Continuous and Discrete Homotopy Operators and the Computation of Conservation Laws

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In memory of Ryan Sayers (1982-2003)

Abstract. We introduce calculus-based formulas for the continuous Euler and homotopy operators. The 1D continuous homotopy operator automates integration by parts on the jet space. Its 3D generalization allows one to invert the total divergence operator. As a practical application, we show how the operators can be used to symbolically compute local conservation laws of nonlinear systems of partial differential equations in multi-dimensions.

Analogous to the continuous case, we also present concrete formulas for the discrete Euler and homotopy operators. Essentially, the discrete homotopy operator carries out summation by parts. We use it to algorithmically invert the forward difference operator. We apply the discrete operator to compute fluxes of differential-difference equations in (1+1) dimensions.

Our calculus-based approach allows for a straightforward implementation of the operators in major computer algebra system, such as *Mathematica* and *Maple*. The symbolic algorithms for integration and summation by parts are illustrated with elementary examples. The algorithms to compute conservation laws are illustrated with nonlinear PDEs and their discretizations arising in fluid dynamics and mathematical physics.

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1. Introduction

This chapter focuses on symbolic methods to compute polynomial conservation laws of partial differential equations (PDEs) in multi-dimensions and differential-difference equations (DDEs, semi-discrete lattices). We only treat (1+1)-dimensional DDEs where time is continuous and the spacial variable has been discretized.

There are several strategies to compute conservation laws of PDEs. Some methods use a generating function [2], which requires the knowledge of key pieces of the Inverse Scattering Transform [1]. Other methods use Noether's theorem to get conservation laws from variational symmetries. More algorithmic methods, some of which circumvent the existence of a variational principle [6, 7, 26, 36], require the solution of a determining system of ODEs or PDEs. Despite their power, only a few of these methods have been implemented in computer algebra systems (CAS), such as *Mathematica*, *Maple*, and *REDUCE*. See [17, 36] for reviews.

The most modern techniques [9] rely on tools from the calculus of variations, including basic operations on vector fields and differential forms. Such tools are available in *Vessiot*, a general purpose suite of *Maple* packages designed by Anderson [10] for computations on jet spaces. The *Vessiot* package `DE_APPLS` offers commands (but no fully automated code) for constructing conservation laws from symmetries by Noether's theorem.

We advocate a direct approach for the computation of conservation laws without recourse to generalized or adjoint symmetries. We use the following procedure: build candidate densities as linear combinations (with undetermined coefficients) of terms that are homogeneous under the scaling symmetry of the PDE. If no such symmetry exists, one is constructed by introducing weighted parameters. Subsequently, use the variational derivative to compute the coefficients, and, finally, use the homotopy operator to compute the flux. Furthermore, our approach can be adapted to nonlinear DDEs [18, 21, 22].

Our method works for evolution equations with polynomial and transcendental terms and does not require a Lagrangian formulation. Built on tools from (variational) calculus and linear algebra, our method is entirely algorithmic and can be implemented in leading CAS. Implementations [17, 18] in *Mathematica* and *Maple* can be downloaded from [13, 20].

Our earlier algorithm [17, 18] worked only for nonlinear PDEs in one spacial variable. In this chapter we present an algorithm that works for systems of PDEs in multi-dimensions that appear in fluid mechanics, elasticity, gas dynamics, general relativity, (magneto-)hydro-dynamics, *etc.*. The new algorithm produces densities in which all divergences and divergence-equivalent terms have been removed.

During the development of our methods we came across tools from the calculus of variations and differential geometry that deserve attention in their own right. These tools are the variational derivative, the higher Euler operators, and the homotopy operator.

To set the stage, we address a few issues arising in multivariate calculus:
(i) To determine whether or not a vector field $\mathbf{F}$ is *conservative*, i.e. $\mathbf{F} = \boldsymbol{\nabla} f$

for some scalar field f, one must verify that $\mathbf{F}$ is *irrotational* or *curl free*, that is $\boldsymbol{\nabla} \times \mathbf{F} = \mathbf{0}$. The field f can be computed via standard integrations [32, p. 518, 522].

(ii) To test if $\mathbf{F}$ is the curl of some vector field $\mathbf{G}$, one must check that $\mathbf{F}$ is *incompressible* or *divergence free*, i.e. $\boldsymbol{\nabla} \cdot \mathbf{F} = 0$. The components of $\mathbf{G}$ result from solving a coupled system of first-order PDEs [32, p. 526].

(iii) To verify whether or not a scalar field f is the divergence of some vector function $\mathbf{F}$, no theorem from vector calculus comes to the rescue. Furthermore, the computation of $\mathbf{F}$ such that $f = \boldsymbol{\nabla} \cdot \mathbf{F}$ is a nontrivial matter. In single variable calculus, it amounts to computing the primitive $F = \int f \, dx$.

