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Abstract

Equidistribution algorithms are designed to generate a grid in conjunction with a numerical solution. The grid is thus adapted to the nature of the solution. With this approach it is feasible to resolve features such as sharp fronts and boundary layers with far fewer grid points than a uniform spacing would dictate. In this work, we analyze equidistribution algorithms from the literature on a simple, one-dimensional, steady, linear, convection-diffusion equation with central or upwind finite differencing. Here, the small diffusion parameter, ϵ, induces an $O(\epsilon)$ boundary layer. A novel feature of our analysis is that no simplifying assumptions are made—the nonlinear algebraic system of equations arising in practice from the finite difference and equidistribution equations is studied directly. For equidistribution based on the first derivative of the solution, we give exact formulas for the grids. For an alternative, smoothed, first derivative algorithm, we find asymptotic (in ϵ) formulas. In this case we show in particular that upwind differences cannot lead to ϵ-uniform convergence, although, depending on the choice of method parameters, this lack of uniformity may not be observable unless ϵ is extremely small. We explain how this result contrasts with previously published numerical and analytical work. For an equidistribution algorithm based on parametrized arc length, we construct solutions that satisfy the finite difference and equidistribution equations to leading order in ϵ, and demonstrate numerically that these approximate solutions are relevant.

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1 Introduction

Equidistribution is an intuitively appealing approach for the numerical solution of differential equations with sharp solutions. We refer to [4, 6] for a range of references in this area. Although effective in practice, especially for problems in one space dimension, equidistribution schemes are not yet supported by a rigorous convergence theory. In this work we analyze popular schemes on a simple test problem. A similar approach is taken in [2, 4, 5], but our analysis has the advantage of dealing with the full algebraic system that determines the numerical solution *and* the grid—we do not require simplifying assumptions that lead to an analytic formula for the grid. We prove three types of result. In section 2, for the simplest first-derivative based equidistribution algorithm, we find exact formulas for the grid. A more general, smoothed, first-derivative algorithm is analyzed in section 3. Here, we are able to derive asymptotic formulas for the grid location. In section 4 we study an arc length based equidistribution algorithm and construct approximate solutions to the resulting nonlinear system. Our main conclusions are summarized in section 5. In the remainder of this section we introduce the algorithms.

We consider the one-dimensional, linear, steady problem

$$u_x = \epsilon u_{xx}, \quad 0 \le x \le 1, \tag{1}$$

where $\epsilon > 0$ is a small parameter, subject to the boundary conditions

$$u(0) = 0, \quad u(1) = 1. \tag{2}$$

The exact solution

$$u(x) = \frac{e^{x/\epsilon} - 1}{e^{1/\epsilon} - 1}, \tag{3}$$

is monotonic, with an $O(\epsilon)$ boundary layer at $x = 1$; see Figure 1.

To apply a finite-difference method to (1)–(2), we require grid points $\{x_j\}_{j=0}^N$, with $0 = x_0 < x_1 < x_2 < \cdots < x_N = 1$. We let U_j denote the numerical approximation to $u(x_j)$ (with $U_0 = 0$ and $U_N = 1$) and introduce $h_j := x_j - x_{j-1}$ for the grid spacings. We also introduce vectors $\mathbf{h} = [h_1, h_2, \ldots, h_N]^T$ and $\mathbf{U} = [U_1, U_2, \ldots, U_{N-1}]^T$. We discretize the diffusion term in (1) using central differences:

$$u_{xx}\big|_{x=x_j} \approx \frac{2}{h_j + h_{j+1}} \left(\frac{U_{j+1} - U_j}{h_{j+1}} - \frac{U_j - U_{j-1}}{h_j} \right). \tag{4}$$

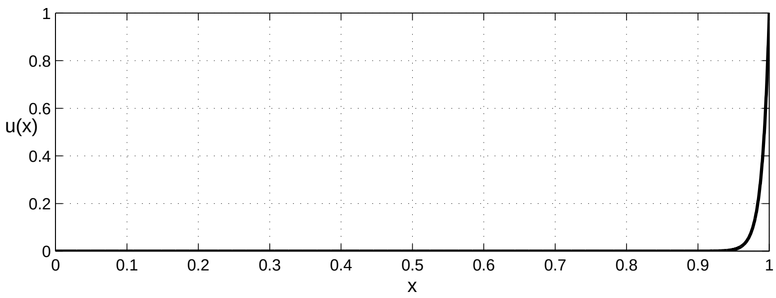

Figure 1: Solution to (1)–(2) for $\epsilon = 10^{-2}$.

For the convection term we consider three different schemes:

$$u_x \Big|_{x=x_j} \approx \frac{U_{j+1} - U_{j-1}}{h_{j+1} + h_j}, \tag{5}$$

$$u_x \Big|_{x=x_j} \approx \frac{1}{2}\left(\frac{U_{j+1} - U_j}{h_{j+1}} + \frac{U_j - U_{j-1}}{h_j}\right), \tag{6}$$

$$u_x \Big|_{x=x_j} \approx \frac{U_j - U_{j-1}}{h_j}. \tag{7}$$

We refer to (5) and (6) as type I and type II central differences, respectively. The scheme (7) is known as an upwind difference. Each finite difference scheme produces a tridiagonal linear system $A(\mathbf{h})\mathbf{U} - \mathbf{b}(\mathbf{h}) = 0$ with

$$A = \begin{bmatrix} b_1 & c_1 & & & & \\ a_2 & b_2 & c_2 & & & \\ & a_3 & b_3 & c_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & c_{N-2} \\ & & & & a_{N-1} & b_{N-1} \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ -c_{N-1} \end{bmatrix}, \tag{8}$$

where for type I differencing we have

$$a_j = \frac{2\epsilon}{h_j} + 1, \quad b_j = -2\epsilon\left(\frac{1}{h_{j+1}} + \frac{1}{h_j}\right), \quad c_j = \frac{2\epsilon}{h_{j+1}} - 1, \tag{9}$$

for type II differencing we have

$$a_j = \frac{1}{2h_j}\left(\frac{4\epsilon}{h_j + h_{j+1}} + 1\right), \quad b_j = -a_j - c_j, \quad c_j = \frac{1}{2h_{j+1}}\left(\frac{4\epsilon}{h_j + h_{j+1}} - 1\right), \tag{10}$$

and for upwinding we have

$$a_j = \frac{2\epsilon}{h_j} + \frac{h_j + h_{j+1}}{h_j}, \quad b_j = -2\epsilon\left(\frac{1}{h_{j+1}} + \frac{1}{h_j}\right) - \frac{h_j + h_{j+1}}{h_j}, \quad c_j = \frac{2\epsilon}{h_{j+1}}. \tag{11}$$

