Differential Equations in MuPAD I: An Object Oriented Environment

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Abstract. We describe an object oriented programming environment for differential equations realised in the computer algebra system *MuPAD*. It serves as a convenient and highly customisable basis for the implementation of sophisticated algorithms and facilitates the interaction between application packages developed by different authors.

1 Introduction

There exist a lot of computer algebra packages for differential equations implementing algorithms for many different tasks. As a simple example, we may take the symmetry analysis of some field theory in physics. Thus our starting point is a Lagrangian and the first step is the derivation of the corresponding Euler-Lagrange equations. The second step consists of setting up the determining system for the symmetry generators of these equations. As these systems tend to be rather large and overdetermined, one will probably need some simplification and completion. As fourth step one might try to solve the determining system. In the fifth step one would like to use the found symmetry generators for a symmetry reduction, preferably to some ordinary differential equations which should finally be solved, too.

For each of these six steps there exist computer algebra packages. However, they have usually been written by different authors. Furthermore, these authors may have had different tasks in their minds and not necessarily precisely the sequence of steps described above. In any case, chances are high that each of the authors implemented his/her

own data structures for differential equations, as no computer algebra system provides standardised ones.¹

Using the output of one package as input for another one requires usually to write some conversion routines between these different data structures. This is not only a tedious and unpleasant task (requiring some information about the interns of the used packages), the conversion is also a time consuming process at runtime. This problem can be largely avoided by using an object oriented approach.

In this report we will present an object oriented programming environment for differential equations realized within the domains package [3] of MuPAD [4,9]. Some years ago, we implemented a similar environment in the computer algebra system AXIOM [10,11]. In comparison, our MuPAD environment is much more user-friendly and many methods are more efficient. Especially, it is now possible to completely hide the usage of domains and categories, so that even users not familiar with object oriented programming can use applications packages based on the domains.

The report is organised as follows. The next section gives a brief introduction into object oriented programming in computer algebra, its realization in *MuPAD* and an overview over our environment. Sects. 3 and 4 describe the functionality of the already provided categories and domains, respectively. They also give some details on the implementation. Finally, we give some conclusions and an outlook in Sect. 5.

2 Overview

2.1 Object Oriented Programming in MuPAD

Object oriented programming in computer algebra has been pioneered by AXIOM [7] (formerly called SCRATCHPAD) and is closely modelled on an abstract algebraic approach to mathematics. Each object is element of a domain (of computation) which in turn belongs to a category. For example, in MuPAD the number 42 may be viewed as an element of the domain Dom::Integer which belongs (among others) to the category Cat::Ring. In addition, there exists the possibility to define axioms, but we will not need this here.

¹ In such a diverse field as differential equations this appears only reasonable, as for different tasks different data structures may be optimal.

Categories provide the possibility to define abstract data types. Their primary task is to specify the methods (or procedures) which each domain belonging to them must contain. For example, each domain in the category Cat::Ring must provide implementations for addition and multiplication of ring elements. A category may contain default implementations for some methods which are inherited by its domains (but the domains may overwrite the default and provide their own implementation).

In our context, categories allow us to abstract certain operations that are always needed in working with differential equations. Then we can provide different concrete implementations in form of domains. An algorithm may now be written in a *generic* form taking such a domain as a parameter. This provides a simple mechanism to exploit special features of certain classes of differential equations without implementing the same algorithm several times.

For example, we may apply an algorithm sometimes to linear and sometimes to nonlinear equations. But certain operations needed in the algorithm can be performed much more efficiently for linear equations. Classically, we could either implement the algorithm in its most general form and thus renounce exploiting the linearity or write two different versions of the algorithm. The first solution is inefficient for linear equations and the second one is tedious and difficult to maintain. In an object oriented environment, we simply develop two different domains for linear and nonlinear equations, respectively. Then we implement the algorithm only once in terms of domain methods and can still fully exploit the linearity when the algorithm is applied to linear equations.

To be fair one should mention that object oriented programming also introduces a certain amount of overhead, especially a higher number of procedure calls. The performance of the object oriented code will usually be lower than that of a specialised version for linear equations. The main advantages are thus for the programmer who obtains a code that is easier to maintain and to reuse and also more flexible to use.

MuPAD provides the necessary tools for object oriented programming within its domains package [3]. All categories are collected within the library Cat, all domains within Dom. In order to address a specific category or domain one uses the operator :: (a notation familiar to C++ programmers). Thus the already mentioned category of all rings is obtained with the call Cat::Ring. The same operator :: is also used

for methods (or procedures) within a domain. If DD is some domain possessing a method method, it is called by DD::method.

A category may have super categories — e.g. Cat::Field is a specialisation of Cat::Ring — from which it inherits all methods. Each domain belongs to at least one category. In addition, it may inherit from one super domain. Any domain may overwrite the inherited implementation of a method.

All domains implemented within the domains package inherit from Dom::BaseDomain (and Cat::BaseCategory). This yields default implementations of a number of basic methods for the generation and the output of domain elements. If DD is a domain, one way to generate an element of it is to call DD::new(...) which can be abbreviated to DD(...). What and how many arguments may be passed depends of course on the domain DD. If wrong arguments are given, DD::new will report an error. By default, DD::new calls the method DD::convert; each domain must provide an implementation of this method. It controls the various ways elements of the domain can be generated. Furthermore, it defines implicitly the internal representation of the domain elements.

For the output of a domain element the method DD::print is used (this is done automatically by MuPAD). By default, DD::print just calls DD::expr which is to some extent the opposite of DD::convert. DD::convert usually takes as arguments some basic MuPAD objects and converts them to an element of DD, whereas DD::expr takes an element of DD and converts it to a basic MuPAD object which can be printed on the screen.

2.2 Structure of our Environment

Our environment consists of two levels. The first one defines differential variables; the second one differential functions. Both levels are specified by a category and we provide a number of domains in both categories (see Fig. 1). Every user can add own domains and still make full use of the environment — as long as the "standards" set for the names and for the semantics of the methods declared by the categories are obeyed.

