Computing with Hamiltonian operators

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Abstract

Hamiltonian operators for partial differential equations are ubiquitous in mathematical models of theoretical and applied physics. In this paper the new Reduce package CDE for computations with Hamiltonian operators is presented. CDE can verify the Hamiltonian properties of skew-adjointness and vanishing Schouten bracket for a differential operator, as well as the compatibility property of two Hamiltonian operators, and it can compute the Lie derivative of a Hamiltonian operator with respect to a vector field. More generally, it can compute with (variational) multivectors, or functions on supermanifolds. This can open the way to applications in other fields of mathematical or theoretical physics.

Keywords: Hamiltonian operators, partial differential equations, integrable systems, Schouten bracket, supermanifolds

Contents

1	Introduction	2
2	Hamiltonian operators and partial differential equations	7
3	Computing with C -differential operators and superfunctions 3.1 CDE and total derivatives	11 11 13
4	Five easy pieces 4.1 Warm-up: tedious large-scale computations	15 18 21 23 26
5	Conclusions	31

1 Introduction

Hamiltonian operators for partial differential equations (PDEs) are one of the most important tools in the modern theory of integrable systems [1, 24, 68], with applications ranging from pure to applied mathematics and physics. Integrable systems are systems of PDEs for which is it possible to construct classes of exact solutions in closed form. A widely accepted characterization of such systems is that they have infinite sequences of symmetries or conserved quantities in involution, or *hierarchies*.¹ Such quantities play a role in the construction of general solutions (see [1, 24, 68]). It is not an easy task to show that a certain PDE has a hierarchy.

Consider a system of PDEs of the form

$$u_t^i = F^i(x^\lambda, u_\sigma^j), \quad i = 1, \dots, n,$$
 (1)

where (u^i) are dependent variables, (t, x^{λ}) are independent variables $(\lambda = 1, \dots, m)$,

$$u_{\sigma}^{i} = \frac{\partial u^{i}}{\partial x^{\sigma_{1}} \cdots \partial x^{\sigma_{m}}}, \quad \sigma \in \mathbb{N}^{m}$$
(2)

(with $u_0^i = u^i$) and F^i is a smooth function of a finite number of arguments. The system (1) is *Hamiltonian* if there exists a linear matrix differential operator (A^{ij}) ,

¹More precisely, they commute with respect to certain bracket operations, see (23)

fulfilling additional properties, such that

$$u_t^i = F^i(x^\lambda, u_\sigma^j) = A^{ij} \frac{\delta H}{\delta u^j},\tag{3}$$

where H is a conservation law density, the *Hamiltonian density*, for the system (1). The properties that make A a Hamiltonian operator are: A is skew-adjoint, $A^* = -A$, and the Schouten bracket of A with itself vanishes, [A, A] = 0. We will come back to those properties in Section 2.

It can be proved [13, 47] that a Hamiltonian operator maps conserved quantities into symmetries. But a Hamiltonian operator alone cannot guarantee the existence of a hierarchy. The fundamental idea of F. Magri [49] was that if a system of PDEs is Hamiltonian with respect to two Hamiltonian operators A_1 , A_2 , then an infinite sequence of conserved quantities could be generated through the recursive definition

$$A_1^{ij} \frac{\delta H_{k+1}}{\delta u^j} = A_2^{ij} \frac{\delta H_k}{\delta u^j}.$$
 (4)

The sequence is made of commuting conserved quantities with respect to a certain bracket operation (see (23)) if and only if the operators A_1 and A_2 are compatible: $[A_1, A_2] = 0$. Of course, we used the Schouten bracket between operators.

We can pose the main computational problems of the Hamiltonian formalism for PDEs.

- 1. Given a system of PDEs of the type $u_t^i = F^i(x^\lambda, u_\sigma^i)$, find a Hamiltonian operator and a Hamiltonian density for the system (direct problem).
- 2. Given a Hamiltonian operator A, find which integrable systems are Hamiltonian with respect to A (inverse problem).
- 3. Given a differential operator, check the properties that make it Hamiltonian: $A^* = -A$ and [A, A] = 0.
- 4. Given a Hamiltonian operator A, change its coordinates in such a way to achieve a certain canonical form (Darboux theorems for Hamiltonian operators).
- 5. Given two Hamiltonian operators A_1 , A_2 , check their compatibility: $[A_1, A_2] = 0$.
- 6. Given a Hamiltonian operator A, compute the set of Hamiltonian operators B which are compatible with A: [A, B] = 0.
- 7. Given a pair of compatible Hamiltonian operators A, B, find a vector field τ such that $B = L_{\tau}A = [\tau, A]$. Here the Lie derivative of A with respect to τ is just the Schouten bracket of the vector field with the operator. This problem is of interest in the theory of Hamiltonian deformations, see subsection 4.5.

While countless papers have been written on the symbolic computation of symmetries and conserved quantities, the literature on symbolic computations with Hamiltonian operators is quite scarce. The same situation holds for publicly available software packages. Possible reasons are that the algorithms for computing with integrability structures, like Hamiltonian, symplectic and recursion operators, are less standard and more involved with respect to those for symmetries and conserved quantities. Another reason might be that few experts in integrable systems have the abilities that are needed to deal with differential operators in a computer algebra system as required for the mathematical problems at hand, and conversely, few experts in computer algebra are also familiar with the mathematics of integrable systems.

A recent book on integrability structures [46] tries to fill the above gaps: it contains, between other material, symbolic computations related to the direct problem (item 1 above). The software package CDE², an official Reduce package [37], is used throughout the book. An extensive review of existing software for integrability structures can be found in the book.

This paper integrates material of [46] in the direction of the solution of the above problems 3–7. It should be remarked that many authors developed software for similar purposes without making it available to the public. That makes their computations much more difficult to reproduce. There are few software packages with similar capabilities that are also in the public domain. We will briefly list them and comment the features that are not already considered in the above mentioned review [46, Section 1.3].

- 1. The Maple package jets [7] contains a module for computing the Schouten bracket of local differential operators. See [46, Section 1.3] for more comments. At the time of writing it seems that the package is no longer available in internet, in particular it is not in the website of the author.
- 2. The Maple package Jets [11], initially developed by Marvan (2003), then also by Baran (2010), has been used for computing Hamiltonian operators for particular differential equations [9, 8, 10, 12]. However, it does not contain any specific feature for integrability structures (like an implementation of the Schouten bracket).
- 3. The Maple package JET [50] can compute with integrability structures, see [46, Section 1.3] for more comments.

The limits of the package are the fact that it can only compute with operators in one independent variable (x) and a partial support of computations with nonlocal (pseudodifferential) operators D_x^{-1} (simplification of such terms cannot always be performed). The recent paper [16] provides an algorithm for the simplification of such expressions; the authors plan to implement the algorithm in computer algebra system (also in CDE) in the near future.

²This is an acronym standing for Calculus on Differential Equations

- 4. The Maple package DifferentialGeometry [2], developed by I. Anderson, is being extended by a library of procedures which are devoted to integrable systems (private communication of I. Anderson to the author). At the moment the library is still not available in Maple.
- 5. The package [5] deserves a mention, in that it is devoted to finding recursion operators for symmetries; however, the kind of computations that are required are different from those considered here, even if the subject is closely related under the mathematical viewpoint (see [46] for a deeper discussion).
- 6. In the framework of the algebraic approach to the Hamiltonian formalism for PDEs [6] the Mathematica packages MasterPVA and WAlg [17] provide procedures for computing the Schouten bracket between local differential operators. The recent paper [16] shows that the algebraic approach to Schouten brackets leads to the same computations and results as more traditional approaches, also for nonlocal operators.

Basically, the only packages that are ready to be used for computations with Hamiltonian operators in a set of problems which is wide enough are the above items 3 and 6. The package JETS is limited by the fact that it can only use operators in one independent variable. The package MasterPVA uses an algebraic formalism which has a completely different nature to formalisms which are more common in the field. Moreover, both the above packages cannot do the computations of items 4 and 7, because the packages lack of capabilities to linearize an operator and take its adjoint, and cannot deal with multivectors. Indeed, Hamiltonian operators are bivectors, and computing with Hamiltonian operators amounts at doing computations for multivectors in the special case of degree 2, see Section 2.

The above limits result from reading the manuals; maybe with some extra programming both packages might include the above capabilities.

The package CDE can compute with operators in an arbitrary number of variables, it uses a standard formalism or the formalism of supermanifolds in order to implement the operators and it can do all computations on Hamiltonian operators that we listed above.

Moreover, CDE is able to deal with Hamiltonian operators as variational multivectors. They are dual to variational forms, exactly as ordinary multivectors on finite-dimensional manifolds are dual to differential forms. Variational forms are endowed by the variational differential (that is the analogue of the de Rham differential of forms on manifolds) and constitute the so-called *variational complex* [64]; variational multivectors are endowed by a bracket operation, the Schouten bracket (which is the analogue of the Schouten-Nijenhuis bracket between ordinary multivectors) [39].

