solutions described in chapter 2, as is the case for true solutions. In chapter 4 we estimate the global order of accuracy for this method applied to a Barenblatt-Pattle solution and to the EUF. In chapter 5 we show that the work required to use this method compares favorably with a finite difference scheme. In chapter 6 we mention directions for future studies emanating from this thesis.

CHAPTER 2

APPROXIMATE SPECTRAL GALERKIN SOLUTIONS

Let Π_N be the space of all polynomials of degree at most N. In section 2.1 we construct approximations to (1.1)-(1.2) in two different ways: the first uses sG methods applied in a straightforward way (*model 1*) and the second seeks to model true solution characteristics (*model 2*). To complete either method one must choose a basis for Π_N from which the trial and test functions will come. We will denote by $\{\phi_i\}_{i=0}^N$ the chosen basis for Π_N. In section 2.2 we discuss two such bases as well as some computational concerns that arise when considering orthogonal bases.

2.1 Model solutions

We formulate two different sG solutions for (1.1)-(1.2). In subsection 2.1.1 we first present the standard spectral Galerkin method. In subsection 2.1.2 we present the second method which builds features of an asymptotically characteristic solution into the resulting numerical solutions.

2.1.1 Model 1

We seek approximate solutions $\tilde{z}$ of the form

$$\tilde{z}(x,t) = \sum_{j=0}^{N} \beta_j(t)\,\phi_j(x)\,. \tag{2.1}$$

We assume that $\tilde{z}(x,t)$ has roots $\tilde{\xi}_\ell(t)$ and $\tilde{\xi}_r(t)$ that comprise the approximate free boundary and which define the support of $\tilde{z}$: $\tilde{\Xi}(t) := \left(\tilde{\xi}_\ell(t), \tilde{\xi}_r(t)\right)$. To determine the $\{\beta_i(t)\}_{i=0}^N$ we force $\tilde{z}$ to satisfy the orthogonality constraints (1.5) with inner product $(f,g)_{\tilde{\Xi}(t)} = \int_{\tilde{\Xi}(t)} f(x)\,g(x)\,dx$:

$$\left(\tilde{z}_t - (\tilde{z}^m)_{xx}, \phi_i\right)_{\tilde{\Xi}(t)} = 0, \tag{2.2}$$

$i = 0, \ldots, N$. We term the numerical solution in (2.1) *model 1.* We will often use the shorthand $p_N(x, t)$ in place of a time-dependent linear combination of the basis functions $\{\phi_i(x)\}_{i=0}^N$ like that found on the right-hand side of (2.1). Though p_N will always represent a polynomial in Π_N, in the sequel we will omit the subscript N for the sake of simplicity of notation.

Let $\tilde{z}_0(x) = \tilde{z}(x, 0)$. We start the method by finding the projection of u_0 in Π_N :

Find $\tilde{z}_0 \in \Pi_N$ such that

$$(u_0 - \tilde{z}_0, \phi_i)_{\Xi(0)} = 0, \tag{2.3}$$

$i = 0, \ldots, N$.

Equations (2.2)-(2.3) give a system of ordinary differential equations and an initial condition. Plugging (2.1) into (2.2)-(2.3) gives

$$\sum_{j=0}^{N} (\phi_j, \phi_i)_{\tilde{\Xi}(t)} \beta_j'(t) = ((p^m)_{xx}, \phi_i)_{\tilde{\Xi}(t)}, \tag{2.4}$$

$$\sum_{j=0}^{N} (\phi_j, \phi_i)_{\Xi(0)} \beta_j(0) = (u_0, \phi_i)_{\Xi(0)}, \tag{2.5}$$

$i = 0, \ldots, N$, where $p \equiv p(x,t)$. These systems can be written in matrix-vector notation,

$$H\boldsymbol{\beta}' = \mathbf{f}(\boldsymbol{\beta}, t), \tag{2.6}$$

$$H\boldsymbol{\beta}_{\mathbf{0}} = \mathbf{f}_{\mathbf{0}}, \tag{2.7}$$

where $\cdot'$ denotes differentiation with respect to time, $\boldsymbol{\beta} = (\beta_i(t)) \in \mathbb{R}^{N+1}$, $\boldsymbol{\beta}_{\mathbf{0}} = (\beta_i(0)) \in \mathbb{R}^{N+1}$, $H = (H(i,j)) \in \mathbb{R}^{(N+1)\times(N+1)}$, $\mathbf{f}(\boldsymbol{\beta}, t) = (f_i) \in \mathbb{R}^{N+1}$, $\mathbf{f}_{\mathbf{0}} = (f_{0,i}) \in \mathbb{R}^{N+1}$,

$$H(i,j) = (\phi_j, \phi_i)_{\widetilde{\Xi}(t)}, \tag{2.8}$$

$$= \int_{\widetilde{\Xi}(t)} \phi_i(x)\,\phi_j(x)\,dx \tag{2.9}$$

$$\begin{aligned}
f_i &= \left((p^m)_{xx}, \phi_i\right)_{\widetilde{\Xi}(t)} \\
&= \left(m(m-1)\,p^{m-2}p_x^2, \phi_i\right)_{\widetilde{\Xi}(t)} \\
&\quad + \left(mp^{m-1}p_{xx}, \phi_i\right)_{\widetilde{\Xi}(t)}, \\
&= m(m-1)\int_{\widetilde{\Xi}(t)} \left(p^{m-2}p_x^2\right)(x,t)\,\phi_i(x)\,dx \\
&\quad + m\int_{\widetilde{\Xi}(t)} \left(p^{m-1}p_{xx}\right)(x,t)\,\phi_i(x)\,dx,
\end{aligned} \tag{2.10}$$

and

$$\begin{aligned}
f_{0,i} &= (u_0, \phi_i)_{\Xi(0)} \\
&= \int_{\Xi(0)} u_0(x)\,\phi_i(x)\,dx,
\end{aligned} \tag{2.11}$$

for $i, j = 0, \ldots, N$.

Though we do not use orthogonal bases for $\{\phi_i\}_{i=0}^N$, we mention a standard technique for determining $\{\beta_i'(t)\}_{i=0}^N$ and $\{\beta_i(0)\}_{i=0}^N$ when $\{\phi_i\}_{i=0}^N$ is orthogonal. If $\{\phi_i\}_{i=0}^N$ is orthogonal with respect to $(f,g)_{\widetilde{\Xi}(t)} = \int_{\widetilde{\Xi}(t)} f(x)\,g(x)\,dx$, then (2.4)-(2.5) gives

$$\beta_i'(t) = f_i / (\phi_i, \phi_i)_{\widetilde{\Xi}(t)}, \tag{2.12}$$

$$\beta_i(0) = f_{0,i} / (\phi_i, \phi_i)_{\Xi(0)}, \tag{2.13}$$

for $i = 0, \ldots, N$.

Remark 2.1. *Note that H is symmetric positive definite. The proof of this follows from the fact that $H(i,j)$ can be considered an inner product of the functions ϕ_j and ϕ_i. That $H(i,j)$ is indeed an inner product can be seen easily. Non-negativity, bi-linearity, symmetry, and that $(0,0)_{\tilde{\Xi}(t)} = \int_{\tilde{\Xi}(t)} 0^2\, dx = 0$ are obvious. To see that $(f,f)_{\tilde{\Xi}(t)} = \int_{\tilde{\Xi}(t)} f^2(x)\, dx = 0$ implies $f(x) = 0$ a.e. on $\tilde{\Xi}(t)$ suppose by way of a contradiction that $f(x) \neq 0$ on some subset $S \subseteq \tilde{\Xi}(t)$, and that $(f,f)_{\tilde{\Xi}(t)} = 0$. Since we are identifying all functions that differ only on sets of measure zero, the measure of S must be nonzero. On S there is $C > 0$ such that $f^2(x) \geq C$ for $x \in S$. Since $S \subseteq \tilde{\Xi}(t)$, $(f,f)_{\tilde{\Xi}(t)} > (f,f)_S > C\mu > 0$, where μ is the non-zero measure of S. This is a contradiction, so $H(i,j)$ is an inner product and H is positive definite.*

Since H is symmetric positive definite, it is possible to find $\boldsymbol{\beta}'$ and $\boldsymbol{\beta_0}$ from (2.6)-(2.7). Letting $\boldsymbol{g} := H^{-1}\mathbf{f}$, we have

$$\boldsymbol{\beta}' = \boldsymbol{g}(\boldsymbol{\beta}, t), \tag{2.14}$$

$$\boldsymbol{\beta_0} = H^{-1}\mathbf{f_0}. \tag{2.15}$$

Finally, to find our approximation $\tilde{z}(x,T)$ we solve the IVP (2.6)-(2.7) using an ODE solver.

We finish this section by discussing some of the properties of the above framework.

In order to enforce boundary conditions, normally one must restrict the set from which our test functions come by constructing a basis of test functions each element of which satisfies the boundary conditions [6]. Numerical experiments (see chapter 4) show that (2.2) is enough to guarantee that free boundaries exist for numerical solutions as long as the time-stepping computation is stable. This is a welcome surprise as the true free boundaries, too, arise naturally: they are not part of the formulation of the PME.

Perhaps several times per time step, the ODE solver used to solve (2.6)-(2.7) will need to compute $\boldsymbol{g} = H^{-1}\mathbf{f}$ in (2.14). Direct methods for this computation requires first factorizing H and next applying backward and forward solves. The backward and forward solves each have $\mathcal{O}\left(N^2\right)$ complexity. For general H, the first step can be done via LU factorization, $H = LU$, L^T, U upper triangular, and has $\frac{2}{3}N^3 + \mathcal{O}\left(N^2\right)$ complexity. For symmetric positive definite H, as is the case for (2.8), the factorization step can be done via Cholesky factorization, $H = R^T R$, R upper triangular, and has $\frac{1}{3}N^3 + \mathcal{O}\left(N^2\right)$ complexity [39].

If we choose an orthogonal basis of Π_N, $\{\phi_i\}_{i=0}^N$, H is diagonal, thereby reducing the running-time complexity of computing $\boldsymbol{g}$ from order $\mathcal{O}\left(N^3\right)$ to $\mathcal{O}\left(N\right)$ and equations (2.4)-(2.5) become equations (2.12)-(2.13). Note that one must still use some quadrature rule to evaluate the inner product with the nonlinear diffusion term, $f_i = \left(\left(p^m\right)_{xx}, \phi_i\right)_{\tilde{\Xi}(t)}$. The factor $\left(\phi_i, \phi_i\right)_{\tilde{\Xi}(t)}$ is available for many bases, or computable in closed-form for some other bases.

The condition of the linear solution problem corresponding to (2.14) that must be computed at each time step, perhaps multiple times per time step, is directly linked to the choice of basis. When a non-orthogonal basis is used, numerical experiments in chapter 4 suggest that the condition number of H grows to problematic sizes for $t \to T$ for fixed N as small as 22. When an orthogonal basis is used H is diagonal, so the condition is ideal. E.g. for the Legendre basis orthonormal with respect to $(f, g)_{\tilde{\Xi}(t)} = \int_{\tilde{\Xi}(t)} f\left(x\right) g\left(x\right)\, dx$, the spectral condition number of H is

$$\kappa\left(H\right) = \frac{\max_i H(i,i)}{\min_i H\left(i,i\right)} = \frac{1}{1} = 1. \tag{2.16}$$

Unfortunately, the full benefit of choosing such a basis cannot be fully realized. We will see that the time-stepping computation becomes unstable because the support of our solutions is time-dependent and because we opted for our inner product also to be linked to this time-dependency. This issue will be more closely examined in subsection 2.2.3, after the model solution in the next subsection has been discussed. There, the reader will see that due to practical concerns we should construct a compromise basis that practically overcomes the difficulties in such a way that allows for stable computation, but where the condition number in (2.16) is not achieved. In subsection 2.2.3 we illustrate such a basis that results in a condition number that is bounded by a very slowly growing function of t for $t \to T$ for fixed N. In chapter 4 we present numerical evidence.

Lastly, solutions to (2.2) conserve the zeroth and first moments, i.e. the mass and center of mass, like solutions of the PME [40]. Fix $t \in \{t_i\}$, where $\{t_i\}$ is the sequence of time steps at which our numerical solution has been computed. Let $w = \tilde{z}$. Substituting (2.1) into (2.2) with $i = 0$, we get

$$\begin{aligned} \left(w_t, \phi_0\right)_{\tilde{\Xi}(t)} &= \left(\left(w^m\right)_{xx}, \phi_0\right)_{\tilde{\Xi}(t)} \\ \int_{\tilde{\Xi}(t)} w_t\left(x,t\right)\,dx &= \int_{\tilde{\Xi}(t)} \left(w^m\right)_{xx}\left(x,t\right)\,dx \\ \int_{\tilde{\Xi}(t)} w_t\left(x,t\right)\,dx &= \left(mw^{m-1}w_x\right)\left(\tilde{\xi}_r\left(t\right),t\right) - \left(mw^{m-1}w_x\right)\left(\tilde{\xi}_\ell\left(t\right),t\right), \end{aligned} \tag{2.17}$$

as long as $\phi_0 \in \Pi_0$. Each term of the right-hand side of (2.17) is zero since $m > 1$, $w_x\left(\tilde{\xi}\left(t\right),t\right) = p_x\left(\tilde{\xi}\left(t\right),t\right) < \infty$, and $w\left(\tilde{\xi}\left(t\right),t\right) = p\left(\tilde{\xi}\left(t\right),t\right) = 0$. The numerical free boundaries in this method are roots of polynomials, so, providing p in (2.1) has roots, $\left|\partial\tilde{\xi}/\partial t\right| < \infty$. The left-hand side of (2.17) is

$$\begin{aligned} \int_{\tilde{\Xi}(t)} w_t\left(x,t\right)\,dx &= -\frac{\partial\tilde{\xi}_r\left(t\right)}{\partial t} w\left(\tilde{\xi}_r\left(t\right),t\right) + \frac{\partial\tilde{\xi}_\ell\left(t\right)}{\partial t} w\left(\tilde{\xi}_\ell\left(t\right),t\right) \\ &\quad + \frac{\partial}{\partial t}\int_{\tilde{\Xi}(t)} w\left(x,t\right)\,dx \\ &= \frac{\partial}{\partial t}\int_{\tilde{\Xi}(t)} w\left(x,t\right)\,dx. \end{aligned}$$

This gives that

$$\frac{\partial}{\partial t}\int_{\widetilde{\Xi}(t)} w\left(x,t\right)\,dx = 0,$$

as needed. A similar argument shows that solutions to (2.2) preserve the center of mass as well. For the sake of simplicity, suppose that $\phi_1 \in \Pi_1 \backslash \Pi_0$. Compute

$$\begin{aligned}
\left(w_t, \phi_1\right)_{\widetilde{\Xi}(t)} &= \left(\left(w^m\right)_{xx}, \phi_1\right)_{\widetilde{\Xi}(t)} \\
\int_{\widetilde{\Xi}(t)} x w_t\left(x,t\right)\,dx &= \int_{\widetilde{\Xi}(t)} x\left(w^m\right)_{xx}\left(x,t\right)\,dx \\
&= \tilde{\xi}_r\left(t\right)\left(w^m\right)_x\left(\tilde{\xi}_r\left(t\right),\,t\right) - \tilde{\xi}_\ell\left(t\right)\left(w^m\right)_x\left(\tilde{\xi}_\ell\left(t\right),\,t\right) \\
&\quad - \int_{\widetilde{\Xi}(t)} \left(w^m\right)_x\left(x,t\right)\,dx \\
&= m\tilde{\xi}_r\left(t\right)\left(w^{m-1}w_x\right)\left(\tilde{\xi}_r\left(t\right),\,t\right) \\
&\quad - m\tilde{\xi}_\ell\left(t\right)\left(w^{m-1}w_x\right)\left(\tilde{\xi}_\ell\left(t\right),\,t\right) \\
&\quad - \left[\left(w^m\right)\left(\tilde{\xi}_r\left(t\right),\,t\right) - \left(w^m\right)\left(\tilde{\xi}_\ell\left(t\right),\,t\right)\right] \\
&= m\tilde{\xi}_r\left(t\right)\cdot 0^{m-1}\cdot w_x\left(\tilde{\xi}_r\left(t\right),\,t\right) \\
&\quad - m\tilde{\xi}_\ell\left(t\right)\cdot 0^{m-1}\cdot w_x\left(\tilde{\xi}_\ell\left(t\right),\,t\right) - 0 \\
&= 0,
\end{aligned}$$

the left-hand side of which is

$$\begin{aligned}
\int_{\widetilde{\Xi}(t)} x w_t\left(x,t\right)\,dx &= -\frac{\partial\tilde{\xi}_r\left(t\right)}{\partial t}\tilde{\xi}_r\left(t\right)w\left(\tilde{\xi}_r\left(t\right),t\right) + \frac{\partial\tilde{\xi}_\ell\left(t\right)}{\partial t}\tilde{\xi}_\ell\left(t\right)w\left(\tilde{\xi}_\ell\left(t\right),t\right) \\
&\quad + \frac{\partial}{\partial t}\int_{\widetilde{\Xi}(t)} x w\left(x,t\right)\,dx \\
&= -0 + 0 + \frac{\partial}{\partial t}\int_{\widetilde{\Xi}(t)} x w\left(x,t\right)\,dx.
\end{aligned}$$

The result then follows. For a general $\phi_1 \in \Pi_1$, we need only write $\phi_1\left(x\right) = ax + b$ for some constants a and b, and carry through the last two arguments separately on both terms on the right-hand side of

$$\left(w_t - \left(w^m\right)_{xx}, \phi_1\right)_{\widetilde{\Xi}(t)} = a\left(w_t - \left(w^m\right)_{xx}, x\right)_{\widetilde{\Xi}(t)} + b\left(w_t - \left(w^m\right)_{xx}, 1\right)_{\widetilde{\Xi}(t)}.$$

Despite the attractive properties detailed above, the above framework suffers from a drawback that we now illustrate. Note that Kamenomostskaya [21] showed that the solution to (1.1)-(1.2) behaves asymptotically like a certain Barenblatt-Pattle solution. Since true solutions tend to the Barenblatt-Pattle solution, we would prefer that $\tilde{z}_x\left(\tilde{\xi}_r(t)-,\, t\right) \to \infty$ as $t \to \infty$ when $m > 2$; while $\tilde{z}_x\left(\tilde{\xi}_r(t)-,\, t\right) < \infty$, since $\tilde{z} \in \Pi_N$, where $\tilde{\xi}_r(t)- = \lim_{x \to \xi_r(t)^-} x$. Analogous remarks apply to the left, free boundary point, $\tilde{\xi}_\ell$. Numerical experiments (see figure 2.1) confirm that numerical solutions indeed suffer in this regard.

We now consider points in the free boundary. Though we will use the right, free boundary point, $\tilde{\xi}_r$, analogous comments apply to the left, free boundary point, $\tilde{\xi}_\ell$. We will use the term *root* because we also want to use the language of *multiplicity* of roots. We will say a root c of function f is *of multiplicity greater than one* if there is a $\gamma > 1$ and a constant $\mathcal{C}$ such that $\lim_{x \to c} f(x)/(x-c)^\gamma = \mathcal{C}$. We do not precisely define what we mean by *nearly of multiplicity greater than one*, except to describe how one observes them in the context of our methods. First, *to perturb a root* is to perturb the coefficients of the polynomial that gave rise to the root in such a way that the perturbation of the root is small. Note that when one perturbs a root of multiplicity greater than one in this way, the root separates into two roots. These roots can both be real, or they can both be complex. The term *root nearly of multiplicity greater than one* refers to the pair of real, perturbed roots that our method evolves to a pair of complex, perturbed roots in a single time step. Note the misnomer: this imprecise definition actually refers to two roots rather than to a single root.

Remark 2.2. *When $1 < m < 2$, the Barenblatt-Pattle solution has roots of multiplicity greater than one. While it is possible for $\tilde{z}$ to have roots of multiplicity greater than one, this situation is computationally undesirable. A root of multi-*

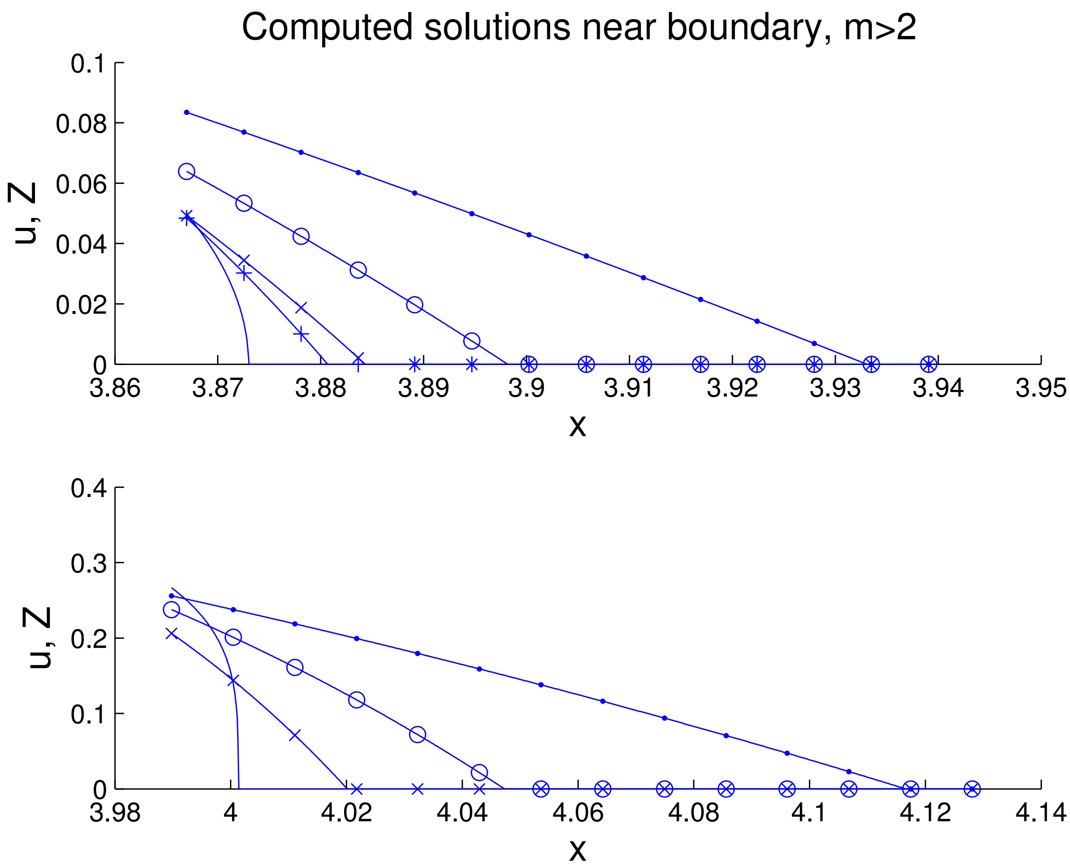

Figure 2.1: Model 1 numerical solutions cannot model the infinite slope at the free boundary of the true solution for $m > 2$. The top panel corresponds to $m = 3$ and the bottom panel corresponds to $m = 5$. Numerical solutions pictured here were computed using model 1 with the modified Legendre basis (see subsection 2.2.4) and RK8. $Z = \tilde{z}$ is our model 1 numerical solution. Markers for curves are $\cdot$ for $N = 8$, o for $N = 14$, $\times$ for $N = 20$, and $+$ for $N = 26$. These are the same functions pictured in the top panels of figure 4.3.

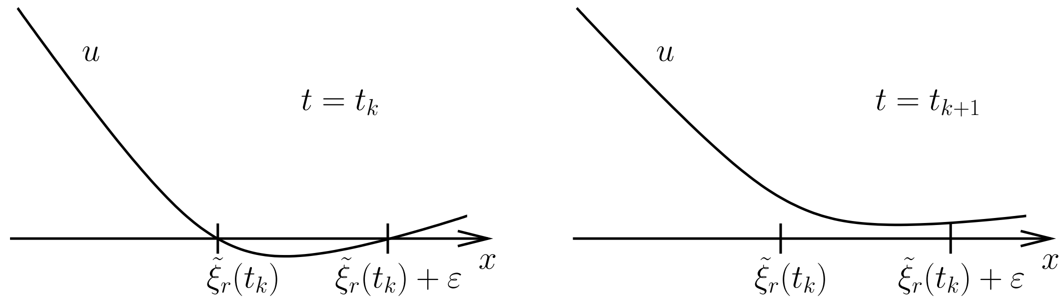

Figure 2.2: A root that is nearly of multiplicity greater than one is lost when a time step is taken. This can also happen if the root is of multiplicity greater than one before the time step is taken. $\varepsilon > 0$ is small.

plicity greater than one, or nearly of multiplicity greater than one, can become two complex roots after a time step. Small perturbations in $\{\beta_i(t)\}_{i=0}^{N}$ *due to rounding errors can cause root-finding routines to find a root of multiplicity greater than one, or nearly of multiplicity greater than one, instead as two complex roots. See figure 2.2. At this point the method would break down since the integrals in* (2.2) *are no longer well-defined.*

2.1.2 Model 2

In this section we describe a method that uses a new model solution form and discuss the motivation of this choice.

We seek approximate solutions $\tilde{u}$ of the form

$$\tilde{u}(x,t) = p^{1/(m-1)}(x,t), \tag{2.18}$$

$$p(x,t) = \sum_{j=0}^{N} \beta_j(t)\,\phi_j(x), \tag{2.19}$$

where $p \in \Pi_N$. We assume that p has roots $\tilde{\xi}_\ell(t)$ and $\tilde{\xi}_r(t)$ that comprise the approximate free boundary and which define the support of $\tilde{u}$: $\widetilde{\Xi}(t) := \left(\tilde{\xi}_\ell(t), \tilde{\xi}_r(t)\right)$. Note that $\widetilde{\Xi}$ is not the same as that used in the previous section. To determine the $\{\beta_i(t)\}_{i=0}^{N}$ we force $\tilde{u}$ to satisfy the orthogonality constraints (1.5) with inner product $(f,g)_{\tilde{\Xi}(t)} = \int_{\tilde{\Xi}(t)} f(x)\, g(x)\; dx$:

$$\left(\tilde{u}_t - (\tilde{u}^m)_{xx}, \phi_i\right)_{\tilde{\Xi}(t)} = 0, \tag{2.20}$$

$i = 0, \ldots, N$. We will refer to $\tilde{u}$ in (2.18)-(2.19) as *model 2*.

We now set initial conditions for (2.20), though below we will supplant this choice with one that is more amenable to solution. We start the method by finding u_0:

Let $\tilde{u}_0(x) \equiv \tilde{u}(x,0)$. Find $\tilde{u}_0 \in \Pi_N$ such that

$$(u_0 - \tilde{u}_0, \phi_i)_{\Xi(0)} = 0, \tag{2.21}$$

$i = 0, \ldots, N$. This is a nonlinear system in $\{\beta_i(0)\}_{i=0}^{N}$ from (2.18)-(2.19).

We mention that we would like to know that $p(x,t) > 0$, for $x \in \widetilde{\tilde{\Xi}}(t)$, for $t = 0$, and similarly for $t > 0$. Numerical experiments suggest that this is true (see chapter 4). Though we do not show that this is the case, we assume it is true in the sequel.

Since $p(x,t) > 0$ for $x \in \widetilde{\tilde{\Xi}}(t)$, we can define an inner product as follows $\langle f,g\rangle_{\tilde{\Xi}(t)} = \frac{1}{m-1}\int_{\tilde{\Xi}(t)} p^{1/(m-1)-1}(x,t)\, f(x)\, g(x)\; dx$, $m > 1$. Below, it will be shown that $\langle\cdot,\cdot\rangle_{\tilde{\Xi}(t)}$ is an inner product.

Plugging (2.18)-(2.19) into (2.20)-(2.21), we get the following system of ordinary differential equations with initial condition

$$H\boldsymbol{\beta}' = \mathbf{f}(\boldsymbol{\beta}, t), \tag{2.22}$$

$$G(\boldsymbol{\beta}_{\mathbf{0}}) = \mathbf{f}_{\mathbf{0}}, \tag{2.23}$$

where $\boldsymbol{\beta} = (\beta_i(t)) \in \mathbb{R}^{N+1}$, $\boldsymbol{\beta}_{\mathbf{0}} = (\beta_i(0)) \in \mathbb{R}^{N+1}$, $H = (H(i,j)) \in \mathbb{R}^{(N+1)\times(N+1)}$,

$G(\boldsymbol{\beta_0}) = (G_i) \in \mathbb{R}^{N+1}$, $\mathbf{f}(\boldsymbol{\beta}, t) = (f_i) \in \mathbb{R}^{N+1}$, $\mathbf{f_0} = (f_{0,i}) \in \mathbb{R}^{N+1}$,

$$H(i,j) = \left(\frac{1}{m-1} p^{1/(m-1)-1} \phi_j, \phi_i\right)_{\widetilde{\Xi}(t)}, \tag{2.24}$$

$$= \frac{1}{m-1} \int_{\widetilde{\Xi}(t)} p^{1/(m-1)-1}(x,t)\, \phi_i(x)\, \phi_j(x)\; dx, \tag{2.25}$$

$$G_i = (\tilde{u}_0, \phi_i)_{\Xi(0)}$$
$$= \int_{\Xi(0)} p^{1/(m-1)}(x,0)\, \phi_i(x)\; dx, \tag{2.26}$$

$$f_i = \left((\tilde{u}^m)_{xx}, \phi_i\right)_{\widetilde{\Xi}(t)}$$
$$= \left(\frac{m}{(m-1)^2} p^{1/(m-1)-1} p_x^2, \phi_i\right)_{\widetilde{\Xi}(t)} + \left(\frac{m}{m-1} p^{1/(m-1)} p_{xx}, \phi_i\right)_{\widetilde{\Xi}(t)} \tag{2.27}$$

$$\begin{aligned} &= \frac{m}{(m-1)^2} \int_{\widetilde{\Xi}(t)} \left(p^{1/(m-1)-1} p_x^2\right)(x,t)\, \phi_i(x)\; dx \\ &\quad + \frac{m}{m-1} \int_{\widetilde{\Xi}(t)} \left(p^{1/(m-1)} p_{xx}\right)(x,t)\, \phi_i(x)\; dx, \end{aligned} \tag{2.28}$$

and

$$f_{0,i} = (u_0, \phi_i)_{\Xi(0)}$$
$$= \int_{\Xi(0)} u_0(x)\, \phi_i(x)\; dx, \tag{2.29}$$

for $i,\, j = 0, \ldots, N$. Note that for this model the mass matrix H depends upon the state of the solution, as well as the value of m, unlike the mass matrix of model 1.

If one used the inner product $\langle \cdot, \cdot \rangle$ defined above then one can write the expressions (2.24) and (2.27) as

$$H(i,j) = \langle \phi_j, \phi_i \rangle_{\widetilde{\Xi}(t)}$$

and

$$f_i = \left\langle \frac{m}{m-1} p_x^2, \phi_i \right\rangle_{\widetilde{\Xi}(t)} + \langle m p p_{xx}, \phi_i \rangle_{\widetilde{\Xi}(t)},$$

respectively. This may aide in a future analysis of the method, where energy methods could prove to be useful.

H in (2.24) is symmetric positive definite. The proof of this follows from the fact that $H(i,j)$ can be considered an inner product of the functions ϕ_j and ϕ_i, with the positive weighting function $\frac{1}{m-1}p^{1/(m-1)-1}$. That $H(i,j) = \langle \phi_i, \phi_j \rangle_{\widetilde{\Xi}(t)}$ is indeed an inner product can be seen easily. Non-negativity, bi-linearity, symmetry, and that $\langle 0, 0 \rangle_{\widetilde{\Xi}(t)} = \int_{\widetilde{\Xi}(t)} \frac{1}{m-1} p^{1/(m-1)-1}(x,t)\, 0^2\, dx = 0$ are obvious. That $\langle f, f \rangle_{\widetilde{\Xi}(t)} = 0$ implies $f(x) = 0$ a.e. on $\widetilde{\Xi}(t)$ follows from our assumption that $p(x,t) > 0$ for $x \in \widetilde{\Xi}(t)$.

Since H is symmetric positive definite, it is possible to find $\boldsymbol{\beta}'$ from (2.22). Letting $\boldsymbol{g} := H^{-1}\mathbf{f}$, (2.22) gives

$$\boldsymbol{\beta}' = \boldsymbol{g}(\boldsymbol{\beta}, t). \tag{2.30}$$

Finally, to find our approximation $\tilde{u}(x,T)$ we solve the IVP (2.22)-(2.23) using an ODE solver.

Recall that $\tilde{u}_0(x) = \tilde{u}(x,0)$ and define $\tilde{v}_0 \in \Pi_{N-2}$ and v_0 through the equations

$$u_0(x) = \left[(\xi_r(0) - x)(x - \xi_\ell(0))\, v_0(x)\right]^{1/(m-1)}, \tag{2.31}$$

$$\tilde{u}_0(x) = \left[(\xi_r(0) - x)(x - \xi_\ell(0))\, \tilde{v}_0(x)\right]^{1/(m-1)}. \tag{2.32}$$

Note that since we know $\Xi(0)$ we use the true interface $\Xi(0)$ as opposed to the approximate interface $\widetilde{\Xi}(0)$.

Note that to find initial conditions for (2.22) we must solve the nonlinear system (2.23). To make this calculation simpler we instead solve a slightly different problem:

Find $\tilde{u}_0 \in \Pi_N$ such that

$$\left(u_0^{m-1} - \tilde{u}_0^{m-1}, \phi_i\right)_{\Xi(0)} \tag{2.33}$$

$i = 0, \ldots, N$. Equation (2.33) gives a linear system the matrix of which has the same form as (2.8), and is thus nonsingular. A linear solve gives $\{\beta_i(0)\}_{i=0}^{N}$ in (2.33).

We can go a step further for setting initial conditions for (2.22). We can use the true initial free boundary information, $\Xi(0)$, if we force $\tilde{u}_0$ to share a common free boundary with u_0. To do this we use the following modified projection rather than that in (2.33):

Find $\tilde{u}_0 \in \Pi_N$ such that

$$(v_0 - \tilde{v}_0, \phi_i)_{\Xi(0)} = 0, \tag{2.34}$$

$i = 0, \ldots, N-2$. Equation (2.34) gives a linear system the matrix of which is similar to that of (2.8) except the matrix in (2.34) is two dimensions smaller. The argument in remark 2.1 shows that the matrix in (2.34) is nonsingular.

For the sake of the completeness, we mention an obvious modification to the other methods for setting initial conditions for (2.22):

Find $\tilde{u}_0 \in \Pi_N$ such that

$$\left(v_0^{1/(m-1)} - \tilde{v}_0^{1/(m-1)}, \phi_i\right)_{\Xi(0)} = 0, \tag{2.35}$$

$i = 0, 1, \ldots, N-2$. This is the nonlinear counterpart to (2.34). Being nonlinear, we do not comment any further on it, except immediately below where we mention its relation to the other methods for setting initial conditions for (2.22).

We finalize our choice of setting initial conditions by choosing (2.34), though before moving on we now make a few comparisons between the different methods of setting initial conditions.

Though each of the systems (2.21), (2.33), (2.34), and (2.35) is heuristically as correct as any of the rest, the systems are not equivalent. Thus, the resulting numerical solutions will not be equal and it is natural to ask about the effects of these different initial conditions.

The linear system (2.33) is preferable to the nonlinear system (2.21) because of the ease of implementing solutions of linear systems as compared to that of implementing solutions of nonlinear systems. The nonlinear system (2.23) results from (2.21). We recast the solution of (2.23) as the solution of $\min_{\boldsymbol{\beta}_0} |\mathbf{f}(\boldsymbol{\beta}_0)|$, where $\mathbf{f}(\boldsymbol{\beta}_0) = G(\boldsymbol{\beta}_0) - \mathbf{f}_0$, and apply the robust and time-tested trust-region Newton's methods for solving unconstrained minimization problems. This general framework uses quadratic information about $\mathbf{f}$ in a way that progresses quickly when such information approximates $\mathbf{f}$ well, and safely when such information poorly models $\mathbf{f}$. It carries the optimal local convergence behavior of Newton's method (quadratic convergence) while precluding its ability to diverge. These methods require computation of first and second derivatives. Let $\mathcal{H} = \left(\frac{\partial}{\partial\beta_i}\frac{\partial\mathbf{f}}{\partial\beta_j}\right)_{i,j=0}^{N}$ be the Hessian matrix, the collection of second order derivatives of $\mathbf{f}$ with respect to the coefficients $\boldsymbol{\beta}$, arranged in the intuitive way. These methods avoid the requirement that $\mathcal{H}$ be positive definite that is required by line search methods that try to use quadratic information about $\mathbf{f}$. Hand computation of the first and second derivatives is tedious but manageable and error-prone. Automatic differentiation could be applied to corroborate hand-calculated and programmed derivatives (see chapter 6). Lastly, a good initial guess will help our method to quickly get into the local convergence behavior regime. Heuristically, the solution of (2.33) is a good initial guess. More on how to solve the unconstrained minimization problem can be learned from [12].

It is natural to compare the error in the solution resulting from (2.33) to the error in the solution resulting from (2.21), though we reserve such questions for future work. These comments also apply when the nonlinear system (2.35) is compared to the linear system (2.34). It is also natural to ask about the effects of using true initial free boundary data. We leave this study to future work as well.

Another warranted study with promise is to check whether an equivalence can be found between computing (2.21) using Gauss-Lobatto quadrature and computing (2.35) using Gauss quadrature with two less nodes, and similarly for (2.33) and (2.34). This seems reasonable since the smallest and largest Gauss-Lobatto quadrature nodes are the endpoints of the interval of integration [17, 8].

One can also modify the problem (2.3) so that the initial interface data, $\Xi(0)$, is used. Recall that $\tilde{z}_0(x) = \tilde{z}(x, 0)$. Analogous to (2.31) and (2.32), we define $\tilde{w}_0 \in \Pi_{N-2}$ and w_0:

$$u_0(x) = (\xi_r(0) - x)(x - \xi_\ell(0))\, w_0(x), \tag{2.36}$$

$$\tilde{z}_0(x) = (\xi_r(0) - x)(x - \xi_\ell(0))\, \tilde{w}_0(x).$$

We thus modify (2.3) so that the initial interface data is used:

Find $\tilde{z}_0 \in \Pi_N$ such that

$$(w_0 - \tilde{w}_0, \phi_i)_{\Xi(0)} = 0, \tag{2.37}$$

$i = 0, \ldots, N-2$.

We close this section by discussing properties of model 2.

