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Numerical Methods for Constructing Solutions of Functional Differential Equations of Pointwise Type

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Abstract: The article discusses construction of traveling wave type solutions for the Frenkel-Kontorova model on the propagation of longitudinal waves. For the first time, based on the existence and uniqueness theorem of traveling wave type solutions, as well as the approximation theorem, a complete family of traveling wave type solutions is constructed in the form of subfamilies of bounded solutions (horizontals) and unbounded solutions (verticals).

Keywords: traveling waves, functional differential equations, equations of mathematical physics, splines, forward-backward differential equation

1. INTRODUCTION

The theory of differential equations with delay, which has developed rapidly in recent decades [1–3], has in many ways acquired a complete form and is now actively used in modeling various objects. Numerical algorithms for solving equations with delay of various types were also developed [4, 5]. At the same time, numerical methods for equations with advanced arguments (and, moreover, with mixed type deviations) are practically not studied, although references to them have been encountered for a long time, mainly in connection with the classification of equations with deviating argument [6]. As a rule, there is a parsing of equations of a particular kind with further obtaining the existence and uniqueness theorems based on the use of the properties of the right-hand side [7] and application of methods, such as the study of the roots of the characteristic quasi-polynomial [8], collocation methods and finite element scheme (expansion of a solution in terms of basis functions of some finite-dimensional space) [9–11] or through the construction of a Hilbert space of the reproducing kernels on the basis of boundary conditions [12].

For equations of a delayed type, as a rule, a well-known initial problem is considered when the initial moment of time coincides with the left end of the interval of equation's domain. Such a statement is characterized by the fact that the initial-boundary conditions are local in nature, and the equation itself can be integrated by the step method. In all other cases, and even more so in the case of functional differential equations of pointwise type (FDEPT) with mixed-type deviations, the initial-boundary conditions are nonlocal in nature.

One of the approaches to the construction of numerical methods for FDEPT is the variational method based on solving the induced optimal control problem (OCP) as an unconditional optimization problem for the residual functional. As noted earlier, the initial-boundary conditions for FDEPT are not local, therefore, the solution of the variational problem for the residual functional cannot be obtained by simple local improvements and requires global optimization. Note that for problems of finite-dimensional optimization there

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are many approaches to finding a global extremum, sufficiently efficient algorithms are built, there are a large number of publications that present precedents for successfully solved problems [13, 14, for example].

At the same time, the task of finding global extremum for OCP remains one of the most acute tasks in the extreme problems theory. Among classical approaches to this task one cannot fail to mention the works [15] and [16]. Some works that apply search and genetic algorithms are also well-known [17, 18]. But unfortunately these efforts have not yet brought about effective algorithms that would be able to solve a wide spectrum of practical problems [19].

One of the ideas in this area is the idea of reducing the optimal control problem to a low-dimensional problem on the reachability set of a controlled system [20]. Unfortunately, the problem of approximating the reachable set in the numerical solution is not much simpler than the problem of finding a global extremum. Nevertheless, the properties of the reachable set known from theoretical studies can be used to construct specialized optimization algorithms for OCP [21]. In particular, the connectivity property of the reachability set allows one to construct a scheme of continuous control variation that leads to the solution of the problem. The idea of using the connectivity property of the reachability set when constructing numerical optimization algorithms belongs to A.G. Chentsov [22].

In the majority of well-known approaches to the construction of non-convex optimization methods, the solution of the problem is divided into two stages: "global", where a wide scan of the variable space is performed, and "local", aimed on local refinement of the obtained solution [14]. The combination of different methods at each stage, as well as the order of the alternation of stages, determines the specific computational algorithm. For mentioned class of problems, we consider a idea of combining both stages in one algorithm package and creating a method that allows one to select and change both the "global scan" procedure and local improvement of the obtained approximate solution at each iteration [23].

2. STATEMENT OF THE INITIAL BOUNDARY-VALUE PROBLEM

The most important goal in FDEPT is the study of the *basic initial-boundary value problem*

$$\dot{x}(t) = f(t, x(q_1(t)), \ldots, x(q_s(t))), \quad t \in B_R, \tag{2.1}$$
$$\dot{x}(t) = \varphi(t), \quad t \in \mathbb{R}\backslash B_R, \quad \varphi(\cdot) \in L_\infty(\mathbb{R}, \mathbb{R}^n), \tag{2.2}$$
$$x(\bar{t}) = \bar{x}, \quad \bar{t} \in \mathbb{R}, \quad \bar{x} \in \mathbb{R}^n. \tag{2.3}$$

where $f : \mathbb{R} \times \mathbb{R}^{ns} \longrightarrow \mathbb{R}^n$ is a mapping of the $C^{(0)}$ class, $q_j(\cdot)$, $j = 1, \ldots, s$, represent diffeomorphisms of the line preserving orientation, and B_R is either the closed interval $[t_0, t_1]$, or closed half-line $[t_0, +\infty)$, or the whole line $\mathbb{R}$.

In the case of a delayed-type equation, for $B_R = [t_0, t_1], [t_0, +\infty), \bar{t} = t_0$, the initial-boundary-value problem becomes a well-known initial problem with the initial function $\zeta(t) = \bar{x} - \int_t^{\bar{t}} \varphi(\tau) d\tau, t \leq \bar{t}$.

The statement of the initial-boundary value problem (2.1)-(2.3) is correct without any restrictions on the type of argument deviations.

Definition 2.1:
The solution to the basic initial-boundary value problem is any absolutely continuous solution of the equation (2.1) *satisfying the boundary condition* (2.2) *and the initial condition* (2.3).

The aim of the FDE research is to study the solution space of the boundary value problem (2.1)-(2.2) for each given boundary function φ, as well as to describe the obstacles due to which the solutions of the boundary value problem (2.1)-(2.2) do not inherit the properties of solutions of ordinary differential equations.