Variational multivectors are implemented in CDE both as differential operators in several arguments and as superfunctions on supermanifolds. This makes CDE unique

within existing software for computing with Hamiltonian operators, also in view of future research with multivectors or in the mathematics and physics of supermanifolds. Indeed, a few packages that can compute with anticommuting (or Grassmann) variables were written so far [18, 36, 61], but none of them has an implementation of all the required capabilities for Hamiltonian operators. At the moment only CDE has an implementation of total derivatives and variational derivatives that act on functions of even or odd field variables and their derivatives. Many calculations that are typical in theoretical physics, like computing the Euler-Lagrange equations of a Lagrangian defined on a supermanifold, computing symmetries and conservation laws for super-differential equations, etc., can be done on a computer by means of CDE, with little or no extra programming. See also [44], where CDIFF, the 'ancestor' of CDE, was used with a non-automatic implementation of total derivatives for computing symmetries of super-differential equations; similar tasks were also considered in [4] with a Maple program.

CDE is implemented in Reduce for several reasons: Reduce is free software, and it was possible to study its internals. As a side outcome of this work, many undocumented parts of Reduce internals were described in the manual [55]. Then, Reduce has been used for decades with its package CDIFF for problems which are closely related to those presented in this paper, in particular by Kersten and the University of Twente research group. Finally, CDE has an easy interface that makes the above problems easy to program, with few commands needed to achieve the result.

Nonlocal Hamiltonian operators are an essential part of integrable systems. At the moment, CDE can quite easily compute the conditions for a nonlocal operator to be Hamiltonian for a given partial differential equation (in the sense of mapping conserved quantities into symmetries), see [46] for examples. However, CDE lack of capabilities for computing Schouten brackets of pseuddifferential operators. In order to fill this gap an algorithm was recently developed [16]. A more advanced geometric approach is in development [45]. We hope to extend the range of CDE to nonlocal operators in a near future.

The structure of the paper is as follows.

In Section 2 we describe multivectors and their calculus, also in terms of superfunctions. The isomorphism between multivectors and superfunctions allows to use a very elegant formula for the Schouten bracket.

In Section 3 we describe the CDE implementation of operators and related computations.

In Section 4 we show examples of nontrivial computations performed with CDE. The examples cover the problems 4–7 listed above. While the corresponding results have already been published elsewhere, the computational methods are a fundamental part of the research effort that led to the scientific results, and have never been published before. They can be of help for similar computations in other mathematical problems. Finally, we present several research-grade problems at the end of each

example. Hopefully, they will motivate the Reader to using CDE in his/her scientific research.

2 Hamiltonian operators and partial differential equations

Let us denote independent variables by x^{λ} , $1 \leq \lambda \leq m$, dependent variables by (u^{i}) , $1 \leq i \leq n$, and derivatives by u^{i}_{σ} (here $\sigma = (\sigma_{1}, \ldots, \sigma_{m})$ is a multiindex representing derivatives with respect to x^{1} σ_{1} times, ..., x^{m} σ_{m} times). For each coordinate x^{λ} the total derivative vector field ∂_{λ} is defined as

$$\partial_{\lambda} = \frac{\partial}{\partial x^{\lambda}} + u^{i}_{\sigma,\lambda} \frac{\partial}{\partial u^{i}_{\sigma}},\tag{5}$$

(the summation convention holds as usual) where σ, λ stands for the multiindex $\sigma + (0, \ldots, 1, \ldots, 0)$, where 1 is at the position λ . Note that if $\sigma = 0$ then $u^i_{\sigma} = u^i$.

Hamiltonian operators are members of a broader family of differential operators, namely, they are *variational multivectors* [13, 34, 57, 39]. Variational multivectors are specific differential operators in total derivatives, or C-differential operators (see [13] for a definition).

Let us define functional m-forms (or Lagrangians) α as volume forms on the space of independent variables whose coefficients depend on $(x^{\lambda}, u_{\sigma}^{i})$:

$$\alpha = \alpha_0(x^{\lambda}, u_{\sigma}^i) dx^1 \wedge \dots \wedge dx^m \tag{6}$$

The space of functional m-forms is denoted by $\bar{\Lambda}^m$. The kernel of the variational derivative of local functionals consists of total divergencies, or functional m-forms of the type $\partial_{\lambda}(\beta^{\lambda})dx^{1}\wedge\cdots\wedge dx^{m}$, where (β^{λ}) , with $1\leq\lambda\leq m$, is a vector function of (x^{μ},u^{j}_{σ}) . Let us denote the space of total divergencies by $d\bar{\Lambda}^{m-1}$. We define the space of local functionals as $\bar{H}^{m}=\bar{\Lambda}^{m}/\bar{d}\bar{\Lambda}^{m-1}$.

A variational multivector is defined to be a skew-symmetric C-differential operator with values in local functionals.

The expression of a variational multivector is

$$\Delta(\psi^1, \dots, \psi^h) = [a^{(\sigma_1 i_1) \cdots (\sigma_h i_h)} \partial_{\sigma_1} \psi^1_{i_1} \cdots \partial_{\sigma_h} \psi^h_{i_h}]. \tag{7}$$

Here, the arguments of Δ are vector-valued functions of the type $\psi = (\psi_i(x^{\lambda}, u^j_{\sigma}))$, and the coefficients $a^{(\sigma_1 i_1)\cdots(\sigma_h i_h)}$ are functions of $(x^{\lambda}, u^j_{\sigma})$ which are skew-symmetric with respect to the interchange of pairs $(\sigma_k i_k)$ and $(\sigma_h i_h)$. The value of Δ , i.e., the right-hand side of (7), is an equivalence class up to total divergencies. Note that we will omit $dx^1 \wedge \cdots \wedge dx^m$ for the sake of brevity.

A variational multivector can be uniquely represented by taking its formal adjoint in one of its arguments (say the last one; see [13] for a geometric definition):

$$\Delta^*(\psi^1, \dots, \psi^{h-1})^i = (-1)^{|\sigma_h|} \partial_{\sigma_h} (a^{(\sigma_1 i_1) \cdots (\sigma_h i)} \partial_{\sigma_1} \psi^1_{i_1} \cdots \partial_{\sigma_{h-1}} \psi^{h-1})$$
(8)

Indeed, it is easy to realize that the above expression is equal to the previous expression (up to a total divergence) and it is divergence-free, i.e., no expression of order zero in one of the arguments can have the form of a total divergence.

The above representation defines an isomorphism between the space of variational h-vectors and the space of vector-valued h-C-differential operators of the form

$$\Box(\psi^1, \dots, \psi^h)^j = b^{j(\sigma_1 i_1) \cdots (\sigma_h i_h)} \partial_{\sigma_1} \psi^1_{i_1} \cdots \partial_{\sigma_h} \psi^h_{i_h}$$
(9)

which are both skew-symmetric with respect to the exchange of arguments and skew-adjoint with respect to each argument [39].

The calculus of variational multivectors consists of obvious operations, like sums and compositions, and of the variational Schouten bracket (or just Schouten bracket for short). The Schouten bracket for variational multivectors was first formulated in wide generality in [34] (see also [39, 42]). Its expression is not implemented in CDE in the language of differential operators.

There is another way to express the bracket which is much more elegant and compact [35] (see also [39, 38, 42]). Let us consider a vector of new dependent variables (p_i) , $1 \le i \le n$. We will assume that the new variables (and hence their derivatives) are Grassmann, or anticommuting, variables, so that we will be dealing with the jet of a superbundle with coordinates $(x^{\lambda}, u^i_{\sigma}, p_{j\tau})$. Then, there is an isomorphism between the space of skew-symmetric vector-valued C-differential operators (9) and the space of vector-valued superfunctions

$$F^{j} = b^{j(\sigma_{1}i_{1})\cdots(\sigma_{h}i_{h})} p_{i_{1}\sigma_{1}}\cdots p_{i_{h}\sigma_{h}}.$$
(10)

In coordinates, the isomorphism is given by

$$b^{j(\sigma_1 i_1)\cdots(\sigma_h i_h)}\partial_{\sigma_1}\psi^1_{i_1}\cdots\partial_{\sigma_h}\psi^h_{i_h} \longrightarrow b^{j(\sigma_1 i_1)\cdots(\sigma_h i_h)}p_{i_1\sigma_1}\cdots p_{i_h\sigma_h}$$
(11)

Of course, if the skew-symmetric C-differential operator is a variational multivector, then the corresponding superfunction is defined up to total divergencies of vector-superfunctions.

