Numerical method for round-error growing estimation.

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Abstract. - In numerical calculating the current-voltage characteristics of Josephson junctions the Runge-Kutta method of the fourth - order accuracy is usually used. The calculations are performed at large time intervals, and at each time step the right-hand sides of the equations are recalculated four times. To shorten the calculating time, using "explicit" scheme of the second order accuracy has been suggested instead of the Runge-Kutta method. In case of \( \tau = h \), estimates of \( \| G^n \| \), guaranting boundedness of round-error grows for all \( n \), have been proved, \( G \) is the operator of trasition from layer to layer; \( \tau, h \) are the grid step sizes in \( t \) and \( x \) respectively. In this work a numerical-analitical algorithm for round-error growing estimation is developd for all \( \tau \leq h \). Their boundedness was stated on the whole interval of IVC calculating long Josephson junctions using the suggested scheme. The calculations were performed on the supercomputer GOVORUN (LIT, JINR) using the REDUCE system.

Keywords. Long Josephson junctions, IVC calculations, finite difference method, round error growth estimation, numerical metod, REDUCE system, supercomputer GOVORUN.

INTRODUCTION

The aim of this work is to demonstrate how one can estimate round error growth by numerical method.

Calculating the current-voltage characteristics of \( n \) long Josephson junctions (LJJ) is related to solving \( n \) nonlinear differential equations. An algorithm was developed that makes it possible to reduce the problem to a single equation of the form

\[
u_{\nu+1} - 2u_{\nu} + u_{\nu-1} = -\beta u_{\nu+1} - u_{\nu-1} - \sin(u_{\nu}) + I_{\nu},
\]

(1)

\( \tau, h \) are the grid step sizes in \( t \) and \( x \) respectively, and \( \gamma = \tau/h \), in what follows, \( \delta = \beta \tau/2 \). The round-error growing estimation is reduced to estimating integrals

\[
I_{n} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \left| \frac{\lambda_{1}^{n} - \lambda_{2}^{n}}{\lambda_{1} - \lambda_{2}} \right| d\phi
\]

1 \( \leq n \leq N \), \( N = t_{\text{max}}/\tau \). Here \( \lambda_{1,2} \) are solutions of the characteristic equation of the considered scheme (1):

\[
\lambda^{2} - 2\frac{1 - 2\gamma^{2}\sin^{2}(\phi/2)}{1 + \delta} \lambda + \frac{1 - \delta}{1 + \delta} = 0,
\]

(2)

\[
\lambda_{1,2} = \frac{1 - 2\gamma^{2}\sin^{2}(\phi/2) \pm \sqrt{\delta^{2} - 4\gamma^{2}\sin^{2}(\phi/2) + 4\gamma^{4}\sin^{4}(\phi/2)}}{1 + \delta}
\]

Note

\[
D_{n} = \frac{\lambda_{1}^{n} - \lambda_{2}^{n}}{\lambda_{1} - \lambda_{2}}.
\]

In real calculations \( N \) values were more than 10000.

1. Reduction of \( I_{n} \) estimation to some classical integral calculation.
After change of variables in $z = 1 - \gamma^2 + \gamma^2 \cos(\phi)$, in (2) we obtain

$$\lambda_{1,2} = \frac{z \pm \sqrt{z^2 + \delta^2 - 1}}{1 + \delta}.$$  

After the corresponding substitution in (3) and a number of algebraic manipulations we find that $D_n$ is polynomial of $n - 1$ power of $z$ with real coefficients:

$$D_n = P_n(z)/(1 + \delta)^{n-1}, \quad P_n = \frac{(z + \sqrt{z^2 + \delta^2 - 1})^n - (z - \sqrt{z^2 + \delta^2 - 1})^n}{2\sqrt{z^2 + \delta^2 - 1}},$$

$$P_n(z) = \sum_{k=1}^{n_c} C_{n-1}^k z^{n-(2k-1)}(z^2 + \delta^2 - 1)^{k-1} \quad (4).$$

Here $n_c$ is integer part of $(n + 1)/2$, $n_c = [(n + 1)/2]$. If $n$ is odd number then polynomials $P_n(z)$ and $P_n^2(z)$ even ones. If $n$ is even number, then $n - (2k - 1)$ is odd number, $P_n(z)$ is odd polynomial but $P_n^2(z)$ is even polynomial.

Remark that $z(0) = 1$, $z(\pi) = 1 - 2\gamma^2$, $dz = -\gamma^2 \sin(\phi) d\phi$,

$$\gamma^2 \cos(\phi) = z - 1 + \gamma^2, \quad \gamma^2 \sin(\phi) = \sqrt{Y(z)}, \quad d\phi = -\frac{dz}{\sqrt{Y(z)}},$$

$$Y(z) = \gamma^4 - (z - 1 + \gamma^2)^2. \quad (5)$$

The problem reduced to calculating the following integrals

$$\frac{1}{\pi} \int_{1-2\gamma^2}^{1} \frac{P_n^2(z)}{\sqrt{Y(z)}} \frac{dz}{\sqrt{Y(z)}}. \quad (6)$$

Remark that $Y(1) = Y(1 - 2\gamma^2) = 0$.

