Computer Assisted Mechanics and Engineering Sciences, 12: 65–81, 2005.

Refined least squares approach to the initial-value problems unstable in the Lyapunov sense[1]

Ryszard Walentyński
Silesian University of Technology, Faculty of Civil Engineering
ul. Akademicka 5, 44-101 Gliwice, Poland

(Received January 7, 2004)

The paper presents application of the Refined Least Squares method to the initial value problems that are instable in the Lyapunov sense. There is shown that the method is not sensitive to this kind of instability. The method is especially useful in search of particular integral of the considered problem. The method has an additional tool to evaluate quality of approximation. The approach is based on minimization of the functional, which square root can is generalized norm L_2 and can be used to estimate global error of approximation. The expected value of the functional is equal to zero. The approximation is satisfactory if both results converge and functional reaches value close to zero. The consideration is illustrated with examples. There are shown initial-value problems which have physical sense and are applicable in mechanics. Whereas numerical approach may fail for these tasks, Refined Least Squares approach returns reliable approximation. The last example presents application of the special feature of the method, which allows neglecting influence of general integral on the solution. The method may be used in sensitivity analysis, search of the problem parameters, verification of numerical methods and an antonymous method in computational physics and mechanics.

1. Introduction

Some problems of mathematical physics and computational mechanics are described with differential equations that are unstable in the Lyapunov sense. It means that small change in the initial or boundary condition results in large change of the computation path. This small change can be caused by round-off error or too big recursion step. The numerical procedures do not have reliable tools to estimate if the result of computation is wrong or not.

The Refined Least Squares method has been implemented within the computer algebra system *Mathematica* [8]. The method has been primarily used to approximate boundary value problems. There was shown in [3] and [4] that it is also applicable to the initial or initial-boundary value tasks.

The paper presents tree examples showing that the Refined Least Squares approach is not sensitive on the Lyapunov instability. Moreover it has an additional tool to estimate a quality of an approximation is provided. This tool is a square root of the minimized functional as it can be regarded a generalized L_2-norm.

Opposite to numerical stepwise approach, it considers problem globally in the whole domain, not step by step. Better approximation is obtained if more approximating functions are considered.

There is shown that the least squares procedure finds first of all a particular integral of the problem. Meantime it tries to satisfy boundary conditions.

There was found that the method has a special feature which allows for a peculiar approach to the boundary conditions. I was found, [5] and [6] that some boundary conditions may be not considered. In this case the method finds a particular integral of the problem or generalized particular integral, called also base solution. This phenomenon, discovered for shells boundary-value problems has been

[1]The paper has been presented at the 15$^{\text{th}}$ International Conference on Computer Methods in Mechanics, Gliwice/Wisła, June 3–6, 2003.

discussed and explained in [7]. There was found that boundary conditions connected with the lowest derivative of the function in the differential equation must be considered obligatory to obtain non singular system of algebraic equations. Other boundary conditions may be neglected. It is especially useful in search of main trend of the function or generalized particular integral.

The fourth example is devoted to illustrate this feature and its application of the differential equation with non-constant coefficients.

2. Method description

The method was described a bit more extensively in [7]. It was designed originally to solve boundary-value problems. Therefore only main elements are presented here with an emphasis on application to initial-value problems.

2.1. Functional

Let us consider a system of n differential equations $e_i == 0$ ("==" denotes "equal to") of n functions $y_k(t)$, describing an initial-value (or boundary-value) problem defined in the domain (period of time) $t \in \langle t_0, t_1 \rangle$. Let $b_k == 0$ be one of m initial (or boundary) condition defined in any moment in the considered period (point of the domain).

For the considered problem we can built the following functional.

$$F := \sum_{i=1}^{n} \int_{t_0}^{t_1} (\alpha_i\, e_i)^2 + \sum_{k=1}^{m} (\beta_k\, b_k)^2 \geq 0, \tag{1}$$

where α_i and β_k are weighting coefficients or weighting functions (":=" denotes definition). Weights play important role in the method. From the formal point of view they provide consistency of physical units in the functional F, definition (1). Next they enable us to moderate convergence path. This problem was remarked in [7] and will be a subject of further research. The most important feature of the method is that under certain conditions some initial or boundary conditions can be neglected by setting appropriate weight to be equal to zero.

2.2. Approximation

We can assume the approximation as a linear combination of p independent functions $u_i(t)$:

$$y_k(t) := \sum_{i=0}^{p} c_{(n\,i+k-1)}\, u_i(t). \tag{2}$$

The functions $u_i(t)$ in definition (2) do not have to satisfy boundary or initial conditions. These conditions are considered within the functional F, definition (1). This is the most important difference to the classical least squares approach. It makes not only the implementation of the method more straightforward but also has some further important consequences.

According to this assumption, the weighted equations $\alpha_k\, e_k$ can be rewritten in the following form:

$$\alpha_k\, e_k(t) == G_k(t) + \sum_{i=0}^{n(p+1)-1} c_i\, K_{ik}(t). \tag{3}$$

Similarly we can do for weighted boundary conditions:

$$\beta_k \, b_k == H_k + \sum_{i=0}^{n(p+1)-1} c_i \, L_{ik}\,(t). \tag{4}$$

Coefficients $K_{ik}\,(t)$, $L_{ik}\,(t)$ standing by decision variables c_i and free elements $G_k\,(t)$, H_k, can be easily extracted from the Eq. (3) and boundary conditions (4), description and implementation is presented in [7].

Another problem is choice of approximating functions $u_i\,(x)$. The best numerical stability and computational speed is obtained with monic Chebyshev polynomials [1], which are weighted Chebyshev polynomials of the first type $T_n\,(t)$ computed according to the following definition:

$$u_i\,(t) := \frac{T_i\left(2\dfrac{t-t_1}{t_0-t_1}-1\right)}{2^{i-1}}. \tag{5}$$

The definition (5) makes that the domain is normalized to the interval $\langle -1,\, 1\rangle$.

2.3. System of algebraic equations

The approximation consists in minimization the functional F, definition (1) with the Ritz method. Unknown coefficients c_i are computed from the system of algebraic equations generated with a minimization condition:

$$\frac{\partial F}{\partial c_i} == 0. \tag{6}$$

For linear problem the system of algebraic equations (6) takes the form:

$$A_{ij}\, c_j == B_i, \tag{7}$$

where elements of the positive definite symmetrical matrix A_{ij} are computed from:

$$A_{ij} := \int_{t_o}^{t_1} \left(\sum_{k=1}^{n} K_{ik}\,(t)\; K_{jk}\,(t) \right) \mathrm{d}t + \sum_{k=1}^{m} L_{ik}\, L_{jk}, \tag{8}$$

where coefficients $K_{ik}\,(t)$, $L_{ik}\,(t)$ are defined in definitions (3) and (4), respectively.