Using the above formalism, if two variational multivectors are represented by the scalar superfunctions F and H (up to total divergencies), then we have the following formula for the Schouten bracket:

$$[F, H] = \left[\frac{\delta H}{\delta u^i} \frac{\delta F}{\delta p_i} - (-1)^{(F+1)(H+1)} \frac{\delta F}{\delta u^i} \frac{\delta H}{\delta p_i} \right]$$
(12)

Here the letters F, H at the exponent of (-1) mean the Grassmann parity of the corresponding superfunction, and $\delta F/\delta u^i$, $\delta F/\delta p_i$,... denote the variational derivatives

$$\frac{\delta F}{\delta u^i} = (-1)^{|\sigma|} \partial_{\sigma} \left(\frac{\partial F}{\partial u^i_{\sigma}} \right), \quad \frac{\delta F}{\delta p_i} = (-1)^{|\sigma|} \partial_{\sigma} \left(\frac{\partial F}{\partial p_{i\sigma}} \right). \tag{13}$$

Note that the derivatives with respect to odd coordinates are odd derivatives, and total derivatives (5) are extended to odd variables as

$$\partial_{\lambda} = \frac{\partial}{\partial x^{\lambda}} + u^{i}_{\sigma,\lambda} \frac{\partial}{\partial u^{i}_{\sigma}} + p_{i\sigma,\lambda} \frac{\partial}{\partial p_{i\sigma}}.$$
 (14)

The square brackets on the right-hand side of (12) mean that we are in an equivalence class, or that the expression in the bracket is considered up to total divergencies of superfunctions.

The above formula is undoubtedly the clearest and most elegant expression of the Schouten bracket. But its clarity has a price to pay: one should be able to compute with Grassmann variables in order to use it. We will see that CDE implements the required capabilities.

Hamiltonian operators are (matrix) differential operators in total derivatives acting on vector-valued functions $\psi = (\psi_i(x^{\lambda}, u^j_{\sigma}))$

$$A(\psi) = A^{ij}\psi_j = a^{i(\sigma j)}\partial_\sigma\psi_j,\tag{15}$$

where $a^{i(\sigma j)}$ are functions of $(x^{\lambda}, u_{\sigma}^{k})$.

The operator A is requested to fulfill two properties:

• A is formally skew-adjoint: $A^* = -A$, where

$$(A^*)^{ij}\psi_j = (-1)^{|\sigma|}\partial_\sigma \left(\psi_j a^{j(\sigma i)}\right) \tag{16}$$

This means that A is a variational bivector represented as (9);

• The Schouten bracket of the operator with itself is zero:

$$[A, A] = 0. (17)$$

In order to compute the Schouten bracket of A, we should first of all represent A as a superfunction. In order to use the isomorphism (11) we need to write A in the form (7). This just means that the isomorphism takes the form

$$a^{i(\sigma j)} \partial_{\sigma} \psi_{i}^{1} \psi_{i}^{2} \longrightarrow a^{i(\sigma j)} p_{j\sigma} p_{i},$$
 (18)

where the product between $p_{j\sigma}p_i$ is the Grassmann product. Then, as the Grassmann parity of A is 2, we have

$$[A, A] = 2 \left[\frac{\delta A}{\delta u^i} \frac{\delta A}{\delta p_i} \right] \tag{19}$$

where $A = a^{i(\sigma j)} p_{j\sigma} p_i$. If we wish to check that the Schouten bracket is zero, we can apply the Euler-Lagrange operator to the expression in the bracket to verify that it is zero.

A partial differential equation in evolutionary form $u_t^i = f^i(x^{\lambda}, u^j, u_{\sigma}^j)$ is said to be *Hamiltonian* with respect to a Hamiltonian differential operator $A = (A^{ij})$ if it exists a local functional H = [h], where $h = h(x^{\lambda}, u_{\sigma}^i)$, such that

$$u_t^i = f^i(x^\lambda, u^j, u_\sigma^j) = A^{ij} \left(\frac{\delta h}{\delta u^j}\right). \tag{20}$$

It can be proved that a Hamiltonian operator satisfies the following equation:

$$\ell_F \circ A = -A \circ \ell_F^*, \tag{21}$$

where ℓ_F is the Fréchet derivative, or linearization, of the function $F = u_t^i - f^i$ that defines the equation, and ℓ_F^* is its formal adjoint:

$$\ell_F(\varphi) = \frac{\partial F^k}{\partial u^i_\sigma} \partial_\sigma \varphi^i, \quad \ell_F^*(\psi) = (-1)^{|\sigma|} \partial_\sigma \left(\frac{\partial F^k}{\partial u^i_\sigma} \psi_k \right), \tag{22}$$

We observe that the kernel of ℓ_F consists of (generalized, or higher) symmetries of the differential equation (20) [13, 57]. A conservation law $\omega = hdt + kdx$ for an evolutionary equation (20) is defined up to trivial quantities of the form $\alpha = \partial_t f dt + \partial_x f dx$, and is uniquely represented by its generating function, or characteristic, $\psi = (\delta h/\delta u^i)$. The kernel of ℓ_F^* contains generating functions, or characteristic vectors, of conserved quantities [13, 20, 57]. Hence, (21) implies that a Hamiltonian operator maps conserved quantities into symmetries.

An extension of this notion for non-evolutionary equations is also available [43], but will not be considered here.

The Poisson bracket of local functionals H = [h] and F = [f] is

$$\{H, F\}_A = \left[\frac{\delta h}{\delta u^i} A^{ij} \frac{\delta f}{\delta u^j} \right]. \tag{23}$$

The Poisson bracket fulfills the properties

$$\{H, F\}_A = -\{F, H\}_A$$
 (24)

$$\{\{H, F\}_A, G\}_A + \{\{G, H\}_A, F\}_A + \{\{F, G\}_A, H\}_A = 0$$
(25)

and it endows the space of functionals with the structure of a Lie algebra. It can be proved that the above properties are direct consequences of the properties (16) and (17), respectively; and conversely, if the bracket defined by a C-differential operator A as in (23) fulfills (24) and (25) then A is a Hamiltonian operator. Of course, the bracket can be computed between generating functions of conserved quantities. Usually, a partial

differential equation is said to be *integrable* if it possesses a sequence of conserved quantities which are in involution with respect to a Poisson bracket.

The integrability of a partial differential equation follows when the equation admits two Hamiltonian formulations (20) for two distinct Hamiltonian operators A_1 , A_2 and respective densities H_1 , H_2 ; the operators are required to be *compatible*, or that their Schouten bracket vanish: $[A_1, A_2] = 0$. In this case, the celebrated theorem by Magri [49] states that the conserved quantities generated by the recurrence formula

$$A_1(\psi_{i+1}) = A_2(\psi_i) \tag{26}$$

are in involution with respect to the Poisson brackets defined by both operators: $\{\psi_i, \psi_{i+1}\}_{A_1} = \{\psi_i, \psi_{i+1}\}_{A_2} = 0, i = 0, 1, 2, \dots$

3 Computing with C-differential operators and superfunctions

We describe the implementation of C-differential operators and superfunctions in CDE and related operations. The exposition differs from that of [46] in that it is aimed at computing with Hamiltonian operators.

Standard Reduce concepts and syntax will not be discussed here; we invite the interested reader to have a look at Reduce's official website [37]. More details on CDE, including a list of all commands, can be found in [46].

3.1 CDE and total derivatives

Starting from independent, dependent and Grassmann, or odd, variables CDE automatically creates the list of derivative coordinates (as symbols). The basic properties of odd variables in CDE, namely the odd product, the odd derivatives and the definition of a supervectorfield, are provided by the package CDIFF (now officially in the Reduce distribution), written by Gragert, Kersten, Post and Roelofs from the University of Twente (Netherlands), which is automatically loaded by CDE.

In a Reduce terminal, load the CDE package by the command load_package cde;. Then a supermanifold is created by the command

```
cde({indep_var,dep_var,odd_var,total_order},{});
```

Here, the first list contains the names of the lists of independent variables, dependent variables, odd variables and the maximal order of derivative coordinates. For example, we might have

```
indep_var:={t,x}; dep_var:={u,v};
odd_var:={p,q}; total_order:=10;
```

The empty list at the second argument of cde is used for the restriction of total derivatives on differential equations (which we will not use in this paper). After the above command the system has distinct lists of even derivatives (u^i_{σ}) and odd derivatives $(p_{j\tau})$ (up to the order total_order) in the form

Note that the symbol v_xt does not exist in CDE (with the above data) for performance reasons. Odd variables can appear in anticommuting products; this is represented as

$$ext(p,p_2tx), ext(p_x,q_t,q_t2x), \dots$$

where p and ext(p) are just the same, while ext(p_2tx,p) is not automatically expanded to -ext(p,p_2tx) for performance reasons; only one of the two symbols is understood by the system. In order to get the correct representation the function

```
odd_product(phi,psi);
```

should be used for the odd product of two superfunctions. The derivative of an expression phi with respect to an odd variable p is achieved by df_odd(phi,p);.