If we introduce notation for a fixed function $\varphi(\cdot)$

$$f_\varphi(t, z_1, \dots, z_s) = \begin{cases} f(t, z_1, \dots, z_s), & t \in B_R, \\ \varphi(t), & t \notin B_R, \end{cases}$$

the boundary value problem (2.1)-(2.3) becomes a Cauchy problem

$$\dot{x}(t) = f_\varphi(t, x(q_1(t)), \dots, x(q_s(t))), \quad t \in \mathbb{R} \tag{2.4}$$

$$x(\bar{t}) = \bar{x}, \quad \bar{t} \in \mathbb{R}, \quad \bar{x} \in \mathbb{R}^n. \tag{2.5}$$

Obviously, in the case $B_R = \mathbb{R}$, the equality $f_\varphi = f$ holds.

In the study of the Cauchy problem (2.4)-(2.5), the role of the group $< q_1, \dots, q_s >$ is very important. Often, instead of such a group, it is useful to consider some wider finitely generated group Q of diffeomorphisms of the line, that is, $< q_1, \dots, q_s > \subseteq Q$. Moreover, we assume that the condition $h_q = \sup_{t \in \mathbb{R}} |q(t) - t| < +\infty$ is satisfied for all elements q of the group Q.

Let's formulate a system of restrictions on the right-hand side $f : \mathbb{R} \times \mathbb{R}^{n \cdot s} \longmapsto \mathbb{R}^n$ of FDEPT (2.1), and on diffeomorphisms $q_j(\cdot), j = 1, \dots, s$:

(a) $f(\cdot) \in C^{(0)}(\mathbb{R} \times \mathbb{R}^{n \cdot s}, \mathbb{R}^n)$;

(b) for any $t, z_j, \bar{z}_j, j = \overline{1, s}$, there is a quasilinear growth

$$\| f(t, z_1, \dots, z_s) \|_{\mathbb{R}^n} \leq M_0(t) + M_1 \sum_{j=1}^{s} \| z_j \|_{\mathbb{R}^n}, \quad M_0(\cdot) \in C^{(0)}(\mathbb{R}, \mathbb{R}),$$

and a Lipschitz condition

$$\| f(t, z_1, \dots, z_s) - f(t, \bar{z}_1, \dots, \bar{z}_s) \|_{\mathbb{R}^n} \leq L_f \sum_{j=1}^{s} \| z_j - \bar{z}_j \|_{\mathbb{R}^n};$$

(c) there exists $\mu^* \in \mathbb{R}_+$ such that

$$M_0(\cdot) \in \mathcal{L}^n_{\mu^*} C^{(0)}(\mathbb{R});$$

(d) the values

$$h_{q_j} = \sup_{t \in \mathbb{R}} |t - q_j(t)|, \quad j = 1, \dots, s,$$

are finite;

(e) with the constant $\mu^* \in \mathbb{R}_+$ from condition (c) the family of functions

$$\tilde{f}_{q, z_1, \dots, z_s}(t) = f(q(t), z_1, \dots, z_s)(\mu^\star)^{h_q}, \quad q \in Q, \quad z_1, \dots, z_s \in \mathbb{R}^n,$$

is equicontinuous on any finite interval.

The continuity condition, growth conditions with respect to the phase variables and time variable, and the Lipschitz condition (conditions $(a) - (b)$) are standard in the theory of ordinary differential equations. In fact, in item (b), the first inequality in the form of the growth condition with respect to the phase variables and time variable is a consequence of the second condition in the form of the Lipschitz condition. Under the Lipschitz constant L_f, the minimum value among the possible values of these constants should be understood. Accordingly, we can assume that $M_1 = L_f$. Moreover, we wrote the first inequality out separately in order to formulate condition (c) for function $M_0(\cdot)$. Condition (c) for function f is related to the study of solutions on the half-line and line, which requires certain restrictions on the time growth of the right-hand side. It should be noted that we can always satisfy condition (d) by making a time change, but we may break condition (c). The last condition (e) is necessary for the right-hand side of the induced infinite-dimensional ordinary differential equation, with the phase space in a suitable Banach space, to easily establish the fact of its Bochner integrability. In fact, condition (e) can be removed, but this leads to further technical complications, as the right-hand side of the induced infinite-dimensional ordinary differential equation will only be measurable, and it will be necessary to establish the fact of its Bochner integrability [24].

The right-hand side $f(\cdot)$ of FDEPT will be considered as an element of the Banach space $V_{\mu^*}(\mathbb{R}\times\mathbb{R}^{ns},\mathbb{R}^n)$ with Lipschitz norm

$$V_{\mu^*}(\mathbb{R}\times\mathbb{R}^{ns},\mathbb{R}^n)=\big\{f(\cdot):f(\cdot)\text{ satisfies the conditions (a)-(d) }\big\},$$
$$\|f(\cdot)\|_{L_{ip}}=\sup_{t\in R}\|f(t,0,\dots,0)(\mu^*)^{|t|}\|_{\mathbb{R}^n}+$$
$$+\sup_{(t,z_1,\dots,z_s,\bar z_1,\dots,\bar z_s)\in\mathbb{R}^{1+2ns}}\frac{\|f(t,z_1,\dots,z_s)-f(t,\bar z_1,\dots,\bar z_s)\|_{\mathbb{R}^n}}{\sum_{j=1}^s\|z_j-\bar z_j\|_{\mathbb{R}^n}},$$

where the parameter $\mu^*\in\mathbb{R}_+$ coincides with the corresponding constant from the condition (c).

Obviously, for the function $f(\cdot)\in V_{\mu^*}(\mathbb{R}\times\mathbb{R}^{ns},\mathbb{R}^n)$ the smallest value of the constant L_f from the Lipschitz condition (the condition (b)) coincides with the value of the second summand in the definition of the norm $f(\cdot)$. In what follows, speaking of the Lipschitz condition, by the constant L_f we mean exactly its smallest value.