Coefficients of the free vector B_i are computed from:

$$B_i := \int_{t_o}^{t_1} \left(\sum_{k=1}^{n} K_{ik}\,(t)\; G_k(t) \right) \mathrm{d}t + \sum_{k=1}^{m} L_{ik}\, H_k, \tag{9}$$

where coefficients $G_k(t)$, H_k are defined in definitions (3) and (4), respectively.

2.4. Additional tool of verification

The functional F, definition (1) is equal to zero if the approximation is an exact solution. Otherwise it is a positive number. It is a generalization of the norm L_2 and can be used to estimate global error of approximation.

3. Examples

The application of the method is illustrated with three examples.

3.1. Example 1

The first example comes from the chapter of the book by Wagon, [2] on pitfalls of numerical analysis. The left hand side of the considered equation $e == 0$ is:

$$e := y'(t) + 2y(t) - \cos(t). \tag{10}$$

The exact solution of the equation (10) is:

$$y(t) := C\, e^{2t} - \frac{2}{5}\cos(t) + \frac{1}{5}\sin(t). \tag{11}$$

Let us consider an initial boundary problem defined with equation (10) in the interval $t \in \langle 0, 3\pi \rangle$ with an initial condition $b == 0$, $b := y(0) + \frac{2}{5}$. The initial problem is unstable in the Lyapunov sense since the general integral of the equation is $y_0(x) := C\, e^{2t}$. Therefore the numerical procedures, also those built in both *Mathematica* and Matlab fails in this case. The exact solution in the considered case is equal to the particular integral:

$$y_p(t) := -\frac{2}{5}\cos(t) + \frac{1}{5}\sin(t), \tag{12}$$

whereas procedure of numerical solution returns approximation that diagram is presented in Fig. 1 and it is wrong due to instability in the Lyapunov sense. Despite advanced numerical algorithms built in the considered computer algebra system the result is returned with no warning. Warnings are usually produced by the system if it has problems with convergence or stability.

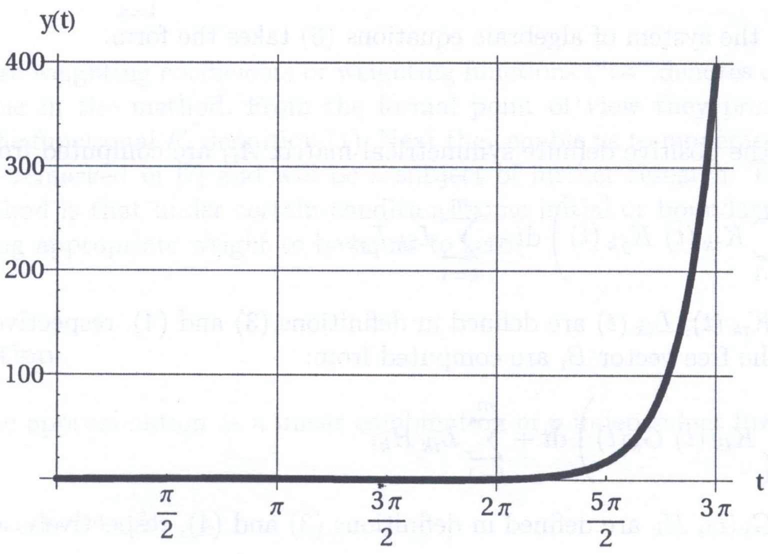

Fig. 1. Numerical approximation

Refined least squares procedure returns approximation which is stable. Approximation with polynomial degree equal to 5, see Fig. 2, is close to exact solution in the most of the domain.

Approximation with higher degrees of polynomials is even better; see Figs. 3 and 4.

The quality of overall approximation can be evaluated by analysis of the square root of the functional (1) $\sqrt{F}$. Its diagram with respect to the polynomial degree is presented in Fig. 5. Its value close to zero informs us about satisfactory convergence.

This example shows that the convergence decides about the approximation quality. The functional F, definition (1) reaches considerably small values much earlier.

