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SOLVING NUMERICALLY EQUATIONS OF EXTREMALS OF VARIATIONAL PROBLEM WITH CONSTRAINTS

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1. Introduction

The known variational problem with constraints (see [1]) consists of the determination of extremals of the functional

$$I=\int_{t_0}^{t_1} L(q,v,t)dt,\quad q=(q_1,\dots,q_n),\quad v=(v_1,\dots,v_n),\quad v_i=\dot q_i=\frac{dq_i}{dt},\quad i=1,\dots,n, \tag{1.1}$$

$$q(t_0)=q^0,\quad q(t_1)=q^1, \tag{1.2}$$

$$f(q,t)=0,\quad f'(q,v,t)=0,\quad f=(f_1,\dots,f_m),\quad f'=(f_{m+1},\dots,f_r),\quad r\le n, \tag{1.3}$$

and can be reduced to the determination of a vector function $q=q(t)$ satisfying simultaneously boundary conditions (1.2), constraint equations (1.3), and the Euler–Lagrange equations

$$\dot q=v,\quad \frac{d}{dt}\frac{\partial L}{\partial v}-\frac{\partial L}{\partial q}=F^T\lambda, \tag{1.4}$$

$$\frac{\partial L}{\partial q}=\left(\frac{\partial L}{\partial q_1},\dots,\frac{\partial L}{\partial q_n}\right),\quad F=(f_{\rho i}),\quad F^T=(f_{i\rho}),\quad f_{\mu i}=\frac{\partial f_\mu}{\partial q_i},\quad f_{\sigma i}=\frac{\partial f_\sigma}{\partial v_i},$$
$$\rho=1,\dots,r,\quad \mu=1,\dots,m,\quad \sigma=m+1,\dots,r.$$

System (1.4) contains the vector of the Lagrange factors $\lambda=(\lambda_1,\dots,\lambda_r)$, which is to be determined via the conditions $\ddot f=0$, $\dot f'=0$. In addition, the manifold $\Omega(t)$ in the space of variables (q,v), which is described by the equations

$$f(q,t)=0,\quad \dot f(q,v,t)=0,\quad f'(q,v,t)=0, \tag{1.5}$$
$$\dot f(q,v,t)\equiv f_q v+f_t,\quad f_q=(f_{\mu i}), f_t=(f_{\mu t}),\quad \mu=1,\dots,m,\quad i=1,\dots,n,$$

is a stable integral manifold of system (1.3), (1.4). However, it is not asymptotically stable and in the numerical solving the system of equations (1.3), (1.4) the deviations from the manifold $\Omega(t)$ will increase as a consequence of errors of the numerical integration.

Equations (1.3), (1.4) compose the system of differential-algebraic equations of index three (DAE-3). The index of the system of DAE is defined (see [2]) by the number exceeding by one the order of the maximal derivative of the constraint equations (1.3), which is necessary for the exclusion of the vector λ from the Euler–Lagrange equations. Recently, the DAE turned to be a subject of intensive investigations (see [2], [3]). The basic problem of these investigations is the provision of an asymptotic stability for the integral manifold $\Omega(t)$. The conditions of stability of

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the integral manifold DAE-2 were formulated in [4]. Possible deviations from constraint equations (1.3), which appear in the numerical solving system (1.3), (1.4), can be bounded. To this end, in Section 2 we introduce the necessary definitions and suggest a method for composing the Euler–Lagrange equations, which makes it possible to restrict the deviations from the constraint equations in the numerical solving the system consisting of equations of extremals and constraint equations. In Section 3 we construct an algorithm of reduction of the system of DAE-3 to a system of DAE-2. In Section 4 we state the conditions of the asymptotic stability of the manifold $\Omega(t)$. Finally, in Section 5 we define conditions which ensure its stability in the numerical solving the DAE-2 by the Euler method and by the Runge–Kutta method.

2. Equations of extremals

During solving system (1.3), (1.4) the constraint equations may turn to be violated even at the initial moment. If we assume that the vector λ is determined via the conditions $\ddot{f} = 0$, $\dot{f}' = 0$, and solve numerically the system of differential equations (1.4) with the initial conditions $q(t_0) = q^0$, $v(t_0) = v^0$, then it may happen that with $t = t_0$ conditions (1.5) will be violated:

$$f(q^0, t_0) = f^0, \quad \dot{f}(q^0, v^0, t_0) = \dot{f}^0, \quad f'(q^0, v^0, t_0) = f'^0.$$