The idea behind equidistribution is to generate the grid along with the numerical solution. A process for finding the grid spacings can be based on the constraints

$$h_{j+1}\left|\frac{U_{j+1}-U_j}{h_{j+1}}\right|^{1/m} = h_j\left|\frac{U_j-U_{j-1}}{h_j}\right|^{1/m}, \quad 1 \le j \le N-1, \tag{12}$$

where $m \ge 1$ is a fixed integer. Here, the interval length h_j is weighted by a finite difference approximation to the first derivative—we require h_j to be small if the first derivative approximation is relatively large. Choosing $m > 1$ makes the effect less dramatic. We refer to (12) as a smoothed first derivative (SFD) strategy. To make $x_N = 1$ we require the extra constraint

$$\sum_{j=1}^{N} h_j = 1. \tag{13}$$

The grid equations (12)–(13) can be written $L(\mathbf{h},\mathbf{U})\mathbf{h} = \mathbf{e}$, where

$$L(\mathbf{h},\mathbf{U}) = \begin{bmatrix} f_1 & -f_2 & & & & \\ & f_2 & -f_3 & & & \\ & & f_3 & -f_4 & & \\ & & & \ddots & \ddots & \\ & & & & f_{N-1} & -f_N \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{e} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ \vdots \\ 0 \\ 1 \end{bmatrix}, \tag{14}$$

with $f_j = |(U_j - U_{j-1})/h_j|^{1/m}$. Overall, the finite difference and grid equations produce a nonlinear algebraic system of $2N-1$ equations in the $2N-1$ unknowns $\{h_j\}_{j=1}^{N}$ and $\{U_j\}_{j=1}^{N-1}$. For convenience, we write the nonlinear system as $G(\mathbf{h},\mathbf{U}) = 0$, where

$$G(\mathbf{h},\mathbf{U}) := \begin{bmatrix} A(\mathbf{h})\mathbf{U} - \mathbf{b}(\mathbf{h}) \\ L(\mathbf{h},\mathbf{U})\mathbf{h} - \mathbf{e} \end{bmatrix}, \tag{15}$$

so $G : \mathbb{R}^N \times \mathbb{R}^{N-1} \mapsto \mathbb{R}^{2N-1}$. Of course, we require positive grid spacings, so $(\mathbf{h},\mathbf{U})$ satisfying $G(\mathbf{h},\mathbf{U}) = 0$ will be regarded as a valid solution only if $h_j > 0$ for all $1 \le j \le N$.

As an alternative to the SFD constraints (12), we also consider

$$h_{j+1}\sqrt{1-\alpha+\alpha\left(\frac{U_{j+1}-U_j}{h_{j+1}}\right)^2} = h_j\sqrt{1-\alpha+\alpha\left(\frac{U_j-U_{j-1}}{h_j}\right)^2}, \quad 1 \le j \le N-1, \tag{16}$$

where $\alpha \in [0,1]$ is a fixed parameter. We refer to (16) as a generalized arc length (GAL) strategy, since for $\alpha = 1/2$ it corresponds to equidistributing an approximation to the solution arc length. Using this strategy in place of (12) we have $f_j = \sqrt{1 - \alpha + \alpha([U_j - U_{j-1}]/h_j))^2}$ in (14). Note that choosing $\alpha = 0$ gives a uniform grid and $\alpha = 1$ corresponds to SFD (12) with $m = 1$.

We remark that throughout this work we consider the parameters N, m and α to be fixed and focus on the case where ϵ is small.

In [4] the upwind finite difference scheme with SFD was analyzed on a problem class that includes (1). In order to establish ϵ-uniform convergence, the authors inserted the exact solution into the grid equations and hence obtained an analytical expression for a grid. This grid, of course, is only an approximation to the one that arises from the full nonlinear system and is independent of the finite difference formula used to solve the differential equation. This idealized analysis showed ϵ-uniform convergence for sufficiently large m, and this was extended to $m \geq 2$ in [2]. A similar analysis for GAL, based on an idealized grid, appears in [5]. Our approach is to study the full nonlinear system and, as we show in section 3, the grid arising in practice may be significantly different from the idealized versions proposed in the literature.

The analysis in [1, section 3.4] is perhaps most closely related to ours. In [1] the authors study a type I central difference scheme for a class of problems with a sharp transition layer. They examine the small ϵ behaviour of the full algebraic system by carefully constructing a solution for $\epsilon = 0$ and then showing that the implicit function theorem is applicable. In this case the small ϵ solutions are $O(\epsilon)$ perturbations of the base solution. Here the grid spacings are $O(1)$ outside the boundary layer and $O(\epsilon)$ in the layer. We have chosen to analyze the full algebraic system in a more direct manner. In section 3 we obtain precise asymptotic expressions for the grid locations. In particular, we find that with upwind differencing the grid spacings are larger than $O(\epsilon)$ in the boundary layer (Result 3.2). This behaviour could not be deduced immediately from the implicit function theorem approach in [1]. In section 4 we construct approximate solutions with small residuals. For type 1 central differences, these solutions are closely related to those found in [1]. However, with upwinding, we have an $O(\epsilon^{\frac{1}{2}})$ grid spacing in the transition between the smooth region and the layer (Result 4.3); so these solutions would not follow immediately from an implicit function theorem analysis.

For convenience in the subsequent analysis, we introduce the further notation $\delta_j := U_j - U_{j-1}$ for solution differences and $D_j := \delta_j / h_j$ for scaled solution differences. Using this notation, we note that with SFD equidistribution, independently of the finite difference formula, we must have $D_j \neq 0$ for all j. (Otherwise, since $h_j > 0$ for all j, (12) gives $D_j \equiv 0$ and hence $U_j \equiv 0$, which contradicts $U_N = 1$.) We also note that upwind differencing (11) may be written

$$D_{j+1} = \left(1 + \frac{h_j + h_{j+1}}{2\epsilon}\right) D_j, \tag{17}$$

and so $D_j > 0$ for all j. This makes clear the well-known result that upwind solutions are monotonic.

2 First Derivative Equidistribution

In the special case of $m = 1$ in (12) or $\alpha = 1$ in (16), the grid equidistribution equations simplify to

$$h_j|D_j| = h_{j+1}|D_{j+1}|. \tag{18}$$

In this case the overall finite difference and grid system can be solved exactly.

Result 2.1 ***Type I differencing***
Suppose type I finite differences are used with SFD *equidistribution and* $m = 1$*. Then for small* ϵ *the grid is unique and satisfies*

$$h_{j+1} = \frac{\epsilon h_j}{h_j + \epsilon}, \quad 1 \le j \le N-1. \tag{19}$$

Further $h_1 = O(1)$*,* $h_2 = \epsilon + O(\epsilon^2)$ *and* $h_{j+1} < h_j$*. The solution* U_j *increases monotonically.*

Proof:
From (8) and (9), the finite difference equations may be written

$$2\epsilon(D_{j+1} - D_j) = h_{j+1}D_{j+1} + h_jD_j. \tag{20}$$

We split (18) into two cases.
Case A: successive D_j's have different sign
If $h_jD_j = -h_{j+1}D_{j+1}$ for any j, then (20) gives $D_j = D_{j+1}$, which is a contradiction. Thus solutions of this type are not possible.
Case B: successive D_j's have same sign
If $h_jD_j = h_{j+1}D_{j+1}$ then (20) reduces to (19). This may be written as a simple recurrence in ϵ/h_j, which solves to give $h_j = \epsilon/(c+j)$, where the constant c is determined by (13). The remaining facts about $\{h_j\}_{j=1}^N$ follow from (19). The common sign of the D_j's must be positive, and so $\{U_j\}_{j=0}^N$ increases monotonically.
∎

Result 2.2 ***Type II differencing***
Suppose type II finite differences are used with SFD *equidistribution and* $m = 1$*. Then for small* ϵ *the grid is unique and satisfies*

$$h_j = \frac{1}{N} + 2(N - 1 - 2(j-1))\epsilon. \tag{21}$$

The solution U_j *is oscillatory (*$\mathrm{sign}(D_j) = -\mathrm{sign}(D_{j+1})$*).*

Proof:

From (8) and (10), the finite difference system may be written

$$\frac{2\epsilon}{h_j + h_{j+1}}(D_{j+1} - D_j) = \frac{1}{2}(D_{j+1} + D_j). \tag{22}$$

We consider two cases for (18).