In this work a numerical-analitical algorithm for calculating $I_n$ on the whole interval of IVC calculating long Josephson junctions is developed.

The well known algorithm (see for instance [5]) had been used in the calculations:

$$\int \frac{P_n^2(z)}{\sqrt{Y(z)}} dz = Q(z)\sqrt{Y(z)} + \kappa \int \frac{dz}{\sqrt{Y(z)}},$$

where polynomial $Q(z)$ and constant $\kappa$ are determining relation

$$P_n^2(z) = Q'(z) Y(z) + \frac{1}{2} Q(z) Y'(z) + \kappa.\quad (7)$$

In the case under consideration (see (5)) the relation determining $Q(z)$, takes the form

$$P_n^2(z) = Q'(z)(-z^2 + 2z(1 - \gamma^2) - (1 - 2\gamma^2)) + Q(z)(-z + (1 - \gamma^2)) + \kappa. \quad (7)$$

As result we have

$$-\frac{1}{\pi} \int_{1}^{1-2\gamma^2} P_n^2(z) \frac{dz}{\sqrt{Y(z)}} = \frac{1}{\pi} \left( Q(z) \sqrt{Y(z)} \right)_{1-2\gamma^2}^{1} + \int_{1-2\gamma^2}^{1} \frac{\kappa dz}{\sqrt{Y(z)}} = \kappa, \quad I_n = \frac{\kappa}{(1 + \delta)^{2(n-1)}}.$$ 

Remark in conclusion that

$$\frac{1}{\pi} \int_{1-2\gamma^2}^{1} \frac{dz}{\sqrt{\gamma^4 - (z - 1 + \gamma^2)^2}} = \frac{1}{\pi} \int_{-1}^{1} \frac{du}{\sqrt{1 - u^2}} = \frac{2}{\pi} \int_{0}^{1} \frac{du}{\sqrt{1 - u^2}} = \frac{2}{\pi} \arcsin(1) = 1.$$
In the process of calculation the change of variables \( z - 1 + \gamma^2 = \gamma^2 u \) was made.

For large \( n \) we had to develop special algorithm to calculate \( P(z) \) coefficients. And odd and even \( n \) cases were considered separately.

2. Algorithm of \( I_n \) calculation, odd \( n \).

This time \( n = 2nc - 1 \), (4) takes the form

\[
P_n(z) = \sum_{k=1}^{nc} C_n^{2k-1} z^{2(nc-k)} (z^2 + \delta^2 - 1)^{k-1}.
\]

After substitution \( z^2 = (\delta^2 - 1)w^2 \), we find

\[
P_n(z) = (\delta^2 - 1)^{nc-1} P_t(w), \quad P_n^2(z) = (\delta^2 - 1)^{n-1} P_t^2(w).
\]

Coefficients of \( P_t(w) \) do not depend on \( \delta \), what gave us possibility to perform the general part of calculations in integer numbers:

\[
P_t(w) = \sum_{k=1}^{nc} C_n^{2k-1} w^{2(nc-k)} (1 + w^2)^{k-1}, \quad P_t^2(w) = \sum_{k=1}^n b_j w^{2(j-1)}.
\]

After changing \( nc - k = \xi - 1 \), we have

\[
P_t(w) = \sum_{\xi=1}^{nc} C_n^{n-2(\xi-1)} w^{2(\xi-1)} (1 + w^2)^{nc-\xi} = \sum_{j=1}^{nc} g_j w^{2(j-1)}, \quad g_j = \sum_{k=1}^j C_n^{n-2(k-1)} C_\xi^{nc-k}.
\]

Here \( \theta \) is determined by relation \( 2(k-1) + 2\theta = 2(j-1) \), \( \theta = j - k \). First \( g_j \) had been calculated right

\[
g_j = \sum_{k=1}^j \frac{n!(nc-k)!}{(2(k-1))!(n-2(k-1))!(j-k)!(nc-j)!}.
\]

In process of numerical experiments some algorithm shortenned calculating time more than 7 times had been found:

\[
g_1 = 1, \quad g_j = \frac{n!}{(n-2(j-1))!(2(j-1))!} \sum_{k=1}^j p(k), \quad 2 \leq j \leq nc - 1, \quad g_{nc} = 2^{n-1},
\]

\[
p(j) = 1, \quad p(k) = p(k+1) \frac{k(2k-1)}{(j-k)(n-2(k-1))} , \quad k = j-1, j-2, \ldots, 1.
\]

When \( g_j \) are found, \( P_n^2(z) \) coefficients are determined in the following way.