One can view this choice of the form of the trial solution $\tilde{u}$ as being the sG solution to a straightforward application of the sG method to the PE. Precisely, consider the following sG method:

Find $V(x,t) = \sum_{j=0}^{N} \eta_j(t)\, \phi_j(x)$ such that

$$\left(V_t - (m-1)\, V V_{xx} - V_x^2,\, \phi_i\right)_{\widetilde{\Omega}(t)} = 0, \tag{2.38}$$

for $i = 0, \ldots, N$, $\{\phi_i\}_{i=0}^{N}$ as before, and $\widetilde{\Omega}(t)$ is the support of V, which we assume to be compact. Then one can show that $V = \frac{m}{m-1}\tilde{u}^{m-1}$ with $\eta_i(t) = \frac{m}{m-1}\beta_i(t)$, for $i = 0, \ldots, N$, where $\{\beta_i\}_{i=0}^{N}$ is from (2.19). To see this suppose $V(x,t) = \sum_{j=0}^{N} \eta_j(t)\,\phi_j(x)$ that satisfies (2.38) is written as $V = \frac{m}{m-1}\tilde{v}^{m-1}$, then

$$
\begin{aligned}
0 &= \left(V_t - (m-1)\,VV_{xx} - V_x^2, \phi_i\right)_{\tilde{\Omega}(t)} \\
&= \left(m\tilde{v}^{m-2}\tilde{v}_t - (m-1)\,\frac{m}{m-1}\tilde{v}^{m-1}\left(m\tilde{v}^{m-2}\tilde{v}_x\right)_x - \left(m\tilde{v}^{m-2}\tilde{v}_x\right)^2, \phi_i\right)_{\tilde{\Omega}(t)} \\
&= \left(m\tilde{v}^{m-2}\tilde{v}_t - m^2\tilde{v}^{m-1}\left((m-2)\,\tilde{v}^{m-3}\tilde{v}_x^2 + \tilde{v}^{m-2}\tilde{v}_{xx}\right) - m^2\tilde{v}^{2m-4}\tilde{v}_x^2, \phi_i\right)_{\tilde{\Omega}(t)} \\
&= \left(m\tilde{v}^{m-2}\tilde{v}_t - m^2\left((m-2)\,\tilde{v}^{2m-4}\tilde{v}_x^2 + \tilde{v}^{2m-3}\tilde{v}_{xx} + \tilde{v}^{2m-4}\tilde{v}_x^2\right), \phi_i\right)_{\tilde{\Omega}(t)} \\
&= \left(m\tilde{v}^{m-2}\tilde{v}_t - m\tilde{v}^{m-2}\left(m\,(m-1)\,\tilde{v}^{m-2}\tilde{v}_x^2 + m\tilde{v}^{m-1}\tilde{v}_{xx}\right), \phi_i\right)_{\tilde{\Omega}(t)} \\
&= \left(m\tilde{v}^{m-2}\left(\tilde{v}_t - m\,(m-1)\,\tilde{v}^{m-2}\tilde{v}_x^2 - m\tilde{v}^{m-1}\tilde{v}_{xx}\right), \phi_i\right)_{\tilde{\Omega}(t)} \\
&= \left(m\tilde{v}^{m-2}\left(\tilde{v}_t - (\tilde{v}^m)_{xx}\right), \phi_i\right)_{\tilde{\Omega}(t)}
\end{aligned}
$$

which is true if and only if $\tilde{v}$ satisfies (1.5). So, $\tilde{v}$ is $\tilde{u}$ from (2.18)-(2.19), if $\eta_i(t) = \frac{m}{m-1}\beta_i(t)$, for $i = 0, \ldots, N$. It should be noted, however, that a different numerical solution would result from using (2.38).

One benefit of this model is that the model solution (2.18)-(2.19) exactly captures the Barenblatt-Pattle solution of equation (1.6):

$$B(x,t) = p^{1/(m-1)}(x,t), \tag{2.39}$$

for $x \in \Xi(t)$. E.g. if $\{\phi_i\}_{i=0}^{N}$ in (2.19) is the standard basis, $\beta_0(t) = At^{-(m-1)/(m+1)}$, $\beta_1(t) = 0$, $\beta_2(t) = -Ct^{-1}$, and $\beta_j(t) = 0$, for $j \geq 3$, in terms of the constants from (1.6). This also happens to be a handicap, too, since it robs us of the only known solution in our class of initial profiles to test against. To remedy this we consider the EUF IVP (1.8)-(1.9) for numerical experimentation (see chapter 4).

As was the case for the method of the previous section, this method does not need to take into account boundary conditions in order to fulfill them. Numerical experiments (see chapter 4) suggest that, when numerical solutions behave well, (2.20) is enough to guarantee that the numerical solutions have free boundaries.

As with model 1 and solutions of (1.1), model 2 conserves the zeroth and first moments. The proofs for model 1 carry through for model 2, except that one must now use slightly more detail to see that $(m\tilde{u}^{m-1}\tilde{u}_x)\left(\tilde{\xi}(t), t\right) = 0$. Under model 2, $m\tilde{u}^{m-1}\tilde{u}_x = \frac{m}{m-1}p^{1/(m-1)}p_x$, so $(m\tilde{u}^{m-1}\tilde{u}_x)\left(\tilde{\xi}(t), t\right) = (m\tilde{u}^{m-1}\tilde{u}_x)\left(\tilde{\xi}(t), t\right)\dot{\tilde{\xi}}(t) = 0$, as well.

Note that as $x \to \tilde{\xi}_r(t)^-$ and as $x \to \tilde{\xi}_\ell(t)^+$, $p \downarrow 0$, so we should justify that such apparent singularities as $p^{1/(m-1)-1}$ in (2.24) and (2.27) are integrable when $m > 2$. We appeal to corollary A.1 and lemma A.6 to show that these integrals are indeed well-defined.

Let us consider the integrand in (2.25) from a computational point of view. For $m = 2$, the exponent $z(m) = 1/(m-1) - 1 = 0$, so H can be computed without resorting to quadrature. Fix $m \neq 2$. In order to successfully integrate the $p^{z(m)}$ factors in (2.25) and (2.28), we should treat the singularities at the free boundaries carefully. To resolve this we calculate said integrals using a Gauss-Jacobi quadrature dependent on $z(m)$. For example, to compute (2.25), we instead compute

$$\int_{\widetilde{\Xi}(t)} \left(\tilde{\xi}_r(t) - x\right)^{z(m)} \left(x - \tilde{\xi}_\ell(t)\right)^{z(m)} f(x)\, \phi_i(x)\, \phi_j(x)\, dx,$$

with

$$f(x) = \left(\tilde{\xi}_r(t) - x\right)^{-z(m)} \left(x - \tilde{\xi}_\ell(t)\right)^{-z(m)} p^{z(m)}(x, t).$$

I.e. the Gauss-Jacobi quadrature parameters α and β are both $z(m)$. Recall that $p(x,t) > 0$ for $x \in \widetilde{\Xi}(t)$, i.e. such singularities in the interior of the numerical support do not exist. When $1 < m < 2$, Gauss-Legendre quadrature suffices, but numerical experiments suggest better results when Gauss-Jacobi quadrature is used in this case too.*

*This is another instance where we do not present numerical experiments. In this case, we omit the poor experiments that lead us to consider using more accurate quadrature methods.

2.2 Bases

We now discuss the effects of the choice of basis functions for the space of test and trial functions for the problem (2.2)-(2.3), $\{\phi_i\}_{i=0}^{N}$. Let $\Omega \subseteq \mathbb{R}$. We will say that a basis $\{\phi_i\}_{i=0}^{N}$ is *orthogonal on* Ω if $(\phi_i, \phi_j)_\Omega := \int_\Omega \phi_i(x)\,\phi_j(x)\,dx = c_i\delta_{i,j}$, for some nonzero constants $\{c_i\}_{i=0}^{N}$, for $i, j = 0, \ldots, N$. The comments in the below sections apply equally to the solution of (2.20), (2.34). We will see that computational concerns guide us from a naive starting point to our ultimate choice of basis functions.

2.2.1 The standard basis

When the standard basis is used for $\{\phi_i\}_{i=0}^{N}$ the resulting method is called the *method of moments*. This choice yields a mass matrix H that is Hankel, i.e. $H(i,j) = R(i+j)$ for some function R [39]. For model 1 we get the well-known, highly ill-conditioned Hilbert matrix [39]. But a similarly ill-conditioned Hankel system results if we use the method of moments for model 2. According to Tyrtyshnikov [38], Hankel matrices have spectral condition numbers bounded below by $3 \cdot 2^{N-5}$. Despite this, we get good results as $N \to \infty$, though there is a value for N where the ill-conditioned nature of such matrices makes accurate numerical resolution impossible. This will be discussed further in chapter 4. The obvious choice is to use an orthogonal basis.

2.2.2 The traditional Legendre basis

It is well-known that the approximation of non-periodic functions on a finite interval is best achieved by eigenfunctions of a singular Sturm-Liouville problem

The experiments presented in chapter 4 use the more accurate quadrature methods.

[5, 13, 17, 37, 8]. The Barenblatt-Pattle solution illustrates that this is the case with solutions of the PME. It is for this reason that we consider Legendre basis functions. Such functions need to be defined on the interval on which they are expected to be orthogonal. Suppose we set our basis functions $\{\phi_i\}_{i=0}^N$ to be Legendre basis functions that are orthogonal on $\Xi(0)$:

$$\phi_i(x) = P_i(y(x)),$$

where

$$y(x) = \left(\frac{\xi_r(0) - \xi_\ell(0)}{2}\right)^{-1}\left(x - \frac{\xi_r(0) + \xi_\ell(0)}{2}\right),$$

$$(P_i, P_j)_I = \frac{2}{2i+1}\delta_{i,j},$$

$(f, g)_I = \int_I f(x)\, g(x)\, dx$, and $I = [-1, +1]$, for $i, j = 0, \ldots, N$. ($\{P_i\}_{i=0}^N$ are the standard Legendre polynomials orthogonal on I . These are available on most computing platforms.) Time-stepping methods for (2.14) or (2.30) must compute inner products defined on $\tilde{\Xi}(t)$, $t > 0$. The orthogonality of this basis is of extremely limited use since $\{\phi_i\}_{i=0}^N$ is not orthogonal on $\tilde{\Xi}(t)$. As we will see shortly, the situation is actually worse.

One might try to remedy the limited applicability of the previously described basis by constructing a basis that is orthogonal at the start of *any* time step. For instance, suppose that times $t = t_i$, $i = 0, \ldots, k$, are times at which (2.2)-(2.3) has been numerically integrated, and that we will now step to time $t = t_{k+1}$. Let

$$y_k(x) = \left(\frac{\tilde{\xi}_r(t_k) - \tilde{\xi}_\ell(t_k)}{2}\right)^{-1}\left(x - \frac{\tilde{\xi}_r(t_k) + \tilde{\xi}_\ell(t_k)}{2}\right),$$

then $\{P_i(y_k(x))\}_{i=0}^N$ is an orthogonal set on $\tilde{\Xi}(t_k)$. We change coordinates of our solution at time t_k with respect to $\{P_i(y_{k-1}(x))\}_{i=0}^N$, $\{\beta_{k-1,i}(t_k)\}_{i=0}^N$, into coordinates of our solution at time t_k with respect to $\{P_i(y_k(x))\}_{i=0}^N$, $\{\beta_{k,i}(t_k)\}_{i=0}^N$. We now step forward to time t_{k+1}. These bases are better than the single basis of

Legendre polynomials orthogonal on $\Xi(0)$, though all the bases considered in this section suffer from a more subtle problem that we discuss in the next section.

2.2.3 Computational domains

We now carefully examine the difference between the analytical expressions that set forth our methods and what is actually computed. Here we will find what causes the basis from the last section to fail in numerical experiments.

Analytically, solutions of (2.2)-(2.3) are defined on $\widetilde{\Xi}$. Through the following construction, we now describe the computational domain on which our solutions are computed, $\widehat{S}$. We will write $\widehat{\Xi}(t)$ for $\left(\hat{\xi}_\ell(t), \hat{\xi}_r(t)\right)$, where $\hat{\xi}$ denotes an approximation to $\tilde{\xi}$ found via a numerical root finding routine.† Let $t_0 = 0$, k be the step size, and $\widehat{\Xi}(0) = \Xi(0)$.‡ For the first step, we solve the IVP ODE arising from (2.2)-(2.3) on $[0, t_1]$ and set $\widehat{S}_0 = \widehat{\Xi}(0) \times [0, t_1]$, where $t_1 = k$. This yields $\{\beta_j(t_1)\}_{j=0}^N$ in (2.1) which we use to find the support of $\tilde{z}(x, t_1)$: $\widehat{\Xi}(t_1)$. If a change in basis is required, we do that at this point. Next solve (2.2) with IC given by $\{\beta_j(t_1)\}_{j=0}^N$ on $(t_1, t_2]$ and set $\widehat{S}_1 = \widehat{\Xi}(t_1) \times (t_1, t_2]$, where $t_2 = 2k$.

Now suppose that, for each $i = 1, ..., n-1$, we have solved (2.2) on $(t_i, t_{i+1}]$, where $t_{i+1} = (i+1)k$ and have set $\widehat{S}_i = \widehat{\Xi}(t_i) \times (t_i, t_{i+1}]$. We now construct $\widehat{S}_n$. We use $\{\beta_j(t_n)\}_{j=0}^N$ in (2.1) to find $\widehat{\Xi}(t_n)$. If a change in basis is required, we do that at this point. Now we solve (2.2) on $(t_n, t_{n+1}]$, where $t_{n+1} = (n+1)k$, and set $\widehat{S}_n = \widehat{\Xi}(t_n) \times (t_n, t_{n+1}]$. We continue until we reach $t = T$. This process defines the truncated domain $\widehat{S}$:

$$\widehat{S} := \bigcup \widehat{S}_i. \tag{2.40}$$

†The methods in this work all rely on algorithms to find the boundary of the support of $\tilde{z}(x, t)$ given $\{\beta_j(t)\}_{j=0}^N$. For all the methods contained in this work, this amounts to finding the roots of the polynomial with coefficients $\{\beta_j(t)\}_{j=0}^N$. Except when we discuss the computational workload of our methods, we omit the details of this procedure.

‡For the sake of simplicity, suppose the step size is constant.

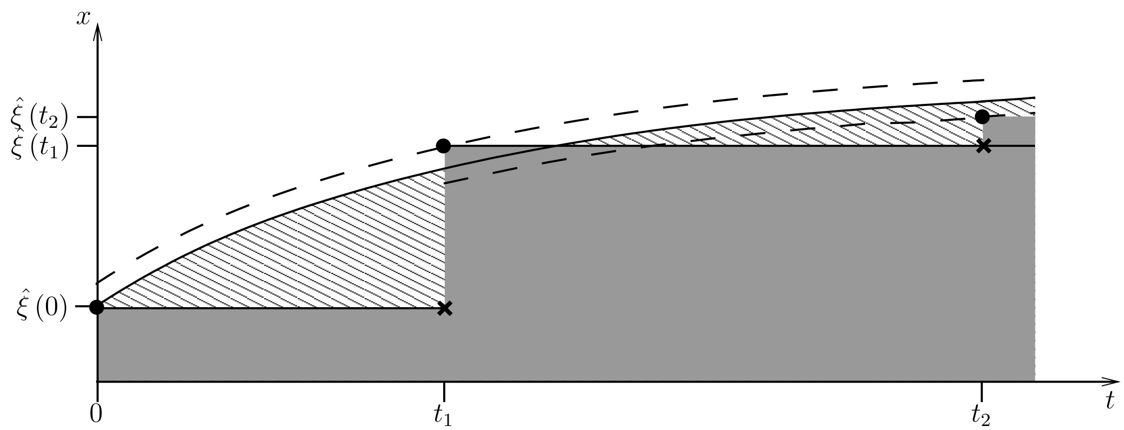

Figure 2.3: Sketch of domains $\widehat{S}$ (shaded), $\widetilde{\widetilde{\Xi}}$ (diagonal-, cross-hatched), and free boundaries of "nearby" solutions (large dashes).

Figure 2.3 shows a typical $\widehat{S}$.

One advantage of using $\widehat{S}$ is that we are computing in the interior of $\widetilde{\widetilde{\Xi}}$, or as near to the interior of $\widetilde{\widetilde{\Xi}}$ as this method allows. Heuristically, our solutions should always be positive in our computing domain since we approximating functions that are positive in their support, Ξ.

Defining our inner products on the interior of the support of u has potential disadvantages for future considerations. Suppose we wanted to handle the joining densities situation illustrated in figure 1.2. Apparently, using this myopic, local view prevents the method "seeing" another density approaching without using some artificial machinery. If we advance the numerical solutions of two disjoint densities, although these two densities must join, as they are each independent of the other, neither will ever suspect the existence of the other. The same deficiency would arise if such a density approached some obstacle, some fixed object, like a insulated wall, that imposes external conditions on our solution.

Numerical experiments with the sequence of Legendre bases orthogonal on the domain at the start of a time step and the computational domain $\widehat{S}$ suggest that time-stepping in this computational regime is unstable. The instability manifests as in remark 2.2. (See figure 2.2). One possible explanation is connected to the domain where we evaluate the orthogonal polynomials.

Suppose that we are at time step t_i and are stepping to time step t_{i+1}. Time stepping routines will need to evaluate the expressions defining our methods for $t \in (t_i, t_{i+1}]$.[§] Let $t \in (t_i, t_{i+1}]$. Using $\widehat{S}$ to evaluate the expressions defining our methods, e.g. inner products defined on $\widetilde{\Xi}(t)$, means that we must evaluate powers or derivatives of expressions like

$$\sum_{j=0}^{N} \beta_j(t)\, \phi_j(x) \tag{2.41}$$

for $x \in \widetilde{\Xi}(t)$. The orthogonal polynomials $\{\phi_i(x)\}_{i=0}^{N}$ in these expressions are orthogonal on $\widehat{\Xi}(t_i)$ and are bounded by one in absolute value for $x \in \widehat{\Xi}(t_i)$. Following from the fact that the roots of each ϕ_i are in $\widehat{\Xi}(t_i)$ [34], $\{\phi_i(x)\}_{i=0}^{N}$ are not bounded in absolute value by one for $x \notin \widehat{\Xi}(t_i)$ as $|x| \to \infty$. In fact, for $x \in \widetilde{\Xi}(t) \setminus \widehat{\Xi}(t_i)$, $\phi_N(x) \to \infty$ as $N \to \infty$. Of course, $|\phi_i(x)| \to \infty$ as $|x| \to \infty$, for fixed $i \in \{0, \ldots, N\}$.

In the next subsection we construct a basis orthogonal on an approximation of $\widetilde{\Xi}(t_{i+1})$, $\breve{\Xi}(t_{i+1})$, for which the containment $\breve{\Xi}(t_{i+1}) \supseteq \widetilde{\Xi}(t)$ holds heuristically. Using this basis ameliorates the situation in practice: we observe stable time-stepping.

[§]Some methods may require $t \in (\tilde{t}_i, \tilde{t}_{i+1}] \supset (t_i, t_{i+1}]$. If implicit methods are used to step in time $\tilde{t}_{i+1} > t_{i+1}$.

2.2.4 The Legendre basis orthogonal with respect to a modified inner product: *the modified Legendre basis*

To guarantee that key computational expressions like (2.41) are evaluated accurately we aim to ensure that $|\phi_i(x)| < 1$ for $t \in (t_i, t_{i+1}]$ and $x \in \widetilde{\breve{\Xi}}(t)$. To do this we approximate $\widetilde{\breve{\Xi}}(t_{i+1})$ and perform computations using a basis that is orthogonal on this approximate support.

We use a differential equation to construct an approximation of $\widetilde{\breve{\Xi}}(t_{i+1})$. Knerr [22] proved that the true free boundaries satisfy the differential equation

$$\xi'(t) = -v_x(\xi(t), t), \tag{2.42}$$

where $v = \frac{m}{m-1}u^{m-1}$, the derivative is a one-sided derivative defined on $\Xi(t)$, and $v_x(\xi(t), t) = \lim_{x\to\xi(t)} v_x(x, t)$, for $x \in \Xi(t)$. We use (2.42) to construct an estimate of $\widetilde{\breve{\Xi}}$, $\breve{S}$. The formal construction of this approximation closely follows that of $\widehat{S}$ except now we show the construction for (2.20), (2.34). The construction for (2.2)-(2.3) or (2.2)-(2.37) is analogous.

We will write $\breve{\Xi}(t)$ for $\left(\breve{\xi}_\ell(t), \breve{\xi}_r(t)\right)$ and $\widehat{\Xi}(t)$ for $\left(\hat{\xi}_\ell(t), \hat{\xi}_r(t)\right)$. Let $t_0 = 0$, k be the constant time step size, and $\hat{\Xi}(0) = \Xi(0)$.

We solve (2.42) on $[0, t_1]$ using Euler's method, where $t_1 = k$. This yields $\breve{\Xi}(t_1)$. We change bases for $\tilde{u}^{m-1}(x,0)$ in (2.18)-(2.19) from coordinates in the Legendre basis orthogonal on $\widehat{\Xi}(0)$ to coordinates in the Legendre basis orthogonal on $\breve{\Xi}(t_1)$. We solve the system of differential equations (2.20), (2.34) on $[0, t_1]$ and set $\breve{S}_0 = \breve{\Xi}(t_1) \times [0, t_1]$. This yields $\left\{\breve{\beta}_j(t_1)\right\}_{j=0}^{N}$ in (2.18)-(2.19) where $\{\phi_j\}_{j=0}^{N}$ are orthogonal on $\breve{\Xi}(t_1)$. We use $\left\{\breve{\beta}_j(t_1)\right\}_{j=0}^{N}$ to find $\widehat{\Xi}(t_1)$.¶ At this point we perform the administrative task of finding and storing appropriate coordinates: we change from coordinates of our solution at time t_1 with respect to the basis orthogonal on

¶As mentioned above, this is done by finding roots of a polynomial. We discuss the method for finding the roots in chapter 5.

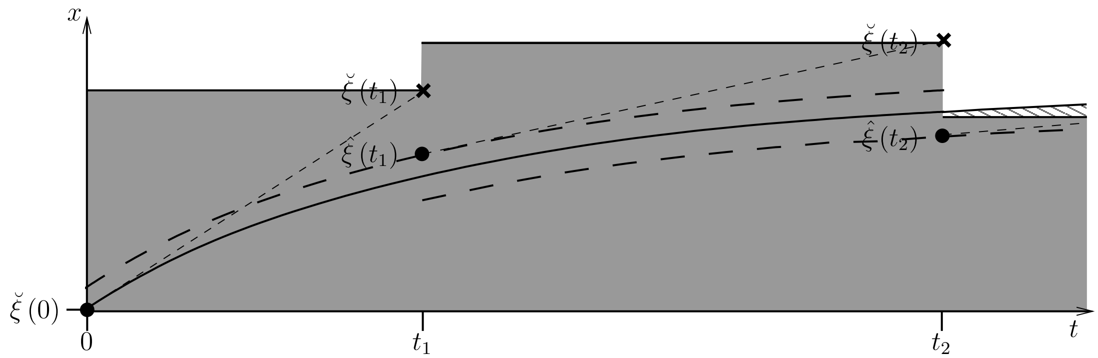

Figure 2.4: Sketch of domains $\breve{S}$ (shaded), $\widetilde{\Xi}$ (diagonal-, cross-hatched, and barely visible), free boundaries of "nearby" solutions (large dashes), and numerical Euler trajectories (small dashes).

$\breve{\Xi}(t_1)$, $\left\{\breve{\beta}_j(t_1)\right\}_{j=0}^{N}$, to coordinates of our solution at time t_1 with respect to the basis orthogonal on $\widehat{\Xi}(t_1)$, $\{\beta_j(t_1)\}_{j=0}^{N}$. We store $\widehat{\Xi}(t_1)$ and $\{\beta_j(t_1)\}_{j=0}^{N}$.

Suppose that, for $i = 1, \ldots, n-1$, we have solved (2.42) on $(t_i, t_{i+1}]$ using Euler's method to get $\breve{\Xi}(t_{i+1})$; changed bases for $\tilde{u}^{m-1}(x, t_i)$ in (2.18)-(2.19) from coordinates in the Legendre basis orthogonal on $\widehat{\Xi}(t_i)$ to coordinates in the Legendre basis orthogonal on $\breve{\Xi}(t_{i+1})$; found $\left\{\breve{\beta}_j(t_{i+1})\right\}_{j=0}^{N}$ in (2.18)-(2.19) by solving the system of differential equations (2.20) on $(t_i, t_{i+1}]$; set $\breve{S}_i = \breve{\Xi}(t_{i+1}) \times (t_i, t_{i+1}]$; found $\widehat{\Xi}(t_{i+1})$; and changed from coordinates of our solution at time t_{i+1} with respect to the basis orthogonal on $\breve{\Xi}(t_{i+1})$ to coordinates of our solution at time t_{i+1} with respect to the basis orthogonal on $\widehat{\Xi}(t_{i+1})$. We repeat this process until we reach $t = T$. This process defines the truncated domain $\breve{S}$:

$$\breve{S} := \bigcup \breve{S}_i. \tag{2.43}$$

Figure 2.4 shows a schematic of one possible $\breve{S}$.

The sequence of bases that are orthogonal on $\breve{\Xi}(t_{i+1})$ that are used for computations (for $t \in (t_i, t_{i+1}]$) will be denoted by the symbol g_i and will be called *the modified Legendre basis*:

$\{g_i\}_{i=0}^{N}$ are such that

$$\int_{\breve{\Xi}(t_{i+1})} g_i(x)\, g_j(x)\, dx = \delta_{i,j}. \tag{2.44}$$

They are related to the standard Legendre polynomials $\{P_i\}_{i=0}^{N}$ that are standard in most computing platforms through

$$g_i(x) = c_i^{-1/2} \left(\frac{\breve{\xi}_r(t_{k+1}) - \breve{\xi}_\ell(t_{k+1})}{2} \right)^{-1/2} P_i(y(x)), \tag{2.45}$$

where $c_i = \frac{2}{2i+1}$, and

$$y(x) = \left(\frac{\breve{\xi}_r(t_{k+1}) - \breve{\xi}_\ell(t_{k+1})}{2} \right)^{-1} \left(x - \frac{\breve{\xi}_r(t_{k+1}) + \breve{\xi}_\ell(t_{k+1})}{2} \right) \tag{2.46}$$

for $i = 0, \ldots, N$. Note that the bases and corresponding coefficients are not those related to the free boundary $\widehat{\Xi}(t_{i+1})$ computed during the administrative stage of each time step.

Note that time-stepping algorithms will compute expressions as in (2.41) for $t \neq t_{i+1}$, consequently even the benefit of diagonal matrices is lost. For example,

$$\int_{\breve{\Xi}(t)} g_i(x)\, g_j(x)\, dx \neq d_i \delta_{i,j},$$

for $i = 0, \ldots, N$, for any sequence of constants $\{d_i\}_{i=0}^{N}$.

Though neither the basis orthogonal on $\widehat{\Xi}(t_i)$ nor the basis orthogonal on $\breve{\Xi}(t_{i+1})$, the modified Legendre basis, makes the H matrices (2.8) or (2.24) diagonal, their condition numbers are greatly improved when the modified Legendre basis is used. More importantly, when the modified Legendre basis is used the time-stepping computations are stable.

In practice we find $\breve{\Xi}(t_{i+1})$ by taking an Euler step. A more complex method for finding $\breve{\Xi}(t_{i+1})$–one that uses information at intermediate times $t \in (t_i, t_{i+1}]$ and would hence require multiple stages or a fixed-point iteration–would necessarily couple the free boundary differential equation (2.42) with the ansatz system (2.20).

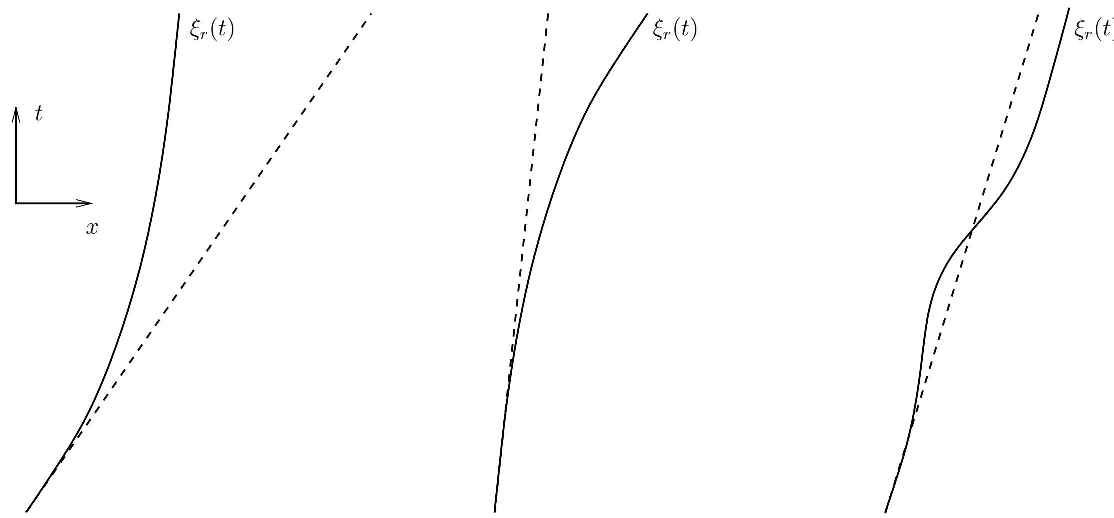

Figure 2.5: Various free boundary curves $\xi_r\,(t)$ (solid) and the associated Euler trajectories (dashed), for $t \in (t_i,\, t_{i+1}]$. The leftmost pictured free boundary curve has $\xi_r''\,(t_i) < 0$, the middle free boundary curve has $\xi_r''\,(t_i) > 0$, while the rightmost free boundary curve has $\xi_r''\,(t_i) < 0$. In the rightmost curve, k is too big, though, so that $\breve{\Xi}\,(t_{i+1}) \not\supseteq \Xi\,(t_i)$. Benilan et al. [3] showed that the middle case cannot occur.

However, this is not necessary: numerical experiments show that no improvement in the error results when the true free boundary, ξ, is used rather than using the free boundary differential equation (2.42) to estimate it. This makes sense since the purpose of using the free boundary differential equation (2.42) is not to accurately approximate the $\widetilde{\Xi}\,(t_{i+1})$, but to try to get some wiggle room about $\widetilde{\Xi}\,(t)$, $t \in (t_i,\, t_{i+1}]$. Consequently, this method should be sufficient as long as

$$\breve{\Xi}\,(t_{i+1}) \supseteq \widetilde{\Xi}\,(t_{i+1})\,, \tag{2.47}$$

which seems to be true though we cannot guarantee it. Heuristically, we have some reasonable expectation that (2.47) holds because of what happens in the true solution. Benilan et al. [3] shows that $\xi_r''\,(t) < 0$ and $-\xi_\ell''\,(t) < 0$, which means that $\xi_r\,(t)$ and $-\xi_\ell\,(t)$ are concave down. It is when $\xi_r\,(t)$ and $-\xi_\ell\,(t)$ are concave down that the Euler step overestimates $\xi_r\,(t+k)$ and $-\xi_\ell\,(t+k)$, for small enough k (see figure 2.5).

CHAPTER 3

CONTRACTION TO THE BARENBLATT-PATTLE SOLUTION

We wish now to prove that small perturbations of Barenblatt-Pattle solutions converge to Barenblatt-Pattle solutions under our semi-discrete computational scheme (2.22) using the standard basis, just as solutions to the PME converge to a Barenblatt-Pattle solution.

Recall that our system

$$H\boldsymbol{\beta}' = \mathbf{f}\left(\boldsymbol{\beta},\, t\right)$$

can be rewritten as

$$\boldsymbol{\beta}' = \mathbf{g}\left(\boldsymbol{\beta},\, t\right) \tag{3.1}$$

where $\mathbf{g}\left(\boldsymbol{\beta},\, t\right) = H^{-1}\mathbf{f}\left(\boldsymbol{\beta},\, t\right)$. Let $\boldsymbol{\beta}^{*}$ be the coefficients of the Barenblatt-Pattle with respect to this basis, and let $\varepsilon > 0$ be small. Let $\boldsymbol{\beta}$ be a solution of (3.1) that can be represented as a small perturbation of $\boldsymbol{\beta}^{*}$, i.e. $\boldsymbol{\beta} = \boldsymbol{\beta}^{*} + \boldsymbol{\delta}$, where $\|\boldsymbol{\delta}\| < \varepsilon$. If we expand the right-hand side of (3.1) in a Taylor series about $\boldsymbol{\beta}^{*}$, we get that

$$\mathbf{g}\left(\boldsymbol{\beta},\, t\right) = \mathbf{g}\left(\boldsymbol{\beta}^{*},\, t\right) + \frac{\partial}{\partial\boldsymbol{\beta}}\mathbf{g}\left(\boldsymbol{\beta}^{*},\, t\right)\boldsymbol{\delta} + o\left(\|\boldsymbol{\delta}\|\right).$$

Then, a first-order approximation is

$$\begin{aligned}
\boldsymbol{\delta}' &= \frac{d}{dt}\boldsymbol{\beta} - \frac{d}{dt}\boldsymbol{\beta}^{*} \\
&= \mathbf{g}\left(\boldsymbol{\beta},\, t\right) - \mathbf{g}\left(\boldsymbol{\beta}^{*},\, t\right) \\
&= \frac{\partial}{\partial\boldsymbol{\beta}}\mathbf{g}\left(\boldsymbol{\beta}^{*},\, t\right)\boldsymbol{\delta}.
\end{aligned}$$

In chapter A we show the calculations needed to show that $\partial\mathbf{g}\left(\boldsymbol{\beta},\, t\right)/\partial\boldsymbol{\beta}$ exists; the results of chapter A are summarized in chapter B. Below we show that the eigenvalues of $\partial\mathbf{g}\left(\boldsymbol{\beta}^{*},\, t\right)/\partial\boldsymbol{\beta}$ are all negative. Our first-order approximation then shows that such perturbations from a Barenblatt-Pattle solution decay to the Barenblatt-Pattle solution. First we show that $\mathbf{g}\left(\boldsymbol{\beta}^{*},\, t\right)$ has a special form.

3.1 Derivative of semi-discrete system for the Barenblatt-Pattle solution

In the following we write the Barenblatt solution (2.39) as $B\left(x,\, t\right) = p\left(x,\, t\right)^{1/(m-1)}$, $p\left(x,\, t\right) = a - cx^2$, where $a = At^{-(m-1)/(m+1)}$, A is a constant, $c = Ct^{-1}$, and $C = \left(m-1\right)/\left(2m\left(m+1\right)\right)$.

Theorem 3.1. *Let the basis for each of the trial and test functions be the standard basis and let the trial solution be as in model* 2 (2.18)-(2.19)*. The derivative,* $\mathbf{g}$*, in the semi-discrete system* (3.1) *has only two nonzero components in the case of the Barenblatt solution. The form of the derivative is*

$$\mathbf{g} = \left(-2mca,\, 0,\, \frac{2m\left(m+1\right)}{m-1}c^2,\, 0,\, \ldots,\, 0\right)^T \tag{3.2}$$

Proof. By corollary A.2 and corollary A.3, H and $\mathbf{f}$ are well-defined. Plugging (3.2) into

$$H\boldsymbol{\beta}' = \mathbf{f}$$

using (B.1) and (B.6) gives the result with a few algebraic manipulations. We need to show that

$$-2mca\int_{\xi_\ell}^{\xi_r}\frac{1}{m-1}p^{\frac{1}{m-1}-1}\left(x\right)x^i\,dx + \frac{2m\left(m+1\right)}{m-1}c^2\int_{\xi_\ell}^{\xi_r}\frac{1}{m-1}p^{\frac{1}{m-1}-1}\left(x\right)x^{i+2}\,dx = \int_{\xi_\ell}^{\xi_r}\left(\frac{m}{\left(m-1\right)^2}p^{\frac{1}{m-1}-1}\left(x\right)p_x^2\left(x\right) + \frac{m}{m-1}p^{\frac{1}{m-1}}\left(x\right)p_{xx}\left(x\right)\right)x^i\,dx$$

Or, that $m/\left(m-1\right)\int_{\xi_\ell}^{\xi_r}p^{1/(m-1)}\left(x\right)x^i f\left(x\right)\,dx = 0$, where

$$f\left(x\right) = -2ca + 2\left(m+1\right)/\left(m-1\right)c^2x^2 - 1/\left(m-1\right)p_x^2\left(x\right) - p\left(x\right)p_{xx}\left(x\right).$$

It is clear that $f(x) \equiv 0$:

$$
\begin{aligned}
f(x) &= -2ca + \frac{2(m+1)}{m-1}c^2x^2 - \frac{1}{m-1}(-2cx)^2 - \left(a - cx^2\right)(-2c) \\
&= -2ca + \frac{2(m+1)}{m-1}c^2x^2 - \frac{4c^2}{m-1}x^2 + 2ca - 2c^2x^2 \\
&= 2\left(\frac{m+1}{m-1} - \frac{2}{m-1} - 1\right)c^2x^2 \equiv 0.
\end{aligned}
$$

■

3.2 Jacobian is upper triangular for the Barenblatt-Pattle: case I

Though the result is true for all $m > 1$, we state the result and organize the proofs in two cases: $1 < m \leq 2$ and $m > 2$, since the case $m > 2$ is much more difficult to establish than the case $1 < m \leq 2$.

Theorem 3.2. *Let $1 < m \leq 2$. In the case of the Barenblatt solution, the Jacobian of $\mathbf{g}$ is upper triangular and banded with bandwidth of three and one entirely zero superdiagonal in the band. To be specific, the form of the Jacobian is*

$$
\frac{\partial \mathbf{g}}{\partial \boldsymbol{\beta}} = \begin{bmatrix}
y(0,0) & 0 & y(0,2) & & & & & \\
 & y(1,1) & 0 & \ddots & & & & \\
 & & y(2,2) & \ddots & y(\ell-2,\ell) & & & \\
 & & & \ddots & 0 & \ddots & & \\
 & & & & y(\ell,\ell) & \ddots & y(N-2,N) & \\
 & & & & & \ddots & 0 & \\
 & & & & & & y(N,N) &
\end{bmatrix}, \tag{3.3}
$$

where

$$
y(\ell-2,\ell) \quad = \quad m\ell(\ell-1)\,a,\ \ell = 2,\ 3,\ ...,\ N, \tag{3.4}
$$

$$y\,(\ell,\,\ell) = -m\left(\ell^2 + \frac{5-m}{m-1}\ell + 2\right)c,\;\ell = 0,\,1,\,...,\,N, \tag{3.5}$$

Though we next state the theorem in the case $m > 2$, we prove this case in section 3.4.

Theorem 3.3. *Let $m > 2$. In the case of the Barenblatt-Pattle solution, the Jacobian of $\mathbf{g}$ is of the same as in theorem 3.2.*

Before the proof of theorem 3.2, we state an important corollary.

Corollary 3.1. *The eigenvalues of $\partial\mathbf{g}/\partial\boldsymbol{\beta}$ are all real and negative.*

Proof. Using the definition of $\partial\mathbf{g}/\partial\boldsymbol{\beta}$ in (3.3)-(3.5), we can easily read off the eigenvalues. They are obviously real. Recalling that $c > 0$, the eigenvalues are negative if we can establish that, for $m > 1$, $\ell^2 + \frac{5-m}{m-1}\ell + 2 > 0$. We establish this fact now.

If $1 < m < 5$, $\ell^2 + \frac{5-m}{m-1}\ell + 2 > 0$ for $\ell > 0$. Suppose $m \geq 5$. We can write $\ell^2 + \frac{5-m}{m-1}\ell + 2 = (\ell - \ell_1)(\ell - \ell_2)$, where $\ell_{1,\,2} \in \mathbb{C}$. Then

$$\ell_{1,\,2} = \frac{(m-5) \pm \sqrt{\Delta}}{2\,(m-1)},$$

where the discriminant $\Delta = -7m^2 + 6m + 17 = (m - m_1)(m - m_2)$, $m_1 = \frac{3-16\sqrt{2}}{7} \approx -1.1877$, and $m_2 = \frac{3+16\sqrt{2}}{7} \approx 2.0448$. This means that for $m \geq 5$, $\Delta < 0$, which means that $\ell_{1,\,2}$ are purely imaginary, which means that $\ell^2 + \frac{5-m}{m-1}\ell + 2$ has no real roots. So, $\ell^2 + \frac{5-m}{m-1}\ell + 2 > 0$, as needed.

■

Next we prove theorem 3.2.

Proof. We will use $\partial_\ell\,[\,\cdot\,]$ to mean $\partial\,[\,\cdot\,]\,/\partial\beta_\ell$, and $\partial\,[\,\cdot\,]$ if the dependence on the index is not useful or to mean the collection of first order derivatives with respect to $\boldsymbol{\beta}$. The idea of this proof is to plug expressions for ∂H, $\mathbf{g}$, H, $\partial\mathbf{g}$, and $\partial\mathbf{f}$ into

$$\frac{\partial H}{\partial\boldsymbol{\beta}}\mathbf{g} + H\frac{\partial\mathbf{g}}{\partial\boldsymbol{\beta}} = \frac{\partial\mathbf{f}}{\partial\boldsymbol{\beta}}, \tag{3.6}$$

from which the identity will fall out. The integrals defining ∂H, H, and $\partial \mathbf{f}$ are well-defined; to see why see subsection A.1.2 for ∂H, subsection A.1.1 for H, and subsection A.2.2 for ∂f. Define $\Delta_\ell = \partial_\ell H \mathbf{g} + H \partial_\ell \mathbf{g} - \partial_\ell \mathbf{f}$. We wish to show that $\Delta_\ell = 0$. We organize the calculations into cases based on m and ℓ. In each case, we will perform algebraic manipulations to arrive at the result. The case $m > 2$ requires more calculation and will therefore be handled separately.