The first level serves mainly as a user interface; the primary task of its domains is to define the format of the used differential variables, i. e. what are their names, how can they be entered, how does the output look like. No real computations happen in these domains besides trivial

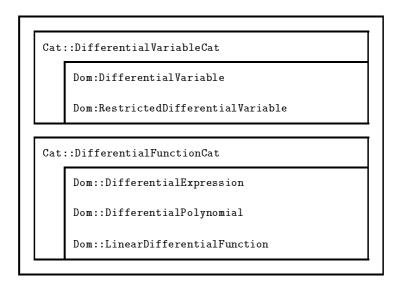


Fig. 1. Implemented domains and categories

ones like determining the order of a derivative. On the other hand, these methods are constantly used and should therefore be rather fast.

The domains in the second level correspond to specific types of differential functions like linear or polynomial ones. Each domain in this category takes as first argument a domain from Cat::DifferentialVariable specifying the differential variables on which the functions may depend. Besides standard arithmetical operations, the domains contain a number of differential methods like total differentiations and some simplification routines. Details will be given in the next two sections.

In a typical application of our environment, one first chooses a domain in Cat::DifferentialVariable. This tells MuPAD what are the independent and dependent variables. Then one chooses a domain in Cat::DifferentialFunction. Usually, this will declare some properties of the differential equations one is working with. With the following input we set the arena for working with arbitrary differential functions in the independent variables x, t and the dependent variable u.

```
>> DV := Dom::DifferentialVariable([x,t],u);
>> DE := Dom::DifferentialExpression(DV);
```

At first sight it might appear rather cumbersome to have to make such explicit declarations, but in extensive computations this pays off in form of much simpler in- and output. In addition, any procedure for differential equations will need the information what are the independent and dependent variables. In the traditional approach, these are passed directly as arguments. In our environment it suffices to define once these domains and any object of them always carries all the information in its datatype.

3 The Categories

The two basic categories underlying our environment are Cat::DifferentialVariable and Cat::DifferentialFunction. Both contain default implementations for many methods. Typically, only a few low level methods need to be written from scratch for implementing a new domain in one of the categories. However, for efficiency reasons it might often be worthwhile to overwrite some default implementations with specialised versions.

3.1 Differential Variables

The main task of Cat::DifferentialVariable is to provide a standardised interface to access the data of differential variables. This includes especially (multi) indices, the type or the order of a differential variable. The category distinguishes three different types of variables (encoded in strings):

- "Indep": This is the type of the *independent variables*. They play a special role in total differentiations and similar operations and carry only one index.
- "Dep": This is the type of the dependent variables (or unknown functions). They also carry only one index.
- "Deriv": This is the type of the derivatives (of the dependent variables with respect to the independent ones). They carry two indices, one of them is a multi or repeated index.

In the literature, one can find two different forms of multi indices. The classical *multi index* notation is mainly used for theoretical works.

If there are n independent variables, a multi index μ is an (ordered) n-tuple $\mu = [\mu_1, \ldots, \mu_n]$ where the entry μ_i denotes the number of differentiations with respect to the i^{th} independent variable. The order q of the corresponding differential variable is given by the length of the multi index $q = |\mu| = \mu_1 + \cdots + \mu_n$. In the second form which we will call, in lack of a better name, repeated index the index I of a q^{th} order derivative is a set of q integers between 1 and n: $I = (i_1, \ldots, i_q)$ where each integer i_k denotes a differentiation with respect to the i_k^{th} independent variable. While in principle the order of the entries in I does not matter, we will usually assume that they are ordered: $i_1 \leq i_2 \cdots \leq i_q$.

Domains in Cat::DifferentialVariable automatically support both notations; the one internally used by a domain is given by the entry notation returning either the string "multi" or "repeated". The auxiliary methods m2r and r2m transform one kind of index into the other one. We refer to the multi or repeated index as the "lower" index of a differential variable; the "upper" index is used to enumerate the independent and dependent variables. This reflects the usual mathematical notation for a derivative:

$$u_{\mu}^{\alpha} = \frac{\partial^{|\mu|} u^{\alpha}}{\partial (x^{1})^{\mu_{1}} \cdots \partial (x^{n})^{\mu_{n}}} = u_{\underbrace{x^{1} \cdots x^{1}}_{\mu_{1} \text{times}}}^{\alpha} \cdots \underbrace{x^{n} \cdots x^{n}}_{\mu_{n} \text{times}}$$
(1)

where we have assumed that there are n independent variables x^i , m dependent variables u^{α} and that $\mu = [\mu_1, \dots, \mu_n]$ is a multi index.

The following alphabetic list contains all the methods and entries which must be implemented in any domain belonging to Cat::DifferentialVariable. For most of them, the category provides a default implementation; in fact, only six methods must be defined explicitly in the domain: index, either multiIndex (if notation returns the value "multi") or repeatedIndex (if notation returns the value "repeated"), notation, numIndVar, numDepVar and vartype. They are marked by an asterisk in the list.

- Methods in Cat::DifferentialVariable

allRepeated(mi): Returns a list of all possible realizations of a given multi index mi as repeated index.

class(dv): Class² of a differential variable dv.

