Lodz University of Technology

Faculty of Electrical, Electronic, Computer and Control Engineering

DOCTORAL THESIS
Extended Abstract

Dariusz Brzeziński MSc Eng.

Problems of Numerical Calculation of Derivatives and Differential Equations of Fractional Orders

Supervisor
Professor Piotr OSTALCZYK PhD Eng.

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Introduction

Fractional calculus can be interpreted as an extension of the concept of derivative operator from integer order n to arbitrary order ν.

English term *fractional calculus* is misleading because it suggests that differentiation and integration orders may assume non-integer values only. The more appropriate description of this branch of mathematics would be differentiation and integration of any order. In practice, both integration as well as differentiation order may assume irrational or rational, real or complex values. In this context derivatives and integrals of integer order can be considered as one of special cases of fractional calculus.

Beginnings of fractional calculus date to the same time as integer order calculus. It came to an existence with the question of consequences of "taking square root of 1^{st} derivative" arose in 1695. However, the first substantial effects of this consideration emerged many years later.

The most important dates in context of the scope of this PhD dissertation are: 1832 and 1876, when Liouville and Riemann, respectively, formulated the definition of fractional derivative and integral and 1867 when Grünwald presented fractional derivative as the limit of a sum.

A significant interest increase for this branch of mathematics can be observed only in the 2^{nd} half of the 20^{th} century: in 1974 the very first book entitled *The Fractional Calculus. Theory and Application of Differentiation and Integration to Arbitrary Order* by Oldham and Spanier was published and the very first conference *International Conference of Fractional Calculus and Its Applications* entirely dedicated to fractional calculus took place around the same time at the University of New Heaven, Connecticut, USA.

Since that time on, the topic became interesting for scientists from various areas of mathematics, physics, chemistry, electrical engineering, economy and biological sciences. Initial works had a pure theoretical character. However, later, can be noticed an intensification of research on practical applications of this tool in physics, technical, biological and economical sciences. In technical sciences, application of fractional calculus is mostly applied for areas of electrical engineering, electronics and control systems as well as signals analysis and processing.

It is worth to mention that the poster entitled *Fractional Calculus: Models, Algorithms, Technology* by Prof. J.A. Tenrerio Machado published in journal Discontinuity, Nonlinearity, and Complexity, 4(4), 2015 lists over 30 application areas of fractional calculus.

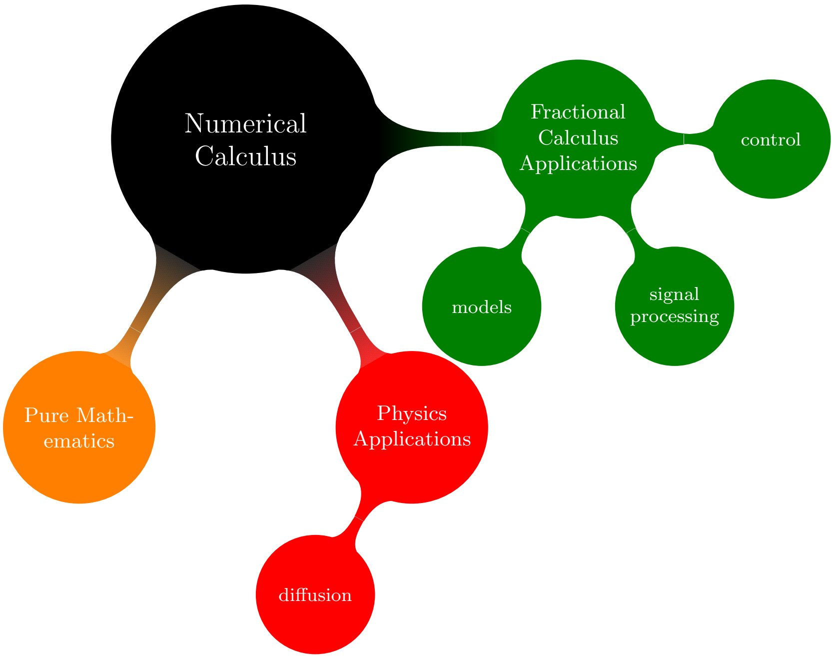

Fig. 1: Application areas for fractional order derivatives and integrals.