In multivariate calculus, all scalar fields f, including the components F_i of vector fields $\mathbf{F} = (F_1, F_2, F_3)$, are functions of the independent variables (x, y, z). In differential geometry one addresses the above issues in much greater generality. The functions f and F_i can now depend on arbitrary functions $u(x, y, z), v(x, y, z)$, *etc.* and their mixed derivatives (up to a fixed order) with respect to the independent variables (x, y, z). Such functions are called *differential functions* [33]. As one might expect, carrying out the gradient-, curl-, or divergence-test requires advanced algebraic machinery. For example, to test whether or not $f = \boldsymbol{\nabla} \cdot \mathbf{F}$ requires the use of the variational derivative (Euler operator) in 3D. The actual computation of $\mathbf{F}$ requires integration by parts. That is where the homotopy operator comes into play.

In 1D problems the continuous total homotopy operator[1] reduces the problem of symbolic integration by parts to an integration with respect to a single auxiliary variable. In 2D and 3D, the homotopy operator allows one to invert the total divergence operator and, again, reduce the problem to a single integration. At the moment, no major CAS have reliable routines for integrating expressions involving *unknown* functions and their derivatives. As far as we know, no CAS offer a function to test if a differential function is a divergence. Routines to symbolically invert the total divergence are certainly lacking.

The continuous homotopy operator is a universal, yet little known, tool that can be applied to many problems in which integration by parts (of arbitrary functions) in multi-variables plays a role. The reader is referred to [33, p. 374] for a history of the homotopy operator. One of the first uses of the homotopy operator in the context of conservation laws can be found in [6, 7] and references therein. A clever argument why the homotopy operator actually works is given in [7, p. 582]. In [5], Anco gives a simple algebraic formula to generate conservation laws of scaling invariant PDEs based on the computation of adjoint symmetries. Like ours, Anco's approach is algorithmic and heavily relies on scaling homogeneity. His approach does not require the use of the homotopy integral formula.

A major motivation for writing this chapter is to demystify the homotopy operators. Therefore, we purposely avoid differential forms and abstract concepts such as the variational bicomplex. Instead, we present calculus formulas for the homotopy operators which makes them readily implementable in major CAS.

[1] Henceforth, homotopy operator instead of total homotopy operator.

By analogy with the continuous case, we also present formulas for the discrete versions of the Euler and homotopy operators. The discrete homotopy operator is a powerful tool to invert the forward difference operator, whatever the application is. It circumvents the necessary summation (by parts) by applying a set of variational derivatives followed by a one-dimensional integration with respect to an auxiliary variable. We use the homotopy operator to compute conserved fluxes of DDEs. Numerous examples of such DDEs are given in [34]. Beyond DDEs, the discrete homotopy operator has proven to be useful in the study of difference equations [24, 30]. To our knowledge, CAS offer no tools to invert the forward difference operator. Our discrete homotopy operator overcomes these shortcomings.

As shown in [24, 30], the parallelism between the continuous and discrete cases can be made rigorous and both theories can be formulated in terms of variational bicomplexes. To make our work accessible to as wide an audience as possible, we do not explicitly use the abstract framework. Aficionados of *de Rham* complexes may consult [8, 9, 11, 27] and [24, 30, 31]. The latter papers cover the discrete variational bicomplexes.

2. Examples of Nonlinear PDEs

We consider nonlinear systems of evolution equations in $(3+1)$ dimensions,

$$\mathbf{u}_t = \mathbf{G}(\mathbf{u}, \mathbf{u}_x, \mathbf{u}_y, \mathbf{u}_z, \mathbf{u}_{2x}, \mathbf{u}_{2y}, \mathbf{u}_{2z}, \mathbf{u}_{xy}, \mathbf{u}_{xz}, \mathbf{u}_{yz}, \dots), \tag{2.1}$$

where $\mathbf{x} = (x, y, z)$ are space variables and t is time. The vector $\mathbf{u}(x, y, z, t)$ has N components u_i. In the examples we denote the components of $\mathbf{u}$ by u, v, w, *etc.*. Subscripts refer to partial derivatives. For brevity, we use $\mathbf{u}_{2x}$ instead of $\mathbf{u}_{xx}$, *etc.* and write $\mathbf{G}(\mathbf{u}^{(n)})$ to indicate that the differential function $\mathbf{G}$ depends on derivatives up to order n of $\mathbf{u}$ with respect to x, y, and z. We assume that $\mathbf{G}$ does not explicitly depend on $\mathbf{x}$ and t. There are no restrictions on the number of components, order, and degree of nonlinearity of the variables in $\mathbf{G}$.

We will predominantly work with polynomial systems, although systems involving one transcendental nonlinearity can also be handled. If parameters are present in (2.1), they will be denoted by lower-case Greek letters.