The right-hand side of the FDEPT (2.1) uniquely defines a pair $(f(\cdot),h)$, where $f(\cdot)$ is an element of the Banach space $V_{\mu^*}(\mathbb{R}\times\mathbb{R}^{ns},\mathbb{R}^n)$, and $h=(h_{q_1},\dots,h_{q_s}),h_{q_j}\geq 0,j=1,\dots,s$, are maximum deviation of the argument from the condition (d), which we will consider as parameters. Therefore, such a right-hand side of the equation will uniquely determine the pair $(L_f;h)$.

We will seek a solution to the FDEPT with a quasilinear right-hand side in a one-parameter family of Banach spaces of functions with a given exponential growth. The exponent is the parameter of the selected family of functions, which is defined as follows

$$\mathcal{L}^n_\mu C^{(k)}(\mathbb{R})=\left\{x(\cdot):x(\cdot)\in C^{(k)}\left(\mathbb{R},\mathbb{R}^n\right),\max_{0\leq r\leq k}\sup_{t\in\mathbb{R}}\|x^{(r)}(t)\mu^{|t|}\|_{\mathbb{R}^n}<+\infty\right\},$$
$$\|x(\cdot)\|^{(k)}_\mu=\max_{0\leq r\leq k}\sup_{t\in\mathbb{R}}\|x^{(r)}(t)\mu^{|t|}\|_{\mathbb{R}^n},\quad k=0,1,\dots,\mu\in(0,+\infty).$$

2.1. Existence and Uniqueness Theorem for the Basic Initial-Boundary Value Problem

In terms of the parameter $\mu\in(0,1)$ and the space $\mathcal{L}^n_\mu C^{(0)}(\mathbb{R})$ we formulate a condition guaranteeing the existence and uniqueness of a solution for the initially-boundary problem.

Theorem 2.1 ([25])**:**
Let function f and diffeomorphisms $q_j(\cdot),j=1,\dots,s$, satisfy the conditions $(a)-(e)$ from the Section 2. If for some $\mu\in(0,\mu^*)\cap(0,1)$ the inequality

$$L_f\sum_{j=1}^s\mu^{-h_{q_j}}<\ln\mu^{-1},\tag{2.6}$$

is satisfied then for any fixed initial-boundary conditions $\bar x\in\mathbb{R}^n,\varphi(\cdot)\in L_\infty(\mathbb{R},\mathbb{R}^n)$ there exists a solution (absolutely continuous) $x(\cdot)\in\mathcal{L}^n_\mu C^{(0)}(\mathbb{R})$ of the basic initial-boundary value problem (2.1)-(2.3). *Such a solution is unique and, as an element of the* *space* $\mathcal{L}_\mu^n C^{(0)}(\mathbb{R})$*, depends continuously on the initial-boundary conditions* $\bar{x} \in \mathbb{R}^n, \varphi(\cdot) \in L_\infty(\mathbb{R}, \mathbb{R}^n)$ *and the right-hand side of the equation (function* $f(\cdot)$*).*

The condition (2.6) is *exact and not improvable*: there are differential equations for which violation of this condition leads to a violation of either the existence of the solution or uniqueness. Note that if the inequality (2.6) has a solution, then there are $\mu_1(L_f; h), \mu_2(L_f; h)$ such that for each solution μ the following condition holds

$$\mu_1(L_f; h) < \mu < \mu_2(L_f; h).$$

3. VARIATIONAL APPROACH TO CONSTRUCTING SOLUTIONS TO THE BASIC INITIAL-BOUNDARY VALUE PROBLEM

We study absolutely continuous solutions of the system

$$F_i(t, \dot{x}(t), x(t+\tau_1), \ldots, x(t+\tau_s)) = 0, \quad i = \overline{1,k}, \quad t \in [t_l, t_r], \tag{3.7}$$

under boundary conditions outside the system definition interval

$$\dot{x}(t) = \varphi_l(t), \quad t \in [t_{ll}, t_l], \tag{3.8}$$

$$\dot{x}(t) = \varphi_r(t), \quad t \in [t_r, t_{rr}], \tag{3.9}$$

as well as initial-boundary conditions on the system definition interval

$$K_m(\dot{x}(\xi), x(\xi_1), \ldots, x(\xi_p)) = 0, \tag{3.10}$$

where $F_i : \mathbb{R} \times \mathbb{R}^n \times \mathbb{R}^{ns} \longrightarrow \mathbb{R}^n, i = \overline{1,k}$, is a mapping of the $C^{(0)}$ class; $\tau_j \in \mathbb{Z}$, $j = \overline{1,s}$; $t_l, t_r \in \mathbb{R};\ t_{ll} = t_l + \min\{0, \tau_1, \ldots, \tau_s\},\ t_{rr} = t_r + \max\{0, \tau_1, \ldots, \tau_s\};\ \varphi_l, \varphi_r : \mathbb{R}^n \longrightarrow \mathbb{R}^n$ are mappings of the $C^{(0)}$ class, defining fixed boundary vector functions; $K_m : \mathbb{R}^n \times \mathbb{R}^{np} \longrightarrow \mathbb{R}^n, m = \overline{1,q}$, is a mapping of the $C^{(0)}$ class; $\xi, \xi_i \in [t_l, t_r], i = \overline{1,p}$, is a fixed set of points on the system definition interval.

We give a formal statement of the optimization problem induced by the initial-boundary-value problem.

Problem A. Find the trajectory $\hat{x}(t)$, which provides a minimum of residual functional

$$I(\hat{x}(t)) = v^{(N)} \left(\sum_{i=1}^{k} \int_{t_l}^{t_r} F_i^2(t, \dot{\hat{x}}(t), \hat{x}(t+\tau_1), \ldots, \hat{x}(t+\tau_s))dt + \int_{t_{ll}}^{t_l} [\dot{\hat{x}}(t) - \varphi_l(t)]^2 dt + \int_{t_r}^{t_{rr}} [\dot{\hat{x}}(t) - \varphi_r(t)]^2 dt \right) + v^{(K)} \sum_{m=1}^{q} K_m^2(\dot{\hat{x}}(\xi), \hat{x}(\xi_1), \ldots, \hat{x}(\xi_p)), \tag{3.11}$$

where $v^{(N)}, v^{(K)} \in \mathbb{R}_+$ are weighting factors.