CDE also defines total derivatives (14) on the given supermanifold, truncated at the order total_order. Total derivatives are distinguished supervector fields; they are defined through a CDIFF function using data that is constructed by CDE. Basically, for each derivative symbol (like u_2tx) in the system the coefficient of the corresponding derivative $\partial/\partial u_{2tx}$ is computed by increasing the multiindex by one in the direction of the corresponding independent variable, and the results are summed up to make (14). The total derivative of a superfunction phi is invoked by td(phi,x); or td(phi,t,x,2);, for example. The syntax closely follows Reduce syntax for standard derivatives df; the above expressions translate to $\partial_x \varphi$ and $\partial_t \partial_x^2 \varphi$, respectively.

Each time that a coefficient in a total derivative has order higher than total_order it is replaced by the identifier letop³, which is a function that depends on all independent variables. After evaluating total derivatives, the result is scanned for the presence of letop. If that is the case the program stops with an error message and the computation must be repeated with a higher value of total_order. If needed, CDE programs can be run by a Linux shell script, rrr.sh, which is included in the package; the script will re-run the program with a higher jet order if a jet order error is met.

The computation of total derivatives can lead to huge expressions. It is possible to disable the expansion of total derivatives by the command noexpand_td(); (and re-enable it by expand_td();).

The command

³In Dutch 'let op' means 'pay attention'

computes the variational derivative $\delta F/\delta w^i$, where F is expr, w^i is the dependent variable dvar and par is the parity of the dependent variable, 0 if even or 1 if odd. The command euler_df(expr) computes all even and odd variational derivatives and returns their values in a list of two lists.

3.2 CDE and C-differential operators

A vector valued C-differential operator (9) must be declared in CDE as follows:

```
mk_cdiffop(opname,num_arg,length_arg,length_target);
```

where

- opname is the name of the operator $(\square \text{ in } (9))$;
- num_arg is the number of arguments (h in (9));
- length_arg is the list of lengths of the arguments, e.g., in (9) one needs a list of h items {k_1,...,k_h}, each corresponding to number of components of the vector functions ψ^j_{ij} to which the operator is applied. In the calculations of this paper we will only use one argument;
- length_target is the number of components of the image vector function (the range of the index j in (9)).

The above parameters of the operator opname are saved in the *property list* of the identifier opname (more comments can be found in [46]). The value of one component of the operator \square on the arguments ψ^1, \ldots, ψ^h is

```
opname(j,i1,...,ih,psi1,...,psih);
```

A vector-valued superfunction (10) must be declared in CDE as follows:

```
mk_superfun(sfname,deg,length_target);
```

where

- sfname is the name of the superfunction (F in (10));
- deg is the degree of the superfunction, e.g., h in (10);
- length_target is the number of components of the image vector (the range of the index j in (10)).

The syntax for one component of the superfunction sfname is

```
sfname(j);
```

CDE can convert C-differential operators with one argument into superfunctions of degree 1 and back:

- conv_cdiff2superfun(cdop,superfun)
- conv_superfun2cdiff(superfun,cdop)

The translation from an operator to a superfunction is easy: it is enough to evaluate all components of the operator on all odd dependent variables. The other direction is more complicated: coefficients $C_i^{j\sigma}$ of odd variables $p_{j\sigma}$ have to be collected from each component i of the superfunction, then a Reduce operator $\operatorname{cdop}(i,j,psi)$ is defined by the sum (with respect to σ) $C_i^{j\sigma}\partial_\sigma\psi$. Here the technical difficulty is defining an operator inside a Reduce procedure, psi being just a formal parameter and not an expression. Indeed, as a data structure, a superfunction is much more easy to handle than a Reduce operator.

The linearization of a purely even vector-function and the adjoint of a C-differential operator with one argument are computed by means of the isomorphism (11). More precisely, given a function $F = F(x^{\lambda}, u^{i}_{\sigma})$ the following superfunctions can be easily computed:

$$\ell_F((p_j))^k = \sum_{i,\sigma} \frac{\partial F^k}{\partial u^i_{\sigma}} p_{i_{\sigma}} \quad \ell_F^*((p_j))_i = (-1)^{|\sigma|} \partial_{\sigma} \left(\frac{\partial F^k}{\partial u^i_{\sigma}} p_{k_{\sigma}} \right)$$
 (27)

and then translated back into C-differential operators using the above conversion utilities.

In CDE a vector function must be introduced as a list of scalar functions

Then its linearization is achieved by the left formula (27) implemented in the command

```
ell_function(fun,lfun);
```

where lfun is automatically declared as a C-differential operator with the appropriate parameters. Moreover, the above command creates a superfunction lfun_sf that corresponds to the C-differential operator lfun.

The command

```
adjoint_cdiffop(lfun,lfun_star);
```

computes the adjoint lfun_star of lfun by the formula on the right of (27) and introduces an equivalent superfunction whose identifier has the suffix _sf: lfun_star_sf.

4 Five easy pieces

Elementary computations with Hamiltonian operators can be found in the CDE section in Reduce's manual [37]. Here, we would like to show the solution of the computational problems that we listed in the Introduction (p. 3, items 4–7) for nontrivial examples. The examples have been published in separate research papers in recent years.

While results are almost all known, a detailed description of the corresponding computations appears here for the first time. The design of effective software for the solution of the mathematical problems that have been considered so far was is a fundamental and nontrivial part of the research activity. It deserves a separate exposition and it might be of interest when trying to solve similar problems. All the examples are provided as Reduce program files in the website of the author http://poincare.unisalento.it/vitolo.

To the authors' knowledge, no other computer algebra computations of this type and level have been published with all details before.

At the end of each example a research problem is presented in order to motivate the Reader to use CDE in his/her research.

4.1 Warm-up: tedious large-scale computations

The associativity equation, or Witten–Dijkgraaf–Verlinde–Verlinde (WDVV) equation was derived in the context of 2D-topological field theory. It consists in an overdetermined system of PDEs with one dependent variable and N independent variables. Nowadays its significance is mostly mathematical. For example, its solutions yield, under mild hypotheses, bi-Hamiltonian systems. See [26] for a mathematical introduction to the equation.

In [29] a bi-Hamiltonian formulation of the WDVV equation in the simplest case N=3 was found. It was only in recent times that such a result was extended to the case N=4, also thanks to CDE [59]. Here we will describe the role of CDE in [59].

In [30] the WDVV equation was rewritten, in the case N=4 (see [26] for details), as a pair of commuting hydrodynamic-type systems

$$a_{y}^{1} = a_{x}^{2}, a_{z}^{1} = a_{x}^{3}, a_{y}^{2} = a_{x}^{4} a_{z}^{2} = a_{x}^{5}, a_{y}^{3} = a_{x}^{5}, and a_{z}^{2} = a_{x}^{6}, a_{y}^{4} = R_{x} and a_{z}^{4} = P_{x}, a_{z}^{4} = P_{x}, a_{z}^{6} = S_{x}, a_{y}^{6} = S_{x} a_{z}^{6} = Q_{x}$$

$$(28)$$

where

$$P = \frac{a^3 a^4 + a^6}{a^1}, \quad R = \frac{2a^5 + a^2 a^4}{a^1}, \quad S = \frac{2a^3 a^5 - a^2 a^6}{a^1},$$

$$Q = (a^5)^2 - a^4 a^6 + \frac{(a^3)^2 a^4 + a^3 a^6 - 2a^2 a^3 a^5 + (a^2)^2 a^6}{a^1}.$$

In [30] (see also [54]) it was proved that the above two systems (28) admit a first-order Dubrovin–Novikov Hamiltonian operator. This is an operator of the type

$$A_1^{ij} = h^{ij}\partial_x + \Gamma_k^{ij}u_x^k. \tag{29}$$

The operator is homogeneous (of degree 1) with respect to a grading which is given by x-derivatives [27]. This implies that the form of the operator is invariant with respect to coordinate transformations of type $\tilde{u}^i = \tilde{u}^i(u^j)$. As a consequence, the coefficients transform as geometric objects: for example, h^{ij} transforms as a contravariant 2-tensor. It can be proved that the Hamiltonian property of the operator is equivalent (here and in what follows $\det(h^{ij}) \neq 0$) to the fact that $(h_{ij}) = (h^{ij})^{-1}$ is a flat pseudo-Riemannian metric and $\Gamma^j_{hk} = -h_{hi}\Gamma^{ij}_k$ are its Christoffel symbols.

