Functional Differentiation of Computer Programs

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Abstract. We present a purely functional implementation of the *computational differentiation* tools — the well known numeric (i.e., not symbolic) techniques which permit one to compute point-wise derivatives of functions defined by computer programs economically and exactly (with machine precision). We show how the use of lazy evaluation permits a transparent and elegant construction of the entire infinite tower of derivatives of higher order for any expressions present in the program. The formalism may be useful in various problems of scientific computing which often demand a hard and ungracious human preprocessing before writing the final code. Some concrete examples are given.

Keywords: Haskell, differentiation, arithmetic, lazy semantics

1. Introduction

The aim of this paper is to show the usefulness of lazy functional techniques in the domain of scientific computing. We present a functional implementacient computation of (point-wise, numeric) derivatives of functions defined tion of the Computational Differentiation techniques which permit an effiby computer programs. A previous version of this work has been presented at plied mathematics. The derivatives are needed for all kind of approximations: analysis of dynamical systems. They permit the computation of geometric properties of curves and surfaces in 3D modelling, image synthesis and animation. In the domain of differential equations, they are used not only directly, but also as an analytic tool for evaluating the numerical stability of a given discrete algorithm. The construction of equations of motion is often based on variational methods, which involve differentiation. Even in discrete tors from the appropriate partition functions, as presented in Knuth, Graham A fast and accurate differentiation is essential for many problems in apgradient methods of equation solving, many sorts of asymptotic expansions, etc. They are needed for optimization and for the sensitivity and stability mathematics the differentiation is useful to compute some combinatorial facthe 1998 International Conference on Functional Programming [14]. and Patashnik's textbook on concrete mathematics [9, Chapter 7].

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1.1. THIS WORK

We are not only interested in the computation of first derivatives, but in implementing a general differentiation operator acting on expressions within a numerical program. We show thus how laziness can be used to define data structures which represent numerical expressions together with all their derivatives

guage Haskell enriched by some generic mathematical operations. It has been tested with the interpreter Hugs[12], and relies on the overloading of arithmetic operations with the aid of type classes. Our basic tools are the corecursive data structures: objects defined by open, non-terminating recursive equations which would overflow the memory if implemented naively in a Our differentiation package is implemented in the purely functional lanwrt. a given independent variable.

The presented approach requires the lazy evaluation strategy which states sonably long history, lazy functional techniques are rarely used in numerical computations. First, they remain relatively unknown to the scientific computtions introduce an overhead which might be considered harmful by those for that a function evaluates its argument only when it needs it. Despite a reaing community. Then, there are some efficiency reasons: the delayed evalua-

Our implementation is not meant as a replacement of highly tuned and efficient low-level numerical programs. The Computational Differentiation packages cited later have been optimized for performance. We show that lazy techniques provide useful coding tools, clear, readable, and semantically very powerful, economising plenty of human time. A few problems rarely whom the computation speed is crucial.

addressed by the standard Computational Differentiation texts, such as the construction of functions defined by differential recurrences, become very easy to code using our lazy approach. This is the main goal of the paper. We assume that the reader is acquainted with the lazy evaluation paradigm, and can follow the Haskell code. Elementary notions of differential calculus and of algebraic structures are also needed for the understanding of our

implementation.

OVERVIEW OF MECHANICAL DIFFERENTIATION TECHNIQUES

There are essentially three ways to compute derivatives of expressions wrt.

some specific variables with the aid of computers.

The approximation by finite differences: $df \to \Delta f = f(x + \Delta x) - f(x)$.

This method may be either inaccurate if Δx is big, or introduce serious cancellation errors if it is too small, so it might be numerically unstable. Sometimes the functions must be sampled many times in order to permit the construction of a decent polynomial interpolant. The complexity of the algorithm may be substantial, and its coding is rather tedious.

pencil/paper/wastebasket. The derivatives, gradients, Jacobians, Hessians, Symbolic computations. This is essentially the "manual", formal method, with a Computer Algebra package substituted for the combined tool: etc. are exact, but the technique is rather costly. The intermediate expression swell might be cumbersome, sometimes overflowing the memory. The generated numerical program is usually unreadable, and needs a good optimizing compiler in order to eliminate all the common subexpressions, which tend to proliferate when symbolic computations are used intensely.

Moreover, it is not obvious how to differentiate expressions which result

from an iterative process or other computations which use non-trivial control structures, so this technique is usually not entirely automatic. The Computational Differentiation (CD) known also as Automatic or Algorithmic Differentiation, which is the subject of this article. Computational Differentiation is a well-established research and engineering domain, see, e.g., [3, 4, 8, 10, 11]. George Corliss also established a comprehensive bibliography [7]. The CD algorithms are numerical, but they yield results as exact as the numerical evaluation of symbolic derivatives. Relatively little has been written about functional programming in this context, most developments appear to be carried out in Fortran, C, or C++. C++ is a natural choice if one wants to exploit the arithmetic operator overloading (see the description of ADOL-C [10]). For languages without overloading, some source code preprocessing is

1.3. COMPUTATIONAL DIFFERENTIATION

usually unavoidable.

The CD idea relies on standard computer arithmetic, and has nothing to do with the symbolic manipulations of data structures representing the alge-

braic formulae. All complicated expressions coded in a standard program-

ming language are composed of simple arithmetic operations and elementary, built-in functions with known differential properties. Of course, a program is not just a numerical expression. It has local variables, iterations, sometimes explicit branching, and other specific control structures, which makes it difficult to differentiate symbolically and automatically a sufficiently complicated code. A symbolic package would have to unfold the loops and to follow the branches — in fact, in general, it would have to interpret the program symbolically. diffalg.tex; 15/09/2000; 3:14; p.3

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But it is always possible to compute all the needed derivatives in parallel

the compositions obey the chain rule: d(f(g(x))) = f'(g(x))d(g(x)). The for all primitive arithmetic operators the derivatives are known, and that all same control structures as in the main computation are used (although not

with the main expressions in an augmented program, taking into account that

We shall restrict the presentation to the univariate case, and we discuss the *direct* or *forward mode* of CD. The alternative, reverse mode is more important for the multi-variate case. A functional implementation of the reverse mode is treated in another paper [18]. The multivariate case in a geometric necessarily in the same way).

1.4. OVERVIEW

framework (differentiation of tensors and exterior forms) is discussed in [17].

The rest of the paper is organized as follows: we begin with the implementation of a simplified framework for computing just the first derivatives, which does not require laziness. For simple usages this variant is more efficient than the full package.

Next we discuss some features of the Haskell class system, and the differences between our framework and the numerical classes belonging to Haskell

We present then a short, elementary introduction to differential algebra, standard libraries.

and we pass to the implementation of our lazy version of it.

The implementation is followed by a collection of non-trivial examples of they show not only how to compute derivatives in a program, but principally applications of the package. They occupy a substantial part of the paper, and how to use them for solving complex programming tasks.

