

**STRONG UNIFORM APPROXIMATION FOR
SOME SINGULARLY PERTURBED DIFFERENTIAL EQUATIONS
ARISING IN CHEMICAL REACTOR THEORY**

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Abstract: A family of singularly perturbed ordinary differential problems that arise from Chemical Reactor Theory introduced among others by O'Malley is under consideration. The numerical stability of this problem is very fragile, very sensitive to the functional space setting particularly to the norm the functional space is equipped with. So the issue of finding an asymptotic solution remains of higher interest since most of those one may find in the literature are not easy to compute or are not of higher order. What we do within the current paper is to make a repeated use of the classical matching technique that is well-known in Asymptotic Analysis to construct, via a strong stable corrector (in a sense to be defined) an easy to compute regular asymptotic solution of any prescribed order. This higher order solution is valid throughout the geometric domain of study.

1 – Introduction

In many problems arising from various fields of physical interest such as biochemical kinetics, plasma physics, mechanical and electrical systems, the observed phenomenon, for example a Mechanical Oscillator or a Chemical Reactor may be described by a differential equation involving a small parameter, say ϵ , affecting the highest derivative term. In the present paper we are focusing our attention on a family of problems that arise in the study of adiabatic tubular chemical flow

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reactors with axial diffusion that is present in the mathematical literature (for example I refer the reader to [19] and the therein references and to other works upto a recent study that is [16]).

From a mathematical point of view the study of such phenomena turns into the study of the attached singularly perturbed problems whose solutions are expected to depict their behaviour.

The numerical study of singularly perturbed differential equations is known to be difficult. Usually two approaches are used to tackle it. A first one, with regard to the failure of many classical numerical methods, is aiming at constructing adapted numerical methods using special meshes or any other special approximation techniques.

Some authors has proposed such schemes that became classical. The interested reader may report to: [6], [1], [21], [14]. In the same field, some new ideas have been proposed these last years. One may find some of those in [3], [7] and [22].

A second approach goes it way through the use of the techniques of Asymptotic Analysis. The asymptotic analysis of ordinary differential equations is largely present in the literature.

As sample of well-known works including pioneering ones we may cite: [24], [19;20], [17], [8], [13], [23], [11], [2]. But it is rare to find easy to compute uniform higher order asymptotic approximation for higher order perturbed differential problems.

Nevertheless in [19;20] and [3;4], explicite approximation solutions have been worked out but those which are higher order approximations are rather representation forms than actual easy to compute solutions.

In the current paper we have made the choice to work from an asymptotic analysis point of view. Namely, we perform the construction of a higher order asymptotic approximation solution in a sense that we call it, according to [3], a Strongly Uniformly or Strongly Stable Asymptotic Approximation.

In fact, adopting the notations in [19;20]; in its more general expression, the family of singularly perturbed problems under our consideration may be written as:

$$(1.1) \quad \begin{cases} L_\epsilon u \equiv \epsilon u'' + a(x) u' + b(x, u) = f, & 0 \leq x \leq 1, \\ B_{\epsilon,0} u = u(0) - \epsilon u'(0) = A, \\ B_{\epsilon,1} u = u(1) + \epsilon u'(1) = B. \end{cases}$$

Setting $\Omega =]0, 1[$, we suppose that for $x \in \bar{\Omega}$

$$(1.2) \quad a(x) \geq \alpha > 0; \quad a \in \mathbf{C}^1(\Omega), \quad b \in \mathbf{C}^1(\Omega \times \mathbf{R}).$$

In [18] and [3;4] it is shown that the stability of the difference operator associated with equations (1.1) is very sensitive to the functional space setting. So that in general, (1.1) is not stable and then is difficult to solve numerically. This legitimates the seek of asymptotic solutions as far as one may find some easy to compute ones.

2 – Setting the problem in the Linear case

The linear singular perturbation problem is derived from (1.1) by taking the function b such that $b(x, u) = b(x) u$.

$\| \cdot \|_\infty$ stands for the Maximum Norm.