The following statement holds.

Proposition 3.1:
Each solution to the initial-boundary value problem (3.7)-(3.10) *is a solution to the optimization Problem A.*

In particular, under the conditions of Theorem 2.1, a solution to the initial-boundary value problem (2.1)-(2.3) exists and is a solution to the corresponding Problem A. In the general case, the converse statement to Proposition 3.1 is false, but, nevertheless, taking into account the uniqueness theorem and also the stability theorem of the solution, in the case of successful construction of a numerical solution, we can speak with high confidence about constructing a solution close to analytical one.

The proposed variational approach to constructing solutions of the basic initial-boundary value problem lies at the basis of the numerical implementation of such solutions. The numerical methods themselves are based on the Ritz method and spline collocation constructions and were implemented in [23, 26]. In order to solve the problem of the class under consideration, the trajectories of the system are discretized on a grid with a constant step, and a generalized residual functional is formulated that includes both the weighted residual of the original differential equation and the residual of the boundary conditions. A spline differentiation technique is used to evaluate the derivatives of the desired trajectories of the system, based on two spline approximation designs: using cubic natural splines and using a special type of spline whose second derivatives at the edges are also controlled using optimized parameters.

3.1. Software Package OPTCON-F

A set of algorithms for local and global optimization was implemented for solving the stated finite-dimensional problems. The used technology includes: an algorithm for sequentially increasing the accuracy of approximation by multiplying the number of nodes in the grid of the discretization; algorithms for the difference evaluation of the derivatives of the functional from the first to the sixth degree of accuracy inclusive; method of successively increasing the precision of spline differentiation. The corresponding software complex (SC) *OPTCON-F* was implemented in the language *C* under the control of operating systems *OS Windows*, *OS Linux* and *Mac OS* using compilers *BCC 5.5* and *GCC*. SC was designed to obtain a numerical solution of boundary value problems, parametric identification problems and optimal control for dynamical systems described by FDEPT [27].

Among the local algorithms included in the SC *OPTCON-F* there are: 1) PARTAN method; 2) Powell-Brent's method; 3) gradient method of confidence intervals; 4) Barzilai-Borwein method; 5) Newton's method with the difference estimate of the Hessian matrix; 6) generalized quasi-Newtonian method; 7) direct-dual method of gradient descent; 8) differential Euler optimization method of the 2nd order; 9) differential Adams optimization method of the 4th order and others.

As algorithms of "closers" there are: 1) adaptive modification of the Hooke-Jeeves method; 2) stochastic search methods in random subspaces of the indicated (2, 3, 4, or 5) dimension; 3) local version of the curvilinear search method.

Non-local algorithms that form the basis of the SC are: 1) "parabolic" method – a combination of coordinate-wise descent with a periodic multistart and a non-local one-dimensional search by the parabola algorithm; 2) non-local method of curvilinear search; 3) Luus-Jaakola method; 4) "forest" method – multivariant adaptive method of random multistart and others.

As part of the work on the SC, taking into account the specifics related to the qualitative properties of FDEPT, the following key results were obtained:

- **Algorithm of construction of "controllable splines" has been developed**. The problem of obtaining a high-precision approximation to the derivative of a function of one variable over a set of values of the function itself, defined on a fixed grid, was investigated. The performed computational experiments showed that in order to achieve good accuracy in estimating derived trajectories for FDEPT systems, it is not possible to use known types of splines ("natural", with additional boundary conditions, Akima splines, etc.). The proposed algorithm is based on the use of derivatives of cubic spline functions.
- **A technology has been developed for approximation of general FDEPT systems using a finite-dimensional unconditional minimization problem**. By analyzing the

behavior of homeomorphisms on the initial (main) time interval, an extended time interval is calculated, for which the discretized grid is constructed. To approximate the initial continuous problem on a fixed grid over time, the Ritz method is used: the trajectories are approximated using controlled spline functions, the coefficients of which are selected by searching for the minimum of the residual functional.

- **A specialized global optimization algorithm was developed, based on the idea of curvilinear search**. To search for the minimum of the non-convex residual functional, a specialized global optimization algorithm has been developed, based on the idea of curvilinear search on the reachable set of a control system produced using a pair of randomly generated "support" controls. Using the property of connectedness, variations in the space of control functions that do not violate the existing constraints are constructed at iterations of the algorithm. This is achieved by direct projection on a parallelepiped. To improve the current approximation, a modification of a non-local one-dimensional search algorithm based on the "parabolic" method is applied [28]. Also, as a globalizing mechanism, a non-local search in random directions is used, repeated many times at each iteration of the algorithm. To solve auxiliary non-convex problems of one-dimensional search, a modification of the stochastic P-algorithm, proposed by A. Zhigljavsky and A. Žilinskas [14], is implemented [29]. To enhance reliability of the proposed method, a periodic random multi-start was provided in the algorithm's construction.
- **An algorithm for the numerical integration of FDEPT systems based on the sequential discretization technique has been developed**. To improve the efficiency of calculations, tools have been implemented to build a sequence of approximative finite-dimensional optimization problems with a growing number of variables. At the same time, solutions obtained at the previous stages of calculations performed on the current discretization grid are projected onto a new grid with an increased number of nodes while preserving the qualitative and quantitative characteristics of the trajectories.
- **The proposed numerical algorithms were tested on a wide range of tasks [27]** with using the principle of "the best of known solutions" [30]. In all considered problems, the proposed algorithm allowed us to find the best known solution. The calculation experiments that have been carried out demonstrate considerably high fidelity of the proposed algorithms.

The above heuristic search algorithm for the solution $\hat{x}(t)$ can be justified on the basis of the existence and uniqueness theorems for initial-boundary value problems for the investigated FDEPT, as well as theorems on approximating solutions of such equations on the whole line by solutions of the initial-boundary value problem on a sequence of expanding intervals. A description of such equations and corresponding results are presented in the following sections.