Let $1 < m < 2$.

Let $\ell = 0$. Here we plug $\partial_0 H$ from (B.3), $\mathbf{g}$ from (3.2), H from (B.1), $\partial_0 \mathbf{g}$ from (3.3)-(3.5), and $\partial_0 \mathbf{f}$ from (B.7) into (3.6) to get

$$\begin{aligned}
\Delta_0 = &\left(\frac{2-m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\, x^i \, dx \right) (-2mca) \\
&+ \left(\frac{2-m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\, x^{i+2} \, dx \right) \left(\frac{2m(m+1)}{m-1} c^2 \right) \\
&+ \left(\frac{1}{m-1} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, x^i \, dx \right) (-2mc) \\
&- \frac{m(2-m)}{(m-1)^3} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\, p_x^2(x)\, x^i \, dx \\
&- \frac{m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, p_{xx}(x)\, x^i \, dx.
\end{aligned}$$

It is clear that $\Delta_0 = m/(m-1)\int_{\xi_\ell}^{\xi_r} p^{1/(m-1)-2}(x)\, x^i f(x)\,dx = 0$, since

$$\begin{aligned}
f(x) &= \frac{-2(2-m)ca}{m-1} + \frac{2(2-m)(m+1)}{(m-1)^2}c^2x^2 - 2cp(x) \\
&\quad - \frac{2-m}{(m-1)^2}p_x^2(x) - \frac{1}{m-1}p(x)\,p_{xx}(x) \\
&= \frac{-2(2-m)ca}{m-1} + \frac{2(2-m)(m+1)}{(m-1)^2}c^2x^2 \\
&\quad - 2cp(x) - \frac{2-m}{(m-1)^2}p_x^2(x) - \frac{1}{m-1}p(x)\,p_{xx}(x) \\
&= \frac{2-m}{m-1}\left(-2ca + \frac{2(m+1)}{m-1}c^2x^2 - \frac{1}{m-1}p_x^2(x)\right) \\
&\quad - p(x)\left(2c + \frac{1}{m-1}p_{xx}(x)\right) \\
&= \frac{2-m}{m-1}\left(-2ca + \frac{2(m+1)}{m-1}c^2x^2 - \frac{1}{m-1}(-2cx)^2\right) \\
&\quad - p(x)\left(2c + \frac{1}{m-1}(-2c)\right) \\
&= \frac{2-m}{m-1}\left(-2ca + 2c^2x^2\right) + 2c\left(\frac{1}{m-1} - 1\right)p(x) \\
&= -\frac{2(2-m)}{m-1}c\left(a - cx^2\right) + 2\frac{(2-m)}{m-1}cp(x) \equiv 0.
\end{aligned}$$

Let $\ell = 1$. Here we plug $\partial_1 H$ from (B.3), $\mathbf{g}$ from (3.2), H from (B.1), $\partial_1\mathbf{g}$ from (3.3)-(3.5), and $\partial_1\mathbf{f}$ from (B.7) into (3.6) to get

$$\begin{aligned}
\Delta_1 = &\left(\frac{2-m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\,x^{i+1}\,dx\right)(-2mca) \\
&+ \left(\frac{2-m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\,x^{i+3}\,dx\right)\left(\frac{2m(m+1)}{m-1}c^2\right) \\
&+ \left(\int_{\xi_\ell}^{\xi_r} \frac{1}{m-1}p^{\frac{1}{m-1}-1}(x)\,x^{i+1}\,dx\right)\left(-\frac{2m(m+1)}{m-1}c\right) \\
&- \frac{m(2-m)}{(m-1)^3}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\,p_x^2(x)\,x^{i+1}\,dx \\
&- \frac{2m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_x(x)\,x^i\,dx - \frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_{xx}(x)\,x^{i+1}\,dx
\end{aligned}$$

It is clear that $\Delta_1 = m/\left(m-1\right)^2 \int_{\xi_\ell}^{\xi_r} p^{1/(m-1)-2}\left(x\right) x^i f\left(x\right)\, dx = 0$, since

$$\begin{aligned}
f\left(x\right) &= -2\left(2-m\right)ca + \frac{2\left(2-m\right)\left(m+1\right)}{m-1}c^2x^2 \\
&\quad - 2\left(m+1\right)cp\left(x\right) - \frac{2-m}{m-1}p_x^2\left(x\right) \\
&\quad - 2p_N\left(x\right)p_x\left(x\right)x^{-1} - p\left(x\right)p_{xx}\left(x\right) \\
&= \left(2-m\right)\left(-2ca + \frac{2\left(m+1\right)}{m-1}c^2x^2 - \frac{1}{m-1}p_x^2\left(x\right)\right) \\
&\quad - p\left(x\right)\left(2\left(m+1\right)c + 2p_x\left(x\right)x^{-1} + p_{xx}\left(x\right)\right) \\
&= \left(2-m\right)\left(-2ca + \frac{2\left(m+1\right)}{m-1}c^2x^2 - \frac{1}{m-1}\left(-2cx\right)^2\right) \\
&\quad - p\left(x\right)\left(2\left(m+1\right)c + 2\left(-2cx\right)x^{-1} + \left(-2c\right)\right) \\
&= \left(2-m\right)\left(-2ca + 2c^2x^2\right) - p\left(x\right)\left(2-m\right)\left(-2c\right) \\
&= \left(2-m\right)\left(-2c\right)\left(a - cx^2\right) - p\left(x\right)\left(2-m\right)\left(-2c\right) \equiv 0
\end{aligned}$$

Let $\ell \geq 2$. Here we plug $\partial_\ell H$ from (B.3), $\mathbf{g}$ from (3.2), H from (B.1), $\partial_\ell \mathbf{g}$ from (3.3)-(3.5), and $\partial_\ell \mathbf{f}$ from (B.7) into (3.6) to get

$$\begin{aligned}
\Delta_\ell = &\left(\frac{2-m}{\left(m-1\right)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}\left(x\right)x^{i+\ell}\,dx\right)\left(-2mca\right) \\
&+ \left(\frac{2-m}{\left(m-1\right)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}\left(x\right)x^{i+\ell+2}\,dx\right)\left(\frac{2m\left(m+1\right)}{m-1}c^2\right) \\
&+ \left(\frac{1}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}\left(x\right)x^{i+\ell-2}\,dx\right)\left(m\ell\left(\ell-1\right)a\right) \\
&+ \left(\frac{1}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}\left(x\right)x^{i+\ell}\,dx\right)\left(-m\left(\ell^2 + \frac{5-m}{m-1}\ell + 2\right)c\right) \\
&- \frac{m\left(2-m\right)}{\left(m-1\right)^3}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}\left(x\right)p_x^2\left(x\right)x^{i+\ell}\,dx \\
&- \frac{2\ell m}{\left(m-1\right)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}\left(x\right)p_x\left(x\right)x^{i+\ell-1}\,dx \\
&- \frac{m}{\left(m-1\right)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}\left(x\right)p_{xx}\left(x\right)x^{i+\ell}\,dx \\
&- \frac{\ell\left(\ell-1\right)m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}\left(x\right)x^{i+\ell-2}\,dx.
\end{aligned}$$

It is clear that $\Delta_\ell = m/(m-1)\int_{\xi_\ell}^{\xi_r} p^{1/(m-1)-2}(x)\, x^{i+\ell} f(x)\, dx = 0$, since

$$\begin{aligned}
f(x) = &-\frac{2(2-m)}{m-1}ca + \frac{2(2-m)(m+1)}{(m-1)^2}c^2x^2 + \ell(\ell-1)\,ap(x)\,x^{-2} \\
&- \left(\ell^2 + \frac{5-m}{m-1}\ell + 2\right)cp(x) - \frac{2-m}{(m-1)^2}p_x^2(x) \\
&- \frac{2\ell}{m-1}p(x)\,p_x(x)\,x^{-1} - \frac{1}{m-1}p(x)\,p_{xx}(x) - \ell(\ell-1)\,p^2(x)\,x^{-2} \\
&= \frac{2-m}{m-1}\left(-2ca + \frac{2(m+1)}{m-1}c^2x^2 - \frac{1}{m-1}p_x^2(x)\right) \\
&+ p(x)\left(\ell(\ell-1)\,ax^{-2} - \left(\ell^2 + \frac{5-m}{m-1}\ell + 2\right)c\right) \\
&+ p(x)\left(-\frac{2\ell}{m-1}p_x(x)\,x^{-1} - \frac{1}{m-1}p_{xx}(x) - \ell(\ell-1)\,p(x)\,x^{-2}\right)
\end{aligned}$$

and

$$\begin{aligned}
f(x) = &\frac{2-m}{m-1}\left(-2ca + \frac{2(m+1)}{m-1}c^2x^2 - \frac{1}{m-1}(-2cx)^2\right) \\
&+ p(x)\left(\ell(\ell-1)\,ax^{-2} - \left(\ell^2 + \frac{5-m}{m-1}\ell + 2\right)c\right) \\
&p(x)\left(-\frac{2\ell}{m-1}(-2cx)\,x^{-1} - \frac{1}{m-1}(-2c) - \ell(\ell-1)\left(a - cx^2\right)x^{-2}\right) \\
&= \frac{2-m}{m-1}\left(-2ca + 2c^2x^2\right) \\
&+ p(x)\left(-\left(\ell^2 + \frac{5-m}{m-1}\ell + 2\right)c + \frac{4\ell c}{m-1} + \frac{2c}{m-1} + \ell(\ell-1)\,c\right) \\
&= -\frac{2(2-m)c}{m-1}\left(a - cx^2\right) \\
&+ cp(x)\left(-\ell^2 - \frac{5-m}{m-1}\ell - 2 + \frac{4\ell}{m-1} + \frac{2}{m-1} + \ell(\ell-1)\right) \\
&= -\frac{2(2-m)c}{m-1}p(x) + cp(x)\,\frac{2(2-m)}{m-1} \equiv 0
\end{aligned}$$

Let $m = 2$.

Let $\ell = 0$. Here we plug $\partial_0 H$ from (B.4), $\mathbf{g}$ from (3.2), H from (B.1), $\partial_0 \mathbf{g}$ from

(3.3)-(3.5), and $\partial_0 \mathbf{f}$ from (B.8) into (3.6) to get

$$\begin{aligned}
\Delta_0 &= \left(-\frac{\xi_r^i}{p_x(\xi_r)} + \frac{\xi_\ell^i}{p_x(\xi_\ell)}\right)(-4ca) + \left(-\frac{\xi_r^{i+2}}{p_x(\xi_r)} + \frac{\xi_\ell^{i+2}}{p_x(\xi_\ell)}\right)\left(12c^2\right) \\
&\quad + \left(\int_{\xi_\ell}^{\xi_r} x^i\,dx\right)(-4c) + 2\left(-2c\xi_r\right)\xi_r^i - 2\left(-2c\xi_\ell\right)\xi_\ell^i - 2\int_{\xi_\ell}^{\xi_r}(-2c)\,x^i\,dx \\
&= \left(-\frac{\xi_r^i}{-2c\xi_r} + \frac{\xi_\ell^i}{-2c\xi_\ell}\right)(-4ca) + \left(-\frac{\xi_r^{i+2}}{-2c\xi_r} + \frac{\xi_\ell^{i+2}}{-2c\xi_\ell}\right)\left(12c^2\right) - 4c\xi_r^{i+1} + 4c\xi_\ell^{i+1} \\
&= \left(-\xi_r^{i-1} + \xi_\ell^{i-1}\right)(2a) + \left(\xi_r^{i+1} - \xi_\ell^{i+1}\right)(6c) - 4c\xi_r^{i+1} + 4c\,(-1)^{i+1}\,\xi_r^{i+1} \\
&= \left(-1 + (-1)^{i-1}\right)2a\xi_r^{i-1} + \left(1 - (-1)^{i+1}\right)6c\frac{a}{c}\xi_r^{i-1} - \left(1 - (-1)^{i-1}\right)4\frac{a}{c}\frac{a}{c}c\xi_r^{i-1} \\
&= -\left(1 - (-1)^{i-1}\right)2a\xi_r^{i-1} + \left(1 - (-1)^{i-1}\right)6a\xi_r^{i-1} - \left(1 - (-1)^{i-1}\right)4a\xi_r^{i-1} \\
&= \left(1 - (-1)^{i-1}\right)(0) = 0
\end{aligned}$$

Let $\ell = 1$. Here we plug $\partial_1 H$ from (B.4), $\mathbf{g}$ from (3.2), H from (B.1), $\partial_1 \mathbf{g}$ from (3.3)-(3.5), and $\partial_1 \mathbf{f}$ from (B.8) into (3.6) to get

$$\begin{aligned}
\Delta_1 &= \left(-\frac{\xi_r^{i+1}}{-2c\xi_r} + \frac{\xi_\ell^{i+1}}{-2c\xi_\ell}\right)(-4ca) + \left(-\frac{\xi_r^{i+3}}{-2c\xi_r} + \frac{\xi_\ell^{i+3}}{-2c\xi_\ell}\right)\left(12c^2\right) \\
&\quad \left(\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,x^{i+1}\,dx\right)(-12c) + 2\left(-2c\xi_r\right)\xi_r^{i+1} - 2\left(-2c\xi_\ell\right)\xi_\ell^{i+1} \\
&\quad - 4\int_{\xi_\ell}^{\xi_r}(-2cx)\,x^i\,dx - 2\int_{\xi_\ell}^{\xi_r}(-2c)\,x^{i+1}\,dx \\
&= \left(\xi_r^i - \xi_\ell^i\right)(-2a) + \left(\xi_r^{i+2} - \xi_\ell^{i+2}\right)(6c) - 4c\xi_r^{i+2} + 4c\xi_\ell^{i+2} \\
&= -\left(1 - (-1)^i\right)2a\xi_r^i + \left(1 - (-1)^i\right)6c\frac{a}{c}\xi_r^i - 4c\frac{a}{c}\xi_r^i + 4c\,(-1)^i\,\frac{a}{c}\xi_r^i \\
&= -\left(1 - (-1)^i\right)2a\xi_r^i + \left(1 - (-1)^i\right)6a\xi_r^i - \left(1 - (-1)^i\right)4a\xi_r^i \\
&= \left(1 - (-1)^i\right)(0) = 0
\end{aligned}$$

Let $\ell \geq 2$. Here we plug $\partial_\ell H$ from (B.4), $\mathbf{g}$ from (3.2), H from (B.1), $\partial_\ell \mathbf{g}$ from

(3.3)-(3.5), and $\partial_\ell \mathbf{f}$ from (B.8) into (3.6) to get

$$\begin{aligned}
\Delta_\ell = &\left(-\frac{\xi_r^{i+\ell}}{-2c\xi_r} + \frac{\xi_\ell^{i+\ell}}{-2c\xi_\ell}\right)(-4ca) + \left(-\frac{\xi_r^{i+\ell+2}}{-2c\xi_r} + \frac{\xi_\ell^{i+\ell+2}}{-2c\xi_\ell}\right)\left(12c^2\right) \\
&\left(\int_{\xi_\ell}^{\xi_r} x^{i+\ell-2}\,dx\right)(2\ell(\ell-1)a) + \left(\int_{\xi_\ell}^{\xi_r} x^{i+\ell}\,dx\right)\left(-2\left(\ell^2+3\ell+2\right)c\right) \\
&+ 2(-2c\xi_r)\,\xi_r^{i+\ell} - 2(-2c\xi_\ell)\,\xi_\ell^{i+\ell} - 4\ell\int_{\xi_\ell}^{\xi_r}(-2cx)\,x^{i+\ell-1}\,dx \\
&- 2\int_{\xi_\ell}^{\xi_r}(-2c)\,x^{i+\ell}\,dx - 2\ell(\ell-1)\int_{\xi_\ell}^{\xi_r}\left(a-cx^2\right)x^{i+\ell-2}\,dx \\
= &\left(-\xi_r^{i+\ell-1}+\xi_\ell^{i+\ell-1}\right)2a + \left(\xi_r^{i+\ell+1}-\xi_\ell^{i+\ell+1}\right)6c \\
&2\ell(\ell-1)\,a\int_{\xi_\ell}^{\xi_r} x^{i+\ell-2}\,dx - 2\left(\ell^2+3\ell+2\right)c\int_{\xi_\ell}^{\xi_r} x^{i+\ell}\,dx \\
&- 4c\xi_r^{i+\ell+1} + 4c\xi_\ell^{i+\ell+1} + 8\ell c\int_{\xi_\ell}^{\xi_r} x^{i+\ell}\,dx \\
&+ 4c\int_{\xi_\ell}^{\xi_r} x^{i+\ell}\,dx - 2\ell(\ell-1)\,a\int_{\xi_\ell}^{\xi_r} x^{i+\ell-2}\,dx \\
&+ 2\ell(\ell-1)\,c\int_{\xi_\ell}^{\xi_r} x^{i+\ell}\,dx \\
= &-\left(1-(-1)^{i+\ell-1}\right)2a\xi_r^{i+\ell-1} + \left(1-(-1)^{i+\ell-1}\right)6c\xi_r^{i+\ell+1} \\
&- \left(2\ell^2+6\ell+4-8\ell-4-2\ell(\ell-1)\right)c\int_{\xi_\ell}^{\xi_r} x^{i+\ell}\,dx \\
&- \left(1-(-1)^{i+\ell+1}\right)4c\xi_r^{i+\ell+1} \\
= &-\left(1-(-1)^{i+\ell-1}\right)2a\xi_r^{i+\ell-1} + \left(1-(-1)^{i+\ell-1}\right)2c\frac{a}{c}\xi_r^{i+\ell-1} = 0
\end{aligned}$$

■

3.3 Barenblatt-Pattle calculations: case II

Let $m > 2$. We will prove some necessary identities. Then we will compute H, ∂H and $\partial \mathbf{f}$ in the Barenblatt-Pattle solution case using the formulas in the summary: (B.2), (B.5), and (B.9)-(B.11). We will then use these to show theorem 3.3.

When $m > 2$, to correctly handle an apparent singularity in some terms it becomes necessary to consider an alternative form of the relevant quantities. The alternative form is that which uses a change of variables to show that the apparent singularity can be successfully integrated.

In the case of the Barenblatt-Pattle solution, we have that $p(x) = a - cx^2$, so that $\beta_0 = a$, $\beta_1 \equiv 0$, $\beta_2 = -c$ and $\beta_i \equiv 0$ for $i \geq 3$. We have simplified the notation from (1.6), where $a = At^{-(m-1)/(m+1)}$ and $c = Ct^{-1}$. In the variables a and c, we have $\xi_r = -\xi_\ell = (a/c)^{1/2}$. Also following is that $p_x(x) = -2cx$, so that $p_x(\xi_r) = -2(ac)^{1/2}$ and $p_x(\xi_\ell) = 2(ac)^{1/2}$. Define degree $N-1$ polynomials q and r such that $p(x) = (x - \xi_\ell)\, q(x)$ and $p(x) = (\xi_r - x)\, r(x)$. One can verify that $q(x) = (ac)^{1/2} - cx$ and $r(x) = (ac)^{1/2} + cx$. From (A.2) of lemma A.2, we get $\partial_\ell \xi_r = a^{(\ell-1)/2} c^{-(\ell+1)/2}/2$ and $\partial_\ell \xi_\ell = (-1)^{\ell+1} a^{(\ell-1)/2} c^{-(\ell+1)/2}/2$.

We will use the following computations to calculate (B.2), (B.5), and (B.9)-(B.11). Using (A.3) and the quantities from the previous paragraph we calculate $\partial_0 [q(\xi_\ell + s^{m-1})]$:

$$\begin{aligned}
\frac{\partial}{\partial \beta_0}\left[q\left(\xi_\ell + s^{m-1}\right)\right] &= \frac{\left(\xi_\ell + s^{m-1}\right)^0 + \frac{\partial \xi_\ell}{\partial \beta_0} p_x\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}} \\
&= \frac{1 - \frac{1}{2} a^{-\frac{1}{2}} c^{-\frac{1}{2}} (-2c)\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}} \\
&= \frac{1 - \xi_\ell^{-1}\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}} \\
&= -\xi_\ell^{-1}
\end{aligned}$$

For general ℓ observe that

$$\begin{aligned}
\frac{\partial \xi_\ell}{\partial \beta_\ell} p_x\left(\xi_\ell + s^{m-1}\right) &= \frac{(-1)^{\ell+1}}{2} a^{\frac{\ell-1}{2}} c^{-\frac{\ell+1}{2}} (-2c)\left(\xi_\ell + s^{m-1}\right) \\
&= (-1)^\ell (-\xi_\ell)^{\ell-1}\left(\xi_\ell + s^{m-1}\right) \\
&= -\xi_\ell^{\ell-1}\left(\xi_\ell + s^{m-1}\right)
\end{aligned}$$

in the case of the Barenblatt-Pattle solution. We can calculate $\partial_\ell [q(\xi_\ell + s^{m-1})]$

for $\ell > 0$ to be:

$$\frac{\partial}{\partial \beta_\ell} q\left(\xi_\ell + s^{m-1}\right) = \frac{\left(\xi_\ell + s^{m-1}\right)^\ell + \frac{\partial \xi_\ell}{\partial \beta_\ell} p_x\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}}$$
$$= \frac{\left(\xi_\ell + s^{m-1}\right)^\ell - \xi_\ell^{\ell-1}\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}}$$

Using this formula for $\ell = 1$ we see that $\partial_1\left[q\left(\xi_\ell + s^{m-1}\right)\right] = 0$. To summarize:

$$\frac{\partial}{\partial \beta_\ell} q\left(\xi_\ell + s^{m-1}\right) = \begin{cases} -\xi_\ell^{-1}, & \ell = 0, \\ 0, & \ell = 1, \\ \frac{\left(\xi_\ell + s^{m-1}\right)^\ell - \xi_\ell^{\ell-1}\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}}, & \ell > 1. \end{cases}$$

Similarly, we use (A.4) to calculate $\partial_0\left[r\left(\xi_r - s^{m-1}\right)\right]$:

$$\frac{\partial}{\partial \beta_0} r\left(\xi_r - s^{m-1}\right) = \frac{\left(\xi_r - s^{m-1}\right)^0 + \frac{\partial \xi_r}{\partial \beta_0} p_x\left(\xi_r - s^{m-1}\right)}{s^{m-1}}$$
$$= \frac{1 + \frac{1}{2} a^{-\frac{1}{2}} c^{-\frac{1}{2}}\left(-2c\right)\left(\xi_r - s^{m-1}\right)}{s^{m-1}}$$
$$= \frac{1 - \xi_r^{-1}\left(\xi_r - s^{m-1}\right)}{s^{m-1}} = \xi_r^{-1}$$

For general ℓ observe that

$$\frac{\partial \xi_r}{\partial \beta_\ell} p_x\left(\xi_r - s^{m-1}\right) = \frac{1}{2} a^{\frac{\ell-1}{2}} c^{-\frac{\ell+1}{2}}\left(-2c\right)\left(\xi_r - s^{m-1}\right) = -\xi_r^{\ell-1}\left(\xi_r - s^{m-1}\right)$$

in the case of the Barenblatt-Pattle solution. From this we can calculate $\partial_\ell\left[r\left(w\right)\right]$, where $w = \xi_r - s^{m-1}$, for $\ell > 0$ to be:

$$\frac{\partial}{\partial \beta_\ell} r\left(\xi_r - s^{m-1}\right) = \frac{\left(\xi_r - s^{m-1}\right)^\ell + \frac{\partial \xi_r}{\partial \beta_\ell} p_x\left(\xi_r - s^{m-1}\right)}{s^{m-1}}$$
$$= \frac{\left(\xi_r - s^{m-1}\right)^\ell - \xi_r^{\ell-1}\left(\xi_r - s^{m-1}\right)}{s^{m-1}}$$

Using this formula for $\ell = 1$ we see that $\partial_1\left[r\left(\xi_r - s^{m-1}\right)\right] = 0$. To summarize:

$$\frac{\partial}{\partial \beta_\ell} r\left(\xi_r - s^{m-1}\right) = \begin{cases} \xi_r^{-1}, & \ell = 0, \\ 0, & \ell = 1, \\ \frac{\left(\xi_r - s^{m-1}\right)^\ell - \xi_r^{\ell-1}\left(\xi_r - s^{m-1}\right)}{s^{m-1}}, & \ell > 1. \end{cases}$$

Since we will need the following quantities note that $q\left(\xi_\ell + s^{m-1}\right) = c\left(-2\xi_\ell - s^{m-1}\right)$ and $r\left(\xi_r - s^{m-1}\right) = c\left(2\xi_r - s^{m-1}\right)$. In general one can see that for the Barenblatt-Pattle solution we have that

$$\begin{aligned}
\frac{\partial}{\partial \beta_\ell} p_x\left(\xi_\ell + s^{m-1}\right) &= \ell\left(\xi_\ell + s^{m-1}\right)^{\ell-1} + \frac{\partial \xi_\ell}{\partial \beta_\ell} p_{xx}\left(\xi_\ell + s^{m-1}\right) \\
&= \ell\left(\xi_\ell + s^{m-1}\right)^{\ell-1} + \frac{(-1)^{\ell+1}}{2} a^{\frac{\ell-1}{2}} c^{-\frac{\ell+1}{2}}\left(-2c\right) \\
&= \ell\left(\xi_\ell + s^{m-1}\right)^{\ell-1} - \xi_\ell^{\ell-1},
\end{aligned} \tag{3.7}$$

$$\begin{aligned}
\frac{\partial}{\partial \beta_\ell} p_x\left(\xi_r - s^{m-1}\right) &= \ell\left(\xi_r - s^{m-1}\right)^{\ell-1} + \frac{\partial \xi_r}{\partial \beta_\ell} p_{xx}\left(\xi_r - s^{m-1}\right) \\
&= \ell\left(\xi_r - s^{m-1}\right)^{\ell-1} + \frac{1}{2} a^{\frac{\ell-1}{2}} c^{-\frac{\ell+1}{2}}\left(-2c\right) \\
&= \ell\left(\xi_r - s^{m-1}\right)^{\ell-1} - \xi_r^{\ell-1}
\end{aligned} \tag{3.8}$$

and

$$\begin{aligned}
\frac{\partial}{\partial \beta_\ell} p_{xx}\left(\xi \pm s^{m-1}\right) &= \ell\left(\ell-1\right)\left(\xi \pm s^{m-1}\right)^{\ell-2} + p_{xxx}\left(\xi \pm s^{m-1}\right)\frac{\partial \xi}{\partial \beta_\ell} \\
&= \ell\left(\ell-1\right)\left(\xi \pm s^{m-1}\right)^{\ell-2} + 0 \cdot \frac{\partial \xi}{\partial \beta_\ell} = \ell\left(\ell-1\right)\left(\xi \pm s^{m-1}\right)^{\ell-2}.
\end{aligned} \tag{3.9}$$

We end this section with a lemma that we will need below.

Lemma 3.1. *If $p \in (0,\, 1)$ and q_1 and q_2 are positive, then*

$$\int_0^1 (1-t)^{p-2}\left(t^{q_1-1} - t^{q_2-1}\right) dt = \frac{p+q_1-1}{p-1} B\left(p,\, q_1\right) - \frac{p+q_2-1}{p-1} B\left(p,\, q_2\right), \tag{3.10}$$

where $B(p,\, q)$ is the beta function:

$$B\left(p,\, q\right) = \int_0^1 (1-t)^{p-1}\, t^{q-1}\, dt.$$

Remark 3.1. *The left hand side of equation* (3.10) *cannot be written as*

$$\int_0^1 (1-t)^{p-2}\, t^{q_1-1}\, dt - \int_0^1 (1-t)^{p-2}\, t^{q_2-1}\, dt$$

since neither of these integrals exist. This is because both integrands behave like $(1-t)^{p-2}$, *as* $t \uparrow 1$, *which grows faster than* $(1-t)^{-1}$, *as* $t \uparrow 1$, *which is not integrable. If this were not the case then the result would follow simply using beta function identities:* $B(p-1,\, q) = (p+q-1)/(p-1)\, B(p,\, q)$.

Proof. The following equation being well-defined, we apply integration by parts

$$\begin{aligned}\frac{q_1}{p-1}B(p,\, q_1) - \frac{q_2}{p-1}B(p,\, q_2) &= \frac{q_1}{p-1}\int_0^1 (1-t)^{p-1}\, t^{q_1-1} \\ &\quad - \frac{q_2}{p-1}\int_0^1 (1-t)^{p-1}\, t^{q_2-1}\, dt \\ &= \int_0^1 \frac{1}{p-1}(1-t)^{p-1}\left(q_1 t^{q_1-1} - q_2 t^{q_2-1}\right) dt \\ &= \frac{1}{p-1}\lim_{t\uparrow 1}(1-t)^{p-1}\left(t^{q_1} - t^{q_2}\right) - 0 \\ &\quad + \int_0^1 (1-t)^{p-2}\left(t^{q_1} - t^{q_2}\right) dt \\ &= \int_0^1 (1-t)^{p-2}\left(t^{q_1} - t^{q_2}\right) dt,\end{aligned}$$

where L'Hôpital's rule shows that the limit is zero. Adding $B(p,\, q_1)$ and subtracting $B(p,\, q_2)$ from both sides we get

$$\begin{aligned}&\frac{q_1+p-1}{p-1}B(p,\, q_1) - \frac{q_2+p-1}{p-1}B(p,\, q_2) \\ &\quad = \int_0^1 (1-t)^{p-2}\left(t^{q_1} - t^{q_2}\right) dt + \int_0^1 (1-t)^{p-1}\left(t^{q_1-1} - t^{q_2-1}\right) dt \\ &\quad = \int_0^1 (1-t)^{p-2}\left(t + (1-t)\right)\left(t^{q_1-1} - t^{q_2-1}\right) dt \\ &\quad = \int_0^1 (1-t)^{p-2}\left(t^{q_1-1} - t^{q_2-1}\right) dt,\end{aligned}$$

as required. ∎

3.3.1 H in the Barenblatt-Pattle case

We begin by introducing some notation. We will use $\tau(k)$, $\mu(k)$, and $\nu(k)$ to denote the following products:

$$\tau(k) = \prod_{s=1}^{k} (2s-1)$$

$$\mu(k) = \prod_{s=1}^{k} [sm - (s-1)]$$

and

$$\nu(k) = \prod_{s=1}^{k} [(2s-1)m - (2s-3)],$$

where we take $\tau(0)$, $\mu(0)$, and $\nu(0)$ to mean empty products producing unity.* Note that τ is a constant, while μ and ν are functions of m.

Recall that $B(p,q)$ denotes the beta function: $\int_0^1 (1-t)^{p-1} t^{q-1}\, dt$. When it is understood that the arguments to the beta function are $1/(m-1)$ and p we will omit the $1/(m-1)$ and write $B(p)$ for $B(1/(m-1), p)$. When it is understood that the arguments to the beta function are $1/(m-1)$ and $1/2$ we will simply write B for $B(1/(m-1), 1/2)$. A change of variables shows that B is symmetric with respect to its arguments, so that $B(1) = \int_0^1 (1-t)^{1-1} t^{\frac{1}{m-1}-1}\, dt = m-1$.

On multiple occasions we will have need to reduce expressions like $B(k+1/2)$ and $B(k)$ for a positive integer k. By repeatedly using the identity $B(p, q+1) =$

*Another notation exists for the numbers $\tau(k)$: some authors use the double factorial notation, $k!!$. We will not use that notation since we will not be using its full connotation which we also omit.

$q/\left(p+q\right)B\left(p,\,q\right)$ we can reduce $B\left(k+1/2\right)$:

$$
\begin{aligned}
&B\left(k+\frac{1}{2}\right)\\
&\qquad=B\left(k-\frac{1}{2}+1\right)=\frac{k-\frac{1}{2}}{\frac{1}{m-1}+k-\frac{1}{2}}B\left(k-\frac{1}{2}\right)=c_1B\left(k-\frac{1}{2}\right)\\
&\qquad=c_1B\left(k-\frac{3}{2}+1\right)=c_1\frac{k-\frac{3}{2}}{\frac{1}{m-1}+k-\frac{3}{2}}B\left(k-\frac{3}{2}\right)=c_1c_3B\left(k-\frac{3}{2}\right)\\
&\qquad=c_1c_3B\left(k-\frac{5}{2}+1\right)=c_1c_3\frac{k-\frac{5}{2}}{\frac{1}{m-1}+k-\frac{5}{2}}B\left(k-\frac{5}{2}\right)=c_1c_3c_5B\left(\frac{1}{m-1},\,k-\frac{5}{2}\right)\\
&\qquad=\cdots=c_1c_3\cdots c_{2k-1}B\left(k-\frac{2k-1}{2}\right)=c_1c_3\cdots c_{2k-1}B
\end{aligned}
$$

where

$$
c_{2i-1}=\frac{k-\frac{2i-1}{2}}{\frac{1}{m-1}+k-\frac{2i-1}{2}}=\frac{\left(2k-2i+1\right)\left(m-1\right)}{\left(2k-2i+1\right)m-\left(2k-2i-1\right)},
$$

for $i=1,\,...,\,k$. So $B\left(k+1/2\right)$ becomes

$$
\begin{aligned}
B\left(k+\frac{1}{2}\right)&=\frac{\Pi_{s=1}^{k}\left(2k-2s+1\right)\left(m-1\right)}{\Pi_{s=1}^{k}\left(\left(2k-2s+1\right)m-\left(2k-2s-1\right)\right)}\cdot B\\
&=\frac{\left(m-1\right)^k\Pi_{s=1}^{k}\left(2s-1\right)}{\Pi_{s=1}^{k}\left(\left(2s-1\right)m-\left(2s-3\right)\right)}\cdot B.
\end{aligned}
$$

The last derivation shows that

$$
B\left(k+\frac{1}{2}\right)=\frac{\left(m-1\right)^k\tau\left(k\right)}{\nu\left(k\right)}\cdot B. \tag{3.11}
$$

Using the same identity, we can also reduce $B\left(k\right)$:

$$
\begin{aligned}
B\left(k\right)&=B\left(k-1+1\right)=\frac{k-1}{\frac{1}{m-1}+k-1}B\left(k-1\right)=d_1B\left(k-1\right)\\
&=d_1B\left(k-2+1\right)=d_1\frac{k-2}{\frac{1}{m-1}+k-2}B\left(k-2\right)=d_1d_2B\left(k-2\right)\\
&=d_1d_2B\left(k-3+1\right)=d_1d_2\frac{k-3}{\frac{1}{m-1}+k-3}B\left(k-3\right)=d_1d_2d_3B\left(k-3\right)\\
&=\cdots=d_1d_2\cdots d_{k-1}B\left(k-\left(k-1\right)\right)=d_1d_2\cdots d_{k-1}\left(m-1\right),
\end{aligned}
$$

where

$$
d_i=\frac{k-i}{\frac{1}{m-1}+k-i}=\frac{\left(k-i\right)\left(m-1\right)}{\left(k-i\right)m-\left(k-i-1\right)}.
$$

We can more compactly write

$$B(k) = \frac{(m-1)^k (k-1)!}{\mu(k-1)}. \tag{3.12}$$

Lemma 3.2. *Let $m > 2$. In the case of the Barenblatt-Pattle solution the mass matrix given in* (B.2) *can be written more simply as*

$$H(i,\,j) = \begin{cases} c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{i+j-1}\frac{(m-1)^{\frac{i+j}{2}-1}\tau\left(\frac{i+j}{2}\right)}{\nu\left(\frac{i+j}{2}\right)}\cdot B, & i+j \text{ even,} \\ 0, & i+j \text{ odd.} \end{cases} \tag{3.13}$$

Proof. To see this we plug the results derived above into (B.2) to compute H in the case of the Barenblatt-Pattle solution:

Plugging the relevant quantities from above into (B.2) we get

$$\begin{aligned} H(i,j) = \int_0^{s^*} & c^{\frac{1}{m-1}-1}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1} z^{i+j}\,ds \\ & + \int_0^{s^\#} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j}\,ds \\ & = \int_0^{s^\#} (-1)^{i+j} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j}\,ds \\ & + \int_0^{s^\#} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j}\,ds \\ = \left(1+(-1)^{i+j}\right) & c^{\frac{1}{m-1}-1}\int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1}\left(\xi_r - s^{m-1}\right)^{i+j}\,ds \end{aligned}$$

If $i+j$ is odd $H(i,\,j)=0$, henceforth we consider only the case when $i+j=2k$, for some $k \in \{0,\,...,\,N\}$. We now change to variables that lead to the closed form of the integrals, $s = (\xi_r - x)^{1/(m-1)}$. This gives that

$$H(i,j) = \frac{2}{m-1}c^{\frac{1}{m-1}-1}\int_0^{\xi_r}\left(\xi_r^2 - x^2\right)^{\frac{1}{m-1}-1} x^{2k}\,dx.$$

Changing variables again, $x = \xi_r y$, we get that

$$H(i,j) = \frac{2}{m-1}c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}-2}\xi_r^{2k+1}\int_0^1\left(1-y^2\right)^{\frac{1}{m-1}-1} y^{2k}\,dy,$$

and yet again, $y = t^{1/2}$, we get that

$$H(i,j) = \frac{1}{m-1} c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{2k-1} \int_0^1 (1-t)^{\frac{1}{m-1}-1} t^{\frac{2k+1}{2}-1}\, dt,$$

which we recognize as a beta integral:

$$H(i,j) = \frac{1}{m-1} c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{2k-1} B\left(\frac{1}{m-1}, k+\frac{1}{2}\right)$$

Using 3.11 we can write H as

$$\begin{aligned} H(i,j) &= \frac{1}{m-1} c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{2k-1} \frac{(m-1)^k \tau(k)}{\nu(k)} \cdot B \\ &= c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{2k-1} \frac{(m-1)^{k-1} \tau(k)}{\nu(k)} \cdot B \\ &= c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{i+j-1} \frac{(m-1)^{\frac{i+j}{2}-1} \tau\left(\frac{i+j}{2}\right)}{\nu\left(\frac{i+j}{2}\right)} \cdot B, \end{aligned}$$

which gives the result. ■

3.3.2 ∂H in the Barenblatt-Pattle case

Lemma 3.3. *Let $m > 2$. In the case of the Barenblatt-Pattle solution the derivative of the mass matrix given in* (B.5) *can be written more simply as, for $i+j=0$,*

$$\frac{\partial H}{\partial \beta_\ell}(0,0) = \begin{cases} c^{\frac{1}{m-1}-2} \xi_r^{\frac{2}{m-1}} \xi_r^{-3} \frac{3-m}{(m-1)^2} \cdot \frac{B}{2}, & \ell = 0, \\ c^{\frac{1}{m-1}-2} \xi_r^{\frac{2}{m-1}} \xi_r^{\ell-3} \frac{(m-1)^{\frac{\ell}{2}-2} \tau\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}-1\right)} \cdot \frac{B}{2}, & \ell \text{ even}, \ \ell \geq 2, \\ 0, & \ell \text{ odd}, \end{cases} \tag{3.14}$$

and, for $i+j \geq 1$,

$$\frac{\partial H}{\partial \beta_\ell}(i,j) = \begin{cases} c^{\frac{1}{m-1}-2} \xi_r^{\frac{2}{m-1}} \xi_r^{i+\ell-3} \frac{(m-1)^{\frac{i+\ell}{2}-2} \tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)} \cdot \frac{B}{2}, & i+\ell \text{ even}, \ j=0, \\ c^{\frac{1}{m-1}-2} \xi_r^{\frac{2}{m-1}} \xi_r^{i+\ell-1} \frac{(m-1)^{\frac{i+\ell}{2}-1} \tau\left(\frac{i+\ell}{2}+1\right)}{\nu\left(\frac{i+\ell}{2}\right)} \cdot \frac{B}{2}, & i+\ell \text{ even}, \ j=2, \\ 0, & i+\ell \text{ odd}, \ j=0,2 \\ \text{not given}, & \text{otherwise}. \end{cases} \tag{3.15}$$

Proof. Let $\mathcal{C} = c^{1/(m-1)-2}\xi_r^{2/(m-1)}\xi_r^{i+\ell}$, $z = \xi_\ell + s^{m-1}$, and $w = \xi_r - s^{m-1}$. Take $i + j \geq 1$. Using (B.5), (A.2), that $z = -w$, and the formulas for $q\left(\xi_\ell + s^{m-1}\right)$, $r\left(\xi_r - s^{m-1}\right)$, and $p_x\left(\xi \pm s^{m-1}\right)$ given above we get

$$\begin{aligned}
\frac{\partial H}{\partial \beta_\ell}(i,\, j) = &-\frac{m-2}{m-1}\left[\int_0^{s^*} c^{\frac{1}{m-1}-2}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{z^\ell - \xi_\ell^{\ell-1}z}{s^{m-1}} z^{i+j}\, ds\right.\\
&\left. + \int_0^{s^\#} c^{\frac{1}{m-1}-2}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^\ell - \xi_r^{\ell-1}w}{s^{m-1}} w^{i+j}\, ds\right]\\
&- (i+j)\left[\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*} c^{\frac{1}{m-1}-1}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1} z^{i+j-1}\, ds\right.\\
&\left. + \frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j-1}\, ds\right]\\
= &-\frac{m-2}{m-1}c^{\frac{1}{m-1}-2}\left[\int_0^{s^*}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{z^{i+j+\ell} - \xi_\ell^{\ell-1}z^{i+j+1}}{s^{m-1}}\, ds\right.\\
&\left. + \int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+j+\ell} - \xi_r^{\ell-1}w^{i+j+1}}{s^{m-1}}\, ds\right]\\
&- (i+j)\, c^{\frac{1}{m-1}-1}\left[\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1} z^{i+j-1}\, ds\right.\\
&\left. + \frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j-1}\, ds\right]\\
= &-\frac{m-2}{m-1}c^{\frac{1}{m-1}-2}\left[(-1)^{i+j+\ell}\int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+j+\ell} - \xi_r^{\ell-1}w^{i+j+1}}{s^{m-1}}\, ds\right.\\
&\left. + \int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+j+\ell} - \xi_r^{\ell-1}w^{i+j+1}}{s^{m-1}}\, ds\right]\\
&+ \frac{i+j}{2}c^{\frac{1}{m-1}-2}\xi_r^{\ell-1}\left[(-1)^{i+j+\ell}\int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j-1}\, ds\right.\\
&\left. + \int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j-1}\, ds\right]\\
= &-\left(1 + (-1)^{i+j+\ell}\right)\frac{m-2}{m-1}c^{\frac{1}{m-1}-2}\int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+j+\ell} - \xi_r^{\ell-1}w^{i+j+1}}{s^{m-1}}\, ds\\
&+ \left(1 + (-1)^{i+j+\ell}\right)\frac{i+j}{2}c^{\frac{1}{m-1}-2}\xi_r^{\ell-1}\int_0^{s^\#}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+j-1}\, ds
\end{aligned} \tag{3.16}$$

From this we see that $\partial H\,(i,\,j) = 0$ if $i+j+\ell$ is odd.