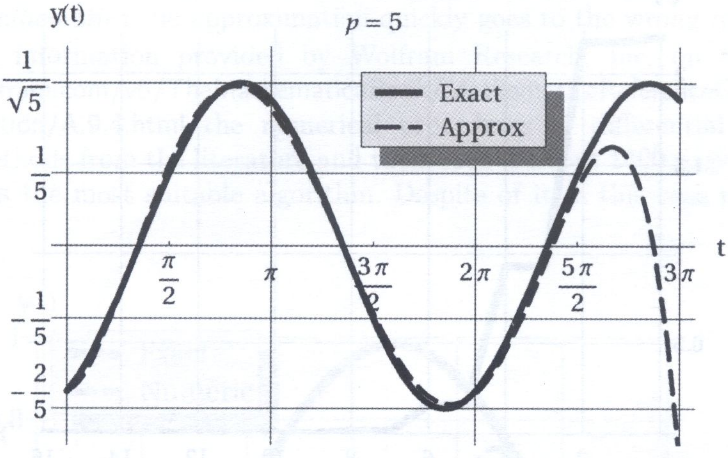

Fig. 2. Least squares approximation, polynomial degree equal to 5

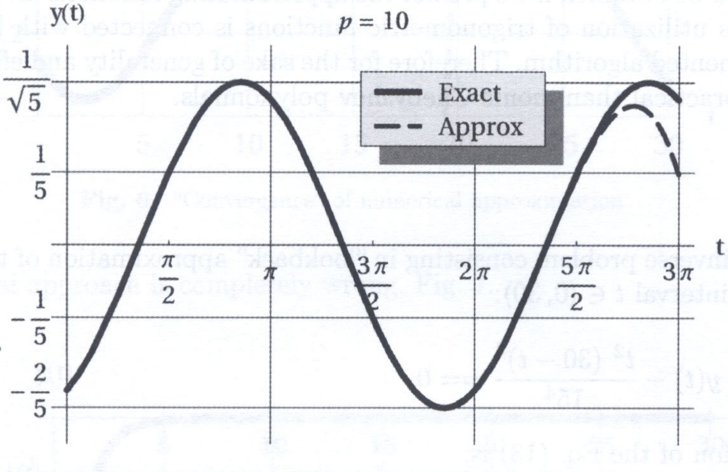

Fig. 3. Least squares approximation, polynomial degree equal to 10

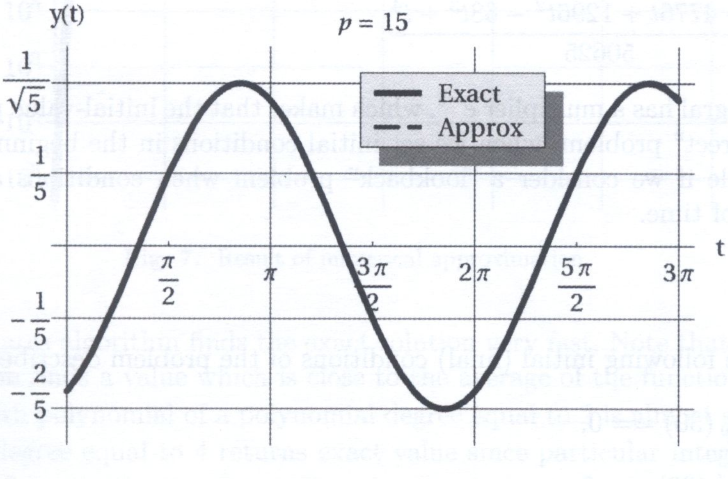

Fig. 4. Least squares approximation, polynomial degree equal to 15

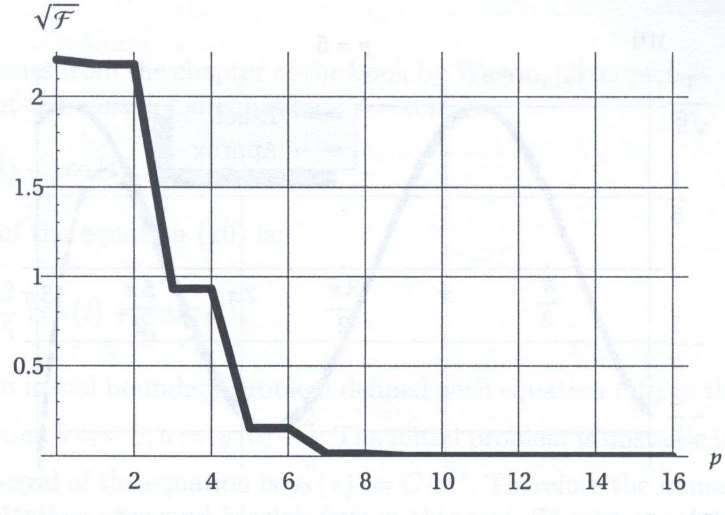

Fig. 5. Convergence of the functional (1) root $\sqrt{F}$ with regard to the polynomial degree

It should be added that the approximation in the considered case would be not only quicker but an exact solution would be obtained if we predict the approximating functions as: $y_1 := \sin(t)$ and $y_1 := \cos(t)$. Nevertheless utilization of trigonometric functions is connected with loss of computational speed of the implemented algorithm. Therefore for the sake of generality and efficiency trigonometric functions are less practical than monic Chebyshev polynomials.

3.2. Example 2

Let us consider an inverse problem consisting in "lookback" approximation of the problem described by Eq. (13) in the interval $t \in \langle 0, 30 \rangle$:

$$y''(t) + 2y'(t) + y(t) - \frac{t^2\,(30-t)^2}{15^4} == 0. \tag{13}$$

The exact solution of the Eq. (13) is:

$$y(t) := (C_1 + C_2\,t)\,e^{-t} + y_p(t), \tag{14}$$

where its particular integral is equal to:

$$y_p\,(t) := \frac{6960 - 4776t + 1296t^2 - 68t^3 + t^4}{50625}. \tag{15}$$

The general integral has a multiplier e^{-t}, which makes that the initial-value problem is stable if we a considering a "direct" problem, when we set initial conditions in the beginning of the considered period and unstable if we consider a "lookback" problem when conditions are set in the end of considered period of time.

3.2.1. Case 1

Let us consider the following initial (final) conditions of the problem described with equation (13):

$$b_1 := y\,(30) - y_p\,(30) == 0, \tag{16}$$

$$b_2 := y'\,(30) - y'_p\,(30) == 0. \tag{17}$$

The exact solution in this case is equal to the particular integral (15). If we apply numerical procedure built-in *Mathematica* the approximation quickly goes to the wrong results, see Fig. 6.

According to the information provided by Wolfram Research, Inc. on their WWW page: http://documents.wolfram.com/v5/TheMathematicaBook/MathematicaReferenceGuide/Some-NotesOnInternalImplementation/A.9.4.html the numerical procedures of differential equations solving cover most known methods from the literature and their code is about 1400 pages long. The routine automatically chooses the most suitable algorithm. Despite of it in this case it fails without any warning, too.

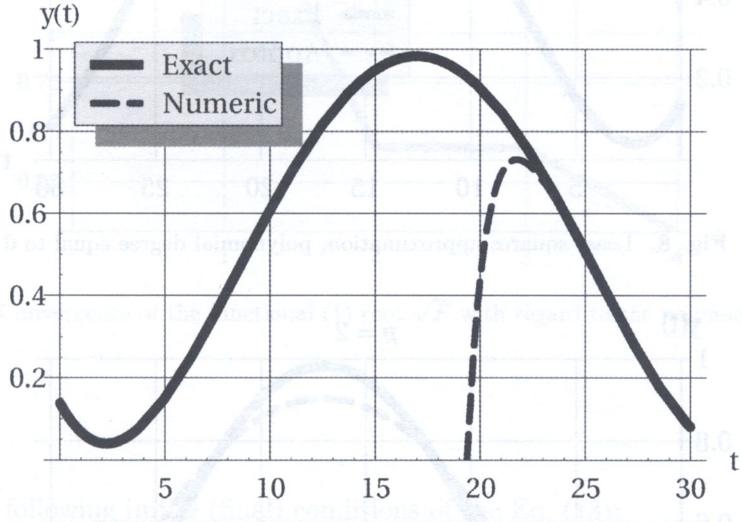

Fig. 6. "Convergence" of numerical approximation

Result of numerical approach is completely wrong, Fig. 7.

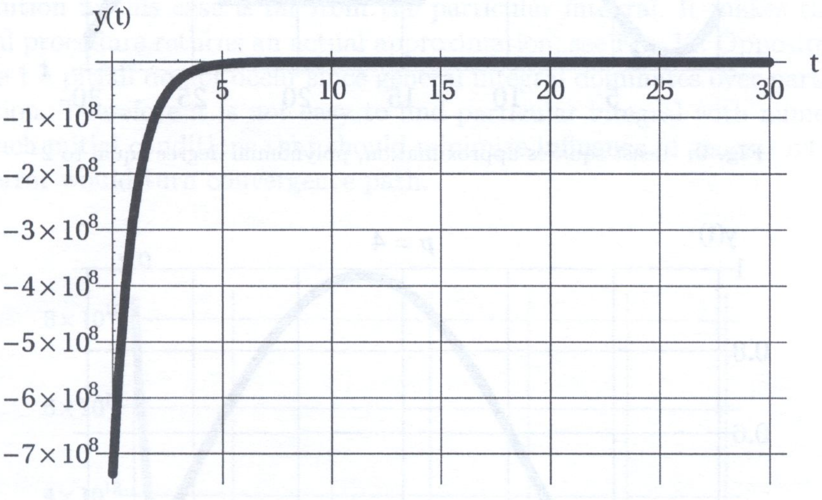

Fig. 7. Result of numerical approximation

Refined Least Squares algorithm finds the exact solution very fast. Note that the approximation with constant function finds a value which is close to the average of the function, see Fig. 8.