Case A: successive D_j's have different sign

If $h_j D_j = -h_{j+1} D_{j+1}$ then multiplying by h_{j+1} in (22) and rearranging gives $h_{j+1} = h_j - 4\epsilon$, which requires $h_j > 4\epsilon$.

Case B: successive D_j's have same sign

If $h_j D_j = h_{j+1} D_{j+1}$ then (22) gives

$$h_{j+1} = -h_j - 2\epsilon + 2\sqrt{\epsilon^2 + 2\epsilon h_j}, \tag{23}$$

which leads to a positive h_{j+1} if and only if $h_j < 4\epsilon$. Note also that (23) then gives $h_{j+1} < -2 + 2\sqrt{\epsilon^2 + 8\epsilon^2} = 4\epsilon$.

Now, we combine the results for cases A and B. First, note that case B cannot hold for all j, since this will give $\sum_{j=1}^{N} h_j < 4N\epsilon < 1$, contradicting (13). Further, if case B holds for $j = k$ then it must hold for all $j > k$ (since case A requires $h_j > 4\epsilon$). The remaining possibilities are: case A holds for all j, or case A holds for $1 \leq j \leq k$ and case B holds for $k+1 \leq j \leq N-1$. However, in the latter circumstance, we have $h_{k+1} < 4\epsilon$, $h_j < 4\epsilon$ for $j > k$ and $h_j = h_{j+1} + 4\epsilon$ for $j < k$, so all h_j are $O(\epsilon)$, which contradicts (13). Thus the only possibility is that case A holds for all j. The expression (21) then follows immediately. ∎

Result 2.3 ***Upwinding***

Suppose upwind finite differences are used with SFD *equidistribution and* $m = 1$. *Then for small* ϵ *the grid is unique with* $h_1 = O(1)$, $h_j < 2\epsilon$ *for* $j > 1$ *and* h_j *monotonic decreasing. The solution* U_j *is monotonic.*

Proof:

Using $h_j D_j = h_{j+1} D_{j+1}$, (17) can be rearranged to give

$$\frac{h_j}{h_{j+1}} = \frac{2\epsilon + h_{j+1}}{2\epsilon - h_{j+1}}.$$

Hence, $h_j < 2\epsilon$ for $j \geq 2$ and the h_j's are monotonic decreasing. Then (13) gives $h_1 = O(1)$. Note that specifying h_1 determines the complete sequence $\{h_j\}_{j=1}^{N}$. Regarding $\sum_{j=1}^{N} h_j$ as a function of h_1 it can be shown that this function increases monotonically, hence there is a unique h_1 that gives (13). ∎

The results above apply to the case where grid selection is based solely on the size of an approximation to the first derivative. Intuitively, we would expect this approach to place all grid points in the boundary layer. Results 2.1 and 2.3 show that this indeed happens for type I central and upwind differences; both give $h_1 = O(1)$ and $h_j = O(\epsilon)$ for $j > 1$. Also, both schemes give monotonic solutions. However, Result 2.2 shows that type II central differencing does not take into account the boundary layer, giving an almost a uniform grid and an oscillatory solution.

Figure 2 illustrates Results 2.1 and 2.3. Here, we have used $N = 19$ and a range of ϵ values from 10^{-1} to 10^{-5}. The upper pair of pictures show how $(1 - h_1)/\epsilon$ varies as a function of ϵ. We see that for both type I and upwind differencing $1 - h_1$ tends to a fixed multiple of ϵ, with the multiple being larger for upwinding. The middle pair of pictures show h_j/ϵ for $2 \leq j \leq N$. We see that as ϵ decreases these grid spacings converge to fixed multiples of ϵ. Finally, the bottom pair of pictures confirm that the $\{U_j\}$ are monotonic.

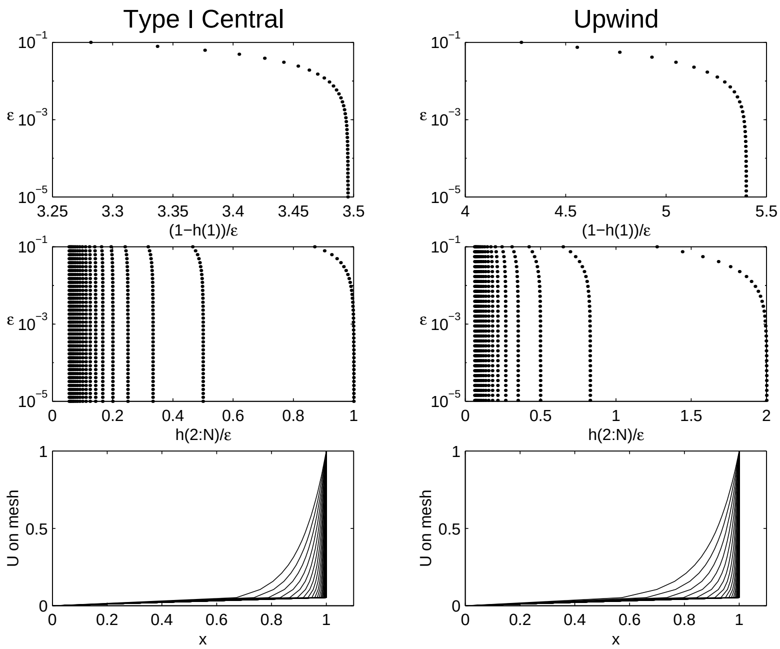

Figure 2: Numerical solutions for SFD with $m = 1$: top row: $(1 - h_1)/\epsilon$; second row: h_j/ϵ for $2 \leq j \leq N$; third row: $\{x_j, U_j\}$.

In the remaining analysis, we consider only type I central and upwind differencing.

3 Smoothed first derivative solutions

We now analyze the general SFD strategy (12). By treating ϵ as a small parameter, we are able to find leading order expressions for the grid spacings.

The grid equations may be written

$$h_j^m |D_j| = h_{j+1}^m |D_{j+1}|, \tag{24}$$

and we recall that $D_j \neq 0$ for all j.

Result 3.1 ***Type 1 differencing***
Suppose type I finite differences are used with SFD *equidistribution. If, for small* ϵ*, a numerical solution exists that is monotonic for* U_j*, then* $h_1 = O(1)$*,* $h_2 < 2\epsilon$ *and the* h_j*'s are monotonic decreasing.*

Proof: It follows from the finite difference equations (20) that

$$D_{j+1} = -D_j \left(\frac{h_j + 2\epsilon}{h_{j+1} - 2\epsilon} \right).$$

Hence, in order for the D_j's to have the same sign we require $h_{j+1} < 2\epsilon$ for $j \geq 1$. Since (13) holds, $h_1 = O(1)$.

