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Numerical and Analitic Solution for the Integrodifferential Equation of Dna Vibrational Dynamics

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Abstract

We analyze the numerical and analytical of solution for the mathematical modelling of DNA vibrational dynamics with relaxing function is studied using an integrodifferential equation which takes past information from the dynamics of DNA based on the Peyrard-Bishop model for vibrational motion of DNA dynamics, some other researchers have tried from the analytical point of view. In addition, we add the boundary conditions and initial data, for that one, we consider the Sobolev spaces and some other result from the theory of functional analysis. We apply the Faedo-Galerkin method in order to obtain the required solution. Using Matlab and Fourier Series, we can obtain numerical solutions as an educational strategy for mathematical research and software development in the areas of bioinformatics.

Keywords: *DNA Vibrational Dynamics, Sobolev Spaces, Faedo-Galerkin Method, Fourier Series, Software Development*

Introduction

Initially, the vibrations of DNA have been analyzed using the discrete nonlinear Klein-Gordon (KG) equations (n=1, 2... N)

$$\ddot{u}_n + V'(u_n) + \mu(2u_n - u_{n-1} - u_{n+1}) = 0, \qquad (1)$$

with $V'(u_n)$ being the derivative of the potential with respect the coordinate u_n wich represents the stretching of DNA and generating its dynamics according to Figure 1 using Matlab and Series de Fourier. (1)

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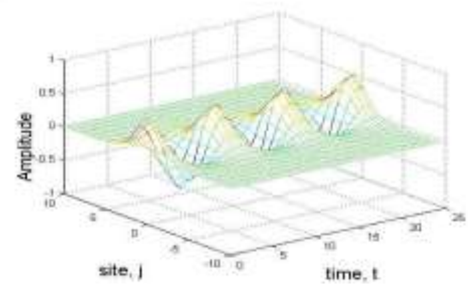

Figure 1. Numerical solution for the equations (0)

In this work we focus on the past of DNA dynamics, which is given by a convolution operation mathematically and transforming the equation into an integrodifferential equation.

Methods

The problem consists of the following model

$$u_{tt} - (l_1 + 3l_2 u_x^2)\, u_{xx} + 2\alpha^2 Du + \int_0^t g(t-s)\big(a(x)u_x(s)\big)_x\, ds = 0\ ,\ \ (0,L)\times(0,+\infty) \qquad (1)$$

$$\begin{cases} u(0,t) = 0 \\ u(L,t) \le d, \qquad a(L)g *\ u_x(L,t) - \big(l_1 u_x(L,t) + l_2 u_x^3(L,t)\big) \le 0 \\ (u(L,t) - d)\,\big(a(L)g *\ u_x(L,t) - (l_1 u_x(L,t) + l_2 u_x^3(L,t)\big) = 0 \end{cases} \qquad (2)$$

$$u(x,0) = u^0(x)\ ,\ u_t(x,0) = u^1(x) \qquad (3)$$

Where, $a\colon [0,L] \to \mathbb{R}$ is such that $a(x) \ge 0$ for all $x \in [0,L]$ (4)

And we assume that the relaxing function satisfies the condition: $g\colon [0,+\infty) \to \mathbb{R}$

$$g(t) \ge 0\ , g'(t) \le 0\ ,\ 0 < M_0 = \ l_1 - \operatorname*{Sup}_{x\in[0,L]} a(x) \int_0^{+\infty} g(s)ds \qquad (5)$$

We recall the convolution $g * h$ as being $\int_0^t g(t-s)h(s)ds$

Consider the subspace $V \subset H^1(0\,,L) \cap W^{1,4}(0,L)$ defined by

$$V = \{u \in H^1(0,L) \cap W^{1,4}(0,L); u(0) = 0\} \qquad (6)$$

with the inner product: $(u,v) = \int_0^L u_x\, v_x dx$ .We also consider some other binary relations:

$$(g \;\square\; h)(t) = \int_0^t g(t-s)|h(t)-h(s)|^2 ds$$

$$(g \quad h)(t) = \int_0^t g(t-s)\{h(t)-h(s)\} ds$$

Then, for every $g\,,h \in C^1(\mathbb{R})$ we have the identity ◇

$$2\,(g\,*h)h' = g' \quad \underset{\square}{h} - g(t)|h|^2 - \frac{d}{dt}\left\{g \quad \underset{\square}{h} - \int_0^t g(s)ds|h|^2\right\} \qquad (7)$$