The class of a derivative with multi index $\mu = [\mu_1, \dots, \mu_n]$ is defined as the smallest index i such that $\mu_i \neq 0$. For an ordered repeated index $I = (i_1, \dots, i_q)$ the class

- depVariables: Returns a list of all dependent variables.
- derivativeOf(dv1,dv2): Checks whether the variable dv1 is a derivative of dv2. If yes, the corresponding multi or repeated index is returned (depending on the notation used by the domain), otherwise the result is an empty list.
- derivatives(q<,cl>): Lists all derivatives up to order q. If a second argument cl is given, all derivatives of order q and class greater than or equal to cl are returned.
- diff(dv,x): "Normal" differentiation where all differential variables are treated as independent; compare with totalDiff and see example in Sect. 4.1.
- dim(q): Counts the dependent variables and the derivatives up to order q.
- dimq(q): Counts the derivatives of order q.
- has(dv,x): Returns TRUE, if dv=x, and FALSE otherwise. Overloads the MuPAD function has.
- indVariables: Returns a list of all independent variables.
- *index(dv): Yields "upper" index of differential variable dv.
- int(dv,i): Tries to integrates the differential variable dv with respect to the independent variable x^i . If this is not possible, FAIL is returned.
- length(dv): Returns 1. Overloads the MuPAD function length.
- m2r(mi): Computes repeated index for given multi index mi.
- makeIndexList(q): Generates all multi indices up to order q.
- *multiIndex(dv): Yields "lower" index of differential variable dv in multi index notation.
- multiRaise(mu,i): Raises the entry i of multi index mu by 1; i may also be a list of indices.
- newMulti(t,i,mi): Generates a new differential variable of the
 type t with index i and multi index mi.
- newRepeated(t,i,ri): Generates a new differential variable of the type t with index i and repeated index ri.

equals i_1 . For an independent variable we define the class to be 0; for a dependent variable as the value of numIndVar.

- *notation: Returns used notation as a string: either "multi" or "repeated".
- *numDepVar: Returns number of dependent variables.
- *numIndVar: Returns number of independent variables.
- order(dv): Computes the order of the differential variable dv.
- orderly: Returns TRUE, if the domain uses an orderly ranking.³
- orderLex(dv1,dv2): Graded reverse lexicographic ranking of the differential variables dv1 and dv2.
- pureLex(dv1,dv2): Purely lexicographic ranking of the differential variables dv1 and dv2.
- r2m(ri): Returns repeated index ri as multi index.
- random(<q>): Returns a random differential variable. The optional parameter q gives the maximal order; default is 6.
- *repeatedIndex(dv): Returns "lower" index of differential variable dv in repeated index notation.
- repeatedRaise(mu,i): Includes the entry i in the repeated index mu; i may also be a list of indices.
- totalDiff(dv,i): Total differentiation of dv with respect to the independent variable with index i (alternatively i may be an independent variable). Compare with diff and see the example in Sect. 4.1.
- *vartype(dv): Returns the type of the differential variable dv (as string).

------ Methods in Cat::DifferentialVariable ------

As one can see, rankings of differential variables should also be implemented in the domains in Cat::DifferentialVariable. Currently, only the purely lexicographic ranking and a graded reverse lexicographic ranking are implemented; the latter one is the default. Different rankings can simply be imposed by overwriting the method _less. Note, however, that the entry orderly should be adapted correspondingly.

Another caveat is that one must be careful with changing dynamically the ranking in a domain DV in Cat::DifferentialVariable. While of course any call to DV::_less will use the new ranking, this

³ A ranking of differential variables is called *orderly*, if variables of higher order are always higher in the ranking than those of lower order.

change might not be noted by domains for differential functions in the variables of DV. Only newly constructed domains will definitely use the new ranking.

3.2 Differential Functions

The basic category for differential functions is called Cat::DifferentialFunction(DV). It takes as argument a domain DV from Cat::DifferentialVariable. All domains belonging to this category represent functions of the variables in DV. The various domains correspond typically to different types of functions, e.g. linear or polynomial ones.

Cat::DifferentialFunction is only a specialisation of the category Cat::AbelianSemiGroup and not of Cat::Rng as one might expect. The reason is that we want to admit domains for linear functions, but these can only be added and not multiplied without loosing their linearity. This also makes difficulties with Jacobians. Normally, the Jacobian is a matrix over the same domain. But MuPAD matrices can be defined only over rings, so something special must be done for linear functions. This problem is discussed in more detail in Sect. 4.4.

Any domain in Cat::DifferentialFunction(DV) should provide (besides the arithmetical operations of a Cat::AbelianSemiGroup) the methods listed in the following table (sorted alphabetically). For most of them a default implementation exists. Only the methods diff, has, indets, solve and subsOne must in any case be newly implemented. They are marked by an asterisk in the list. Concrete examples for the use the methods can be found in the next section.

ullet Methods in Cat::DifferentialFunction

autoreduce(sys): Autoreduction of the list sys of differential functions. Note that reduction includes (total) differentiations in contrast to simplification.

autosimplify(sys): Autosimplification of the list sys of differential functions. Note that simplification is a purely algebraic operation, i.e. no derivatives of the functions in sys are used.

class(df): This is a simple lift of the corresponding method in DV; it returns the maximal class of the highest order differential variables contained in the differential function df.

- *diff(df,x): Partial differentiation of the differential function df with respect to the variable x. Compare with totalDiff!
- diffSubs(df,dv=e): In a differential substitution not only the differential variable dv but also all its derivatives are substituted by the expression e and its total derivatives.
- eval(df,sol): Evaluates the differential function df for some given functions. The list sol must have as many entries as there are dependent variables, and each entry must be a function of the independent variables only. These functions (and their total derivatives) are substituted in df for the differential variables.
- *has(df,dv): Returns TRUE, if the differential variable dv effectively occurs in the differential function df.
- *indets(df<,DiffVars>): Returns a set with all the indeterminates occurring in the differential function df. With the option DiffVars only those indeterminates are returned which are elements of DV, i.e. no parameters (see the example in Sect. 4.2).
- isConst(df): Returns TRUE, if the differential function df does not depend on any differential variable.
- jacobian(sys): Computes the Jacobian of the differential functions contained in the list sys.
- jacobianType: This entry returns the data type of the Jacobian matrices computed by the method jacobian (some MuPAD matrix domain).
- leader(df): Returns the leading derivative of the differential
 function df. The ranking is implicitly defined by the method
 _less of the domain DV.
- linear: This entry returns TRUE or FALSE depending on whether or not the functions represented by the domain are linear.
- multiDiff(df): Computes with as few differentiations as possible several derivatives of the same differential function df.
- multiSubs(df,dv1=e1<,dv2=e2,...>): Substitutes the differential variables dv1,dv2,... by the expressions e1,e2,... in the differential function df using the method subsOne.

order(df): Returns the maximal order of the differential variables effectively appearing in df.

polynomial: This entry returns TRUE or FALSE depending on whether or not the functions represented by the domain are polynomial.