Fractional order operators of differentiation and integration are non-local operators. This property builds many advantages. However, it increases, among others, the difficulty level of their numerical calculations, because it requires the inclusion of functions values from an entire integration interval.

Fractional order derivatives and integrals can be calculated using well known definitions and formulas by applying numerical methods. However, problems associated with them has not been solved entirely, especially in context of accuracy of calculations and methods of its assessment.

The integrands in Riemann/Liouville and Caputo formulas are fast-changing and include singularity at the end of integration interval. There is also general lack of mathematical formulas for their exact values. On the other hand, Grünwald-Letnikov formula requires a huge amount of coefficients for calculations with accuracy greater than four decimal places (relative error smaller than 10^{-04} calculated in respect to exact values).

Effectiveness of fractional derivatives and integrals practical applications can be increased by improving their computational accuracy. Thus, increasing it is the main scope of this PhD dissertation.

Accuracy assessment is crucial in the process of an algorithm development and evaluation of its efficiency and proper operation. An effective accuracy assessment based on error calculation in case of fractional order derivatives and integrals computations is difficult due to general lack of availability of analytical formulas for their exact values. They are accessible only for exponential, trigonometric, power and step functions. Therefore, another goal of this PhD dissertation is to develop versatile accuracy assessment criteria, which can be applied with any function.

One of many important applications of fractional calculus is finding solutions of differential equations of fractional orders. Unfortunately, many of them pose problems in this context. Therefore, searching for new effective and stable numerical algorithms for finding their solutions became the very important task for many computer scientist around the world.

For this purpose can be applied algorithms developed for classical numerical analysis. However, they must be modified for this new task.

Laplace Transform proved to be a very effective tool for finding solutions of linear fractional order differential equations. An obtained solution by using Laplace Transform requires to be inverted to time depended solution. This is done by applying Inverse Laplace Transform. When analytical inversion formula does not exist or is difficult to obtain, numerical approximation of Inverse Laplace Transform is commonly performed.

Due to existence of large amount of algorithms of numerical approximation of Inverse Laplace Transform, it is crucial to evaluate them for accuracy and versatility in context of, among others, solution of linear fractional order differential equations.

Numerical calculations of fractional order derivatives and integrals and their computer applications, which are considered in the scope of this PhD dissertation, required skillful joining of computer science branches: algorithmics and programming with mathematics as well as theoretical and practical knowledge about the numerical integration.

The difficulty of the problems selected to be solved to prove the theses of the PhD dissertation required the development of new algorithms and the adaptation of some existing ones. It made mandatory to apply a novelty programming technology known as *infinite precision computing* as well. It enables using arbitrary precision for computations.

The application of arbitrary precision enabled increasing the accuracy many times in comparison to the application of standard double precision for computations. It also mitigated the influence of mathematical operations rounding on final results.

The importance of elimination of limited precision in computer calculations was best presented by Toshio Fukushima in *The Astronomical Journal* in 2001 by giving the following example: "In the days of powerful computers, the errors of numerical integration are the main limitation in the research of complex dynamical systems, such as the long-term stability of our solar system and of some exoplanets [...]" and gives an example where using double precision leads to an accumulated round-off error of more than 1 radian for the solar system.

Theses of the PhD Dissertation

There have been defined the following theses:

1. In the scope of fractional-order differentiation and integration, the application of (i) an independent variable substitution in an integrand and (ii) adaptation of the Gauss-Jacobi Quadrature weight function increase significantly the final accuracy of numerical calculations

2. In the scope of fractional-order numerical integration and differentiation, the use of the concatenation rules for the generalized operators makes possible to assess the accuracy of numerical calculations for any function

3. Application of the Talbot or the De Hoog algorithm of the numerical Inverse Laplace Transform leads to solutions of linear fractional order differential equations with high accuracy.