2. Overloading and Differentiation; First Approach

of a numerical value of an expression and the value of the derivative of the In this section we introduce an "extended numerical" structure: a combination same expression at the same point. We may declare

type Dx = (Double, Double)

where only for simplicity of presentation we restrict the base type to **Double**. In principle we can use any number domain rich enough for our needs. This domain should be at least a ring (a field if we need division).

derivation variable which is represented as something like (2.71828, 1.0). Since we are not doing symbolic calculations, the variable does not need to The elementary objects which are injected into the calculations are either explicit constants, for example (3.14159,0.0), or the (independent) have a particular name. From the above we see that constants are objects

whose derivatives vanish, and the variable (henceforth always referred to through the italic typesetting), has the derivative equal to 1. The value x in From the mathematical point of view we have constructed a specific ex-(x, x') will be called the "main" value.

tension of the basic domain. All objects (e, p) with $p \neq 0$ are algebraically independent of constants (e, 0). The augmented arithmetic defined below ensures this property, and shows that the subset of constants is closed under all arithmetic operations.

2.1. OVERLOADED ARITHMETIC

In order to construct procedures which can use the type Dx we declare the following numerical operator instances:

```
(x,a)+(y,b) = (x+y, a+b)
                          = (x-y, a-b)
                          (x,a)-(y,b)
```

$$(\alpha - \alpha \cdot \lambda - \alpha) = (\alpha \cdot \lambda) - (\alpha \cdot \alpha)$$

$$(x,a) \cdot (y,b) = (x*y, x*b+a*y)$$

$$negate(x,a) = (negate x, negate a)$$

= (x/y, (a*y-x*b/(y*y))

or, for the reciprocal:

(x,a)/(y,b)

recip
$$(x,a) = (w, (negate a)*w*w)$$
 where $w=recip x$
We define also two auxiliary functions which help to construct the constants and the $variable$.

dCst z = (z, 0.0)

$$acst z = (z, 0.0)$$

 $avar z = (z, 1.0)$

(Conv. of numeric, real constants) from Double z = dCst zNow all rational functions, e.g.,

$$f x = (z + 3.0*x)/(z - 1.0)$$
 where $z=x*(2.0*x*x + x)$

called with an appropriate argument, say, £ (dvar 2.5) compute the main

value and its derivative. The user does not need to change the definition of the function. The following properties of Haskell are essential here:

- The type inference is automatic and polymorphic. The compiler is able to deduce that £ accepts an argument of any type which admits the
 - multiplication, addition, etc. The same function can be used for normal
- floating numbers.
- The numerical constants are automatically "lifted": 3.0 in the source is
- compiled as the polymorphic expression (fromDouble 3.0), whose type depends on the context.
 - We implement also the chain rule, which for every function demands the functions may then be easily lifted to the **Dx** domain. Here are some examples: knowledge of its derivative form, for example $sin \to cos$. All elementary

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```
(recip x means I/x)
dlift f f' (x,a) = (f x , a * f' x)
                                                                                                                              sqrt = dlift sqrt ((0.5 /) . sqrt)
                                                                                                     dlift cos (negate . sin)
                                                                                                                                                        log = dlift log recip
                                                   = dlift exp exp
                                                                            dlift sin cos
                                                                                                         II
                                                                               II
                                                                             sin
                                                                                                        GOS
```

and now the following program

0.521095). The call ch (dcst 0.5) calculates the main value, but its computes automatically the hyperbolic sine together with the hyperbolic cosine for any concrete value, here for x = 0.5. The value of res is (1.12763,

derivative is equal to zero. The expression sqrt (cos (dvar 1.0)) computes also the value $-0.572388 = -\sin x/(2\sqrt{\cos x})$ for x = 1. If a function is discontinuous or non-differentiable, this formalism might return an unsatisfactory answer. For example, if we define abs x = if x>0 then x else -x, the derivative at zero is equal to -1, if the test x>0, with the appropriately overloaded (<) operator, uses the main value only.

2.2. USAGE OF THE HASKELL CLASS SYSTEM

The above presentation of the arithmetic operations over pairs of numbers is simplified. In a concrete implementation in Haskell the overloading must follow the discipline of its type system, where all generic operations are declared within classes, and all datatypes which accept those operations are instances of these classes. The standard Haskell library (Prelude) specifies square root, and other elementary functions, etc. Our package does not use these classes. We found it more natural to introduce a modified "algebraic and is more suitable for the definition of arithmetic operations over intricate several arithmetic classes: Num for objects which can be added or multiplied, Fractional where the division is declared, Floating with the exponential, style" library, which corresponds to the classical mathematical hierarchy, mathematical objects.

fines the addition and the subtraction, Monoid for multiplication, Group for division, etc. Some more involved operations are made generic within such classes as Ring for structures which can be added and multiplied, Field which adds the division to a ring, or **module** which abstracts over a multiplithe multiplication of a vector or of a polynomial by a numeric constant). The conversion of the standard numbers: fromInt, fromDouble into constants Our modified Prelude contains such type classes as AddGroup which decation of a complex object by an element of an underlying basic domain (e.g.

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to the algebraic hierarchy.

Some classes in Haskell permit to specify generic operations over composite data structures independently of the type of elements of these structures. If then Constr alone may be an instance of a constructor class. A canonical example of such a class is Functor. This class declares a generic mapping functional **fmap** which applies some function to all the elements, and constructs a structurally equivalent compound. In particular, it transforms a list **Constr a** is a compound type parameterized by the type **a** of its elements, $[\ldots x_k, \ldots]$ into the list of applications $[\ldots f(x_k), \ldots]$. The current version of our class **Module** is also a constructor class, and the multiplication of a compound by an elementary object uses fmap. A closely related constructor class vspace introduces a generic division operation of a compound by an element of the basic domain. In future versions of our package these classes will probably be converted into multi-parametric type classes with dependencies (see the Hugs manual [12]).

3. Differential Algebra and Lazy Towers of Derivatives

The only language attributes really needed in the example above were:

1. the possibility to overload the arithmetic operators, and

so it may have been implemented in almost any serious language, for example in C++, and of course it has been done, e.g., in such packages as ADOL-C or TADIFF [10, 3]. We can extract the derivatives from the expressions, and code some mixed type arithmetics as well, involving normal expressions and the pairs (z,z') together. However, this approach is not homogeneous, and the extensions needed to get the second derivative, etc. are a little inconvenient.

lazily — a data structure which represents an expression e belonging to an infinitely extended domain. It contains the principal numeric value e_0 , and the values of all its derivatives: $\{e_0, e', e'', e^{(3)} \dots\}$, without any truncation explicitly present within the code. We construct a complete arithmetic for these structures, and we show how to lift the elementary functions and their We propose thus to skip all the intermediate stages, and to define

The remaining of this section is structured as follows: we propose first an easy formal introduction to differential algebras, then we define our lazy data defining thus a particular instance of differential algebra. We show how to use structures, and we construct the appropriate overloaded arithmetic operations, these operations, and we discuss some less evident properties of the system. compositions.

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3.1. WHAT IS A DIFFERENTIAL ALGEBRA?

The theory of the domain called Differential Algebra was developed mainly This term often denotes the branch of mathematics devoted to the algebraic analysis of differential equations, but here it is the name of a mathematical by Ritt [22] and Kolchin, see also a more recent book by Kaplanski [13].

For the moment let us forget that the concrete computer representation of numbers is necessarily truncated, that the operations may be inexact, etc. The meaning of the arithmetic operations (the correctness of the division, of the

square root, etc.) in the extended domain is inherited from the basic domain.

We begin with some field equipped with standard arithmetic operations

is always zero. Indeed, the linearity and the Leibniz rule prove immediately

that for the ring of integers 0' = 1' = 0, and from $(a^{-1}a) = 1$ it follows purely algebraically that $(a^{-1})' = -a'/a^2$. For a computer scientist it means that all numbers are constants. This basic field must be extended in order to Calculating derivatives within a simple polynomial extension: A[x] of any field A is well known and described in many books on algebra, e. g., Bourbaki's [5]. We know also how to compute derivatives in the rational extension

generate non-trivial derivatives.

braic indeterminate, some "x" which may be represented symbolically in the program. This is usually the way the interactive Computer Algebra packages proceed. However, it is obvious that if we know the mathematical structure of the manipulated expressions, often no symbols are needed: a polynomial may be represented just as a list of its coefficients, a rational expression as a

A(x). These extensions can be considered as based on adjoining of an alge-

 $(+, \times, /)$. To this set of operations we add one more, the *derivation*: an internal mapping $a \to a'$ which is linear: (a+b)' = a' + b', obeys the Leibniz rule: (ab)' = a'b + ab', and some continuity properties. It is straightforward to prove that for the field of rational numbers the derivation is trivial, the result

pair of polynomials, and the construction of a commutative algebra on such data structures is a school exercise.

functions to its data, and the construction of an appropriate extension is more involved. The symbolic extensions are possible, but they are costly, and much A practical computer program may apply all algebraic and transcendental

representing the expressions.

Our approach is minimalistic, as local as possible. We just want to com-

pute the numeric values of the expressions for a given input, and the values

of some derivatives. We do not know a priori how many derivatives might be

local) object. The derivation becomes a structural operation on data objects

for any value of the "variable" x; it behaves as a symbolic functional (non-

more powerful than usually needed in a numerical program: a polynomial data structure permits to compute the value of the represented polynomial

needed, so we require that our differential algebra is closed, in the sense that

For any new element x introduced into the domain we have to provide x', x'', $x^{(3)}$, etc. — in fact, the possibility of an infinite number of algebraically independent objects, as there is a priori no reason that an x' should the derivation becomes an internal operation in the domain of expressions. be algebraically dependent on x (although it might be true in some cases).

adjoins explicitly its derivative e', and by necessity all the higher derivatives as well. Kaplanski in [13] discusses the model where the basic domain is exoperator is just the mapping $e_n \to e_{n+1}$. Our model is conceptually similar to entities, but we do not use indeterminates. Structurally the program operates We propose thus that to any expression e (a numerical value) the program tended by an infinite number of indeterminates. Every item e (renamed as e_0) of the basic domain is accompanied by $e_1 \equiv e'$, $e_2 \equiv e''$, etc. The derivation this one in the sense that we add explicitly an infinite number of independent

on infinite, lazy lists whose elements are a priori independent.

3.2. THE DATA AND BASIC MANIPULATIONS

The data type we shall work with belongs to an infinite co-recursive domain Dif a parameterized by any basic type a, which is an instance of all needed arithmetic classes, normally it should be a field. Usually it will be **Double**, but rationals or complex numbers are also possible.

could be represented by (D x (D 0 (C))) —a purely co-recursive structure without terminating clause, but adding explicit constants is much more efficient. The first field is the value of the numerical expression itself, In this data the c variant represents constants. It is redundant, and $(c \times x)$ and the second is the tower of all its derivatives, beginning with the first.

the type a onto Dif a belongs to the class of numbers only if the type a itself Here are the numeric conversion functions, and the definition of constants and of the variable. The "=>" construct below means that the embedding of belongs to this class.

instance Number a => Number (Dif a) where fromDouble
$$x = C$$
 (fromDouble x) (et