Take $i+j+\ell$ to be even.

$$\begin{aligned}
&\left(\mathcal{C}^{\frac{1}{m-1}-2}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}\,(i,\,j) \\
&= -\frac{2\,(m-2)}{m-1} \int_0^{s^\#} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{\left(\xi_r - s^{m-1}\right)^{i+j+\ell} - \xi_r^{\ell-1}\left(\xi_r - s^{m-1}\right)^{i+j+1}}{s^{m-1}}\,ds \\
&\qquad + (i+j)\,\xi_r^{\ell-1} \int_0^{s^\#} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} \left(\xi_r - s^{m-1}\right)^{i+j-1}\,ds
\end{aligned}$$

After using the change of variables $s = (\xi_r - x)^{1/(m-1)}$ we get that the last equation is

$$\begin{aligned}
&= -\frac{2\,(m-2)}{m-1} \cdot \frac{1}{m-1} \int_0^{\xi_r} \left(\xi_r^2 - x^2\right)^{\frac{1}{m-1}-2} \left(x^{i+j+\ell} - \xi_r^{\ell-1} x^{i+j+1}\right)\,dx \\
&\qquad + (i+j)\,\xi_r^{\ell-1} \cdot \frac{1}{m-1} \int_0^{\xi_r} \left(\xi_r^2 - x^2\right)^{\frac{1}{m-1}-1} x^{i+j-1}\,dx
\end{aligned}$$

Using the change of variables $x = \xi_r y$ we get

$$\begin{aligned}
&\left(\frac{1}{m-1}\mathcal{C}^{\frac{1}{m-1}-2}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}\,(i,\,j) \\
&\quad = -\frac{2\,(m-2)}{m-1} \cdot \xi_r^{\frac{2}{m-1}-4} \xi_r^{i+j+\ell} \xi_r \int_0^1 \left(1-y^2\right)^{\frac{1}{m-1}-2} \left(y^{i+j+\ell} - y^{i+j+1}\right)\,dy \\
&\qquad + (i+j)\,\xi_r^{\ell-1} \cdot \xi_r^{\frac{2}{m-1}-2} \xi_r^{i+j-1} \xi_r \int_0^1 \left(1-y^2\right)^{\frac{1}{m-1}-1} y^{i+j-1}\,dy
\end{aligned}$$

Making the last change of variables, $y = t^{1/2}$, we get

$$\begin{aligned}
\mathcal{E}^{-1}\frac{\partial H}{\partial \beta_\ell}\,(i,\,j) &= -\frac{2\,(m-2)}{m-1} \cdot \frac{1}{2} \int_0^1 (1-t)^{\frac{1}{m-1}-2} \left(t^{\frac{i+j+\ell+1}{2}-1} - t^{\frac{i+j+2}{2}-1}\right)\,dt \\
&\quad + (i+j) \cdot \frac{1}{2} \int_0^1 (1-t)^{\frac{1}{m-1}-1}\, t^{\frac{i+j}{2}-1}\,dt,
\end{aligned} \tag{3.17}$$

where $\mathcal{E} = \mathcal{C}\xi_r^{j-3}/\,(m-1)$. The second term of this equation can be written as $(i+j)\,B\,((i+j)\,/2)\,/2$. Taking p, q_1, and q_2 from lemma 3.1 as $1/\,(m-1)$, $(i+j+\ell+1)\,/2$, and $(i+j+2)\,/2$, respectively, we can write the first term of (3.17) can be written as

$$\frac{(i+j+\ell+1)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+j+\ell+1}{2}\right) - \frac{(i+j+2)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+j+2}{2}\right).$$

Using these we write (3.17) as

$$\mathcal{E}^{-1}\frac{\partial H}{\partial \beta_\ell}(i,\, j) = \frac{(i+j+\ell+1)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+j+\ell+1}{2}\right) - \frac{(i+j+2)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+j+2}{2}\right) + \frac{i+j}{2} B\left(\frac{i+j}{2}\right). \tag{3.18}$$

The form of $\mathbf{g}$ informs us that our calculations of ∂H can be restricted to $\partial H\,(:,\,[0,\,2])$. We proceed only with $j=0$ and $j=2$ cases:

$$\begin{aligned}\left(\frac{1}{m-1}\mathcal{C}\xi_r^{-3}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}(i,\, 0) &= \frac{(i+\ell+1)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+\ell+1}{2}\right) - \frac{(i+2)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+2}{2}\right) + \frac{i}{2} B\left(\frac{i}{2}\right) \\ &= \frac{(i+\ell-1)\,m-(i+\ell-3)}{2(m-1)} B\left(\frac{i+\ell+1}{2}\right) - \frac{im-(i-2)}{2(m-1)} B\left(\frac{i+2}{2}\right) + \frac{i}{2} B\left(\frac{i}{2}\right)\end{aligned}$$

and

$$\begin{aligned}\left(\frac{1}{m-1}\mathcal{C}\xi_r^{-1}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}(i,\, 2) &= \frac{(i+\ell+3)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+\ell+3}{2}\right) - \frac{(i+4)(m-1)+2(2-m)}{2(m-1)} B\left(\frac{i+4}{2}\right) + \frac{i+2}{2} B\left(\frac{i+2}{2}\right) \\ &= \frac{(i+\ell+1)\,m-(i+\ell-1)}{2(m-1)} B\left(\frac{i+\ell+3}{2}\right) - \frac{(i+2)\,m-i}{2(m-1)} B\left(\frac{i+4}{2}\right) + \frac{i+2}{2} B\left(\frac{i+2}{2}\right).\end{aligned}$$

Since $i+j+\ell$ is even and $j=0$ or $j=2$, $i+\ell$ must be even.

Suppose both i and ℓ are even and write $i = 2k_1$ for some $k_1 \in \{1, ..., \lfloor N/2 \rfloor\}$ and $\ell = 2k_2$ for some $k_2 \in \{0, ..., \lfloor N/2 \rfloor\}$. Let $j = 0$ and compute $\partial H(i, 0)$:

$$\begin{aligned}
&\left(\frac{1}{m-1}\mathcal{C}\xi_r^{-3}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}(i, 0) \\
&\qquad = \frac{(i+\ell-1)m - (i+\ell-3)}{2(m-1)} B\left(k_1 + k_2 + \frac{1}{2}\right) \\
&\qquad\qquad - \frac{im - (i-2)}{2(m-1)} B(k_1+1) + \frac{i}{2} B(k_1)
\end{aligned}$$

$$\begin{aligned}
&= \frac{(2k_1+2k_2-1)m - (2k_1+2k_2-3)}{2(m-1)} \cdot \frac{(m-1)^{k_1+k_2}\tau(k_1+k_2)}{\nu(k_1+k_2)} \cdot B \\
&\qquad - \frac{2k_1 m - (2k_1-2)}{2(m-1)} \cdot \frac{(m-1)^{k_1+1} k_1!}{\mu(k_1)} + \frac{2k_1}{2} \cdot \frac{(m-1)^{k_1}(k_1-1)!}{\mu(k_1-1)},
\end{aligned}$$

where we have applied (3.11) and (3.12). We can further rewrite $\partial H(i, 0)$:

$$\begin{aligned}
\left(\mathcal{C}\xi_r^{-3}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}(i,\, 0) &= \frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2)}{\nu(k_1+k_2-1)} \cdot \frac{B}{2} \\
&\quad - \frac{(m-1)^{k_1-1} k_1!}{\mu(k_1-1)} + \frac{(m-1)^{k_1-1} k_1!}{\mu(k_1-1)} \\
&= \frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2)}{\nu(k_1+k_2-1)} \cdot \frac{B}{2},
\end{aligned}$$

or

$$\left(\mathcal{C}\xi_r^{-3}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}(i,\, 0) = \frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)} \cdot \frac{B}{2}.$$

Let $j = 2$ and compute $\partial H(i, 2)$:

$$\begin{aligned}
&\left(\frac{1}{m-1}\mathcal{C}\xi_r^{-1}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}(i,\, 2) \\
&\qquad = \frac{(i+\ell+1)m - (i+\ell-1)}{2(m-1)} B\left(k_1 + k_2 + \frac{3}{2}\right) \\
&\qquad\qquad - \frac{(i+2)m - i}{2(m-1)} B(k_1+2) + \frac{i+2}{2} B(k_1+1)
\end{aligned}$$

$$= \frac{(2k_1+2k_2+1)\,m-(2k_1+2k_2-1)}{2\,(m-1)} \cdot \frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)} \cdot B$$
$$- \frac{(2k_1+2)\,m-2k_1}{2\,(m-1)} \cdot \frac{(m-1)^{k_1+2}\,(k_1+1)!}{\mu\,(k_1+1)} + \frac{2k_1+2}{2} \cdot \frac{(m-1)^{k_1+1}\,k_1!}{\mu\,(k_1)},$$

where we have applied (3.11) and (3.12). We can further rewrite $\partial H\,(i,2)$:

$$\begin{aligned}
\left(\mathcal{C}\xi_r^{-1}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}\,(i,2) &= \frac{(m-1)^{k_1+k_2-1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2)} \cdot \frac{B}{2} \\
&\quad - \frac{(m-1)^{k_1}\,(k_1+1)!}{\mu\,(k_1)} + \frac{(m-1)^{k_1}\,(k_1+1)!}{\mu\,(k_1)}. \\
&= \frac{(m-1)^{k_1+k_2-1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2)} \cdot \frac{B}{2},
\end{aligned}$$

or

$$\left(\mathcal{C}\xi_r^{-1}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}\,(i,2) = \frac{(m-1)^{\frac{i+\ell}{2}-1}\,\tau\left(\frac{i+\ell}{2}+1\right)}{\nu\left(\frac{i+\ell}{2}\right)} \cdot \frac{B}{2}.$$

Suppose both i and ℓ are odd and write $i = 2k_1+1$ for some $k_1 \in \{1, ..., \lfloor (N-1)/2 \rfloor\}$ and $\ell = 2k_2+1$ for some $k_2 \in \{0, ..., \lfloor (N-1)/2 \rfloor\}$. Let $j = 0$ and compute $\partial H\,(i,0)$:

$$\begin{aligned}
&\left(\frac{1}{m-1}\mathcal{C}\xi_r^{-3}\right)^{-1} \frac{\partial H}{\partial \beta_\ell}\,(i,0) \\
&\qquad = \frac{(i+\ell-1)\,m-(i+\ell-3)}{2\,(m-1)} B\left(k_1+k_2+\frac{3}{2}\right) \\
&\qquad\qquad - \frac{im-(i-2)}{2\,(m-1)} B\left(k_1+\frac{3}{2}\right) + \frac{i}{2} B\left(k_1+\frac{1}{2}\right)
\end{aligned}$$

$$= \frac{(2k_1+2k_2+1)\,m-(2k_1+2k_2-1)}{2\,(m-1)} \cdot \frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)} \cdot B$$
$$- \frac{(2k_1+1)\,m-(2k_1-1)}{2\,(m-1)} \cdot \frac{(m-1)^{k_1+1}\,\tau\,(k_1+1)}{\nu\,(k_1+1)} \cdot B + \frac{i}{2} \cdot \frac{(m-1)^{k_1}\,\tau\,(k_1)}{\nu\,(k_1)} \cdot B,$$

where we have applied (3.11). We can further rewrite $\partial H\left(i,0\right)$:

$$\begin{aligned}\left(\mathcal{C}\xi_r^{-3}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}\left(i,\,0\right) &= \frac{\left(m-1\right)^{k_1+k_2-1}\tau\left(k_1+k_2+1\right)}{\nu\left(k_1+k_2\right)}\cdot\frac{B}{2}\\ &\quad-\frac{\left(m-1\right)^{k_1-1}\tau\left(k_1+1\right)}{\nu\left(k_1\right)}\cdot\frac{B}{2}+i\cdot\frac{\left(m-1\right)^{k_1-1}\tau\left(k_1\right)}{\nu\left(k_1\right)}\cdot\frac{B}{2}\\ &= \frac{\left(m-1\right)^{k_1+k_2-1}\tau\left(k_1+k_2+1\right)}{\nu\left(k_1+k_2\right)}\cdot\frac{B}{2}\\ &\quad-i\frac{\left(m-1\right)^{k_1-1}\tau\left(k_1\right)}{\nu\left(k_1\right)}\cdot\frac{B}{2}+i\cdot\frac{\left(m-1\right)^{k_1-1}\tau\left(k_1\right)}{\nu\left(k_1\right)}\cdot\frac{B}{2}\\ &= \frac{\left(m-1\right)^{k_1+k_2-1}\tau\left(k_1+k_2+1\right)}{\nu\left(k_1+k_2\right)}\cdot\frac{B}{2},\end{aligned}$$

or

$$\left(\mathcal{C}\xi_r^{-3}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}\left(i,\,0\right)=\frac{\left(m-1\right)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}\cdot\frac{B}{2}.$$

In the last sequence of reductions we used that

$$\tau\left(k_1+1\right)=\left[2\left(k_1+1\right)-1\right]\tau\left(k_1\right)=\left(2k_1+1\right)\tau\left(k_1\right)=i\tau\left(k_1\right).$$

Let $j=2$ and compute $\partial H\left(i,2\right)$:

$$\begin{aligned}&\left(\frac{1}{m-1}\mathcal{C}\xi_r^{-1}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}\left(i,\,2\right)\\ &\quad=\frac{\left(i+\ell+1\right)m-\left(i+\ell-1\right)}{2\left(m-1\right)}B\left(k_1+k_2+\frac{5}{2}\right)\\ &\qquad-\frac{\left(i+2\right)m-i}{2\left(m-1\right)}B\left(k_1+\frac{5}{2}\right)+\frac{i+2}{2}B\left(k_1+\frac{3}{2}\right)\end{aligned}$$

$$\begin{aligned}&=\frac{\left(2k_1+2k_2+3\right)m-\left(2k_1+2k_2+1\right)}{2\left(m-1\right)}\cdot\frac{\left(m-1\right)^{k_1+k_2+2}\tau\left(k_1+k_2+2\right)}{\nu\left(k_1+k_2+2\right)}\cdot B\\ &-\frac{\left(2k_1+3\right)m-\left(2k_1+1\right)}{2\left(m-1\right)}\cdot\frac{\left(m-1\right)^{k_1+2}\tau\left(k_1+2\right)}{\nu\left(k_1+2\right)}\cdot B+\frac{i+2}{2}\cdot\frac{\left(m-1\right)^{k_1+1}\tau\left(k_1+1\right)}{\nu\left(k_1+1\right)}\cdot B,\end{aligned}$$

where we have applied (3.11). We can further rewrite $\partial H\left(i,2\right)$:

$$\begin{aligned}\left(\mathcal{C}\xi_r^{-1}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}\left(i,2\right) &= \frac{\left(m-1\right)^{k_1+k_2}\tau\left(k_1+k_2+2\right)}{\nu\left(k_1+k_2+1\right)}\cdot\frac{B}{2}\\ &\quad-\frac{\left(m-1\right)^{k_1}\tau\left(k_1+2\right)}{\nu\left(k_1+1\right)}\cdot\frac{B}{2}+\left(i+2\right)\frac{\left(m-1\right)^{k_1}\tau\left(k_1+1\right)}{\nu\left(k_1+1\right)}\cdot\frac{B}{2}\end{aligned}$$

$$
\begin{aligned}
=&\frac{(m-1)^{k_1+k_2}\,\tau\left(k_1+k_2+2\right)}{\nu\left(k_1+k_2+1\right)}\cdot\frac{B}{2}-(i+2)\,\frac{(m-1)^{k_1}\,\tau\left(k_1+1\right)}{\nu\left(k_1+1\right)}\cdot\frac{B}{2}\\
&+(i+2)\,\frac{(m-1)^{k_1}\,\tau\left(k_1+1\right)}{\nu\left(k_1+1\right)}\cdot\frac{B}{2}\\
=&\frac{(m-1)^{k_1+k_2}\,\tau\left(k_1+k_2+2\right)}{\nu\left(k_1+k_2+1\right)}\cdot\frac{B}{2},
\end{aligned}
$$

or

$$
\left(\mathcal{C}\xi_r^{-1}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}\left(i,2\right)=\frac{(m-1)^{\frac{i+\ell}{2}-1}\,\tau\left(\frac{i+\ell}{2}+1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot\frac{B}{2}.
$$

In the last sequence of reductions we used that

$$
\tau\left(k_1+2\right)=\left[2\left(k_1+2\right)-1\right]\tau\left(k_1+1\right)=\left(2k_1+3\right)\tau\left(k_1+1\right)=\left(i+2\right)\tau\left(k_1+1\right).
$$

To summarize, when $i+j\geq 1$:

$$
\begin{aligned}
&\partial_\ell H\left(i,0\right)=\mathcal{C}\xi_r^{-3}\frac{(m-1)^{\frac{i+\ell}{2}-2}\,\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}\cdot\frac{B}{2},i+\ell\text{ even},\\
&\partial_\ell H\left(i,2\right)=\mathcal{C}\xi_r^{-1}\frac{(m-1)^{\frac{i+\ell}{2}-1}\,\tau\left(\frac{i+\ell}{2}+1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot\frac{B}{2},i+\ell\text{ even},\\
&\partial_\ell H\left(i,0\right)=0,\ i+\ell\text{odd},\\
&\partial_\ell H\left(i,2\right)=0,\ i+\ell\text{odd}.
\end{aligned}
$$

Take $i+j=0$. Using (B.5) and the relevant quantities above we get

$$
\begin{aligned}
\frac{\partial H}{\partial\beta_\ell}\left(0,\,0\right)=&\frac{1}{2}\left(1+(-1)^\ell\right)\frac{1}{m-1}a^{\frac{1}{m-1}-1}c^{-1}\xi_r^{\ell-1}\\
&-\frac{m-2}{m-1}c^{\frac{1}{m-1}-2}\left[\int_0^{s^*}\left(-2\xi_\ell-s^{m-1}\right)^{\frac{1}{m-1}-2}\frac{z^\ell-\xi_\ell^{\ell-1}z}{s^{m-1}}\,ds\right.\\
&\left.+\int_0^{s^\#}\left(2\xi_r-s^{m-1}\right)^{\frac{1}{m-1}-2}\frac{w^\ell-\xi_r^{\ell-1}w}{s^{m-1}}\,ds\right]\\
=&\frac{1}{2}\left(1+(-1)^\ell\right)\frac{1}{m-1}c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\\
&-\frac{m-2}{m-1}c^{\frac{1}{m-1}-2}\left[(-1)^\ell\int_0^{s^\#}\left(2\xi_r-s^{m-1}\right)^{\frac{1}{m-1}-2}\frac{w^\ell-\xi_r^{\ell-1}w}{s^{m-1}}\,ds\right.\\
&\left.+\int_0^{s^\#}\left(2\xi_r-s^{m-1}\right)^{\frac{1}{m-1}-2}\frac{w^\ell-\xi_r^{\ell-1}w}{s^{m-1}}\,ds\right]
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{2}\left(1+(-1)^{\ell}\right)\frac{1}{m-1}c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3} \\
&\quad -\left(1+(-1)^{\ell}\right)\frac{m-2}{m-1}c^{\frac{1}{m-1}-2}\int_0^{s^{\#}}\left(2\xi_r-s^{m-1}\right)^{\frac{1}{m-1}-2}\frac{w^{\ell}-\xi_r^{\ell-1}w}{s^{m-1}}\,ds
\end{aligned}
\tag{3.19}
$$

If ℓ is odd, then (3.19) says $\partial_\ell H(0,0)=0$. If ℓ is even, then (3.19) is the same as (3.16) with $i=j=0$, and the first term in the last expression added. In light of this, we use (3.17) to say that

$$
\begin{aligned}
&\left(\frac{1}{m-1}c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}(0,\,0) \\
&\qquad = 1-\frac{2(m-2)}{m-1}\cdot\frac{1}{2}\int_0^1(1-t)^{\frac{1}{m-1}-2}\left(t^{\frac{\ell+1}{2}-1}-t^{1-1}\right)dt.
\end{aligned}
$$

Applying lemma 3.1, with $p=1/(m-1)$, $q_1=(\ell+1)/2$ and $q_2=1$, we get that the last equation

$$
\begin{aligned}
&= 1+\left(\frac{1}{m-1}-1+\frac{\ell+1}{2}\right)B\left(\frac{\ell+1}{2}\right)-\left(1+\frac{1}{m-1}-1\right)B(1) \\
&= 1+\frac{(\ell-1)m-(\ell-3)}{2(m-1)}B\left(\frac{\ell+1}{2}\right)-\frac{1}{m-1}(m-1) \\
&= \frac{1}{2}\cdot\frac{1}{m-1}\left[(\ell-1)m-(\ell-3)\right]B\left(\frac{\ell+1}{2}\right).
\end{aligned}
$$

Suppose that $\ell=0$ then the last equation shows that

$$
\frac{\partial H}{\partial\beta_0}(0,\,0)=c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{-3}\frac{3-m}{(m-1)^2}\cdot\frac{B}{2}. \tag{3.20}
$$

For $\ell\geq 1$, the term $B((\ell+1)/2)$ can be handled as before. Write $\ell=2k$, for $k\in\{1,\,...,\,\lfloor N/2\rfloor\}$, and use (3.11), then $B((\ell+1)/2)=B(k+1/2)=(m-1)^k\tau(k)[\nu(k)]^{-1}\cdot B$. Plugging this in we get that

$$
\begin{aligned}
\left(\frac{1}{m-1}c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}(0,0) &= \frac{1}{2}\frac{(2k-1)m-(2k-3)}{m-1}\cdot\frac{(m-1)^k\tau(k)}{\nu(k)}\cdot B \\
\left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\right)^{-1}\frac{\partial H}{\partial\beta_\ell}(0,0) &= \frac{(m-1)^{k-2}\tau(k)}{\nu(k-1)}\cdot\frac{B}{2} \\
\frac{\partial H}{\partial\beta_\ell}(0,0) &= c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\frac{(m-1)^{\frac{\ell}{2}-2}\tau\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}-1\right)}\cdot\frac{B}{2}.
\end{aligned}
$$

Note that using $\ell=0$ in this last equation does not give (3.20).This shows the result. ■

3.3.3 ∂f in the Barenblatt-Pattle case

Lemma 3.4. *Let $m > 2$. In the case of the Barenblatt-Pattle solution the derivative of the load vector given in* (B.9)-(B.11) *can be written more simply as*

$$\frac{\partial \mathbf{f}}{\partial \beta} = \begin{cases} 2i\,(i-1)\,mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B, & i+\ell \text{ even,} \\ 0, & \text{otherwise.} \end{cases} \tag{3.21}$$

Proof. We use (B.9) of the summary. First we calculate ∂I_1. Take $i \geq 1$. Using the formulas (B.10), (A.2), and the formulas for $q\left(\xi_\ell + s^{m-1}\right)$, $r\left(\xi_r - s^{m-1}\right)$, $p_x\left(\xi \pm s^{m-1}\right)$ and $p_{xx}\left(\xi \pm s^{m-1}\right)$ given above, we get

$$\begin{aligned}
\frac{\partial I_1}{\partial \beta_\ell}(i) = &-\frac{m\,(m-2)}{(m-1)^2}\left[\int_0^{s^*} c^{\frac{1}{m-1}-2}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-2}(-2cz)^2\,\frac{z^\ell - \xi_\ell^{\ell-1}z}{s^{m-1}}z^i\,ds\right. \\
&\left.+\int_0^{s^\#} c^{\frac{1}{m-1}-2}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2}(-2cw)^2\,\frac{w^\ell - \xi_r^{\ell-1}w}{s^{m-1}}w^i\,ds\right] \\
&+\frac{2\ell m}{m-1}\left[\int_0^{s^*} c^{\frac{1}{m-1}-1}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1}(-2cz)\,z^{i+\ell-1}\,ds\right. \\
&\left.+\int_0^{s^\#} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1}(-2cw)\,w^{i+\ell-1}\,ds\right] \\
&+\frac{2m}{m-1}\frac{c^{-1}}{2}\left[\xi_\ell^{\ell-1}\int_0^{s^*} c^{\frac{1}{m-1}-1}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1}(-2cz)\,(-2c)\,z^i\,ds\right. \\
&\left.+\xi_r^{\ell-1}\int_0^{s^\#} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1}(-2cw)\,(-2c)\,w^i\,ds\right] \\
&+\frac{im}{m-1}\frac{c^{-1}}{2}\left[\xi_\ell^{\ell-1}\int_0^{s^*} c^{\frac{1}{m-1}-1}\left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1}(-2cz)^2\,z^{i-1}\,ds\right. \\
&\left.+\xi_r^{\ell-1}\int_0^{s^\#} c^{\frac{1}{m-1}-1}\left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1}(-2cw)^2\,w^{i-1}\,ds\right]
\end{aligned}$$

$$
\begin{aligned}
= -\frac{4m\,(m-2)}{(m-1)^2} c^{\frac{1}{m-1}} \Bigg[& \int_0^{s^*} \left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{z^{i+\ell+2} - \xi_\ell^{\ell-1} z^{i+3}}{s^{m-1}}\, ds \\
& + \int_0^{s^\#} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+\ell+2} - \xi_r^{\ell-1} w^{i+3}}{s^{m-1}}\, ds \Bigg] \\
- \frac{4\ell m}{m-1} c^{\frac{1}{m-1}} \Bigg[& \int_0^{s^*} \left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1} z^{i+\ell}\, ds \\
& + \int_0^{s^\#} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+\ell}\, ds \Bigg] \\
+ \frac{4m}{m-1} c^{\frac{1}{m-1}} \Bigg[& \xi_\ell^{\ell-1} \int_0^{s^*} \left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1} z^{i+1}\, ds \\
& + \xi_r^{\ell-1} \int_0^{s^\#} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+1}\, ds \Bigg] \\
+ \frac{2im}{m-1} c^{\frac{1}{m-1}} \Bigg[& \xi_\ell^{\ell-1} \int_0^{s^*} \left(-2\xi_\ell - s^{m-1}\right)^{\frac{1}{m-1}-1} z^{i+1}\, ds \\
& + \xi_r^{\ell-1} \int_0^{s^\#} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+1}\, ds \Bigg]
\end{aligned}
$$

$$= -\frac{4m\,(m-2)}{(m-1)^2} c^{\frac{1}{m-1}} \left[(-1)^{i+\ell} \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+\ell+2} - \xi_r^{\ell-1} w^{i+3}}{s^{m-1}}\, ds \right.$$

$$\left. + \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{w^{i+\ell+2} - \xi_r^{\ell-1} w^{i+3}}{s^{m-1}}\, ds \right]$$

$$- \frac{4\ell m}{m-1} c^{\frac{1}{m-1}} \left[(-1)^{i+\ell} \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+\ell}\, ds \right.$$

$$\left. + \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+\ell}\, ds \right]$$

$$+ \frac{4m}{m-1} c^{\frac{1}{m-1}} \xi_r^{\ell-1} \left[(-1)^{i+\ell} \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+1}\, ds \right.$$

$$\left. + \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+1}\, ds \right]$$

$$+ \frac{2im}{m-1} c^{\frac{1}{m-1}} \xi_r^{\ell-1} \left[(-1)^{i+\ell} \int_0^{s^{*}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+1}\, ds \right.$$

$$\left. + \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} w^{i+1}\, ds \right]$$

Taking $i+\ell$ to be odd gives that $\partial_\ell I_1(i) = 0$. Take $i+\ell$ to be even, then

$$\left(\frac{4m}{m-1} c^{\frac{1}{m-1}}\right)^{-1} \frac{\partial I_1}{\partial \beta_\ell}(i) =$$

$$- \frac{2\,(m-2)}{m-1} \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-2} \frac{\left(\xi_r - s^{m-1}\right)^{i+\ell+2} - \xi_r^{\ell-1} \left(\xi_r - s^{m-1}\right)^{i+3}}{s^{m-1}}\, ds$$

$$- 2\ell \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} \left(\xi_r - s^{m-1}\right)^{i+\ell} ds$$

$$+ (i+2)\, \xi_r^{\ell-1} \int_0^{s^{\#}} \left(2\xi_r - s^{m-1}\right)^{\frac{1}{m-1}-1} \left(\xi_r - s^{m-1}\right)^{i+1} ds.$$

Changing variables using $s = (\xi_r - x)^{1/(m-1)}$ we get

$$\left(\frac{4m}{(m-1)^2} c^{\frac{1}{m-1}}\right)^{-1} \frac{\partial I_1}{\partial \beta_\ell}(i) = -\frac{2\,(m-2)}{m-1} \int_0^{\xi_r} \left(\xi_r^2 - x^2\right)^{\frac{1}{m-1}-2} \left(x^{i+\ell+2} - \xi_r^{\ell-1} x^{i+3}\right) dx$$

$$- 2\ell \int_0^{\xi_r} \left(\xi_r^2 - x^2\right)^{\frac{1}{m-1}-1} x^{i+\ell}\, dx$$

$$+ (i+2)\, \xi_r^{\ell-1} \int_0^{\xi_r} \left(\xi_r^2 - x^2\right)^{\frac{1}{m-1}-1} x^{i+1}\, dx.$$

Changing variables again, using $x = \xi_r y$, we get

$$\left(\frac{4m}{(m-1)^2}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_1}{\partial \beta_\ell}(i)$$
$$= -\frac{2(m-2)}{m-1}\int_0^1 \left(1-y^2\right)^{\frac{1}{m-1}-2}\left(y^{i+\ell+2}-y^{i+3}\right)dy$$
$$-2\ell\int_0^1 \left(1-y^2\right)^{\frac{1}{m-1}-1}y^{i+\ell}\,dy$$
$$+(i+2)\int_0^1 \left(1-y^2\right)^{\frac{1}{m-1}-1}y^{i+1}\,dy.$$

Changing variables one last time, using $y = t^{1/2}$, we get

$$\left(\frac{2m}{(m-1)^2}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_1}{\partial \beta_\ell}(i)$$
$$= -\frac{2(m-2)}{m-1}\int_0^1 (1-t)^{\frac{1}{m-1}-2}\left(t^{\frac{i+\ell+3}{2}-1}-t^{\frac{i+4}{2}-1}\right)dt$$
$$-2\ell\int_0^1 (1-t)^{\frac{1}{m-1}-1}t^{\frac{i+\ell+1}{2}-1}\,dt$$
$$+(i+2)\int_0^1 (1-t)^{\frac{1}{m-1}-1}t^{\frac{i+2}{2}-1}\,dt.$$

Using lemma 3.1 with $p = 1/(m-1)$, $q_1 = (i+\ell+3)/2$ and $q_2 = (i+4)/2$, we get

$$\left(\frac{2m}{(m-1)^2}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_1}{\partial \beta_\ell}(i) = 2\left(\frac{i+\ell+3}{2}+\frac{2-m}{m-1}\right)B\left(\frac{i+\ell+3}{2}\right)$$
$$-2\left(\frac{i+4}{2}+\frac{2-m}{m-1}\right)B\left(\frac{i+4}{2}\right)$$
$$-2\ell B\left(\frac{i+\ell+1}{2}\right)+(i+2)B\left(\frac{i+2}{2}\right)$$

$$\begin{aligned}=&2\frac{(i+\ell+1)m-(i+\ell-1)}{2(m-1)}B\left(\frac{i+\ell+3}{2}\right)-2\frac{(i+2)m-i}{2(m-1)}B\left(\frac{i+4}{2}\right)\\&-2\ell B\left(\frac{i+\ell+1}{2}\right)+(i+2)B\left(\frac{i+2}{2}\right).\end{aligned} \tag{3.22}$$

From this point we case on the parity of i.

Let $i = 2k_1$ for some $k_1 \in \{1, ..., \lfloor N/2 \rfloor\}$, then only even ℓ correspond to nonzero $\partial_\ell I_1(i)$ and we write $\ell = 2k_2$ for some $k_2 \in \{0, ..., \lfloor N/2 \rfloor\}$. Then (3.22) can be rewritten as

$$\begin{aligned}
=&2\frac{(i+\ell+1)m-(i+\ell-1)}{2(m-1)}B\left(k_1+k_2+\frac{3}{2}\right)-2\frac{(i+2)m-i}{2(m-1)}B(k_1+2)\\
&-2\ell B\left(k_1+k_2+\frac{1}{2}\right)+(i+2)B(k_1+1).
\end{aligned}$$

Using (3.11) and (3.12) this can be rewritten

$$\begin{aligned}
=&2\frac{(2k_1+2k_2+1)m-(2k_1+2k_2-1)}{2(m-1)}\cdot\frac{(m-1)^{k_1+k_2+1}\tau(k_1+k_2+1)}{\nu(k_1+k_2+1)}\cdot B\\
&-2\frac{(2k_1+2)m-2k_1}{2(m-1)}\cdot\frac{(m-1)^{k_1+2}(k_1+1)!}{\mu(k_1+1)}\\
&-2\ell\cdot\frac{(m-1)^{k_1+k_2}\tau(k_1+k_2)}{\nu(k_1+k_2)}\cdot B+(2k_1+2)\frac{(m-1)^{k_1+1}k_1!}{\mu(k_1)}
\end{aligned}$$

$$\begin{aligned}
&\left(2mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_1}{\partial\beta_\ell}(i)\\
&\quad=\frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2+1)}{\nu(k_1+k_2)}\cdot B-2\frac{(m-1)^{k_1-1}(k_1+1)!}{\mu(k_1)}\\
&\qquad\quad-2\ell\cdot\frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2)}{\nu(k_1+k_2)}\cdot B+2\frac{(m-1)^{k_1-1}(k_1+1)!}{\mu(k_1)}
\end{aligned}$$

$$\begin{aligned}
&=\frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2+1)}{\nu(k_1+k_2)}\cdot B-2\ell\cdot\frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2)}{\nu(k_1+k_2)}\cdot B\\
&=(i-\ell+1)\frac{(m-1)^{k_1+k_2-2}\tau(k_1+k_2)}{\nu(k_1+k_2)}\cdot B\\
&=(i-\ell+1)\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B,
\end{aligned}$$

or

$$\frac{\partial I_1}{\partial\beta_\ell}(i)=2(i-\ell+1)mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B. \tag{3.23}$$

In the last sequence of reductions we used that

$$\frac{\tau\left(k_1+k_2+1\right)}{\tau\left(k_1+k_2\right)}=2\left(k_1+k_2+1\right)-1=2k_1+2k_2+1=i+\ell+1.$$

Let $i=2k_1+1$ for some $k_1\in\{0,\ ...,\ \lfloor(N-1)/2\rfloor\}$, then only odd ℓ correspond to nonzero $\partial_\ell I_1(i)$ and we write $\ell=2k_2+1$, and $k_2\in\{0,\ ...,\ \lfloor(N-1)/2\rfloor\}$. Then (3.22) can be rewritten as

$$\begin{aligned}
&\left(\frac{2m}{(m-1)^2}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_1}{\partial\beta_\ell}(i)\\
&\quad=\frac{(i+\ell+1)\,m-(i+\ell-1)}{m-1}B\left(\frac{i+\ell+3}{2}\right)-\frac{(i+2)\,m-i}{m-1}B\left(\frac{i+4}{2}\right)\\
&\qquad\qquad-2\ell B\left(\frac{i+\ell+1}{2}\right)+(i+2)\,B\left(\frac{i+2}{2}\right)\\
&\quad=\frac{(i+\ell+1)\,m-(i+\ell-1)}{m-1}B\left(k_1+k_2+\frac{5}{2}\right)-\frac{(i+2)\,m-i}{m-1}B\left(k_1+\frac{5}{2}\right)\\
&\qquad\qquad-2\ell B\left(k_1+k_2+\frac{3}{2}\right)+(i+2)\,B\left(k_1+\frac{3}{2}\right)
\end{aligned}$$

$$
\begin{aligned}
&= \frac{(2k_1+2k_2+3)\,m-(2k_1+2k_2+1)}{m-1}\cdot\frac{(m-1)^{k_1+k_2+2}\,\tau\,(k_1+k_2+2)}{\nu\,(k_1+k_2+2)}\cdot B\\
&\quad-\frac{(2k_1+3)\,m-(2k_1+1)}{m-1}\cdot\frac{(m-1)^{k_1+2}\,\tau\,(k_1+2)}{\nu\,(k_1+2)}\cdot B\\
&\quad-2\ell\cdot\frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)}\cdot B+(i+2)\cdot\frac{(m-1)^{k_1+1}\,\tau\,(k_1+1)}{\nu\,(k_1+1)}\cdot B\\
&= \frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+2)}{\nu\,(k_1+k_2+1)}\cdot B-\frac{(m-1)^{k_1+1}\,\tau\,(k_1+2)}{\nu\,(k_1+1)}\cdot B\\
&\quad-2\ell\cdot\frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)}\cdot B+(i+2)\cdot\frac{(m-1)^{k_1+1}\,\tau\,(k_1+1)}{\nu\,(k_1+1)}\cdot B\\
&= (i+\ell+1)\,\frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)}\cdot B\\
&\qquad\qquad\qquad\qquad-(i+2)\,\frac{(m-1)^{k_1+1}\,\tau\,(k_1+1)}{\nu\,(k_1+1)}\cdot B\\
&\quad-2\ell\cdot\frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)}\cdot B+(i+2)\cdot\frac{(m-1)^{k_1+1}\,\tau\,(k_1+1)}{\nu\,(k_1+1)}\cdot B\\
&= (i-\ell+1)\,\frac{(m-1)^{k_1+k_2+1}\,\tau\,(k_1+k_2+1)}{\nu\,(k_1+k_2+1)}\cdot B\\
&= (i-\ell+1)\,\frac{(m-1)^{\frac{i+\ell}{2}}\,\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B,
\end{aligned}
$$

or

$$
\frac{\partial I_1}{\partial\beta_\ell}(i)=2\,(i-\ell+1)\,mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\,\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B. \tag{3.24}
$$

In the last sequence of reductions we used that

$$
\frac{\tau\,(k_1+k_2+2)}{\tau\,(k_1+k_2+1)}=2\,(k_1+k_2+2)-1=2k_1+2k_2+3=i+\ell+1,
$$

and that

$$
\frac{\tau\,(k_1+2)}{\tau\,(k_1+1)}=2\,(k_1+2)-1=2k_1+3=i+2.
$$

Note that (3.23) and (3.24) are equal.