$\mathbf{L}^1(\Omega)$ stands for the Lebesgue space of absolute integrable functions over Ω , and $\mathbf{L}^2(\Omega)$ is the Lebesgue Space of Square Integrable functions defined on Ω . The norms over these classical Lebesgue function spaces are set to be respectively:

$$|f|_1 = \int_{\Omega} |f(x)| dx \quad \text{and} \quad |f|_2 = \left(\int_{\Omega} |f(x)|^2 dx \right)^{\frac{1}{2}} .$$

$\mathbf{H}^1(\Omega)$ denotes the Sobolev Space of the functions which, with their first derivatives are lying in $\mathbf{L}^2(\Omega)$. The norm in $\mathbf{H}^1(\Omega)$ is set to be:

$$\|f\|_1 = \text{Max}(|f|_2, |f'|_2) .$$

Then, we consider the following linear singular perturbation problem:

$$(2.1) \quad \begin{cases} L_\epsilon u \equiv \epsilon u'' + a(x) u' + b(x) u = f, & x \in \Omega , \\ B_{\epsilon,0} u = u(0) - \epsilon u'(0) = A , \\ B_{\epsilon,1} u = u(1) + \epsilon u'(1) = B . \end{cases}$$

Hypothesis (1.2) becomes:

$$(2.2) \quad a(x) \geq \alpha > 0, \quad a, b \in \mathbf{C}^1(\Omega) .$$

It is known from [19] that under hypothesis (2.2) Problem (2.1) has a unique solution which exhibits a boundary layer phenomenon near the point $x = 0$.

A key tool we are using in the sequel is an a-priori estimate from [18] that is used in [4] (see theorem 1.2 at page 633) to set up the notion of Strong Stability.

We set the Weighted Sobolev Norm to be:

$$\|v\| = \|v\|_\infty + \|v'\|_\infty .$$

In the sequel, we are making use of a definition from [3;4] which is:

Definition 2.1. We say that the set $(L_\epsilon, B_{\epsilon,0}, B_{\epsilon,1})$ is strongly Uniformly Stable in the sense of Gartland Jr. if there exist two constants C and ϵ_0 such that:

$$\|v\| \leq C \left(|L_\epsilon v|_1 + |B_{\epsilon,0} v| + |B_{\epsilon,1} v| \right)$$

for $0 < \epsilon \leq \epsilon_0$, and all sufficiently smooth v . \square

We, then have the following result:

Theorem 2.1. Under hypothesis (2.2), the set $(L_\epsilon, B_{\epsilon,0}, B_{\epsilon,1})$ that defines Problem (2.1) is Strongly Uniformly Stable. \blacksquare

3 – Construction of the Uniformly Stable Solution

With regard to what precedes, we define a corrector in the following sense

Definition 3.1. Consider two auxiliary operators $B_{\epsilon,0}$ and $B_{\epsilon,1}$ such that $(L_\epsilon, B_{\epsilon,0}, B_{\epsilon,1})$ is strongly uniformly stable in the sense of Gartland. A regular function, say θ_q is said to be a Strong Stable q -th order Corrector or a Strongly Uniformly Stable Corrector for u solution of Problem (2.1) with respect to $(L_\epsilon, B_{\epsilon,0}, B_{\epsilon,1})$ if:

$$(H.1) \quad \text{Max} \left(|B_{\epsilon,0} w|, |B_{\epsilon,1} w| \right) \leq C \cdot \epsilon^q$$

where $w = u - (\bar{u}_q + \theta_q)$ and \bar{u}_q is a q -th order outer expansion to u (see below).

The regular function $Y_q = \bar{u}_q + \theta_q$ will be said a strongly Stable q -th order approximation solution to u if, in addition to inequality (H.1), the following inequality holds true:

$$(H.2) \quad |L_\epsilon w|_1 \leq C \cdot \epsilon^q .$$

C stands for various constants that are independent of ϵ . \square

We start by setting up u_q the q -th order outer expansion or regular expansion to u .