In our example, the first-order Dubrovin–Novikov Hamiltonian operator for (28) is

$$A_{1}^{ij} = \begin{pmatrix} 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ a^{1} & a^{2} & a^{3} & a^{4} & a^{5} & a^{6} \\ -1 & 0 & 0 & 0 & 0 & 0 \\ a^{2} & a^{4} & a^{5} & R & P & S \\ 2a^{3} & 2a^{5} & 2a^{6} & 2P & 2S & 2Q \end{pmatrix} \partial_{x} + \partial_{x} \begin{pmatrix} 0 & 0 & a^{1} & -1 & a^{2} & 2a^{3} \\ 0 & -1 & a^{2} & 0 & a^{4} & 2a^{5} \\ 0 & 0 & a^{3} & 0 & a^{5} & 2a^{6} \\ -1 & 0 & a^{4} & 0 & R & 2P \\ 0 & 0 & a^{5} & 0 & P & 2S \\ 0 & 0 & a^{6} & 0 & S & 2Q \end{pmatrix}.$$
(30)

In [59] it was proved that the above two systems (28) are indeed bi-Hamiltonian, as they also admit the compatible Dubrovin–Novikov type third-order Hamiltonian operator [25] (see subsection 4.2)

$$A_2^{ij} = \partial_r (g^{ij}\partial_r + c_k^{ij}a_r^k)\partial_r, \tag{31}$$

where we assume that $det(g^{ij}) \neq 0$, and if we set $(g_{ij}) = (g^{ij})^{-1}$, then

$$g_{ik}(\mathbf{a}) = \begin{pmatrix} (a^4)^2 & -2a^5 & 2a^4 & -(a^1a^4 + a^3) & a^2 & 1\\ -2a^5 & -2a^3 & a^2 & 0 & a^1 & 0\\ 2a^4 & a^2 & 2 & -a^1 & 0 & 0\\ -(a^1a^4 + a^3) & 0 & -a^1 & (a^1)^2 & 0 & 0\\ a^2 & a^1 & 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$
(32)

The coefficients c_k^{ij} are given by the formula [31]

$$c_{skm} = \frac{1}{3}(g_{sm,k} - g_{sk,m}),\tag{33}$$

where $c_{ijk} = g_{iq}g_{jp}c_k^{pq}$. The condition $[A_2, A_2] = 0$ is ensured by the properties [31, 62]

$$g_{mk,s} + g_{ks,m} + g_{ms,k} = 0, (34)$$

$$c_{msk,l} = -g^{pq}c_{pml}c_{qsk}. (35)$$

In [59] CDE was used to check that $[A_1, A_2] = 0$. Indeed, for few types of Dubrovin–Novikov operators (like first, second and third-order operators) it is known that the vanishing of the Schouten bracket is equivalent to some tensorial conditions on the coefficients of the operators. However, at the moment of writing, tensorial conditions of compatibility of a first order and a third-order Dubrovin-Novikov operator are not known. Hence, the only way to check that $[A_1, A_2] = 0$ is a direct computation. This is a very long and tedious task which is not instructive at all: a typical computation for a machine.

Here we describe the implementation of the calculation of $[A_1, A_2] = 0$. The program file is w6c_biham and can be found at the web page of the author http://poincare.unisalento.it/vitolo.

In Reduce, load the package CDE, then declare the input variables and call cde:

```
indep_var:={x};
dep_var:={a,b,c,d,ee,f};
odd_var:={p,q,r,s,tt,u};
total_order:=10;
cde({indep_var,dep_var,odd_var,total_order},{});
```

Then we define two matrices whose entries are: the metric of the first-order operator (in upper indices) hul(i,j), and the metric of the third-order operator (in lower indices) gl3(i,j). We define two operators, gamma_hi_con(i,j) that contains the expression $\Gamma_k^{ij}u_x^k$ and c_hi_con(i,j) that contains the expression $c_k^{ij}u_x^k$. The operator A_1 is defined as

```
mk_cdiffop(aa1,1,{6},6);
for all i,j,psi let aa1(i,j,psi)=
   hu1(i,j)*td(psi,x)+gamma_hi_con(i,j)*psi;

and the operator A2 is defined as:
   mk_cdiffop(aa2,1,{6},6);
   for all i,j,psi let aa2(i,j,psi) =
   td(
   gu3(i,j)*td(psi,x,2)+c_hi_con(i,j)*td(psi,x)
   ,x);

We convert them into superfunctions, according with (11)
   conv_cdiff2superfun(aa1,aa1_sf);
   conv_cdiff2superfun(aa2,aa2_sf);
```

We take their adjoint by cde and make the following simple skew-adjointness test:

```
adjoint_cdiffop(aa1,aa1_star);
for i:=1:length(dep_var) do
  if aa1_sf(i) + aa1_star_sf(i) neq 0 then
   write "Warning: non-skew-adjoint operator!";
```

and analogously for aa2. Then, we convert the operators into bivectors, according with (9)

```
conv_genfun2biv(aa1_sf,biv1);
conv_genfun2biv(aa2_sf,biv2);
```

Finally, we should check whether the Schouten bracket of the two operators is zero. We can even compute all possible Schouten brackets, to check the Hamiltonian property of the two operators:

```
iszero_schouten_bracket(biv1,biv1,thr11b);
iszero_schouten_bracket(biv1,biv2,thr12b);
iszero_schouten_bracket(biv2,biv2,thr22b);
```

the results are lists of zeros, and the computation takes a negligible time on a contemporary laptop of average computing power.

1 Problem. When forming WDVV equations an essential parameter is the number N of independent variables. It is an opinion of the author that WDVV equations might have a bi-Hamiltonian formalism for an arbitrary value of N. It is a recent discovery that the same holds for another system of PDEs that is of fundamental importance in the geometric theory of integrable systems, the oriented associativity equation, in the case N=3 [15].

The Readers might wish to try to find a bi-Hamiltonian formalism for the WDVV system in the easiest unknown case N = 5, to corroborate (or negate!) the above conjecture. The recommended literature for this problem is [29, 33, 59].

4.2 Finding Darboux coordinates

A natural problem of the theory of Hamiltonian operators is: given a Hamiltonian operator A, find coordinates such that the operator takes the form $A^{ij} = \eta^{ij}\partial_x$, where (η^{ij}) is a constant matrix. The corresponding coordinates are said to be Darboux coordinates of A. The problem of finding Darboux coordinates for Hamiltonian operators was considered by many authors so far, like [3, 53, 52, 56], where scalar Hamiltonian operators have been considered.

Darboux coordinates for operators A_1 of the type (29) always exist: they are flat coordinates for the flat pseudo-Riemannian metric h_{ij} . This means that a point transformation (which is not always easy to find in concrete examples) is enough to transform an operator of type (29) to $A^{ij} = \eta^{ij}\partial_x$.

A more difficult problem is finding Darboux coordinates for higher-order Dubrovin–Novikov operators. These operators were introduced in [25]. In the third-order case they have the form

$$A^{ij} = g^{ij}\partial_x^3 + b_k^{ij}u_x^k\partial_x^2 + (c_k^{ij}u_{xx}^k + c_{km}^{ij}u_x^k u_x^m)\partial_x + d_k^{ij}u_{xxx}^k + d_{km}^{ij}u_{xx}^k u_x^m + d_{kmn}^{ij}u_x^k u_x^m u_x^n.$$
 (36)

where coefficients are functions of (u^i) . It can be proved that the coefficient $-g_{js}d_k^{is}$ transforms like a linear connection that is symmetric and flat by the Hamiltonian property. The operator (36) can be rewritten in flat coordinates of $-g_{js}d_k^{is}$ as in (31). This means that the operator is completely determined by its leading term (g^{ij}) using (33). The pseudo-Riemannian metric (g_{ij}) is in bijective correspondence with certain projective varieties, see [31, 32, 33]. In particular, in the case of 3 dependent variables u^1 , u^2 , u^3 the operators are divided in 6 classes with respect to reciprocal transformations of the following projective type

$$d\tilde{x} = (a_0^0 + a_i^0 u^i) dx, \qquad d\tilde{t} = dt, \qquad \tilde{u}^i = \frac{a_0^i + a_j^i u^j}{a_0^0 + a_i^0 u^j}, \tag{37}$$

where a_j^i , a_j^0 , a_0^i , a_0^0 are constants. The 6 projective classes of operators are

$$g^{(1)} = \begin{pmatrix} (u^2)^2 + c & -u^1u^2 - u^3 & 2u^2 \\ -u^1u^2 - u^3 & (u^1)^2 + c(u^3)^2 & -cu^2u^3 - u^1 \\ 2u^2 & -cu^2u^3 - u^1 & c(u^2)^2 + 1 \end{pmatrix},$$

$$g^{(2)} = \begin{pmatrix} (u^2)^2 + 1 & -u^1u^2 - u^3 & 2u^2 \\ -u^1u^2 - u^3 & (u^1)^2 & -u^1 \\ 2u^2 & -u^1 & 1 \end{pmatrix}, \quad g^{(3)} = \begin{pmatrix} (u^2)^2 + 1 & -u^1u^2 & 0 \\ -u^1u^2 & (u^1)^2 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$g^{(4)} = \begin{pmatrix} -2u^2 & u^1 & 0 \\ u^1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad g^{(5)} = \begin{pmatrix} -2u^2 & u^1 & 1 \\ u^1 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad g^{(6)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