Now, using (24), we may rearrange (20) to give

$$\frac{h_{j+1}^m}{h_j^m} = \frac{2\epsilon - h_{j+1}}{2\epsilon + h_j}, \quad 1 \leq j \leq N-1,$$

which shows that the h_j's are monotonic. ∎

Result 3.2 ***Upwinding***
Suppose upwind finite differences are used with SFD *equidistribution for* $m > 1$*. If, for sufficiently small* ϵ*, a numerical solution exists then there is a constant* C *such that*

$$\tfrac{1}{2}\epsilon^{1-(\frac{m-1}{m})^{j-1}} \leq h_j \leq C\epsilon^{1-(\frac{m-1}{m})^{j-1}}, \quad j = 1, 2, \ldots, N.$$

Proof: Using $D_j > 0$ and substituting (24) into (17) gives

$$h_{j+1}^m = h_j^m \frac{2\epsilon}{2\epsilon + h_j + h_{j+1}}, \tag{25}$$

which shows that $\{h_j\}$ decreases monotonically. It then follows from (13) that $1/N \leq h_1 \leq 1$. We will write this in the form

$$B_1\epsilon^{\rho_1} \leq h_1 \leq C_1\epsilon^{\rho_1},$$

where $\rho_1 = 0$, $B_1 = 1/N$ and $C_1 = 1$. Using (25) with $j = 1$ then gives

$$h_2^m \leq h_1^m \frac{2\epsilon}{h_1} = 2h_1^{m-1}\epsilon \leq 2C_1^{m-1}\epsilon^{(m-1)\rho_1+1}.$$

So

$$h_2 \leq C_2\epsilon^{\rho_2},$$

where $C_2 = (2C_1^{m-1})^{1/m}$ and $\rho_2 = ((m-1)\rho_1 + 1)/m$. Since $1 > \rho_2 > \rho_1$ we have, for sufficiently small ϵ, $2\epsilon + h_1 + h_2 \le 2h_1$. So, in (25),

$$h_2^m \ge h_1^m \frac{2\epsilon}{2h_1} = h_1^{m-1}\epsilon \ge B_1^{m-1}\epsilon^{(m-1)\rho_1+1}.$$

This gives

$$h_2 \ge B_2 \epsilon^{\rho_2},$$

with $B_2 = B_1^{(m-1)/m}$. Proceeding by induction, suppose that

$$B_j \epsilon^{\rho_j} \le h_j \le C_j \epsilon^{\rho_j}, \quad 1 \le j \le k, \tag{26}$$

for constants $\{B_j, C_j, \rho_j\}_{j=1}^k$, with $1 > \rho_k > \rho_{k-1} > \cdots > \rho_1 = 0$. Then (25) gives

$$h_{k+1}^m \le h_k^m \frac{2\epsilon}{h_k} = 2h_k^{m-1}\epsilon \le 2C_k^{m-1}\epsilon^{(m-1)\rho_k+1}.$$

So

$$h_{k+1} \le C_{k+1}\epsilon^{\rho_{k+1}},$$

where $C_{k+1} = (2C_k^{m-1})^{1/m}$ and $\rho_{k+1} = ((m-1)\rho_k + 1)/m$. Since $1 > \rho_{k+1} > \rho_k$ we have, for sufficiently small ϵ, $2\epsilon + h_k + h_{k+1} \le 2h_k$. So, in (25),

$$h_{k+1}^m \ge h_k^m \frac{2\epsilon}{2h_k} = h_k^{m-1}\epsilon \ge B_k^{m-1}\epsilon^{(m-1)\rho_k+1}.$$

This gives

$$h_{k+1} \ge B_{k+1}\epsilon^{\rho_{k+1}},$$

with $B_{k+1} = B_k^{(m-1)/m}$. Hence, by induction, (26) holds for all k.

Note that $\rho_{j+1} = ((m-1)\rho_j + 1)/m$, so ρ_{j+1} is a weighted average of ρ_j and 1. Using $\rho_1 = 0$, it follows that

$$\rho_j = 1 - ((m-1)/m)^{j-1}.$$

Setting $C = \max_j C_j$ completes the upper bound. For the lower bound, note that $B_j \ge B_1$ for all j. Since $h_1 = 1 - \sum_{j=2}^N h_j = 1 - O(\epsilon^{\rho_2})$, we may take B_1 to be arbitrarily close to 1—for definiteness, we have chosen the value 1/2. ∎

Taking the limit as $m \to 1$ in Result 3.2 gives $h_1 = O(1)$ and $h_j = O(\epsilon)$ for $j \ge 2$, which agrees with Result 2.3. Generally, for $m > 1$, Result 3.2 shows that the grid spacing at the right-hand boundary satisfies

$$h_N \ge \tfrac{1}{2}\epsilon^{1-(\frac{m-1}{m})^{N-1}}. \tag{27}$$

Hence, for fixed $m > 1$ and N, and sufficiently small ϵ, there are no grid points in the $O(\epsilon)$ boundary layer. Intuitively, we would expect that the finite difference scheme cannot then resolve the boundary layer accurately, in the sense that any natural interpolation process that produces a global solution from the discrete date $\{x_j, U_j\}_{j=0}^N$ will have a large error in the layer. We now show that this is indeed the case for piecewise constant and piecewise linear interpolation.

We first show that, since x_{N-1} is outside the boundary layer, $u(x_{N-1})$ is exponentially small.

Lemma 3.3 *Suppose upwind finite differences are used with* SFD *equidistribution for fixed $m > 1$ and N. Let $\gamma = \gamma(m, N) = (\frac{m-1}{m})^{N-1} > 0$. If, for sufficiently small ϵ, a numerical solution exists then*

$$\log\left(u(x_{N-1})\right) \leq \log(2) - \frac{1}{2\epsilon^{\gamma}}.$$

Proof: We know from Result 3.2 that, for sufficiently small ϵ, $x_{N-1} = 1 - h_N \leq 1 - \frac{1}{2}\epsilon^{1-\gamma}$. Hence, in (3),

$$u(x_{N-1}) \leq u(1 - \tfrac{1}{2}e^{1-\gamma}) = \frac{e^{\frac{1-\frac{1}{2}\epsilon^{1-\gamma}}{\epsilon}} - 1}{e^{1/\epsilon} - 1} \leq \frac{e^{\frac{1-\frac{1}{2}\epsilon^{1-\gamma}}{\epsilon}}}{\frac{1}{2}e^{1/\epsilon}} = 2e^{-\frac{1}{2}\epsilon^{-\gamma}}.$$

Taking logs gives the required result. ∎

Result 3.4 *Suppose upwind finite differences are used with* SFD *equidistribution for fixed $m > 1$ and N. Let $\bar{u}(x)$ denote either a piecewise constant or a piecewise linear interpolant to $\{x_j, U_j\}_{j=0}^N$. If, for sufficiently small ϵ, a numerical solution exists then*

$$\max_{[0,1]}|u(x) - \bar{u}(x)| \geq \frac{1}{4}. \tag{28}$$

Proof: In the case where $\bar{u}(x)$ is piecewise constant, consider the interval $[x_{N-1}, 1]$. We know that $u(x_N) = 1$ and yet, from Lemma 3.3, $u(x_{N-1})$ is exponentially small. Hence, whatever constant value $\bar{u}(x)$ takes in this interval it must be in error by at least $1/4$ at one of the endpoints.