$\bar{u}_q = \sum_{i=0}^q \epsilon^i u_i$ where the coefficient functions u_i , $0 \leq i \leq q$, are defined by:

$$(3.1) \quad a u'_0 + b u_0 = f, \quad a u'_i + b u_i = -u''_{i-1}, \quad 1 \leq i \leq q$$

under some initial conditions that are:

$$(3.2) \quad u_0(1) = B, \quad u_i(1) = -u'_{i-1}(1), \quad 1 \leq i \leq q.$$

We state:

Theorem 3.1. *There exists a regular function U such that:*

$$(3.3) \quad \begin{cases} L_\epsilon U \equiv \epsilon U'' + a(x)U' + b(x)U = -\epsilon^{q+1}u''_q, \\ B_{\epsilon,0}U = U(0) - \epsilon U'(0) = A + \alpha_\epsilon, \\ B_{\epsilon,1}U = U(1) + \epsilon U'(1) = \epsilon^{q+1}u'_q(1), \end{cases}$$

where: $A = u(0) - \epsilon u'(0)$;

$$\begin{aligned} \alpha_\epsilon &= -\bar{u}_q(0) + \epsilon \bar{u}'_q(0) \\ &= -u_0(0) - \epsilon(u_1(0) - u'_0(0)) - \epsilon^2(u_2(0) - u'_1(0)) \\ &\quad - \epsilon^3(u_3(0) - u'_2(0)) - \dots - \epsilon^q(u_q(0) - u'_{q-1}(0)) + \epsilon^{q+1}u'_q(0). \end{aligned}$$

Proof: Set $U = u - \bar{u}_q$.

• Calculation of $L_\epsilon U$

From (3.1) we get:

$$L_\epsilon u_0 = \epsilon u''_0 + a u'_0 + b u_0 = f + \epsilon u''_0$$

and, for $1 \leq i \leq q$:

$$L_\epsilon u_i = \epsilon u''_i + a u'_i + b u_i = -u''_{i-1} + \epsilon u''_i,$$

$$\epsilon^i L_\epsilon u_i = -\epsilon^i u''_{i-1} + \epsilon^{i+1} u''_i.$$

Hence

$$L_\epsilon \bar{u}_q = \sum_{i=0}^q \epsilon^i L_\epsilon u_i = f + \epsilon u''_0 + \sum_{i=1}^q (-\epsilon^i u''_{i-1} + \epsilon^{i+1} u''_i) = f + \epsilon^{q+1} u''_q.$$

Which identity, by virtue of the equality $U = u - \bar{u}_q$, leads to:

$$L_\epsilon U = L_\epsilon u - L_\epsilon \bar{u}_q = f - f - \epsilon^{q+1} u''_q = -\epsilon^{q+1} u''_q$$

which is the first equality of the system (3.3).

- Calculation of $B_{\epsilon,0}U = U(0) - \epsilon U'(0)$.

We have:

$$\bar{u}_q(0) - \epsilon \bar{u}'_q(0) = u_0(0) + \sum_{i=1}^q \epsilon^i (u_i(0) - u'_{i-1}(0)) - \epsilon^{q+1} u'_q(0) .$$

We set:

$$-\alpha_\epsilon = u_0(0) + \sum_{i=1}^q \epsilon^i (u_i(0) - u'_{i-1}(0)) - \epsilon^{q+1} u'_q(0) .$$

So:

$$U(0) - \epsilon U'(0) = u(0) - \epsilon u'(0) - (\bar{u}_q(0) - \epsilon \bar{u}'_q(0)) = A + \alpha_\epsilon .$$

- Calculation of $B_{\epsilon,1}U = U(1) + \epsilon U'(1)$. We have:

$$\bar{u}_q(1) + \epsilon \bar{u}'_q(1) = u_0(1) + \sum_{i=1}^q \epsilon (u_i(1) + u'_{i-1}(1)) + \epsilon^{q+1} u'_q(1) .$$

According to equation (3.2), it comes that:

$$\bar{u}_q(1) + \epsilon \bar{u}'_q(1) = B + \epsilon^{q+1} u'_q(1) ,$$

then we conclude that:

$$\begin{aligned} U(1) + \epsilon U'(1) &= u(1) + \epsilon u'(1) - (\bar{u}_q(1) + \epsilon \bar{u}'_q(1)) \\ &= B - B - \epsilon^{q+1} u'_q(1) \\ &= -\epsilon^{q+1} u'_q(1) . \blacksquare \end{aligned}$$

Next, we state:

Theorem 3.2. *There exists a regular function W such that W is a $q+1$ -th order corrector to u based only on the outer expansion \bar{u}_q at the exclusion of the inner expansion.*

Proof: We consider a regular expansion, say $\bar{\beta}_q$ such that:

$$\bar{\beta}_q = \sum_{i=0}^q \epsilon^i \beta_i \quad \text{where } \beta_i(x) = (x-1)^2 t_i, \quad t_i \in \mathbf{R}, \quad 0 \leq i \leq q .$$