Take $i=0$. In this case (B.10) picks up the boundary term

$$
\frac{m}{(m-1)^2}\beta_0^{\frac{1}{m-1}-1}\beta_1^2\left[\frac{\xi_\ell^\ell}{\theta_\ell}-\frac{\xi_r^\ell}{\theta_r}\right]
$$

and loses the last term. So, we can reuse the above computations. First we note that the boundary term has no contribution since the factor β_1 is zero as this is the coefficient of x in the Barenblatt-Pattle solution. We pick up the computation for this case at equation (3.22). Note that $\partial_\ell I_1(0) = 0$ if $i + \ell = \ell$ is odd. Take $i + \ell = \ell$ to be even, then

$$\begin{aligned}
&\left(\frac{4m}{(m-1)^2} c^{\frac{1}{m-1}} \xi_r^{\frac{2}{m-1}} \xi_r^{\ell-1}\right)^{-1} \frac{\partial I_1}{\partial \beta_\ell}(0) \\
&= \frac{(\ell+1)m - (\ell-1)}{2(m-1)} B\left(\frac{\ell+3}{2}\right) - \frac{2m}{2(m-1)} B(2) - \ell B\left(\frac{\ell+1}{2}\right) + B(1) \\
&\qquad = \frac{(\ell+1)m - (\ell-1)}{2(m-1)} B\left(\frac{\ell+3}{2}\right) - \ell B\left(\frac{\ell+1}{2}\right), \qquad (3.25)
\end{aligned}$$

where we have used the facts $B(2) = (m-1)^2/m$ and $B(1) = m-1$.

Let $\ell = 2k$, for some $k \in \{0, ..., \lfloor N/2 \rfloor\}$, then (3.25) can be rewritten as

$$\begin{aligned}
&\left(\frac{4m}{(m-1)^2} c^{\frac{1}{m-1}} \xi_r^{\frac{2}{m-1}} \xi_r^{\ell-1}\right)^{-1} \frac{\partial I_1}{\partial \beta_\ell}(0) \\
&\qquad = \frac{(\ell+1)m - (\ell-1)}{2(m-1)} B\left(k+\frac{3}{2}\right) - \ell B\left(k+\frac{1}{2}\right)
\end{aligned}$$

Using (3.11) and (3.12) this can be rewritten

$$\begin{aligned}
&= \frac{(2k+1)m - (2k-1)}{2(m-1)} \cdot \frac{(m-1)^{k+1}\tau(k+1)}{\nu(k+1)} \cdot B - \ell \frac{(m-1)^k \tau(k)}{\nu(k)} \cdot B \\
&= \frac{1}{2} \cdot \frac{(m-1)^k \tau(k+1)}{\nu(k)} \cdot B - \ell \cdot \frac{(m-1)^k \tau(k)}{\nu(k)} \cdot B \\
&= \frac{\ell+1}{2} \cdot \frac{(m-1)^k \tau(k)}{\nu(k)} \cdot B - \ell \cdot \frac{(m-1)^k \tau(k)}{\nu(k)} \cdot B \\
&= -\frac{\ell-1}{2} \cdot \frac{(m-1)^k \tau(k)}{\nu(k)} \cdot B,
\end{aligned}$$

or

$$\frac{\partial I_1}{\partial \beta_\ell}(0) = -2(\ell-1) m c^{\frac{1}{m-1}} \xi_r^{\frac{2}{m-1}} \xi_r^{\ell-1} \frac{(m-1)^{\frac{\ell}{2}-2} \tau\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}\right)} \cdot B.$$

Note that this is a special case of (3.23) or (3.24), which are equal.

We now calculate ∂I_2. Suppose $\ell \geq 2$, then we get

$$\begin{aligned}\frac{\partial I_2}{\partial \beta_\ell}(i) &= \frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, p_{xx}(x)\, x^{i+\ell}\, dx \\ &\quad + \frac{\ell(\ell-1)m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x)\, x^{i+\ell-2}\, dx \\ &= -\frac{2mc}{(m-1)^2}\int_{\xi_\ell}^{\xi_r}\left(a-cx^2\right)^{\frac{1}{m-1}-1} x^{i+\ell}\, dx \\ &\quad + \frac{\ell(\ell-1)m}{m-1}\int_{\xi_\ell}^{\xi_r}\left(a-cx^2\right)^{\frac{1}{m-1}} x^{i+\ell-2}\, dx,\end{aligned} \tag{3.26}$$

the integrands of which are odd if $i+\ell$ is odd and even when $i+\ell$ is even. This says that $\partial_\ell I_2(i) = 0$ if $i+\ell$ is odd. Take $i+\ell$ even, then the last equation

$$\begin{aligned}&= -\frac{4m}{(m-1)^2}c^{\frac{1}{m-1}}\int_0^{\xi_r}\left(\xi_r^2-x^2\right)^{\frac{1}{m-1}-1} x^{i+\ell}\, dx \\ &\quad + \frac{2\ell(\ell-1)m}{m-1}c^{\frac{1}{m-1}}\int_0^{\xi_r}\left(\xi_r^2-x^2\right)^{\frac{1}{m-1}} x^{i+\ell-2}\, dx \\ &= -\frac{4m}{(m-1)^2}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}-2}\xi_r^{i+\ell+1}\int_0^1\left(1-y^2\right)^{\frac{1}{m-1}-1} y^{i+\ell}\, dy \\ &\quad + \frac{2\ell(\ell-1)m}{m-1}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\int_0^1\left(1-y^2\right)^{\frac{1}{m-1}} y^{i+\ell-2}\, dy\end{aligned}$$

$$\begin{aligned}&\left(\frac{m}{m-1}c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_2}{\partial \beta_\ell}(i) \\ &= -\frac{2}{m-1}\int_0^1 (1-t)^{\frac{1}{m-1}-1} t^{\frac{i+\ell+1}{2}-1}\, dt + \ell(\ell-1)\int_0^1 (1-t)^{\frac{1}{m-1}} t^{\frac{i+\ell-1}{2}-1}\, dt \\ &\quad = -\frac{2}{m-1}B\left(\frac{i+\ell+1}{2}\right) + \ell(\ell-1)B\left(\frac{1}{m-1}+1,\ \frac{i+\ell-1}{2}\right) \\ &= -\frac{2}{m-1}B\left(\frac{i+\ell+1}{2}\right) + \frac{2\ell(\ell-1)}{(i+\ell-1)m-(i+\ell-3)}B\left(\frac{i+\ell-1}{2}\right)\end{aligned} \tag{3.27}$$

Using (3.11) we have

$$B\left(\frac{i+\ell+1}{2}\right) = \frac{(m-1)^{\frac{i+\ell}{2}}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B$$

and

$$B\left(\frac{i+\ell-1}{2}\right) = \frac{(m-1)^{\frac{i+\ell}{2}-1}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}\cdot B.$$

Using these we get that (3.27) is

$$= -\frac{2}{m-1}\frac{(m-1)^{\frac{i+\ell}{2}}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B$$
$$+\frac{2\ell(\ell-1)}{(i+\ell-1)m-(i+\ell-3)}\cdot\frac{(m-1)^{\frac{i+\ell}{2}-1}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}\cdot B$$

$$\left(mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\right)^{-1}\frac{\partial I_2}{\partial\beta_\ell}(i)$$
$$=-2\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B+2\ell(\ell-1)\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B$$
$$=-2(i+\ell-1)\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B+2\ell(\ell-1)\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B$$
$$=-2\left[i-(\ell-1)^2\right]\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B,$$

or

$$\frac{\partial I_2}{\partial\beta_\ell}(i)=-2\left[i-(\ell-1)^2\right]mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B, \quad (3.28)$$

Suppose that $\ell=0,1$, then the second term in (3.26) is absent and the calculations can be reused with this taken into account. When $i+\ell$ is odd, $\partial_\ell I_2(i)=0$, and when $i+\ell$ is even,

$$\frac{\partial I_2}{\partial\beta_\ell}(i)=-2mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B.$$

Note that this is a special case of (3.28).

We now add $\partial_\ell I_1$ in (3.24) and $\partial_\ell I_2$ in (3.28)

$$\frac{\partial\mathbf{f}}{\partial\beta_\ell}(i)=\frac{\partial I_1}{\partial\beta_\ell}(i)+\frac{\partial I_2}{\partial\beta_\ell}(i)$$
$$=2(i-\ell+1)mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B$$
$$-2\left[i-(\ell-1)^2\right]mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B$$
$$=2\Upsilon mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B,$$

where $\Upsilon = (i - \ell + 1)(i + \ell - 1) - \left[i - (\ell - 1)^2\right] = i(i-1)$ since

$$\tau\left(\frac{i+\ell}{2}\right) = (i + \ell - 1)\,\tau\left(\frac{i+\ell}{2} - 1\right).$$

This finishes the proof. ■

3.4 Jacobian is upper triangular for the Barenblatt-Pattle: case II

We now prove theorem 3.3.

Proof. As before we define $\Delta_\ell = \partial_\ell H\mathbf{g} + H\partial_\ell\mathbf{g} - \partial_\ell\mathbf{f}$ and we want to show that $\Delta_\ell = 0$. We will break the proof into cases on ℓ and i. The strategy is simple and the same for any of the below cases, plug $\partial_\ell H$ from (3.15); $\mathbf{g}$ from (3.2); H from (3.13); $\partial_\ell\mathbf{g}$ from (3.3)-(3.5); and $\partial_\ell\mathbf{f}$ from (3.21) into (3.6) and simplify.

In the first case all terms are wiped out by zeros. This case can be viewed as six subcases. Suppose that either

1. $\ell = 0$, $i \geq 1$, and i odd;
2. $\ell = 1$, and $i = 0$;
3. $\ell = 1$, $i \geq 2$, and i even;
4. $\ell \geq 2$, ℓ even, $i \geq 1$, and i odd;
5. $\ell \geq 2$, ℓ odd, $i = 0$; or
6. $\ell \geq 2$, ℓ odd, $i \geq 2$, and i even.

For any of these cases, we get (term four is not present for cases 1, 2, and 3)

$$\begin{aligned}\Delta_\ell(i) &= \frac{\partial H}{\partial \beta_\ell}(i,\,0)\,\mathbf{g}(0) + \frac{\partial H}{\partial \beta_\ell}(i,\,2)\,\mathbf{g}(2)\\ &\quad + H(i,\,\ell)\frac{\partial \mathbf{g}}{\partial \beta_\ell}(\ell) + H(i,\,\ell-2)\frac{\partial \mathbf{g}}{\partial \beta_\ell}(\ell-2) - \frac{\partial \mathbf{f}}{\partial \beta_\ell}(i)\\ &= 0\cdot\mathbf{g}(0) + 0\cdot\mathbf{g}(2) + 0\cdot\frac{\partial \mathbf{g}}{\partial \beta_\ell}(\ell) + 0\cdot\frac{\partial \mathbf{g}}{\partial \beta_\ell}(\ell-2) - 0 = 0.\end{aligned}$$

We must check the remaining cases:

7. $\ell = 0$, $i = 0$;

8. $\ell = 0$, $i \geq 2$, and i even;

9. $\ell = 1$, $i \geq 1$, and i odd;

10. $\ell \geq 2$, ℓ even, and $i = 0$;

11. $\ell \geq 2$, ℓ even, $i \geq 2$, and i even; and

12. $\ell \geq 2$, ℓ odd, $i \geq 1$, and i odd;

Case 7. In this case we get

$$\begin{aligned}\Delta_0(0) &= \frac{\partial H}{\partial \beta_0}(0,\,0)\,\mathbf{g}(0) + \frac{\partial H}{\partial \beta_0}(0,\,2)\,\mathbf{g}(2) + H(0,\,0)\frac{\partial \mathbf{g}}{\partial \beta_0}(0) - \frac{\partial \mathbf{f}}{\partial \beta_0}(0)\\ &= \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{-3}\frac{3-m}{(m-2)^2}\cdot\frac{B}{2}\right)(-2mca)\\ &\quad + \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{-1}\frac{(m-1)^{-1}\tau(1)}{\nu(0)}\cdot\frac{B}{2}\right)\left(\frac{2m(m+1)}{m-1}c^2\right)\\ &\quad + \left(c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{-1}\frac{(m-1)^{-1}\tau(0)}{\nu(0)}\cdot B\right)\left(-m\left(0^2+\frac{5-m}{m-1}\cdot 0+2\right)c\right)\\ &\quad - 0\end{aligned}$$

Using that $\tau(0) = \tau(1) = 1$, $\nu(0) = 1$ and $\xi_r^2 = a/c$; dividing Δ_0 by $\mathcal{C}_1 = c^{1/(m-1)}\xi_r^{2/(m-1)}\xi_r^{-1}$; and simplifying gives

$$\mathcal{C}_1^{-1}\Delta_0(0) = -\frac{3-m}{(m-2)^2} + \frac{m+1}{(m-1)^2} - \frac{2}{m-1} = 0$$

Case 8. In this case we get

$$
\begin{aligned}
\Delta_0(i) &= \frac{\partial H}{\partial \beta_0}(i,\,0)\,\mathbf{g}(0) + \frac{\partial H}{\partial \beta_0}(i,\,2)\,\mathbf{g}(2) + H(i,\,0)\,\frac{\partial \mathbf{g}}{\partial \beta_0}(0) - \frac{\partial \mathbf{f}}{\partial \beta_0}(i) \\
&= \left(c^{\frac{1}{m-1}-2} \xi_r^{\frac{2}{m-1}} \xi_r^{i-3} \frac{(m-1)^{\frac{i}{2}-2}\,\tau\left(\frac{i}{2}\right)}{\nu\left(\frac{i}{2}-1\right)} \cdot \frac{B}{2} \right)(-2mca) \\
&\quad + \left(c^{\frac{1}{m-1}-2} \xi_r^{\frac{2}{m-1}} \xi_r^{i-1} \frac{(m-1)^{\frac{i}{2}-1}\,\tau\left(\frac{i}{2}+1\right)}{\nu\left(\frac{i}{2}\right)} \cdot \frac{B}{2} \right)\left(\frac{2m(m+1)}{m-1} c^2 \right) \\
&\quad + \left(c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{i-1} \frac{(m-1)^{\frac{i}{2}-1}\,\tau\left(\frac{i}{2}\right)}{\nu\left(\frac{i}{2}\right)} \cdot B \right)\left(-m\left(0^2 + \frac{5-m}{m-1}\cdot 0 + 2\right) c \right) \\
&\quad - 2i(i-1)\,mc^{\frac{1}{m-1}} \xi_r^{\frac{2}{m-1}} \xi_r^{i-1} \frac{(m-1)^{\frac{i}{2}-2}\,\tau\left(\frac{i}{2}-1\right)}{\nu\left(\frac{i}{2}\right)} \cdot B
\end{aligned}
$$

Using that

$$
\frac{\tau\left(\frac{i}{2}+1\right)}{\tau\left(\frac{i}{2}\right)} = i+1 \qquad\qquad \frac{\tau\left(\frac{i}{2}\right)}{\tau\left(\frac{i}{2}-1\right)} = i-1
$$

and

$$
\frac{\nu\left(\frac{i}{2}\right)}{\nu\left(\frac{i}{2}-1\right)} = (i-1)\,m - (i-3)\,;
$$

dividing Δ_0 by

$$
\mathcal{C}_2 = c^{\frac{1}{m-1}-1} \xi_r^{\frac{2}{m-1}} \xi_r^{i-3} \frac{(m-1)^{\frac{i}{2}-2}\,\tau\left(\frac{i}{2}\right)}{\nu\left(\frac{i}{2}\right)} \cdot Bm,
$$

and simplifying gives

$$
\begin{aligned}
\mathcal{C}_2^{-1}\Delta_0(i) &= [(i-1)\,m - (i-3)]\,(-a) + c\xi_r^2\,(m-1)\,(i+1)\,\frac{(m+1)}{m-1} \\
&\quad + \xi_r^2\,(m-1)\,(-2c) - 2i\,(i-1)\,c\xi_r^2 \frac{1}{i-1}.
\end{aligned}
$$

Dividing by $a = c\xi_r^2$, and simplifying gives

$$
\begin{aligned}
(a\mathcal{C}_2)^{-1}\,\Delta_0(i) &= -\left[(i-1)\,m - (i-3)\right] + (m+1)\,(i+1) - 2\,(m-1) - 2i \\
&= 0
\end{aligned}
$$

Case 9. In this case we get

$$\begin{aligned}
\Delta_1(i) &= \frac{\partial H}{\partial \beta_1}(i,0)\,\mathbf{g}(0) + \frac{\partial H}{\partial \beta_1}(i,2)\,\mathbf{g}(2) + H(i,1)\frac{\partial \mathbf{g}}{\partial \beta_1}(1) - \frac{\partial \mathbf{f}}{\partial \beta_1}(i) \\
&= \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{i-2}\frac{(m-1)^{\frac{i+1}{2}-2}\tau\left(\frac{i+1}{2}\right)}{\nu\left(\frac{i+1}{2}-1\right)}\cdot\frac{B}{2}\right)(-2mca) \\
&\quad + \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{i}\frac{(m-1)^{\frac{i+1}{2}-1}\tau\left(\frac{i+1}{2}+1\right)}{\nu\left(\frac{i+1}{2}\right)}\cdot\frac{B}{2}\right)\left(\frac{2m(m+1)}{m-1}c^2\right) \\
&\quad + \left(c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{i}\frac{(m-1)^{\frac{i+1}{2}-1}\tau\left(\frac{i+1}{2}\right)}{\nu\left(\frac{i+1}{2}\right)}\cdot B\right)\left(-m\left(1^2+\frac{5-m}{m-1}\cdot 1+2\right)c\right) \\
&\quad - 2i(i-1)\,mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i}\frac{(m-1)^{\frac{i+1}{2}-2}\tau\left(\frac{i+1}{2}-1\right)}{\nu\left(\frac{i+1}{2}\right)}\cdot B.
\end{aligned}$$

Dividing Δ_1 by

$$\mathcal{C}_3 = c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{i}\frac{(m-1)^{\frac{i+1}{2}-2}\tau\left(\frac{i+1}{2}\right)}{\nu\left(\frac{i+1}{2}\right)}\cdot Bm,$$

we get

$$\begin{aligned}
\mathcal{C}_3^{-1}\Delta_1(i) &= \xi_r^{-2}\frac{\nu\left(\frac{i+1}{2}\right)}{\nu\left(\frac{i+1}{2}-1\right)}(-a) + c\frac{\tau\left(\frac{i+1}{2}+1\right)}{\tau\left(\frac{i+1}{2}\right)}(m+1) \\
&\quad - 2c(m+1) - 2i(i-1)\,c\frac{\tau\left(\frac{i+1}{2}-1\right)}{\tau\left(\frac{i+1}{2}\right)}.
\end{aligned}$$

Divide this by $c = a\xi_r^{-2}$ and use

$$\frac{\nu\left(\frac{i+1}{2}\right)}{\nu\left(\frac{i+1}{2}-1\right)} = im-(i-2), \qquad \frac{\tau\left(\frac{i+1}{2}+1\right)}{\tau\left(\frac{i+1}{2}\right)} = i+2,$$

and

$$\frac{\tau\left(\frac{i+1}{2}\right)}{\tau\left(\frac{i+1}{2}-1\right)} = i,$$

to get

$$\begin{aligned}
(c\mathcal{C}_3)^{-1}\Delta_1(i) &= -(im-(i-2)) + (i+2)(m+1) - 2(m+1) - 2i(i-1)\frac{1}{i} \\
&= 0.
\end{aligned}$$

Case 10. In this case we get

$$\begin{aligned}
\Delta_\ell(0) &= \frac{\partial H}{\partial \beta_\ell}(0,\,0)\,\mathbf{g}(0) + \frac{\partial H}{\partial \beta_\ell}(0,\,2)\,\mathbf{g}(2) + H(0,\,\ell)\,\frac{\partial \mathbf{g}}{\partial \beta_\ell}(\ell) \\
&\quad + H(0,\,\ell-2)\,\frac{\partial \mathbf{g}}{\partial \beta_\ell}(\ell-2) - \frac{\partial \mathbf{f}}{\partial \beta_\ell}(0) \\
&= \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\frac{(m-1)^{\frac{\ell}{2}-2}\,\tau\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}-1\right)}\cdot\frac{B}{2}\right)(-2mca) \\
&\quad + \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-1}\frac{(m-1)^{\frac{\ell}{2}-1}\,\tau\left(\frac{\ell}{2}+1\right)}{\nu\left(\frac{\ell}{2}\right)}\cdot\frac{B}{2}\right)\left(\frac{2m\,(m+1)}{m-1}c^2\right) \\
&\quad + \left(c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-1}\frac{(m-1)^{\frac{\ell}{2}-1}\,\tau\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}\right)}\cdot B\right)\left(-m\left(\ell^2+\frac{5-m}{m-1}\ell+2\right)c\right) \\
&\quad + \left(c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell-3}\frac{(m-1)^{\frac{\ell}{2}-2}\,\tau\left(\frac{\ell}{2}-1\right)}{\nu\left(\frac{\ell}{2}-1\right)}\cdot B\right)(m\ell\,(\ell-1)\,a) \\
&\quad - 0.
\end{aligned}$$

Dividing $\Delta_\ell(0)$ by

$$\mathcal{C}_3 = c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{\ell}\frac{(m-1)^{\frac{\ell}{2}-2}\,\tau\left(\frac{\ell}{2}-1\right)}{\nu\left(\frac{\ell}{2}\right)}\cdot Bm,$$

and substituting $a = \xi_r^2 c$ we get

$$\begin{aligned}
\mathcal{C}_3^{-1}\Delta_\ell(0) &= -\xi_r^{-1}\frac{\tau\left(\frac{\ell}{2}\right)}{\tau\left(\frac{\ell}{2}-1\right)}\cdot\frac{\nu\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}-1\right)} + \xi_r^{-1}(m+1)\,\frac{\tau\left(\frac{\ell}{2}+1\right)}{\tau\left(\frac{\ell}{2}-1\right)} \\
&\quad - \xi_r^{-1}(m-1)\left(\ell^2+\frac{5-m}{m-1}\ell+2\right)\frac{\tau\left(\frac{\ell}{2}\right)}{\tau\left(\frac{\ell}{2}-1\right)} + \ell\,(\ell-1)\,\xi_r^{-1}\frac{\nu\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}-1\right)}.
\end{aligned}$$

Using that

$$\frac{\tau\left(\frac{\ell}{2}\right)}{\tau\left(\frac{\ell}{2}-1\right)} = \ell-1, \qquad \frac{\tau\left(\frac{\ell}{2}+1\right)}{\tau\left(\frac{\ell}{2}-1\right)} = (\ell+1)\,(\ell-1),$$

and

$$\frac{\nu\left(\frac{\ell}{2}\right)}{\nu\left(\frac{\ell}{2}-1\right)} = (\ell-1)\,m-(\ell-3)\,;$$

and dividing by ξ_r^{-1} gives

$$\begin{aligned}\left(\xi_r^{-1}\mathcal{C}_3\right)^{-1}\Delta_\ell(0) &= -(\ell-1)\left[(\ell-1)m-(\ell-3)\right]+(m+1)(\ell+1)(\ell-1)\\ &-(m-1)\left(\ell^2+\frac{5-m}{m-1}\ell+2\right)(\ell-1)+\ell(\ell-1)\left[(\ell-1)m-(\ell-3)\right]\\ &= 0.\end{aligned}$$

Cases 11 and 12. These cases can be combined since $i+\ell$ is even. In these cases we get

$$\begin{aligned}\Delta_\ell(i) = {} & \frac{\partial H}{\partial\beta_\ell}(i,0)\,\mathbf{g}(0)+\frac{\partial H}{\partial\beta_\ell}(i,2)\,\mathbf{g}(2)+H(i,\ell)\frac{\partial\mathbf{g}}{\partial\beta_\ell}(\ell)\\ &+H(i,\ell-2)\frac{\partial\mathbf{g}}{\partial\beta_\ell}(\ell-2)-\frac{\partial\mathbf{f}}{\partial\beta_\ell}(i)\end{aligned}$$

$$\begin{aligned}= & \left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-3}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}\cdot\frac{B}{2}\right)(-2mca)\\ &+\left(c^{\frac{1}{m-1}-2}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-1}\tau\left(\frac{i+\ell}{2}+1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot\frac{B}{2}\right)\left(\frac{2m(m+1)}{m-1}c^2\right)\\ &+\left(c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-1}\tau\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B\right)\left(-m\left(\ell^2+\frac{5-m}{m-1}\ell+2\right)c\right)\\ &+\left(c^{\frac{1}{m-1}-1}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-3}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}\cdot B\right)(m\ell(\ell-1)a)\\ &-\left(2i(i-1)mc^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot B\right)\end{aligned}$$

Dividing $\Delta_\ell(i)$ by

$$\mathcal{C}_4 = c^{\frac{1}{m-1}}\xi_r^{\frac{2}{m-1}}\xi_r^{i+\ell-1}\frac{(m-1)^{\frac{i+\ell}{2}-2}\tau\left(\frac{i+\ell}{2}-1\right)}{\nu\left(\frac{i+\ell}{2}\right)}\cdot Bm,$$

and using that $\xi_r^2 = ac^{-1}$ we get

$$\begin{aligned}\mathcal{C}_4^{-1}\Delta_\ell(i) = & -\frac{\tau\left(\frac{i+\ell}{2}\right)}{\tau\left(\frac{i+\ell}{2}-1\right)}\cdot\frac{\nu\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}+(m+1)\frac{\tau\left(\frac{i+\ell}{2}+1\right)}{\tau\left(\frac{i+\ell}{2}-1\right)}\\ &-\left(\ell^2+\frac{5-m}{m-1}\ell+2\right)(m-1)\frac{\tau\left(\frac{i+\ell}{2}\right)}{\tau\left(\frac{i+\ell}{2}-1\right)}+\ell(\ell-1)\frac{\nu\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)}-2i(i-1)\end{aligned}$$

Using that

$$\frac{\tau\left(\frac{i+\ell}{2}\right)}{\tau\left(\frac{i+\ell}{2}-1\right)} = i+\ell-1, \qquad \frac{\tau\left(\frac{i+\ell}{2}+1\right)}{\tau\left(\frac{i+\ell}{2}-1\right)} = (i+\ell+1)\,(i+\ell-1)\,,$$

and

$$\frac{\nu\left(\frac{i+\ell}{2}\right)}{\nu\left(\frac{i+\ell}{2}-1\right)} = (i+\ell-1)\,m-(i+\ell-3)\,,$$

gives

$$\begin{aligned}
\mathcal{C}_4^{-1}\Delta_\ell\,(i) = &-(i+\ell-1)\,[(i+\ell-1)\,m-(i+\ell-3)] \\
&+(m+1)\,(i+\ell+1)\,(i+\ell-1)-\left(\ell^2+\frac{5-m}{m-1}\ell+2\right)(m-1)\,(i+\ell-1) \\
&+\ell\,(\ell-1)\,[(i+\ell-1)\,m-(i+\ell-3)]-2i\,(i-1) \\
&= 0. \qquad \blacksquare
\end{aligned}$$

CHAPTER 4

NUMERICAL EXPERIMENTS

We now evaluate the application of the models and bases from chapter 2 to (1.1)-(1.2). We give a brief overview of other methods and make general remarks concerning our methods. We then describe our numerical experiments to determine the order of accuracy for method 1, then method 2.

We give a quick snapshot of some previous studies of numerical methods for the PME. Graveleau and Jamet [14] solve the PE (1.7) by a splitting into the hyperbolic v_x^2 and parabolic $(m-1)\,vv_{xx}$ terms and using finite differences (FD). Tomoeda and Mimura [35] modify the method of [14] by solving the hyperbolic part by using a Rakine-Hugoniot jump condition. Di Benedetto and Hoff [9] adapt [14] by incorporating numerical solutions of the free boundary. Hoff [18] overcomes the parabolic stability condition on the mesh in [9] by including a viscosity parameter.

In another line of research, Berger et al. [4] used the non-linear Chernoff formula to solve linear approximations schemes applied to (1.1). Following this approach, others made extensions and contributed to error estimates: Magenes et al. [25] provide error estimates and show that using numerical integration preserves convergence, while Nochetto and Verdi [28] prove near-optimal error estimates. Unsatisfied with the performance of the method in [25], Jager and Kacur [19] improve the method by using a transformation and by using a relaxation parameter that incorporates the location of the free boundary. Pop and Yong [33] solve the PME by perturbing the IC rather than nonlinear diffusion coefficients as in [19], to marginally better success.

In order to demonstrate the effectiveness of their models, these authors commonly solved (1.1)-(1.2) with Barenblatt-Pattle initial conditions. It is not uncommon to demonstrate a method's effectiveness by overlaying plots of true and computed solutions or free boundaries. At this level of measure of accuracy, the methods in this dissertation compare favorably: when a graph of a numerical solution generated by our methods and the corresponding true solution are overlaid upon one another the naked eye cannot discern a difference (See the top panels of figure 4.1 and figure 4.3). For those methods described in the papers mentioned above, it is valid to use the Barenblatt-Pattle solution since it cannot be expressed exactly in terms of the numerical solution. For model solution $\tilde{z}$ of (2.1)-(2.2), (2.37), we can use the Barenblatt-Pattle solution as a benchmark since the Barenblatt-Pattle solution is not included as one of the solutions. Figure 4.3 shows that while the numerical solutions converge to the true solution, the errors decay slowly, more so near the free boundary where a boundary layer can be seen to develop as $m \to \infty$. For model solution $\tilde{u}$ of (2.18)-(2.20), (2.34), the Barenblatt-Pattle solution is part of the model solution. In this case one should realize that observed errors result from the quadrature of inner products, from the inversion of linear systems, and from time-stepping, but not from the discrete nature of the approximate solution.

4.1 Experimentally determining global order of accuracy: PME

We experimentally determined the rate at which the error decays in order to evaluate models and bases. The experiment was set up as follows: we computed each of the model solutions $\tilde{z}$ and $\tilde{u}$ of equations (2.1)-(2.2), (2.37) and (2.18)-(2.20), (2.34), respectively; each using the standard basis then *the modified Legendre basis*. Recall that we will refer to the modified Legendre basis constructed in subsection 2.2.4 as the modified Legendre basis (MLB). We used 4th- and 8th-order Runge-Kutta methods to numerically solve the semi-discrete systems in time: (2.6) in the case of model 1 and (2.22) in the case of model 2. For initial conditions we used

$$u_0(x,\, t) = B(x,\, t + t_0) \tag{4.1}$$

of (1.6) with $A = 1$, $C = (m-1)/(2m(m+1))$ and t_0 such that the $\xi_r(0) = -\xi_\ell(0) = 3$: $t_0 = \left(\xi_r(0)\sqrt{C/A}\right)^{m+1}$.

For each combination of model, basis, and time-stepping method, we proceeded as follows: for a fixed degree N in (2.1) and in (2.19), we shrank the time step size parameter k until a particular error level, to be described below, was reached. Labeling this value of k by $k_{opt} = k_{opt}(N)$, we fitted this experimental relationship between k_{opt} and N. The error corresponding to each pair $(N, k_{opt}(N))$, e_{opt}, was then used to determine an experimental relationship between k_{opt} and the errors.

Before we can define k_{opt} we must introduce the best approximation (BA) and its error. For both models and bases, the BA uses both the true solution and true free boundary to approximate u and ξ. Let $t \in [0, T]$. We will omit the dependence on t in our notation: $\xi \equiv \xi(t)$, $c_j \equiv c_j(t)$, $d_j \equiv d_j(t)$. Let

$$d_i = \int_{\Xi(t)} f(B(x,t))\, \phi_i(x)\; dx, \tag{4.2}$$

for $i = 0, \ldots, N-2$, where B is the true Barenblatt-Pattle solution corresponding to (4.1), $\{\phi_i\}_{i=0}^{N}$ is orthonormal on $\Xi(t)$,

$$f(r) = \frac{r}{(\xi_r - x)(x - \xi_\ell)}$$

for model 1 and

$$f(r) = \frac{r^{m-1}}{(\xi_r - x)(x - \xi_\ell)}$$

for model 2.

In the case of model 1, the BA is given by

$$\tilde{z}_{BA}(x) = \sum_{j=0}^{N} c_j \phi_j(x),$$
$$\tilde{w}_{BA}(x) = \sum_{j=0}^{N-2} d_j \phi_j(x)$$

where $\{c_i\}_{i=0}^N$ are computed from $\{d_i\}_{i=0}^N$ in (4.2) so that

$$\tilde{z}_{BA}(x) = (\xi_r - x)(x - \xi_\ell)\,\tilde{w}_{BA}(x).$$

In the case of model 2, the BA is given by

$$\tilde{u}_{BA}(x) = \left[\sum_{j=0}^{N} c_j \phi_j(x)\right]^{1/(m-1)},$$
$$\tilde{v}_{BA}(x) = \sum_{j=0}^{N-2} d_j \phi_j(x)$$

where $\{c_i\}_{i=0}^N$ are computed from $\{d_i\}_{i=0}^N$ in (4.2) so that

$$\tilde{u}_{BA}^{m-1}(x) = (\xi_r - x)(x - \xi_\ell)\,\tilde{v}_{BA}(x).$$

For either model, in the case of standard basis the coordinates $\{c_i\}_{i=0}^N$ are further converted to coordinates with respect to the standard basis $\{x^i\}_{i=0}^N$, $\{\tilde{c}_i\}_{i=0}^N$, so that

$$\sum_{j=0}^{N} c_j \phi_j(x) = \sum_{j=0}^{N} \tilde{c}_j x^j.$$

Practically, the above procedures for determining $\{d_j\}_{i=0}^N$ amount to solving

$$(w - \tilde{w}_{BA}, \phi_i)_{\Xi(t)} = 0,$$

in the case of model 1 and

$$(v - \tilde{v}_{BA}, \phi_i)_{\Xi(t)} = 0,$$

for $i = 0, \ldots, N-2$, in the case of model 2, where w and v are defined implicitly, like w_0 and v_0 in (2.36) and (2.31), respectively,

$$\begin{aligned} B(x,t) &= (\xi_r - x)(x - \xi_\ell)\, w(x), \\ &= \left[(\xi_r - x)(x - \xi_\ell)\, v(x)\right]^{1/(m-1)}. \end{aligned}$$

With the BA defined for both models, we set the errors to be

$$e^1_{BA} = \left\| z_{BA}(\,\cdot\,, T) - B(\,\cdot\,, T)\right\|$$

and

$$e^2_{BA} = \left\| u_{BA}(\,\cdot\,, T) - B(\,\cdot\,, T)\right\|,$$

where $\|\cdot\|$ is the L_2-norm over $\Xi(T) \cup \widehat{\Xi}(T)$. Recall that $\widehat{\Xi}(T)$ is the "administrative" numerical support that is retained from time step to time step. Furthermore, let

$$e^1 = \left\| \tilde{z}(\,\cdot\,, T) - B(\,\cdot\,, T)\right\|$$

and

$$e^2 = \left\| \tilde{u}(\,\cdot\,, T) - B(\,\cdot\,, T)\right\|.$$

Note that the superscripts denote labels, rather than powers and that we will use e_{BA} and e when the model is irrelevant.

The following procedure was used to assign to each N a k_{opt}. For each N, we shrunk k until an $e \approx e_{BA}$. The value of k for which this happened was labeled k_{opt}. Sometimes, shrinking k produced e that shrunk but never achieved the size of e_{BA}. In these cases, we labeled that k for which the error was minimal by k_{opt}. We label the error corresponding to each k_{opt} by e_{opt}. When we need to distinguish between which model produced the error we use a superscript: e^1_{opt} and e^2_{opt}.

Two kinds of instabilities were observed during these trials. Considering the semi-discrete systems (2.14) and (2.30), we apply the terms *stability* and *Eigenvalue* *stability (e-stability)* as Trefethen does in his monograph [37]. Specifically, the terms *stability* and *Eigenvalue stability (e-stability)* apply to ODE systems and answer the following two questions that arise when performing an experiment that aims to experimentally determine the accuracy of a method:

stability: For fixed t, do numerical solutions remain bounded as $k \downarrow 0$?

e-stability: For fixed k, do numerical solutions remain bounded as $t \to \infty$?

For fixed N and k, consider trying to step in time from $t = 0$ to $t = T$. The numerical method crashed if the time step size parameter k was too large. Specifically, there is a value of the time step size parameter k_{comp} where the numerical method did not run to completion if $k > k_{comp}$. In these cases there is a t_{crash} such that for $t < t_{crash}$ the numerical solution exists, while for $t > t_{crash}$ the polynomial component of the model solution loses roots (see remark 2.2 and figure 2.2), at which point the definitions of the method do not make sense. This is most likely caused by the time-stepping method.

Recall that $\mathbf{g}$ is the symbol denoting the derivative in a semi-discrete system: (2.14) and (2.30). Eigenvalue stability of these semi-discrete systems might be better understood by the first order approximation $\partial \mathbf{g}\left(\boldsymbol{\beta}, t\right) / \partial \boldsymbol{\beta}$, (see chapter 3). We did not investigate the second order terms, though they can be important. Trefethen [37] illustrates how the behavior of such higher-order terms can reveal more structure (in the form of instability). Roughly*, the containment of the point spectrum of $\mathbf{g}$ in the stability region of the time-stepping method (e.g. RK4, RK8, or leap frog) will dictate stability constraints on the time-stepping solution of the semi-discrete system [37, 17]. For linear systems convergence and stability are nearly equivalent, though this need not be the case for nonlinear systems. Modes (basis functions) corresponding to eigenvalues not contained (at least roughly) in

*modulo a factor of the step size parameter k

the stability region of the time-stepping method will not be bounded.

Now, suppose that $k < k_{comp}$ so that marching in time from $t = 0$ to $t = T$ is possible for all $k \downarrow 0$. As mentioned in subsection 2.1.2, the numerical methods naturally define numerical free boundaries when the methods are used in this stable regime of k. However, for some N it happens that as $k \downarrow 0$, e grows from a minimum. In such cases the numerical solution is equal to a "nearby" errant approximant. The bottom panel of figure 4.1 shows typical behavior of such errant solutions. As $k \downarrow 0$ the errors in these approximants could grow to troublesome sizes.

We now present results from experiments on each combination of model numerical solution and the two bases: the standard basis and the modified Legendre basis. We fit the resulting data in order to experimentally determine the order of accuracy.

First we verify the observations made in chapter 2 about the effect of the choice of basis on the numerical solution. Table 4.1 shows the poor performance of the standard basis. In this case, the error e^2_{opt} tracks the order 10^{-15} error e^2_{BA}, until $N = 12$ where e^2_{opt} grows unboundedly as $N \to \infty$. When $N \geq 12$ the condition of the matrices is large enough to affect numerical solution and e^2_{opt} begins to grow unboundedly away from e^2_{BA}. Also, the error e^1_{opt} tracks the order 10^{-2} error e^1_{BA}, until $N = 22$ where the method breaks down. Table 4.1 also shows how nicely-conditioned the linear solution of the semi-discrete systems becomes when the modified Legendre basis (MLB) is used. Indeed, for either model, using the modified Legendre basis instead of the standard basis allows for accurate resolution of numerical solutions for larger N: e_{opt} tracks or is smaller than e_{BA}.

