Automated symbolic calculations in nonequilibrium thermodynamics

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A R T I C L E   I N F O

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A B S T R A C T

We cast the Jacobi identity for continuous fields into a local form which eliminates the need to perform any partial integration to the expense of performing variational derivatives. This allows us to test the Jacobi identity definitely and efficiently and to provide equations between different components defining a potential Poisson bracket. We provide a simple Mathematica™ notebook which allows to perform this task conveniently, and which offers some additional functionalities of use within the framework of nonequilibrium thermodynamics: reversible equations of change for fields, and the conservation of entropy during the reversible dynamics.

Program summary

Program title: Poissonbracket.nb
Catalogue identifier: AEGW_v1_0
Program summary URL: http://cpc.cs.qub.ac.uk/summaries/AEGW_v1_0.html
Program obtainable from: CPC Program Library, Queen’s University, Belfast, N. Ireland
No. of lines in distributed program, including test data, etc.: 227952
No. of bytes in distributed program, including test data, etc.: 268918
Distribution format: tar.gz
Programming language: Mathematica™ 7.0
Computer: Any computer running Mathematica™ 6.0 and later versions
Operating system: Linux, MacOS, Windows
RAM: 100 MB
Classification: 4.2, 5, 23
Nature of problem: Testing the Jacobi identity can be a very complex task depending on the structure of the Poisson bracket. The Mathematica™ notebook provided here solves this problem using a novel symbolic approach based on inherent properties of the variational derivative, highly suitable for the present tasks. As a by product, calculations performed with the Poisson bracket assume a compact form.
Solution method: The problem is first cast into a form which eliminates the need to perform partial integration for arbitrary functionals at the expense of performing variational derivatives. The corresponding equations are conveniently obtained using the symbolic programming environment Mathematica™.
Running time: For the test cases and most typical cases in the literature, the running time is of the order of seconds or minutes, respectively.

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1. Introduction

In the modeling of gases, liquids, soft matter, glasses, and materials in general, continuous fields are ubiquitous for describing the material behavior. For example, nonisothermal hydrodynamics can be described in terms of the densities of linear momentum, mass, and internal energy. While the corresponding evolution equations are well known for the simplest systems, the modeling task becomes more fascinating, and more complicated, upon describing materials with internal microstructure. For example, the
microstructure of polymeric liquids, liquid crystals, and colloidal suspensions is described by conformation tensors or distribution functions. While it is needless to say that the corresponding microstructure is time-dependent, the question of formulating the evolution equations warrants special attention. To that end, techniques can be used that have emerged in the field of nonequilibrium thermodynamics [1,2]. In these techniques, two brackets (or corresponding operators) are used to capture the reversible and irreversible contributions, respectively, to the evolution equations.

The operator related to the reversible dynamics, a Poisson operator, must satisfy the Jacobi identity [3]. The latter is related to the time-structure invariance of the dynamics (see Section 2 below). It is well documented in the literature that while the Jacobi identity imposes severe conditions on the dynamics [2,4–6] it is from all the properties on the Poisson operator the one that is most tedious to implement. Implementation here refers not only to verifying the Jacobi identity, but more so to the constructive improvement of inconsistent dynamics as to comply with the Jacobi identity. A decade ago, a symbolic computational package [7] has been developed to check the Jacobi identity. However, the corresponding code suffered from being inefficient, and eventually not converging to a final result. A manual rearrangement of integrals – resulting due to the underlying approach – was typically required, and success therefore not guaranteed. The calculation of the Jacobi identity is particularly tedious for theories involving continuous fields, we are thus focusing on this more challenging case from an orthogonal viewpoint which allows to bring remaining uncertainties to an end. For discrete finite-dimensional cases [8], the formerly developed program [7] should remain useful.

In the present paper, we derive a local equivalent to the classical Jacobi identity for functionals. We propose a symbolic computational method that does not only prove validity or invalidity of the Jacobi identity under all circumstances. It consists of a few lines of code, operates efficiently, and does not require any additional package or manual post-processing. Using the proposed software, apparently tedious calculations related to the Poisson bracket will become highly transparent. For these reasons, it should now become a convenient task to actually improve on erroneous reversible dynamics in an efficient, computational way. Entropy and information content remains unaltered by purely reversible processes. The entropy gradient has to therefore lie in the nullspace of the thermodynamic Poisson operator. As a by-product of the treatment proposed in this manuscript, the related degeneracy condition is conveniently tested. Within the same approach, equations of change for the fields, and the Poisson operator itself will be obtained directly from the Poisson bracket.

The manuscript is organized as follows. In Section 2, the properties of Poisson brackets are discussed, particularly so the Jacobi identity, degeneracy condition, and Poisson operator. Local formalizations of the Jacobi identity and other local formalizations are derived and stated in Section 3. The main points of the method and accompanying software are summarized in Section 4. After some brief installation notes for the software in Section 5, the features and proper use of the Mathematica™ notebook are presented in Section 6. Specific examples are given in Section 7.