```
dCst x = C xdVar x = D x 1.0
```

(The compiler should lift automatically the numeric constants, so $\mathbf{D} \times \mathbf{1.0}$ should be treated as $\mathbf{D} \times (\mathbf{C} \ \mathbf{1.0})$.

The derivation operator is declared within the class Diff:

("a" is a type of differentiable objects) (the derivation operator) class Diff a where df :: a->a

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```
(numbers are constants)
                                                                  (lifting proc.)
                                                                instance Number a=>Diff (Dif a) where
instance Diff Double where
                                                                                                     df (C_{-}) = C_{0.0}
```

The equality (instance of the class Eq) for our data is semi-defined. The in-

(just a selector)

equality can be in principle discovered after a finite number of comparisons, but the (==) operator may loop forever, as always with infinite lists. We define it only for "main" values. This is unavoidable, the equality of symbolic expressions is ill-defined as well, and Computer Algebra has to cope with this primeval sin. (The equality of floating-point numbers is also somewhat dubious and may lead to non-portability of programs, but those issues cannot be discussed here.)

3.3. ARITHMETIC

The definitions below construct the overloaded arithmetic operations for the **Dif** objects. The presentation is simplified. The subtraction is almost a clone The Dif data type being a list-like structure, is a natural Functor, with the of the addition, the lifting of operators to the constant subfield is routine.

generalized (fmap) functional defined almost trivially. From the multiplication rule it follows that the operation df is a derivation. The algorithm for the reciprocal shows the power of the lazy semantics — the corresponding (truncated) strict algorithm would be much longer.

```
("mappable" composite types)
                                                                                                                                                                                                                                                                                                                                                                                                                                         C \times + D Y Y' = D (x+Y) Y' (and symmetrically D+C)
                                                                                                                                                                                                                                                                                                                                                        instance AddGroup a => AddGroup (Dif a) where
                                                                                         fmap f (D x x') = D (f x) (fmap f x')
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        D \times x' + D y y' = D (x+y) (x'+y')
  instance Functor Dif where
                                                                                                                                   instance Module Dif where
                                                                                                                                                                                                                            instance VSpace Dif where
                                                 fmap f (C \times) = C (f \times)
                                                                                                                                                                               x \times x = fmap(x^*) s
                                                                                                                                                                                                                                                                      s > / x = fmap (/x) s
                                                                                                                                                                                                                                                                                                                                                                                                       C \times + C Y = C (x+Y)
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       neg = fmap neg
```

instance (Monoid a, AddGroup a) => Monoid (Dif a) where

C x * C Y = C (x*y

(and symmetrically ...)

```
p@(D \times x') * q@(D Y Y') = D (x*Y)(x'*q+p*Y') (Leibnizrule)
```