Let K be the subset of V given by $K = \{u \in V; u(L) \le d\}$ (8)

Definition 1. We say that the function $u(x,t)$ defined in $[0,L]\times[0,T]$ is a weak solution for (1)-(3) if the following properties hold

$$u \in L^\infty(0,T;K) \cap W^{1,\infty}(0,T;L^4(0,L)) \cap C^1\big([0,T];H^{-1/2}(0,L)\big)$$

$$-\int_0^T\int_0^L u_t(v_t-u_t)\,dxdt + \int_0^T\int_0^L [l_1u_x + l_2u_x^3 - a(x)g *\, u_x](v_x-u_x)\,dxdt$$

$$+$$

$$+2\alpha^2 D\int_0^T\int_0^L u(v-u)\,dxdt \ge -\int_0^L u_t(T)\big(v(T)-u(T)\big)\,dx + \int_0^L u^1(x)(v(0)-u^0(x))\,dx$$

$$u(x,0) = u^0(x)\,,\ u_t(x,0) = u^1(x)$$

We assume that the following properties hold

P1) If $u^0 \in H^2(0\,,L)\cap V$, $u^1 \in V$, and (4) , (5) is verified. In addition, the compatibility relation holds

$l_1u_x^0(L) + l_2[u_x^0(L)]^3 = -\frac{1}{\varepsilon}[u^0(L)-d]^+ - \varepsilon u^1(L)$ for all $\varepsilon > 0$. Then we have

$u \in \cap_{k=0}^2 W^{1,\infty}\big(0,T;H^{2-k}(0,L)\big)\cap W^{1,4}(0,L)$

P2) Let $a \in C[0,L]$ and $g \in C[0,+\infty)$ satisfying ≥ 0 , $\|a\|_{C[0,L]}\int_0^t g(s)ds < 1/l_1$

If $v \in L^\infty(0\,,T;V)\cap W^{1,\infty}(0,T;L^4(0,L))$, is a solution of the equation (1)

Then, we have $g *\ v \in\ L^\infty(0,T;H^2(0,L))\cap V$

P3) Let $(u^m)_{m\in\mathbb{N}}$ be a sequence of functions such that

$u^m,\ u_t^m \in \cap_{k=0}^2 W^{1,\infty}\big(0,T;H^{2-k}(0,L)\big)\cap W^{1,4}(0,L)$, $u_{tt}^m \in L^\infty(0,T;L^2(0,L))$

satisfying $u_{tt}^m - (l_1 + 3l_2(u_x^m)^2)\,u_{xx}^m = f^m$. Furthermore, is verified

$$\|u^m\|_{L^\infty(0,T;W^{1,4}(0,L))} + \|u_t^m\|_{L^\infty(0,T;L^2(0,L))} + \|f^m\|_{L^2((0,L)\times(0,T))} \le C$$

Where C is a constant independent of m.We also assume that

$u^m \rightharpoonup u$ weak star in $L^\infty(0,T;W^{1,4}(0,L))$

$u_t^m \rightharpoonup u_t$ weak star in $L^\infty(0,T;L^2(0,L))$. Then we have

$$\lim_{m\to\infty} sup \int_0^T \int_0^L |u_t^m|^2 - [l_1|u_x^m|^2 + l_2|u_x^m|^4]\, dxdt \le \int_0^T \int_0^L |u_t|^2 - [l_1|u_x|^2 + l_2|u_x|^4]\, dxdt$$

Results and Discussions

Theorem. If $u^0 \in K$, $u^1 \in L^2(0,L)$, and (4) , (5) is verified. Then there exists a weak solution of the equation (1)-(3).