After introducing potential coordinates $u^i = b_x^i$ the operator (31) takes the form

$$A^{ij} = -\left(g^{ij}\partial_x + c_k^{ij}b_{xx}^k\right),\tag{38}$$

where coefficients are functions of (b_x^i) . It can be proved [59, 33] that each of the above metrics can be factorized as $g_{ij} = \varphi_{\alpha\beta}\psi_i^{\alpha}\psi_j^{\beta}$, where $(\varphi_{\alpha\beta})$ is a constant non-degenerate symmetric matrix and ψ_i^{α} are linear functions of the field variables: $\psi_i^{\alpha} = \psi_{im}^{\alpha}u^m + \omega_i^{\alpha}$, where $\psi_{im}^{\alpha} = -\psi_{mi}^{\alpha}$. In [33] we proved that n Casimirs exist for every operator in the form (38). More precisely, we proved that the functions $C^{\alpha} = (\frac{1}{2}\psi_{mk}^{\alpha}b_x^k + \omega_m^{\alpha})b^m$ satisfy

$$A^{ij}\frac{\delta C^{\alpha}}{\delta b^j} = 0. (39)$$

The above Casimirs turn out to be Darboux coordinates for $g^{(4)}$ and $g^{(5)}$. In order to prove that, we use the change of coordinates formula (see, e.g., [53, 56])

$$\tilde{A} = \ell_C \circ A \circ \ell_C^*, \tag{40}$$

where C is the Casimir vector function. The proof that \hat{A} will be of Darboux type can be done by CDE. We refer to the program file casimir. We start by

```
indep_var:={x};
dep_var:={b1,b2,b3};
odd_var:={p1,p2,p3};
total_order:=6;
```

and call cde, then we load the metric

```
g_5:=mat(( - 2*b2_x,b1_x,1),(b1_x,1,0),(1,0,0));
g13:=g_5;
gu3:=g13**(-1);
```

and define the operator $c_k i_c con(i,j)$ with the values of the expression $c_k^{ij} b_{xx}^k$ (see the source file) and introduce the operator A as

The Casimirs of the operator A are:

```
operator casimir;
casimir(1):=b1;
casimir(2):=b2;
casimir(3):=b3 + b1_x*b2;
```

We linearize the vector function casimir and define its adjoint:

```
f_dar:=for i:=1:ncomp collect casimir(i);
ell_function(f_dar,ldar);
adjoint_cdiffop(ldar,ldar_star);
```

The formula (40) is easily implemented:

```
mk_cdiffop(ta,1,{3},3);
for all i,j,psi let ta(i,j,psi)=
  for k:=1:ncomp sum for h:=1:ncomp sum
   ldar(i,k,a(k,h,ldar_star(h,j,psi)));
```

The result can be converted into a superfunction for a better presentation

```
conv_cdiff2superfun(ta,ta_sf);
```

we have

```
ta_sf(1);
    p3_x
ta_sf(2);
    p2_x
ta_sf(3);
    p1_x
```

that confirms that the above choice of Casimirs is a set of Darboux coordinates for A. In particular,

$$\tilde{A} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \partial_x. \tag{41}$$

Note that this is a proper differential substitution, i.e., a transformation that depends on derivatives of the dependent variables.

2 Problem. Proving that the nonlocal Casimirs are Darboux coordinates for $g^{(4)}$ is not a problem [41, 40]. However, the author did not manage to prove a similar result for the metrics $g^{(1)}$, $g^{(2)}$, $g^{(3)}$ and the metric of the third-order operator in subsection 4.1. Note that the equation (40), where $\tilde{A} = \eta^{ij}\partial_x$, η^{ij} is a constant matrix and C is an unknown vector function, is non-linear with respect to C; the resulting system of equations on C can be difficult to solve, even by using a simplified ansatz. The interested Reader might wish to consider this as a possible research problem.

4.3 Compatibility of third-order operators

A compatible pair A_1 , A_2 of Hamiltonian operators immediately leads to new integrable systems. The standard way to construct them is to solve the equation for Casimirs of A_1 :

$$A_1^{ij} \frac{\delta C}{\delta u^j} = 0, \tag{42}$$

where C is an unknown function of (u^k) . If there are at least n independent solutions of the above equations, they can be used as new coordinates (\tilde{u}^i) . In most cases the new coordinates are *not* Casimirs of A_2 , and define an integrable hierarchy through Magri's recursion (26).

For this reason, an interesting question that can be posed is: if we consider all possible pairs of homogeneous third-order Hamiltonian operators A_1 , A_2 , both from our list on page 19 (in the form (31)), will there be compatible pairs? The answer is: yes, but only in a rather trivial sense. The details are in the following table:

		$g^{(2)}$	$g^{(3)}$	$g^{(4)}$	$g^{(5)}$	$g^{(6)}$
$g^{(1)}$	y*	n	n	n	n	n
$g^{(2)}$	n	У	n	n	n	n
$g^{(3)}$	n	n	У	У	n	n
$g^{(4)}$	n	n	У	У	n	n
$g^{(5)}$	n	n	n	n	У	n
$g^{(6)}$	n	n	n	n	n	у

The notation is: n for non compatible, y for compatible, y^* for compatible under additional conditions. More particularly, the operators coming from $g^{(3)}$ and $g^{(4)}$ are indeed the direct sum of a 2×2 block and the one-dimensional operator ∂_x^3 , and the 2×2 blocks are known to be compatible [31]. Operators A_1 and A_2 coming from $g^{(1)}$ are compatible if and only if the value of the constants c in both operators is the same; so, we have no new compatible pairs besides the known ones.

The code for the above computation is rather simple (file compat3rd). We define an operator by

```
mk_cdiffop(aa1,1,{ncomp},ncomp);
for all i,j,psi let aa1(i,j,psi) =
td(
   gu3_1(i,j)*td(psi,x,2) + c_hi_con_1(i,j)*td(psi,x)
   ,x
);
```

and another operator aa2 with a different metric gu3_2(i,j), and then convert both to superfunctions and bivectors:

```
conv_cdiff2superfun(aa1,aa1_sf);
conv_cdiff2superfun(aa2,aa2_sf);
conv_genfun2biv(aa1_sf,biv_aa1);
conv_genfun2biv(aa2_sf,biv_aa2);
```

Finally, we compute the Schouten bracket and require that the three-vector is a total divergence:

```
schouten_bracket(biv_aa1,biv_aa2,th12);
eth12:=euler_df(th12(1));
templ:=for each el in eth12 join el;
sb_coeff:=splitext_list(templ);
sb_num_coeff:=for each el in sb_coeff collect num el;
sb_allcoeff:=splitvars_list(sb_num_coeff,all_parametric_der);
```

The list eth12 contains all variational derivatives with respect to even and odd coordinates of the Schouten bracket, the list sb_coeff contains all coefficients of odd variable

expressions, the list sb_num_coeff contains the numerators of the previous expressions, and the list sb_allcoeff contains the coefficients of monomials of even variables. It is easy to deduce the above results.

Despite the fact that the result is negative, it is new and the above computational scheme can be used for more interesting computations. The above computation would clearly be very hard with pen and paper.

3 Problem. The above computation is not a well-posed problem under the geometric viewpoint. Indeed, if A and B are two third-order Hamiltonian operators of the type (31) then only one of them (say A) can be brought to one of the forms (4.2); the other will be again of the form (31) but the leading term will not necessarily be in the list (4.2).

It is an open problem to check if there are any compatible pairs A, B, where A is one of the operators in the above list and B is another operator from the same list after a transformation of type (37).

4.4 Finding compatible operators

In this subsection we will address the following problem: given a Hamiltonian operator A, find all Hamiltonian operators B that are compatible with A. As it is known (see also the beginning of the previous subsection), compatible pairs of Hamiltonian operators yield integrable systems [49]. Usually, the answer is provided for specified forms of the unknown operator B.

We consider the above problem in the following formulation: given a third-order local homogeneous Hamiltonian operator R find all first-order homogeneous Hamiltonian operators P that are compatible with R: [P,R]=0. This problem was completely solved in the case n=2 in [48]. In this case there is an affine classification of third-order homogeneous Hamiltonian operators [31]: they are the three operators R_1 , R_2 , R_3 respectively determined by the three pseudo-Riemannian metrics

$$g^{(1)} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad g^{(2)} = \begin{pmatrix} -2u^2 & u^1 \\ u^1 & 0 \end{pmatrix}, \quad g^{(3)} = \begin{pmatrix} (u^2)^2 + 1 & -u^1u^2 \\ -u^1u^2 & (u^1)^2 \end{pmatrix}.$$

One of the results from [48] is that P_1 is a Hamiltonian operator compatible with R_3 if and only if

$$g_1^{11} = c_1 u^1 + c_2 u^2 + c_3, (43a)$$

$$g_1^{12} = c_4 u^1 - \frac{c_2}{2u^1} + \frac{c_3 u^2}{u^1} + \frac{c_2 (u^2)^2}{2u^1}, \tag{43b}$$

$$g_1^{22} = 2c_4u^2 + \frac{c_1}{u^1} + \frac{c_5u^2}{u^1} - \frac{c_1(u^2)^2}{u^1} + c_6, \tag{43c}$$

where g_1^{ij} are the coefficients of the metric of the first-order operator P_1 (of the form (29)) together with the algebraic conditions

$$c_2c_5 + 2c_1c_3 = 0$$
, $c_2c_6 - 2c_3c_4 = 0$, $c_1c_6 + c_4c_5 = 0$. (44)