Approximation with polynomial of a polynomial degree equal to 2 is almost satisfactory, Fig. 9.

Polynomial with degree equal to 4 returns exact value since particular integral is a polynomial of that degree, Fig. 10.

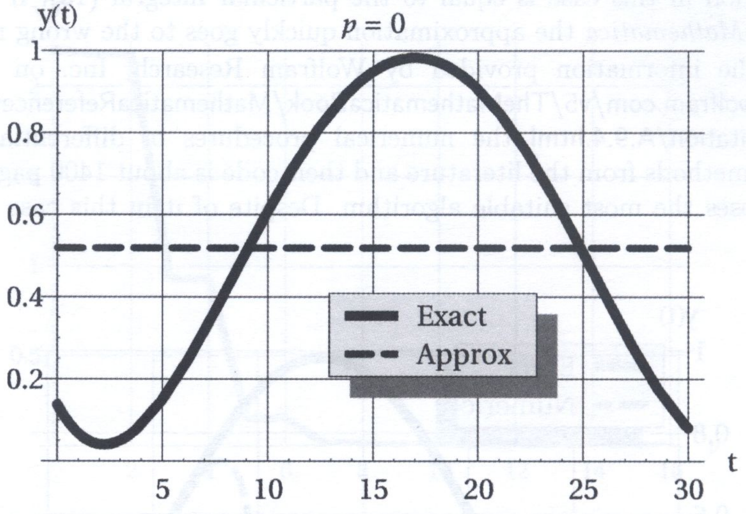

Fig. 8. Least squares approximation, polynomial degree equal to 0

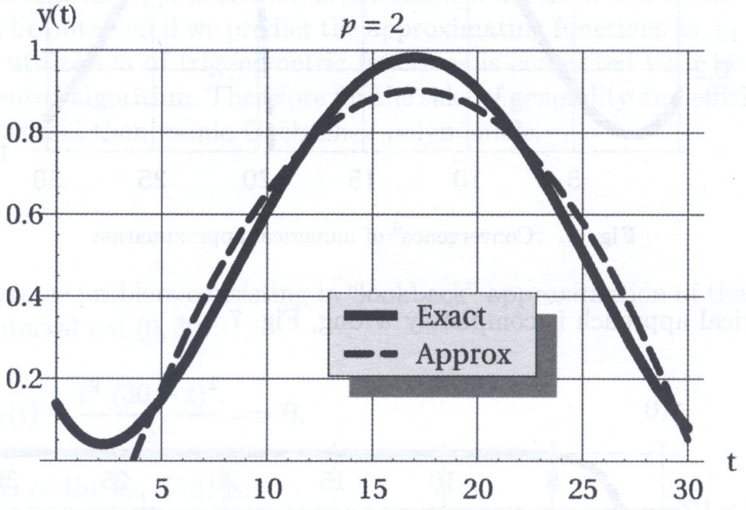

Fig. 9. Least squares approximation, polynomial degree equal to 2

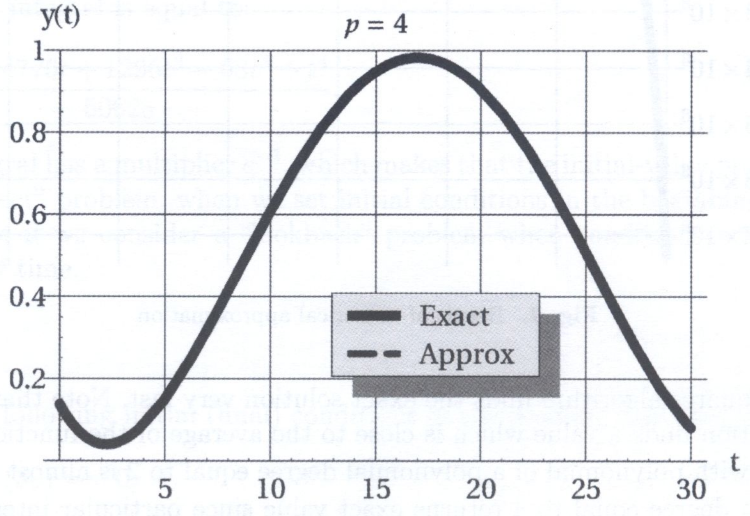

Fig. 10. Least squares approximation, polynomial degree equal to 4

Additional information about convergence is provided by a value of the functional root $\sqrt{F}$, definition (1). It reaches value equal to zero for polynomial degree equal to 4, Fig. 11.

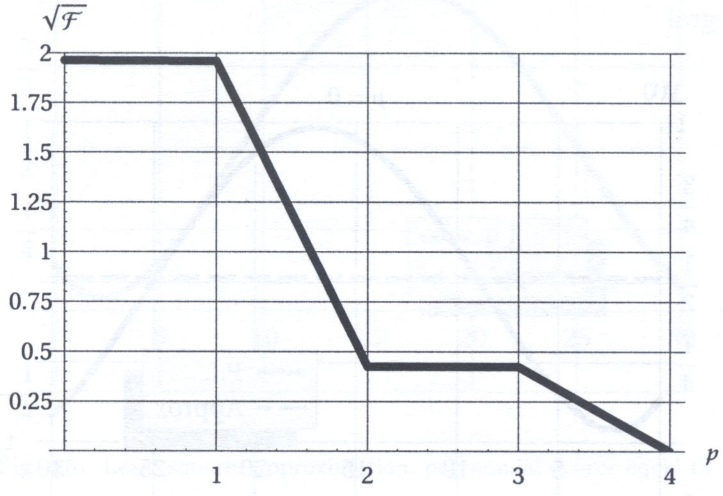

Fig. 11. Convergence of the functional (1) root $\sqrt{F}$ with regard to the polynomial degree

3.2.2. Case 2

Let us consider the following initial (final) conditions of the Eq. (13):

$$b_1 := y\,(30) == 0, \tag{18}$$

$$b_2 := y'\,(30) == 0. \tag{19}$$

The exact solution in this case is far from the particular integral. It makes that *Mathematica* built-in numerical procedure returns an actual approximation, see Fig. 12. Opposite to the previous case and example 1 a pitfall do not occur since general integral dominates over particular one in the considered equation. Therefore it is not easy to find particular integral with numerical procedure, despite setting such initial conditions that should minimize influence of general integral, since even small round-off error would turn convergence path.