Even if the initial data satisfy exactly equations (1.5), the posterior accumulation of errors of the numerical integration will inevitably lead us to the growth of deviations from the constraint equations. By means of introduction of the corresponding correction into the difference scheme for solving system (1.3), (1.4), the deviations from the constraint equations (1.3) can be restricted. In order to estimate the deviations from equations (1.5) we write the constraint equations in the form of the equalities

$$f_\mu(q, t) = \alpha_\mu, \quad \dot{f}_\mu(q, v, t) = \alpha_{m+\mu}, \quad f_\sigma(q, v, t) = \alpha_{m+\sigma}. \tag{2.1}$$

The right-hand sides of equations (2.1) are chosen as the solutions $\alpha_\gamma = \alpha_\gamma(t)$ of the differential equations

$$\dot{\alpha}_\gamma = \varphi_\gamma(\alpha, q, v, t), \quad \varphi_\mu = \alpha_{m+\mu}, \quad \alpha = (\alpha_1, \dots, \alpha_{m+r}), \quad \varphi_\gamma(0, q, v, t) = 0, \quad \gamma = 1, \dots, m + r, \tag{2.2}$$

which are considered together with the equations of extremals (1.4) and satisfy the initial conditions

$$q_i(t_0) = q_i^0, \quad v_i(t_0) = v_i^0, \quad \alpha_\mu(t_0) = f_\mu^0, \quad \alpha_{m+\mu}(t_0) = \dot{f}_\mu^0, \quad \alpha_{m+\sigma}(t_0) = f_\sigma^0, \tag{2.3}$$
$$f_\mu^0 = f_\mu(q^0, t_0), \quad \dot{f}_\mu^0 = \sum_{i=1}^n f_{\mu i}(q^0, t_0) v_i^0 + f_{\mu t}(q^0, t_0), \quad f_\sigma^0 = f_\sigma(q^0, v^0, t_0).$$

The right-hand sides of system (2.2) can be chosen so that its trivial solution $\alpha_1 = \dots = \alpha_{r+m} = 0$ be asymptotically stable (see [4]). However, even in this case the deviations from the constraint equations within the numerical integration of equations (1.4), (2.2) can increase (see [2]). The stabilization of the constraint equations (1.3) in the numerical integration can be ensured at the expense of constraints imposed upon the right-hand sides of equations of system (2.2). In what follows we will prove that the use of constraint equations (2.1), (2.2) does not change the structure of equations (1.4); however, it leads us to change of the expressions of the vector λ which is composed by the Lagrange factors.

Definition 1. Conditions (2.1) imposed upon the functions $q_1(t), \dots, q_n(t)$ and their derivatives $v_1(t), \dots, v_n(t)$, are called *equations of program constraints*, while conditions (2.2) satisfied by their right-hand sides $\alpha_1(t), \dots, \alpha_{m+r}(t)$, — *equations of perturbation of constraints.*

Definition 2. The integral manifold $\Omega(t)$ of system (1.4), described by equations (1.5), is called a *stable integral manifold* if, for any ε, a δ exists such that for all initial values (2.3) which satisfy the condition $\|\alpha^0\| \le \delta$, for all $t > t_0$ the inequality will be valid $\|\alpha(t)\| \le \varepsilon$; we will use the term an *asymptotically integral manifold* if it is stable and $\lim\limits_{t\to\infty} \|\alpha(t)\| = 0$.

Theorem 1. *In order for the functions* $q_i = q_i(t)$, $i = 1, \dots, n$, *to determine the extremals of functional* (1.1) *under constraints* (1.3), (2.3), $f^0_\mu = f^0_\mu = 0$, $\mu = 1, \dots, m$, $f^0_\sigma = 0$, $\sigma = m+1, \dots, r$, *it is necessary that they satisfy the system of equations* (1.4), (2.1), (2.2).

Proof. The stationarity condition

$$\delta \int_{t_0}^{t_1} (L + \lambda^T \widehat{f})dt = 0, \quad \widehat{f} = (f_1, \dots, f_r),$$

of functional (1.1) on the extremals satisfying conditions (2.1), (2.2), leads us to the known inequality

$$\int_{t_0}^{t_1} (\delta L + \lambda^T \delta \widehat{f})dt = 0. \tag{2.4}$$

The expression for the vector λ is determined by the technique of varying the functions f_μ and f_σ. Let us put (see [5]):

$$\delta f_\mu = \sum_{i=1}^n \frac{\partial f_\mu}{\partial q_i}\delta q_i, \quad \delta f_\sigma = \sum_{i=1}^n \frac{\partial f_\sigma}{\partial v_i}\delta q_i. \tag{2.5}$$