4. EXISTENCE AND UNIQUENESS THEOREM FOR SOLITON SOLUTIONS IN THE PROBLEM OF LONGITUDINAL VIBRATIONS OF AN INFINITE HOMOGENEOUS ROD

We consider a problem from the theory of plastic deformation, in which solutions of the traveling wave type for the following system are studied

$$m\ddot{y}_i(t) = y_{i+1}(t) - 2y_i(t) + y_{i-1}(t) + \Phi(y_i(t)),\ i \in \mathbb{Z},\ y_i \in \mathbb{R},\ t \in \mathbb{R}, \quad (4.12)$$
$$y_i(t+\tau) = y_{i+1}(t), \quad \tau \geq 0. \quad (4.13)$$

We will study such a system under the most weak conditions on the potential $\Phi(\cdot)$ in the form of the Lipschitz condition. The Lipschitz constant will be denoted by L_Φ. We formulate a theorem on the existence and uniqueness of a traveling wave type solution (soliton solution),

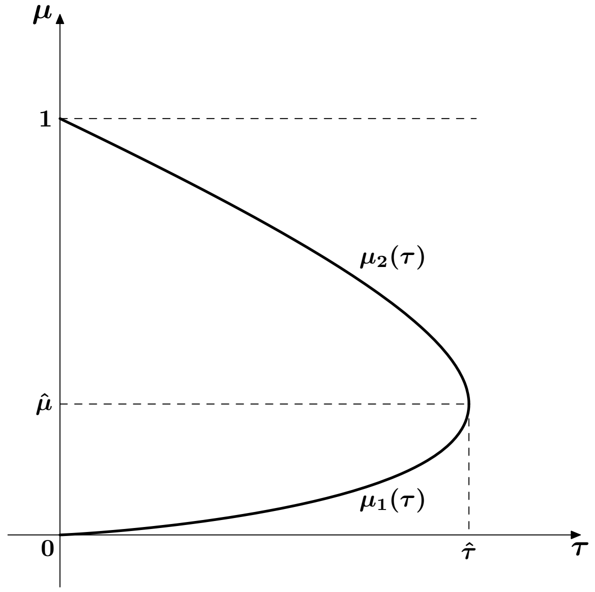


Fig. 4.1. Graphs of functions $\mu_1(\tau), \mu_2(\tau)$

based on the correspondence of traveling-wave type solutions of the infinite-dimensional system (4.12)-(4.13) to the solutions of the induced FDEPT [24], reduced to a first-order system

$$\begin{aligned} &\dot{x}_1(t) = x_2(t), \quad x \in \mathbb{R}^2, \quad x = (x_1, x_2)', \quad t \in \mathbb{R}, \\ &\dot{x}_2(t) = m^{-1}\big(x_1(t+\tau) - 2x_1(t) + x_1(t-\tau) + \Phi(x_1(t))\big), \end{aligned} \tag{4.14}$$

as well as the existence and uniqueness theorem for solutions to such equations (Theorem 2.1).

To do this, we consider a transcendental equation with respect to two variables $\tau \in [0, +\infty)$ and $\mu \in (0, 1)$

$$C\tau\left(2\mu^{-1} + 1\right) = \ln \mu^{-1}, \tag{4.15}$$

where

$$C = \max\{1; 2m^{-1}\sqrt{L_\Phi^2 + 2}\}.$$

The set of solutions of the equation (4.15) is described by functions $\mu_1(\tau), \mu_2(\tau)$ given in Fig. 4.1.

If we denote the right-hand side of the system (4.14) by f, then relations $\mu_1(L_f; h) = \sqrt[\tau]{\mu_1(\tau)}$ and $\mu_2(L_f; h) = \sqrt[\tau]{\mu_2(\tau)}$ will be valid, where $L_f = C, h = (\tau, \tau)$.

For each $\mu \in (0, 1)$ we define the phase space of the infinite-dimensional equation (4.12)as a Hilbert space of sequences with the corresponding norm

$$\mathcal{K}^2_{\mathbb{Z}2\mu} = \{\kappa : \kappa = \{z_i\}_{-\infty}^{+\infty}, \quad z_i \in \mathbb{R}^2, \quad i \in \mathbb{Z}, \quad \sum_{i\in\mathbb{Z}} \|z_i\|^2_{\mathbb{R}^2} \mu^{2|i|} < +\infty\}.$$

Theorem 4.1 ([24]):
Let the potential Φ satisfy the Lipschitz condition with constant L_Φ. Then, for any initial values $\bar{i} \in \mathbb{Z}, a, b \in \mathbb{R}, \bar{t} \in \mathbb{R}$, and characteristics $\tau > 0$ satisfying the condition

$$0 < \tau < \hat{\tau},$$

for the initial system of differential equations (4.12) *there exists a unique solution of the traveling wave type* $\{y_i(\cdot)\}_{-\infty}^{+\infty}$ *with characteristic* τ *such that it satisfies the initial conditions* $y_{\bar{i}}(\bar{t}) = a, \dot{y}_{\bar{i}}(\bar{t}) = b$. *For any parameter* $\mu \in (\mu_1(\tau), \mu_2(\tau))$ *the vector function*

$$\omega(t) = \{(y_i(t), \dot{y}_i(t))'\}_{-\infty}^{+\infty}$$

belongs to the space $\mathcal{K}^2_{\mathbb{Z}2\mu}$ *for any* $t \in \mathbb{R}$, *and the function*

$$\rho(t) = \|\omega(t)\|_{2\mu}$$

belongs to the space $\mathcal{L}^1_{\sqrt[\tau]{\mu}} C^{(1)}(\mathbb{R})$. *Such a solution depends continuously on the initial values* $a, b \in \mathbb{R}$, *as well as on the mass* m.

Theorem 4.1 not only guarantees the existence of a solution but also determines the limitation of its possible growth both in time t and in coordinates $i \in \mathbb{Z}$ (over space). It is obvious that for each $0 < \tau < \hat{\tau}$ the space $\mathcal{K}^2_{\mathbb{Z}2(\mu_2(\tau)-\varepsilon)}$, for small $\varepsilon > 0$, is much narrower than the space $\mathcal{K}^2_{\mathbb{Z}2(\mu_1(\tau)+\varepsilon)}$. The theorem guarantees the existence of a solution in narrower spaces and uniqueness in wider spaces.