In the piecewise linear case, consider $\hat{x} = (x_{N-1} + 1)/2$. Since $U_{N-1} > 0$ and $U_N = 1$ we have $\bar{u}(\hat{x}) = (u_{N-1} + 1)/2 \geq 1/2$. However, as in the proof of Lemma 3.3, we can show that $u(\hat{x})$ is exponentially small, and so $\bar{u}(\hat{x}) - u(\hat{x}) \geq 1/4$. ∎

Figure 3 illustrates Results 3.2 and 3.4 for the case $N = 19$, $m = 7$ with a range of ϵ values between 10^{-1} and 10^{-12}. In each case, we generated a grid by making use of the analysis in the proof of Result 3.2. Given h_1, we computed h_2, h_3, ..., h_N in sequence; h_{j+1} was found by solving the polynomial equation given by (25) using MATLAB's `roots` [9]. In this way $\sum_{j=1}^N |h_j|$ was regarded as a function of h_1 alone, say $f(h_1)$. The remaining nonlinear equation $f(h_1) = 1$ was solved with MATLAB's `fzero`. The left-hand picture shows h_N/ϵ^β, where $\beta = 1 - ((m-1)/m)^{N-1} \approx 0.94$, as a solid line and h_N/ϵ as a dashed line. We see that h_N/ϵ^β appears to be bounded, whereas h_N/ϵ grows unboundedly for small ϵ, as predicted by Result 3.2. A least squares fit of the parameters c_1, c_2 in $\log(h_N) = c_1 \log(\epsilon) + c_2$ gave $c_1 = 0.928$ with a 2-norm residual of 5.6×10^{-3}. The right-hand picture shows the error at x_{N-1} (solid) and the error in the piecewise linear interpolant at $(x_{N-1}+1)/2$ (dashed). We see that as ϵ is reduced all mid-nodal accuracy is lost, although the gridpoint error ultimately improves. The $O(1)$ error at $x = (x_{N-1}+1)/2$ agrees with Result 3.4. The numerical results for $x = x_{N-1}$ emphasize that it is possible for a numerical method to resolve the boundary layer inadequately and yet still have good accuracy at each gridpoint.

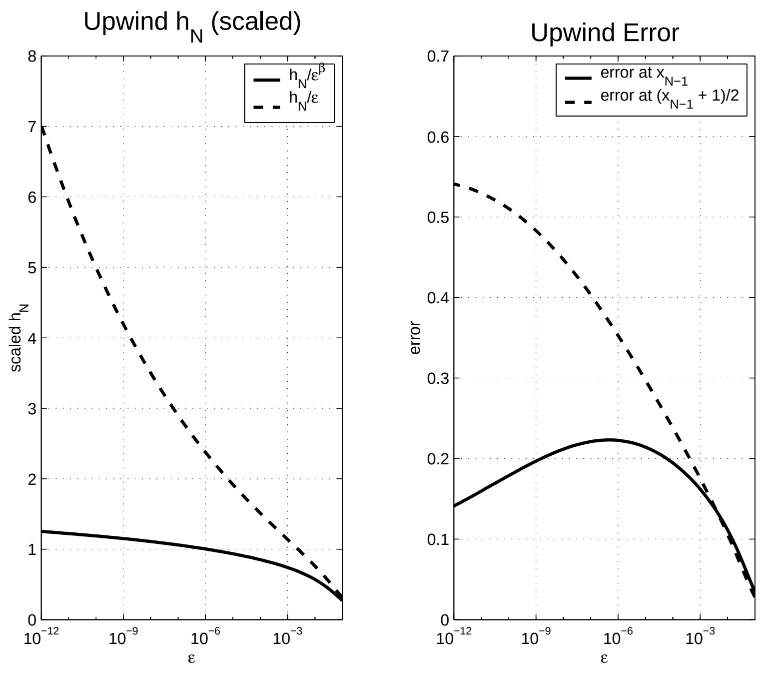

Figure 3: Behaviour of h_N and the error for upwind with SFD: $N = 19$, $m = 7$, $10^{-12} \le \epsilon \le 10^{-1}$, $\beta = 1 - (6/7)^{18} \approx 0.94$.

In contrast to Result 3.4, the following result can be inferred from [2, Theorem 10] (which generalizes analysis in [4]):

Theorem 3.5 (Mackenzie, 1999) *Consider the upwind scheme on (1) with grid spacings h_j chosen to exactly equidistribute $(du/dx)^{1/m}$, with some $m \ge 2$, for the exact solution (3). Then letting $\bar{u}(x)$ denote either the piecewise constant or the piecewise linear interpolant to $\{x_j, U_j\}_{j=0}^N$, the error satisfies*

$$\max_{[0,1]} |u(x) - \bar{u}(x)| \le \frac{C}{N}, \tag{29}$$

where the constant C is independent of ϵ.

We note that the convergence behaviours described by (28) and (29) are not compatible. The ϵ-uniform convergence bound (29) holds under the assumption that the exact solution is equidistributed (in which case an analytic formula is available for the grid). Result 3.4 shows that when this assumption is discarded, the solution obtained with the grid that arises in practice has an error of $O(1)$ *for sufficiently small* ϵ. We conclude that it can be misleading to study the behaviour of numerical schemes on analytically defined grids that are designed to be representative of grids that arise in practice. However, we emphasize that the analysis in [2, 4] is backed up by numerical experimentation; see, for example Table 2 (B) in [4] where for $m = 2$ and $\epsilon = 10^{-4}$ the errors on the analytically defined and practically computed grids are virtually identical. In our numerical experiments, as expected from (27), we found it necessary to take either N small or m large in order to observe the non-uniform convergence effect in Result 3.4 for a value of ϵ at which (1) is a physically reasonable model. We also emphasize that our computations for Figure 3 used specific information about the constraints that determine the grid. A general nonlinear system solver may give different results for small ϵ due to the inherent ill-conditioning.

Overall, however, Result 3.4 makes it clear that it can be dangerous to draw general conclusions from insights obtained via idealized assumptions.

4 Leading order residuals with generalized arc length

In this section we construct families of leading order residual solutions for GAL equidistribution. In the case of type I central differences, these solutions have $G(\mathbf{h}, \mathbf{U}) = O(\epsilon)$, whereas for upwinding they have $G(\mathbf{h}, \mathbf{U}) = O(\epsilon^{\frac{1}{2}})$. We then show that these approximate solutions are relevant in the sense that when they are fed as initial data into a nonlinear equation solver, they lead to exact solutions (to within rounding error) of the same form.