Then, taking into account conditions (2.5), equalities $\delta q(t_0) = \delta q(t_1) = 0$, we obtain

$$\delta L = E^T(L)\delta q, \quad E(L) = \frac{d}{dt}\frac{\partial L}{\partial v} - \frac{\partial L}{\partial q},$$

and, taking into account the notation in (1.4), we represent equality (2.4) in the form

$$\int_{t_0}^{t_1} (-E^T(L) + \lambda^T F)\delta q \, dt = 0. \tag{2.6}$$

Condition (2.6) is fulfilled if

$$(E^T(L) - \lambda^T F)\delta q = 0. \tag{2.7}$$

From (2.1), (2.5) the equality follows

$$F\delta q = \delta\widehat{\alpha}, \quad \widehat{\alpha} = (\alpha_1, \dots, \alpha_m, \alpha_{2m+1}, \dots, \alpha_{m+r}), \tag{2.8}$$

which represents a system of linear algebraic equations with respect to the components of the vector δq with a rectangular matrix of coefficients. It was proved in [6] that the general solution of equation (2.8) is determined by the expression

$$\delta q = [FC]\delta s + F^+\delta\widehat{\alpha}, \tag{2.9}$$

where $[FC]$ is the vector product of the vectors $f_{1q}, \dots, f_{mq}, f_{m+1v}, \dots, f_{rv}$, which form the rows of the matrix F and arbitrary vectors $c_{r+1}, \dots, c_{n-1}$, which compose the matrix $C = (c_{\beta i})$, $\beta = r+1, \dots, n-1$, $F^+ = F^T(FF^T)^{-1}$, δs is an arbitrary small scalar value. The component a_{1k} of the vector product $a_1 = [a_2 a_3 \dots a_n]$ is calculated as the value of the determinant whose first row is composed by zeros except for unit at the k-th place; remaining rows are components of the vectors $a_2, a_3, \dots, a_n$.

By substituting the value (2.9) into (2.7) and taking into account the identities $F[FC] \equiv 0$, $FF^+ \equiv I_r$, where I_r is the unit matrix of order r, we obtain

$$E^T(L)[FC]\delta s + (E^T(L)F^+ - \lambda^T I_r)\delta\widehat{\alpha} = 0. \tag{2.10}$$

Since both the scalar δs and the vector $\delta\widehat{\alpha}$ are arbitrary, from (2.10) the equalities follow

$$E(L) = F^T k, \quad k = \lambda, \tag{2.11}$$

which are equivalent to system of equations (1.4).

Thus, if the functions $q_i = q_i(t)$, $i = 1, \dots, n$, satisfying the initial conditions (2.3), are extremals of functional (1.1), then they must represent the corresponding solution of system of equations (2.11) with the vector λ, defined via equalities (2.1), (2.2).

3. Reducing DAE-3 to system of DAE-2

System of equations (2.1)–(2.3), (2.11) represents a system of DAE-3. With an appropriate choice of the vector λ by means of a change of variables the DAE-3 can be reduced to a system of DAE-2 which can be reduced to a system of first order differential equations, which admits particular integrals determined by constraint equations (1.5).

Theorem 2. *System* (2.11) *with the vector* $\lambda = \lambda(q, v, t)$ *determined with regard for* (2.1), (2.2), *can be represented by the system of first order differential equations*

$$\dot{x} = v^{\tau}(x, t) + J(x, t) g(x, t), \tag{3.1}$$

which admits the particular integrals

$$g(x, t) = 0, \quad g = (f_1, \dots, f_m, \dot{f}_1, \dots, \dot{f}_m, f_{m+1}, \dots, f_r). \tag{3.2}$$

Proof. Let us calculate the expression in the left-hand side of equation (2.11) and then represent system (1.4) in the form

$$\frac{dq}{dt} = v, \quad \frac{dv}{dt} = M^{-1}(F^T\lambda - \gamma), \tag{3.3}$$

$$M = (m_{jh}), \quad m_{jh} = \frac{\partial^2 L}{\partial v_j \partial v_h}, \quad j, h = 1, \dots, n,$$

$$\gamma = (\gamma_1, \dots, \gamma_n), \quad \gamma_h = \sum_{j=1}^{n} \frac{\partial^2 L}{\partial v_h \partial q_j} v_j + \frac{\partial^2 L}{\partial v_h \partial t} - \frac{\partial L}{\partial q_h}.$$