2. Reversible dynamics from the perspective of nonequilibrium thermodynamics

2.1. Poisson bracket

A Poisson bracket describing the reversible dynamics is in the focus of our interest. With the yet unspecified total energy $E$, the reversible evolution of an observable $A$ can be written in the form

$$\frac{d}{dt} A = \{A, E\},$$

where $\{., .\}$ denotes a bi-linear Poisson bracket. Such a Poisson bracket must satisfy the anti-symmetry condition

$$\{A, B\} = -\{B, A\}$$

for arbitrary observables $A$ and $B$. This condition ensures that the total energy is not changed by the reversible dynamics, i.e., $dE/dt = 0$. The second criterion for valid Poisson brackets is its so-called time-structure invariance for arbitrary energies. This criterion states that reversibly evolving a bracket $\{A, B\}$ amounts to the same as evolving the arguments $A$ and $B$ of the bracket, i.e.,

$$\frac{d}{dt} \{A, B\} = \{\{A, B\}, E\}$$

and

$$\{\frac{d}{dt} A, B\} + \{A, \frac{d}{dt} B\} = \{\{A, E\}, B\} + \{A, \{B, E\}\}$$

should be equal. Denoting the total energy by $C$ and using the anti-symmetry property (2a) one obtains the Jacobi condition (or Jacobi identity) in its most common appearance,

$$\{\{ABC\}, 0\} \equiv A, \{B, \{C, A\}\} + \{C, \{A, B\}\} = 0,$$

for arbitrary observables $A$, $B$, and $C$. We have abbreviated the cyclic sum over nested brackets by $\{ABC\}$.

In nonequilibrium thermodynamics, since the reversible dynamics also must not alter the entropy $S$ of the (closed) system, one obtains as an additional constraint for thermodynamic Poisson brackets the degeneracy condition [1]

$$\{A, S\} = 0,$$

for an arbitrary observable $A$.

Confirming the Jacobi identity (2b) is the most time-consuming step in many practical applications of nonequilibrium thermodynamics as compared to (2a), (2c) or the conditions on the irreversible bracket (irrelevant in the present context, and thus not shown). This holds particularly true if field variables are included in the description. In that case the observables are integrals. For the remainder of the paper, we restrict our attention to the calculation-intensive case of continuous field variables. The discrete case is adsorbed as a special case ($Q=0$ in Eq. (4)) below.

2.2. Poisson operator for field theories

Let us denote by $x = x(r) \in \mathbb{R}^d$ the fields of interest at position $r \in \mathbb{R}^d$. Since the Poisson bracket is antisymmetric and bi-linear in the observables $A$ and $B$, one can write

$$\{A, B\} = \int \frac{\delta A}{\delta x(r)} \cdot \mathcal{L}(r) \cdot \frac{\delta B}{\delta x(r)} \, dr = -\{B, A\},$$

(3)

where the so-called Poisson operator $\mathcal{L}$, uniquely characterized by the bracket, is a linear operator, $\delta A/\delta x$ denotes the functional derivative with respect to the continuous field $x(r)$, and $\cdot$ denotes the regular scalar product in $\mathbb{R}^d$. Throughout this manuscript we assume integrals $\int dr$ to extend over the whole $\mathbb{R}^d$ space, and boundary terms to vanish. Generally, $\mathcal{L} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a vector-valued (linear) differential operator defined by $n \times n$ matrices $L^{(q)}$,

$$\mathcal{L}(r) = \sum_{q=0}^Q L^{(q)} \nabla^q,$$

(4)

where $\nabla$ is a tensor whose $d^q$ components are all partial derivative operators with respect to $r$ of order $q$, and $Q$ is the finite upper limit on the order of derivatives, $q \leq Q$. We explicitly restrict
our attention to finite $Q$ in order to address local and weakly-nonlocal theories, but not discuss strongly nonlocal field theories. For most typical cases, $Q = 1$ \cite{1,2,4,9–31}. The derivative operators $
abla^L$ act on everything that appears to the right of $\mathcal{L}$. The tensors $L^{ij}$ may depend explicitly on $r$, however, most often they are space-dependent through the fields $x(r)$ and their derivatives \cite{9–11,13–25,28–61}. Except for (4), throughout the entire manuscript an argument $r$ implies that the corresponding function depends on position only explicitly and that there is no dependence on the fields $x(r)$ or on their derivatives. So, the above defined operator (4) is the only exception to this rule.

Note that the properties (2) on the Poisson bracket imply non-trivial restrictions on the Poisson operator $\mathcal{L}$ and its defining matrices $L^{ij}$, which we are going to derive. Since conditions (2a), (2c) are significantly more straightforward to implement as compared to the Jacobi identity (2b), we concentrate exclusively on the latter in the sequel. The comparably trivial antisymmetry condition (2a), in particular, translates into the conditions $L^{ij} = (L^{ij})^T$ and $L^{i0} = (L^{i1})^T$ for the case of $Q = 1$. These relations between the matrices characterizing first order $\mathcal{L}$ are inherently related to vanishing boundary terms of the integral (3).

### 2.3. The Jacobi identity for field theories

Let us first highlight the difficulty of proving the Jacobi identity for given bracket $(A, B)$. In order to test the condition (2b) for a given bracket it is sufficient to use linear test functionals (see Appendix A for details).

$$A = \int \sum_{i=1}^{n} a_i(r) x_i(r) \, dr,$$

$$B = \int \sum_{j=1}^{n} b_j(r) x_j(r) \, dr,$$

$$C = \int \sum_{k=1}^{n} c_k(r) x_k(r) \, dr,$$

with $3n$ arbitrary functions $a_i, b_j, c_k$, and $x_i$ denoting the $i$-th component of the fields $x$. Upon inserting (5) into (2b), the Jacobi identity then assumes the form

$$\{ ABC \}_{\mathcal{L}} = \int \sum_{i,j,k=1}^{n} \left[ a_i(r) L_{ij}(r) \frac{\delta}{\delta x_k(r)} \int b_j(r') L_{jk}(r') c_k(r') \, dr' \right. + b_j(r) L_{jk}(r) \frac{\delta}{\delta x_i(r)} \int c_k(r') L_{ik}(r') a_i(r') \, dr' \right.$

$$+ c_k(r) L_{ik}(r) \frac{\delta}{\delta x_j(r)} \int a_i(r') L_{ij}(r') b_j(r') \, dr' \left. \right] \, dr = 0. \quad (6)$$

For differential operators $\mathcal{L}$ the functional derivative of the inner bracket, i.e., of the $r'$-integral in (6), acts only on the prefactors $L^{ij}$. It can thus be seen that the functional derivative of the inner bracket is a local function of $r$. In other words, $\{ ABC \}_{\mathcal{L}}$ contains actually only an integral over $r$, which is the representative scenario for all local field theories.