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```
instance (Eq a, Monoid a, Group a, AddGroup a)
                                                                                                                                                    ip = D (recip x) (neg x' * ip*ip)
                                                                                                              recip (D x x') = ip where
                                                                      recip (C x) = C (recip x)
                                                                                                                                                                                C \times / C Y = C (x/Y)
                                   Group (Dif a) where
                                                                                                                                                                                                                               \mathbf{p} / \mathbf{C} \mathbf{y} = \mathbf{p} > / \mathbf{y}
```

```
(de l'Hôpital!)
                                                                                                                  otherwise = D (x/y) (x'/q - p*y'/(q*q))
                                                                          x==0.0 && y==0.0 = x'/y'
                                    p@(D \times x') / q@(D y y')
C \times / p = x * \times recip p
```

(we have used the de l'Hôpital rule, which may not be what the user wishes.)

ing" to the programmer, because they are calculated (lazily) anyway, but if used, they do consume the processor time, since they force the evaluation of The generalized expressions belong to a differential field. One can add, divide or multiply them, one can calculate the derivatives, which costs "noththe deferred thunks.

One can also define the elementary algebraic and transcendental functions acting on such expressions. We begin with a general lifting functional. Then ity, we have defined there the square root as well.) We omit trivial clauses, we propose some optimizations for the standard transcendental functions, exp, sin, etc. (They are declared within a new class Transcen. For simpliclike exp(Cx) = C(expx).

```
(univariate function lifting)
                                     D (f x) (x' * dlift fq p)
dlift (f:fq) p@(D \times x') =
```

Transcen a, Group (Dif a)) => Transcen (Dif a) where instance (Number a, Monoid a, AddGroup a, Group a,

```
sin = dlift (cycle[sin,cos,(neg . sin),(neg . cos)])
                                                                                                                                                                                                                                                                                                                                                                                                                                                              cos = dlift (cycle[cos,(neg . sin),(neg . cos),sin])
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           the list of all its formal derivatives is given, for example (exp, exp, ...) for the
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     exponential, or (\sin, \cos, -\sin, -\cos, \sin...) for the sine. The definitions of
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           in an extremely compact way. Such definitions in TADIFF [3], where a
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         The function dlift lifts any univariate function to the Dif domain, provided
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       the exponent and of the logarithm have been optimized, although the function
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 dlift could have been used. The self-generating lazy sequences are coded
exp(Dxx') = r where r = D(exp x)(x'*r)
                                                                                                                                                                                                                             r = D (sqrt x) ((from Double 0.5*>x')/r)
                                                                                                                                                                                                                                                                                                           (sin/cos: Use generic lifting, (for instruction))
                                                                     \log p@(D \times x') = D (\log x) (x'/p)
                                                                                                                                                       sqrt (D \times x') = r \text{ where}
```

more classical approach is presented, are much longer. In [15, 16] we have shown how the lazy formulation simplifies the coding of infinite power series arithmetic as compared to the commonly used vector style, (see for example Knuth [20]). We see here a similar shortening of algorithms. Our definition of the hyperbolic cosine still works, and gives an infinite sequence beginning with ch and followed by all its derivatives at a given point. The following function, applicable for small z:

```
lnga z = (z-0.5)*log z - z + 0.9189385 + 0.0833333/
                                                                                                                             (z + 1.0115231/(z + 1.517474/(z + 2.26949/z)))))
                                                          (z + 0.033333/(z + 0.2523809/(z + 0.525606/
```

called as, say, lnga (dvar 1.8) produces the logarithm of the Euler Γ function, together with the digamma ψ , trigamma, etc., needed sometimes in the same program: -0.071084, 0.284991, 0.736975, -0.523871, 0.722494, $-1.45697, 3.83453, \ldots$ One should not exaggerate: the errors in higher derivatives will increase, because the original continuous fraction expansion taken

from the Handbook of Mathematical Functions [1], is an approximation only, and this formula has not been specifically designed to express the derivatives. We get the same error as if we had differentiated symbolically the expression, and constructed the numerical program thereof. The value of $\psi^{(3)}(x)$ has still

several digits of precision.

3.4. SOME FORMAL REMARKS

We cannot include here the proofs of the correctness of the overloaded arith-

- indeterminates to the basic domain. In our case, if the n-th derivative of list are some numerical values, it is obvious that $e^{(n)}$ is independent of We have mentioned that Kaplanski in [13] constructed a formal differential algebra by explicit adjoining of an infinite sequence of independent an expression is a list $e^{(n)} = [p_n, p_{n+1}, \ldots]$, where the elements of the metic, but some formal observations may be useful.
- It can be shown that our definitions are co-recursively sane. Such definitions as the exponential are presented for efficiency as self-referring data

 $e^{(n-1)}$; the latter adds another independent value in front of the list.

is a generalized *unfold*. All proofs that, e.g. (e/f) defines the inverse of structures, but we see that $\exp(D\;x\;x') = D\;(\exp x)\;(x'\cdot \exp(D\;x\;x'))$ multiplication, that $\log(\exp(e)) = e$, etc., are almost trivial.

3.5. PRACTICAL OBSERVATIONS

We recapitulate here the basic properties of the presented computational frame-

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If the definition of a function is autonomous, without external black-

out any extra programming effort. It suffices to call this function with box entities, the computation of all derivatives is fully automatic, withappropriately overloaded arguments.

- The derivatives are computed exactly, i.e., up to machine precision. There derivative than for the main expression (unless it is a polynomial). If is no propagation of instabilities other than the standard error propagation through normalization, truncation after multiplication etc. The putation, since usually more arithmetic operations are needed for the roundoff errors might grow a little faster than those of the "main" com
 - the main numerical outcome of the program is an approximation, e.g., the result of an iterative process, the error of the derivative depends on the behaviour of the iterated expression in the neighbourhood of the
- The generalization to vector or tensor objects depending on scalar variables is straightforward, it fact nothing new is needed, provided the standard commutative algebra has been implemented.
 - The efficiency of the method is good. The manual, analytic, highly tuned differentiation may be faster because a human may recognize the possibility of some global simplification, but the automatic symbolic differen-

a symbolic formula may be differentiated only once, and then evaluated be competitive, because treating independently the "main" formula and tiation techniques are far behind: symbolic differentiation of graph-like numerically for many arguments, but even then, the CD techniques may structures, simplification, shared sub-expression handling — these operations increase the computational complexity considerably. Obviously,

its derivative may inhibit the optimization of shared sub-expressions.

A few words on control structures are needed. The computation of the the standard operators ==, <, >= etc. check only the main values, and cisions are based on numerical relations: if a==b then ... else ..., and if a and b are lifted, we have to define the arithmetic relations of equality, inferiority etc., even if they are imperfect. In our package ignore the derivatives. To handle them the user has to write his own derivatives follow the normal control thread. But sometimes the de-

ical answer. The space leaks induced by these deferred closures might be tional objects whose evaluation produces eventually (upon demand) a numer-

dangerous. The reader should not think that he can compute 1000 derivatives of a complex expression using our lazy towers, unless the program finds

However, all deferred numerical operations generate closures or thunks, func-

_

keeps references to all global values used in its definition, and the lazy towers grow with the order of the derivative. We know that symbolic algebraic manipulations suffer from the intermediate expression swell that may render it In our framework we have "just" lists of numbers, but a similar difficulty impossible to calculate too high order derivatives of complicated expressions.

some specific shortcuts preventing the proliferation of thunks, since a closure

overflow it would be more efficient to use a truncated, strict variant of the In order to increase the package performance, and to prevent the memory

method, sketched in Section 2, provided we know how many derivatives are needed. The code generated by packages written in C++ will be faster.

rithm does not discover it automatically, and it blindly computes one of the possible values, by following the control thread of the program. This strategy may be or may be not what the user wishes, in such circumstances the tal extension of our package, replacing normal numbers by a non-standard arithmetics which includes "infinity" and "undefined", and which permits the usage of such objects as the Heaviside step function, but this direction leads towards the symbolic calculus, which we tried to avoid in this work. In If a function is discontinuous, e.g., defined segment-wise, the CD algotechnique cannot be fully automatic. We have constructed a small experimen-

3.6. IS LAZINESS INDISPENSABLE?

general, the user would have to treat limit cases as carefully as he would do it

It is possible to implement the derivation in a strict language which permits overloading, but the truncation code is more complicated and error-prone, although the resulting program might be faster. (The standard CD packages

We have reimplemented the CD in Scheme (Rice University MzScheme [21])

are of course based on strict semantics.) A combined strategy is also possible.

only these thunks which are really needed occupy the memory, and the Hugs strictness analyser is not ideal. However, the coding is much more tedious, and the code is longer.

using lazy streams constructed with explicit thunks. The speed of the resulting program is comparable with the fully lazy solution tested under Hugs. Some execution-time space efficiency seems to be gained, since in Scheme A more thorough comparison of performances is difficult, because Scheme

is a dynamically typed language. Moreover, some of our algorithms (for

example the definition of the exponential) exploit self-referring variables;

this requires that either the concerned definitions contain unreadable combistructs must be implemented as macros. This may not be portable. Despite the standardisation of macros in the Revised(5) Report on the Algorithmic Lannations of thunks and recursive binding constructs (letrec), or those con-

guage Scheme[19], currently used dialects of Scheme often use their own syntactic extensions. A fully lazy language, especially with a good type system is much easier to use.

4. Some Applications

The application domain covered by the cited literature on CD is very wide, graphy, up to biostatistics. The authors not only used CD packages in order to get concrete results, but they have thoroughly analyzed the behaviour of their algorithms, and several non-trivial optimisation techniques have been ranging from nuclear reactor diagnostics, through meteorology and oceano-

The examples in this section demonstrate how the lazy semantics bridges

computational problems, and effective algorithms. The following issues are the gap between intricate equations which are natural formulations of many We show how to code the solution of differential recurrences of any

- order, and how to construct a function defined by these recurrences. This is a standard technique for symbolic manipulation, but rarely found in a
- We show how to automatically differentiate functions defined implicitly. numerical context.
- Such issues are rarely addressed by the CD literature, although the mathematics involved is rather elementary, and many scientific computations,

e.g., the asymptotic expansions exploit them very intensely.

- If a function obeys a differential equation, its formal solution as se-
- ries can often be obtained by iterated differentiation. If the equation is singular, a naive algorithm breaks down, and the automation of the process may be difficult. We show how to deal with such an equation by using a particular implicitization thereof. transforming it into
- We develop an asymptotic expansion known as the WKB approximation

in quantum theory. This example shows an interplay between lazy dif-

ferentiation, and lazy power series, whose terms "bootstrap" themselves in a highly co-recursive manner. Finally, in the last example construct the Stirling approximation of the This is a "torture test" of our package, which shows that sometimes a good deal of human preprocessing is necessary in order to apply lazy factorial, using the Laplace (steepest descent) asymptotic expansion. techniques to non-trivial cases. diffalg.tex; 15/09/2000; 3:14; p.15

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RECURRENTLY DEFINED FUNCTIONS

envelope of the oscillator corresponds to the classical distribution. But we Suppose that we teach Quantum Mechanics, and we wish to plot a highorder Hermite function, say $H_{24}(x)$ in order to show that the wave-function insist on using only the fact that $H_0(x) = \exp(-x^2/2)$, and that

$$H_n(x) = \frac{1}{\sqrt{2n}} \left(x H_{n-1}(x) - \frac{dH_{n-1}(x)}{dx} \right).$$
 (1)

We do not want to see the polynomial of degree 24, we need just numerical values to be plotted. It suffices to code

```
hr n x = (x*z - df z)/(sqrt(fromInteger (2*n)))
                                                                                      hr 0 \times = \exp(\text{neg } \times \times \times / \text{ fromDouble 2.0})
                                                                                                                                                                                     where z=hr (n-1) x
                                     D cc _{-} = hr n (dVar _{x})
herm n \times = cc where
```

(some normalization factors are omitted here), and to launch, say, map (herm 24) [-10.0, -9.95 .. 10.0] before plotting the obtained sequence.

any other recurrence, but this one works in practice without problems. The efficiency of the differential recurrences is as good as any other method. The This example is a bit contrived, we could use the Rodrigues formula, or generation of the 400 numbers in the example above takes less than 20 sec on a 400MHz/130MB PC with 6MCells of heap space allotted to Hugs, which but this first stage is much more costly. Maple using the equivalent procedure (and reusing all lower-order forms) chokes before n=24. Other recurrence is a Haskell interpreter, and thus much slower than the compiled code would be. Mapping the explicit, symbolically computed form would be much faster, schemes are more suitable.

4.2. Lambert function

We find the Taylor expansion around zero of the Lambert function defined implicitly by the equation

$$W(z)e^{W(z)} = z, (2)$$

equations have closed solutions in terms of W. Corless et al. [6] discuss the existence and the analyticity properties of this function. The differentiation without using any symbolic data. This function is used in many branches of computational physics and in combinatorics. Many interesting differential of (2) gives

$$\frac{dz}{dW} = e^W(1+W) \qquad \left(=\frac{z}{W}(1+W) \text{ for } z \neq 0\right)$$
(3)

gives a one-line code for the McLaurin sequence of W, knowing that W(0) = $\left(= \frac{W}{z} \frac{1}{1+W} \right)$ $\frac{dW}{dz} = \frac{e^{-W}}{1+W}$ whose inverse

4

producing the following numerical sequence: 0.0, 1.0, -2.0, 9.0, -64.0, 625.0, wl = D 0.0 (exp (neg wl)/(1.0+wl))

-7776.0, 117649.0, -2097152,..., which agrees with the known theoretical

values: $W^{(n)}(0) = (-n)^{n-1}$.

If we insert the formula (4) into any program which calculates numerically W(x) for any $x \neq 0$, (for example using the Newton or Haley approximation [6]) we obtain all its derivatives at any point.

Can we use the second, apparently cheaper form of (4) which does not use solution, passing from $Y = \exp(-W)$ to Y = W/z at z = 0 loses some the exponential? For $z \neq 0$ naturally yes, provided we knew independently recursive definitions effective. In the example above, there is no immediate information, we do not know any more that the value of Y(0) = 1. We can the value of W(z). But lazy algorithms sometimes need some intelligent reformulation in order to transform equations in algorithms, and to make coadd it by hand, and we get for the derivative

$$Y' = -Y (Y + zY')$$
 or $Y' = \frac{-Y^2}{1 + zY}$. (5)

Both forms are implementable now, and the first, recursive, is faster, because the differentiation of a fraction is more complex. We just have to introduce an auxiliary function ζ which multiplies an expression f by the variable z at z = 0. The resulting "main value" vanishes, but the result is non-trivial:

from which we can reconstruct the derivatives of W = zY in one line.

4.3. A SINGULAR DIFFERENTIAL EQUATION

shorter than an approach using arrays, indices and truncations. In some cases The previous example shows also how to code the Taylor expansion of any function satisfying a (sufficiently regular) differential equation. There is nothing algorithmically specific in the lazy approach, only the coding is much it is possible to treat also singular equations. The function u(x) defined by

$$u(x^2)=x^{-\nu}J_{\nu}(x)$$
 obeys the equality
$$f'(x)=-\frac{1}{\nu+1}\left(x^2f''(x)+\frac{1}{4}f(x)\right) \ , \tag{6}$$

which is implicit: needing f and f'' to compute f', and singular at x=0(although this singularity is not dangerous). We may apply now our $\zeta(w)$ trick. By putting for simplicity ν equal to zero, and replacing $x^2f''(x)$ by $\zeta(\zeta(f''))$ in (6), we obtain f = 1.0, -0.25, 0.0625, -0.140625, 0.878906, $-10.7666, 218.024, \dots$ for