In particular, if $L = \frac{1}{2} v^T M v - V(q)$, $m_{jh} = m_{jh}(q)$, $j, h = 1, \dots, n$ (see [5]), then

$$\gamma_h = \sum_{k,j=1}^{n} \gamma_{kj,h} v_k v_j - \frac{\partial V}{\partial q_h}, \quad \gamma_{kj,h} = \frac{1}{2}(m_{hk,j} + m_{jh,k} - m_{kj,h}), \quad m_{jh,s} = \frac{\partial m_{jh}}{\partial q_s}.$$

Let us write system of equations (2.1)–(2.2) as follows

$$f(q, t) = y, \quad \dot{f}(q, v, t) = \dot{y}, \quad f'(q, v, t) = y', \tag{3.4}$$

$$\frac{dy}{dt} = \dot{y}, \quad \frac{d\dot{y}}{dt} = A_{10} y + A_{11} \dot{y} + A_{12} y', \quad \frac{dy'}{dt} = A_{20} y + A_{21} \dot{y} + A_{22} y', \tag{3.5}$$

$$A_{\alpha\beta} = A_{\alpha\beta}(x, t), \quad \alpha = 1, 2, \quad \beta = 0, 1, 2.$$

In particular, if the matrices $A_{\alpha\beta}$, $\alpha = 1, 2$, $\beta = 0, 1, 2$, are constant block-diagonal, then system (3.5) corresponds to a linear combination of equations of constraints and their derivatives, which was suggested in [7].

We introduce the notation

$$x = (q, v), \qquad w = (v, -\gamma), \qquad g = (f, \dot{f}, f'),$$

$$N = \begin{pmatrix} I_n & 0_{n,n} \\ 0_{n,n} & M \end{pmatrix}, \quad D = \begin{pmatrix} 0_{m,n} & f_q \\ 0_{r-m,n} & f'_v \end{pmatrix}, \quad G = \begin{pmatrix} f_q & f_v \\ \dot{f}_q & \dot{f}_v \\ f'_q & f'_v \end{pmatrix}, \tag{3.6}$$

where I_n is the unit matrix, $0_{m,n}$ the $m\times n$-matrix composed by zeros, and write system (3.3)–(3.5) in the form of the controllable system

$$\dot{x} = N^{-1}w + N^{-1}D^T\lambda \tag{3.7}$$

with the control vector λ corresponding to the equation of program constraints

$$g(x,t) = \alpha, \quad \alpha = (y, \dot{y}, y'), \tag{3.8}$$

and the equation of perturbation of constraints

$$\dot{\alpha} = \widetilde{A}\alpha, \quad \widetilde{A} = \begin{pmatrix} 0_{m,m} & I_m & 0_{m,r-m} \\ A_{10} & A_{11} & A_{12} \\ A_{20} & A_{21} & A_{22} \end{pmatrix}. \tag{3.9}$$

The differentiation of expression (3.8) with regard for notation (3.6) and equations (3.7), (3.9) leads to the equality

$$G\dot{x} + g_t = \widetilde{A}g, \tag{3.10}$$

which consists of the evident identity $\dot{f} - f_q v - f_t \equiv 0$ and the equation for determination of the vector λ of the Lagrange factors of system (3.3)–(3.5):

$$S\lambda = Ag - s, \quad S = FM^{-1}F^T, \tag{3.11}$$

$$A = \begin{pmatrix} A_{10}A_{11}A_{12} \\ A_{20}A_{21}A_{22} \end{pmatrix}, \quad s = \begin{pmatrix} \dot{f}_q v - f_q M^{-1}\gamma + \dot{f}_t \\ f'_q v - f'_v M^{-1}\gamma + f'_t \end{pmatrix}.$$

Substituting into (3.7) the solution $\lambda = S^{-1}(Ag - s)$ of equation (3.11), we obtain equation (3.1) which in its right-hand side contains the vector $\dot{x}^r = N^{-1}(w - D^T S^{-1}s)$ and the matrix $J = N^{-1}D^T S^{-1}A$, which satisfy the equalities

$$G\dot{x}^r \equiv (\dot{f}, 0_{r1}), \quad GJ = (0_{m,m+r}, A). \tag{3.12}$$

From (3.10), (3.12) it follows that the vector $\dot{x}^r$ up to an arbitrary factor c can be represented by the vector product $\dot{x}^r = c[GC]$, $J = G^+A$, i.e., equation (3.1) is contained in a set of systems of differential equations (see [4]):

$$\dot{x} = c[GC] + G^+(Ag - g_t), \quad G^+ = G^T W^{-1}, \quad W = GG^T,$$

and the equality is fulfilled $\dot{g} = Ag$.