While the thermodynamics of boundaries and its coupling to the bulk thermodynamics has been studied in some applications \cite{57}, most applications of nonequilibrium thermodynamics is concentrated on studying the time-evolution of the bulk. In these latter cases, in order to satisfy the Jacobi identity $\{ ABC \}_{\mathcal{L}} = 0$, the integrand does not have to be zero. Under the condition of negligible boundary terms, $\{ ABC \}_{\mathcal{L}} = 0$ if the integrand is the divergence of a vector field. The physical argument for negligible boundary terms can be two-fold. Either, all fields fall-off sufficiently fast towards the domain boundary, or one is only interested in a local theory. In either case, the neglect of boundary terms means that in proving the Jacobi identity, one can make use of partial integrations at will, until one eventually arrives at a vanishing or divergence-type integrand of $\{ ABC \}_{\mathcal{L}}$. For a computational implementation of the Jacobi identity, any arbitrariness carries the danger of a poor or even absent convergence, unless a unique rule is given for what partial integrations are desirable and which should be omitted.

### 3. Local formulation of the Jacobi identity

The strategy we propose for testing the Jacobi condition is very simple and ideally suited for symbolic computation. It is based on the observation that $\{ ABC \}_{\mathcal{L}}$ is an integral which has to vanish for arbitrary $a_i(r)$, in particular. If we were able to factorize the whole integrand such that $a_i(r)$ ends up to be a global prefactor, the remaining integrand has to vanish identically, for all $r$. The factorization of an arbitrary integrand of an integral whose surface terms vanish, and whose integrand is linear in $a_i(r)$, is done by means of the variational derivative with respect to $a_i$. The Jacobi identity (2b) for brackets, and also the equivalent one using linear test functionals (6) are thus both identical with a set of $n$ equations for fields $x, \mathcal{N}^q \rightarrow \mathcal{N}^{q'}$

$$\frac{\delta \{ ABC \}_{\mathcal{L}}}{\delta a_i(r)} = 0, \quad i = 1, \ldots, n, \text{ for any } r \in \mathcal{R} \quad (7)$$

with $\{ ABC \}_{\mathcal{L}}$ defined in (2b) and with $A = \int \sum a_i(r) x_i(r) \, dr$. We may call (7) the local formulation of the Jacobi identity for field theories. $\{ ABC \}_{\mathcal{L}} = 0$ for arbitrary $A$, which obviously implies condition (7), but more importantly, condition (7) also implies $\{ ABC \} = 0$. Because formulation (7) and the reader’s confidence on its validity is central to the approach (and tools) to be presented, we are going to put it on a more formal basis below. Step 1. While (7) applied to the linear ansatz (5)–(6) has eliminated the arbitrary observable $A$, it still contains $B$ and $C$. In Step 2 below we explain how to furthermore eliminate $B$ and $C$ as this helps to read off conditions for the fields, or equivalently, conditions for matrices $L^{ij}$ to be fulfilled if the Jacobi identity remains non-satisfied. For the case $Q = 1$ we have worked out (7) with (5) manually in Appendix B. The result is a large set of conditions for matrices, Eqs. (B.5), which is behind the apparently simpler condition (7).

Step 1. To make our line of argument leading to (7) transparent, we briefly remind the reader of the functional derivative as relevant for the present context. Let us consider an arbitrary differential operator $\mathcal{L}(r)$ such as (4), and introduce the functional

$$F \{ f \} = \int \mathcal{L}(r) \cdot f(r) \, dr$$

for a function $f(r) \in \mathcal{R}$. Its variational derivative $\frac{\delta F \{ f \}}{\delta f(r)}$ is given by

$$\frac{\delta F}{\delta f(r)} = \sum_{q=0}^{Q} (-1)^q \nabla^q \left( \mathcal{L}(r) \cdot f(r) \right) \frac{\delta f(r)}{\delta f(r)}$$

$$\sum_{q=0}^{Q} (-1)^q \nabla^q \mathcal{L}^{(q)}(r, x, \nabla x, \nabla^2 x, \ldots), \quad (9)$$

thus independent on $f$, but via matrices $L^{(q)}$ a function of $r, x$, and its gradients. By means of integration by parts one arrives at the useful identity

$$F \{ f \} = \int \mathcal{L}(r) \cdot f(r) \, dr = \int f(r) \cdot \frac{\delta F \{ f \}}{\delta f(r)} \, dr. \quad (10)$$
which holds if surface terms vanish. As a result, one finds the equivalence
\[ \forall \mathbf{f} \quad F[f] = 0 \iff \frac{\delta F[f]}{\delta f} = 0. \]  
(11)

It can be shown that the identity (11) holds not only for the functional of the special form (8), but rather for all functionals of integral-type that are linear in \( \mathbf{f} \). As applied to the verification of the Jacobi identity (6) with \( F = [ABC] \), and arbitrary test functions \( a_i(r), b_j(r), \) and \( c_k(r) \), Eq. (10) can be used by replacing \( f \) by vector \( \mathbf{a} \), whose components are the \( a_i \)'s. Since the Jacobi identity must be satisfied for all choices for the functions \( a_i(r) \), we conclude that the Jacobi identity is strictly identical with the set of conditions (7). It should be worthwhile mentioning that the local formulation of the Jacobi identity (7) remains valid if the arbitrary functionals belong to some subset within the space of functionals (such as those constructed by scalar invariants of a tensor \( \mathbf{x} \)). This follows immediately from (11) where the linearity of the test functions in \( \mathbf{x} \), cf. (5a), does not matter.