Formulated theses has been successfully proved. Next, there are presented the most important results and conclusions.

Thesis 1

There exist several definitions and formulas for fractional order derivatives and integrals calculations. The methods of their accuracy increase presented in this PhD dissertation only apply to: (i) Riemann-Liouville fractional integral, (ii) Caputo fractional order derivative and its equivalent Riemann-Liouville fractional derivative and (iii) Grünwald-Letnikov fractional differ-integral.

In cases of (i) and (ii), there is applied classical numerical integration known from numerical analysis of integer orders. In case of (iii) fractional order derivatives and integrals are approximated by applying finite differences using formulas for backward sums and differences.

The low accuracy problem of fractional order derivatives and integrals computations for Riemann-Liouville/Caputo formulas can be reduced to the problem of integrating the kernel of the integrand in these formulas. It is difficult to integrate due to the presence of singularity on the end of integration interval, which is preceded by rapid and stiff increase of integrand's values.

This problem can not be solved by applying the numerical methods and techniques common for integer order derivatives and integrals calculations in their existing form. Accessible accuracy of calculations is low - relative error calculated in respect to exact values can range from 1% to even 200-300% dependently on an applied numerical method of integration, calculated fractional order and type of function.

The general concept of the problem effective solution is that (i) either the integrand must be transformed to fit into a selected numerical method requirements for high accuracy integration or (ii) a numerical method of integration must be adapted to handle with high accuracy the integrand with particular difficult feature.

In case of (i) two effective methods were developed and implemented using C++ programming language; wherein, in case of the 2^{nd} method, due to well known flaws of the double precision computer arithmetic and to be able to achieve the highest accuracy, C++ language capabilities had to be enhanced by applying the *infinite* precision. For this purpose, the GNU MPFR arbitrary precision library is selected.

In case of (ii), one effective method was developed and C++ was selected for its implementation. Wherein, the double precision implementation accuracy increase was incremented by the use of the GNU MPFR library.

The methods are as follows:

1. For (i) - analytical transformation of the integrand in the formulas via independent variable substitution prior numerical integration with three custom functions. They were proposed to adapt the integrand to the requirements for high accuracy integration by applying selected Gauss quadratures
2. For (i) - transformation of the integrand via independent variable substitution as a numerical quadrature using the Double Exponential Quadrature. There were developed the method of its construction, its application for fractional order derivatives and integrals computations and solutions for numerical implementation issues
3. For (ii) - Gauss-Jacobi Quadrature is selected due its capabilities to deal with the integrands equipped with singularities at the end of integration intervals. However, its weight function and the default integration interval had to be adapted during the quadrature construction and application.

The conclusions for this part are as follows:

Analytical integrand transformation prior numerical integration is very effective and can increase accuracy of numerical integration many times, depending on particular substitution selected according to the requirements of a particular Gauss quadrature - relative error can be reduced up to 10^{-16} in respect to the exact values. However, the method is arduous, because it requires manual transformation of each integrand prior the integration.

Transformation of the integrand via independent variable substitution as a numerical quadrature enables omitting the arduous manual transformation part of the integrand and automating the whole substitution and integration process.

The employed numerical quadrature is the Double Exponential Quadrature, which is built upon the Double Exponential Transformation (it joins the transformation of the integrand using hyperbolic functions and the trapezoidal rule for the integration). The Transformation has not been used before for fractional order derivatives and integrals computations. Its double precision implementation reduces relative errors calculated with respect to the exact values up to 0.01 for the most fractional orders. Its high-precision variables implementation enables incrementing this computational accuracy dozens of times (relative error reduced up to 10^{-50} in respect to the exact values). However, to achieve this increase, the precision of computations had to be increased to 1500, and in cases of some orders to 5000 digits due to underflows occurrence during the integration of the transformed integrand. They occurred at both ends of the transformed integrand, wherein their distance from the zero contributed the most for the integration accuracy. Nevertheless, the high-precision implementation can still be easily run on moderate class computer.