If $f_t = 0$, $g = (f, \dot{f})$, then by assuming

$$\dot{g} = -\gamma L(ZL)^{-1}g, \quad Z = \begin{pmatrix} F & 0 \\ v^T F_{q^T} & F \end{pmatrix}, \quad L = \begin{pmatrix} F^T & 0 \\ 0 & F^T \end{pmatrix}, \quad F = f_q,$$

we arrive at a system investigated in [2].

4. Stability of constraints

In [4], conditions of asymptotic stability of the integral manifold $\Omega(t)$ of system of differential equations (3.1), which is given by equation (3.2), were formulated. The realized transformation of DAE-3 (1.4), (2.1), (2.2) to DAE-2 allows us to use the known criteria for definition of the conditions of asymptotic stability of the integral manifold $\Omega(t)$ of system (1.4), (2.1), (2.2). At the moment t we define the distance $\rho(x, \Omega(t))$ between a point $x \in R_{2n}$ of the space of variables $(q_1, \dots, q_n, v_1, \dots, v_n)$ and the integral manifold $\Omega(t) \in R_{2n}$ by the equality $\rho(x, \Omega(t)) = \|\alpha(t)\|$, $\|\alpha\| = \sqrt{\alpha^T\alpha}$. Then from either asymptotic, or exponential stability of the trivial solution $\alpha_1 = \dots = \alpha_{r+m} = 0$ of system (2.2) either asymptotic, or exponential stability of the integral manifold $\Omega(t)$ of system (2.11), respectively, follows.

For system (3.9) with a constant matrix $\widetilde{A}$ the following theorem is valid.

Theorem 3. *If* $\rho(x,\Omega(t)) = \|\alpha(t)\|$ *and all the roots of the characteristic equation* $D(\varkappa) \equiv \det(\widetilde{A} - \varkappa I_{m+r}) = 0$ *of system* (3.9) *have negative real parts, then the integral manifold* $\Omega(t)$ *of system* (3.7) *is asymptotically stable.*

Using the method of Lyapunov's functions, we can formulate the condition of the asymptotic stability of the manifold $\Omega(t)$.

Theorem 4. *If* $\rho(x,\Omega(t)) = \|\alpha(t)\|$ *and for the equations of perturbation of constraints* (3.9) *a function* $V(\alpha,x,t)$ *of fixed sign exists admitting an infinitesimal upper limit, whose derivative* $\dot{V}(\alpha,x,t)$, *calculated via equations* (3.7), (3.9), *is a fixed sign function with the opposite sign, then the integral manifold* $\Omega(t)$ *of system* (3.7) *is asymptotically stable.*

In particular, if $2V = \alpha^T L\alpha$, $L = L^T = (l_{ij})$, $i,j = 1,\dots,m+r$, is a positively definite quadratic form with constant coefficients, then $\dot{V} = \alpha^T L\widetilde{A}\alpha$, and one can apply Sylvester's criterion of the positive definiteness of the quadratic form $-\dot{V} = \alpha^T A'\alpha$, $A' = -L\widetilde{A} = (a'_{ij})$:

$$a'_{11}(x,t) \geq \varepsilon > 0, \quad \begin{vmatrix} a'_{11}(x,t) & a'_{12}(x,t) \\ a'_{21}(x,t) & a'_{22}(x,t) \end{vmatrix} \geq \varepsilon > 0, \dots, \begin{vmatrix} a'_{11}(x,t) & \dots & a'_{1,m+r}(x,t) \\ \dots & \dots & \dots \\ a'_{m+r,1}(x,t) & \dots & a'_{m+r,m+r}(x,t) \end{vmatrix} \geq \varepsilon > 0.$$

If upon the variables q, v only constraints of the form $f'(q,v,t) = 0$ are imposed, then $m = 0$, $\widetilde{A} = A_{22}(x,t)$ and one can apply the theorem about the exponential stability of the manifold $\Omega(t)$ (see [8]) of system (3.7).

Theorem 5. *If*

1) $\rho(x,\Omega(t)) = \|\alpha(t)\|$, $\alpha(t) = f'(x,t)$;
2) $\dot{\alpha} = -k(x,t)W(x,t)L\alpha$, *the scalar function* $k(x,t)$ *is bounded from below*: $k(x,t) \geq k_0 > 0$, $W = f'_v(f'_v)^T$, *the matrix* L *is constant and satisfies Sylvester's conditions*;
3) $w_0 > 0$ *exists such that for all* $x = x(t) \in \Omega_h(t)$, $t \geq t_0$, *where* $\Omega_h(t)$ *is an* h*-neighborhood of the manifold* $\Omega(t)$, *the inequality is fulfilled* $\alpha^T W(x,t)\alpha \geq w_0^2\|\alpha\|^2$;
4) l_1 *and* l_m *are the least and the most eigenvalues of the matrix* L, *respectively,* $\gamma = g(x_0,t_0)\sqrt{l_m/l_1}$, $\beta = k_0 w_0 l_1^2/l_m$,

then the integral manifold $\Omega(t)$ *of system* (3.7) *is exponentially stable and the condition is fulfilled* $\sqrt{\alpha^T(t)\alpha(t)} \leq \gamma e^{-\beta(t-t_0)}$.