5. APPROXIMATION OF THE SOLUTION OF A FUNCTIONAL DIFFERENTIAL EQUATION DEFINED ON THE LINE BY SOLUTIONS OF AN INITIAL-BOUNDARY VALUE PROBLEM WITH EXPANDING INTERVALS OF THE DEFINITION

Next, we consider soliton solutions of the system, which will be implemented as solutions of the induced functional differential equations defined on the whole line. For the numerical integration of such an equation, one should be able to approximate the solutions of such an equation by the solutions of initial-boundary value problems defined on an expanding family of finite intervals. This section is devoted to this problem.

Let's consider the initial boundary value problem

$$\dot{x}(t) = f(t, x(t + \tau_1), \ldots, x(t + \tau_s)), \quad t \in B_R, \tag{5.16}$$
$$\dot{x}(t) = \varphi(t), \quad t \in \mathbb{R}\backslash B_R, \quad \varphi(\cdot) \in L_\infty(\mathbb{R}, \mathbb{R}^n), \tag{5.17}$$
$$x(\bar{t}) = \bar{x}, \quad \bar{t} \in \mathbb{R}, \quad \bar{x} \in \mathbb{R}^n, \tag{5.18}$$

where $\tau_j \in \mathbb{R}$. We formulate again the theorem on the continuous dependence on the initial-boundary conditions. We define a Banach space of functions with weight

$$\mathcal{L}^n_\mu L_\infty(\mathbb{R}) = \left\{ \varphi(\cdot) : \varphi(\cdot) \in L_\infty(\mathbb{R}, \mathbb{R}^n), \sup_{t\in\mathbb{R}} vrai \|\varphi(t)\mu^{|t|}\|_{\mathbb{R}^n} < +\infty \right\}, \quad \mu \in (0, 1)$$

and norm

$$\|\varphi(\cdot)\|_\mu = \sup_{t\in\mathbb{R}} vrai \|\varphi(t)\mu^{|t|}\|_{\mathbb{R}^n}.$$

If in the boundary condition (5.17), starting with some sufficiently large $k \in \mathbb{Z}_+$ with the condition $B_R \subset [-k, k]$, the boundary condition $\varphi(\cdot) \in L_\infty(\mathbb{R})$ replace outside the interval $B_R \subset [-k, k]$ so that the new boundary function $\tilde{\varphi}(\cdot)$ satisfies the condition $\tilde{\varphi}(\cdot) \in \mathcal{L}^n_\mu L_\infty(\mathbb{R})$, then the corresponding solution $\tilde{x}(\cdot)$ of the boundary value problem on $B_R \subset [-k, k]$ will match the original solution $x(\cdot)$.

We are going to formulate a proposition on the approximation of solutions of an initial-boundary value problem defined on the whole line by solutions of the initial-boundary value problem defined on the interval $[-k, k]$ as $k \to +\infty$. We consider the initial-boundary value problem on the whole line $B_R = \mathbb{R}$

$$\dot{x}(t) = f(t, x(t+\tau_1), \ldots, x(t+\tau_s)), \quad t \in \mathbb{R}, \tag{5.19}$$
$$x(\bar{t}) = \bar{x}, \quad \bar{t} \in \mathbb{R}, \quad \bar{x} \in \mathbb{R}^n, \tag{5.20}$$

where $\tau_j \in \mathbb{R}, j = 1, \ldots, s, j = 1, \ldots, s$. For each $k \in \mathbb{Z}$ we consider the initial-boundary value problem on a finite interval $B_R = [-k, k]$

$$\dot{x}(t) = f(t, x(t+\tau_1), \ldots, x(t+\tau_s)), \quad t \in [-k, k], \tag{5.21}$$
$$\dot{x}(t) = \varphi(t), \quad t \in \mathbb{R}\backslash[-k, k], \quad \varphi(\cdot) \in \mathcal{L}_1^n L_\infty(\mathbb{R}), \tag{5.22}$$
$$x(\bar{t}) = \bar{x}, \quad \bar{t} \in \mathbb{R}, \quad \bar{x} \in \mathbb{R}^n. \tag{5.23}$$

Theorem 5.1 ([31]):
Let the map $f(\cdot)$ satisfies the conditions $(a) - (d)$. If for $\mu \in (0, \mu^\star) \cap (0, 1)$ the inequality

$$L_f \sum_{j=1}^{s} \mu^{-|\tau_j|} < \ln \mu^{-1} \tag{5.24}$$

holds, and $(\mu_1(L_f; h), \mu_2(L_f; h))$ is the maximum solution interval for the inequality (5.24)*, then for any $\bar{x} \in \mathbb{R}^n, \varphi(\cdot) \in \mathcal{L}_1^n L_\infty(\mathbb{R})$, the solution $\hat{x}(\cdot)$ of the initial-boundary value problem* (5.19)-(5.20)*, as an element of the space $\mathcal{L}_\mu^n C^{(0)}(\mathbb{R})$, is approximated by solutions $\hat{x}_k(\cdot)$ of the initial-boundary value problem* (5.21)–(5.23) *as $k \to +\infty$. Moreover, for any arbitrarily small ε, $0 < \varepsilon < \mu_2 - \mu_1$ there is $C_{f\varphi\varepsilon}$ such that the following estimate is true*

$$\|\hat{x}(\cdot) - \hat{x}_k(\cdot)\|_\mu^{(0)} \le C_{f\varphi\varepsilon} \left(\frac{\mu_1(L_f; h)}{\mu_2(L_f; h) - \varepsilon} \right)^k .$$

From the estimate it follows that the convergence rate will be the higher, the more the $\mu_1(L_f; h)$ and $\mu_2(L_f; h)$ values will differ from each other, the difference between them is inversely proportional to the value of $L_f \max_{1 \le j \le s} |\tau_j|$.