Both methods proved to be effective under the condition of finding and applying substitution function which transforms the integrand into one which matches the very requirements for high-computation of a selected method of integration.

Gauss-Jacobi Quadrature application with adapted weight function and integration interval using standard double precision for the computations enables reducing relative error of fractional order derivatives and integrals up to 10^{-14} in respect to the exact values. Programming it using high precision variables and corresponding mathematical functions reduces this relative error up to 10^{-120} independently of calculated fractional order, integration interval and type of function. It is also very efficient method which requires for this accuracy only at maximum 32 sampling points of function. For the relative error reduction up to 10^{-50} it is required only 4-8 sampling points. It is worth mention that derivatives and integrals of fractional orders near 0 and 1, which calculation of is not accessible by applying any other method of numerical integration, can be calculated with the same efficiency and accuracy as fractional orders of moderate computational difficulty, e.g. 0.5.

Some additional studies on accuracy increase of fractional order derivatives and integrals computations involved the Grünwald-Letnikov formula application. They were not placed in the theses though they are in the scope of the dissertation.

The Grünwald-Letnikov formula uses fractional order backward differences and sums for fractional order derivatives and integrals computations. Its algorithm consists of summation of function values and some coefficients which values converge to 0.

Due to the importance of unchanged function values for the correct calculations, a function can not be transformed or modified in order to increase accuracy of computations.

The general concept of solutions for the accuracy and the efficiency problems by applying the Grünwald-Letnikov formula took a different approach and involved the application of: (i) a different but equivalent method of summation and the use of different coefficients (with different properties), (ii) different schemas for a function discretization and more than one function's value per step in summation.

In case of (i), the application of Horner's schema added some crucial capability to the Grünwald-Letnikov method to operate with significantly increased efficiency and accuracy with decreased amount of coefficients.

Case (ii) and (iii) involved the application of central and forward point discretization schemas and a discretization schema with 2 or 3 points per step in summation.

The conclusion for this part is that by applying of the methods (i), (ii) and (iii), it is possible to compute fractional derivatives and integrals with 4 or more times higher accuracy with drastically reduced amount of coefficients than it is in case of the application of the default Grünwald-Letnikov formula form. However, the accuracy increase still depends on the characteristics of a function, which feature is forced by the summation algorithm and the properties of the coefficients.

A demanding case, when there is to calculate a low order of fractional derivative/integral for a high frequency periodic function, which bounding box is either constant or increasing, requires - in case of the default Grünwald-Letnikov formula - the calculation and the multiplication of over 2 billion of coefficients for the relative error calculated in respect to the exact values to be reduced up to 10^{-8}. The developed methods application enables reducing this amount to one hundred thousand.

Thesis 2

Problem included in the 2^{nd} thesis of the dissertation concerns the accuracy assessment of fractional order derivatives and integrals computations.

The accuracy assessment is the crucial component of programming because it enables examining a program proper operation and its accuracy.

Common approach to the accuracy assessment requires an exact value for the error calculation. In case of fractional order derivative and integral computations, the accuracy assessment is difficult due to general lack of formulas for their exact values.

The general solution concept of the problem developed for proving the 2^{nd} thesis assumes that the accuracy assessment is possible for computation of fractional order derivative or integral for any function.

The solution has been accomplished by applying: (i) the concatenation rules for generalized fractional order operators of differentiation and integration and (ii) fractional order differentiation and integration of Mittag-Leffler special function.

The practical meaning of (i) is that the n-times concatenation of fractional operators which orders sum is an integer greater than zero enables assessing the accuracy of computation in respect to classical first derivative and integral of the first orders' values or if the order equals zero - in respect to value of function.

In case of (ii), Mittag-Leffler function is applied for the accuracy assessment of fractional order derivatives and integrals.