The crucial aspect of the local formulation (7) is the fact that it actually constitutes a well-defined and unique recipe to perform partial integrations, as exemplified by Eqs. (9)–(11), positioning the function \( a_i(r) \) all to the left in the integrand of the Jacobi integral (6). As we have explained earlier, such a clear strategy for performing integrations by parts is a prerequisite for the design of an efficient computational tool for the analytical verification of the Jacobi identity.

**Step 2.** Just in case the Jacobi condition (7) with (6) is not satisfied, it leaves us with a problem with terms bi-linear in the test functions \( b_j(r) \) and \( c_k(r) \) which should all vanish. In turn, for given \( \mathcal{L} \), the expression \( \delta[ABC]_\alpha/\delta a_\alpha(r) \) can be written as a power series in terms of the quantities \( \nabla^q b_j(r) \) and \( \nabla^q c_k(r) \) with \( 0 \leq q, p \leq Q \). Since from a local perspective, these \( p \)- and \( q \)-th order derivatives contain, with one important exception, independent information about the functions \( b_j(r) \) and \( c_k(r) \), the Jacobi identity (7) is equivalent to
\[ \frac{\partial}{\partial \nabla^q b_j(r)} \frac{\partial}{\partial \nabla^q c_k(r)} \frac{\delta[ABC]_\alpha}{\delta a_\alpha(r)} = 0, \]
\[ 1 \leq i \leq j \leq k \leq n, \quad p, q \geq 0, 1, \ldots, Q. \]  
(12)

The exception concerns second and higher order derivatives of \( b \) or \( c \). The terms \( \nabla^q b_j \) and \( \nabla^q c_k \), both components of \( \nabla^2 \mathbf{x} \), are identical. Accordingly, only the symmetrized sum of the corresponding prefactors must vanish. By means of this straightforward procedure (above Steps 1 and 2), we have eliminated all test functionals and all integrals from the Jacobi identity for local and weakly-nonlocal field theories.

### 3.1. Further local calculations of interest

The time-evolution (1), can be employed to write evolution equations for the fields \( \mathbf{x} \). Using the chain rule for an arbitrary functional \( A[\mathbf{x}] \), one finds
\[ \frac{\partial}{\partial t} \mathbf{x}_i(r) = \sum_{l=1}^{n} \mathcal{L}_l(r) \frac{\delta E}{\delta \mathbf{x}_i(r)}, \quad i = 1, \ldots, n \]  
(13)

which requires the Poisson operator \( \mathcal{L} \) rather than the Poisson bracket \( \{ \cdot , \cdot \} \) at first glance. On the other hand, once the Poisson bracket is entered in the symbolic code for verification of the Jacobi identity, one may ask whether one can formulate the evolution \( \mathcal{L}[\mathbf{x}]/\partial t \) directly in terms of the Poisson bracket. Indeed, inserting \( A_t = \int a(\mathbf{x}) \mathbf{x}_i(r) \mathbf{d}r \) into the bracket, and subsequent variational derivative with respect to \( a(r) \), one has
\[ \frac{\partial}{\partial t} \mathbf{x}_i(r) = \frac{\delta}{\delta a(r)} \{ A_t, E \}. \]  
(14)

Therefore, once the Jacobi identity is checked, the symbolic computational tool presented in the next section can be used to output also the reversible evolution equations, as needed in further numerical studies of the model at hand. Similarly, the degeneracy condition (2c) can be equivalently written in a local formulation as
\[ \sum_{l=1}^{n} \mathcal{L}_l(r) \frac{\delta S}{\delta \mathbf{x}_i(r)} = 0, \]  
and for the present purpose as
\[ \frac{\delta}{\delta a(r)} \{ A_t, S \} = 0. \]  
(15)

With regard to the local formulations (13)–(15) an important reminder is in place. We have pointed out earlier that in local field theories partial integrations in the bracket formulation can be performed at will since boundary terms are irrelevant. However, this arbitrariness is absent in the local equations (13)–(15) because the functional derivative \( \delta/\delta a(r) \) gives preference to one very specific representation of the brackets. That specific representation is the one in which the function \( a_i(r) \) is isolated on the left-end of the integrand, in analogy to the position of the function \( f \) in the last equation of (10).

The above calculations rely on the representation (3) with (4), i.e., on the derivative operators acting exclusively on the functional derivative of \( B \). However, the anti-symmetry of the bracket can be appreciated only indirectly, e.g., after performing integrations by parts and neglecting boundary terms. In order to enforce the anti-symmetry by construction, in the literature it is also common to write the bracket in the form
\[ \{ A, B \} = \int \frac{\delta A}{\delta x(r)} \frac{\delta B}{\delta x(r)} \mathcal{K}(r) \mathbf{d}r \]
\[ \quad - \int \frac{\delta B}{\delta x(r)} \frac{\delta A}{\delta x(r)} \mathcal{K}(r) \mathbf{d}r, \]  
with another differential operator \( \mathcal{K} \). Eq. (16) differs from (3) by boundary terms. It is generally nontrivial to read off \( \mathcal{L} \) or its matrices \( \mathbf{L}^{(q)} \) from \( \mathcal{K} \) without any effort. However, using the symbolic toolbox that we provide, this task is overtaken by a single operation. Particularly, the action of a Poisson-operator \( \mathcal{L} \) itself, applied to arbitrary \( b(r) \) is uniquely obtained from the bracket via
\[ \mathcal{L}[b(r)] = \frac{\delta}{\delta a(r)} \{ A_t, B \} \]  
(17)

with \( A_t = \int a(\mathbf{x}) \mathbf{x}_i(r) \mathbf{d}r \) and \( B_t = \int b(\mathbf{x}) x_i(r) \mathbf{d}r \). This formulation allows us to read off the matrices \( L^{(q)} \) and its components \( L^{(q)}_{ij} \) from a given bracket via
\[ L^{(q)} = \frac{\partial \mathcal{L}(b)}{\partial \nabla^q b}. \quad L^{(q)}_{ij} = \frac{\partial \mathcal{L}(b)}{\partial \nabla^q b} \frac{\delta}{\delta a(r)} \{ A_t, B_t \}. \]  
(18)