Proof.

First of all, we consider the penalized problem

$$u_{tt}^\varepsilon - (l_1 + 3l_2(u_x^\varepsilon)^2)\, u_{xx}^\varepsilon + 2\alpha^2 D u^\varepsilon + \int_0^t g(t-s)\big(a(x)u_x^\varepsilon(s)\big)_x\, ds = 0, (0,L) \times (0,+\infty) \qquad (9)$$

$$\begin{cases} u^\varepsilon(0,t) = 0 \\ a(L)g * u_x^\varepsilon(L,t) - \left(l_1 u_x^\varepsilon(L,t) + l_2\left(u_x^\varepsilon(L,t)\right)^3\right) = \frac{1}{\varepsilon}[u^\varepsilon(L,t) - d]^+ + \varepsilon u_t^\varepsilon(L,t) \ , \varepsilon > 0 \\ u^\varepsilon(x,0) = u^{\varepsilon,0}(x) , \qquad u_t^\varepsilon(x,0) = u^{\varepsilon,1}(x) \end{cases} \qquad (10)$$

On the other hand, we define the following spaces

$$W = \{u \in H^2(0,L) \cap V; u(0) = 0 ,\ u_x(L) = 0\}$$

$$W_d = \{u \in H^2(0,L) \cap V; u(0) = 0 ,\ u_x(L) = 0 , u(L) = d\}$$

Where, W is dense in V while $W \cap H_0^1(0,L)$ is dense in $H_0^1(0,L)$.

Hence, we suppose that for the initial conditions $(u^{\varepsilon,0})_{\varepsilon>0}$ and $(u^{\varepsilon,1})_{\varepsilon>0}$ is verified the following convergences

$u^{\varepsilon,0} \longrightarrow u^0$ in V

$u^{\varepsilon,1} \longrightarrow u^1$ in $L^2(0,L)$, as ε goes to zero. Where

$u^{\varepsilon,0} \in W$, $u^{\varepsilon,1} \in H_0^1(0,L)$ if $u^0(L) < d$

$u^{\varepsilon,0} \in W_d$, $u^{\varepsilon,1} \in H_0^1(0,L)$ if $u^0(L) = d$

We recall that $u^{\varepsilon,0}$ and $u^{\varepsilon,1}$ satisfy the compatibility condition given in (P1).So that we assume u^ε as being the strong solution the penalized problem (9) , (10).

Multiplying the equation (9) by u_t^ε and after integration on $(0,L)$, we obtain

$$\frac{1}{2}\frac{d}{dt}\left\{\int_0^L |u_t^\varepsilon|^2 + \left[l_1|u_x^\varepsilon|^2 + \frac{l_2}{2}|u_x^\varepsilon|^4\right] + 2\alpha^2 D|u^\varepsilon|^2\right\} - \left(l_1 u_x^\varepsilon(L,t) + l_2\left(u_x^\varepsilon(L,t)\right)^3\right)u_t^\varepsilon(L,t) +$$

$$+\int_0^L\int_0^t g(t-s)\left(a(x)u_x^\varepsilon(s)\right)_x u_t^\varepsilon(s)\,ds\,dx = 0$$

From the above relation (7) applied to the last integral, we deduce from the previous equality

$$\frac{1}{2}\frac{d}{dt}\left\{\int_0^L |u_t^\varepsilon|^2 + \left[l_1|u_x^\varepsilon|^2 + \frac{l_2}{2}|u_x^\varepsilon|^4\right] + 2\alpha^2 D|u^\varepsilon|^2\right\} - \left(l_1 u_x^\varepsilon(L,t) + l_2\left(u_x^\varepsilon(L,t)\right)^3\right)u_t^\varepsilon(L,t) +$$

$$+a(L)[g * u_x^\varepsilon(L,t)]u_t^\varepsilon(L,t) + \frac{1}{2}\frac{d}{dt}\left\{\int_0^L a(x)\, g \quad u_x^\varepsilon dx - \int_0^L a(x)\int_0^t g(s)ds\,|u_x^\varepsilon|^2 dx\right\} -$$

$$-\frac{1}{2}\int_0^L a(x)\, g' \;\square\; u_x^\varepsilon dx + \frac{1}{2}g(t)\int_0^L a(x)\,|u_x^\varepsilon|^2 dx = 0$$