We are interested in solutions that respect the existence of the boundary layer. We see from Figure 1 that, at least visually, the true solution roughly consists of two straight line sections. Considering how the arc length of such a solution can be equidistributed leads to the idea of a numerical solution where, for some M, the grid is uniform for $j \leq M$ and the solution differences are uniform for $j \geq M$. We formalize this in the following definition.

Definition 4.1 *A* (r, h, δ) uniform partition *is a pair* $\mathbf{h}, \mathbf{U}$ *such that* $h_j \equiv h$ *for* $1 \leq j \leq M$ *and* $\delta_j \equiv \delta$ *for* $M + 1 \leq j \leq N$*, with* r *given by* $r := (\frac{N-M}{M})^2$.

Result 4.2 ***Type 1 differencing***
Suppose type I finite differences are used with GAL *equidistribution.*

Given any even M for which $r < \frac{\alpha}{1-\alpha}$ there exist two distinct (r,h,δ) uniform partitions for which $G(\mathbf{h},\mathbf{U}) = O(\epsilon)$. These partitions have $h = 1/M$, $h_{M+1} = K\epsilon$, where $K(>1)$ may take either of the two positive values

$$K_{\pm} = \frac{2}{1 \pm \sqrt{1 - (\frac{1-\alpha}{\alpha})r}} \tag{30}$$

and

$$h_{j+1} = \frac{\epsilon h_j}{h_j + \epsilon}, \quad M+1 \leq j \leq N-1. \tag{31}$$

They also have $\delta_{j+1} = -\delta_j + O(\epsilon)$ for $1 \leq j \leq M-1$, $\delta = \frac{1}{N-M}$ and $\delta_M = \delta(\frac{2}{K} - 1) + O(\epsilon)$. Taking $K = K_+$ or $K = K_-$ produces the two solutions.

Given any odd M for which $r < \frac{\alpha}{1-\alpha} + \frac{1}{M^2}$ there exist two distinct (r,h,δ) uniform partitions for which $G(\mathbf{h},\mathbf{U}) = O(\epsilon)$. These partitions have $h = 1/M$, $h_{M+1} = K\epsilon$, where $K(>1)$ may take either of the two positive values

$$K_{\pm} = \frac{2\left[(1 - M\sqrt{r} + \frac{\alpha M^2}{1-\alpha}) \pm \frac{M}{1-\alpha}\sqrt{\alpha(1 - M^2 r + \alpha(M^2(1+r) - 1))}\right]}{(M\sqrt{r} - 1)^2} \tag{32}$$

and

$$h_{j+1} = \frac{\epsilon h_j}{h_j + \epsilon}, \quad M+1 \leq j \leq N-1. \tag{33}$$

They also have $\delta_{j+1} = -\delta_j + O(\epsilon)$ for $1 \leq j \leq M-1$, $\delta = \frac{1-\delta_M}{N-M}$ and $\delta_M = \left(1 + (\frac{1}{N-M})(\frac{2}{K} - 1)\right)^{-1} \left(\frac{1}{N-M}\right)\left(\frac{2}{K} - 1\right) + O(\epsilon)$. Taking $K = K_+$ or $K = K_-$ produces the two solutions.

Proof We consider first the case where M is even. We prove existence by constructing the solution over the smooth region and the boundary layer and then patching the two solutions across the interface.

Smooth region: $1 \leq j \leq M-1$

Setting $h_j \equiv h = 1/M$, the finite difference equations give (for $h > 2\epsilon$)

$$D_{j+1} = -D_j \left(\frac{h + 2\epsilon}{h - 2\epsilon}\right), \quad 1 \leq j \leq M-1.$$

This shows that $\delta_{j+1} = -\delta_j + O(\epsilon)$ for $1 \leq j \leq M-1$. Specifying δ_M determines $\{\delta_j\}_{j=1}^{M-1}$ and thus $\{U_j\}_{j=1}^{M}$. Note that since M is even, we have $U_M = O(\epsilon)$. To simplify the remaining analysis, we perturb U_M to the value zero. (This has no effect on the residual in the finite difference equations, to leading order). The grid equations (16) for $1 \leq j \leq M-1$ are satisfied to $O(\epsilon)$ because

$$(1-\alpha)h_j^2 + \alpha\delta_j^2 = (1-\alpha)h^2 + \alpha\delta_M^2 + O(\epsilon), \quad 1 \leq j \leq M-1.$$

Boundary layer: $M+1 \le j \le N$
Setting $\delta_j \equiv \delta = 1/(N-M)$ for $M+1 \le j \le N$, the finite difference equations give (31). We will let $h_{M+1} = K\epsilon$ for some constant K. The remaining values $\{h_j\}_{j=M+2}^N$ and $\{U_j\}_{j=M+1}^N$ are then completely determined. Note that $h_j = O(\epsilon)$ for $M+1 \le j \le N$. The grid equations (16) for $M+1 \le j \le N$ are satisfied to leading order since

$$(1-\alpha)h_j^2 + \alpha\delta_j^2 = O(\epsilon^2) + \alpha\delta^2 \quad M+1 \le j \le N,$$

and also (13) holds to $O(\epsilon)$.
Interface: $j = M$
It remains to satisfy the finite difference and grid equation at $j = M$. We still have δ_M and K at our disposal. The finite difference equation at $j = M$ gives

$$\delta_M = \delta \left(\frac{\frac{2\epsilon}{h_{M+1}} - 1}{\frac{2\epsilon}{h} + 1} \right) = \delta \left(\frac{2}{K} - 1 \right) + O(\epsilon). \tag{34}$$

Applying the grid equation at $j = M$ and using (34) gives

$$(1-\alpha)h^2 + \alpha\delta^2 \left(\frac{2}{K} - 1 \right)^2 = \alpha\delta^2 + O(\epsilon).$$

Using $h = 1/M$, $\delta = 1/(N-M)$ and $r = ((N-M)/M)^2 = (h/\delta)^2$, we obtain

$$r = \frac{\alpha}{1-\alpha} \left(1 - \left(\tfrac{2}{K} - 1 \right)^2 \right).$$

Given any $r < \alpha/(1-\alpha)$ we can satisfy this condition with the two choices (30). This completes the construction for M even.

The proof for M odd proceeds similarly.
Smooth region: $1 \le j \le M-1$
The results follow as in the case for M even. Note that since M is odd, we have $U_M = \delta_M + O(\epsilon)$. To simplify the remaining analysis, we perturb U_M to the value δ_M. (This has no effect on the residual in the finite difference equations, to leading order). The grid equations (16) for $1 \le j \le M-1$ are satisfied to $O(\epsilon)$ as before.
Boundary layer: $M+1 \le j \le N$
Setting $\delta_j \equiv \delta = (1-\delta_M)/(N-M)$ for $M+1 \le j \le N$, the finite difference equations give (33). The remaining analysis follows as before.
Interface: $j = M$
It remains to satisfy the finite difference and grid equations at $j = M$. We still have δ_M and K at our disposal.

The finite difference equation at $j = M$ gives

$$\delta_M = \delta \left(\frac{\frac{2\epsilon}{h_{M+1}} - 1}{\frac{2\epsilon}{h} + 1} \right) = \delta \left(\frac{2}{K} - 1 \right) + O(\epsilon). \tag{35}$$

This can be rearranged to give δ_M as displayed in the statement of the result.