As already mentioned, these matrices borrow some basic symmetry features and are interrelated to each other due to the anti-symmetry of the bracket. It should be also worthwhile mentioning that, while there are infinitely many possible \( \mathcal{K} \) giving rise to the same bracket, there is only a single unique \( \mathcal{L} \).

### 4. Summary and conclusion

By means of the straightforward procedure outlined in Section 3 we have eliminated all test functionals and all integrals from the Jacobi identity for local and weakly-nonlocal field theories. In particular, we do not need to perform any explicit integration by parts. If all the independent equations are identically fulfilled, the Jacobi identity is fulfilled; contrary, if only a single one of the equations is invalid, the Jacobi identity has been disproven. This allows to disprove the Jacobi identity by citing a single equation between the fields, or, in a more constructive fashion, to use the equations in order to adjust open parameters defining \( \mathcal{L} \).
The accompanying software basically starts from an arbitrary bracket \((A, B)\) and implements (7) with (5a) in two alternate fashions ("sequential" vs "all-in-one") and optionally (12) ("bc-free"). While both of these fashions calculate nested Poisson brackets and subsequently determine the functional derivative, one may alternatively wish to examine the implications of the Jacobi identity directly on the matrices \(L^{(0)}\) of \(L\) in (4) themselves. For the special case of \(Q = 1\) we provide exactly this variant, where the matrices \(L^{(0)}\) are extracted from a given bracket, and where we test (12) after having inserted \([ABC]_{\rho}\) manually. This leaves us with an \(ABC\)-free Jacobi condition in terms of the matrices \(L^{(0)}\), given in Appendix B. There is only a single advantage of this latter variant: it is the least memory-consuming representation of the Jacobi condition. However, it is restricted so far to the potential of Poisson operators containing first derivatives only. The local form of the Jacobi identity (7), on the other hand, remains generally applicable.

We have furthermore demonstrated how other local expressions such as the equations of change for fields, the degeneracy condition, or the Poisson operator itself are obtained from the bracket via variational derivative. Possible future extensions of the simple program could include the friction matrix, the corresponding irreversible equations of change, and a structure-preserving numerical solution [58] of the time-dependent equations.

5. Installation notes

Start Mathematica\textsuperscript{TM} 6 or later versions and open the notebook (.nb) file. Execute a command by pressing the (shift return) keys. The commands of the notebook can also be copied to an ascii file and then executed in batch mode (unix, linux) via \texttt{<ascii-file>}

6. User’s guide

The Mathematica\textsuperscript{TM} notebook is kept very simple in order to allow a user to easily add additional functionalities. At the same time it is powerful and offers a solution to deal with eventually more time-consuming applications. The notebook has essentially four parts:

6.1. Overhead

Here you just load Mathematica\textsuperscript{TM}’s VariationalD and define our \texttt{NoSimplify} command. It is essential that \texttt{VariationalD} is operational before entering any other part of the accompanying notebook. \texttt{NoSimplify} renders obsolete upon manually replacing the build-in \texttt{VariationalD}, cf. footnote.1 \texttt{VariationalD} we use to perform variational derivatives, \texttt{\[\delta A\]} with arbitrary integrand \(f(r, x, Vx, \nabla^2 x, \ldots)\) and arbitrary function \(g(r)\), such as \(a(r), b(r), \) or \(c_i(r)\). Please note that the first argument of Mathematica\textsuperscript{TM}’s VariationalD is the integrand, rather than the entire integral. To our experience the direct use of the matrices \(L^{(0)}\) is often the most efficient way. However, when the matrices \(L^{(0)}\) are extracted from a given bracket, and where we test (12) after having inserted \([ABC]_{\rho}\) manually. This leaves us with an \(ABC\)-free Jacobi condition in terms of the matrices \(L^{(0)}\), given in Appendix B. There is only a single advantage of this latter variant: it is the least memory-consuming representation of the Jacobi condition. However, it is restricted so far to the potential of Poisson operators containing first derivatives only. The local form of the Jacobi identity (7), on the other hand, remains generally applicable.

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We provide the above-mentioned alternate ways for testing the Jacobi identity for the Poisson bracket already defined in 6.2. by just executing the unmodified commands available in this section. It is also possible to manually evaluate a Poisson bracket via \texttt{PB[A, B]} with arbitrary functions \(A\) and \(B\). Within the notebook, one has to just specify densities \(A\) and \(B\) as follows

\[
A = \int f(r) \, dr \equiv A = f@r
\]

where \(f\) is an arbitrary, symbolic object. Accordingly, Mathematica\textsuperscript{TM}’s \texttt{Integrate} command does not appear anywhere within the notebook.