Before moving one we mention some patterns that occur in $\kappa(t)$ when the modified Legendre basis is used. If we fix N and k and watch $\kappa(t)$ as the time-

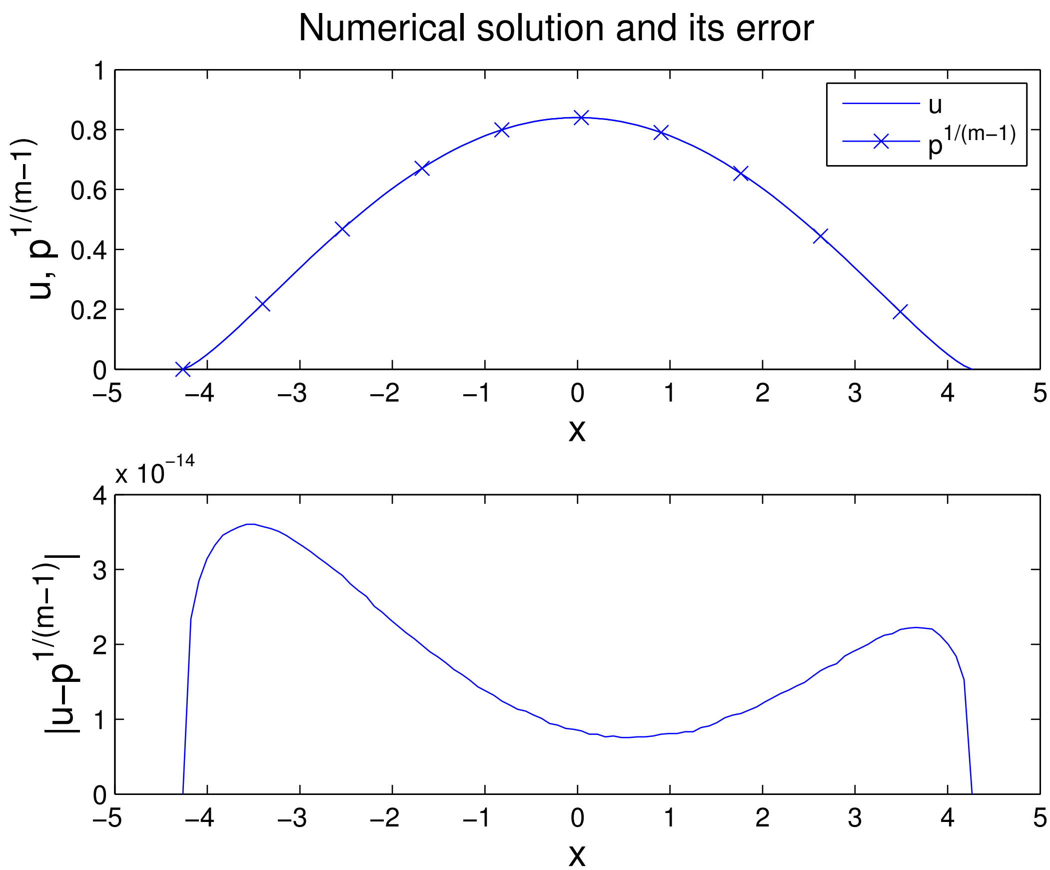

Figure 4.1: Errant numerical solution matches quite well, but the error shows that the numerical solution is actually a "nearby" function. Note that the method should be programmed to take advantage of the symmetry of the problem because the numerical method does not respect parity in such solutions. This example is for $m = 1.75$, $N = 16$, and $k = 1/17 < k_{opt} = 1/15$ where model 2 and the modified Legendre basis are used.

Table 4.1: Spectral condition number of mass matrices in (2.8) and (2.24) for $t = 1$. Here, $m = 1.75$, RK8 and $k = k_{opt}$. DNC means that k_{opt} could not be found in the range of k we searched.

	model 1		model 2	
N	standard	MLB	standard	MLB
4	3.8019e+04	1.3948	2.5423e+04	2.1578
6	1.5381e+07	1.8074	8.7008e+06	2.6276
8	7.6870e+09	2.0336	3.9832e+09	3.0522
10	4.6062e+12	2.0266	2.2333e+12	3.4508
12	2.9987e+15	2.1153	1.3667e+15	3.8688
14	2.0192e+18	2.1713	8.7300e+17	4.2527
16	8.7910e+20	2.2083	7.3380e+23	4.6288
18	7.4063e+24	2.2337	1.1067e+26	4.9246
20	1.9060e+26	2.2521	3.2192e+29	5.2992
22	DNC	2.2983	1.5077e+30	5.5729
24	DNC	2.3039	DNC	5.8693
26	DNC	2.3083	DNC	6.1594

stepping method marches through $[0, T]$, we see that $\kappa(t)$ is a bounded function. See figure 4.2. $\kappa(t)$ dips for t within a timestep of RK8, at its so-called stages. This pattern persists as $N \to \infty$. When model 1 is used, the scale of $\kappa(t)$ grows like $\mathcal{O}(N)$, with a small constant, as $N \to \infty$. As $m \to \infty$, the dipping pattern changes to a backslash-shaped (\) sawtooth function and the scaling pattern persists as $N \to \infty$. When model 2 is used and $m = 1.75$, $\kappa(t)$ is a backslash-shaped sawtooth function. As $N \to \infty$ a sag develops in the sawtooth and the scale grows to about 90. When model 2 is used and $m = 3$ or $m = 5$, $\kappa(t)$ is a forward slash-shaped sawtooth function. As $N \to \infty$ a sag develops in the sawtooth and the scale grows to about 120.

As mentioned, applying model 2 to Barenblatt-Pattle initial conditions results in errors on the order of machine epsilon regardless of the value of $N \geq 2$. This is expected since there is no approximation error in the numerical solution form in this case. Here, the only sources of error are from the use of quadrature and from time-stepping, the former of which includes solution of linear systems. Since this

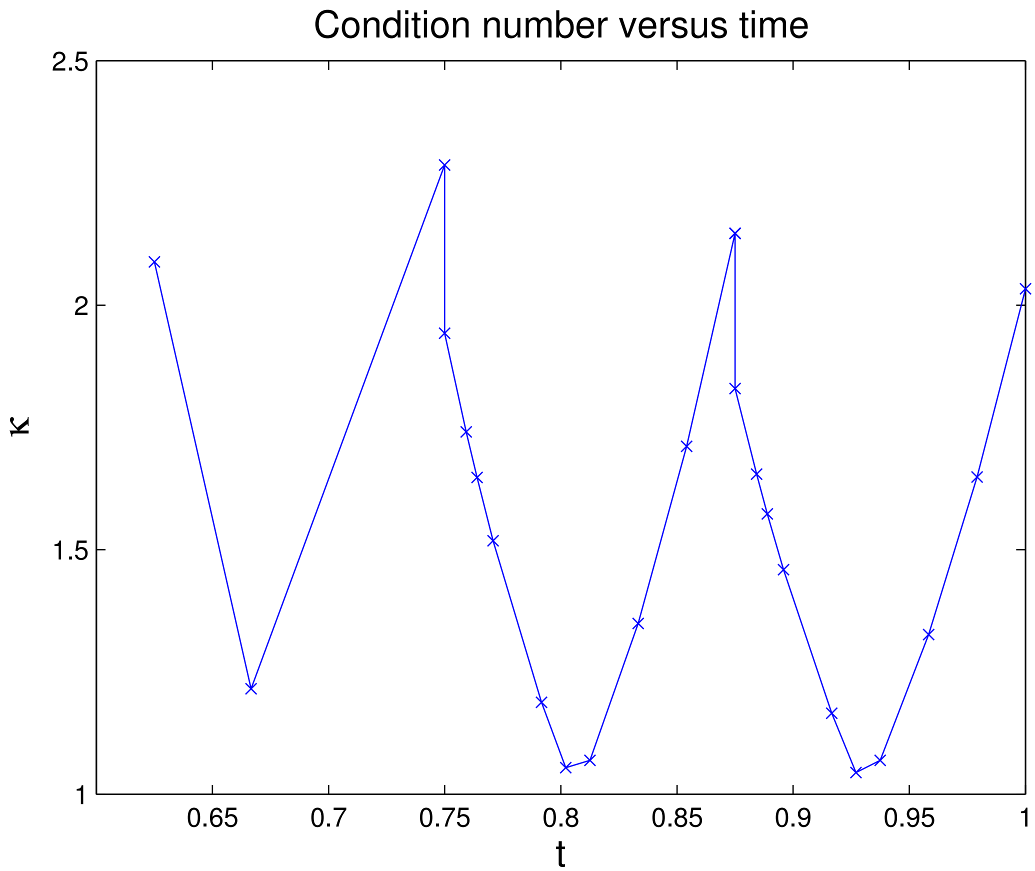

Figure 4.2: The spectral condition number of matrices in (2.8), $\kappa(t)$, when using the modified Legendre basis constructed in subsection 2.2.4 for $t \in \{t_i\}$, and where t_i are the thirty largest time values used by RK8. The condition number is bounded as a function of time. Here, $m = 1.75$, $N = 8$, and $k = 1/8$. Note the drop and rise of the condition number within the last two steps of the time stepping method. Within each time step RK8 evaluates the derivative in the semi-discrete system at 13 stages/times, 10 of which are unique.

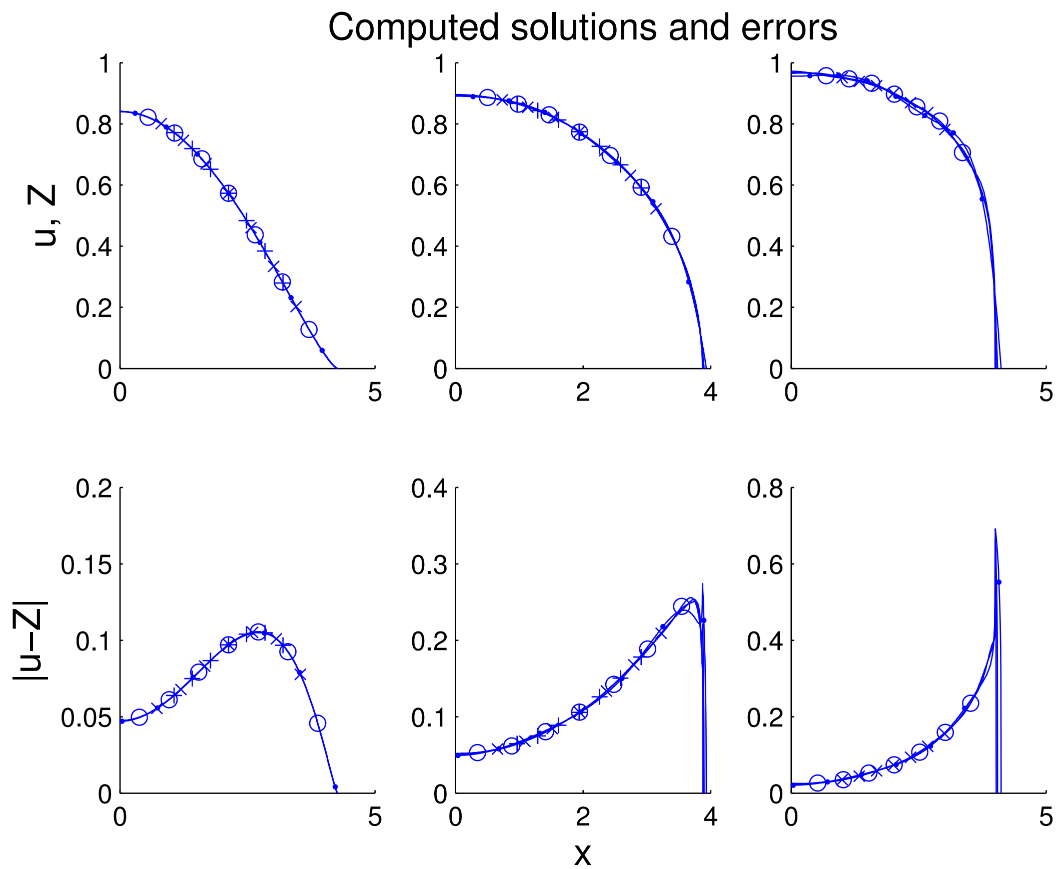

Figure 4.3: Model 1 solutions and their errors as $m \to \infty$. Columns 1, 2, and 3 correspond to $m = 1.75$, $m = 3$, $m = 5$, respectively. Note that a boundary layer forms as $m \to \infty$. $Z = \tilde{z}$ is our model 1. Markers for curves are $\cdot$ for $N = 8$, o for $N = 14$, $\times$ for $N = 20$, and $+$ for $N = 26$. The functions pictured in the two right-most panels in the top row of panels are the same functions pictured in figure 2.1.

does not test model 2's ability we confine our remarks to model 1. As the standard basis restricts our ability to use large N, we also limit our remarks to the use of the modified Legendre basis.

Figure 4.3 shows model 1 solutions and their errors for a selection of m values as $m \to \infty$. Our results are drawn from these solutions.

Fix m to be 1.75, 3, or 5. Consider data corresponding to either k_{opt} or e_{opt}: a set of tuples $(N, k_{opt}(N))$ or $(N, e_{opt}(N))$, for $N = 4, \ldots, 26$. We fit this data

Table 4.2: Fitting parameters α and C in $k_{opt} = CN^{-\alpha}$ and $e_{opt} = CN^{-\alpha}$ as $m \to \infty$.

	$m = 1.75$		$m = 3$		$m = 5$	
k_{opt}	1.8107,	4.8152	1.8999,	2.8831	1.6000,	2.9314×10^{-1}
e_{opt}	1.7975,	4.3092×10^{-1}	1.8834,	1.1152	1.4023,	1.5208

Table 4.3: Estimated order of accuracy p in $e_{opt} = Ck_{opt}^p$. C is 9.0523×10^{-2}, 3.9038×10^{-1}, and 4.4581, for $m = 1.75$, $m = 3$, and $m = 5$, respectively.

$m = 1.75$	$m = 3$	$m = 5$
0.9927	0.9913	0.8764

to a power model, $CN^{-\alpha}$, an exponential model, $C\alpha^N$, and an exponential model with geometric rate r, $C\alpha^{N^r}$, to determine which fits best. We then used the proper fittings to estimate p in $e_{opt} = Ck_{opt}^p$. In each case a power model was most appropriate. This led to the following estimates

$$\begin{aligned} k_{opt} &= C_1 N^{-\alpha_1}, \\ e_{opt} &= C_2 N^{-\alpha_2}, \\ &= C_3 k_{opt}^p, \end{aligned}$$

where $C_3 = C_2 C_1^{-\alpha_1/\alpha_2}$ and $p = \alpha_2/\alpha_1$. Table 4.2 shows the fitting parameters and table 4.3 shows the pattern in the estimated global order of accuracy as $m \to \infty$.

4.2 Experimentally determining global order of accuracy: EUF

We next investigate the global order of accuracy of the fully discrete method when time-stepping with RK4 and RK8. We present an instance of the initial value EUF problem (1.8)-(1.9). Suppose w is the solution of this problem for a given φ and initial condition, w_0. We compute a sequence of sG solutions $\{\tilde{w}\}_{N=0}^{\infty}$. We fit numerical data to the error model $\|w(\cdot, T) - \tilde{w}(\cdot, T)\| = Ck^p$, where

$k = O(f(N)) \to 0$ as $N \to \infty$, $\|\cdot\|$ is an L_2-norm, and where we determine f experimentally.

We compute a sG solution $\tilde{w}$ to the EUF IVP (1.8)-(1.9) with

$$\varphi(u) = -u - \sqrt{a^2 - u^2} \arccos\left(\frac{u}{a}\right) + \frac{\pi}{2} a, \tag{4.3}$$

$$a \equiv a(t) = a_0 b_0^{-1} \left(2t + b_0^{-2}\right)^{-1/2}, \tag{4.4}$$

$$a_0 = \frac{1}{2} M b_0, \tag{4.5}$$

$$b_0 = \frac{\pi}{2} \xi_r^{-1}(0), \tag{4.6}$$

$M = \int_{\xi_\ell(0)}^{\xi_r(0)} w_0(x)\, dx$, and $\Xi(0) := (\xi_\ell(0), \xi_r(0))$ is the support of w_0. If $w_0(x) = a_0 \cos(b_0 x)$, then $w(x,t) = a(t) \cos(b(t)x)$, where $b(t) = \left(2t + b_0^{-2}\right)^{-1/2}$. With such initial profiles $\frac{\partial}{\partial t} \int_{\xi_\ell(t)}^{\xi_r(t)} w(x,t)\, dx = 0$ for any, $t \geq 0$.

Our numerical solution $\tilde{w}$ will take the form

$$\tilde{w}(x,t) = \sum_{j=0}^{N} \beta_j(t) \phi_j(x).$$

The basis $\{\phi_i\}_{i=0}^N$ is as in subsection 2.2.4, orthogonal on an approximation to the support at time $t = k$, where k is the time step used in the semi-discrete system solver. The approximate support is gotten by using a differential equation (given explicitly below) analogous to (2.42). Assume that $\tilde{w}$ has roots $\tilde{\xi}(t)$ that comprise the approximate free boundary and which define the support of $\tilde{w}$: $\tilde{\Xi}(t) := \left(\tilde{\xi}_\ell(t), \tilde{\xi}_r(t)\right)$. Let $\tilde{w}_0(x) = \tilde{w}(x,0)$ and define $\tilde{q}_0 \in \Pi_{N-2}$ and q_0 implicitly such that

$$w_0(x) = (\xi_r(0) - x)(x - \xi_\ell(0))\, q_0(x),$$

$$\tilde{w}_0(x) = (\xi_r(0) - x)(x - \xi_\ell(0))\, \tilde{q}_0(x).$$

The coefficients $\{\beta_i\}_{i=0}^N$ are determined by forcing $\tilde{w}$ to satisfy the weak formulation of (1.8)-(1.9), (4.3)-(4.6):

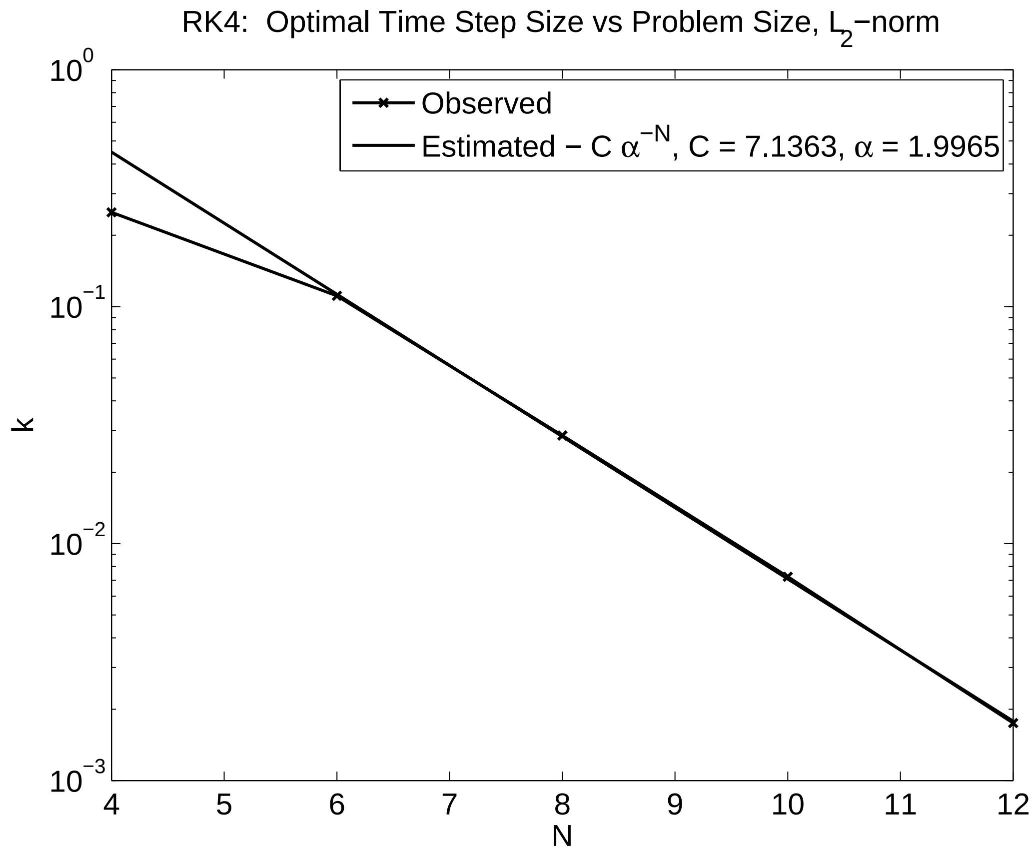

Figure 4.4: Optimal k versus N where e and e_{BA} are measured in the L_2 norm.

Find $\tilde{w} \in \Pi_N$ such that

$$\left(\tilde{w}_t - \varphi\left(\tilde{w}\right)_{xx}, \phi_i\right)_{\widetilde{\Xi}(t)} = 0, \tag{4.7}$$

for $i = 2, \ldots, N$, and

$$\left(q_0 - \tilde{q}_0, \phi_i\right)_{\Xi(0)} = 0 \tag{4.8}$$

for $i = 2, \ldots, N-2$. We have lost two degrees of freedom by setting $\widetilde{\Xi}(0) = \Xi(0)$.

Suppose that $\boldsymbol{\gamma_0} = \left(\gamma_j(0)\right) \in \mathbb{R}^{N-1}$ is the vector of the coordinates of q with respect to the basis $\{\phi_i\}_{i=0}^{N}$. To solve (4.7)-(4.8) we first solve (4.8) by finding $\boldsymbol{\gamma_0}$ such that

$$\sum_{j=0}^{N-2} \left(\phi_j, \phi_i\right)_{\Xi(0)} \gamma_j(0) = \left(q_0, \phi_i\right)_{\Xi(0)}$$

or, in matrix-vector notation,

$$H\boldsymbol{\gamma_0} = \mathbf{f_0}, \tag{4.9}$$

where $H = (H(i,j)) \in \mathbb{R}^{(N-1)\times(N-1)}$, $\mathbf{f_0} = (f_{0,i}) \in \mathbb{R}^{N-1}$,

$$\begin{aligned} H(i,j) &= (\phi_j, \phi_i) \\ &= \int_{\Xi(0)} \phi_j(x)\,\phi_i(x)\; dx. \end{aligned}$$

and

$$f_{0,i} = \int_{\Xi(0)} \frac{w_0(x)\,\phi_i(x)}{(\xi_r(0) - x)(x - \xi_\ell(0))}\, dx.$$

Note that $H(i,j) \neq \delta_{i,j}$ since $\{\phi_i\}_{i=0}^N$ is not orthogonal on $\Xi(0)$ but on $\breve{\Xi}(k)$.

To solve (4.7) we find $\{\beta_i(k)\}_{i=0}^N$ by plugging $v = \tilde{w}$ into (4.7) where $v_t(x,t) = \sum_{j=0}^N \beta_j'(t)\,\phi_j(x)$ and

$$\varphi(v)_{xx} = \frac{\arccos(v/a)}{\sqrt{a^2 - v^2}}\left(vv_{xx} + v_x^2\right) + \frac{\arccos(v/a)}{\left(v^2 - a^2\right)^{3/2}} v^2 v_x^2 - \frac{v}{a^2 - v^2} v_x^2$$

In order to find the approximation to $\Xi(t+k)$, $\widetilde{\breve{\Xi}}(t+k)$, we use the differential equation satisfied by the free boundary curve [22]

$$\xi'(t) = -\nu_x(\xi(t), t), \tag{4.10}$$

where $\nu = \psi(v)$, $\psi(s) = \int_0^s \varphi'(z)\, z^{-1}\, dz$. So, $\nu_x = \psi'(v)\, v_x$.

Thus,

$$\nu_x = \frac{\arccos(v/a)}{\sqrt{a^2 - v^2}} v_x \tag{4.11}$$

Using the generalized velocity, ν_x, (4.11) and the numerical form in (4.10) we get

$$\begin{aligned} \xi' &= -\frac{\arccos(v(\xi)/a)}{\sqrt{a^2 - v(\xi)^2}} v_x(\xi) \\ &= -\frac{\arccos(0/a)}{\sqrt{a^2 - 0^2}} v_x(\xi) \\ &= -\frac{\pi}{2a} v_x(\xi). \end{aligned}$$

Table 4.4: Fitting parameters α and C in $k_{opt} = C\alpha^{-N}$ for each time stepping method and for each norm.

	RK4		RK8	
L_2	1.9965,	7.1363	1.5651,	7.2492
L_∞	1.9997,	7.3000	1.6028,	8.6773

We use this to take an Euler step

$$\breve{\xi}(t+k) = \xi(t) - k\frac{\pi}{2a}v_x(\xi(t))$$

to find $\breve{\Xi}(t+k)$.

Let $w_{BA}(x,T)$ be the solution to (4.8) with w_0 replaced with $w(x,T)$, let $e = \|w(\cdot,T) - \tilde{w}(\cdot,T)\|$ and $e_{BA} = \|w(\cdot,T) - w_{BA}(\cdot,T)\|$, where $\|\cdot\|$ is the L_2-norm over $\Xi(T) \cup \widehat{\Xi}(T)$. As a check we also computed L_∞-norms over $\Xi(T) \cup \widehat{\Xi}(T)$. For each time stepping scheme, RK4 and RK8, for each norm, L_2 and L_∞, and for each N, we determined the smallest k such that $e \approx e_{BA}$ and called this value of the time step size parameter k_{opt}. We refer to the e corresponding to the k_{opt} by e_{opt}. We fitted this data to a power model, $k_{opt} = CN^{-\alpha}$, and to an exponential model, $k_{opt} = C\alpha^{-N}$. In each case, the exponential relationship fit better. Figure 4.4 exemplifies how well the data fits the model for each time stepping method and norm. Table 4.4 shows the results.

For each time stepping scheme and for each norm, using the exponential relationship between k_{opt} and N given in Table 4.4 we found $\tilde{w}(\cdot,T)$ and fitted e_{opt} to three different models: $e_{opt} = CN^{-\alpha}$, $e_{opt} = C\alpha^{-N}$, and $e_{opt} = C\alpha^{-N^r}$. The first model did not fit as well as the second and the degree to which the third model improved upon the second was marginal: for each time stepping scheme and norm, r was 0.99 or 1.00, and the coefficient of determination of the least squares fit was $R^2 = 1.00$ for both models. Table 4.5 shows the results.

Using these relationships we can determine the global order of accuracy for

Table 4.5: Fitting parameters α and C in $e_{opt} = C\alpha^{-N}$ for each time stepping method and for each norm.

	RK4		RK8	
L_2	14.5859,	6.6850	14.1236,	4.2821×10
L_∞	14.1284,	3.3419×10	15.7573,	1.0338×10^2

Table 4.6: Estimated order of accuracy p in $e_{opt} = Ck_{opt}^p$ for each time stepping method and for each norm.

	RK4	RK8
L_2	3.8763	5.9110
L_∞	3.8214	5.8448

each time stepping scheme and norm. Table 4.6 shows the results.

CHAPTER 5

RUNNING-TIME ANALYSIS

We now examine the time-consuming aspects of the algorithm. We briefly discuss those aspects of the time stepping iteration that are particularly costly. We will see that, asymptotically, the number of flops required for one time step is $\mathcal{O}(N^3)$ in the degree of the polynomial expansion. We will see that the spectral method outperforms the Hoff method in terms of the global amount of work: $\frac{1}{k}\left(\log\left(\frac{1}{k}\right)\right)^3$ compared to $\frac{1}{k^2}$. For the spectral method, the nature of the exponential relationship between the problem size N and the time step size k obviates reductions of per-time-step workload.

In the time stepping iteration we must perform the following costly operations: finding the free boundary, changing basis coordinates, computing a dense matrix of discrete inner products, and solving a dense linear system. In the sequel the number of quadrature points, ν, is $\mathcal{O}(N)$ and we are always considering $N \to \infty$. At a few points I point out where the $\mathcal{O}(N^3)$ complexity for one time step may be reduced, but do not put much emphasis since the main result still holds if one time step required $\mathcal{O}(N^p)$ for any $p < \infty$.

Finding the free boundary amounts to finding roots of a polynomial equation. We solve this using a polynomial root finder, which solves an eigenvalue problem or a generalized eigenvalue problem and takes $\mathcal{O}(N^3)$ flops. One way to reduce this is to use NM. Each Newton iteration requires evaluation of polynomial expansion of the pressure $\sum \beta_j \phi_j(x)$ and its derivative. These require $\mathcal{O}(N^2)$ flops and may be reduced to $\mathcal{O}(N \log N)$ if the appropriate technology exists, as is mentioned below. Using the root at the previous time step as a seed should allow for optimal quadratic convergence of NM, which translates into $\mathcal{O}(N^2)$ complexity. This is plausible since Knerr [22] proved bounds on maximal growth of the free boundary of the PME and particular generalizations of it that include the generalized PME of the previous chapter.

At each step we must change coordinates of the solution at time t, $\beta(t)$, from coordinates with respect to Legendre basis functions orthogonal on $\Xi(t)$ to coordinates with respect to Legendre basis functions orthogonal on $\tilde{\Xi}(t+k)$. We considered three methods for doing this. One reduces to solving a dense linear system and two others construct dense, upper triangular transformations matrices for use in a less costly matrix-vector multiply.

The first algorithm could take advantage of the high degree of interdependence between the matrices from one time step and the next, in terms of starting guesses for iterative methods. This may be successfully exploited to reduce the cost of this operation to $o(N^3)$.

The first of the last two methods, implements the closed form transformation, but turns out to be unstable in practice. We will omit this method from further discussion.

The second of the last two algorithms numerically integrates the inner products which make up the entries of the transformation matrix. Each of these requires $\mathcal{O}(Np(N))$ flops since we numerically integrate the inner products which make up its entries, where $p(N)$ is the time required to evaluate a polynomial expressed in non-exponential basis functions. Evaluating the functions in the inner products at the quadrature nodes requires $\mathcal{O}(N^2)$ flops to compute, i.e. $p(N) = \mathcal{O}(N^2)$. If FFT technology for non-exponential basis functions exists this might reduce the computation to $\mathcal{O}(N^2 \log N)$ flops.

Forming H from (2.6) or (2.22) requires $\mathcal{O}(N^3)$ since , for each entry, we are numerically integrating inner products of functions which cost $\mathcal{O}(N^2)$ to evaluate at the quadrature nodes. As discussed above this may be lowered with FFT-like technology.

Finally computing the derivative in (2.6) or (2.22) requires solving a dense linear system which requires $\mathcal{O}(N^3)$ flops. This matrix is symmetric so these methods enjoy Cholesky's partial reduction in work and stability. Investigating the interdependence between derivatives at one time step and derivatives at the next time step may reveal more structure that could be used to advantage in the context of iterative methods.

The method of Hoff [18] is a finite difference method that sidesteps the normal parabolic mesh condition needed for stability. In the paper Hoff proves convergence and gives bounds on the rate of convergence. This method performs a linear solve with a tridiagonal matrix, so requires only $\mathcal{O}(N)$ flops per iteration. Convergence is guaranteed for $k = \mathcal{O}(h)$. Since $h = \mathcal{O}(N^{-1})$, we that the total complexity $\mathcal{O}(MN) = \mathcal{O}(k^{-1}k^{-1}) = \mathcal{O}(k^{-2})$.

The total complexity for the spectral method is $\mathcal{O}(MN^3) = \mathcal{O}\left(k^{-1}\left(\log k^{-1}\right)^3\right)$ which grows asymptotically slower than Hoff's $\mathcal{O}(k^{-2})$.

CHAPTER 6

FUTURE WORK

We list some ideas for future work that range from highly pertinent to this work, to interesting questions for future investigations or extensions to this work.

From the first category:

- As mentioned in section 2.1.2, our numerical form (2.18)-(2.19) can be considered a spectral method for the pressure equation (1.7). We can reconsider some of the questions that were left unanswered in light of this interpretation of our numerical form.

- Can we prove a comparison principle for solutions of the semidiscrete system (2.22)? This would prove that our method stays positive if $\tilde{z}(x, 0) > 0$, $\forall x \in \Xi(t)$. Similarly for $\tilde{u}$.

- Estimate the accuracy in approximating $(u^m)_{xx}$ with numerical form (2.18)-(2.19). This is usually done using linearity of the functional being approximated and by estimating the error by summing the tail of the infinite expansion. See [10, 8].

- Study the eigensystem of model 2 that uses the modified Legendre basis. In particular, that those solutions contract to the Barenblatt would not be surprising, but the form of the decay will be interesting.

- Get a better understanding of the dependence of the time-step on the stability. This will undoubtedly involve the shape of the stability region of the time stepper used to solve the discrete system (2.14), as well as the eigenvalues of the derivative from this discrete system, $\mathbf{g}$. And similarly for the semidiscrete system (2.30).

- Let $\mathbf{f}$ be a multivariate vector-valued function and consider computing derivatives of the i^{th} component of $\mathbf{f}$, $\mathbf{f}(i)$. We collect the first derivatives of $\mathbf{f}(i)$

with respect to the coefficients $\boldsymbol{\beta}$ into vector known as the gradient of $\mathbf{f}\,(i)$, $\nabla \mathbf{f}\,(i)$. Similarly, the collection of second derivatives of $\mathbf{f}\,(i)$ with respect to the coefficients $\boldsymbol{\beta}$ are arranged in a matrix known as the Hessian, $\nabla^2 \mathbf{f}\,(i)$. Given the code to compute $\mathbf{f}$, automatic differentiation produces code to compute $\nabla \mathbf{f}\,(i)$ and $\nabla^2 \mathbf{f}\,(i)$. These are necessary, e.g., for trust-region Newton's methods mentioned in the solution of (2.23). These methods require the computation of the vector $s = -\left[\nabla^2 \mathbf{f}\,(i)\right]^{-1} \nabla \mathbf{f}\,(i)$, called the Newton direction. As mentioned in the solution of (2.23), we can use automatic differentiation to produce the code that computes $\nabla \mathbf{f}\,(i)$ and $\nabla^2 \mathbf{f}\,(i)$, and use them to corroborate our own implementations of our hand-computed gradients and Hessians. For more about automatic differentiation see [15].

- Extend the method to higher dimensions. Begin by applying it to the radial formulation of the PME.

Interesting questions for future investigations:

- Consider solving the system that explicitly keeps the free boundary as part of the unknown. For instance, if we plug $\tilde{w}$

$$\tilde{w}^{m-1} = (\xi_r - x)(x - \xi_\ell) \sum_{j=0}^{N} \beta_j(t)\, \phi_j(x)$$

  into (1.5). The mass matrix divides the DE into two coupled subsystems: one for the free boundary curves and one for the coefficients. How does the free boundary equation of Knerr (2.42) fit in? Can we prove that the matrix system analogous to (2.6) is nonsingular? One obvious benefit is that we do not need to find roots of a polynomial to find the free boundary at each step.

- Apply the ideas from this work to other PDE with free boundaries. This dissertation work started by trying to numerically solve a nonlinear diffusion PDE with a free boundary found in the Mainguy and Coussy [26].

- Solve the joining nonzero densities problem where two disjoint supports eventually join.

APPENDIX A

CALCULATIONS

We summarize the calculations used in determining the derivatives involved in the differential identity in (3.6). The free boundaries ξ_ℓ and ξ_r used in the sequel are the roots of sG solution of section 2.1.2. For the most part, calculations will be for the case when the trial and test functions bases are each the standard basis. In some places we use a more general setting where stipulations on the basis are relaxed.

We note the following changes of variables, which will prove useful. For $x \in [\xi_\ell, 0]$, we let $s = (x - \xi_\ell)^{1/(m-1)}$, so that $(m-1)\, s^{m-2}\, ds = dx$, $s \downarrow 0$ as $x \downarrow \xi_\ell$ and $s \uparrow (-\xi_\ell)^{1/(m-1)}$ as $x \uparrow 0$. Let $s^* = (-\xi_\ell)^{1/(m-1)}$. For $x \in [0, \xi_r]$, we let $s = (\xi_r - x)^{1/(m-1)}$, so that $-(m-1)\, s^{m-2}\, ds = dx$, $s \downarrow 0$ as $x \uparrow \xi_r$ and $s \uparrow \xi_r^{1/(m-1)}$ as $x \downarrow 0$. Let $s^{\#} = \xi_r^{1/(m-1)}$.

Now we note the following rewriting of p that isolates the singularities at the interface. Define q and r such that $p(x) = (x - \xi_\ell)\, q(x) = (\xi_r - x)\, r(x)$, where $q, r \in \Pi_{N-1}$. In the case where each of the trial and test function bases is the standard basis, $q(x) = \sum_{i=0}^{N-1} \alpha_i x^i$, $\alpha_i = \sum_{j=0}^{N-1-i} \xi_\ell^j \beta_{i+j+1}$, $r(x) = \sum_{i=0}^{N-1} \gamma_i x^i$, and $\gamma_i = -\sum_{j=0}^{N-1-i} \xi_r^j \beta_{i+j+1}$. The quantities $\xi_\ell + s^{m-1}$ and $\xi_r - s^{m-1}$ will appear often enough that we will use the shorthands z and w for them: $z = \xi_\ell + s^{m-1}$ and $w = \xi_r - s^{m-1}$. Also, we will use the following notations: $\theta_\ell = p_x(\xi_\ell)$, $\theta_r = p_x(\xi_r)$, and $\theta = p_x(\xi)$. Also, $\chi_I(x)$ is the indicator function: $\chi_I(x) = 1$ if $x \in I$ and

$\chi_I(x) = 0$ if $x \notin I$

A.1 Mass matrix, H, and its derivatives

A.1.1 Mass matrix, H

Let p and $\tilde{u}$ be as in (2.18)-(2.19). Then the mass matrix, H, in (2.24) is

$$H(i, j) = \frac{1}{m-1} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, \phi_j(x)\, \phi_i(x)\, dx, \tag{A.1}$$

where the trial and test functions $\{\phi_i\}$ form a basis of Π_N. In the course of writing down such formulas, we must be cautious that we are not writing nonsense. That is, we must ensure that the integrals involved exist. In this chapter, we address this point.

We now give sufficient conditions for a keystone integral to exist.

Lemma A.1. *If q and r are such that $0 < q(x), r(y) < \infty$, for $x \in [\xi_\ell, 0]$ and $y \in [0, \xi_r]$, then*

$$A = \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, dx < \infty,$$

for all $m > 1$.

Proof. Take $m \in (1, 2)$, then $1/(m-1) - 1$ is positive. Since $p(x)$ is bounded for $x \in [\xi_\ell, \xi_r]$, we have $M < \infty$ such that

$$A < M^{\frac{1}{m-1}-1} \int_{\xi_\ell}^{\xi_r} dx < \infty.$$

Take $m = 2$, then $A = \int_{\xi_\ell}^{\xi_r} dx < \infty$. Take $m > 2$, then $1/(m-1) - 1$ is negative. Since q and r are bounded away from zero and infinity, we have an $0 < M < \infty$ such that $q^{1/(m-1)-1}(x), r^{1/(m-1)-1}(y) < M$, for $x \in [\xi_\ell, 0]$ and $y \in [0, \xi_r]$. Proceeding with this estimate we have

$$
\begin{aligned}
A &= \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\ dx = \int_{\xi_\ell}^{0} p^{\frac{1}{m-1}-1}(x)\ dx + \int_{0}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\ dx \\
&= \int_{\xi_\ell}^{0} (x-\xi_\ell)^{\frac{1}{m-1}-1} q^{\frac{1}{m-1}-1}(x)\ dx + \int_{0}^{\xi_r} (\xi_r - x)^{\frac{1}{m-1}-1} r^{\frac{1}{m-1}-1}(x)\ dx \\
&\leq M \int_{\xi_\ell}^{0} (x-\xi_\ell)^{\frac{1}{m-1}-1}\ dx + M \int_{0}^{\xi_r} (\xi_r - x)^{\frac{1}{m-1}-1}\ dx \\
&= M(m-1)\left[(-\xi_\ell)^{\frac{1}{m-1}} - 0^{\frac{1}{m-1}} + \xi_r^{\frac{1}{m-1}} - 0^{\frac{1}{m-1}}\right] < \infty,
\end{aligned}
$$

since $1/(m-1) > 0$. ■

From this follows the result we are after:

Corollary A.1. *H given in* (A.1) *is well-defined.*

Proof. To see this, we use that for $x \in [\xi_\ell, \xi_r]$, we have that any $\phi_i(x)$ will be bounded as each is a polynomial on a bounded set: $|\phi_i(x)| < M$, for some $0 < M < \infty$. Applying lemma A.1 we get that

$$
H(i, j) \leq \frac{M^2}{m-1} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\ dx < \infty. \quad ■
$$

Corollary A.2. *H given in* (A.1) *with $\{\phi_i(x)\} = \{x^i\}$ is well-defined.*

Proof. Such ϕ_i are particular examples of those described in the proof of corollary A.1. ■

We will need the following preliminary calculations in the sequel.