```
fp = neg (0.25*besf + zeta (zeta (df fp)))
besf = D 1.0 fp where
```

because the second derivative is protected twice from being touched by the reduction of the auto-referential expression $\pm p$. In [15] we have used a similar trick to generate the power series solution of the Bessel equation.

4.4. WKB EXPANSION

the wave function in Quantum Mechanics. We start with a generalized wave Our next exercise presents a way of generating and handling functions defined by intricate differential identities in the domain of power series in some small perturbation parameter (not the differentiation variable). We derive higher order terms for the Wentzel-Kramers-Brillouin approximation, as presented in the textbook [2], and useful for some quasi-classical approximation to

equation

$$\epsilon^2 y'' = Q(x)y. \tag{7}$$

velopment of y in ϵ . Within the standard WKB formalism y is represented with ϵ very small. The essential singularity at zero prevents a regular de-

$$y \approx \exp\left(\frac{1}{\epsilon} \sum_{n=0}^{\infty} \epsilon^n S_n(x)\right)$$
 (8)

integration irrelevant for our discussion), and $\exp(S_1) = 1/\sqrt{S'_0}$, which has Inserting (8) into (7) generates a chain of coupled recurrent equalities satisfied by S_n . The lowest approximation is $S_0' = \pm \sqrt{Q}$, (which needs an explicit profited from the fact that the coefficients S_{2n+1} are directly integrable.

We propose the following expansion, which separates the odd and the even powers of ϵ . The coefficients of proportionality, and the necessity to combine linearly the two solutions differing by the sign of \sqrt{Q} are omitted.

$$y \approx \exp\left(\frac{1}{\epsilon}S_0 + U(x,\epsilon^2) + \epsilon V(x,\epsilon^2)\right)$$
 (9)

Injecting this formula into the equation (7) gives the following differential identities:

$$U' = \frac{-1}{2} \frac{S_0'' + \epsilon^2 V''}{S_0' + \epsilon^2 V'}$$
 or $e^U = \frac{1}{\sqrt{S_0' + \epsilon^2 V}}$

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and

$$V' = \frac{-1}{2S_0'} \left(U'^2 + U'' + \epsilon^2 V'^2 \right) . \tag{11}$$

These cross-referencing definitions seem intricate, but they constitute an effective lazy algorithm. The aim of this section is to show how to code U(x)and V'(x). The last one has to be integrated using other methods.

Until now we never really needed all derivatives of a function, and the

Here, in order to get one numerical value of, say V'(x), we need the second reduction of the lazy chain stopped always after a finite number of steps. derivative of U, which needs the second and the third derivative of V, etc. The point is that U and V should be treated as series in ϵ^2 , and the higher derivatives of U and V appear only in higher-order terms, which make the co-recursive formulae effective.

We have thus to introduce some lazy techniques of power series manipula-

tion. This topic has been extensively covered elsewhere, e.g., in our own work [15]. We review here the basics. The series $U(z) = u_0 + u_1 z + u_2 z^2 + \cdots$ u2,...]. The linear operations: term-wise addition and multiplication by a scalar are easy (zip with (+), and map). The multiplication algorithm $u_0v_0+z(u_0\overline{v}+v_0\overline{u}+z\overline{u}\overline{v})=u_0v_0+z(v_0\overline{u}+U\overline{v}).$ For the reciprocal is a simple recurrence. If we represent $U(z) = u_0 + z\overline{u}$, then $U \cdot V =$ W=1/U (with $u_0\neq 0$) we have $w_0=1/u_0$, and $\overline{w}=-w_0\overline{u}/U$, (with the symbolic variable z implicit) is represented as a lazy list [u0, u1,

which result from $U \cdot W = 1$. The differentiation and integration need only some multiplicative zips with factorials, and an integration constant. The elementary functions such as $W = \exp(U)$ may use the following technique: W'=U'W, and thus $W=\exp(u_0)+\int U'W\,dz$, which is a known algorithm, see the Knuth's book [20], although its standard presentation is not The terms u_i need not be numbers. They may belong to the domain \mathbf{Dif} . or on the contrary, our differential field may be an extension of the series do-

main, i.e., the "values" present within the Dif structure are not Doubles, but series. The first variant is used here. Hence we have a doubly lazy structure, and we need an extension of the differentiation operator over the variable xwhich is a lazy list representing a series over ϵ . In this domain it suffices to In our actual implementation series are not lists, but similar, specific data structures with (:>) as the chaining infix constructor, and a constant z representing the zero (empty) series, more efficiently than an infinite list of zeros. taylor p = tlr 1 (fromInteger 1) p where
tlr _ f (C x) = (x*f) :> Z
tlr m f (D x q)=(x*f):>tlr (m+1) (f/fromInteger m) Any **Dif** expression p may be converted into its Taylor series by define df = map df, or, more explicitly df (u0:uq) = df u0 : df uq

Ö

We may test the WKB algorithm and generate the approximation to the Airy function which is the solution of the equation (7) for Q(x) = x, for some Then we define s0'=sqrt q and s0'' = df s0', and the equations (10) numerical values of x. We fix the value of the variable, e. g. $\mathbf{q} = \mathbf{d}\mathbf{var}$ 1.0. and (11) may be coded as