*solve(df,dv): Tries to solve the differential function df for the differential variable dv.

*subsOne(df,dv=e): Substitutes the expression e for the differential variable dv in the differential function df.

totalDiff(df,x):⁴ Total differentiation of the differential function df with respect to the independent variable x. This implies the use of the chain rule in contrast to partial differentiations with diff.

Variables: This entry returns the domain DV.

- Methods in Cat::DifferentialFunction

Of importance are here the distinctions made between autoreduction and autosimplification and between partial and total differentiation. If we are given a differential function $\phi(x,u,p)$ where x represents the independent, u the dependent variables and p the derivatives, then the method diff computes the usual partial derivatives $\partial \phi/\partial x$, $\partial \phi/\partial u$, or $\partial \phi/\partial p$. If ϕ depends in addition on some parameters a, diff can also compute derivatives with respect to them. In contrast, the total differentiation is defined only for independent variables. Using multi-index notation for the derivatives, it is given by

$$D_{x^{i}}\phi = \frac{\partial\phi}{\partial x^{i}} + \sum_{\alpha} \frac{\partial\phi}{\partial u^{\alpha}} p_{i}^{\alpha} + \sum_{\alpha,\mu} \frac{\partial\phi}{\partial p_{\mu}^{\alpha}} p_{\mu+1_{i}}^{\alpha}$$
 (2)

where p_i^{α} is a short hand for the derivative with a multi index μ where all entries are zero except μ_i which is one (i.e. $\mu_j = \delta_{ji}$) and $p_{\mu+1_i}^{\alpha}$ represents the derivative with a multi index given by μ and μ_i raised by one. Thus if we take $\phi = u_x$, then $\partial \phi/\partial x = 0$ (and the result of a corresponding diff call will be zero), as ϕ does not depend explicitly on x. If we want to take into account the implicit dependency of u_x on x, we must use the total differentiation provided by totalDiff which uses the chain rule and will return $D_x \phi = u_{xx}$.

⁴ A default implementation is provided only for the case that the domain is a ring.

Autosimplification is a purely algebraic operation. Its main goal is to eliminate all algebraic dependencies between the differential functions in a given list. Here u_{xx} and u_x are considered as algebraically independent, as they are distinct differential variables. Autoreduction eliminates in addition differential dependencies. A simple application of the chain rule yields $D_x(\sin u_x) = u_{xx}\cos u_x$, so the functions $u_{xx}\cos u_x$ and $\sin u_x$ are differentially dependent although they are algebraically independent. autoreduce therefore eliminates $u_{xx}\cos u_x$ from the list $[u_{xx}\cos u_x, \sin u_x]$, whereas autosimplify leaves it unchanged.

autoreduce and autosimplify will furthermore try to put the given list of functions in a kind of triangular form: each function in the output should have a different leading derivative. Ideally, these leading derivatives are completely eliminated from all other functions. Note that no general algorithm exists for the autoreduction or -simplification of arbitrary differential functions. Such algorithms can be given only for special classes of functions, e.g. for linear functions where autosimplification reduces to Gaussian elimination or for polynomials where Gröbner bases [2] can be used.

The default implementations of autoreduce and autosimplify in Cat::DifferentialFunction apply a simple heuristic relying essentially on the domain method solve. Each equation is solved for its leading derivative and then this derivative is eliminated in all other equations by substitution. This process continues, until no further eliminations can be performed. Obviously, for arbitrary differential functions it cannot be guaranteed that one can always solve for the leading derivatives and thus it is not sure that the remaining functions are indeed algebraically (or even differentially) independent.

Finally, some words are necessary to explain the approach taken for the implementation of the method subs. It is intended to free programmers from having to write code for argument checking and multiple substitutions each time they write a new domain belonging to Cat::DifferentialFunction. The categorical method multiSubs handles these tasks; however, it uses for a single replacement the method subsOne which has to be provided by each domain. Consequently, subs should be defined in the domain as subs:=dom::multiSubs. As the default implementation in Dom::BaseDomain overwrites any categorical one, one cannot proceed this way directly in Cat::DifferentialFunction.

4 The Domains

With categories alone one cannot perform any computations. Therefore our environment provides already a number of instances, namely two domains for differential variables and three domains for differential functions. The latter ones cover the three most important types of functions: linear functions, polynomials and general expressions. The distinction between polynomials and general expressions is of interest for performance reasons. MuPAD possesses a special built-in data type DOM_POLY for polynomials and executes both arithmetical and differential operations much faster for polynomials than for general expressions.

In the sequel we will briefly describe these five provided domains. As their basic functionality is inherited from the categories, we will discuss only those methods which are specific for a given domain. In addition, we will give some indications on the underlying representation and the implementation of some important methods.

4.1 Differential Variables

The main domain for differential variables is Dom::DifferentialVariable. It may be considered as the simultaneous implementation of two different domains distinguished by the arguments they take. In the first usage, Dom::DifferentialVariable is given as arguments two lists (if a list has only one entry, one may omit the list brackets) with the names of the independent and the dependent variables, respectively. In the second usage, a domain with indexed variables is generated. Here one gives as arguments indexed identifiers like x[3] in order to obtain the variables x_1, x_2, x_3 . Thus two different ways to generate a domain with three independent and two dependent variables are

```
>> DV := Dom::DifferentialVariable([x,y,z],[u,v]):
>> IDV := Dom::DifferentialVariable(x[3],u[2]):
```

The two so generated domains DV and IDV differ especially in their internally used representations: DV is based on *repeated index* notation and IDV on *multi index* notation, as one can see from the following two lines of output.