We provide the above-mentioned alternate ways for testing the Jacobi identity (see Section 4), a sequential versus a parallel one (Tools I and II, respectively). The sequential version inserts functions \(A_i = \int a(r)x_i(r) \, dr\) and \(B_j = \int b(r)x_j(r) \, dr\) and \(C_k = \int c(r)x_k(r) \, dr\) into \(\int f(r) \, dr\) for each possible, sorted triple \((i, j, k)\) separately. The parallel version “all-in-one” uses vectors \(\{a, b, c\}\) and inserts \(A_i = \int a(r)x_i(r) \, dr\) and \(B_j = \int b(r) \cdot x_j(r) \, dr\), and \(C_k = \int c(r) \cdot x_k(r) \, dr\) into \(\int f(r) \, dr\). Both versions are ultimately equivalent, however, they may differ in execution speed. The user should feel free to choose. Both versions report about the success of the Jacobi test.

\[1\] If Mathematica\textsuperscript{TM}’s \texttt{VariationalCalculus}' Package is unavailable, it could also be implemented manually as follows: \texttt{VariationalD}[F_, Q_, \ldots] := Sum[(-1)^n D[D[F, Q], {r, n}], {r, 1, \ldots}, {n, 0, 10}], and similarly for the high-dimensional case, where \(r\) is a vector.

\[2\] In principle, one could also use for \(A\) a combination of terms, \(A = \int a(r) \cdot x(r) \, dr\). However, upon the differentiation \(\texttt{\\Delta ABC}_{\rho}\), all but one term will drop out. In order to avoid unnecessarily long expressions during the computations, we therefore rather use \(A_i = \int a(r)x_i(r) \, dr\) instead.
If the Jacobi identity is not fulfilled, our Mathematica\textsuperscript{TM} tools provide a relationship in terms of the fields $x$ or parameters appearing within the Poisson bracket, which must be obeyed in order to allow for a successful Jacobi test. This relationship, which we save for the users convenience in variables JacobiCondition\textsuperscript{[12]} still contain the functions $b$ and $c$ and their derivatives. The independently vanishing conditions for the preferred ones can be read off conveniently using our bcFree\textsuperscript{[JacobiCondition\textsuperscript{[12]]}} command (Tool III). The (bc)-containing or (bc)-free conditions can hence be used equivalently as a guideline to modify the bracket.

For the case of Poisson operators falling into the $Q = 1$ class, we offer an implementation of the Jacobi identity \textsuperscript{[B.5]} derived in Appendix B with Tool IV. While Tool IV is the least elegant to test the Jacobi identity, it is by construction the least memory consuming version of it and as such, might find its application.

6.4. Applications

Besides testing the Jacobi identity we can use the Poisson bracket to perform some more trivial operations. Examples are given in the Application section of the notebook. They contain the evaluation of the Poisson bracket for user-defined functionals, or the components of the Poisson operator $\mathcal{L}$. After entering the energy density in the form MyEnergy=\ldots the equation of change for the $t$th field variable $x_t$ is displayed using EquationOfChange\textsuperscript{[1]}. which is defined via \textsuperscript{[14]}. The notebook allows to choose long or short output format. The latter version of it and as such, might find its application.

7. Test runs

7.1. Test run I: Classical $d$-dimensional hydrodynamics

The characteristics are as follows:

- Space coordinates $r = \{r_1, \ldots, r_d\} \in \mathbb{R}^d$
- State variables $x = \{u(r), \rho(r), \theta(r), Q(r), A(r)\}$ where $Q$ is symmetric, $Q = Q^T$.
- Half the Poisson bracket according to the notation of Eqs. (16), (22) contains the contributions

$$aKb[1][\ldots, B_\ldots] = -\frac{\delta A}{\delta u_i(r)} u_j(r) \left( \frac{\partial \delta B}{\partial \delta u_i(r)} \right),$$

$$aKb[2][\ldots, B_\ldots] = -\frac{\delta A}{\delta u_i(r)} \rho(r) \left( \frac{\partial \delta B}{\partial \delta \rho(r)} \right),$$

$$aKb[3][\ldots, B_\ldots] = -\frac{\delta A}{\delta e(r)} \left( \frac{\partial \delta B}{\partial \delta e(r)} \right),$$

$$aKb[4][\ldots, B_\ldots] = -\frac{\delta A}{\delta e(r)} \rho(r) \left( \frac{\partial \delta B}{\partial \delta \rho(r)} \right) \left( \sum_{i=1}^{d} \frac{\partial}{\partial \delta u_i(r)} \right).$$

(25)

- Energy density $u(r)/2 + e(r)$
- Entropy density $s(\rho(r), e(r))$

For a snapshot of the corresponding Mathematica\textsuperscript{TM} notebook, the reader is referred to Fig. 1.

7.2. Test run 2: Tensorial ($Q$) and scalar ($A$) structural variable

This is example is adapted from \textsuperscript{[1]}, pp. 113–115. The characteristics are as follows:

- Space coordinates $r = \{r_1, \ldots, r_d\} \in \mathbb{R}^d$
- State variables $x = \{u(r), \rho(r), s(r), Q(r), A(r)\}$ where $Q$ is symmetric, $Q = Q^T$
- Half the Poisson bracket according to the notation of Eqs. (16), (22) contains the contributions

$$aKb[1][\ldots, B_\ldots] = -\frac{\delta A}{\delta u_i(r)} u_j(r) \left( \frac{\partial \delta B}{\partial \delta u_i(r)} \right),$$

$$aKb[2][\ldots, B_\ldots] = \frac{\delta A}{\delta Q_{jk}(r)} Q_{ik}(r) \left( \frac{\partial \delta B}{\partial \delta Q_{jk}(r)} \right) + \frac{\delta A}{\delta u_i(r)} \left( \frac{\partial \delta B}{\partial \delta u_j(r)} \right),$$

$$aKb[3][\ldots, B_\ldots] = \frac{\delta A}{\delta A} \left[ \frac{\partial \delta B}{\partial \delta \rho(r)} \right],$$

$$\quad + g_{jk}(Q, A) \left( \frac{\partial \delta B}{\partial \delta \rho(r)} \right) \left( \sum_{i=1}^{d} \frac{\partial}{\partial \delta u_i(r)} \right).$$

(26)

with tensor $g(Q, A)$,

$$g = g_1 Q + g_2 1 + g_3 Q^{-1}. \quad (27)$$

The functions $g_i = g_i(1, 2, 3, A)$ remain unspecified in terms of the invariants of $Q$: $Q_1 = \text{tr}(Q)$, $Q_2 = \text{det}(Q)$, and $Q_3 = -\text{tr}(Q^{-1})$.