6. CONSTRUCTION OF THE COMPLETE FAMILY OF TRAVELING WAVE TYPE SOLUTIONS IN THE FRENKEL-KONTOROVA MODEL

Considering periodic functionals for the model from the section 4, we obtain the Frenkel-Kontorova model from the theory of plastic deformation. In this case, taking the functional $\Phi(y) = A\sin(By), A, B \in \mathbb{R}$

$$m\ddot{y}_i(t) = y_{i+1}(t) - 2y_i(t) + y_{i-1}(t) + Asin(By_i(t)),\ i \in \mathbb{Z},\ y_i \in \mathbb{R},\ t \in \mathbb{R}, \tag{6.25}$$
$$y_i(t+\tau) = y_{i+1}(t), \quad \tau > 0, \tag{6.26}$$

we construct solutions of the traveling wave type with characteristic τ. As noted earlier, the space of traveling wave type solutions for such a system coincides with the space of solutions of the FDEPT system

$$\begin{aligned} \dot{x_1}(t) &= \tau x_2(t), \quad t \in \mathbb{R}, \\ \dot{x_2}(t) &= \tau m^{-1}[x_1(t+1) - 2x_1(t) + x_1(t-1) + A\sin(Bx_1(t))]. \end{aligned} \tag{6.27}$$

Moreover, there is a correspondence of solutions according to the rule

$$y_i(t) = x(\tau^{-1}t + i).$$

We will construct numerical solutions of the system (6.27) using the approximation Theorem 5.1.

6.1. Numerical experiments

Next, the results of the computational experiments on the study of initial-boundary value problems for systems of FDEPT using *OPTCON-F* software will be presented. Before demonstrating the examples, it is necessary to make a number of significant observations:

(a) in the SC *OPTCON-F*, the possibility of satisfying the condition of uniform boundedness of the derivative is realized. The maximum deviation from zero is determined by the Lipschitz constant of the right side of the equation, by the parameter μ, and also by the deviations of the argument;

(b) numerical integration on an interval with initial-boundary conditions is realized as an integration process with given boundary conditions at the left end and procedures for minimizing deviations from the boundary conditions at the right end for the solution constructed with observance of the restrictions from the preceding item;

(c) in the obtained theorem on approximating solutions of the original equation on the whole line by solutions on expanding finite intervals $[-k, k]$, the only restriction on the boundary conditions themselves is the condition for their uniform boundedness. In particular, we choose the zero boundary condition;

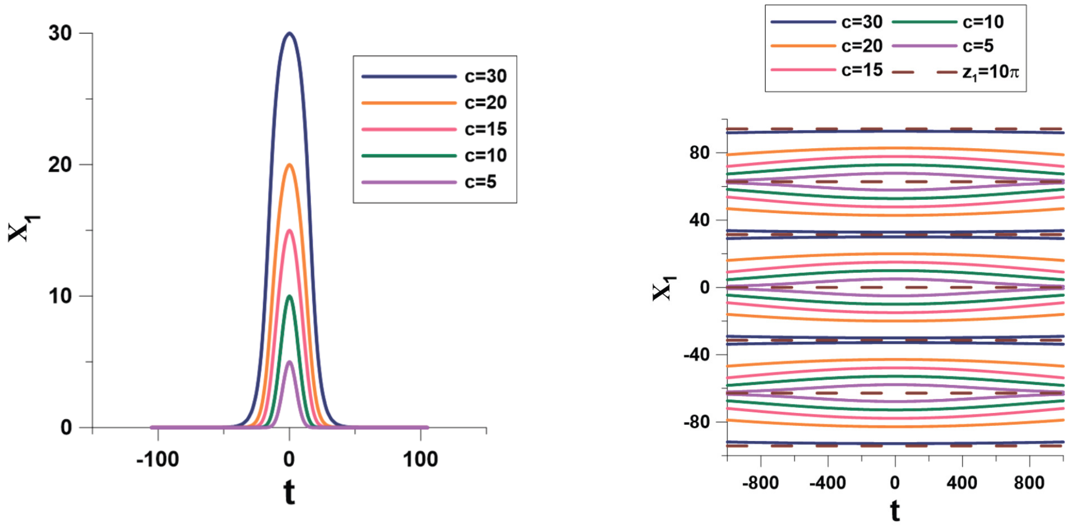
(d) we note that the obtained condition for the existence of a solution of the traveling wave type is just a sufficient condition. Therefore, solutions of the traveling wave type can also be numerically constructed for $\tau > \hat{\tau}$. Nevertheless, many of the central conditions of the presented theory are "exact", that is, there are examples of equations for which violation of the indicated conditions leads to the lack of solutions;

(e) in the SC *OPTCON-F* there is the possibility of sequential application of various algorithms within the framework of constructing a solution for one task. Thus, the constructed intermediate solution in the previous step becomes the starting solution ("baseline") for the following algorithm. In this case, such an implementation does not prevent the global search algorithms from "popping out" of the local solution. Separately, we note the presence of a programming module that allows predetermining the order of application of algorithms, as well as the construction of complex chain of steps (conditional statements, loops, etc.) depending on the current or historical values of a number parameters (for example, error estimation or number of iterations). For the examples presented below, in addition to the basic global optimization algorithm described in Section 1, the following scheme was used in cycle: the generalized quasi-Newtonian and Powell-Brent's methods (with bi-directional line search along each dimension) were used alternately, and after the error changed by less than 10^{-p} the adaptive modification of the Hooke-Jeeves method was used l times (p and l are computable functions on the basis of the loop iteration number, as well as the Lipschitz constants of the equation itself and a number of other technical characteristics). The stopping criterion depended on the number of iterations in the first part of the cycle, as well as the current error estimate and its dynamics;

(f) in view of all the points listed above, as well as stochastic elements in the applied algorithms, the presented value of the residual functional (RF, i.e. error of a numerical solution) can not be used to estimate the theoretical rate of convergence.