Dom::DifferentialVariable supports several notations for the inand output of differential variables. One is of course the standard Mu-PAD notation using diff. Alternatively one may use the D operator. However, for most purposes the most convenient notation is a rather condensed one mimicking the usual mathematical notation as good as possible using only ASCII characters. Here dependent variables always appear without arguments; for derivatives one uses the same symbols as for the dependent variables but uses them now as function names with a list of the independent variables with respect to which differentiations occur as argument. Finally, one may use the generic methods newMulti and newRepeated defined in Cat::DifferentialVariable not requiring any knowledge of variable names. The following five input lines all generate the same differential variable u_{xy} (we show the output only once, as it is of course always the same).

As one can see, for better readability the output of Dom::DifferentialVariable uses always the condensed notation. If one wants to convert back to one of the other input forms one can use the method convert_to with the options "diff" and "D", respectively. The arguments of the remaining two calls could be retrieved with the methods vartype, index, multiIndex or repeatedIndex, resp.

Finally, it is possible to obtain the output as TEX; all domains in our environment are compatible with the MuPAD-TEX interface in the generate library. Again a condensed notation is used and not full differential quotients.

The following example shows the difference between the two methods diff and totalDiff: whereas the former one treats all differential variables as independent of each other and thus returns either 1 or 0, the latter one represents the total differentiation one needs for prolonging differential equations and similar operations.

As $x \neq u_{xy}$, the first call returns 0. The second call adds a differentiation with respect to x. This is demonstrated in the third line where the "difference" between u_{xy} and u_{xxy} is computed as a repeated index. If the domain IDV had been used for this example, the result would have been the corresponding multi index, [1,0,0], as determined by the auxiliary method r2m in the last line.

The internal representation of the domain Dom::DifferentialVariable is straightforward. It consists of five slots: (i) the type of the

variable, (ii) the upper index, (iii) the lower index (or the empty list, if no lower index exists), (iv) the order and (v) the class of the variable. (iv) and (v) are not really necessary, however, it turned out that for many computations it is advantageous to store this information in the representation instead of computing it newly each time it is needed. Especially, comparisons with respect to the graded lexicographic order (our default ranking) are speeded up considerably.

The domain Dom::RestrictedDifferentialVariable is typically used for constructing coefficient domains of linear or polynomial functions (see Sects. 4.3 and 4.4) or by domains representing solutions of differential equations. It takes as first argument another domain in Cat:: DifferentialVariable and imposes then some restrictions, specified by the second argument, on the variables. A typical example for such a restriction is that only independent variables are admitted.

Five different possibilities are provided for specifying the restriction. They always take the form of an equality where the left hand side denotes the type of restriction:

Types: Here one specifies the types of the differential variables which are admitted. If several types are allowed, a set with their names must be passed.

Order: If the order of the admitted variables is specified, then instead of an equality one might also use an inequality. Thus it is possible to generate domains containing either only derivatives up to a prescribed order or alternatively only derivatives of higher order.

InSet: In this case one specifies a set with all the differential variables admitted by the domain.

OutSet: This is just the converse of the last case; a set with all the variables *not* admitted is passed.

Crit: This represents the most general case where a criterion procedure is passed. This procedure should take a differential variable as argument and return TRUE or FALSE depending on whether or not the variable belongs to the domain.

It is not possible to combine these options. If, for instance, one wants to prescribe simultaneously the type and the order, one must write a criterion procedure and use the last possibility. The actually imposed restriction of a domain RDV:=Dom::RestrictedDifferentialVariable(DV,...) can be retrieved with the method mode. Its possible results are:

```
["Indep"]: RDV contains all the independent variables of DV.
["Less/Greater",q]: RDV contains all differential variables of order
less resp. greater than q (for example, in case of the restriction
    Types={"Indep","Dep"} RDV::mode returns ["Less",1]).
["General"]: All other cases.
```

4.2 Differential Expressions

Our most general domain for differential functions is called Dom::DifferentialExpression(DV). It is essentially a lift of the basic MuPAD type DOM_EXPR to the category Cat::DifferentialFunction and thus allows for computations with arbitrary differential expressions.

In order to avoid the need to always explicitly generate a domain DV belonging to Cat::DifferentialVariable, it is also possible to specify the domain via one or two optional arguments. These options contain essentially the arguments passed to the constructor Dom::DifferentialVariable or Dom::RestrictedDifferentialVariable, respectively. Thus in the following example the domain DE represents general differential expressions in the independent variables x, y, z, the dependent variables u, v and their derivatives. In contrast, the domain RDE represents only functions of the independent variables and consequently the attempt to generate a function of the dependent variable u yields an error. The automatically generated domain for the differential variables can be retrieved with the method Variables.

Besides the methods specified in the category Cat::Differential-Function some basic *MuPAD* functions have been lifted to Dom::DifferentialExpression. This includes eval,⁵ normal, simplify, radsimp, combine and rewrite. For efficiency reasons, the default implementations of many methods in Cat::DifferentialFunction have been replaced by special versions.

The representation consists of two slots: the first one contains usually an element of the basic domain DOM_EXPR, the second one a set of differential variables, i.e. elements of DV. All differential variables appearing in the differential expression are contained in this set. However, in general the set will contain some further variables. While it is very useful for many operations to have such a set stored in the representation, it turned out that it is inefficient to always eliminate redundant variables (it is a rather expensive operation to check whether an element of DOM_EXPR effectively depends on a given variable).

Note that this second slot also affects tests for equality. It is a well-known problem in computer algebra that no normal representation exists for general expressions, i.e. it is not always possible to decide whether or not an expression is zero. In Dom::DifferentialExpression it may furthermore happen that two expressions look equal, as the have the same element of DOM_EXPR in their first slot (which determines the output), but still a check for equality returns FALSE, as one of them has redundant elements in the set in the second slot. In such cases the domain method equal will return TRUE.