\[
P_n^2(z) = \sum_{k=1}^n b_k (\delta^2 - 1)^{n-k} z^{2(k-1)}, \text{where}
\]

\[
b_k = \sum_{l=1}^k g_l g_{k-l+1}, \text{ for } k \leq nc, \quad b_k = \sum_{l=k}^{nc} g_l g_{k-l+1}, \text{ for } k > nc.
\]

In particular we have \( b_1 = 1, b_n = 2^{2(n-1)} \), It followes fro relation (6), that \( Q(z) \) is polynomial of \( 2n-3 \) degree:

\[
Q(z) = \sum_{k=1}^{n-1} (a_k z^{2k-1} + c_k z^{2(k-1)}), \quad Q'(z) = \sum_{k=1}^{n-1} (2k-1) a_k z^{2(k-1)} + \sum_{k=2}^{n-1} 2(k-1) c_k z^{2k-3}.
\]
And we calculate step by step

\[ a_{n-1} = -\frac{b_n}{2(n-1)}; \quad c_{n-1} = a_{n-1}(1 - \gamma^2)(2 + \frac{1}{2n-3}); \]

\[ a_{k-1} = -a_k(1 - 2\gamma^2) - \frac{b_k(\delta^2 - 1)^{n-k} + a_k(1 - 2\gamma^2)}{2(k-1)} + c_k(2 + \frac{1}{2(k-1)})(1 - \gamma^2), \]

\[ c_{k-1} = a_{k-1}(2 + \frac{1}{2k-3})(1 - \gamma^2) - c_k(1 + \frac{1}{2k-3})(1 - 2\gamma^2), \quad k = n-1, \ldots, 2. \]

After \( a_1, c_1 \) are determined, we calculate \( I_n \) easily. Taking in account that

\[ P_n^2(0) = (\delta^2 - 1)^{n-1}, \quad Q(0) = c_1, \quad Q'(0) = a_1, \quad Y(0) = -1 + 2\gamma^2, \quad Y'(0) = 2(1 - \gamma^2), \]

we obtain that relation (7) with \( z = 0 \) takes the form

\[ P_n^2(0) = (-1 + 2\gamma^2)a_1 + (1 - \gamma^2)c_1 + \kappa, \]

hence,

\[ \kappa = (1 - 2\gamma^2)a_1 - (1 - \gamma^2)c_1 + (\delta^2 - 1)^{n-1}, \quad I_n = \kappa/(1 + \delta)^{2(n-1)}. \]

3. Algorithm of \( I_n \) calculation, even \( n \).

This time

\[ P_n(z) = z \sum_{k=1}^{\infty} C_n^{2k-1} z^{2(n-1)}(z^2 + \delta^2 - 1)^{k-1}. \]

Acting similarly to the case of odd \( n \), we find

\[ P_n^2(z) = \sum_{k=1}^{n-1} b_k(\delta^2 - 1)^{n-k-1} z^{2k}, \]

\[ Q(z) = \sum_{k=1}^{n-1} (a_k z^{2k-1} + c_k z^{2(k-1)}). \]

After \( a_1, c_1 \) values are determined, we calculate \( I_n \). Taking in account that

\[ P_n^2(0) = 0, \quad Q(0) = a_1, \quad Q'(0) = c_1, \quad Y(0) = 1 - 2\gamma^2, \quad Y'(0) = 2(1 - \gamma^2), \]

we obtain that with \( z = 0 \) the relation (7) takes the form

\[ 0 = -(1 - 2\gamma^2)a_1 + (1 - \gamma^2)c_1 + \kappa, \]

hence,

\[ \kappa = (1 - 2\gamma^2)a_1 - (1 - \gamma^2)c_1, \quad I_n = \kappa/(1 + \delta)^{2(n-1)}. \]

Boundedness of the round errors on whole IVC time interval calculation guarantees reliability of the numerical results obtained using the suggested difference scheme. Norms of \( G^n \) depend on \( A^n(e^{i\phi}) \) norms, \( \|A^n(e^{i\phi})\| \leq 7 + 5\|D_n\| \).
On Fig.1 Graph of $\|D_n\| = \sqrt{T_n}$, $n \leq 10000$, refering to $\tau = h = 0.1$, $t_{max} = 1000$ is presented.

On Fig.2 asterisks mark $\|D_n\|$ values near the pick on Fig.1. $\|D_n\|$ reaches maximal value at $n = 63$, $\|D_{63}\| = 4.5586...$ It has been proved analyticaly that $\|D_n\| < 9.525$ for all $n$. 
On Fig. 3 graphs of $\|D_n\|$, $n \leq 5000$, are presented. Lower graph refers to the case $\tau = h = 0.1$ Middle one - to the case $\tau = h = 0.05$ and upper - to $h = 0.05$, $\tau = h/5$. 