We consider dynamical system in the following form:

$$\begin{cases} \dot{x}_1(t) = 0.15x_2(t), \\ \dot{x}_2(t) = 0.15 \times 100^{-1}(x_1(t+1) - 2x_1(t) + x_1(t-1) + 500\sin(0.1x_1(t))), \end{cases}$$
$$t \in \mathbb{R}, \tag{6.28}$$
initial conditions
$$\begin{cases} x_1(0) = c, \\ x_2(0) = 0. \end{cases}$$



(a) Trajectories of $x_1(t)$ for the system (6.29)

(b) Trajectories of $x_1(t)$ for the system (6.28)

Fig. 6.2. Trajectories of $x_1(t)$ at different c

Here, with respect to the system (6.27), we have $A = 500, B = 0.1, \tau = 0.15, m = 100$, and the equality (4.15) takes the form

$$0.003\sqrt{2502}(2\mu^{-1} + 1) = \ln \mu^{-1}$$

and has on the interval $(0, 1)$ two solutions with approximate values $\mu_1(0.15) = 0,22$ and $\mu_2(0.15) = 0,424191$ (the exact values are expressed in terms of the Lambert W-function and can't be written out in quadratures).

Taking into account the impossibility of considering the numerical solution of the system on an infinite interval, we introduce the parameter k and the corresponding family of expanding initial-boundary value problems

$$\begin{cases} \dot{x}_1(t) = 0.15x_2(t), \\ \dot{x}_2(t) = 0.15 \times 100^{-1}(x_1(t+1) - 2x_1(t) + x_1(t-1) + 500\sin(0.1x_1(t))), \end{cases}$$

$t \in [-k, k]$,

boundary conditions

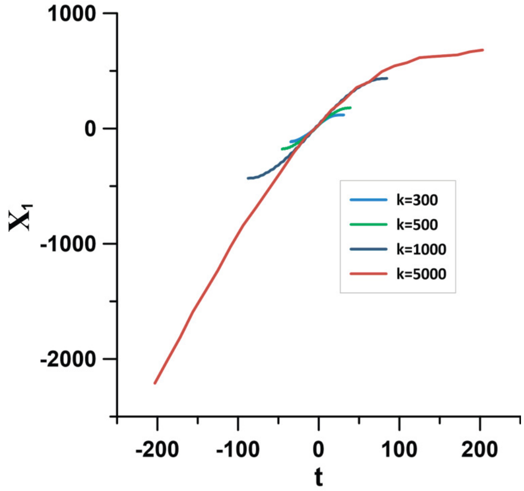
$$\begin{cases} \dot{x}_1(t) = 0, \\ \dot{x}_2(t) = 0, \end{cases} \quad t \in (-\infty, -k] \cup [k, +\infty), \tag{6.29}$$

initial conditions

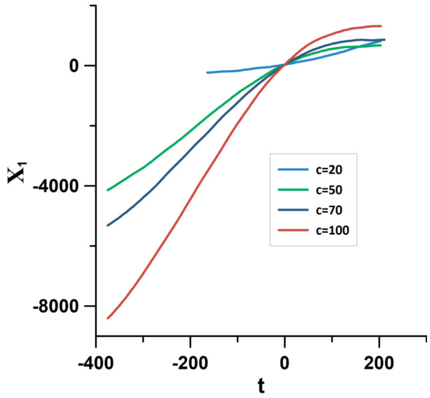
$$\begin{cases} x_1(0) = c, \\ x_2(0) = 0. \end{cases}$$

According to the Theorem 5.1, convergence is guaranteed under any given essentially bounded boundary conditions. In the system (6.29), the simplest boundary function is chosen, the identity zero. Thus, the solution of the system (6.29) converges (according to the metric of the space $\mathcal{L}^n_\mu C^{(0)}(\mathbb{R})$ for $\mu \in (\mu_1(0.15), \mu_2(0.15))$) to the solution of the system (6.28) as $k \to \infty$.

Since the equation (6.27) is autonomous, the solution space of such equation is invariant with respect to time-variable shifts. On the other hand, from the periodicity of the right-hand side with respect to the $x_1(t)$ it follows that the solution space of such equation is invariant



(a) Trajectories of $x_1(t)$ at different k



(b) Trajectories of $x_1(t)$ at different c

Fig. 6.3. Unbounded trajectories of $x_1(t)$

with respect to a shift in $x_1(t)$ for a period equal to $\frac{2\pi}{B}$. Therefore, it suffices to consider a family of solutions of the initial system (6.28) with a value of initial conditions $x_1(0)$ from zero to the value of the period. Nevertheless, the stationary solutions $x_1(t)$ are repeated each half-period $\frac{\pi}{B}$. Since the right-hand side of the equation is an odd function with respect to the $x_1(t)$, the solution space of such equation can withstand the reflection transformation with respect to the axis t. Hence, it is sufficient to construct trajectories $x_1(t)$ in the strip from zero to the half-period. Figure 6.2 shows the graphs $x_1(t)$ for different values of the parameter $c = x_1(0)$ for both the system (6.29) and the initial system (6.28) (the values of c are reduced to half-period). Note that Fig. 6.2 shows the complete family of bounded graphs $x_1(t)$ (up to the above transformations) from the space $\mathcal{L}_\mu^n C^{(0)}(\mathbb{R})$ for $\mu \in (\mu_1(0.15), \mu_2(0.15))$.

At the same time, for some initial conditions, there are only unbounded $x_1(t)$. Figure 6.3a demonstrates the evolution of such an unbounded graph $x_1(t)$ with increasing k for the initial conditions $x_1(0) = \frac{\pi}{B}, x_2(0) = 50$. Figure 6.3b, in turn, shows a one-parameter family of unbounded graphs $x_1(t)$ for $x_1(0) = \frac{\pi}{B}$ and different values of $x_2(0) = c$.

7. CONCLUSION

The construction of numerical solutions of the traveling wave type for the Frenkel-Kontorova model on the propagation of longitudinal waves using the developed software package was demonstrated. For this model, a complete family of traveling wave solutions was constructed.

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