While the first slot usually contains an expression, there exist a few further possibilities. The simplest ones are that the differential expression is actually just a number (i. e. an element of one of the basic domain DOM_INT, DOM_RAT or DOM_FLOAT) or an identifier (which is considered by Dom::DifferentialExpression as a parameter). In all these cases, the second slot contains an empty set, thus we have a normal representation for them. A differential expression may also consist just of a differential variable; then the first slot contains this variable. The last possibility is an element of the domain Dom::DifferentialFunction(DV).

⁵ Note that called with one argument eval yields the lifted kernel function and with two arguments the method specified in Cat::DifferentialFunction.

⁶ In general, it is a good strategy to use the domain method equal instead of the boolean operator = in order to compare elements of domains without a canonical representation.

This special domain is a (hopefully only temporary) hack around a problem with the differentiation of undetermined expressions. If (using the domain DE of our example above) an expression of the form F(x,y,z,u,v) is differentiated with respect to one of its arguments, i.e. with respect to a differential variable, MuPAD uses its differential operator D to represent the result. Unfortunately, it will try in subsequent computations repeatedly to simplify the result, although there is obviously nothing to simplify. In larger calculations (especially in Lie symmetry theory) this can waste surprisingly much computing time.

As an alternative, one may use the domain Dom::Differential-Function(DV) to represent such expressions. Then the differentiation is a completely formal operation (as it should be) and no subsequent evaluation attempts will happen. A user will almost never work directly with this domain, as Dom::DifferentialExpression provides an interface with the method arbFunction. The following example demonstrates the difference in the execution times of a simple differentiation: using internally Dom::DifferentialFunction is usually between two and three times faster.

We can now provide concrete examples for some of the procedures specified in the category Cat::DifferentialFunction. We start with the method indets and demonstrate the meaning of the option DiffVar for the expression de defined above. Without this option the parameters a, b are returned, too; otherwise only the differential variables are returned.

```
>> DE::indets(de);
>> DE::indets(de,DiffVars);
```

Next we give an example for the computation of a Jacobian. We wrote a special domain $\mathtt{Dom::SparseMatrix}$ for representing Jacobians. It has a number of particularities. As the name already indicates, it is specialised to sparse matrices, as differential functions appearing in applications are typically sparse, i.e. they do depend only on a small subset of all possible differential variables up to a given order. Secondly, the columns of such matrices are labelled not by integers but by differential variables. In the following MuPAD commands we first define a system consisting of two differential functions, $u_{xx} - u_{yy}$ and $v_z + v_{xxx} + vv_x$. Then we determine its Jacobian jac and the domain of jac. In the last line we extract all column labels of jac.

One can see here how the columns are indexed by the occurring differential variables sorted in descending order (the ranking determined by the method _less of the used domain for differential variables — compare with Sect. 4.1). Dom::SparseMatrix has three parameters: DV for labelling the columns, DE for the matrix entries and a boolean function for ordering the elements of DV. In the case of Jacobians the

columns are always ordered decreasingly with respect to the order _less of the domain DV. Thus the first column of the matrix corresponds always to the leading derivative.

The following three methods have in common that they require several derivatives of the same differential function. In order to minimise the number of differentiations needed to compute these derivatives, the auxiliary procedure derivativeTree of the DETools library is used. It determines for a given set of multi indices a tree whose leaves represent the wanted derivatives. One can read off this tree in which order the differentiations should take place. A simple heuristic algorithm is used to determine the tree; it will be described in more detail in [1].

The method multiDiff takes a differential function and a list of multi indices and returns the total derivatives of the function with respect to the indices. eval substitutes functions (of the independent variables) for the dependent variables and their derivatives in a given differential expression de. A typical use is to check whether the functions form actually a solution of the differential equation de=0. eval uses internally multiDiff to determine the needed derivatives. The functions given as arguments should be elements of a domain of differential functions over the independent variables only (i. e. over Dom::Restricted-DifferentialVariable(DV, Types="Indep"). But in interactive calls automatic conversions are performed, so that one can simply enter:

diffSubs is similar to eval but more general: it substitutes an arbitrary differential expression for a single dependent variable or derivative and all of its derivatives.

4.3 Differential Polynomials

Dom::DifferentialPolynomial can be used to generate domains representing differential functions which are polynomial in some or all differential variables. In the simplest call the constructor takes only one argument: a domain DV from Cat::DifferentialVariable. Then one obtains a domain which represents classical differential polynomials with constant coefficients, i. e. functions which are polynomial in the dependent variables and the derivatives and which do not depend at all on the independent variables. The domain Dom::Rational is used as coefficient ring.

One may also explicitly specify a coefficient ring R as second argument of the constructor. If the ring R belongs to the category Cat:: DifferentialFunction, so that we have variable coefficients, its differential variable domain (obtainable with R::Variables) must be of the form RDV:=Dom::RestrictedDifferentialVariable(DV,...) where the dots stand for the chosen form of restriction (see Sect. 4.1). The functions contained in the so generated domain are polynomial in all differential variables of DV which are *not* admitted in RDV. The entry coeffRing returns the domain R, while the entry constCoeff signals whether constant coefficients are used.

For users unwilling to create domains for differential variables and the coefficient ring it is also possible to obtain differential polynomials in a way similar to that described in Sect. 4.2, by giving variables and restrictions directly as right hand sides of the options Vars=[...] and Rest=[...]. Here the restrictions apply to the coefficient ring; if they are missing, constant coefficients with dependent variables and derivatives in the terms are used.