5. Numerical solving the equations of extremals

Equations (1.4), (2.1), (2.2), even if the asymptotic stability of the manifold $\Omega(t)$ is ensured, cannot guarantee in the numerical solving the necessary accuracy of the fulfillment of equality (1.5). For the estimation of the accuracy of the numerical solution of equations of extremals we will use the system of DAE-2, represented by equations (3.1), (3.2).

Assume that the initial values t_0, x^0, for which $\|g^0\| = \sup\limits_i |g_i^0| < \varepsilon$, $g(x^0,t_0) = g^0$, are known and equation (3.1) has been constructed admitting an asymptotically stable integral manifold $\Omega(t)$ given by equation (3.2). Assuming $a = A(x,t)g$ and using the right-hand side of system (3.1), we construct the difference equation

$$x^{k+1} = x^k + \tau v^k, \quad x^k = x(t_k), \quad t_{k+1} = t_k + \tau, \quad v = v^\tau(x,t) + J(x,t)g(x,t). \qquad (5.1)$$

Theorem 6. *Constants* α, τ_1, ε *and a matrix* $A(x,t)$ *exist such that, under the fulfillment of the inequalities*

1) $\|g^0\| \leq \varepsilon$;
2) $\tau \leq \tau_1$;
3) $\|E + \tau A(x,t)\| \leq \alpha < 1$;
4) $\frac{\tau_1^2}{2}\|g^{(2)}\| \leq (1-\alpha)\varepsilon$, $g^{(2)} = v^T g_{xx} v + 2g_{xt} + g_{tt}$,

the solution of difference equation (5.1) *satisfies the condition*

$$\|g^k\| \le \varepsilon \quad \forall k = 1, \dots, K. \tag{5.2}$$

Proof. We assume that for solving equation (3.1) the difference scheme (5.1) is used and conditions 1)–4) are fulfilled. Suppose that condition (5.2) is fulfilled for a certain value of k and represent the vector $g^{k+1} = g(x^{k+1}, t_{k+1})$ by the expansion into the series

$$g^{k+1} = g^k + g^k_x \Delta x^k + g^k_t \tau + \frac{\tau^2}{2} g^{(k2)}, \quad \Delta x^k = \tau v^k, \tag{5.3}$$

$$g^{(k2)} = (g_1^{(k2)}, \dots, g_{m+r}^{(k2)}), \quad g_\gamma^{(k2)} = \frac{1}{2\tau^2}\Big(\sum_{p,q} \widetilde{g}^{(k)}_{\gamma,pq} \Delta x^k_p \Delta x^k_q + 2\tau \sum_p \widetilde{g}^{(k)}_{\gamma,pt} \Delta x^k_p + \tau^2 \widetilde{g}^{(k)}_{\gamma,tt}\Big),$$

$\widetilde{g}^{(k)}_{\gamma,pq}$, $\widetilde{g}^{(k)}_{\gamma,pt}$, $\widetilde{g}^{(k)}_{\gamma,tt}$ are values of the partial derivatives $\frac{\partial^2 g_\gamma}{\partial x_p \partial x_q}$, $\frac{\partial^2 g_\gamma}{\partial x_p \partial t}$, $\frac{\partial^2 g_\gamma}{\partial t^2}$, calculated for $x = x^k + \Theta \Delta x^k$, $t = t_k + \theta\tau$. The matrix $\Theta = (\theta_{jl})$, $0 \le \theta_{jl} \le 1$, and the scalar θ, $0 \le \theta \le 1$, take values corresponding to the intermediary values of the derivatives.