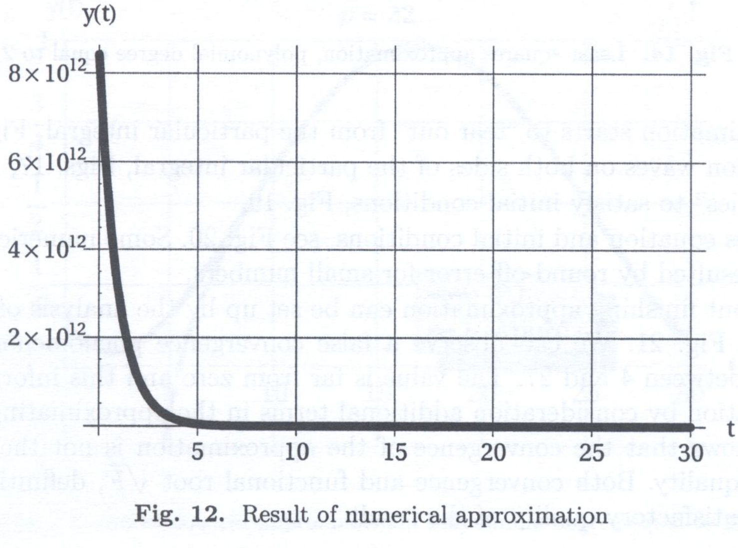

Fig. 12. Result of numerical approximation

The Refined Least Squares procedure finds particular integral, first. Figures 13, 14, 15 show beginning of the approximation. The approximate solution (`Approx`) is compared to the particular equation (`P.I.`) As we can observe in Fig. 15 for $p == 4$ the approximation converges almost exactly to the particular integral.

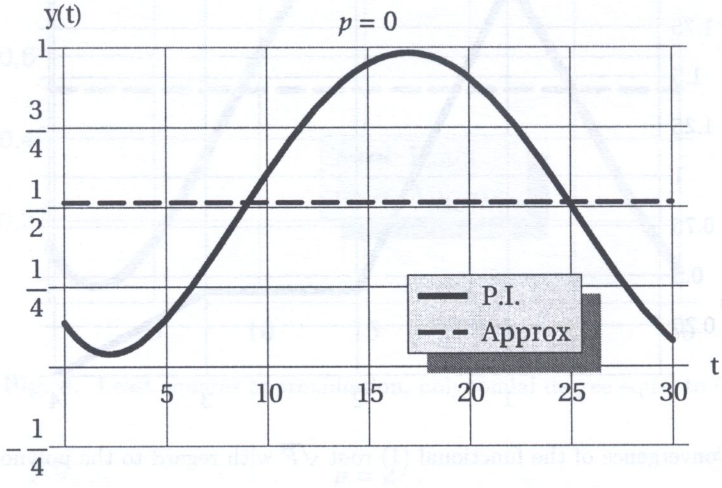

Fig. 13. Least squares approximation, polynomial degree equal to 0

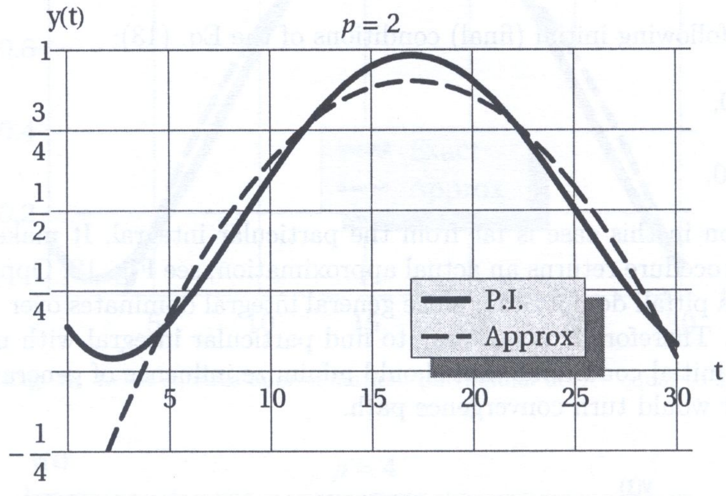

Fig. 14. Least squares approximation, polynomial degree equal to 2

Then the approximation starts to "tear out" from the particular integral, Fig. 16.

The approximation waves on both sides of the particular integral, Figs. 17, 18 and 19.

Afterwards it "tries" to satisfy initial conditions, Fig. 19.

Finally it satisfies equation and initial conditions, see Fig. 20. Some numerical instability visible on the drawing is resulted by round-off error for small numbers.

The decision about finishing approximation can be set up by the analysis of the functional root $\sqrt{F}$, definition (1), Fig. 21. We can observe a false convergence phenomenon in the interval of polynomial degree between 4 and 27. The value is far from zero and this informs us that we must continue approximation by consideration additional terms in the approximating polynomial.

This example shows that the convergence of the approximation is not the unique criterion of the approximation quality. Both convergence and functional root $\sqrt{F}$, definition (1) close to zero informs about the satisfactory quality of the result.