Since

$$\beta'_i(x) = 2t_i(x-1)$$

then it is obvious that

$$(3.4) \quad \bar{\beta}_q(1) + \epsilon \bar{\beta}'_q(1) = 0 .$$

The coefficients t_i which values identification are a part of the trouble to shoot will be determined later. We need now to calculate $\bar{\beta}_q(0) + \bar{\beta}'_q(0)$. We have $\beta_i(0) = t_i$ and $\beta'_i(0) = -2t_i$ which, put together lead to $\bar{\beta}_q(0) = \sum_{i=0}^q \epsilon^i t_i$ and $\bar{\beta}'_q(0) = -2 \left(\sum_{i=0}^q \epsilon^i t_i \right)$ so, we obtain:

$$(3.5) \quad \bar{\beta}_q(0) - \epsilon \bar{\beta}'_q(0) = (1 + 2\epsilon) \left(\sum_{i=0}^q \epsilon^i t_i \right) .$$

We set $(1 + 2\epsilon) \left(\sum_{i=0}^q \epsilon^i t_i \right) = \bar{B}$ and $V = U - \bar{\beta}_q = u - \bar{u}_q - \bar{\beta}_q$. We state:

Lemma 3.1. *The function V such that $V = U - \bar{\beta}_q = u - \bar{u}_q - \bar{\beta}_q$ satisfies:*

$$(3.6) \quad \begin{cases} L_\epsilon V = -\epsilon^{q+1} u''_q - L_\epsilon \bar{\beta}_q, & 0 \leq x \leq 1, \\ B_{\epsilon,0} V = V(0) - \epsilon V'(0) = A + \alpha_\epsilon - \bar{B}, \\ B_{\epsilon,1} V = V(1) + \epsilon V'(1) = \epsilon^{q+1} u'_q(1), \end{cases}$$

where

$$(3.7) \quad \begin{cases} L_\epsilon \bar{\beta}_q = \sum_{i=0}^q L_\epsilon \beta_i = \sum_{i=0}^q \epsilon^i t_i c, \\ c = 2\epsilon + 2(x-1)a(x) + (x-1)^2 b(x). \end{cases}$$

Proof:

- Calculation of $L_\epsilon V$.

From

$$\beta_i = (x-1)^2 t_i ,$$

and reminding that:

$$L_\epsilon u = \epsilon u'' + a u' + b u ,$$

the equalities:

$$\beta'_i = 2t_i(x-1)$$

$$\beta''_i = 2t_i$$

lead to

$$L_\epsilon \beta_i = t_i \left(2\epsilon + 2a(x-1) + b(x-1)^2 \right) = t_i c$$

hence $L_\epsilon \bar{\beta}_q$ is given by equation (3.7).

From equality $V = U - \bar{\beta}_q$, we get:

$$L_\epsilon V = L_\epsilon U - L_\epsilon \bar{\beta}_q = -\epsilon^{q+1} u_q'' - L_\epsilon \bar{\beta}_q$$

by virtue of Theorem 3.1.

- Calculation of $B_{\epsilon,0}V$

$$B_{\epsilon,0}V = U(0) - \epsilon U'(0) - \left(\bar{\beta}_q(0) - \epsilon \bar{\beta}'_q(0) \right) = A + \alpha_\epsilon - \bar{B}$$

by virtue of Theorem 3.1 and equation (3.5).

- Calculation of $B_{\epsilon,1}V$

$$B_{\epsilon,1}V = U(1) + \epsilon U'(1) + \left(\bar{\beta}_q(1) + \epsilon \bar{\beta}'_q(1) \right) = \epsilon^{q+1} u_q'(1)$$

by virtue of Theorem 3.1 and equation (3.4). ■

The next step on the way to our goal is to work out an asymptotic outer expansion to V . We state:

Lemma 3.2. *There exists a regular function H_q which coincides with a q -th order outer expansion to V . Moreover the regular function W such that $W = V - H_q$ satisfies:*

$$(3.8) \quad \begin{cases} L_\epsilon W = \mathcal{O}(\epsilon^{q+1}), \\ W(0) - \epsilon W'(0) = \mathcal{O}(\epsilon^{q+1}), \\ W(1) + \epsilon W'(1) = \mathcal{O}(\epsilon^{q+1}). \end{cases}$$

Proof: We set

$$H_q = \sum_{i=0}^q \epsilon^i t_i h_i$$

where the scalars t_i are the same from the definition of β_i and the coefficient functions h_i are to be determined by matching, with regard to the parameter ϵ , the same power terms in $L_\epsilon V$ in one hand and in $L_\epsilon H_q$ in an other hand. We know $L_\epsilon V$ from equation (3.7) and it remains to work out $L_\epsilon H_q$.