The choice of the internal representation of Dom::Differential-Polynomial requires some explanations of how polynomial arithmetics is performed in MuPAD. The basic polynomial type is DOM_POLY. An element of it consists of three operands: the expression representing the polynomial, the list of variables and the domain of the coefficients. Polynomials are created by a call of the kernel function poly with these three arguments (if the the coefficient ring is omitted, DOM_EXPR is the default). In order to utilise the fast polynomial addition and multiplication provided by the MuPAD kernel, the variable lists and

coefficient rings of the operands must coincide. If the variable set is known *a priori* and if it is finite, this poses no problem.

In the case of differential polynomials, however, we have an infinite number of variables. Thus the variable lists of polynomials must be compared and adapted before adding or multiplying them and one loses some of the benefits of the faster arithmetics. In order to decrease the number of changes of the variable lists to a minimum, we chose the following approach: the internal representation of an element of Dom:: DifferentialPolynomial consists of three slots.

REP=poly			VARS	ORD
expr	VARSP	R		

The first slot contains the polynomial as an element of DOM_POLY which in turn consists again of three slots as mentioned above. For the variable list VARSP we take *all* differential variables up to the order given by the third slot ORD. The slot VARS holds a superset of the set of all differential variables effectively occurring in expr (similar to the second slot in the representation of Dom::DifferentialExpression).

The variable lists are adapted only before two polynomials are added or multiplied. The values of ORD are compared. If the polynomials are of different order, the one of lower order is converted into list representation by the kernel function poly2list. The auxiliary function addZterms augments the exponent vectors by the necessary zeros (the number of which is determined by the methods dim and dimq from Dom::DifferentialVariable); the result is changed back to a polynomial by another call of poly. For the same reasons as in Sect. 4.2 no adaptation of the variable list is performed on the result, i.e. if a variable is cancelled, it still appears in the list VARSP and the set VARS. This might also lead to a too high value of ORD.

All the points mentioned in the previous section on normalised expressions thus also apply for differential polynomials. The removal of superfluous variables from VARS, the determination of the correct value for ORD and the truncation of VARSP via a further auxiliary method remZterms can be enforced by the method normalPoly.

⁷ It consists of a list of monomials, each of them again being a list of two elements: the coefficient (from the domain R) and the *exponent vector*, which is a list of integers where each entry holds the degree of the corresponding element in the variable list.

Dom::DifferentialPolynomial is also a member of the category Cat::Polynomial. There are two reasons why we do not use Dom:: DistributedPolynomial or one of its descendants for the representation. Adaptations of the variable lists are done there before and after each operation and we simply did not succeed in making this domain work with differential variables. So a great deal of methods had to be implemented in Dom::DifferentialPolynomial anew, making the code rather large. Currently, it works only with restrictions possessing mode=["Less",q] or mode=["Indep"] (which is internally treated as ["Less",0]). The case mode=["Greater",q] requires a completely different implementation, as the variable lists are now finite, and for mode=["General"], certain methods, e.g. totalDiff, have to be changed. Since these cases rarely turn up in applications, they have been deferred until needed. The same applies for Dom::LinearDifferentialFunction (see Sect. 4.4).

The convert routine of Dom::DifferentialPolynomial takes either one or two arguments; in the latter case, the first argument holds the polynomial in dense list representation and the second argument is the variable list. With the following commands, first a domain DP is constructed which represents differential functions which are polynomial in all derivatives and where the coefficients can be arbitrary expressions in the independent and dependent variables (the order of a dependent variable is 0). Then an element p of this domain is generated using a list notation. Of course, it would have been also possible to enter p directly in standard MuPAD notation.

If convert is given merely one argument, any *MuPAD* expression that can be converted into a differential polynomial is allowed. Especially, Dom::DifferentialPolynomial provides methods to convert to

and from all other currently existing domains in the category Cat:: DifferentialFunction.

As arithmetical operations the methods of a (commutative) ring have been implemented: _plus, _negate and _mult. They use the respective fast polynomial kernel operations as described above. All methods required by the category Cat::Polynomial (and some more) have also been lifted from the corresponding polynomial functions. This includes multcoeffs, mapcoeffs, coeff, lcoeff, tcoeff, nthcoeff, nterms, lterm, nthterm, lmonomial, nthmonomial, mainvar, degreevec, degree, evalp as well as the methods for Gröbner bases, gbasis and normalf. If working with a monomial ordering other than the default DegreeOrder note that the variable list itself is ordered according to how DV::derivatives returns its result. Currently, this means a DegreeOrder ranking on the variables.

An important polynomial operation for many applications is pseu-dodivision. It is used, for example, in (differential) algebra in the computation of characteristic sets [8]. The procedure pseudoRemainder takes as argument two differential polynomials f and g and a differential variable g such that deg(f,g) > deg(g,g) > 0. It returns a list [r,q,d,s] such that $d^sf = qg + r$ where g is the leading coefficient of g and g and g and g are g and g are g and g are g and g are g are g and g are g and g are g and g are g are g are g are g are g are g and g and g are g are g are g are g are g are g and g are g are g are g are g are g and g are g are g and g are g are g are g are g and g are g a

Finally, implementations for all the deferred methods of Cat::DifferentialFunction are provided. diff uses the operator for polynomial differentiation Dpoly. solve can only solve for differential variables appearing linearly (this can be checked by the method isLinear); in all other cases, it returns FAIL. A completely new implementation is given for totalDiff. It turned out that the approach via the Jacobian taken in Cat::DifferentialFunction is inferior to working directly on the list representation.

The following comparison of the execution times for the addition and the total differentiation of two random polynomials in Dom::DifferentialPolynomial and Dom::DifferentialExpression, respectively, demonstrates very clearly the usefulness of having a special domain for differential polynomials.

The differences in the execution times are so drastic, because we are dealing with rather large polynomials: dp1 is here of total degree 97 in 58 differential variables up to order 5 and consists of 18 terms; dp2 is of degree 60 in 51 differential variables also up to order 5 and consists of 13 terms. For smaller examples and if differential polynomials of differing orders are treated the speedup is usually smaller due to overheads, but nevertheless it is clearly worthwhile to use polynomial arithmetics whenever possible.