To evaluate the effectiveness and precision of the accuracy assessment of both solutions: (i) a numerical algorithm for fractional order operators concatenation has been developed and implemented, separately for integration methods which use equally-spaced nodes and for Gauss quadratures, (ii) the formulas for Mittag-Leffler function with one, two and three parameters using series expansion has been developed, wherein the algorithm made possible to calculate the function value with arbitrary selected accuracy. Both tasks has been accomplished by using C++, the double precision as well as high-precision variables and corresponding functions. The latter was required due to the fact that the testbed for effectiveness of the accuracy assessment were the methods of fractional order derivatives and integrals computations developed for proving the thesis 1 of this PhD dissertation.

The conclusion for this part is that fractional order operators concatenation can be effectively applied to assess accuracy of fractional order derivatives and integrals computations for any function. However, how precisely the accuracy can be assessed depends on how a particular method of numerical integration handles the decreasing amount of information about a function in a given interval. Such a situation occurs when transiting from an input function in a continuous form to a discrete one.

Gauss quadratures require full information about the function in a given interval to give accurate results. In case of theirs, the accuracy assessment is precise to 6-7 decimal places. The application of high-precision variables does not make it more precise.

In case of quadratures with equally-spaced nodes as for example the Double Exponential Quadrature, that uses the trapezoidal rule for integration, the accessible accuracy of computations can be fully assessed by applying maximum threefold fractional order operators concatenation.

The computational accuracy of simple algorithmic methods, as for example the Grünwald-Letnikov method, can be precisely assessed by applying even four or more-fold fractional order operators concatenation.

The advantage of the developed accuracy assessment method is its versatility, i.e. the accuracy assessment can now be successfully established for fractional derivatives and integrals computations of any function. Although, in the worst scenario the accuracy can be assessed accurately only for 6-7 decimal places, it is an obvious advantage in case of fractional order derivatives calculations of function, which lacks exact values formulas.

Thesis 3

The Laplace Transform proved to be a valuable tool for solving linear differential equations. Due to some of its properties, it is possible to apply it for finding solutions of fractional linear differential equations. These solutions have to be inverted by applying the Inverse Laplace Transform.

When an inversion formula does not exist or is difficult to obtain, numerical approximation of the Inverse Laplace Transform is commonly conducted.

The 3^{rd} thesis of the dissertation concerns the accuracy of numerical approximation of the Inverse Laplace Transform in context of test sets, which include inversion problems associated with fractional calculus.

Numerical approximation of the Inverse Laplace Transform is a challenging task. There exist multiple algorithms presenting various approaches to the inversion problem. Their accuracy capabilities are unknown regarding the scope of the evaluation. Additionally, the formula of the Inverse Laplace Transform includes difficult for computer implementation multiplication by exponential function of time which leads to overflows and high-inaccurate results, if directly used.

The general solution concept of the problem is as follows: (i) select the most effective algorithms of numerical approximation of the Inverse Laplace Transform, (ii) implement them using more than one programming language, (iii) solve the problems of computer implementation by applying arbitrary precision libraries, (iv) select for the inversion accuracy evaluation test sets consisting of problems, which are difficult to invert due to general computational problems, problems, which are associated with fractional calculus and solutions of important fractional order linear differential equations obtained by applying the Laplace Transform.

To evaluate the effectiveness of the solutions: (i) there were selected 7 algorithms representing almost all approaches to numerical approximation of the Inverse Laplace Transform based on the literature of the subject, and (ii) programmed using C++ and Python programming languages, (iii) solving most of the critical programming issues by applying the GNU MPFR arbitrary precision library for C++ and mpmath for Python, (iv) evaluation the algorithms using test sets, which included problems difficult to invert due to general computational problems, associated with fractional calculus and 5 solutions of important linear, fractional differential equations, which were selected from the literature of the subject.

The conclusions for this part are as follows:

Numerical approximation of the Inverse Laplace Transform is a very effective tool for inverting with high accuracy solutions found by applying the Laplace Transform.

The selection which numerical algorithm is to apply, is to be made on the basis of the particular inversion problem.

The same inverse problem can be often correctly and accurately inverted by applying more than one algorithm.

The Talbot algorithm is the most accurate and versatile of all. However, it requires the input of singularities coordinates, which calculation can be difficult and hinder its effective application.