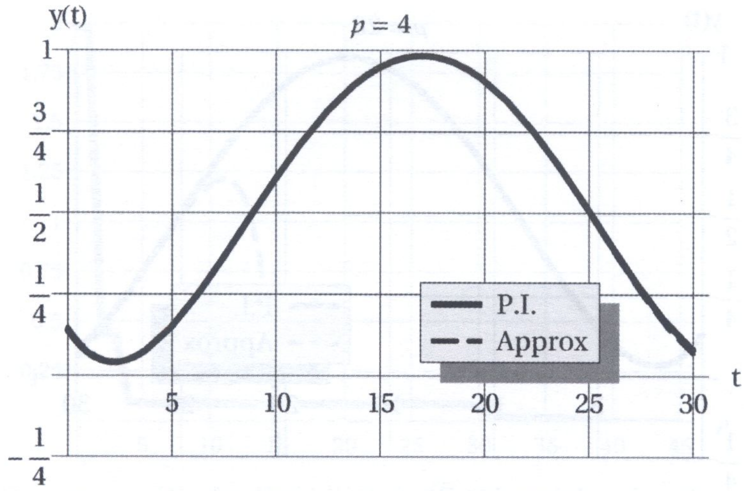

Fig. 15. Least squares approximation, polynomial degree equal to 4

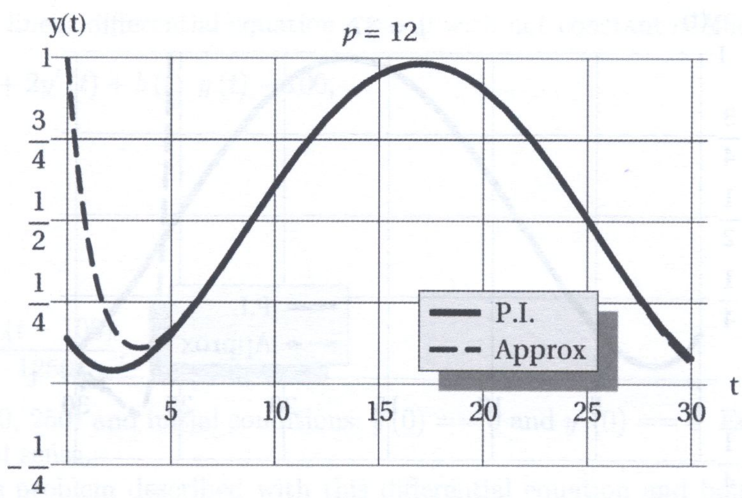

Fig. 16. Least squares approximation, polynomial degree equal to 12

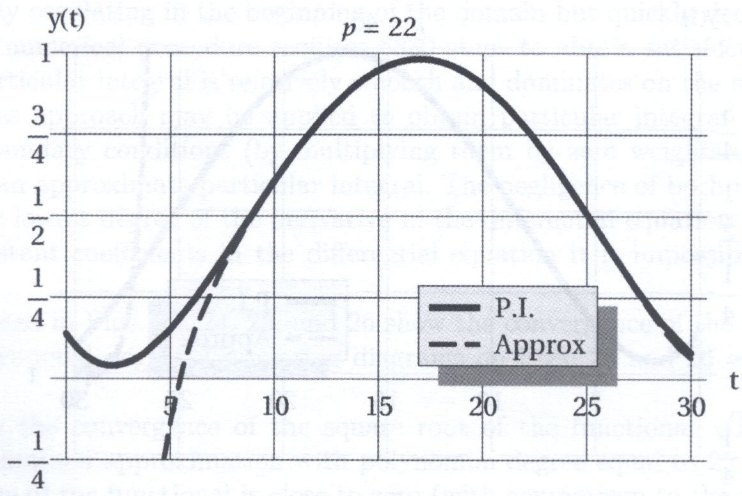

Fig. 17. Least squares approximation, polynomial degree equal to 22

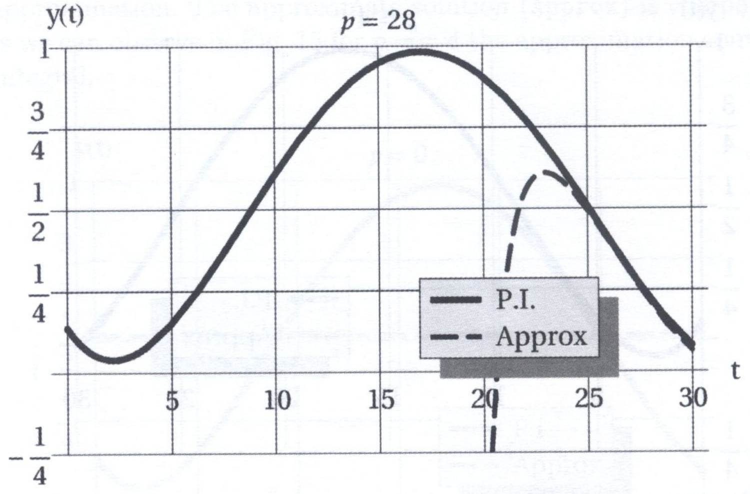

Fig. 18. Least squares approximation, polynomial degree equal to 28

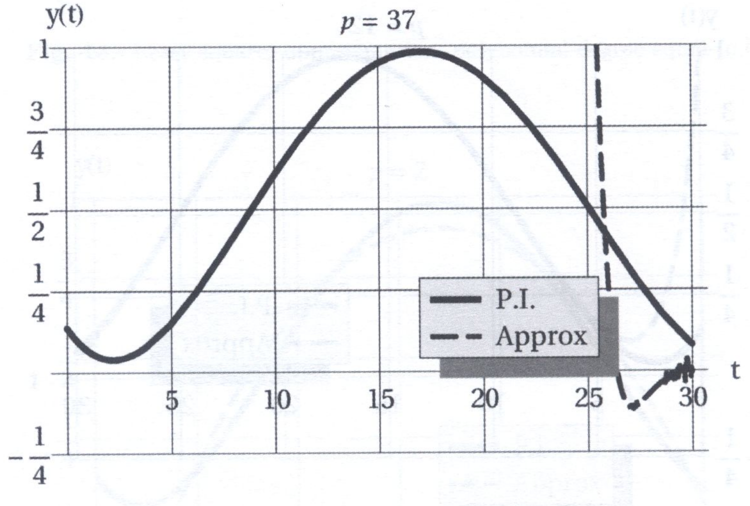

Fig. 19. Least squares approximation, polynomial degree equal to 37

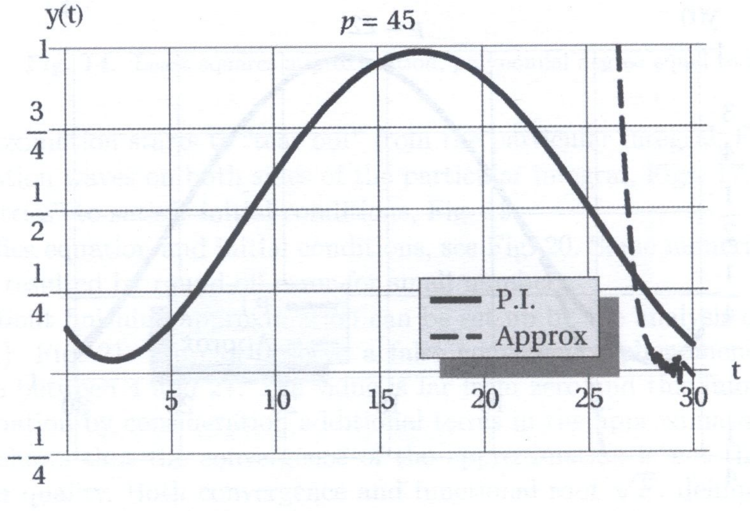

Fig. 20. Least squares approximation, polynomial degree equal to 45

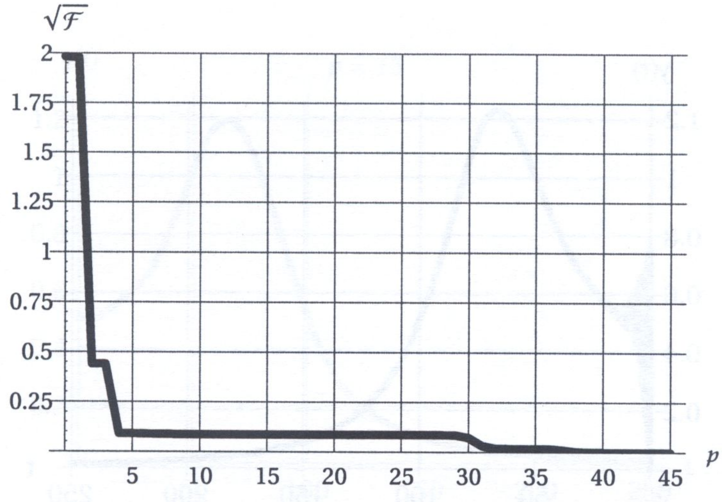

Fig. 21. Convergence of the functional (1) root $\sqrt{F}$ with regard to the polynomial degree