4.4 Linear Differential Functions

Dom::LinearDifferentialFunction is in many respects similar to Dom::DifferentialPolynomial but for linear instead of polynomial functions. For the arguments exactly the same rules apply. The linearity concerns only those differential variables which are not admitted in the coefficients. As it is not preserved under multiplication, this domain belongs only to the category Cat::LeftModule(R), where R denotes again the coefficient ring, and not to Cat::PartialDifferentialRing as all the other domains in Cat::DifferentialFunction.

Another difference lies in the behaviour of the method jacobian. Usually, it returns a matrix whose entries are of the same type as the differential function. For linear functions this is not possible, as the matrix domains of *MuPAD* require a ring for the entries. In domains generated by Dom::LinearDifferentialFunction the method jacobian

computes the Jacobian only with respect to those variables in which the functions are linear and returns a matrix over the coefficient ring R.

One must also be cautious with total differentiations. For constant coefficients or if the coefficient ring has the restriction mode=["Indep"] no problems arise. In all other cases, differentiation of the coefficients may yield nonlinear terms in variables in which the function should be linear. Hence for all other restrictions totalDiff returns an error.

Linear differential functions are finite sums with summands of the form coefficient times differential variable and possibly one single element of the coefficient ring to which we refer in the sequel as the inhomogeneity (or "right hand side", if we think of differential equations). Consequently, we let Dom::LinearDifferentialFunction(DV,R) inherit its representation from the domain Dom::FreeModule(R,DV) supplying finite linear combinations of elements from DV over the ring R and add an additional slot for the inhomogeneity. The representation consists thus of one slot for storing a list containing all monomials in the form [coefficient,variable] and one slot for the inhomogeneity. The presence of the latter makes it necessary to reimplement many of the methods provided by Dom::FreeModule.

The method **convert** either accepts a list of pairs consisting of an element of the coefficient ring and a differential variable, optionally extended by a coefficient representing the inhomogeneity, or any expression that can be legally converted into a linear differential function. For example, we can generate linear differential functions with variable coefficients as follows:

In order to check whether or not a linear differential function possesses an inhomogeneity, the method isHomogeneous can be used; the inhomogeneous term itself is extracted with inhomogeneity:

The implemented arithmetical methods are those specified in the category Cat::LeftModule(R):_plus,_negate and _mult, where the latter means the scalar multiplication with elements of the ring R. Due to the similarity of the internal representation with the one used by polynomials, the polynomial methods mentioned in Sect. 4.3 are also provided by Dom::LinearDifferentialFunction. They differ slightly from the corresponding MuPAD functions:

- lterm and nthterm directly return the corresponding differential variable.
- coeff returns a list of all the coefficients of the linear differential function given as argument; if a differential variable is passed as second argument, the result is only its coefficient.
- In addition, the methods tterm and tmonomial for determining the lowest term and monomial as well as terms returning a list of all terms have been implemented.

Since no entry one exists in Dom::DifferentialVariable, it is not possible to represent a constant term. Hence any method which should return the constant term returns FAIL instead. Nevertheless, the inhomogeneity counts as a term when determining their number with nterms.

Of the methods specified in Cat::DifferentialFunction, a new version of totalDiff is provided; the above made restrictions on when this procedure works apply. solve can solve only for those differential variables in which the function is linear and returns FAIL otherwise.

The domain contains some additional methods written in view of upcoming applications. These include the following ones:⁸

changeIndVars(ldf,newVars,NewFromOld<,LDF>): This method performs a change of the independent variables in the linear differential function ldf. The names of the new variables are given in the list newVars and expressions of the new variables in terms of the old ones in the list NewFromOld. The optional argument LDF specifies the domain of the output, although there is a default one.

changeDepVars(ldf,newVars,OldFromNew<,LDF>): The same for the dependent variables. Note however that for this method the old variables have to be given in terms of the new ones.

makeMatrix, makeSystem: These methods convert between a list of linear differential functions and its coefficient matrix. The matrix domain is identical to the one used for the Jacobian (i.e. the domain Dom::SparseMatrix(DV,R)). Inhomogeneities of the functions are ignored in the conversion.

As a simple example we consider a change of the independent variables in the linear function 1f2 introduce above. The second line shows the automatically generated output domain.

⁸ The first two methods have been supplied by Jay Belanger (Truman University).

5 Conclusions and Outlook

In this report we presented a programming environment for differential equations. We have not considered any serious application; but two packages for the completion of systems of differential equations and for Lie symmetry analysis built upon our environment will be described in two further reports of this series [5,6]. Their implementations will demonstrate some of the advantages and the flexibility of the object oriented approach to computer algebra.

Most general purpose computer algebra systems do not really use data types and even where they do, it is not very transparent to the user. The other extreme is a strongly typed system like AXIOM where the user must declare the type of each object (or must hope that the system can infer the type which is often very time consuming). This can be very inconvenient, especially if one just want to do some quick computations. MuPAD tries to combine these two approaches by distinguishing between basic types and the domains in the domains package. The user can enter some expressions without bothering about their types and perform all kinds of computations. But he can also work in a strongly typed environment for more sophisticated tasks. Bridges between the basic types and domains are provided by the methods convert and expr which each domain should possess.

The topic of a fourth report [1] in this series will be a new MuPAD library DETools. It allows users which are deterred by concepts like categories or domains to use sophisticated methods like those contained in the symmetry and the completion package; the library acts here as an interface that automatically chooses appropriate domains. In addition, it contains many others methods for solving, manipulating or visualising differential equations. A lot of them are again based on the environment described in this report.

All the categories and domains mentioned in this report will be contained in the forthcoming release 2.0 of MuPAD. Unfortunately, our environment cannot be used with the current version 1.4 of MuPAD due to some changes in the language.

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