- Calculation of $L_\epsilon H_q$

From the equality $H_q = \sum_{i=0}^q \epsilon^i t_i h_i$, we draw obviously that:

$$L_\epsilon H_q = \sum_{i=0}^q \left(\epsilon^{i+1} t_i h_i'' + \epsilon^i t_i (a h_i' + b h_i) \right) .$$

So the matching yields:

$$(3.9a) \quad \begin{cases} a h_0' + b h_0 = -c , \\ \begin{cases} t_i (a h_i' + b h_i) = -t_{i-1} h_{i-1}'' - t_i c , \\ 1 \leq i \leq q . \end{cases} \end{cases}$$

The equations (3.9a) have to be supplemented with some boundary or initial conditions to make well posed problems out about the determination of the functions h_i .

- Determination of the boundary conditions attached to the function h_i .

One has:

$$(3.10a) \quad \begin{aligned} H_q(1) + \epsilon H_q'(1) &= \\ &= t_0 h_0(1) + \sum_{i=1}^q \left(\epsilon^i (t_i h_i(1) + t_{i-1} h_{i-1}'(1)) \right) + \epsilon^{q+1} t_q h_q'(1) \end{aligned}$$

and

$$(3.11) \quad \begin{aligned} H_q(0) - \epsilon H_q'(0) &= \\ &= t_0 h_0(0) + \sum_{i=1}^q \left(\epsilon^i (t_i h_i(0) - t_{i-1} h_{i-1}'(0)) \right) - \epsilon^{q+1} t_q h_q'(0) . \end{aligned}$$

We are imposing such boundary conditions on the function h_i so that:

$$|H_q(1) + \epsilon H_q'(1)| = \mathcal{O}(\epsilon^{q+1}) .$$

Such condition is fulfilled under:

$$(3.9b) \quad \begin{cases} h_0(1) = 0 , \\ \begin{cases} t_i h_i(1) + t_{i-1} h_{i-1}' = 0 , \\ 1 \leq i \leq q . \end{cases} \end{cases}$$

More precisely, under conditions (3.9b), we get:

$$(3.10b) \quad H_q(1) + \epsilon H_q'(1) = \epsilon^{q+1} t_q h_q'(1) .$$

Then the coefficient functions h_i are fully determined by putting together the equations (3.9a) and (3.9b).

- Calculation of $L_\epsilon W$:

Since H_q is the q -th order outer expansion to V then, according to Theorem 3.1 we have:

$$(3.12a) \quad L_\epsilon W = -\epsilon^{q+1} t_q h_q'' - \epsilon^{q+1} u_q'' .$$

- Calculation of $B_{\epsilon,0} W$:

We have:

$$W(0) - \epsilon W'(0) = V(0) - \epsilon V'(0) - \left(H_q(0) - \epsilon H_q'(0) \right) .$$

Referring to

$$V(0) - \epsilon V'(0) = A + \alpha_\epsilon - \bar{B}$$

and to equation (3.11), we conclude that:

$$(3.12b) \quad \begin{aligned} W(0) - \epsilon W'(0) &= g \\ &= A - u_0(0) - t_0 - t_0 h_0(0) \\ &\quad - \sum_{i=1}^q \epsilon^i \left(u_i(0) - u_0'(0) + 2t_i + t_i h_i(0) - t_{i-1} h_{i-1}'(0) \right) \\ &\quad + \epsilon^{q+1} \left(u_q'(0) - 2t_q + t_q h_q'(0) \right) . \end{aligned}$$

- Calculation of $B_{\epsilon,1} W$:

We have:

$$W(1) + \epsilon W'(1) = V(1) + \epsilon V'(1) - \left(H_q(1) + \epsilon H_q'(1) \right) .$$