Let us set up the computation in CDE; we describe the program file compat13. After initialization, we define an operator $\mathtt{hul_op}$ that contains the leading term of the unknown operator P_1 : $\mathtt{hul_op(i,j)}$:= $\mathtt{hul_ij}$ where $\mathtt{hul_ij}$ depends on dependent variables only. We also define an operator gamma_hi in such a way that

- 1. gamma_hi(i,j,k):=gamma_hi_ijk for i < j
- 2. gamma_hi(i,i,k):=(1/2)*df(hu1_op(i,i),part(dep_var,k))
- 3. gamma_hi(j,i,k):= gamma_hi(i,j,k) + df(hu1_op(i,j),part(dep_var,k)) for i > j

Indeed, we can use the linear part of the Hamiltonian properties for an operator of the form (29) as given in [21] in order to reduce the number of unknowns: they are

$$\Gamma_k^{ij} + \Gamma_k^{ji} = \partial_k g_1^{ij} \tag{45}$$

Then, we introduce an operator gamma_hi_con such that gamma_hi_con(i,j) contains the expression $\Gamma_k^{ij}u_x^k$. Now, we define the first-order operator

```
mk_cdiffop(aa1,1,{2},2);
for all i,j,psi let aa1(i,j,psi)=
  hu1_op(i,j)*td(psi,x)+gamma_hi_con(i,j)*psi;
```

(here aa1 stands for P_1) and from the metric

```
matrix g2_3(2,2);
g2_3(1,1):=b2**2 + 1;
g2_3(1,2):= - b1*b2;
g2_3(2,1):=g2_3(1,2);
g2_3(2,2):=b1**2;
g13:=g2_3;
```

construct the third-order operator

```
mk_cdiffop(aa2,1,{2},2);
for all i,j,psi let aa2(i,j,psi) =
td(
gu3(i,j)*td(psi,x,2)+c_hi_con(i,j)*td(psi,x)
,x);
```

(here aa2 stands for R_3). After converting the operators into bivectors

```
\begin{split} & \operatorname{conv\_cdiff2superfun(aa1,sym1)}; \\ & \operatorname{conv\_cdiff2superfun(aa2,sym2)}; \\ & \operatorname{conv\_genfun2biv(sym1,biv1)}; \\ & \operatorname{conv\_genfun2biv(sym2,biv2)}; \\ & \operatorname{it\ can\ be\ easily\ checked\ that\ } [R_3,R_3] = 0; \\ & \operatorname{schouten\_bracket(biv2,biv2,sb22)}; \\ & \operatorname{euler\_df(sb22(1))}; \\ & \operatorname{The\ compatibility\ equation\ } [P_1,R_3] = 0 \ \text{is\ found\ by} \\ & \operatorname{schouten\_bracket(biv1,biv2,sb12)}; \\ & \operatorname{comp12:=euler\_df(sb12(1))}; \\ \end{split}
```

Then, we solve the above equation. To do that, we first define an operator equ whose values are the 4 components of the equation, then use a CDE procedure that takes all coefficients of all monomials of odd coordinates in the equations and put them in the values equ(5), equ(6), ... of the operator:

the solution is (43) (after renaming the constants); we are also able to determine the Christoffel symbols Γ_k^{ij} in terms of the same constants. We should require the further condition

$$g^{is}\Gamma_s^{jk} = g^{js}\Gamma_s^{ik} \tag{46}$$

in order to obtain the symmetry of Γ^i_{jk} and the fact that Γ^i_{jk} are the Christoffel symbols of the Levi-Civita connection of g_1^{ij} . It turns out that the metric in (43) and the symbols Γ^{ij}_k satisfy the above equation without further conditions. Moreover, we must require the flatness of the metric g_1^{ij} ; that amounts to the algebraic equations (44).

In [48] we also prove that there are pencils of compatible first-order operators inside the space of solutions of the above problem. Unpublished computations with CDE show that such pencils continue to exist in the case n=3 and n=4, thus providing multi-parameter spaces of Miura-inequivalent integrable systems according with the mechanism which was first discovered in [58]. Such results would be very hard to achieve without computer-assisted calculations.

4 Problem. Find the list of all pencils of compatible first-order operators that are compatible with a fixed third-order operator in the case n = 3 or n = 4. Use the classification of third-order operators provided in [31, 32].

4.5 Computing Lie derivatives

Given a pair of compatible Hamiltonian operators A_1 , A_2 , it happens in many cases that there exists a vector field

$$\tau = \tau^i \frac{\partial}{\partial u^i}, \quad \text{where} \quad \tau^i = \tau^i(x^\lambda, u^i_\sigma),$$
 (47)

such that $A_2 = L_{\tau}A_1 = [\tau, A_1]$, where the bracket is obviously the Schouten bracket. This is more than just a curiosity: it is an essential feature of the perturbative approach to the classification of integrable systems in 1 + 1 dimensions initiated in [22]. Indeed, consider a Hamiltonian deformation of a first-order homogeneous Hamiltonian operator P_0 of the type (29)

$$P_{\epsilon} = P_0 + \epsilon P_1 + \epsilon^2 P_2 + \cdots \tag{48}$$

i.e., a one-parameter family of Hamiltonian operators P_{ϵ} where each of the summands P_1, P_2, \ldots is homogeneous of increasing degree. Then, it can be proved under some reasonable assumptions (see [19, 51]) that the deformation is always trivial, in the sense that there exists a vector field τ such that $P_{\epsilon} = L_{\tau}P_0$; this implies the existence of a formal diffeomorphism φ_{ϵ} such that $P_{\epsilon} = \ell_{\varphi_{\epsilon}} \circ P_0 \circ \ell_{\varphi_{\epsilon}}^*$. See [63] for a detailed exploration on Lie derivative and compatibility for Hamiltonian operators.

More generally, any Hamiltonian operator P_0 defines a map $d_{P_0} = [P_0, \cdot]$ which is a differential: $d_{P_0}^2 = 0$. The Hamiltonian cohomology, or Lichnerowicz-Poisson cohomology of d_{P_0} measures the presence of operators which are compatible with P_0 and are not the Lie derivative of P_0 , so that they are not deformable back to P_0 .

Another interesting feature of the Lie derivative is that it is useful to find topological hierarchies. Topological hierarchies are related with the theory of Gromov-Witten invariants, the theory of singularities and other topics; for more details, see [23]. In [28]

it was proved that if two Hamiltonian operators A_1 and A_2 of the type (48) fulfilling some further property define a topological hierarchy if and only if they are an *exact Poisson pencil*. The latter condition is, by definition, the existence of a vector field τ such that

$$A_2 = L_{\tau} A_1, \qquad L_{\tau} A_2 = L_{\tau}^2 A_1 = 0.$$
 (49)

Hence, for the above reasons (and more) it is natural to pose the question: given two compatible Hamiltonian operators A_1 , A_2 find a vector field τ (if it exists!) such that $A_2 = L_{\tau}A_1$.

In this paper we will consider two such calculations: one is for the bi-Hamiltonian pair of the KdV-equation, from [19], and the other is for the bi-Hamiltonian pair of the WDVV equation [26] presented as a hydrodynamic-type system [60].

Let us start with the KdV equation; the calculation is in the file kdv_lieder . After the initialization, we define the two well-known Hamiltonian operators A_1 and A_2

and consider the vector field τ as a degree 1 variational multivector tau and superfunction tau_sf

```
mk_cdiffop(tau,1,{1},1);
for all phi let tau(1,phi) = (- (1/2)*u**2 - (1/2)*u_2x)*phi;
mk_superfun(tau_sf,1,1);
tau_sf(1):= (- (1/2)*u**2 - (1/2)*u_2x)*p;
```

Then, we convert the above operators into the corresponding bivectors

```
conv_cdiff2superfun(a1,s1);

conv_cdiff2superfun(a2,s2);

conv_genfun2biv(s1,biv1);

conv_genfun2biv(s2,biv2);

and we compute the Schouten bracket [\tau, A_2]:
```

```
schouten_bracket(tau_sf,biv1,l_tau_biv1);
l_tau_biv1(1);
```

The result is not the same as biv2(1); however, they coincide in the variational cohomology, as they should:

euler_df(l_tau_biv1(1) - biv3(1));

{{0},{0}};

the latter being the list of the variational derivatives with respect to even (u) and odd (p) coordinates.