From the relation (10) , multiplying by $u_t^\varepsilon(L,t)$, we see that

$\left[a(L)g * u_x^\varepsilon(L,t) - \left(l_1 u_x^\varepsilon(L,t) + l_2\left(u_x^\varepsilon(L,t)\right)^3\right)\right]u_t^\varepsilon(L,t) = \left\{\frac{1}{\varepsilon}[u^\varepsilon(L,t) - d]^+ + \varepsilon u_t^\varepsilon(L,t)\right\}u_t^\varepsilon(L,t) =$

$$= \frac{1}{2}\frac{d}{dt}\left\{\frac{1}{\varepsilon}|[u^\varepsilon(L,t) - d]^+|^2\right\} + \varepsilon|u_t^\varepsilon(L,t)|^2$$

Substituting into the previous equation, we have

$$\frac{1}{2}\frac{d}{dt}\left\{\int_0^L |u_t^\varepsilon|^2 + \left[l_1|u_x^\varepsilon|^2 + \frac{l_2}{2}|u_x^\varepsilon|^4\right] + 2\alpha^2 D|u^\varepsilon|^2 + \frac{1}{\varepsilon}|[u^\varepsilon(L,t) - d]^+|^2\right\} =$$

$$= \frac{1}{2}\int_0^L a(x)\, g' \;\square\; u_x^\varepsilon dx - \frac{1}{2}g(t)\int_0^L a(x)\,|u_x^\varepsilon|^2 dx - \varepsilon|u_t^\varepsilon(L,t)|^2$$

Which is equivalent to the expression

$$\frac{d}{dt}E_\varepsilon(t,u^\varepsilon) = \frac{1}{2}\int_0^L a(x)\, g' \;\square\; u_x^\varepsilon dx - \frac{1}{2}g(t)\int_0^L a(x)\,|u_x^\varepsilon|^2 dx - \varepsilon|u_t^\varepsilon(L,t)|^2$$

Integrating on $(0,t)$, we obtain

$\square$

$$E_\varepsilon(t,u^\varepsilon) \le E_\varepsilon(0,u^\varepsilon) + \frac{1}{2}\int_0^T\int_0^L a(x)\, g' \quad u_x^\varepsilon dx - \frac{1}{2}\int_0^T\int_0^L g(t)a(x)\,|u_x^\varepsilon|^2 dxdt$$
$$-\,\varepsilon\int_0^T |u_t^\varepsilon(L,t)|^2 dt$$

Since $(4),(5)$ is verified and from the hypothesis of the initial conditions, it yields

$E_\varepsilon(t,u^\varepsilon)$ is bounded in $L^\infty(0,T)$, therefore, we can extract a subsequence that we will still denote with the same subscript, such that

$u^\varepsilon \rightharpoonup u$ weak star in $L^\infty(0,T;V)$

$u_t^\varepsilon \rightharpoonup u_t$ weak star in $L^\infty(0,T;L^2(0,L))$

And by the property (P2), we have

$g *\ u_x^\varepsilon$ is bounded in $L^\infty(0,T;H^1(0,L))$. On the other hand

$(g *\ u_x^\varepsilon)_t = g(0)\ u_x^\varepsilon + g' *\ u_x^\varepsilon$ is bounded in $L^\infty(0,T;L^2(0,L))$. For a result of compactness, we deduce that

$$g *\ u_x^\varepsilon \longrightarrow g *\ u_x \quad \text{in } L^\infty(0,T;L^2(0,L)) \qquad (11)$$