3.2.3. Example 3

Let us consider the linear differential equation $e == 0$ with not constant coefficients:

$$e := a(t)\ y''(t) + 2y'(t) + b(t)\ y(t) - 100, \tag{20}$$

where:

$$a(t) := \frac{t}{50} + 4, \tag{21}$$

and

$$b(t) := 200 - \frac{t^2(t-100)}{1250}, \tag{22}$$

in the interval $t \in \langle 0, 250 \rangle$ and initial conditions: $y(0) == 0$ and $y'(0) == 0$. Equation of that type may have a physical sense.

The initial-value problem described with this differential equation and boundary conditions is stable in the Lyapunov sense but the domain is relatively long, with comparison of the period of the free vibrations, which can be estimated as $T \approx 1.2$. Value of T has been estimated analyzing the diagram of the approximated solution in the interval $t \in \langle 0, 10 \rangle$ (not shown in the paper). Therefore the solution is highly oscillating in the beginning of the domain but quickly decay to the particular integral. Thus, the numerical procedure requires 6830 steps to obtain satisfactory approximation, see Fig. 22. The particular integral is relatively smooth and dominates on the most of the domain.

The least squares approach may be applied to obtain particular integral of equation (20). If we neglect both boundary conditions (by multiplying them by zero weights in the functional F, definition (1)) we can approximate particular integral. The negligence of both boundary conditions is possible since the lowest degree of the derivative in the differential equation is equal to zero.

Due to non constant coefficients in the differential equation it is impossible to find its closed solution.

Diagrams presented in Figs. 23, 24, 25, and 26 show the convergence of the approximation with enlargement of polynomial degree. Comparing diagrams on Figs. 25 and 26 we find that they do not differ a lot.

Figure 28 shows the convergence of the square root of the functional $\sqrt{F}$, definition (1). It confirms that the obtained approximation with polynomial degree equal to 25 is satisfactory since respective to it value of the functional is close to zero (with comparison to the value of the approximation with the polynomials of lower degrees).