Further, taking into account the equality $\dot{g} = A(x,t)g$, we write expression (5.3) as follows

$$g^{k+1} = (E + \tau A^k) g^k + \frac{\tau^2}{2} g^{(k2)}.$$

By estimating the right-hand side of expression (5.3) with regard for 1)–4), we obtain

$$\|g^{k+1}\| \le \|E + \tau A^k\| \, \|g^k\| + \frac{1}{2}\tau^2 \|g^{(k2)}\| \le \alpha\varepsilon + (1-\alpha)\varepsilon = \varepsilon.$$

Let us define the conditions which should be imposed upon the right-hand side of equations (3.9) in order to guarantee the accuracy in (5.2) within the numerical solving the equation (3.1) by the Runge–Kutta method. We will approximate the solution of equation (3.1) by the difference scheme of the second order of accuracy

$$x^{k+1} = x^k + \Delta x^k, \tag{5.4}$$

$$\Delta x^k = \tau(1-\sigma) v^k + \sigma \overline{v}^k, \quad \sigma > 0, \tag{5.5}$$

$$\overline{v}^k = v(\overline{x}^k, t_k + \alpha\tau), \quad \alpha > 0, \tag{5.6}$$

$$\overline{x}^k = x_k + \alpha\tau v^k, \quad v = v^\tau(x,t) + J(x,t) g(x,t), \tag{5.7}$$

α, σ are the parameters of the difference scheme. The initial conditions are assumed to satisfy the inequality $\|g^0\| \le \varepsilon$.

Let us represent the vector g^{k+1} in the form of the sum of the powers Δx^k, τ

$$g^{k+1} = g^k + g^k_x \Delta x^k + g^k_t \tau + \frac{1}{2}((\Delta x^k)^T g^k_{x^T x} \Delta x^k + 2 g^k_{xt} \Delta x^k \tau + g^k_{tt}\tau^2) + R_g^{(k3)}, \tag{5.8}$$

$$R_g^{(k3)} = (R_{g1}^{(k3)}, \dots, R_{g,m+r}^{(k3)}),$$

$$R_{g\gamma}^{(k3)} = \frac{1}{3!}\Big(\sum_{p,q,r} \widetilde{g}^{(k)}_{\gamma,pqr} \Delta x^k_p \Delta x^k_q \Delta x^k_r + 3\tau \sum_{p,q} \widetilde{g}^{(k)}_{\gamma,pqt} \Delta x^k_p \Delta x^k_q + 3\tau^2 \sum_p \widetilde{g}^{(k)}_{\gamma,ptt} \Delta x^k_p + \tau^3 \widetilde{g}^{(k)}_{\gamma,ttt}\Big),$$

$\widetilde{g}^{(k)}_{\gamma,pqr}$, $\widetilde{g}^{(k)}_{\gamma,pqt}$, $\widetilde{g}^{(k)}_{\gamma,ptt}$, $\widetilde{g}^{(k)}_{\gamma,ttt}$ are the values of the partial derivatives $\frac{\partial^3 g_\gamma}{\partial x_p \partial x_q \partial x_r}$, $\frac{\partial^3 g_\gamma}{\partial x_p \partial x_q \partial t}$, $\frac{\partial^3 g_\gamma}{\partial x_p \partial t^2}$, $\frac{\partial^3 g_\gamma}{\partial t^3}$, calculated for $x = x^k + \Theta\Delta x^k$, $t = t_k + \theta\tau$. From (5.5), (5.6) the equality follows $\Delta x^k = \tau((1-\sigma)v^k + \sigma v(x^k + \alpha\tau v^k, t_k + \alpha\tau))$, which after expansion into series can be represented as follows

$$\Delta x^k = \tau(v^k + \alpha\sigma\tau \dot{v}^k) + R_v^{(k3)}, \tag{5.9}$$

$$R_v^{(k3)} = (R_{v1}^{(k3)}, \dots, R_{vn}^{(k3)}),$$

$$R_{vj}^{(k3)} = \frac{1}{2!}\alpha^2\sigma\tau^2\Big(\sum_{p,q} \widetilde{v}^{(k)}_{j,pq} v^k_q v^k_q + 2\sum_p \widetilde{v}^{(k)}_{j,pt} v^k_p + \widetilde{v}^{(k)}_{j,tt}\Big),$$

$\widetilde{v}^{(k)}_{j,pq}$, $\widetilde{v}^{(k)}_{j,pt}$, $\widetilde{v}^{(k)}_{j,tt}$ are the values of the partial derivatives $\frac{\partial^2 v_j}{\partial x_p \partial x_q}$, $\frac{\partial^2 v_j}{\partial x_p \partial t}$, $\frac{\partial^2 v_j}{\partial t^2}$, calculated for $x = x^k + \Theta\Delta x^k$, $t = t_k + \theta\tau$.