From the equation (9), we see that u_{tt}^ε is bounded in $L^\infty(0,T;H^{-1}(0,L))$, once more time from the compactness, we have

$$u^\varepsilon \longrightarrow u \quad \text{in } C^0\big(0,T;H^{1-\delta}(0,L)\big) \qquad (12)$$

$$u_t^\varepsilon \longrightarrow u_t \quad \text{in } L^\infty\big(0,T;H^{-\delta}(0,L)\big)\text{, for all } \delta > 0 \qquad (13)$$

Multiplying the equation (9) by $v(x,t) - u^\varepsilon(x,t)$, with

$v \in L^\infty(0,T;K) \cap W^{1,\infty}(0,T;L^4(0,L))$ and integrating by part on $(0,L)\times(0,T)$, we have

$$-\int_0^T\int_0^L u_t^\varepsilon(v_t - u_t^\varepsilon)dxdt + \int_0^L u_t^\varepsilon(T)\big(v(T) - \ u^\varepsilon(T)\big)dx\ - \int_0^L u^{\varepsilon,1}(v(0) - \ u^{\varepsilon,0})dx +$$

$$+\int_0^T\int_0^L (l_1 u_x^\varepsilon + l_2(u_x^\varepsilon)^3)(v_x - u_x^\varepsilon)dxdt$$
$$-\int_0^T \left(l_1 u_x^\varepsilon(L,t) + l_2\big(u_x^\varepsilon(L,t)\big)^3\right)\big(v(L) - \ u^\varepsilon(L,t)\big)dt +$$

$$+2\alpha^2 D\int_0^T\int_0^L u^\varepsilon(v-u^\varepsilon)dxdt+\int_0^T\int_0^L g*\left(a(x)u_x^\varepsilon(s)\right)_x(v-u^\varepsilon)dxdt=0$$

Which is equivalent to the following expression

$$-\int_0^T\int_0^L u_t^\varepsilon(v_t-u_t^\varepsilon)dxdt+\int_0^L u_t^\varepsilon(T)\left(v(T)-\ u^\varepsilon(T)\right)dx\ -\int_0^L u^{\varepsilon,1}(v(0)-\ u^{\varepsilon,0})dx+$$

$$+\int_0^T\int_0^L(l_1u_x^\varepsilon+l_2(u_x^\varepsilon)^3)(v_x-u_x^\varepsilon)dxdt$$

$$-\int_0^T\left(l_1u_x^\varepsilon(L,t)+l_2\left(u_x^\varepsilon(L,t)\right)^3\right)\left(v(L)-\ u^\varepsilon(L,t)\right)dt+$$

$$+2\alpha^2 D\int_0^T\int_0^L u^\varepsilon(v-u^\varepsilon)dxdt-\int_0^T\int_0^L g*\left(a(x)u_x^\varepsilon(s)\right)(v_x-u_x^\varepsilon)dxdt+$$

$$+\int_0^T g*\left(a(L)u_x^\varepsilon(L,t)\right)\left(v(L,t)-\ u^\varepsilon(L,t)\right)dt=0$$

Making use of the equation (10), we obtain

$$-\int_0^T\int_0^L u_t^\varepsilon(v_t-u_t^\varepsilon)dxdt+\int_0^T\int_0^L(l_1u_x^\varepsilon+l_2(u_x^\varepsilon)^3)(v_x-u_x^\varepsilon)dxdt+$$

$$+2\alpha^2 D\int_0^T\int_0^L u^\varepsilon(v-u^\varepsilon)dxdt-\int_0^T\int_0^L g*\left(a(x)u_x^\varepsilon(s)\right)(v_x-u_x^\varepsilon)dxdt=-$$

$$=-\int_0^L u_t^\varepsilon(T)\left(v(T)-\ u^\varepsilon(T)\right)dx+\int_0^L u^{\varepsilon,1}(v(0)-\ u^{\varepsilon,0})dx-$$

$$-\frac{1}{\varepsilon}\int_0^T\left([u^\varepsilon(L,t)-d]^++\varepsilon^2u_t^\varepsilon(L,t)\right)\left(v(L)-\ u^\varepsilon(L,t)\right)dt$$