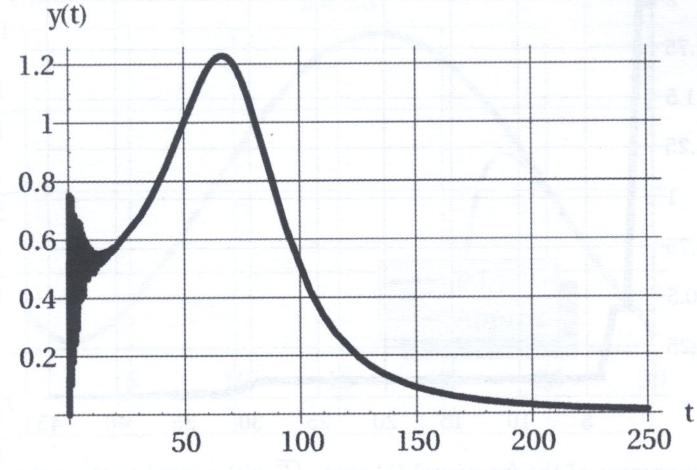

Fig. 22. Result of numerical approximation

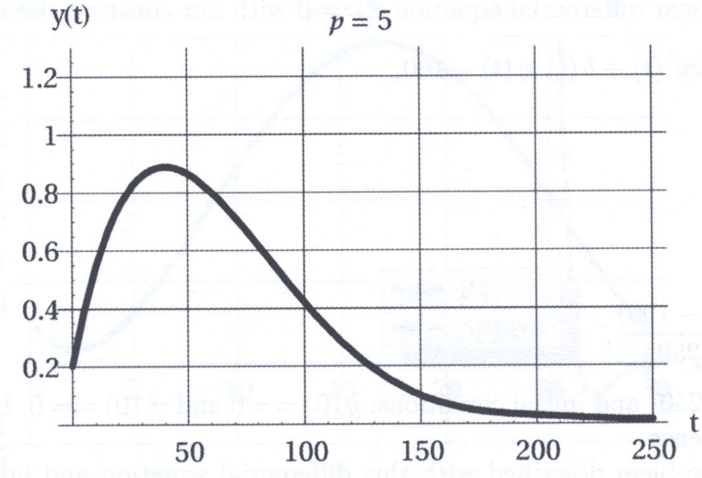

Fig. 23. Least squares approximation, polynomial degree equal to 5

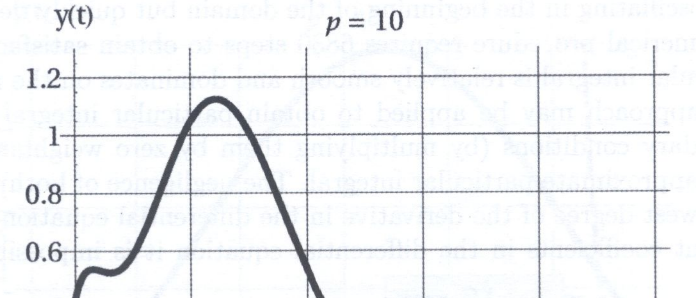

Fig. 24. Least squares approximation, polynomial degree equal to 10

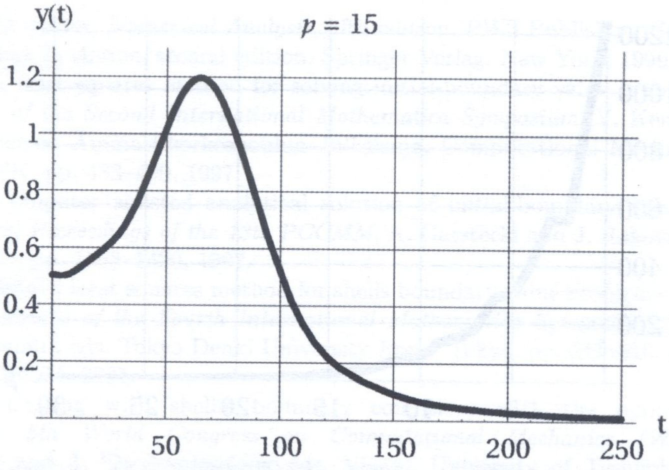

Fig. 25. Least squares approximation, polynomial degree equal to 15

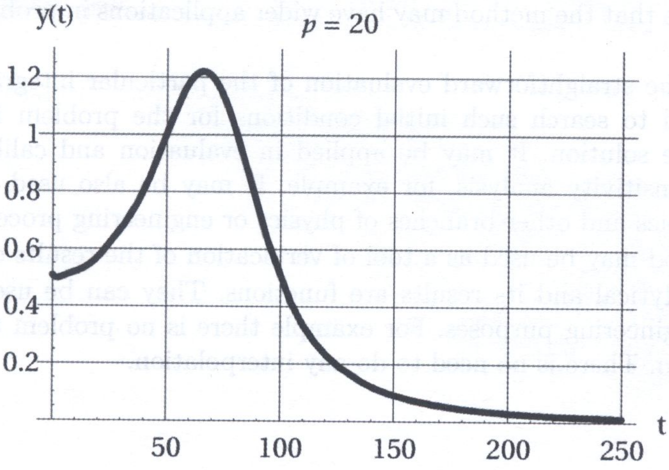

Fig. 26. Least squares approximation, polynomial degree equal to 20

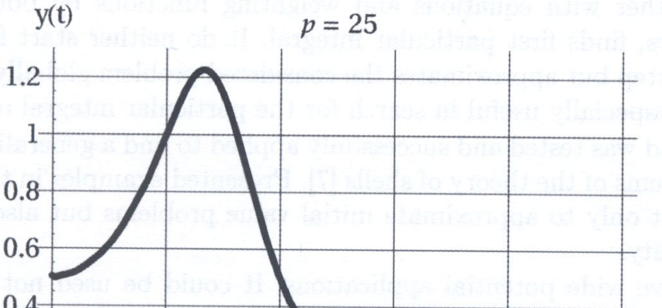

Fig. 27. Least squares approximation, polynomial degree equal to 25

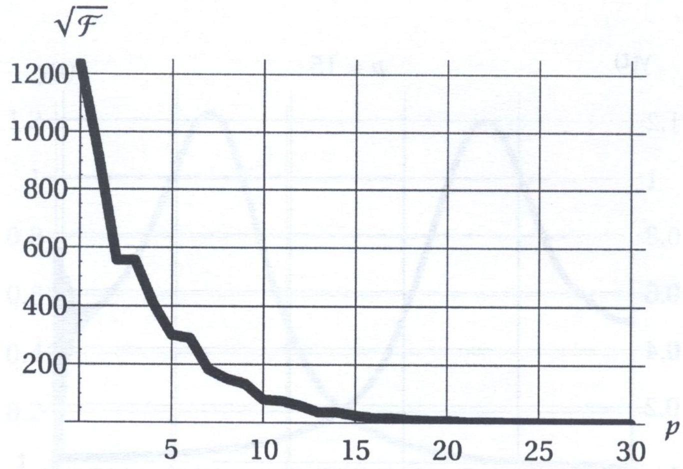

Fig. 28. Convergence of the functional (1) root $\sqrt{F}$ with regard to the polynomial degree

4. Other applications

The last example shows that the method may have wider applications in problems of computational physics and mechanics.

The possibility of the straightforward evaluation of the particular integral for the initial-value problems may be used to search such initial conditions for the problem to avoid influences of general integral on the solution. It may be applied in evaluation and calibration of parameters of the problem and sensitivity analysis, for example. It may be also used in designing scientific experiments of mechanics and other branches of physics or engineering processes.

Moreover the method may be used as a tool of verification of the results of other methods.

The method is analytical and its results are functions. They can be used directly for further computational and engineering purposes. For example there is no problem to find a derivative or integrating the function. There is no need to do any interpolation.

5. Conclusions

Presented examples proves that the refined least squares approach is not sensitive to instability in the Lyapunov sense. The presented approach to the method, where boundary or initial conditions are approximated together with equations and weighting functions by boundary conditions are relatively small numbers, finds first particular integral. It do neither start from initial conditions nor find points step by step but approximates the considered problem globally in the whole domain. Due to that it may be especially useful in search for the particular integral of the problem.

Originally the method was tested and successfully applied to find a generalized particular integral for ill-conditioned problems of the theory of shells [7]. Presented examples in this contribution shows that it may be used not only to approximate initial value problems but also avoid problems with another kind of instability.

The method can have wide potential applications. It could be used not only to verify results of numerical and asymptotic approaches, but also may become an alternative to them. This thesis should be supported by further research, of course.

The method is analytical indeed, but it becomes computer one thanks to computer algebra systems and could be applied for approximation of ill-conditioned tasks of mechanics.

The method has an additional tool for verification of the approximation quality. It is a value of the functional (1) root $\sqrt{F}$ which is a generalization of L_2-norm. Completed with analysis of convergence it produces answer about reliability of an approximation.

References

[1] R. L. Burden and J. D. Faires, *Numerical Analysis*, fifth edition. PWS Publishing Company, Boston, 1993.

[2] S. Wagon, *Mathematica in Action*, second edition. Springer-Verlag, New York, 1999.

[3] R. A. Walentyński, A least squares method for solving initial-boundary value problems. *Innovations in Mathematics, Proceedings of the Second International Mathematica Symposium*, V. Keränen, P. Mitic. and A. Hietamäki, eds. Rovaniemen Ammattikorkeakoulun Julkaisuja, Computational Mechanics Publications, Boston, MA; Southampton, UK, pp. 483–490, 1997.

[4] R. A. Walentyński, Computer assisted analytical solution of initial-boundary value problems. In: *Computer Methods in Mechanics, Proceedings of the 13th PCCMM*, A. Garstecki and J. Rakowski, eds. Poznań University of Technology, Poznań, pp. 1363–1400, 1997.

[5] R. A. Walentyński, Refined least squares method for shells boundary value problems. In: *Symbolic Computation: New Horizons, Proceedings of the Fourth International Mathematica Symposium*, Y. Tazawa, S. Sakakibara, S. Ohashi and Y. Uemura eds. Tokyo Denki University Press, Tokyo, pp. 511–518, electronic extended version on the conference CDROM, 2001.

[6] R. A. Walentyński, Dealing with shell's boundary conditions with the refined least squares method. Proceedings of the *5th World Congress on Computational Mechanics (WCCM V)*, H. A. Mang, F. G. Rammerstorfer and J. Eberhardsteiner, eds. Vienna University of Technology, Vienna, pp. 10, 2002 http://wccm.tuwien.ac.at/publications/Papers/fp80303.pdf

[7] R. A. Walentyński, *Application of Computer Algebra in Symbolic and Boundary-Value Problems of Theory of Shells.* Silesian University of Technology Press, Civil Engineering (100)1587, Gliwice, 2003.

[8] S. Wolfram, *The Mathematica Book*, fourth edition. Cambridge University Press and Wolfram Research, Inc., New York and Champaign, 1999.