- Energy density $u^2/2 + e(\rho, s, Q, A)$
- Entropy density $s(r)$ is amongst the variables

The notebook allows to specify $g$. Predefined is the special case of $g_2 = g_3 = 0$, i.e., $g = g_1 Q$. While the Jacobi identity is seen to be fulfilled for $g_1 = f(t_1)$, it is not fulfilled, e.g., for $g_3 = f(t_2)$. These simple cases are meant to demonstrate the capability of the software. More generally, it has been proven in \textsuperscript{[1]} that the Jacobi identity is satisfied if the following conditions are met:

$$g_1 \frac{\partial g_2}{\partial A} - g_2 \frac{\partial g_1}{\partial A} = 2 \frac{\partial g_1}{\partial t_2} - \frac{\partial g_2}{\partial t_1},$$

$$g_1 \frac{\partial g_3}{\partial A} - g_3 \frac{\partial g_1}{\partial A} = 2 \frac{\partial g_1}{\partial t_3} - \frac{\partial g_3}{\partial t_1},$$

$$g_2 \frac{\partial g_3}{\partial A} - g_3 \frac{\partial g_2}{\partial A} = 2 \frac{\partial g_2}{\partial t_3} - \frac{\partial g_3}{\partial t_2}. \quad (28c)$$

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Appendix A. Jacobi identity: Justification for using linear test functionals

We give a proof that for checking the Jacobi identity it is sufficient to use test functionals that are linear in the fields $x$. To
that end, we introduce the abbreviations 
\[ x_1 = x_1(r), \quad \mathcal{L}_{ij} = \mathcal{L}_{ij}(r). \]
For the further calculations, it is convenient to write the Jacobi identity in the form (using the anti-symmetry property of the bracket)

\[
\{A, \{B, C\}\} - \{B, \{A, C\}\} + \{C, \{A, B\}\},
\]

i.e.,

\[
\{A, \{B, C\}\} = \int \frac{\delta A}{\delta x_1} \frac{\delta^2}{\delta x_2 \delta x_3} \mathcal{L}_{jk} \frac{\delta C}{\delta x_k} \, dr \, dr' - \int \frac{\delta B}{\delta x_1} \frac{\delta^2}{\delta x_2 \delta x_3} \mathcal{L}_{jk} \frac{\delta C}{\delta x_k} \, dr \, dr' + \int \frac{\delta C}{\delta x_1} \frac{\delta^2}{\delta x_2 \delta x_3} \mathcal{L}_{jk} \frac{\delta B}{\delta x_k} \, dr \, dr'.
\] (A.2)

The functional derivative of the inner integral will lead in general to three contributions, one of which is proportional to the functional derivative of \( \mathcal{L}_{jk} \), whereas the other two contributions are associated to the second order functional derivatives of the test functionals. We are going to test whether these second order functional derivatives have an effect on the verification of the Jacobi identity. Collecting in (A.2) all contributions proportional to the second derivative of the functional \( A \), we obtain

\[
\{A, \{B, C\}\} = -\int \int \left( \frac{\delta B}{\delta x_1} \frac{\delta^2}{\delta x_2 \delta x_3} \mathcal{L}_{jk} \frac{\delta C}{\delta x_k} \right) \, dr \, dr' + \int \int \left( \frac{\delta C}{\delta x_1} \frac{\delta^2}{\delta x_2 \delta x_3} \mathcal{L}_{jk} \frac{\delta B}{\delta x_k} \right) \, dr \, dr'.
\] (A.3)

Since the Poisson operator \( \mathcal{L} \) is anti-symmetric, we can rewrite this expression as

\[
\{A, \{B, C\}\} = \int \int \left( \mathcal{L}_{ij} \frac{\delta^2}{\delta x_i \delta x_j} \mathcal{L}_{jk} \frac{\delta C}{\delta x_k} \right) \, dr \, dr' - \int \int \left( \mathcal{L}_{ij} \frac{\delta^2}{\delta x_i \delta x_j} \mathcal{L}_{jk} \frac{\delta B}{\delta x_k} \right) \, dr \, dr'.
\] (A.4)

Because the second functional derivative of \( A \) is symmetric with respect to interchanging \( (j, r) \leftrightarrow (j', r') \), we obtain \( \{A, \{B, C\}\} = 0 \). In other words, the second order derivatives of \( A \) are irrelevant for the verification of the Jacobi identity, which also holds true for \( B \) and \( C \). In turn, this means that it is sufficient (although not
necessary) to use test functionals $A$, $B$, and $C$ that are linear in the fields $x$.