The De Hoog algorithm is equally accurate - in most cases - to the Talbot method and it does not require the input of singularities coordinates. Thus, it can be considered as a replacement for the Talbot algorithm when singularities locations are not possible to input.

The Abate and Whitt algorithm is advised for inversions of problems which time depended solutions are periodic functions.

C++ and Python, used alongside for programming, have equal capabilities. However, the algorithms are shorter and simpler to code using Python. Still, due to their compactness, there are no significant accuracy or speed differences between both languages implementations. Although, they confirm each other the evaluation results.

Numerical approximation of the Inverse Laplace Transform is difficult to program, especially by applying the standard double precision due to the multiplication by the exponential term included in the inversion formula. If it is incompetently programmed, it can lead to a large increase in the total error from even small numerical and finite precision errors. Thus, it requires the application of high-precision variables and the corresponding mathematical libraries for programming.

Appendices

Extensiveness of the research conducted for the purpose of proving the theses of the PhD dissertation made possible to find solutions of three additional problems:

1. The dependency of numerical calculations accuracy on an amount of coefficients used with the Grünwald-Letnikov formula
2. Application of *Calculation Tail Length* and different discretization schemas for mitigation of time and memory shortages influence on accuracy in real time microprocessor calculations
3. The Double Exponential Transformation as an equivalent replacement for major Gauss quadratures in context of integration accuracy.

The Grünwald-Letnikov formula computational accuracy of fractional order derivatives and integrals depends on an amount of coefficients used during calculations. Their amount required for a set accuracy depends in turn on characteristics of a function (shape, frequency) and fractional order which is to calculate.

Conducted research results enable concluding that:

The monotonicity of a function is the main factor which influences the computational accuracy. If a function is monotonically increasing there is required fewer coefficients to complete the calculations with a set accuracy than in the case of a function which is monotonically decreasing.

The order of fractional derivative or integral influences an amount of the coefficients required for a set accuracy as well. Low orders computations require generally more coefficients.

However, this is the frequency of a periodic function which has the enormous influence on an coefficients amount required for the accuracy: it increases intensively with the frequency of a function. If additionally a bounding box is of increasing or constant character and there is low order or fractional derivative to compute, the amount of required coefficients could reach many millions.

Time and memory limitations in real-time microprocessor calculations resulted from various coefficients amount requirements for a set accuracy in case of a particular type of a function can decrease computational accuracy.

The application of *simplified* variants of the Grünwald-Letnikov formula and its equivalent Horner form as *the calculation tail* can help to mitigate it.

The investigation of *the calculation tail* of variable *length* influence on numerical calculations accuracy led to conclusions that only in case of Horner's simplified variant removal of significant amount coefficients without accuracy loss is possible, i.e. removing 5% to 30% of coefficients required for a set accuracy does not decrease it over assumed level more than by 0.1%.

It was confirmed by the comparison of the computer simulation results with identical calculations conducted with the help of a real-time DSP system.

Additionally, changing the discretization schema to central point in the Grünwald-Letnikov algorithm requires only minimal changes in code. Then, it guarantees multiple times higher computational accuracy with up to thousand times reduced requirements for the coefficients application.

Gauss quadratures are the ultimate tools for high-accuracy numerical integration of difficult integrands (improper integrals, integrals with endpoint singularities). However, they have strict application conditions and are complex to compute. In a nutshell, they cannot be applied as a tool of general application.

The Double Exponential Transformation with appropriate substitution expression enables calculating these difficult integrals with similar or higher accuracy (with slightly more sampling points due to the Trapezoidal Rule application) than commonly applied Gauss-Laguerre, Gauss-Hermite, Gauss-Chebyshev, Gauss-Jacobi, Gauss-Legendre or even Gauss-Kronrod Quadratures. It was proved by direct comparing the integration accuracy.

Future research directions:

Development of an numerical algorithm of fractional order differential equations using the Gauss-Jacobi Quadrature. Implicit collocation points methods, in which the solution of differential equation is approximated by applying polynomial are the most effective tools of this type.