On the other hand,

$$-\frac{1}{\varepsilon}\int_0^T [u^\varepsilon(L,t)-d]^+[v(L,t)-d]-[u^\varepsilon(L,t)-d]^+(\ u^\varepsilon(L)-d)dt \geq 0$$

So that, we obtain from the last equality

$$-\int_0^T\int_0^L u_t^\varepsilon(v_t-u_t^\varepsilon)dxdt+\int_0^T\int_0^L (l_1u_x^\varepsilon+l_2(u_x^\varepsilon)^3)(v_x-u_x^\varepsilon)dxdt+$$

$$+2\alpha^2 D\int_0^T\int_0^L\ u^\varepsilon(v-u^\varepsilon)dxdt-\int_0^T\int_0^L g*\left(a(x)u_x^\varepsilon(s)\right)(v_x-u_x^\varepsilon)dxdt\geq -$$

$$\geq -\int_0^L u_t^\varepsilon(T)\big(v(T)-\ u^\varepsilon(T)\big)dx$$

$$+\int_0^L u^{\varepsilon,1}(v(0)-\ u^{\varepsilon,0})dx-\int_0^T \varepsilon u_t^\varepsilon(L,t)\big(v(L,t)-\ u^\varepsilon(L,t)\big)dt$$

Of the strong convergences (11)-(13), we have

$$\int_0^L u_t^\varepsilon(T)\big(v(T)-\ u^\varepsilon(T)\big)dx=\langle u_t^\varepsilon(T),v(T)-\ u^\varepsilon(T)\rangle_{H^{-1/2}\times H^{1/2}}$$

$$\longrightarrow \langle u_t(T),v(T)-\ u(T)\rangle_{H^{-1/2}\times H^{1/2}}$$

$$\int_0^T\int_0^L g*\left(a(x)u_x^\varepsilon(s)\right)(v_x-u_x^\varepsilon)dxdt\longrightarrow\int_0^T\int_0^L g*\left(a(x)u_x(s)\right)(v_x-u_x)dxdt$$

For all $v\in H^{1/2}(0,L)$.

Hence, taking the upper limit and from the property (P3), we get the inequality

$$-\int_0^T\int_0^L u_t(v_t-u_t)\,dxdt+\int_0^T\int_0^L [l_1u_x+l_2u_x^3-a(x)g*\ u_x](v_x-u_x)\,dxdt$$

$$+$$

$$+2\alpha^2 D\int_0^T\int_0^L u(v-u)\,dxdt\geq -\int_0^L u_t(T)\big(v(T)-u(T)\big)\,dx+\int_0^L u^1(x)(v(0)-u^0(x))\,dx$$

And from the relations (12) and (13), we obtain $u(x,0)=u^0(x)$, $u_t(x,0)=u^1(x)$

Finally, to obtain $u(L,t) \in K$ for all $t \in [0,T]$. We recall that

$[u^{\varepsilon}(L,t) - d]^{+} \longrightarrow [u(L,t) - d]^{+}$ on $[0,T]$. On the other hand , $E_{\varepsilon}(t, u^{\varepsilon})$ is bounded in $L^{\infty}(0,T)$. So that, we have

$\frac{1}{\sqrt{\varepsilon}}[u^{\varepsilon}(L,t) - d]^{+}$ is bounded in $L^{\infty}(0,T)$, which implies that $[u(L,t) - d]^{+} = 0$. Hence, we deduce $u(L,t) \leq d$, therefore $u(L,t) \in K$ for all $t \in [0,T]$.

Conclusions

We have achieved a result of existence through of Faedo-Galerkin method's as long as we have used multiplicative techniques. The penalized problem played a fundamental role such as shown by the main result theorem. Using Matlab and Fourier Series, we can obtain numerical solutions as an educational strategy for mathematical research and software development in the areas of bioinformatics.

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