A.1.1.1 Preliminary calculations

All subsequent calculations will hold for general polynomials.

We will need the following lemma to continue.

Lemma A.2. *If the bases for the trial and test functions are both the standard basis and that* $p_x(\xi) \neq 0$, *then*

$$\frac{\partial \xi}{\partial \beta_\ell} = -\frac{\xi^\ell}{\theta} \tag{A.2}$$

$$\frac{\partial}{\partial \beta_\ell}\left[q\left(\xi_\ell + s^{m-1}\right)\right] = \frac{\left(\xi_\ell + s^{m-1}\right)^\ell - \theta_\ell^{-1}\xi_\ell^\ell p_x\left(\xi_\ell + s^{m-1}\right)}{s^{m-1}} \tag{A.3}$$

$$\frac{\partial}{\partial \beta_\ell}\left[r\left(\xi_r - s^{m-1}\right)\right] = \frac{\left(\xi_r - s^{m-1}\right)^\ell - \theta_r^{-1}\xi_r^\ell p_x\left(\xi_r - s^{m-1}\right)}{s^{m-1}} \tag{A.4}$$

$$\frac{\partial}{\partial \beta}\left[p_x\left(\xi \pm s^{m-1}\right)\right] = \ell\left(\xi \pm s^{m-1}\right)^{\ell-1} - \frac{\xi^\ell}{\theta}p_{xx}\left(\xi \pm s^{m-1}\right) \tag{A.5}$$

$$\frac{\partial}{\partial \beta}\left[p_{xx}\left(\xi \pm s^{m-1}\right)\right] = \ell\left(\ell-1\right)\left(\xi \pm s^{m-1}\right)^{\ell-2} - \frac{\xi^\ell}{\theta}p_{xxx}\left(\xi \pm s^{m-1}\right). \tag{A.6}$$

Proof. The formulas follow from using the definitions of p, q, r, p_x, and p_{xx}.

Equation (A.2). The equation giving $\partial\xi$ follows from implicitly differentiating the equation $p(\xi) = 0$ with respect to β:

$$\begin{aligned}
0 &= \frac{d}{d\beta_\ell}p(\xi) \\
&= \frac{d}{d\beta_\ell}\sum_{k=0}^{N}\beta_k\xi^k \\
&= \sum_{k=1}^{N}\beta_k k\xi^{k-1}\frac{\partial \xi}{\partial \beta_\ell} + \xi^\ell \\
&= p_x(\xi)\frac{\partial \xi}{\partial \beta_\ell} + \xi^\ell.
\end{aligned}$$

Now solve for $\partial_\ell \xi$. This shows (A.2).

Equations (A.3), (A.4). To calculate the term $\partial\left[q\left(\xi_\ell + s^{m-1}\right)\right]$, substitute $\xi_\ell + s^{m-1}$ in q's defining equation, $p\left(\xi_\ell + s^{m-1}\right) = s^{m-1}q\left(\xi_\ell + s^{m-1}\right)$, and differentiate to get

$$
\begin{aligned}
s^{m-1}\frac{\partial}{\partial\beta_\ell}\left[q\left(\xi_\ell+s^{m-1}\right)\right] &= \sum_{j=0}^{N}\frac{\partial\beta_j}{\partial\beta_\ell}\left(\xi_\ell+s^{m-1}\right)^j+\sum_{j=1}^{N}\beta_j\cdot j\left(\xi_\ell+s^{m-1}\right)^{j-1}\frac{\partial\xi_\ell}{\partial\beta_\ell}\\
&= \left(\xi_\ell+s^{m-1}\right)^\ell+\frac{\partial\xi_\ell}{\partial\beta_\ell}p_x\left(\xi_\ell+s^{m-1}\right),
\end{aligned}
$$

so that dividing by s^{m-1} and using (A.2) gives (A.3). We can derive (A.4) for $\partial\left[r\left(\xi_r-s^{m-1}\right)\right]$ in a similar way. This shows (A.3) and (A.4).

Equation (A.5). Proceeding as above,

$$
\begin{aligned}
\frac{\partial}{\partial\beta_\ell}\left[p_x\left(\xi\pm s^{m-1}\right)\right] &= \frac{\partial}{\partial\beta_\ell}\sum_{j=1}^{N}j\beta_j\left(\xi\pm s^{m-1}\right)^{j-1}\\
&= \sum_{j=1}^{N}j\frac{\partial\beta_j}{\partial\beta_\ell}\left(\xi\pm s^{m-1}\right)^{j-1}+\sum_{j=1}^{N}j\beta_j\frac{\partial}{\partial\beta_\ell}\left[\left(\xi\pm s^{m-1}\right)^{j-1}\right]\\
&= \ell\left(\xi\pm s^{m-1}\right)^{\ell-1}+\sum_{j=1}^{N}j\beta_j\cdot(j-1)\left(\xi\pm s^{m-1}\right)^{j-2}\frac{\partial\xi}{\partial\beta_\ell}\\
&= \ell\left(\xi\pm s^{m-1}\right)^{\ell-1}-\frac{\xi^\ell}{p_x(\xi)}p_{xx}\left(\xi\pm s^{m-1}\right),
\end{aligned}
$$

where we used (A.2) in the final equality. This shows (A.5).

Equation (A.6). We use the same methodology:

$$
\begin{aligned}
\frac{\partial}{\partial\beta_\ell}\left[p_{xx}\left(\xi\pm s^{m-1}\right)\right] &= \frac{\partial}{\partial\beta_\ell}\sum_{j=2}^{N}j(j-1)\beta_j\left(\xi\pm s^{m-1}\right)^{j-2}\\
&= \sum_{j=2}^{N}j(j-1)\frac{\partial\beta_j}{\partial\beta_\ell}\left(\xi\pm s^{m-1}\right)^{j-2}+\sum_{j=2}^{N}j(j-1)\beta_j\frac{\partial}{\partial\beta_\ell}\left[\left(\xi\pm s^{m-1}\right)^{j-2}\right]\\
&= \ell(\ell-1)\left(\xi\pm s^{m-1}\right)^{\ell-2}+\sum_{j=3}^{N}j(j-1)\beta_j\cdot(j-2)\left(\xi\pm s^{m-1}\right)^{j-3}\frac{\partial\xi}{\partial\beta_\ell}\\
&= \ell(\ell-1)\left(\xi\pm s^{m-1}\right)^{\ell-2}-\frac{\xi^\ell}{p_x(\xi)}p_{xxx}\left(\xi\pm s^{m-1}\right).
\end{aligned}
$$

This shows (A.6) and completes the lemma. ■

A.1.2 Derivatives of H: Introduction

For the remainder of section A.1 we set $\{\phi_i\}$ to be the standard basis. With the question of existence of H settled in corollary A.1 and in corollary A.2, we take a derivative of H:

$$\begin{aligned}\frac{\partial H}{\partial \beta_\ell}(i,\, j) = \frac{1}{m-1}\frac{\partial \xi_r}{\partial \beta_\ell} p^{\frac{1}{m-1}-1}(\xi_r)\, \xi_r^{i+j} - \frac{1}{m-1}\frac{\partial \xi_\ell}{\partial \beta_\ell} p^{\frac{1}{m-1}-1}(\xi_\ell)\, \xi_\ell^{i+j} \\ + \frac{1}{m-1}\left(\frac{1}{m-1}-1\right)\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\, x^{i+j+\ell}\, dx.\end{aligned} \tag{A.7}$$

Notice that the above equation may not make sense for $m > 2$; in this case, the boundary terms seem to blow up because $p(\xi) = 0$ and the exponent, $1/(m-1) - 1$, is negative. Likewise, the integral $\int_{\xi_\ell}^{\xi_r} p^{1/(m-1)-2}(x)\, dx$ has a singularity at the interface that may not be integrable, since the exponent, $1/(m-1) - 2$, is smaller than -1. We address these issues in the following sections. The calculation is broken into several cases and steps:

1. ∂H, $m \in (1,\, 2]$ in section A.1.2.1
2. $\partial H = \partial J_1 + \partial J_2$, $m \in (2,\, \infty)$ in section A.1.2.2
   (a) ∂J_1 in section A.1.2.3
   (b) ∂J_2 in section A.1.2.4

A.1.2.1 Derivatives of H, $1 < m \leq 2$

Putting $1 < m < 2$ in (A.7) we see that because $|\partial \xi|$ and $|\xi|$ are bounded, $p(\xi) = 0$ and the exponent $1/(m-1) - 1$ is positive, the boundary terms are zero:

$$\frac{\partial H}{\partial \beta_\ell}(i,\, j) = \frac{2-m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\, x^{i+j+\ell}\, dx.$$

This integral exists because $|p(x)|$ and $|x|^\alpha$, $\alpha > 0$, are bounded and the exponent $1/(m-1) - 2$ is positive for $m \in (1,\, 2)$. This formula is recounted in equation (B.3) of the summary.

Putting $m = 2$ in (A.1) gives

$$H(i,\, j) = \int_{\xi_\ell}^{\xi_r} x^{i+j}\, dx = \frac{1}{i+j+1}\left(\xi_r^{i+j+1} - \xi_\ell^{i+j+1}\right).$$

Taking a derivative of this and using (A.2) gives (B.4) of the summary.

A.1.2.2 Derivatives of $H, m > 2$

Set $m > 2$. To resolve the potential issues observed in this case, we rewrite $H(i,\, j)$ as integrals over the intervals $[\xi_\ell,\, 0]$ and $[0,\, \xi_r]$, change variables, and use q and r in order to show that the effects of the apparent singularity in (A.7) are negligible:

$$H = J_1 + J_2,$$

where

$$J_1(i,\, j) = \frac{1}{m-1}\int_{\xi_\ell}^{0} p^{\frac{1}{m-1}-1}(x)\, x^{i+j}\, dx \tag{A.8}$$

and

$$J_2(i,\, j) = \frac{1}{m-1}\int_{0}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, x^{i+j}\, dx. \tag{A.9}$$

We want to calculate ∂H, which can be written as

$$\frac{\partial H}{\partial \beta} = \frac{\partial J_1}{\partial \beta} + \frac{\partial J_2}{\partial \beta}.$$

We calculate ∂J_1 in section A.1.2.3 and ∂J_2 in section A.1.2.4. The calculations of ∂J_1 and ∂J_2 are completely analogous to each other. Lemmas A.4 and A.5 establish that ∂J_1 and ∂J_2 are well-defined, respectively, and depend on lemma A.3 which we show next.

We now consider the existence of the integrals in (A.15) and (A.18). To establish the existence of those integrals with q^α and r^α, $\alpha = 1/(m-1) - 1$, we require that q and r be bounded away from zero. To establish the existence of the remaining integrals, those with q^α, r^α, $\alpha = 1/(m-1) - 2$, we require the strict positivity q and r and that q and r be such that

$$\mathcal{C}\left(1+\xi_\ell^{-1}x\right) \le q\left(x\right), \text{ as } x \downarrow \xi_\ell, \tag{A.10}$$

and

$$\mathcal{C}\left(1+\xi_r^{-1}x\right) \le r\left(x\right), \text{ as } x \uparrow \xi_r, \tag{A.11}$$

for some positive constant $\mathcal{C}$. Note that such $\mathcal{C} > 0$ can be found if we have strict positivity of $q\left(x\right)$, for $x \in [\xi_\ell,\, 0]$, and $r\left(y\right)$, for $y \in [0,\, \xi_r]$.

Lemma A.3. *The integrals in* (A.15) *and* (A.18) *are well-defined provided that* $q\left(x\right) > 0$*, for* $x \in [\xi_\ell,\, 0]$*, and* $r\left(y\right) > 0$*, for* $y \in [0,\, \xi_r]$*.*

Proof. We will write $\theta_\ell = p_x\left(\xi_\ell\right)$ and $\theta_r = p_x\left(\xi_r\right)$. We first take care of the second integrals in (A.15) and (A.18). Since q and r are bounded away from zero, there is an $M < \infty$ such that

$$q^{\frac{1}{m-1}-1}\left(\xi_\ell + s^{m-1}\right)\left|\left(\xi_\ell + s^{m-1}\right)^{i+j-1}\right| < M$$

and

$$r^{\frac{1}{m-1}-1}\left(\xi_r - t^{m-1}\right)\left|\left(\xi_r - t^{m-1}\right)^{i+j-1}\right| < M,$$

for $s \in [0,\, s^*]$ and $t \in \left[0,\, s^{\#}\right]$, respectively. Then we have

$$\int_0^{s^*} q^{\frac{1}{m-1}-1}\left(\xi_\ell + s^{m-1}\right)\left(\xi_\ell + s^{m-1}\right)^{i+j-1} ds \le M\int_0^{s^*} ds < \infty$$

and

$$\int_0^{s^{\#}} r^{\frac{1}{m-1}-1}\left(\xi_r - s^{m-1}\right)\left(\xi_r - s^{m-1}\right)^{i+j-1} ds \le M\int_0^{s^{\#}} ds < \infty.$$

We next show the result for the first integral in (A.15). Change variables using $s = \left(x - \xi_\ell\right)^{1/(m-1)}$, then again using $x = \xi_\ell y$ and yet again using $y = t^{1/2}$:

$$\begin{aligned}
A &:= \int_0^{s^*} s^{-(m-1)} q^{\frac{1}{m-1}-2}\left(\xi_\ell + s^{m-1}\right)\left[\theta_\ell\left(\xi_\ell + s^{m-1}\right)^\ell - \xi_\ell^\ell p_x\left(\xi_\ell + s^{m-1}\right)\right] ds \\
&= \frac{1}{m-1}\int_{\xi_\ell}^0 \left(x-\xi_\ell\right)^{\frac{1}{m-1}-2} q^{\frac{1}{m-1}-2}\left(x\right)\left[\theta_\ell x^\ell - \xi_\ell^\ell p_x\left(x\right)\right] dx \\
&= \frac{1}{m-1}\left(-\xi_\ell\right)^{\frac{1}{m-1}-2}\xi_\ell^{\ell+1}\int_1^0 \left(1-y\right)^{\frac{1}{m-1}-2} q^{\frac{1}{m-1}-2}\left(\xi_\ell y\right)\left[\theta_\ell y^\ell - p_x\left(\xi_\ell y\right)\right] dy \\
&= \mathcal{C}_0\int_1^0 \left(1-t^{\frac{1}{2}}\right)^{\frac{1}{m-1}-2} q^{\frac{1}{m-1}-2}\left(\xi_\ell t^{\frac{1}{2}}\right)\left[\theta_\ell t^{\frac{\ell}{2}} - p_x\left(\xi_\ell t^{\frac{1}{2}}\right)\right] t^{\frac{1}{2}-1}\, dt,
\end{aligned}$$

where $\mathcal{C}_0 = 2^{-1} \cdot (m-1)^{-1} (-\xi_\ell)^{1/(m-1)-2} \xi_\ell^{\ell+1}$. Since (A.10) holds, changing variables, there is a $t^* \in (0,\, 1)$ such that

$$\mathcal{C} \left(1 + t^{\frac{1}{2}}\right) \le q\left(\xi_\ell t^{\frac{1}{2}}\right),\ \forall t \in (t^*,\, 1)\,. \tag{A.12}$$

Write $|A| \le A_1 + A_2$, where

$$A_1 = |\mathcal{C}_0| \int_0^{t^*} \left(1 - t^{\frac{1}{2}}\right)^{\frac{1}{m-1}-2} q^{\frac{1}{m-1}-2}\left(\xi_\ell t^{\frac{1}{2}}\right) \left|\theta_\ell t^{\frac{\ell}{2}} - p_x\left(\xi_\ell t^{\frac{1}{2}}\right)\right| t^{\frac{1}{2}-1}\, dt$$

and

$$A_2 = |\mathcal{C}_0| \int_{t^*}^{1} \left(1 - t^{\frac{1}{2}}\right)^{\frac{1}{m-1}-2} q^{\frac{1}{m-1}-2}\left(\xi_\ell t^{\frac{1}{2}}\right) \left|\theta_\ell t^{\frac{\ell}{2}} - p_x\left(\xi_\ell t^{\frac{1}{2}}\right)\right| t^{\frac{1}{2}-1}\, dt.$$

Then, since $0 < q(x)\,,\ |p_x(x)| < \infty$, there is an $0 < M < \infty$ such that

$$q^{\frac{1}{m-1}-2}\left(\xi_\ell t^{\frac{1}{2}}\right) \left|\theta_\ell t^{\frac{\ell}{2}} - p_x\left(\xi_\ell t^{\frac{1}{2}}\right)\right| < M,$$

with which we can say that

$$\begin{aligned} A_1 &\le \mathcal{C}_1 \int_0^{t^*} \left(1 - t^{\frac{1}{2}}\right)^{\frac{1}{m-1}-2} t^{-\frac{1}{2}}\, dt \\ &= 2\mathcal{C}_1 \int_0^{\sqrt{t^*}} (1-u)^{\frac{1}{m-1}-2}\, du < \infty, \end{aligned}$$

where $\mathcal{C}_1 = M\,|\mathcal{C}_0|$. Using (A.12) we have

$$\begin{aligned} A_2 &\le \mathcal{C}_2 \int_{t^*}^{1} (1-t)^{\frac{1}{m-1}-2} \left|\theta_\ell t^{\frac{\ell}{2}} - p_x\left(\xi_\ell t^{\frac{1}{2}}\right)\right| t^{\frac{1}{2}-1}\, dt \\ &\le \mathcal{C}_1 \int_{t^*}^{1} (1-t)^{\frac{1}{m-1}-2} \left|\sum_{k=1}^{N} k\beta_k \xi_\ell^{k-1}\left(t^{\frac{k-1}{2}} - t^{\frac{\ell}{2}}\right)\right| t^{\frac{1}{2}-1}\, dt \\ &= \mathcal{C}_1 \int_{t^*}^{1} (1-t)^{\frac{1}{m-1}-2}\, t^{\frac{1}{2}-1}\, |\rho(t)|\, dt, \end{aligned} \tag{A.13}$$

where $\mathcal{C}_2 = \mathcal{C}^{1/(m-1)-2}\,|\mathcal{C}_0|$ and

$$\begin{aligned} |\rho(t)| &= \left|\sum_{k=1}^{\ell} k\beta_k \xi_\ell^{k-1} t^{\frac{\ell-k}{2}}\left(1 - t^{\frac{k}{2}}\right) - t^{\frac{\ell}{2}} \sum_{k=1}^{N-\ell-1} k\beta_k \xi_\ell^{k-1}\left(1 - t^{\frac{k}{2}}\right)\right| \\ &\le \sum_{k=1}^{\ell} k\,|\beta_k|\,\left|\xi_\ell^{k-1}\right| t^{\frac{\ell-k}{2}}\left(1 - t^{\frac{k}{2}}\right) + t^{\frac{\ell}{2}} \sum_{k=1}^{N-\ell-1} k\,|\beta_k|\,\left|\xi_\ell^{k-1}\right|\left(1 - t^{\frac{k}{2}}\right) \\ &\le \mathcal{C}_3 \sum_{k=1}^{\ell} t^{\frac{\ell-k}{2}}\left(1 - t^{\frac{k}{2}}\right) + \mathcal{C}_3 t^{\frac{\ell}{2}} \sum_{k=1}^{N-\ell-1} \left(1 - t^{\frac{k}{2}}\right), \end{aligned}$$

where $\mathcal{C}_3 = NBC$, $B = \max_k |\beta_k|$, $C = \max_k \left|\xi_\ell^{k-1}\right|$. Note that

$$
\begin{aligned}
|\rho(t)| &\leq \begin{cases} \mathcal{C}_3 N \cdot t^{\frac{\ell}{2}} \left(1 - t^{\frac{N-\ell-1}{2}}\right), & \ell = 0, \ldots, \left\lfloor \frac{N-1}{2} \right\rfloor, \\ \mathcal{C}_3 N \left(1 - t^{\frac{\ell}{2}}\right), & \ell = \left\lfloor \frac{N-1}{2} \right\rfloor + 1, \ldots, N. \end{cases} \\
&\leq \mathcal{C}_4 \left(1 - t^{\frac{N}{2}}\right),
\end{aligned}
\tag{A.14}
$$

where $\mathcal{C}_4 = \mathcal{C}_3 N$. Since $m > 2$,, $1 - 1/(m-1) \in (0, 1)$, so there is $\gamma \in (1 - 1/(m-1), 1)$ such that

$$1 - t^{\frac{N}{2}} \leq (1-t)^\gamma, \ \forall t \in (t^*, 1),$$

and t^* is the same as that above. Using this and (A.14) in (A.13) we get that

$$
\begin{aligned}
A_2 &\leq \mathcal{C}_5 \int_{t^*}^1 (1-t)^{\frac{1}{m-1}-2} t^{\frac{1}{2}-1} \left(1 - t^{\frac{N}{2}}\right) dt \\
&\leq \mathcal{C}_5 \int_{t^*}^1 (1-t)^{\gamma + \frac{1}{m-1}-2} t^{\frac{1}{2}-1} \, dt \\
&\leq \mathcal{C}_5 \int_0^1 (1-t)^{\gamma + \frac{1}{m-1}-2} t^{\frac{1}{2}-1} \, dt \\
&= \mathcal{C}_5 B \left(\gamma + \frac{1}{m-1} - 1, \frac{1}{2}\right),
\end{aligned}
$$

where $\mathcal{C}_5 = \mathcal{C}_1 \mathcal{C}_4$ and $B(p, q)$ is the beta function. The beta function is positive and finite for $p, q > 0$. Similar considerations give

$$\int_0^{s^\#} s^{-(m-1)} r^{\frac{1}{m-1}-2} \left(\xi_r - s^{m-1}\right) \left[\theta_r \left(\xi_r - s^{m-1}\right)^\ell - \xi_r^\ell p_x \left(\xi_r - s^{m-1}\right)\right] ds < \infty.$$

$\blacksquare$

A.1.2.3 Subcalculation one: ∂J_1

Lemma A.4. *Suppose condition* (A.10) *holds, then*

$$\begin{aligned}\frac{\partial J_1}{\partial \beta_\ell}(i,\, j) = {} & \frac{1}{m-1} \cdot \frac{\xi_\ell^\ell}{\theta_\ell} \beta_0^{\frac{1}{m-1}-1} \chi_{\{0\}}(i+j) \\ & - \frac{m-2}{m-1} \cdot \frac{1}{\theta_\ell} \int_0^{s^*} q^{\frac{1}{m-1}-2}(z) \frac{\theta_\ell z^\ell - \xi_\ell^\ell p_x(z)}{s^{m-1}} z^{i+j}\, ds \\ & - (i+j) \frac{\xi_\ell^\ell}{\theta_\ell} \int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\, z^{i+j-1}\, ds.\end{aligned} \tag{A.15}$$

Note: the derivation of this formula shows that the integral in the last term need only make sense when $i+j \geq 1$.

Proof. Assume that $i+j \geq 1$. Changing variables in (A.8) gives

$$\begin{aligned}J_1(i,\, j) &= \frac{1}{m-1} \int_{\xi_\ell}^{0} p^{\frac{1}{m-1}-1}(x)\, x^{i+j}\, dx \\ &= \frac{1}{m-1} \int_0^{s^*} p^{\frac{1}{m-1}-1}\left(\xi_\ell + s^{m-1}\right) \left(\xi_\ell + s^{m-1}\right)^{i+j} (m-1)\, s^{m-2}\, ds \\ &= \int_0^{s^*} \left(s^{m-1} q\left(\xi_\ell + s^{m-1}\right)\right)^{\frac{1}{m-1}-1} \left(\xi_\ell + s^{m-1}\right)^{i+j} s^{m-2}\, ds \\ &= \int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\, z^{i+j}\, ds\end{aligned}$$

Taking a derivative of J_1 we get

$$\begin{aligned}\frac{\partial J_1}{\partial \beta_\ell}(i,\, j) = {} & \partial_{11} - \partial_{12} \\ & + \int_0^{s^*} \left(\frac{1}{m-1} - 1\right) q^{\frac{1}{m-1}-2}(z) \frac{\partial}{\partial \beta_\ell}\left[q(z)\right] z^{i+j}\, ds \\ & + \int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\,(i+j)\, z^{i+j-1} \frac{\partial \xi_\ell}{\partial \beta_\ell}\, ds,\end{aligned} \tag{A.16}$$

where

$$\begin{aligned}\partial_{11} &= \frac{\partial(s^*)}{\partial \beta_\ell} q^{\frac{1}{m-1}-1}(0)\, 0^{i+j} \\ &= -\frac{1}{m-1} (-\xi_\ell)^{\frac{1}{m-1}-1} \frac{\partial \xi_\ell}{\partial \beta_\ell} \left(\frac{\beta_0}{-\xi_\ell}\right)^{\frac{1}{m-1}-1} 0^{i+j} \\ &= -\frac{1}{m-1} \frac{\partial \xi_\ell}{\partial \beta_\ell} \beta_0^{\frac{1}{m-1}-1} 0^{i+j}\end{aligned}$$

and

$$\begin{aligned}\partial_{12} &= \frac{\partial (0)}{\partial \beta_\ell} q^{\frac{1}{m-1}-1}(\xi_\ell)\, \xi_\ell^{i+j} \\ &= 0 \cdot q^{\frac{1}{m-1}-1}(\xi_\ell)\, \xi_\ell^{i+j}.\end{aligned}$$

We have calculated $q(0)$ in ∂_{11} by taking $x = 0$ in the identity $p(x) = (x - \xi_\ell)\, q(x)$. Considering the second boundary term, we see that $\partial_{12} = 0$, since $0 < q(\xi_\ell) < \infty$.

Using (A.2) and that $i + j \geq 1$, the first boundary term ∂_{11} can be calculated as

$$\partial_{11} = -\frac{1}{m-1}\left(-\frac{\xi_\ell^\ell}{p_x(\xi_\ell)}\right) \beta_0^{\frac{1}{m-1}-1} \cdot 0 = 0.$$

Using (A.3), (A.2), and that the boundary terms are zero in (A.16) gives that

$$\begin{aligned}\frac{\partial J_1}{\partial \beta_\ell}(i,\, j) = &-\frac{m-2}{m-1}\int_0^{s^*} q^{\frac{1}{m-1}-2}(z)\, \frac{z^\ell - \theta_\ell^{-1}\xi_\ell^\ell p_x(z)}{s^{m-1}} z^{i+j}\, ds \\ &- (i+j)\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\, z^{i+j-1}\, ds\end{aligned}$$

Assume that $i + j = 0$. In this case $J_1(0,\, 0) = \int_0^{s^*} q^{1/(m-1)-1}(z)\, ds$. Taking a derivative gives that

$$\frac{\partial J_1}{\partial \beta_\ell}(0,\, 0) = \partial_{11} - \partial_{12} + \int_0^{s^*}\left(\frac{1}{m-1} - 1\right) q^{\frac{1}{m-1}-2}(z)\, \frac{\partial}{\partial \beta_\ell}[q(z)]\, ds, \qquad \text{(A.17)}$$

where

$$\begin{aligned}\partial_{11} &= \frac{\partial (s^*)}{\partial \beta_\ell} q^{\frac{1}{m-1}-1}(0) \\ &= -\frac{1}{m-1}(-\xi_\ell)^{\frac{1}{m-1}-1}\frac{\partial \xi_\ell}{\partial \beta_\ell}\left(\frac{\beta_0}{-\xi_\ell}\right)^{\frac{1}{m-1}-1} \\ &= -\frac{1}{m-1}\frac{\partial \xi_\ell}{\partial \beta_\ell}\beta_0^{\frac{1}{m-1}-1}\end{aligned}$$

and

$$\begin{aligned}\partial_{12} &= \frac{\partial (0)}{\partial \beta_\ell} q^{\frac{1}{m-1}-1}(\xi_\ell) \\ &= 0 \cdot q^{\frac{1}{m-1}-1}(\xi_\ell).\end{aligned}$$

We have calculated $q(0)$ in ∂_{11} by taking $x=0$ in the identity $p(x)=(x-\xi_\ell)\,q(x)$. Considering the second boundary term, we see that $\partial_{12}=0$, since $0<q(\xi_\ell)<\infty$.

Using (A.3), (A.2), and that $\partial_{12}=0$ in (A.17) gives that

$$\begin{aligned}
\frac{\partial J_1}{\partial \beta_\ell}(0,\,0) &= -\frac{1}{m-1}\frac{\partial \xi_\ell}{\partial \beta_\ell}\beta_0^{\frac{1}{m-1}-1} \\
&\quad -\frac{m-2}{m-1}\int_0^{s^*} q^{\frac{1}{m-1}-2}(z)\,\frac{z^\ell-\theta_\ell^{-1}\xi_\ell^\ell p_x(z)}{s^{m-1}}\,ds \\
&= \frac{1}{m-1}\frac{\xi_\ell^\ell}{\theta_\ell}\beta_0^{\frac{1}{m-1}-1} \\
&\quad -\frac{m-2}{m-1}\int_0^{s^*} q^{\frac{1}{m-1}-2}(z)\,\frac{z^\ell-\theta_\ell^{-1}\xi_\ell^\ell p_x(z)}{s^{m-1}}\,ds
\end{aligned}$$

This completes the result. ■

A.1.2.4 Subcalculation two: ∂J_2

Lemma A.5. *Suppose condition* (A.11) *holds, then*

$$\begin{aligned}
\frac{\partial J_2}{\partial \beta_\ell}(i,\,j) &= -\frac{1}{m-1}\cdot\frac{\xi_r^\ell}{\theta_r}\beta_0^{\frac{1}{m-1}-1}\chi_{\{0\}}(i+j) \\
&\quad -\frac{m-2}{m-1}\cdot\frac{1}{\theta_r}\int_0^{s^\#} r^{\frac{1}{m-1}-2}(w)\,\frac{\theta_r w^\ell-\xi_r^\ell p_x(w)}{s^{m-1}}w^{i+j}\,ds \\
&\quad -(i+j)\,\frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#} r^{\frac{1}{m-1}-1}(w)\,w^{i+j-1}\,ds.
\end{aligned} \tag{A.18}$$

Note: the derivation of this formula shows that the integral in the last term need only make sense when $i+j\geq 1$.

Proof. Assume $i+j\geq 1$. These calculations will proceed much the same as those for ∂J_1. We proceed to rewrite J_2 by changing variables:

$$J_2(i,\,j)=\int_0^{s^\#} r^{\frac{1}{m-1}-1}(w)\,w^{i+j}\,ds.$$

We calculate a derivative of J_2 to be

$$\frac{\partial J_2}{\partial \beta_\ell}(i,\, j) = \partial_{21} - \partial_{22} + \int_0^{s^\#} \left(\frac{1}{m-1} - 1\right) r^{\frac{1}{m-1}-2}(w) \frac{\partial}{\partial \beta_\ell}[r(w)]\, w^{i+j}\, ds + \int_0^{s^\#} r^{\frac{1}{m-1}-1} \left(\xi_r - s^{m-1}\right)(i+j)\left(\xi_r - s^{m-1}\right)^{i+j-1} \frac{\partial \xi_r}{\partial \beta_\ell}\, ds, \tag{A.19}$$

where

$$\begin{aligned}\partial_{21} &= \frac{\partial\left(s^\#\right)}{\partial \beta_\ell} r^{\frac{1}{m-1}-1}(0)\, 0^{i+j} \\ &= \frac{1}{m-1} \xi_r^{\frac{1}{m-1}-1} \frac{\partial \xi_r}{\partial \beta_\ell} \left(\frac{\beta_0}{\xi_r}\right)^{\frac{1}{m-1}-1} 0^{i+j} \\ &= \frac{1}{m-1} \frac{\partial \xi_r}{\partial \beta_\ell} \beta_0^{\frac{1}{m-1}-1} 0^{i+j}\end{aligned}$$

and

$$\begin{aligned}\partial_{22} &= \frac{\partial(0)}{\partial \beta_\ell} r^{\frac{1}{m-1}-1}(\xi_r)\, \xi_r^{i+j} \\ &= 0 \cdot r^{\frac{1}{m-1}-1}(\xi_r)\, \xi_r^{i+j}.\end{aligned}$$

We have calculated $r(0)$ in ∂_{21} by taking $x = 0$ in the identity $p(x) = (\xi_r - x)\, r(x)$. Considering the second boundary term, we see that $\partial_{22} = 0$, since $0 < r(\xi_r) < \infty$.

Using (A.2) and that $i + j \geq 1$, the first boundary term ∂_{21} can be calculated as

$$\partial_{21} = \frac{1}{m-1}\left(-\frac{\xi_r^\ell}{p_x(\xi_r)}\right) \beta_0^{\frac{1}{m-1}-1} \cdot 0 = 0.$$

Using (A.4), (A.2), and that the boundary terms are zero in (A.19) we get

$$\begin{aligned}\frac{\partial J_2}{\partial \beta_\ell}(i,\, j) = &-\frac{m-2}{m-1} \int_0^{s^\#} r^{\frac{1}{m-1}-2}(w) \frac{w^\ell - \theta_r^{-1} \xi_r^\ell p_x(w)}{s^{m-1}} w^{i+j}\, ds \\ &- (i+j) \frac{\xi_r^\ell}{\theta_r} \int_0^{s^\#} r^{\frac{1}{m-1}-1}(w)\, w^{i+j-1}\, ds\end{aligned}$$

Assume that $i + j = 0$. In this case $J_2(0,\, 0) = \int_0^{s^\#} r^{1/(m-1)-1}(w)\, ds$. Taking a derivative gives that

$$\frac{\partial J_2}{\partial \beta_\ell}(0,\, 0) = \partial_{21} - \partial_{22} + \int_0^{s^\#} \left(\frac{1}{m-1} - 1\right) r^{\frac{1}{m-1}-2}(w) \frac{\partial}{\partial \beta_\ell}[r(w)]\, ds, \tag{A.20}$$

where

$$
\begin{aligned}
\partial_{21} &= \frac{\partial\left(s^{\#}\right)}{\partial\beta_\ell} r^{\frac{1}{m-1}-1}(0) \\
&= \frac{1}{m-1}\xi_r^{\frac{1}{m-1}-1}\frac{\partial\xi_r}{\partial\beta_\ell}\left(\frac{\beta_0}{\xi_r}\right)^{\frac{1}{m-1}-1} \\
&= \frac{1}{m-1}\frac{\partial\xi_r}{\partial\beta_\ell}\beta_0^{\frac{1}{m-1}-1}
\end{aligned}
$$

and

$$
\begin{aligned}
\partial_{22} &= \frac{\partial(0)}{\partial\beta_\ell} r^{\frac{1}{m-1}-1}(\xi_r) \\
&= 0\cdot r^{\frac{1}{m-1}-1}(\xi_r).
\end{aligned}
$$

We have calculated $r(0)$ in ∂_{21} by taking $x=0$ in the identity $p(x)=(\xi_r-x)\,r(x)$. Considering the second boundary term, we see that $\partial_{22}=0$, since $0<r(\xi_r)<\infty$.

Using (A.4), (A.2), and that $\partial_{22}=0$ in (A.20) we get that

$$
\begin{aligned}
\frac{\partial J_2}{\partial\beta_\ell}(0,\,0) &= \frac{1}{m-1}\frac{\partial\xi_r}{\partial\beta_\ell}\beta_0^{\frac{1}{m-1}-1} \\
&\quad - \frac{m-2}{m-1}\int_0^{s^{\#}} r^{\frac{1}{m-1}-2}(w)\,\frac{w^\ell-\theta_r^{-1}\xi_r^\ell p_x(w)}{s^{m-1}}\,ds \\
&= -\frac{1}{m-1}\cdot\frac{\xi_r^\ell}{\theta_r}\beta_0^{\frac{1}{m-1}-1} \\
&\quad - \frac{m-2}{m-1}\int_0^{s^{\#}} r^{\frac{1}{m-1}-2}(w)\,\frac{w^\ell-\theta_r^{-1}\xi_r^\ell p_x(w)}{s^{m-1}}\,ds
\end{aligned}
$$

This completes the result. ■

Now that ∂J_1 and ∂J_2 have been shown to be well-defined, we combine the results of lemmas A.4 and A.5 to give (B.5) of the summary.

A.2 Load vector, f, and its derivatives

A.2.1 Load vector, f

Let p and $\tilde{u}$ be as in (2.18)-(2.19). Then the load vector, $\mathbf{f}$, in (2.27) is

$$
\begin{aligned}
f_i &= \int_{\xi_\ell}^{\xi_r} m\,(m-1)\,\tilde{u}^{m-2}(x)\,\tilde{u}_x^2(x)\,\phi_i(x)\;dx \\
&\quad + \int_{\xi_\ell}^{\xi_r} m\tilde{u}^{m-1}(x)\,\tilde{u}_{xx}(x)\,\phi_i(x)\;dx \\
&= \frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_x^2(x)\,\phi_i(x)\;dx \\
&\quad + \frac{m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x)\,p_{xx}(x)\,\phi_i(x)\;dx.
\end{aligned}
\tag{A.21}
$$

We write $\mathbf{f} = I_1 + I_2$, with

$$
I_1(i) = \frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_x^2(x)\,\phi_i(x)\;dx
$$

and

$$
I_2(i) = \frac{m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x)\,p_{xx}(x)\,\phi_i(x)\;dx.
$$

We should be sure that these formulas make sense.

Lemma A.6. *The integrals in I_1 and I_2 in the definition of $\mathbf{f}$ are well-defined.*

Proof. Since $\phi_i(x)$ is a polynomial defined on a bounded domain $\phi_i(x) \in L^\infty(\Xi(t))$, for any fixed t. Similarly, $p_x(x) \in L^\infty(\Xi(t))$. Finally, since we have seen from lemma A.1 that $p^{1/(m-1)-1}(x) \in L^1(\Xi(t))$, we have that the integral in $I_1 < \infty$. To see that I_2 is well-defined we point out that since $1/(m-1) > 0$ for all $m > 1$ and $p(x)$, $p_{xx}(x)$ and $\phi_i(x)$ are bounded for $x \in \Xi(t)$, there is an $0 < M < \infty$ such that

$$
I_2(i) \le M\int_{\xi_\ell}^{\xi_r} dx < \infty.
$$

■

Corollary A.3. *If $\{\phi_i(x)\} = \{x^i\}$, $\mathbf{f}$ is well-defined.*

Proof. The arguments made for lemma A.6 hold. ■

A.2.2 Derivatives of f

For the remainder of section A.2 we set $\{\phi_i\}$ to be the standard basis. $\mathbf{f}$ being well-defined, we calculate $\partial\mathbf{f}$. The calculation is broken into several cases and steps:

1. $\partial\mathbf{f}$, $m \in (1,\, 2)$ in section A.2.3
2. $\partial\mathbf{f}$, $m = 2$ in section A.2.4
3. $\partial\mathbf{f} = \partial I_1 + \partial I_2$, $\partial I_1 = \partial J_1 + \partial J_2$, $m \in (2,\, \infty)$ in section A.2.5
   (a) ∂J_1 in section A.2.5.1
   (b) ∂J_2 in section A.2.5.2

A.2.3 Derivatives of f, $1 < m < 2$

Lemma A.7. *Let $1 < m < 2$.*

$$\begin{aligned}\frac{\partial f_i}{\partial \boldsymbol{\beta}_\ell} = {} & \frac{m\,(2-m)}{(m-1)^3}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\,p_x^2(x)\,x^{i+\ell}\,dx \\ & + \frac{2\ell m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_x(x)\,x^{i+\ell-1}\,dx \\ & + \frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_{xx}(x)\,x^{i+\ell}\,dx \\ & + \frac{\ell\,(\ell-1)\,m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x)\,x^{i+\ell-2}\,dx.\end{aligned}$$

Note: the derivation of this formula shows that the integral in the second term need only make sense when $\ell \geq 1$. Similarly, the integral in the fourth term need only make sense when $\ell \geq 2$.