The grid equation at $j = M$ is, using (35),

$$(1-\alpha)h^2 + \alpha\delta^2 \left(\frac{2}{K} - 1\right)^2 = \alpha\delta^2 + O(\epsilon).$$

Using $h = 1/M$, $\delta = (1-\delta_M)/(N-M)$ and $r = ((N-M)/M)^2 = (h(1-\delta M)/\delta)^2$, we obtain

$$r = \frac{\alpha(1-\delta_M)^2}{1-\alpha} \left(1 - \left(\tfrac{2}{K} - 1\right)^2\right).$$

For any $r < \alpha/(1-\alpha) + 1/M^2$ this constraint is satisfied by the two choices (32). This completes the construction. ∎

The interval $[0, x_M]$ corresponds to the smooth region and $[x_M, 1]$ to the boundary layer. It follows from (31) that $1 - x_M = O(\epsilon)$, so these approximate numerical solutions have the layer width qualitatively correct. Also, the solution is monotone in the boundary layer. However, $O(1)$ oscillations are present in the smooth region. The oscillatory solution is sawtoothed about the x-axis. The teeth point downwards for $K = K_+$ and upwards for $K = K_-$. The amplitude of the oscillations is the same for K_+ and K_-, but the size of the first grid space in the layer is smaller for K_- than for K_+. In the commonly used case $\alpha = \frac{1}{2}$, Result 4.2 says that if we ask for any ratio $r < 1$—that is, we ask for more spaces in the smooth region than the boundary layer—then two distinct leading order solutions exist.

In Figure 4, the circles denote the leading order residual solution constructed in Result 4.2 for the case $\epsilon = 10^{-7}$, $\alpha = \frac{1}{2}$, $N = 19$, $M = 12$ and $K = K_+$ in (30). We then supplied this approximate solution as an initial guess to a nonlinear equation solver. This solver was written in MATLAB [9] by M. Reichelt and L. F. Shampine [7] and is based on the FORTRAN code MINPACK [3]. We specified a tolerance of 10^{-12} in the convergence criterion for the solver. The resulting solution is plotted with crosses. It is clear that the approximate solution from Result 4.2 is close to a solution that can be computed in practice. Figure 5 repeats the experiment with $K = K_-$, and the same conclusions apply.

Result 4.3 ***Upwinding***
Suppose upwind differences are used with GAL *equidistribution. Given any M for which $r = \frac{\alpha}{1-\alpha}$ there is a (r, h, δ) uniform partition with $G(\mathbf{h}, \mathbf{U}) = O(\epsilon^{\frac{1}{2}})$. These partitions have $h = 1/M$, $h_{M+1} = K\epsilon^{\frac{1}{2}}$, where $K > 0$ is any constant, and for $j \geq M+2$ the h_j's are $O(\epsilon)$ and monotonic decreasing. Also, $\delta_j = O(\epsilon^{\frac{1}{2}+M-j})$ for $1 \leq j \leq M$, $\delta = \frac{1}{N-M}$ and $\delta_M = \delta\frac{2\epsilon^{\frac{1}{2}}}{K} + o(\epsilon^{\frac{1}{2}})$.*

Proof As for Result 4.2, we prove existence by construction.

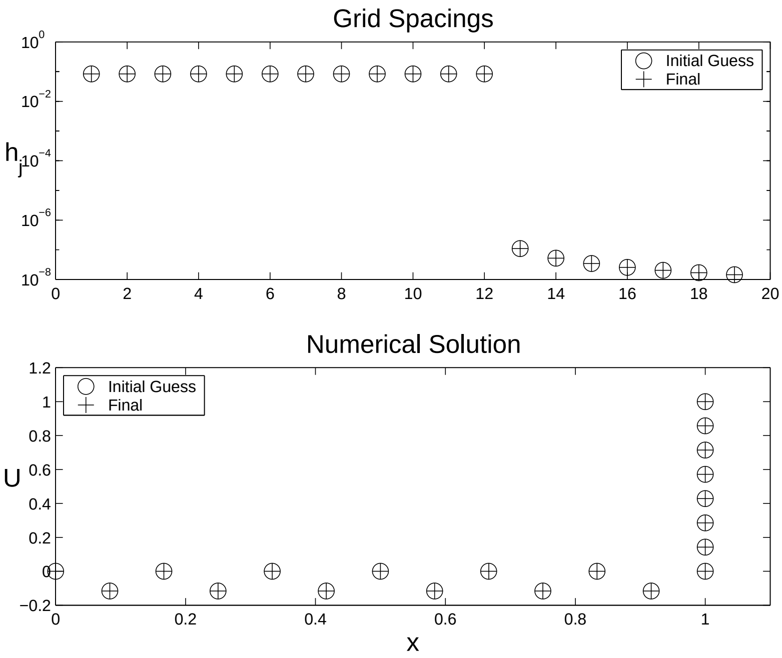

Figure 4: Leading order solution from Result 4.2 using $K = K_+$ (circles), and computed solution (crosses).

Smooth region: $1 \leq j \leq M-1$
Setting $h_j \equiv h = 1/M$, the finite difference equations give

$$D_{j+1} = D_j \left(1 + \frac{h}{\epsilon}\right), \quad 1 \leq j \leq M-1.$$

It follows from (36) below that $\delta_M = O(\epsilon^{\frac{1}{2}})$, and hence $\delta_j = O(\epsilon^{\frac{1}{2}+M-j})$ for $1 \leq j \leq M-1$. Specifying δ_M determines $\{\delta_j\}_{j=1}^{M-1}$ and thus $\{U_j\}_{j=1}^{M}$. The grid equations (16) for $1 \leq j \leq M-1$ are then satisfied to $O(\epsilon^{\frac{1}{2}})$ because

$$(1-\alpha)h_j^2 + \alpha\delta_j^2 = (1-\alpha)h^2 + O(\epsilon^{\frac{1}{2}}), \quad 1 \leq j \leq M-1.$$

Boundary layer: $M+1 \leq j \leq N$
Setting $\delta_j \equiv \delta = 1/(N-M)$ for $M+1 \leq j \leq N$, the finite difference equations give

$$h_{j+1} = \frac{-(h_j + 2\epsilon) + \sqrt{(h_j+2\epsilon)^2 + 8\epsilon h_j}}{2}, \quad M+1 \leq j \leq N-1.$$

We let $h_{M+1} = K\epsilon^{\frac{1}{2}}$ for some constant K. The remaining values $\{h_j\}_{j=M+2}^{N}$ and $\{U_j\}_{j=M+1}^{N}$ are then completely determined. Note that $h_j = O(\epsilon)$ for $M+2 \leq$