Appendix B. ABC-free Jacobi identity for first order $\mathcal{L}$

Starting out with a given antisymmetric bracket $\{A, B\}$, the components of the corresponding $\mathcal{L}$-operator are uniquely obtained via Eq. (17),

$$\mathcal{L}_{i j}(b) = \frac{\delta}{\delta a_i(r)} \left( A_i, B_j \right),$$

(B.1)

with $A_i = \int \varphi(r) x_i(r) \, d\mathbf{r}$ and $B_i = \int \varphi(r) x_i(r) \, d\mathbf{r}$. Let us consider a differential operator $\mathcal{L}$ which defines an antisymmetric bracket and contains no higher than first spatial derivatives of the fields $x_i(r) : \mathbb{R}^d \rightarrow \mathbb{R}^d$. This corresponds to $Q = 1$ in our more general form (4). Accordingly, the operator is fully characterized by $d + 1$ square matrices $L_{ij}(r, x, \nabla x)$ and $L_{ij} \cdots \cdots (r, x, \nabla x)$, all of rank $n$. For the operator components we explicitly have

$$\mathcal{L}_{ij}(b) = L_{ij}^0 b + \sum_{\mu=1}^d L_{ij}^{\mu} \frac{\partial b}{\partial x_\mu},$$

(B.2)

where $\nabla_\mu \equiv \partial / \partial x_\mu$. The matrix elements are obtained for a given bracket via particular choices of $b$ in Eq. (B.2), or also Eq. (B.1).

$$L_{ij}^0 = \mathcal{L}_{ij}(1),$$

(B.3a)

$$L_{ij}^{\mu} = \mathcal{L}_{ij}(r, r) - r \mu_0 L_{ij}, \quad \mu = 1, \ldots, d.$$  

(B.3b)

According to (7) and in order to derive an ABC-free version of the Jacobi identity we need to first evaluate $\delta \{ABC\} / \delta a_i(r)$. To this end we insert the above $\mathcal{L}$ into three nested brackets with $A = \int \varphi(r) \, d\mathbf{r}$ etc. such as with $(b_{ij} = \nabla_\mu)$,

$$\left\{ A, \{B, C\} \right\} = \int a_i \left( L_{ij}^0 + L_{ij}^{\mu} \frac{\partial b}{\partial x_\mu} \right) \frac{\delta}{\delta x_i(r)} \left[ b_{jk} L_{ij}^0 + b_{j} c_{k} L_{ij}^{\mu} \right] \, d\mathbf{r} \, dr$$

where we have just applied the product rule of differentiation, and where some additional terms stemming from the underlined term have been skipped and abbreviated by the dots. The notation $\delta L_{ij} / \delta x_i$ here stands for $\delta L_{ij} / \delta x_i = \partial L_{ij} / \partial x_i - \nabla_\mu / \partial x_i \nabla_\mu x_i$, where $L_i$ is not an operator, but a matrix containing functions. Using corresponding expressions for $\{B, C\}$ and $\{A, B\}$ and collecting terms derivative-free in $a_i$ after partial integration, or equivalently, performing a variational derivative with respect to $a_i$, and subsequent partial derivative with respect to all the (independent, symmetrized) components of $(\nabla b_i(r)) x_{kj}$ leads to a set of five ABC-free equations for the fields, which have to be pointwise fulfilled. These equations equivalent with the Jacobi identity for the case of first order $\mathcal{L}$ read

$$0 = \left( \frac{\partial L_{ij}^0}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} \right) + (\mu \rightarrow \nu),$$

(B.5a)

$$0 = L_{ij}^0 \frac{\partial L_{ij}^0}{\partial x_i} + L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i},$$

(B.5b)

$$0 = L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} + L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} + (\mu \rightarrow \nu),$$

(B.5c)

$$0 = L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} - L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} + \frac{\partial L_{ij}^{\mu}}{\partial x_i} \nabla_i \frac{\partial L_{ij}^{\mu}}{\partial x_i},$$

(B.5d)

$$0 = \left( \frac{\partial L_{ij}^0}{\partial x_i} + L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} \right) - \frac{\partial L_{ij}^{\mu}}{\partial x_i} + \frac{\partial L_{ij}^{\mu}}{\partial x_i} \nabla_i \frac{\partial L_{ij}^{\mu}}{\partial x_i}.$$  

(B.5e)

In deriving the ABC-free Jacobi identity (B.5) we made use of the identities $\nabla_\mu L_{ij} = L_{ij}^{\mu} = L_{ij}^{\mu}$ as it follows from the assumed antisymmetry of the underlying bracket. Condition (B.5a) results from the term containing second spatial derivatives of $b_{ij} \dagger c_{kl}$ or $c_{ij} \dagger b_{kl}$, so that only one of them is actually independent. Conditions (B.5b), (B.5c) and (B.5d) arise from terms containing $b_{ij} \dagger c_{kl}$, $b_{ij} \dagger c_{kl}$ and $c_{ij} \dagger b_{kl}$, respectively. The fifth condition (B.5e) stems from terms preceded by $c_{ij} \dagger b_{kl}$. Some of the terms appearing in (B.5) are visible in (B.4), others have cancelled out with the corresponding terms from the remaining two nested brackets. The set (B.5) stands for $(1 + \partial^2)$th order equations, or less if one restricts to sorted $i \leq j \leq k$ which is sufficient. Einstein summation convention applies in (B.5). We remind the reader that all matrix elements appearing in (B.5) are given in terms of an antisymmetric bracket $\{A, B\} = -\{B, A\}$ via (B.3) with (B.1). For the case of zeroth order $\mathcal{L} = L^0$ with antisymmetric $L^0$ and $L^0 / \partial x = 0$, the only nontrivial condition remaining from the Jacobi conditions (B.5) is Eq. (B.3c). It reduces to the ABC-free Jacobi identity stated in textbooks, cf. [62].

$$L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} + L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} + L_{ij}^{\mu} \frac{\partial L_{ij}^{\mu}}{\partial x_i} = 0.$$  

(B.6)

References