Proof. Take $1 < m < 2$ in (A.21). Taking a derivative of $\mathbf{f}$, we get $\partial\mathbf{f} = \partial I_1 + \partial I_2$. These terms may be written as $\partial I_1 = \partial_{11} + \partial_{12} + \partial I_{11} + \partial I_{12}$ and $\partial I_2 = \partial_{21} + \partial_{22} +$

$\partial I_{21}+\partial I_{22}$, where

$$\partial_{11}+\partial_{12}=\frac{m}{(m-1)^2}\frac{\partial \xi_r}{\partial \beta_\ell}p^{\frac{1}{m-1}-1}(\xi_r)\,p_x^2(\xi_r)\,\xi_r^i-\frac{m}{(m-1)^2}\frac{\partial \xi_\ell}{\partial \beta_\ell}p^{\frac{1}{m-1}-1}(\xi_\ell)\,p_x^2(\xi_\ell)\,\xi_\ell^i, \tag{A.22}$$

$$\frac{\partial I_{11}}{\partial \beta_\ell}(i)=\frac{m(2-m)}{(m-1)^3}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}-2}(x)\,p_x^2(x)\,x^{i+\ell}\,dx, \tag{A.23}$$

$$\begin{aligned}\frac{\partial I_{12}}{\partial \beta_\ell}(i)&=\frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}-1}(x)\,\frac{\partial}{\partial \beta_\ell}\left[p_x^2(x)\right]x^i\,dx\\&=\frac{2m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}-1}(x)\,p_x(x)\,\frac{\partial}{\partial \beta_\ell}\left[p_x(x)\right]x^i\,dx\\&=\frac{2\ell m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}-1}(x)\,p_x(x)\,x^{i+\ell-1}\,dx,\end{aligned} \tag{A.24}$$

$$\partial_{21}+\partial_{22}=\frac{m}{m-1}\frac{\partial \xi_r}{\partial \beta_\ell}p^{\frac{1}{m-1}}(\xi_r)\,p_{xx}(\xi_r)\,\xi_r^i-\frac{m}{m-1}\frac{\partial \xi_\ell}{\partial \beta_\ell}p^{\frac{1}{m-1}}(\xi_\ell)\,p_{xx}(\xi_\ell)\,\xi_\ell^i, \tag{A.25}$$

$$\frac{\partial I_{21}}{\partial \beta_\ell}(i)=\frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}-1}(x)\,p_{xx}(x)\,x^{i+\ell}\,dx, \tag{A.26}$$

and

$$\begin{aligned}\frac{\partial I_{22}}{\partial \beta_\ell}(i)&=\frac{m}{m-1}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}}(x)\,\frac{\partial}{\partial \beta_\ell}\left[p_{xx}(x)\right]x^i\,dx\\&=\frac{\ell(\ell-1)\,m}{m-1}\int_{\xi_\ell}^{\xi_r}p^{\frac{1}{m-1}}(x)\,x^{i+\ell-2}\,dx.\end{aligned} \tag{A.27}$$

The boundary terms $\partial_{11}+\partial_{12}$ and $\partial_{21}+\partial_{22}$ vanish since $|\partial\xi|$, $|p_x(\xi)|$, $|p_{xx}(\xi)|$ and ξ are finite, $p(\xi)=0$ and the exponents $1/(m-1)-1$ and $1/(m-1)$ are positive.

Note that when $\ell=0$, $\partial p_x\equiv\partial p_{xx}\equiv 0$ because the coefficient of the constant term of p, β_0, appears in neither p_x nor p_{xx}. Similarly, when $\ell=1$, $\partial p_{xx}\equiv 0$, because the coefficient of the linear term of p, β_1, does not appear in p_{xx}. This gives that $\partial_0 I_{12}(i)=0$, when $\ell=0$, which is consistent with (A.24). Similarly, $\partial_\ell I_{22}(i)=0$, when $\ell\le 1$, which is consistent with (A.27). The integrals defining $\partial_\ell I_{12}(i)$, for $\ell\ge 1$, $\partial_\ell I_{21}$, for all ℓ, and $\partial_\ell I_{22}$, for $\ell\ge 2$, exist because the functions

$p(x)$, $|p_x(x)|$, $|p_{xx}(x)|$ and x^α, $\alpha \geq 0$, are bounded on the interval $\Xi(t)$ and because the exponents $1/(m-1)-1$ and $1/(m-1)$ are positive. The relevant integral arising from ∂I_{11}, $\int_{\xi_\ell}^{\xi_r} p^{1/(m-1)-2}(x)\,dx$, also appears in ∂H and was shown to exist in the case $1 < m < 2$. ■

The results of lemma A.7 are collected in (B.7) of the summary.

A.2.4 Derivatives of f, $m = 2$

Lemma A.8. *Let* $m = 2$.

$$\frac{\partial f_i}{\partial \boldsymbol{\beta}_\ell} = -2\theta_r \xi_r^{i+\ell} + 2\theta_\ell \xi_\ell^{i+\ell} + 4\ell \int_{\xi_\ell}^{\xi_r} p_x(x)\, x^{i+\ell-1}\,dx$$
$$+ 2\int_{\xi_\ell}^{\xi_r} p_{xx}(x)\, x^{i+\ell}\,dx + 2\ell(\ell-1)\int_{\xi_\ell}^{\xi_r} p(x)\, x^{i+\ell-2}\,dx,$$

Note: the derivation of this formula shows that the integral in the third term need only make sense when $\ell \geq 1$. *Similarly, the integral in the fifth term need only make sense when* $\ell \geq 2$.

Proof. Putting $m = 2$ in (A.21) gives $\mathbf{f} = I_1 + I_2$, where

$$I_1(i) = 2\int_{\xi_\ell}^{\xi_r} p_x^2(x)\, x^i\,dx$$

and

$$I_2(i) = 2\int_{\xi_\ell}^{\xi_r} p(x)\, p_{xx}(x)\, x^i\,dx.$$

We compute $\partial_\ell I_1$ for the cases $\ell = 0$ and $\ell \geq 1$, then compute $\partial_\ell I_2$ for the cases $\ell \leq 1$ and $\ell \geq 2$.

Taking the derivative of I_1 gives

$$\frac{\partial I_1}{\partial \beta_\ell}(i) = 2\frac{\partial \xi_r}{\partial \beta_\ell} p_x^2(\xi_r)\,\xi_r^i - 2\frac{\partial \xi_\ell}{\partial \beta_\ell} p_x^2(\xi_\ell)\,\xi_\ell^i + 4\int_{\xi_\ell}^{\xi_r} p_x(x)\,\frac{\partial}{\partial \beta_\ell}[p_x(x)]\, x^i\,dx,$$

the boundary terms of which are well-defined since $|\partial\xi|$, $p_x(\xi)$, and ξ have bounded ranges.

Assume that $\ell = 0$. The coefficient β_0, of p_x, is identically zero, which gives that $\partial_0 I_1 (i) = 2\partial_0 \xi_r p_x^2 (\xi_r) \xi_r^i - 2\partial_0 \xi_\ell p_x^2 (\xi_\ell) \xi_\ell^i$.

Then

$$\begin{aligned}
\frac{\partial I_1}{\partial \beta_0} (i) &= 2\partial_0 \xi_r p_x^2 (\xi_r) \xi_r^i - 2\partial_0 \xi_\ell p_x^2 (\xi_\ell) \xi_\ell^i \\
&= 2 \left(-\frac{\xi_r^0}{p_x (\xi_r)} \right) p_x^2 (\xi_r) \xi_r^i - 2 \left(-\frac{\xi_\ell^0}{p_x (\xi_\ell)} \right) p_x^2 (\xi_\ell) \xi_\ell^i \\
&= -2p_x (\xi_r) \xi_r^i + 2p_x (\xi_\ell) \xi_\ell^i.
\end{aligned}$$

Assume that $\ell \geq 1$. We get

$$\frac{\partial I_1}{\partial \beta_\ell} (i) = -2p_x (\xi_r) \xi_r^{i+\ell} + 2p_x (\xi_\ell) \xi_\ell^{i+\ell} + 4\ell \int_{\xi_\ell}^{\xi_r} p_x (x) x^{i+\ell-1} \, dx.$$

Regardless, the integral appearing in ∂I_1 is well-defined since $|p_x (x)|$ and x^α, $\alpha \geq 0$, are bounded on the interval $\Xi (t)$.

We now compute ∂I_2. Taking the derivative of I_2 gives $\partial I_2 = \partial_{21} + \partial_{22} + \partial I_{21} + \partial I_{22}$, where

$$\partial_{21} + \partial_{22} = 2\frac{\partial \xi_r}{\partial \beta_\ell} p (\xi_r) p_{xx} (\xi_r) \xi_r^i - 2\frac{\partial \xi_r}{\partial \beta_\ell} p (\xi_\ell) p_{xx} (\xi_\ell) \xi_\ell^i,$$

$$\frac{\partial I_{21}}{\partial \beta_\ell} (i) = 2 \int_{\xi_\ell}^{\xi_r} p_{xx} (x) x^{i+\ell} \, dx$$

and

$$\frac{\partial I_{22}}{\partial \beta_\ell} (i) = 2 \int_{\xi_\ell}^{\xi_r} p (x) \frac{\partial}{\partial \beta_\ell} [p_{xx} (x)] x^i \, dx.$$

The boundary terms, $\partial_{21} + \partial_{22}$, vanish since $p (\xi) = 0$ and because $|\partial \xi|$, $|p_{xx} (\xi)|$, and ξ have bounded ranges. The integral in ∂I_{21} is well-defined because $|p_{xx} (x)|$ and x^α, $\alpha \geq 0$, are bounded functions over $\Xi (t)$. When $\ell = 0, 1$, the term $\partial_\ell I_{22}$ is identically zero since the coefficients β_0 and β_1, of p_{xx}, are identically zero. This means that when $\ell = 0, 1$, we have

$$\frac{\partial I_2}{\partial \beta_\ell} (i) = 2 \int_{\xi_\ell}^{\xi_r} p_{xx} (x) x^{i+\ell} \, dx$$

and when $\ell \geq 2$, we have

$$\frac{\partial I_2}{\partial \beta_\ell}(i) = 2\int_{\xi_\ell}^{\xi_r} p_{xx}(x)\, x^{i+\ell}\, dx + 2\ell(\ell-1)\int_{\xi_\ell}^{\xi_r} p(x)\, x^{i+\ell-2}\, dx.$$

■

The results of lemma A.8 are summarized in (B.8) of the summary.

A.2.5 Derivatives of f, $m > 2$

We calculate the derivative to be $\partial \mathbf{f} = \partial I_1 + \partial I_2$, where $\partial I_1 = \partial_{11} + \partial_{12} + \partial I_{11} + \partial I_{12}$ and $\partial I_2 = \partial_{21} + \partial_{22} + \partial I_{21} + \partial I_{22}$, and where $\partial_{11} + \partial_{12}$, ∂I_{11}, ∂I_{12}, $\partial_{21} + \partial_{22}$, ∂I_{21}, and ∂I_{22} are defined in equations (A.22)-(A.27).

Take $m > 2$. The boundary terms (A.22) appear to blow up because $p(\xi) = 0$ and the exponent, $1/(m-1) - 1$, is negative. Likewise, the first integral term (A.23) has an apparent singularity at the interface that may not be integrable, since the exponent, $1/(m-1) - 2$, is smaller than -1 and $p(x) \to 0$ as $|x - \xi| \to 0$ for $x \in \Xi(t)$.

Lemma A.9. *Let $m > 2$. $\partial \mathbf{f} = \partial I_1 + \partial I_2$, where ∂I_1 and ∂I_2 are given by:*[*]

$$
\begin{aligned}
\frac{\partial I_1}{\partial \beta_\ell}(i) = {} & \frac{m}{(m-1)^2} \beta_0^{\frac{1}{m-1}-1} \beta_1^2 \left[\frac{\xi_\ell^\ell}{\theta_\ell} - \frac{\xi_r^\ell}{\theta_r} \right] \chi_{\{0\}}(i) \\
& - \frac{m(m-2)}{(m-1)^2} \left[\frac{1}{\theta_\ell} \int_0^{s^*} \left(q^{\frac{1}{m-1}-2} p_x^2 \right)(z) \frac{\theta_\ell z^\ell - \xi_\ell^\ell p_x(z)}{s^{m-1}} z^i \, ds \right. \\
& \qquad \left. + \frac{1}{\theta_r} \int_0^{s^\#} \left(r^{\frac{1}{m-1}-2} p_x^2 \right)(w) \frac{\theta_r w^\ell - \xi_r^\ell p_x(w)}{s^{m-1}} w^i \, ds \right] \\
& + \frac{2\ell m}{m-1} \left[\int_0^{s^*} \left(q^{\frac{1}{m-1}-1} p_x \right)(z) z^{i+\ell-1} \, ds \right. \\
& \qquad \left. + \int_0^{s^\#} \left(r^{\frac{1}{m-1}-1} p_x \right)(w) w^{i+\ell-1} \, ds \right] \\
& - \frac{2m}{m-1} \left[\frac{\xi_\ell^\ell}{\theta_\ell} \int_0^{s^*} \left(q^{\frac{1}{m-1}-1} p_x p_{xx} \right)(z) z^i \, ds \right. \\
& \qquad \left. + \frac{\xi_r^\ell}{\theta_r} \int_0^{s^\#} \left(r^{\frac{1}{m-1}-1} p_x p_{xx} \right)(w) w^i \, ds \right] \\
& - \frac{im}{m-1} \left[\frac{\xi_\ell^\ell}{\theta_\ell} \int_0^{s^*} \left(q^{\frac{1}{m-1}-1} p_x^2 \right)(z) z^{i-1} \, ds \right. \\
& \qquad \left. + \frac{\xi_r^\ell}{\theta_r} \int_0^{s^\#} \left(r^{\frac{1}{m-1}-1} p_x^2 \right)(w) w^{i-1} \, ds \right].
\end{aligned}
$$

$$
\begin{aligned}
\frac{\partial I_2}{\partial \beta_\ell}(i) = {} & \frac{m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x) p_{xx}(x) x^{i+\ell} \, dx \\
& + \frac{\ell(\ell-1) m}{m-1} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x) x^{i+\ell-2} \, dx.
\end{aligned}
$$

Note: the derivation of this formula shows that the integrals in the third term in $\partial_\ell I_1$ need only make sense when $\ell \geq 1$. Similarly, the integrals in the fifth term of $\partial I_1(i)$ need only make sense when $i \geq 1$, and the integral in the second term of $\partial_\ell I_2$ need only make sense when $\ell \geq 2$.

Proof. We address ∂I_2 then ∂I_1. The formulas for ∂I_2 are well-defined: The boundary terms (A.25) are zero since $|\partial \xi|$ is bounded $|\xi|$, $|p_{xx}(\xi)| < \infty$, the exponent $1/(m-1)$ is positive for all $m > 1$, and $p(\xi) = 0$. The second integral (A.27)

[*]Recall that $\chi_I(x)$ is the indicator function on the set I.

exists because $1/(m-1) > 0$ and $|x|$, $|p(x)| < \infty$, for $x \in \Xi(t)$. Likewise, the first integral (A.26) exists as $p_{xx}(x)\, x^{i+\ell} \in L^{\infty}(\Xi(t))$ and $p^{1/(m-1)-1}(x) \in L^{1}(\Xi(t))$, as has been shown in lemma A.1. So our results from the case $1 < m < 2$ carry over: If $\ell \leq 1$, then

$$\frac{\partial I_2}{\partial \beta_\ell}(i) = \frac{m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, p_{xx}(x)\, x^{i+\ell}\, dx.$$

If $\ell \geq 2$, then

$$\begin{aligned} \frac{\partial I_2}{\partial \beta_\ell}(i) &= \frac{m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, p_{xx}(x)\, x^{i+\ell}\, dx \\ &\quad + \frac{\ell(\ell-1)\, m}{m-1} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x)\, x^{i+\ell-2}\, dx. \end{aligned}$$

Now we address ∂I_1. Rewrite I_1 as $I_1 = J_1 + J_2$, where

$$\begin{aligned} J_1(i) &= \int_{\xi_\ell}^{0} \frac{m}{(m-1)^2} p^{\frac{1}{m-1}-1}(x)\, p_x^2(x)\, x^i\, dx \\ &= \int_0^{s^*} \frac{m}{m-1} q^{\frac{1}{m-1}-1}\left(\xi_\ell + s^{m-1}\right) p_x^2\left(\xi_\ell + s^{m-1}\right)\left(\xi_\ell + s^{m-1}\right)^i\, ds \\ &= \int_0^{s^*} \frac{m}{m-1}\left(q^{\frac{1}{m-1}-1} p_x^2\right)(z)\, z^i\, ds \qquad \text{(A.28)} \end{aligned}$$

and

$$\begin{aligned} J_2(i) &= \int_{0}^{\xi_r} \frac{m}{(m-1)^2} p^{\frac{1}{m-1}-1}(x)\, p_x^2(x)\, x^i\, dx \\ &= \int_0^{s^\#} \frac{m}{m-1} r^{\frac{1}{m-1}-1}\left(\xi_r - s^{m-1}\right) p_x^2\left(\xi_r - s^{m-1}\right)\left(\xi_r - s^{m-1}\right)^i\, ds \\ &= \int_0^{s^\#} \frac{m}{m-1}\left(r^{\frac{1}{m-1}-1} p_x^2\right)(w)\, w^i\, ds. \qquad \text{(A.29)} \end{aligned}$$

The calculation of ∂J_1 is in lemma A.10 of subsection A.2.5.1. The calculation of ∂J_2 is completely analogous to that of ∂J_1 and is in lemma A.11 of subsection A.2.5.2. We combine the results of these lemmas to get ∂I_1 as above.

That every integral in these formulas is well-defined can be seen as before. By judiciously choosing factors of the integrand to bound from above we arrive at integrals the existence of which was established above. ■

The results of lemma A.9 are summarized in (B.9)-(B.11) of the summary.

A.2.5.1 Subcalculation one: ∂J_1

Lemma A.10. *Let $m > 2$.*

$$\begin{aligned}\frac{\partial J_1}{\partial \boldsymbol{\beta}_\ell}(i) &= \frac{m}{(m-1)^2} \cdot \frac{\xi_\ell^\ell}{\theta_\ell} \beta_0^{\frac{1}{m-1}-1} \beta_1^2 \chi_{\{0\}}(i) \\ &\quad - \frac{m(m-2)}{(m-1)^2} \cdot \frac{1}{\theta_\ell} \int_0^{s^*} \left(q^{\frac{1}{m-1}-2} p_x^2\right)(z) \frac{\theta_\ell z^\ell - \xi_\ell^\ell p_x(z)}{s^{m-1}} z^i \, ds \\ &\quad + \frac{2\ell m}{m-1} \int_0^{s^*} \left(q^{\frac{1}{m-1}-1} p_x\right)(z) z^{i+\ell-1} \, ds \\ &\quad - \frac{2m}{m-1} \cdot \frac{\xi_\ell^\ell}{\theta_\ell} \int_0^{s^*} \left(q^{\frac{1}{m-1}-1} p_x p_{xx}\right)(z) z^i \, ds \\ &\quad - \frac{im}{m-1} \cdot \frac{\xi_\ell^\ell}{\theta_\ell} \int_0^{s^*} \left(q^{\frac{1}{m-1}-1} p_x^2\right)(z) z^{i-1} \, ds.\end{aligned}$$

Note: the derivation of this formula shows that the integral in the third term need only make sense when $\ell \geq 1$. Similarly, the integral in the last term need only make sense when $i \geq 1$.

Proof. Taking a derivative of (A.28) we have

$$\frac{\partial J_1}{\partial \beta_\ell} = \partial_{11} - \partial_{12} + L_1 + L_2 + L_3, \tag{A.30}$$

where

$$\begin{aligned}
\partial_{11} &= \frac{\partial\left(s^*\right)}{\partial\beta_\ell}\frac{m}{m-1}q^{\frac{1}{m-1}-1}\left(0\right)p_x^2\left(0\right)0^i \\
&= -\frac{1}{m-1}\left(-\xi_\ell\right)^{\frac{1}{m-1}-1}\frac{\partial\xi_\ell}{\partial\beta_\ell}\frac{m}{m-1}\left(\frac{\beta_0}{-\xi_\ell}\right)^{\frac{1}{m-1}-1}p_x^2\left(0\right)0^i \\
&= -\frac{m}{\left(m-1\right)^2}\frac{\partial\xi_\ell}{\partial\beta_\ell}\beta_0^{\frac{1}{m-1}-1}p_x^2\left(0\right)0^i, \qquad \text{(A.31)}\\
\partial_{12} &= \frac{\partial\left(0\right)}{\partial\beta_\ell}\frac{m}{m-1}q^{\frac{1}{m-1}-1}\left(\xi_\ell\right)p_x^2\left(\xi_\ell\right)\xi_\ell^i \\
&= 0\cdot\frac{m}{m-1}q^{\frac{1}{m-1}-1}\left(\xi_\ell\right)p_x^2\left(\xi_\ell\right)\xi_\ell^i \\
&= 0, \qquad \text{(A.32)}\\
L_1\left(i\right) &= \frac{m}{m-1}\int_0^{s^*}\frac{\partial}{\partial\beta_\ell}\left[q^{\frac{1}{m-1}-1}\left(z\right)\right]p_x^2\left(z\right)z^i\,ds \\
&= \frac{m}{m-1}\int_0^{s^*}\left(\frac{1}{m-1}-1\right)q^{\frac{1}{m-1}-2}\left(z\right)\frac{\partial}{\partial\beta_\ell}\left[q\left(z\right)\right]p_x^2\left(z\right)z^i\,ds, \qquad \text{(A.33)}\\
L_2\left(i\right) &= \frac{m}{m-1}\int_0^{s^*}q^{\frac{1}{m-1}-1}\left(z\right)\frac{\partial}{\partial\beta_\ell}\left[p_x^2\left(z\right)\right]z^i\,ds \\
&= \frac{m}{m-1}\int_0^{s^*}q^{\frac{1}{m-1}-1}\left(z\right)\left(2\right)p_x\left(z\right)\frac{\partial}{\partial\beta_\ell}\left[p_x\left(z\right)\right]z^i\,ds \qquad \text{(A.34)}
\end{aligned}$$

and

$$L_3\left(i\right) = \frac{m}{m-1}\int_0^{s^*}q^{\frac{1}{m-1}-1}\left(z\right)p_x^2\left(z\right)iz^{i-1}\frac{\partial\xi_\ell}{\partial\beta_\ell}\,ds. \qquad \text{(A.35)}$$

Consider the boundary term ∂_{11} (A.31). Take $i\geq 1$. Using (A.2) and that $|\partial\xi|$ is bounded in (A.31) we get that $\partial_{11}=0$. If $i=0$, we use (A.2) in (A.31) to get

$$\begin{aligned}
\partial_{11} &= -\frac{m}{\left(m-1\right)^2}\left(-\frac{\xi_\ell^\ell}{\theta_\ell}\right)\beta_0^{\frac{1}{m-1}-1}\beta_1^2 \\
&= \frac{m}{\left(m-1\right)^2}\cdot\frac{\xi_\ell^\ell}{\theta_\ell}\beta_0^{\frac{1}{m-1}-1}\beta_1^2.
\end{aligned}$$

Consider the second boundary term ∂_{12} given by (A.32). As $q\left(\xi_\ell\right)$, $p_x\left(\xi_\ell\right)$, and ξ_ℓ are all finite, we see that $\partial_{12}=0$.

Consider L_1. We use (A.3) and (A.2) in (A.33) to get

$$L_1\left(i\right) = -\frac{\left(m-2\right)m}{\left(m-1\right)^2}\int_0^{s^*}q^{\frac{1}{m-1}-2}\left(z\right)\frac{z^\ell-\theta_\ell^{-1}\xi_\ell^\ell p_x\left(z\right)}{s^{m-1}}p_x^2\left(z\right)z^i\,ds.$$

Consider L_2. We use (A.5) and (A.2) in (A.34) to get

$$\begin{aligned} L_2(i) &= \frac{2\ell m}{m-1}\int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\,p_x(z)\,z^{i+\ell-1}\,ds \\ &\quad + \frac{2m}{m-1}\cdot\frac{\partial\xi_\ell}{\partial\beta_\ell}\int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\,(p_x p_{xx})(z)\,z^i\,ds \\ &= \frac{2\ell m}{m-1}\int_0^{s^*}\left(q^{\frac{1}{m-1}-1}p_x\right)(z)\,z^{i+\ell-1}\,ds \\ &\quad - \frac{2m}{m-1}\cdot\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*}\left(q^{\frac{1}{m-1}-1}p_x p_{xx}\right)(z)\,z^i\,ds. \end{aligned}$$

Consider L_3. Taking $i=0$ in (A.28) shows that L_3 will not be present in this case. Take $i \geq 1$. Using (A.2) in (A.35) we have

$$L_3(i) = -\frac{m}{m-1}\cdot\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\,p_x^2(z)\,iz^{i-1}\,ds.$$

This gives the result. ■

A.2.5.2 Subcalculation two: ∂J_2

Lemma A.11. *Let $m>2$.*

$$\begin{aligned} \frac{\partial J_2}{\partial\boldsymbol{\beta}_\ell}(i) &= -\frac{m}{(m-1)^2}\cdot\frac{\xi_r^\ell}{\theta_r}\beta_0^{\frac{1}{m-1}-1}\beta_1^2\chi_{\{0\}}(i) \\ &\quad - \frac{m(m-2)}{(m-1)^2}\cdot\frac{1}{\theta_r}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-2}p_x^2\right)(w)\,\frac{\theta_r w^\ell - \xi_r^\ell p_x(w)}{s^{m-1}}w^i\,ds \\ &\quad + \frac{2\ell m}{m-1}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-1}p_x\right)(w)\,w^{i+\ell-1}\,ds \\ &\quad - \frac{2m}{m-1}\cdot\frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-1}p_x p_{xx}\right)(w)\,w^i\,ds \\ &\quad - \frac{im}{m-1}\cdot\frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-1}p_x^2\right)(w)\,w^{i-1}\,ds. \end{aligned}$$

Note: the derivation of this formula shows that the integral in the third term need only make sense when $\ell \geq 1$. Similarly, the integral in the last term need only make sense when $i \geq 1$.

Proof. Taking a derivative of (A.29) we have

$$\frac{\partial J_2}{\partial \beta_\ell} = \partial_{21} - \partial_{22} + R_1 + R_2 + R_3, \tag{A.36}$$

where

$$\begin{aligned}
\partial_{21} &= \frac{\partial \left(s^{\#}\right)}{\partial \beta_\ell} \frac{m}{m-1} r^{\frac{1}{m-1}-1}(0)\, p_x^2(0)\, 0^i \\
&= \frac{1}{m-1} \xi_r^{\frac{1}{m-1}-1} \frac{\partial \xi_r}{\partial \beta_\ell} \frac{m}{m-1} \left(\frac{\beta_0}{\xi_r}\right)^{\frac{1}{m-1}-1} p_x^2(0)\, 0^i \\
&= \frac{m}{(m-1)^2} \frac{\partial \xi_r}{\partial \beta_\ell} \beta_0^{\frac{1}{m-1}-1} p_x^2(0)\, 0^i, && \text{(A.37)} \\
\partial_{22} &= \frac{\partial(0)}{\partial \beta_\ell} \frac{m}{m-1} r^{\frac{1}{m-1}-1}(\xi_r)\, p_x^2(\xi_r)\, \xi_r^i \\
&= 0 \cdot \frac{m}{m-1} r^{\frac{1}{m-1}-1}(\xi_r)\, p_x^2(\xi_r)\, \xi_r^i \\
&= 0, && \text{(A.38)} \\
R_1(i) &= \frac{m}{m-1} \int_0^{s^{\#}} \frac{\partial}{\partial \beta_\ell} \left[r^{\frac{1}{m-1}-1}(w)\right] p_x^2(w)\, w^i\, ds \\
&= \frac{m}{m-1} \int_0^{s^{\#}} \left(\frac{1}{m-1} - 1\right) r^{\frac{1}{m-1}-2}(w) \frac{\partial}{\partial \beta_\ell} [r(w)]\, p_x^2(w)\, w^i\, ds, && \text{(A.39)} \\
R_2(i) &= \frac{m}{m-1} \int_0^{s^{\#}} r^{\frac{1}{m-1}-1}(w) \frac{\partial}{\partial \beta_\ell} \left[p_x^2(w)\right] w^i\, ds \\
&= \frac{m}{m-1} \int_0^{s^{\#}} r^{\frac{1}{m-1}-1}(w)\, (2)\, p_x(w) \frac{\partial}{\partial \beta_\ell} [p_x(w)]\, w^i\, ds && \text{(A.40)}
\end{aligned}$$

and

$$R_3(i) = \frac{m}{m-1} \int_0^{s^{\#}} r^{\frac{1}{m-1}-1}(w)\, p_x^2(w)\, i w^{i-1} \frac{\partial \xi_r}{\partial \beta_\ell}\, ds. \tag{A.41}$$

Consider the boundary term ∂_{21} (A.37). Take $i \geq 1$. Using (A.2) and that $|\partial \xi|$ is bounded in (A.37) we get that $\partial_{21} = 0$. If $i = 0$, we use (A.2) in (A.37) to get

$$\begin{aligned}
\partial_{21} &= \frac{m}{(m-1)^2} \left(-\frac{\xi_r^\ell}{\theta_r}\right) \beta_0^{\frac{1}{m-1}-1} \beta_1^2 \\
&= -\frac{m}{(m-1)^2} \cdot \frac{\xi_r^\ell}{\theta_r} \beta_0^{\frac{1}{m-1}-1} \beta_1^2.
\end{aligned}$$

Consider the second boundary term ∂_{22} given by (A.38). As $r(\xi_r)$, $p_x(\xi_r)$, and ξ_r are all finite, we see that $\partial_{22} = 0$.

Consider R_1. We use (A.4) and (A.2) in (A.39) to get

$$R_1(i) = -\frac{m(m-2)}{(m-1)^2} \int_0^{s^\#} r^{\frac{1}{m-1}-2}(w) \left[\frac{w^\ell - \theta_r^{-1} \xi_r^\ell p_x(w)}{s^{m-1}} \right] p_x^2(w) w^i \, ds.$$

Consider R_2. We use (A.5) and (A.2) in (A.40) to get

$$\begin{aligned} R_2(i) &= \frac{2\ell m}{m-1} \int_0^{s^*} r^{\frac{1}{m-1}-1}(w) p_x(w) w^{i+\ell-1} \, ds \\ &\quad + \frac{2m}{m-1} \frac{\partial \xi_r}{\partial \beta_\ell} \int_0^{s^\#} r^{\frac{1}{m-1}-1}(w) (p_x p_{xx})(w) w^i \, ds \\ &= \frac{2\ell m}{m-1} \int_0^{s^\#} r^{\frac{1}{m-1}-1}(w) p_x(w) w^{i+\ell-1} \, ds \\ &\quad - \frac{2m}{m-1} \frac{\xi_r^\ell}{\theta_r} \int_0^{s^\#} r^{\frac{1}{m-1}-1}(w) (p_x p_{xx})(w) w^i \, ds. \end{aligned}$$

Consider R_3. Taking $i = 0$ in (A.29) shows that R_3 will not be present in this case. Take $i \geq 1$. Using (A.2) in (A.41) we have

$$R_3(i) = -\frac{m}{m-1} \frac{\xi_r^\ell}{\theta_r} \int_0^{s^\#} r^{\frac{1}{m-1}-1}(w) p_x^2(w) i w^{i-1} \, ds.$$

This proves the result. ■

APPENDIX B

SUMMARY OF FORMULAS

The following is a summary of the formulas for H, $\mathbf{f}$, and their derivatives computed in appendix A. Recall that $\theta_r = p_x(\xi_r)$, and $\theta_\ell = p_x(\xi_\ell)$ for p as in (2.18)-(2.19), that $z = \xi_\ell + s^{m-1}$, $w = \xi_r - s^{m-1}$, that $s^* = (-\xi_\ell)^{1/(m-1)}$, $s^\# = \xi_r^{1/(m-1)}$, that $\chi_I(x)$ is the indicator function on the set I, and that $q \in \Pi_{N-1}$ and $r \in \Pi_{N-1}$ are defined such that $p(x) = (x - \xi_\ell)\, q(x) = (\xi_r - x)\, r(x)$. All indices run through $0, \ldots, N$.

B.1 H formulas

$$\boxed{H(i,\, j) = \frac{1}{m-1} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\, x^{i+j}\, dx} \tag{B.1}$$

$$\begin{aligned} \boxed{H(i,\, j)} &= \int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\, z^{i+j}\, ds \\ &\quad + \int_0^{s^\#} r^{\frac{1}{m-1}-1}(w)\, w^{i+j}\, ds \end{aligned} \tag{B.2}$$

B.1.1 ∂H, $1 < m < 2$

$$\boxed{\frac{\partial H}{\partial \beta_\ell}(i,\, j) = \frac{2-m}{(m-1)^2} \int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}(x)\, x^{i+j+\ell}\, dx} \tag{B.3}$$

B.1.2 ∂H, $m = 2$

$$\boxed{\frac{\partial H}{\partial \beta_\ell}(i,\, j) = -\theta_r^{-1} \xi_r^{i+j+\ell} + \theta_\ell^{-1} \xi_\ell^{i+j+\ell}} \tag{B.4}$$

B.1.3 ∂H, $m > 2$

$$\boxed{\frac{\partial H}{\partial \beta_\ell}(i,j)} = \frac{1}{m-1}\beta_0^{\frac{1}{m-1}-1}\left[\frac{\xi_\ell^\ell}{\theta_\ell} - \frac{\xi_r^\ell}{\theta_r}\right]\chi_{\{0\}}(i+j)$$
$$- \frac{m-2}{m-1}\left[\frac{1}{\theta_\ell}\int_0^{s^*} q^{\frac{1}{m-1}-2}(z)\,\frac{\theta_\ell z^\ell - \xi_\ell^\ell p_x(z)}{s^{m-1}} z^{i+j}\,ds\right.$$
$$\left. + \frac{1}{\theta_r}\int_0^{s^\#} r^{\frac{1}{m-1}-2}(w)\,\frac{\theta_r w^\ell - \xi_r^\ell p_x(w)}{s^{m-1}} w^{i+j}\,ds\right] \tag{B.5}$$
$$- (i+j)\left[\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*} q^{\frac{1}{m-1}-1}(z)\,z^{i+j-1}ds\right.$$
$$\left. + \frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#} r^{\frac{1}{m-1}-1}(w)\,w^{i+j-1}ds\right]$$

The derivation of this shows that the integrals in the last term need only make sense when $i + j \geq 1$.

B.2 f formulas

$$\boxed{f_i = \int_{\xi_\ell}^{\xi_r}\left[\frac{m}{(m-1)^2}p^{\frac{1}{m-1}-1}(x)\,p_x^2(x) + \frac{m}{m-1}p^{\frac{1}{m-1}}(x)\,p_{xx}(x)\right]x^i\,dx} \tag{B.6}$$

B.2.1 ∂f, $1 < m < 2$

$$\begin{aligned}\boxed{\frac{\partial f_i}{\partial \beta_\ell}} &= \frac{m\left(2-m\right)}{\left(m-1\right)^3}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-2}\left(x\right)p_x^2\left(x\right)x^{i+\ell}\,dx \\ &+ \frac{2\ell m}{\left(m-1\right)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}\left(x\right)p_x\left(x\right)x^{i+\ell-1}\,dx \\ &+ \frac{m}{\left(m-1\right)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}\left(x\right)p_{xx}\left(x\right)x^{i+\ell}\,dx \\ &+ \frac{\ell\left(\ell-1\right)m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}\left(x\right)x^{i+\ell-2}\,dx\end{aligned} \tag{B.7}$$

The derivation of this shows that the integral in the second term need only make sense when $\ell \geq 1$. Similarly, the integral in the last term need only make sense when $\ell \geq 2$.

B.2.2 ∂f, $m = 2$

$$\begin{aligned}\boxed{\frac{\partial f_i}{\partial \beta_\ell}} &= -2p_x\left(\xi_r\right)\xi_r^{i+\ell} + 2p_x\left(\xi_\ell\right)\xi_\ell^{i+\ell} + 4\ell\int_{\xi_\ell}^{\xi_r} p_x\left(x\right)x^{i+\ell-1}\,dx \\ &+ 2\int_{\xi_\ell}^{\xi_r} p_{xx}\left(x\right)x^{i+\ell}\,dx + 2\ell\left(\ell-1\right)\int_{\xi_\ell}^{\xi_r} p\left(x\right)x^{i+\ell-2}\,dx\end{aligned} \tag{B.8}$$

The derivation of this shows that the integral in the third term need only make sense when $\ell \geq 1$. Similarly, the integral in the last term need only make sense when $\ell \geq 2$.

B.2.3 ∂f, $m > 2$

$$\boxed{\frac{\partial \mathbf{f}}{\partial \beta} = \frac{\partial I_1}{\partial \beta} + \frac{\partial I_2}{\partial \beta}} \tag{B.9}$$

$$
\begin{aligned}
\boxed{\frac{\partial I_1}{\partial \beta_\ell}(i)} &= \frac{m}{(m-1)^2}\beta_0^{\frac{1}{m-1}-1}\beta_1^2\left[\frac{\xi_\ell^\ell}{\theta_\ell}-\frac{\xi_r^\ell}{\theta_r}\right]\chi_{\{0\}}(i) \\
&\quad - \frac{m(m-2)}{(m-1)^2}\left[\frac{1}{\theta_\ell}\int_0^{s^*}\left(q^{\frac{1}{m-1}-2}p_x^2\right)(z)\,\frac{\left[\theta_\ell z^\ell-\xi_\ell^\ell p_x(z)\right]z^i}{s^{m-1}}\,ds\right. \\
&\qquad\qquad \left. +\frac{1}{\theta_r}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-2}p_x^2\right)(w)\,\frac{\left[\theta_r w^\ell-\xi_r^\ell p_x(w)\right]w^i}{s^{m-1}}\,ds\right] \\
&\quad + \frac{2\ell m}{m-1}\left[\int_0^{s^*}\left(q^{\frac{1}{m-1}-1}p_x\right)(z)\,z^{i+\ell-1}\,ds\right. \\
&\qquad\qquad \left. +\int_0^{s^\#}\left(r^{\frac{1}{m-1}-1}p_x\right)(w)\,w^{i+\ell-1}\,ds\right] \\
&\quad - \frac{2m}{m-1}\left[\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*}\left(q^{\frac{1}{m-1}-1}p_xp_{xx}\right)(z)\,z^i\,ds\right. \\
&\qquad\qquad \left. +\frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-1}p_xp_{xx}\right)(w)\,w^i\,ds\right] \\
&\quad - \frac{im}{m-1}\left[\frac{\xi_\ell^\ell}{\theta_\ell}\int_0^{s^*}\left(q^{\frac{1}{m-1}-1}p_x^2\right)(z)\,z^{i-1}\,ds\right. \\
&\qquad\qquad \left. +\frac{\xi_r^\ell}{\theta_r}\int_0^{s^\#}\left(r^{\frac{1}{m-1}-1}p_x^2\right)(w)\,w^{i-1}\,ds\right]
\end{aligned} \tag{B.10}
$$

$$
\begin{aligned}
\boxed{\frac{\partial I_2}{\partial \beta_\ell}(i)} &= \frac{m}{(m-1)^2}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}-1}(x)\,p_{xx}(x)\,x^{i+\ell}\,dx \\
&\quad + \frac{\ell(\ell-1)m}{m-1}\int_{\xi_\ell}^{\xi_r} p^{\frac{1}{m-1}}(x)\,x^{i+\ell-2}\,dx
\end{aligned} \tag{B.11}
$$

The derivation of $\partial_\ell I_1$ shows that the integrals in the third term need only make sense when $\ell \geq 1$. Similarly, the integrals in the last term of $\partial I_1(i)$ need only make sense when $i \geq 1$ and the integral in the last term of $\partial_\ell I_2$ need only make sense when $\ell \geq 2$.

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