The consecutive calculation of the right-hand side of (5.8) with regard for (5.9) makes it possible to express g^{k+1} via g^k, x^k, t_k, A^k, $\dot{A}^k$. To this end we substitute into (5.8) expression (5.9)

$$g^{k+1} = g^k + \tau(g^k_x(v^k + \alpha\sigma\tau\dot{v}^k + R^{(k3)}_v) + g^k_t) + \frac{\tau^2}{2}((v^k + \alpha\sigma\tau\dot{v}^k + R^{(k3)}_v)^T g^k_{x^T x}(v^k + \alpha\sigma\tau\dot{v}^k + R^{(k3)}_v) + \\ + 2g^k_{xt}(v^k + \alpha\sigma\tau\dot{v}^k + R^{(k3)}_v) + g^k_{tt}) + R^{(k3)}_g \quad (5.10)$$

and represent (5.10) as follows

$$g^{k+1} = g^k + \tau(g^k_x v^k + g^k_t) + \alpha\sigma\tau^2(g_x\dot{v})^k + \frac{\tau^2}{2}((v^k)^T g^k_{x^T x} v^k + 2g^k_{xt} v^k + g^k_{tt}) + R^{(k3)}, \quad (5.11)$$

$$R^{(k3)} = \tau g^k_x R^{(k3)}_v + \frac{\tau^2}{2}(\alpha\sigma\tau\dot{v}^k + R^{(k3)}_v)^T g^k_{x^T x}(\alpha\sigma\tau\dot{v}^k + R^{(k3)}_v) + \\ + \tau^2(v^{k^T} g^k_{x^T x}(\alpha\sigma\tau\dot{v}^k + R^{(k3)}_v) + g^k_{xt}(\alpha\sigma\tau\dot{v}^k + R^{(k3)}_v)) + R^{(k3)}_f.$$

Next, taking into account the equalities

$$\dot{g} = A(x,t)g, \quad (g_x\dot{v}) = \ddot{g} - ((v)^T g_{x^T x} v + 2g_{xt} v + g_{tt}),$$

from (5.11) we will have the expression

$$g^{k+1} = (E + \tau A^k + \tau^2\alpha\sigma((A^k)^2 + \dot{A}^k))g^k + \frac{\tau^2}{2}(1 - 2\alpha\sigma)((v^k)^T g^k_{x^T x} v^k + 2g^k_{xt} v^k + g^k_{tt}) + R^{(k3)}. \quad (5.12)$$

Let us choose the parameters α, σ so that $2\alpha\sigma = 1$. Then from (5.12) it follows

$$g^{k+1} = \Big(E + \tau A^k + \frac{1}{2}\tau^2((A^k)^2 + \dot{A}^k)\Big)g^k + R^{(k3)}. \quad (5.13)$$

Theorem 7. *If to solve equation* (3.1) *we use the Runge–Kutta difference scheme of the second order of accuracy* (5.4)–(5.7), *and for all* $x = x_k$, $t = t_k$, $k = 1, \dots, K$, *the values* τ, $q > 0$, α, σ, $R^{(k3)}$, g^0, $A(x,t)$ *satisfy the conditions*
1) $\|g^0\| \le \varepsilon$;
2) $2\alpha\sigma = 1$;
3) $\|R^{(k3)}\| \le (1 - q)\varepsilon$;
4) $\|E + \tau A^k + \frac{1}{2}\tau^2((A^k)^2 + \dot{A}^k)\| \le q < 1$,
then inequality (5.2) *is fulfilled for all* $k = 1, \dots, K$.

Proof. If inequality (5.2) is valid for a certain k, then from the estimate for the right-hand side of expression (5.13) it follows that the inequality will also be valid:

$$\|g^{k+1}\| \le \Big\|E + \tau A^k \frac{1}{2}\tau^2((A^k)^2 + \dot{A}^k)\Big\| \, \|g^k\| + \|R^{(k3)}\| \le q\varepsilon + (1 - q)\varepsilon = \varepsilon.$$

Let us recall that, for computations by the difference scheme (5.4)–(5.7), the two variants are usually applied

$$1) \ \ \sigma = 1, \ \alpha = \frac{1}{2}: \ \overline{x}^k = x^k + \frac{\tau}{2}v(x^k, t_k), \ \ x^{k+1} = x^k + \tau v\Big(\overline{x}^k, t_k + \frac{\tau}{2}\Big),$$

$$2) \ \ \sigma = \frac{1}{2} \ \ \alpha = 1: \ \overline{x}^k = x^k + \tau v(x^k, t_k), \ \ x^{k+1} = x^k + \frac{\tau}{2}(v(x^k, t_k) + v(\overline{x}^k, t_k)).$$

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