```
where a shifted addition operator a +:> b which represents a+\epsilon^2b is defined
                                                                        v' = p \text{ where } p = ((-0.5)/s0') *>(u'^2 + df u' +:> p*p)
u' = (-0.5)*>(s0'': df v')/(s0': v')
```

$$(a+ba) <: 0a = d <:+ (pa <: 0a)$$

and (*>) multiplies a series by a scalar. Now u' is a series whose elements belong to the data type Dif, but we do not need the derivatives, only the main values, so we construct a function £ which returns this main value

nal solution. The generation and exponentiation of u, and the integration of from the Dif sequence. One application of map f to the series u' suffices to obtain -0.25, -0.234375, -1.65527, -28.8208, -923.858, -47242.1, -152.83, -6271.45, -391094.0, -3.44924e+007, etc., and this is our fi- \mathbf{v}' give for a sufficiently small ϵ a good numerical precision. This result is known. Our aim was to prove that the result can be obtained in a very totic expansions, for example the saddle-point techniques which also generate -3.52963e+006, etc. while \mathbf{v}' produces -0.15625, -0.539551, -6.31905, few lines of user-written code, without any symbolic variables. Other asympunwieldy formulae may be implemented with equal ease.

4.5. SADDLE-POINT APPROXIMATION

We want the asymptotic evaluation of

$$I(x) = \int f(t)e^{-x\varphi(t)}dt , \qquad (12)$$

for $x \to \infty$, knowing that $\varphi(t)$ has one minimum inside the integration interval, (see [2], or any other similar book on mathematical methods for scent) are extremely important in natural and technical sciences. It consists physicists). The Laplace method and its variants (saddle point, steepest de-

in expanding φ about the position of this minimum $p: \varphi'(p) = 0$. Then

 $\varphi(t) = \varphi(p) + \varphi''(p)(t-p)^2/2 + R(t)$, and evaluating the integral

$$I(x) = e^{-x\varphi(p)} \int e^{-x\varphi''(p)(t-p)^2/2} f(t) e^{-x(t-p)^3 R}$$
, (13)

considering the expansion of $f(t) \exp(-x(t-p)^3 R)$ as polynomial correction to the main Gaussian contribution around the point where the maximum

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is assumed. R is a series in (t-p), beginning with the constant $\varphi'''/31$.

Analytically we get

$$= \sqrt{\frac{2\pi}{x\varphi''}} e^{-x\varphi} \left\{ f + \frac{1}{x} \left(\frac{f''}{2\varphi''} - \frac{f\varphi^{(w)}}{8(\varphi'')^2} - \frac{f'\varphi'''}{4(\varphi'')^2} + \frac{f'\varphi'''}{24(\varphi'')^3} \right) + \frac{1}{x^2} \left(\cdots \right) \cdots \right\}$$
(14)

where f, φ and their derivatives are taken at p. The next terms need a good dose of patience. Even an attempt to program this expansion using some Computer Algebra package is a serious task, and the resulting formula is finite number of particles involved. Is it possible to compute the expansion terms without analytic manipulation? The problem is that the expressions here are bivariate, and all the expansions mix the dependencies on x and t, so We begin with computing $\varphi(t)$ as a series at p (in the Dif domain), extracting difficult to read. These terms are often necessary, for example in computations in nuclear physics or quantum chemistry, where x is proportional to a we obtain a series of series. We have to disentangle it, because we want the dependence on x to remain parametric: x should not appear in the expansion. the constant $\varphi_0 = \varphi(p)$, $\varphi''/2$ and the series R with its coefficient $(t-p)^3$:

$$phi0 :> \frac{1}{2} :> ah :> r = taylor phi$$

Henceforth we do not care about $\exp(\varphi_0)$ nor about the normalization, we compute only the asymptotic series. Expanding the exponential and multiplying it by $f: \mathbf{u} = \text{fmap} (\mathbf{f} *) \text{ exp} (\mathbf{Z} :> \text{neg } \mathbf{r} :> \mathbf{Z}) \text{ we get}$

$$U = \sum_{n=0}^{\infty} x^{n} (t-p)^{3n} U_{n} (t-p) , \qquad (15)$$

where U_n is a series in (t-p). It suffices to integrate (15) with a Gaussian, $1)!!/(ax)^m$, where $(2m-1)!! = 1 \cdot 3 \cdot 5 \cdots (2m-1)$. Here is the program but this is easy: $I_m = \int \exp(-xat^2/2)t^{2m}dt$ is equal to $\sqrt{2\pi/ax}\cdot(2m-$

which computes the Gaussian integral of a series v multiplied by $(t-p)^m$:

```
otherwise=t:>cf(k+2)((t*fromInteger k)/a)
                                                                                                                                                                                                                    ig (c0:>cq) (v0 :> vq) = v0*c0 :> ig cq (stl vq)
                                                                                                                        let cf k t | k<mm = cf (k+2) ((t*fromInteger k)/a)
                                        odd mm = igauss a (mm+1) vq
igauss a mm v@(_:>vq)
                                                                                        otherwise =
```

where **stl** is the series tail, ig is the internal iterator, and cf computes the series of coefficients $(2m-1)!!/a^m$. We keep with each term an additional number m_0 , the least power of 1/a (and subsequently of 1/x) of the resulting

in (mm 'div' 2, ig (cf 1 (fromInteger 1)) v)

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Laurent series. Applying this function to our series of series U, after having restored the coefficient $(t-p)^{3n}$:

we obtain a sum of the form

$$\sum_{n=0}^{\infty} x^n G_n\left(\frac{1}{x}\right) , \quad \text{where} \quad G_n\left(\frac{1}{x}\right) = \sum_{m=0}^{\infty} g_{nm} (1/x)^m \quad (16)$$

The resulting infinite matrix must be re-summed along all diagonals above and including the main diagonal, in order to get coefficients of $(1/x)^{m-n}$. It is easy to prove that the sum is always finite, because the factor $(t-p)^{3n}$ makes m_0 grow faster than n. The re-summation algorithm uses m_0 in order to "shift right" the next added term, and if it can prove that there is nothing more to be added, emits the partial result, and *lazity* recurs. here is the final part of the program:

```
(strict sum. step)
                                                                                                                                                                                  (lazy iteration)
                                                                                        rs m0 g0@(ghd :> gtl) gq@((m1,g1) :> grst)
                                            rs _ Z ((m1,g1) :> grst) = rs m1 g1 grst
resum ((m0,g0) :> gq) = rs m0 g0 gq where
                                                                                                                                                                                  otherwise = ghd :> rs (m0+1) gtl gq
                                                                                                                                      m1==m0+1 = rs m1 (g0+g1) grst
```

finalResult = resum (dseries a u)

In order to test the formula we may take $\varphi = z - \log(z)$ at z = 1, and we obtain in less than 4 seconds the well known Stirling approximation for the

$$n! = \int t^n \exp(-t)dt \approx n^{(n+1)} \int \exp(-n(z - \log z))dz . \tag{17}$$

The first terms of the asymptotic sequence in (1/n) are

(18	
5246819	75246796800
163879	$^{\circ}$ 2488320° 209018880°
	2488320
-139	51840
	288
	$\frac{1}{12}$, $\frac{288}{288}$,

5. Conclusions

The present work belongs to a longer suite of papers in which we try to demonstrate the applicability of modern functional programming paradigms ally dominated by low-level coding techniques, since the computational efficiency is considered primordial, and although one often needs here elaborate to the realm of scientific computing [15, 16, 17, 18]. This domain is usunumerical methods, sophisticated algorithmisation tools are rare. This is partly due to the lack of sufficiently powerful abstraction mechanisms in standard languages used for numerical computations, such as C or Fortran. The path between an analytical formula and its implementation in a numerical context is often long. Human time is precious, and Computer Algebra packages are often exploited. Symbolic computations are often needed piler only, and never looked upon by a human. For many years it was typical for insight, people like to see the analytical form of their numerical formulae. However, it is not unfrequent that the symbolic algebra is applied in despair, just to generate some huge expressions consumed by the Fortran or C comof many computations involving differentiation.

know now how to compute efficiently and exactly the numerical derivatives of The development of Computational Differentiation tools changed that. We expressions without passing through the symbolic stage. Several highly tuned packages adapted to C, C++ and Fortran exist, and their popularity steadily increases, although they do not always integrate smoothly with existing nu-

It was not our aim to propose a replacement for these packages. However, on the methodological side our ambition was a little bigger. The specificity merical software.

unknown) number of times. This makes it possible and easy to code functions defined by differential recurrences. No explicit truncation of The derivation operation exists in the program at the same footing as all standard arithmetic procedures. It can be applied an arbitrary (a priori the derivation orders, synchronisation of powers, etc. are needed. Laziof our contribution may be summarized as follows:

ness liberates the user from the major part of the algorithmisation bur-

- suffices to load a very short library of overloaded, extended arithmetic The usage of our package is extremely simple and straightforward. It methods, and to declare in a few places in the program that a given identitifier corresponds to the differentiation variable. Polymorphism, and the automatic type inference of Haskell does the rest.

Thanks to the Haskell class system, the extended arithmetics remains valid for any basic domain, not only for floating-point reals. No changes

structs some specific arithmetic operations for polynomials or ratios of are needed in order to compute complex derivatives. If the user conpolynomials, the lifting of these operations to the differential ring or field becomes almost automatic.

implementations of functional languages is far from ideal. The examples we The exercise of the lazy style of programming needs some experience, and the conceptual work involved may be substantial. The efficiency of current

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mula), but they are generic, presented modularly, and their discussion is fairly have presented are intricate (there are easier ways to compute the Stirling forcomplete. To us there is plenty of evidence that lazy functional languages, erties of operations in complicated mathematical domains, have a nice future which permit better than many others to concentrate upon the algebraic propin the area of applied mathematics.

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References

- Abramowitz Milton, Stegun Irene, eds. Handbook of Mathematical Functions, Dover Publications, (1970).
 - Bender Carl, Orszag Steven, Advanced Mathematical Methods for Scientists and
 - Bendtsen Claus, Stauning Ole, TADIFF, a flexible C++ package for automatic differentiation, Tech. Rep. IMM-REP-1997-07, Dept. of Mathematical Modelling, Technical University of Denmark, Lyngby, (1997). Engineers, McGraw-Hill, (1978).
- Berz Martin, Bischof Christian, Corliss George, Griewank Andreas, eds., Computational differentiation: techniques, applications and tools, Second SIAM International

- Workshop on Computational Differentiation, Proceedings in Applied Mathematics 89,
 - Corless Robert, Gonnet Gaston, Hare D.E.G., Jeffrey D.J., Knuth Donald, On the Lambert W function, Advances in Computational Mathematics 5 (1996), pp. 329-359. See Bourbaki Nicolas, Algebra, Springer (1989).
 - also the documentation of the Maple SHARE Library.
- Corliss George, Automatic differentiation bibliography, originally published in the SIAM Proceedings of Automatic Differentiation of Algorithms: The-
- ory, Implementation and Application, ed. by G. Corliss and A. Griewank, (1991), but many times updated since then. Available from the netlib archives

liinwww.ira.uka.de/bibliography/Math/auto.diff.html .See also

(www.netlib.org/bib/all_brec.bib), and in other places, e.g.

Graham Ronald, Knuth Donald, Patashnik Oren, Concrete Mathematics, Addison-Max-Planck-Institut für Meteorologie, (1996), ACM TOMS in press.

Giering Ralf, Kaminski Thomas, Recipes for adjoint code construction, Tech. Rep. 212,

∞.

- Wesley, Reading, MA, (1989).
- Griewank Andreas, Juedes David, Mitev Hristo, Utke Jean, Vogel Olaf, Walther Andrea, 10.
- ADOL-C: A Package for the Automatic Differentiation of Algorithms Written in C/C++, ACM TOMS, 22(2) (1996), pp. 131–167, Algorithm 755.
- Hovland Paul, Bischof Christian, Spiegelman Donna, Cosella Mario, Efficient derivative codes through automatic differentiation and interface contraction: an application in biostatistics, SIAM J. on Sci. Comp. 18, (1997), pp. 1056–1066.

25

- diffalg.tex; 15/09/2000; 3:14; p.24
- - site Karczmarczuk Jerzy, Functional Differentiation of Computer Programs, Proceedings, Jones Mark P., The Hugs 98 User Manual, available from the Web http://www.haskell.org/hugs together with the full distribution of Hugs. Kaplansky Irving, An Introduction to Differential Algebra, Hermann, Paris (1957).
- Karczmarczuk Jerzy, Generating power of lazy semantics, Theoretical Computer Sci-(1998), pp. 195–203. 15.

III ACM SIGPLAN International Conference on Functional Programming, Baltimore,

Karczmarczuk Jerzy, Functional programming and mathematical objects, Proceedings, Functional Programming Languages in Education, FPLE'95, Lecture Notes in ence **187**, (1997), pp. 203–219. 16.

Computer Science, vol. 1022, Springer, (1995), pp 121-137.

the Haskell Workshop, Colloquium PLI 2000, Montreal, (September 2000), available Karczmarczuk Jerzy, Adjoint Codes in Functional Framework, informal presentation at Workshop on Functional Programming, Stirling, (September 1999).

Karczmarczuk Jerzy, Functional coding of differential forms, talk at the 1-st Scottish

Knuth Donald, The Art of Computer Programming, vol. 2: Seminumerical Algorithms, www.cs.indiana.edu/scheme-repository/. 20.

on the Algorithmic Language Scheme, available from the Scheme Repository:

Kelsey Richard, Clinger William Rees Jonathan (editors), Revised(5) Report from the author: www.info.unicaen.fr/~karczma/arpap/revdiff.pdf

- Addison-Wesley, Reading, (1981).
- Rice University PLT software site, http://www.cs.rice.edu/CS/PLT.

- Ritt Joseph, Differential Algebra, Dover, N.Y., (1966).



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