From Lemma 3.1, we take:

$$V(1) + \epsilon V'(1) = \epsilon^{q+1} u_q'(1)$$

and from equation (3.10b), we have

$$H_q(1) + \epsilon H_q'(1) = \epsilon^{q+1} t_q h_q'(1)$$

so that, we get:

$$(3.12c) \quad W(1) + \epsilon W'(1) = \epsilon^{q+1} \left(u_q'(1) - t_q h_q'(1) \right) .$$

Put together, equations (3.12a), (3.12b) and (3.12c) lead to the system:

$$(3.12) \quad \begin{cases} L_\epsilon W = -\epsilon^{q+1} t_q h_q'' - \epsilon^{q+1} u_q'' , \\ W(0) - \epsilon W'(0) = g , \\ W(1) + \epsilon W'(1) = \epsilon^{q+1} (u_q'(1) - t_q h_q'(1)) , \end{cases}$$

where g is given by (3.12b). This leads to the conclusion that equations (3.8) holds true. ■

Next we state:

Theorem 3.2. *We set*

$$\theta_q = \bar{u}_q + \bar{\beta}_q + H_q .$$

We assume that:

$$(3.13) \quad \begin{cases} h_i(0) \neq -1 , \\ 0 \leq i \leq q . \end{cases}$$

Then there exists a unique $(q+1)$ -tuple $[t_0, t_1, \dots, t_q]$ that makes a Uniformly Stable q -th order Solution to u out of the regular function θ_q . More precisely, we have:

$$\| \| (u - \theta_q) \| \| \leq C \epsilon^{q+1}$$

where C is a constant that is independent of ϵ .

Proof: From equations (3.12), we have:

$$W(0) - \epsilon W'(0) = g .$$

We assume that conditions (3.13) hold true. The following setting:

$$\begin{cases} t_0 = (A - u_0(0) - 1)/(h_0(0) + 1) , \\ \begin{cases} t_i = (u_i(0) - u_{i-1}'(0) + 2t_{i-1} - t_{i-1} h_{i-1}'(0))/(h_i(0) + 1) , \\ 1 \leq i \leq q , \end{cases} \end{cases}$$

turns g to be such that

$$g = \epsilon^{q+1} (u_q'(0) - 2t_q + t_q h_q'(0)) .$$

Which means, among others, that

$$(3.14) \quad |g| = \mathcal{O}(\epsilon^{q+1}) .$$

Then equations (3.12) can be rewritten as:

$$(3.12bis) \quad \begin{cases} L_\epsilon W = -\epsilon^{q+1} t_i h_i'' , \\ W(0) - \epsilon W'(0) = \epsilon^{q+1} \left(u'_q(0) - 2t_q + t_q h'_q(0) \right) , \\ W(1) + \epsilon W'(1) = \epsilon^{q+1} \left(u'_q(1) - t_q h'_q(1) \right) . \end{cases}$$

we have:

$$W = V - H_q = u - (\bar{u}_q + \bar{\beta}_q + H_q) = u - \theta_q .$$

One has just to replace, into equations (3.12bis) W with $u - \theta_q$ and to, straight-way apply Theorem 2.1 knowing that

$$\text{Max} \left[|L_\epsilon u - \theta_q|, |B_{\epsilon,0} u - \theta_q|, |B_{\epsilon,1} u - \theta_q| \right] \leq C \epsilon^{q+1}$$

with C a constant independent of ϵ . ■

An easy consequence of Theorem 3.2 is:

Corollary 3.1. *We assume the hypotheses of Theorem 3.2. In addition, we assume that the functions u , \bar{u}_q , H_q belong to $C^\infty(\Omega)$. Then the following statement holds true:*

$$u^{(i)}(x) = \bar{u}_q^{(i)}(x) + \bar{\beta}_q^{(i)}(x) + H_q^{(i)}(x) + \mathcal{O}(\epsilon^{q-i+1})$$

for $x \in \Omega$, for $0 \leq i \leq q$. ■

Remark 3.1. Via linearization technics (e.g. the Newton Method of Quasi-linearization); the non-linear case that occurs when $b = b(x, u)$ can be turned into a sequence of linear problems to be solved as above. □

We may observe that:

Remark 3.2. The coefficient functions u_i of \bar{u}_q and h_i of H_q are obtained from similar equations so they can be computed in parallel. □

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