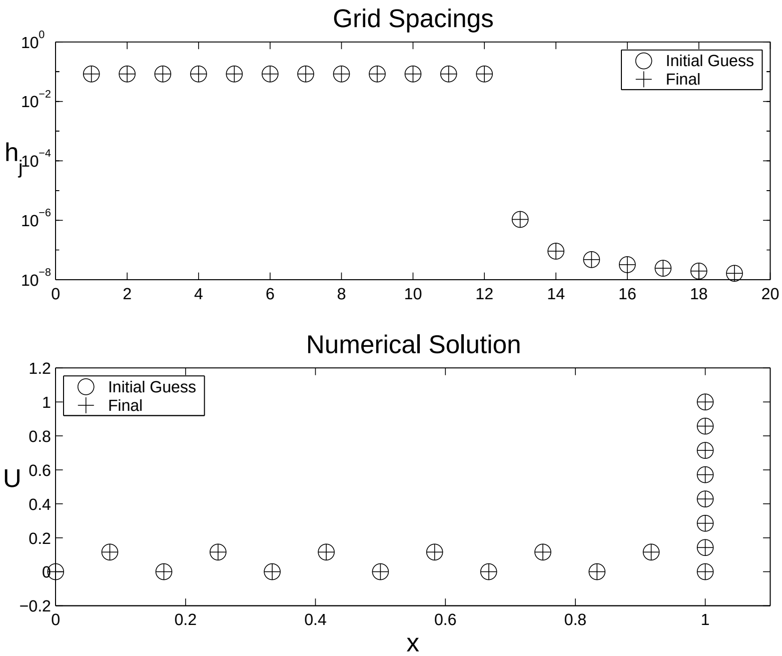

Figure 5: Leading order solution from Result 4.2 using $K = K_-$ (circles), and computed solution (crosses).

$j \leq N$ and the h_j's are monotonic decreasing. The grid equations (16) for $M+1 \leq j \leq N$ are satisfied to leading order since

$$(1-\alpha)h_j^2 + \alpha\delta_j^2 = O(\epsilon) + \alpha\delta^2 \quad M+1 \leq j \leq N,$$

and (13) holds to $O(\epsilon^{\frac{1}{2}})$.

Interface: $j = M$

It remains to satisfy the finite difference and grid equations at $j = M$. We still have δ_M and K at our disposal.

The finite difference equation at $j = M$ gives

$$\delta_M = \delta\left(\frac{\frac{2\epsilon}{h_{M+1}}}{\frac{2\epsilon}{h}+1}\right) = \delta\frac{2\epsilon^{\frac{1}{2}}}{K} + o(\epsilon^{\frac{1}{2}}). \tag{36}$$

The grid equation at $j = M$ is, using (36),

$$(1-\alpha)h^2 = \alpha\delta^2 + O(\epsilon). \tag{37}$$

Inserting $h = 1/M$, $\delta = 1/(N-M)$ and $r = ((N-M)/M)^2 = (h/\delta)^2$, we satisfy this to leading order with

$$r = \frac{\alpha}{1-\alpha}. \tag{38}$$

This completes the construction. ∎

In Result 4.3 we see that $1 - x_{M+1} = O(\epsilon)$, so the equidistribution scheme successfully places points in the boundary layer.

In the case $\alpha = \frac{1}{2}$, Result 4.3 applies when $r = 1$, that is, there is an equal number of spaces in the smooth region and the boundary layer, which requires N even.

In Figure 6, the circles denote the leading order solution constructed in Result 4.3 for the case $\epsilon = 10^{-7}$, $\alpha = \frac{1}{2}$, $N = 20$, $M = 10$ and $K = 1$. We then supplied this approximate solution as an initial guess to a nonlinear equation solver, as for Figures 4 and 5. The resulting solution is plotted with crosses. The approximate solution is seen to have the same qualitative form as the one that is computed by the solver. The interface grid spacing h_{M+1} has moved slightly—this is inevitable since we chose K arbitrarily. To confirm the $h_{M+1} \approx K\epsilon^{\frac{1}{2}}$ prediction of Result 4.3, we repeated this experiment for $\epsilon = 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}$ and computed a least squares solution of $\log h_{M+1} = \log(K) + a\log(\epsilon)$. This gave $\log(K) = 0.3969$ and $a = 0.4929$ with a 2-norm residual of 0.0293.

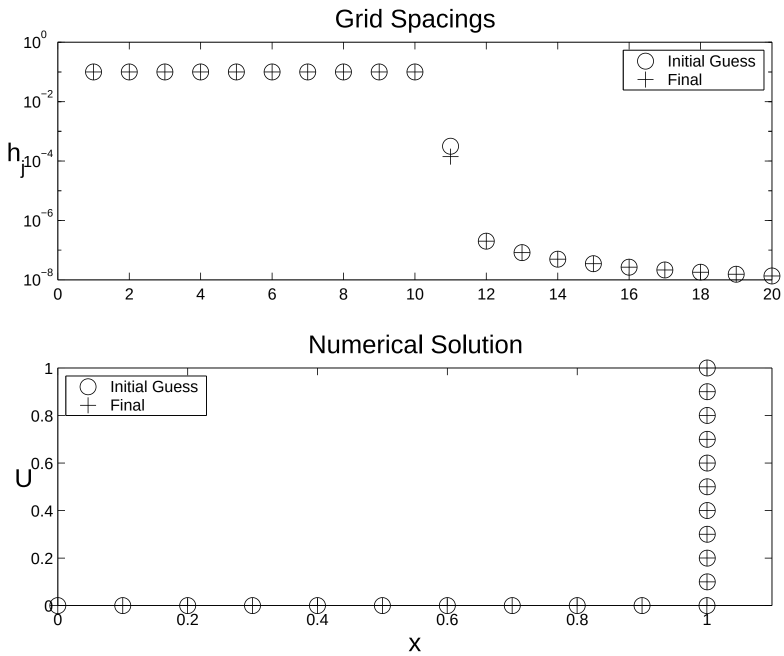

Figure 6: Leading order solution from Result 4.3 with $K = 1$ (circles), and computed solution (crosses).

5 Conclusions

Our overall conclusion in this work is that the grid depends on *both the equidistribution algorithm and the finite difference formula.* In section 2 we saw dramatically different grids occurring for SFD with $m = 1$ in the case of type I and type II central differencing. Section 3 showed that general SFD equidistribution puts grids points in the boundary layer when type I central differences are used, but misses the layer (and consequently does not give ϵ-uniform convergence) with upwinding. In section 4 we saw that GAL equidistribution induces an $O(\epsilon^{\frac{1}{2}})$ grid spacing at the interface between the smooth region and the boundary layer—a feature that is not present with type I central differencing.

Our approach was to analyze the algorithms directly on the widely-studied test problem (1). We emphasize that the upwind analysis in sections 3 and 4 involved quantities larger than $O(\epsilon)$, and hence our results would not follow from straightforward application of the implicit function theorem.

Result 3.4 was perhaps our most surprising result, showing that despite previous numerical and analytical evidence to the contrary, upwind differencing with a smoothed first derivative equidistribution scheme is not ϵ-uniform convergent. It would thus be of interest to look for an alternative equidistribution scheme for upwind differencing that is both effective in practical tests and provably ϵ-uniform convergent on (1).

Another negative feature that showed up in our work was the lack of uniqueness identified in Results 4.2 and 4.3. (This effect was also pointed out for central differences in [1].) The existence of many solutions to a steady problem may be particularly harmful when a related time-dependent problem is to be integrated to steady state. The numerical experiments in [8] indicate that complicated dynamics can arise in practice in the time-dependent case, and an extension of the approach used here may explain some of the effects.

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