It is known that the simplest WDVV equation: $f_{ttt} = f_{xxt}^2 - f_{xxx}f_{xtt}$ can be rewritten as a hydrodynamic-type system by introducing new variables $a^1 = a = f_{xxx}$, $a^2 = b = f_{xxt}$, $a^3 = c = f_{xtt}$, namely:

$$a_t = b_x, \quad b_t = c_x, \quad c_t = (b^2 - ac)_x.$$
 (50)

It was proved in [29] that the above system is bi-Hamiltonian, with (compatible) operators

$$A_{1} = \begin{pmatrix} -\frac{3}{2}\partial_{x} & \frac{1}{2}\partial_{x}a & \partial_{x}b \\ \frac{1}{2}a\partial_{x} & \frac{1}{2}(\partial_{x}b + b\partial_{x}) & \frac{3}{2}c\partial_{x} + c_{x} \\ b\partial_{x} & \frac{3}{2}\partial_{x}c - c_{x} & (b^{2} - ac)\partial_{x} + \partial_{x}(b^{2} - ac) \end{pmatrix},$$

$$(51)$$

$$A_{2} = \begin{pmatrix} 0 & 0 & \partial_{x}^{3} \\ 0 & \partial_{x}^{3} & -\partial_{x}^{2}a\partial_{x} \\ \partial_{x}^{3} & -\partial_{x}a\partial_{x}^{2} & \partial_{x}^{2}b\partial_{x} + \partial_{x}b\partial_{x}^{2} + \partial_{x}a\partial_{x}a\partial_{x} \end{pmatrix}.$$
 (52)

We can rewrite the system and the operators in flat coordinates u^k of the leading term of the operator A_1 (as a flat pseudo-Riemannian contravariant metric):

$$a = u^{1} + u^{2} + u^{3}, \quad b = -\frac{1}{2}(u^{1}u^{2} + u^{2}u^{3} + u^{3}u^{1}), \quad c = u^{1}u^{2}u^{3},$$
 (53)

the operator A_1 becomes $A_1^{ij} = K^{ij}\partial_x$, where

$$(K^{ij}) = \frac{1}{2} \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{pmatrix},$$

and the system (50) takes the form

$$u_t^i = \frac{1}{2}(u^j u^k - u^i u^j - u^i u^k)_x, \tag{54}$$

where i, j, k are three distinct indices. Note that flat coordinates u^i of the first operator A_1 make the expression of the second operator A_2 much more complicated with respect to the initial coordinates a, b, c.

It is proved in [60] that the coordinate expression of τ is

$$\tau = -K^{in}L_n \frac{\partial}{\partial u^i}, \quad \text{where} \quad L_n = \left(\frac{1}{2}G_{nm}u_x^m + R_{nm}u_x^m\right)_x - \frac{1}{2}L_{nsm}u_x^s u_x^m. \tag{55}$$

In the above formula we have:

- 1. $-\frac{1}{2}L_{nsm}u_x^su_x^m$ are 3 conserved densities of the system (54) with coordinate expressions (note that $L_{ijk} = L_{ikj}$):
 - (a) when $j \neq 1$ and $k \neq 1$ or when j = k = 1

$$L_{1jk} = \frac{((u^1 - u^2) + (u^1 - u^3))(u^a - u^b)(u^c - u^d)}{2(u^1 - u^2)^3(u^1 - u^3)^3},$$
 (56)

where (a, j, b), (c, d, k) are triplets of distinct indices with a < b, c < d;

(b) when (1, j, k) are a triplet of distinct indices

$$L_{11k} = -\frac{(u^1 - u^k)^2 + (u^1 - u^j)^2}{2(u^1 - u^k)^2(u^1 - u^j)^3}.$$
 (57)

- (c) when $i \neq 1$ the expressions of L_{ijk} are obtained by a cyclic permutation of the above expressions.
- 2. G_{nm} is the leading term of the symplectic operator $B_{ij} = -K_{ip}A_2^{pq}K_{qj}$ (see [60]), and it is a pseudo-Riemannian metric; the coordinate expression of the inverse matrix (G^{ij}) is simpler:

$$G^{ii} = -\frac{1}{4}(u^i - u^j)(u^i - u^k), \quad G^{ij} = -\frac{1}{4}(u^i - u^j)^2.$$
 (58)

3. R_{pm} is a two-form whose expression is

$$R_{ij} = -\frac{1}{3} \left(\frac{1}{(u^i - u^j)(u^i - u^k)} - \frac{1}{(u^j - u^i)(u^j - u^k)} \right), \tag{59}$$

where i, j, k are distinct indices.

Let us describe the computation that leads to directly proving the equality $L_{\tau}A_1 = A_2$ (file w3c_lagrep3). We initialize the jet space with

```
indep_var:={x};
dep_var:={u1,u2,u3};
odd_var:={p1,p2,p3};
total_order:=10;
ncomp:=length(dep_var);
```

We load the third-order operator A_2 as in subsection 4.1, then we set up the change of variables with its Jacobian:

```
a:=u1 + u2 + u3;
a_x:=td(a,x);
b:=-1/2*(u1*u2 + u2*u3 + u3*u1);
b_x:=td(b,x);
c:=u1*u2*u3;
c_x:=td(c,x);
a_uqs:={a,b,c};

matrix jac(ncomp,ncomp);
for i:=1:ncomp do
   for j:=1:ncomp do jac(i,j):=df(part(a_uqs,i),part(dep_var,j));
jacinv:=jac**(-1);
```

We can use the following formula to change coordinates to the operator A_2 :

$$A_2^{ij}(\mathbf{u}) = \frac{\partial u^i}{\partial a^n} A_2^{nm}(\mathbf{a}) \frac{\partial u^j}{\partial a^m},\tag{60}$$

implemented as

```
mk_cdiffop(taa2,1,{3},3);
for all i,j,psi let taa2(i,j,psi)=
  (for h:=1:ncomp sum
      (for k:=1:ncomp sum jacinv(i,h)*aa2(h,k,jacinv(j,k)*psi))
  );
```

Obviously, taa2 is the operator A_2 in the coordinates u^i . The various tensors G_{mn} , R_{mn} and L_{nmp} can be obtained from the coefficients of the operator taa2 (see the file w3c_lagrep3). The operator l_n can be defined in such a way that the expression of l_n(n) will be L_n . Then we define the operator A_1 (in coordinates u^i)

```
matrix kap(ncomp,ncomp),kapinv(ncomp,ncomp);
kap:=(1/2)*mat((1,-1,-1),(-1,1,-1),(-1,-1,1));
kapinv:=kap**(-1);

mk_cdiffop(taa1,1,{3},3);
for all i,j,psi let taa1(i,j,psi) =
kap(i,j)*td(psi,x);

and vector field \(\tau\), with its conversion to an operator and a superfunction
mk_cdiffop(tau,1,{3},1);
for all i,phi let tau(i,1,phi)=
    (for j:=1:ncomp sum - kap(i,j)*l_n(j))*phi;
mk_superfun(tau_sf,1,1);
tau_sf(1):=for i:=1:ncomp sum tau(i,1,part(odd_var,i));
```

After the conversion of the Hamiltonian operators to bivectors:

```
\label{eq:conv_cdiff2superfun(taa1,taa1_sf);} $$ conv_cdiff2superfun(taa2,taa2_sf);$ $$ conv_genfun2biv(taa1_sf,biv1);$ $$ conv_genfun2biv(taa2_sf,biv2);$ $$ we can compute the Lie derivative $L_{\tau}A_1$ as the Schouten bracket $[\tau,A_1]$ $$ schouten_bracket(tau_sf,biv1,l_tau_biv1);$ $$ and check that the result coincides with biv2 in the variational cohomology: $$ euler_df(l_tau_biv1(1) - biv2(1));$ $$
```

Beware: the computation takes 18 hours and 8GB RAM on a (not too fast) compute server.

- **5 Problem.** Repeat the above computation for the bi-Hamiltonian pair of the WDVV equation in the case N = 4 [59]. Can the computation be successfully carried out for the oriented associativity equation [15]?
- **6 Remark.** A few simple examples of computations of Schouten bracket can be found in the CDE manual (which is part of the official Reduce manual).

We did not show any calculation of Schouten bracket between operators in more than one independent variable due to space constraints. CDE has this capability, the interested Reader can find one simple example (provided by Casati) in the CDE manual. More non-trivial examples, with applications to Hamiltonian and bi-Hamiltonian cohomology, are computed (also by CDE) in the recent paper [14].

5 Conclusions

In this paper we deliberately did not deal with nonlocal operators, i.e., operators which contain expressions with ∂_x^{-1} . At the moment, the only publicly available software for computations of Schouten bracket between nonlocal operators is the Maple package JET, but it has some limitations: indeed, it cannot always simplify expressions that contain ∂_x^{-1} . Recently, an algorithm for bringing such expression to a canonical form has been introduced [16], and we plan to implement it as an additional module of CDE in the near future. An extension of the odd variable formalism for the Schouten bracket of nonlocal operators is in progress [45].

An interesting perspective of application of CDE could be in theoretical physics, wherever supermanifolds play a role. Indeed, CDE can do every calculation on jets of superbundles (see [39, 42, 47]). This means, for example, Euler–Lagrange expressions of superfunctions, symmetries and conserved quantities of super-differential equations, etc.. Hence, it could be of help in complex computations in supersymmetric mechanics and field theories.

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