Example 2.1. The coupled Korteweg-de Vries (cKdV) equations [1],

$$u_t - 6\beta u u_x + 6 v v_x - \beta u_{3x} = 0, \qquad v_t + 3 u v_x + v_{3x} = 0, \tag{2.2}$$

where β is a nonzero parameter, describes interactions of two waves with different dispersion relations. System (2.2) is known in the literature as the Hirota-Satsuma system. It is completely integrable [1, 23] when $\beta = \frac{1}{2}$.

Example 2.2. The sine-Gordon (sG) equation [12, 29], $u_{2t} - u_{2x} = \sin u$, can be written as a system of evolution equations,

$$u_t = v, \quad v_t = u_{2x} + \sin u. \tag{2.3}$$

This system occurs in numerous problems of mathematics and physics, ranging from surfaces with constant mean curvature to superconductivity.

Example 2.3. The (2+1)-dimensional shallow-water wave (SWW) equations [14],

$$\begin{aligned}&\mathbf{u}_t + (\mathbf{u}\cdot\boldsymbol{\nabla})\mathbf{u} + 2\boldsymbol{\Omega}\times\mathbf{u} = -\boldsymbol{\nabla}(h\theta) + \tfrac{1}{2}h\boldsymbol{\nabla}\theta,\\ &\theta_t + \mathbf{u}\cdot(\boldsymbol{\nabla}\theta) = 0, \quad h_t + \boldsymbol{\nabla}\cdot(h\mathbf{u}) = 0,\end{aligned} \tag{2.4}$$

describe waves in the ocean using layered models. Vectors $\mathbf{u} = u(x,y,t)\mathbf{i}+v(x,y,t)\mathbf{j}$ and $\boldsymbol{\Omega} = \Omega\mathbf{k}$ are the fluid and angular velocities, respectively. $\mathbf{i}$, $\mathbf{j}$, and $\mathbf{k}$ are unit vectors along the x, y, and z-axes. $\theta(x,y,t)$ is the horizontally varying potential temperature field and $h(x,y,t)$ is the layer depth. The dot $(\cdot)$ stands for Euclidean inner product and $\boldsymbol{\nabla} = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j}$ is the gradient operator. System (2.4) is written in components as

$$\begin{aligned}&u_t + uu_x + vu_y - 2\Omega v + \tfrac{1}{2}h\theta_x + \theta h_x = 0,\ v_t + uv_x + vv_y + 2\Omega u + \tfrac{1}{2}h\theta_y + \theta h_y = 0,\\ &\theta_t + u\theta_x + v\theta_y = 0, \quad h_t + hu_x + uh_x + hv_y + vh_y = 0.\end{aligned} \tag{2.5}$$

3. Key Definitions–Continuous Case

Definition 3.1. System (2.1) is said to be *dilation invariant* if it is invariant under a scaling (dilation) symmetry.

Example 3.2. The cKdV system (2.2) is invariant under the scaling symmetry

$$(x,t,u,v) \to (\lambda^{-1}x, \lambda^{-3}t, \lambda^2 u, \lambda^2 v), \tag{3.1}$$

where λ is an arbitrary scaling parameter.

Definition 3.3. We define the *weight*[2], W, of a variable as the exponent p in λ^p which multiplies the variable.

Example 3.4. We will replace x by $\lambda^{-1}x$. Thus, $W(x) = -1$ or $W(\partial/\partial x) = 1$. From (3.1), we have $W(\partial/\partial t) = 3$ and $W(u) = W(v) = 2$ for the cKdV equations.

Definition 3.5. The *rank* of a monomial is defined as the total weight of the monomial. An expression is *uniform in rank* if its monomial terms have equal rank.

Example 3.6. All monomials in *both* equations of (2.2) have rank 5. Thus, (2.2) is uniform in rank.

Weights of dependent variables and weights of $\partial/\partial x, \partial/\partial y$, *etc.* are assumed to be non-negative and rational. Ranks must be positive natural or rational numbers. The ranks of the equations in (2.1) may differ from each other. Conversely, requiring uniformity in rank for each equation in (2.1) allows one to compute the weights of the variables (and thus the scaling symmetry) with linear algebra.

[2]For PDEs modeling physical phenomena, the weights are the remnants of physical units after non-dimensionalization.

Example 3.7. For the cKdV equations (2.2), one has

$$\begin{aligned} W(u) + W(\partial/\partial t) &= 2W(u) + 1 = 2W(v) + 1 = W(u) + 3, \\ W(v) + W(\partial/\partial t) &= W(u) + W(v) + 1 = W(v) + 3, \end{aligned}$$

which yields $W(u) = W(v) = 2$, $W(\partial/\partial t) = 3$, leading to (3.1).

Dilation symmetries, which are special Lie-point symmetries, are common to many nonlinear PDEs. However, non-uniform PDEs can be made uniform by extending the set of dependent variables with auxiliary parameters with appropriate weights. Upon completion of the computations one equates these parameters to 1.

Example 3.8. The sG equation (2.3) is not uniform in rank unless we replace it by

$$u_t = v, \quad v_t = u_{2x} + \alpha \sin u, \quad \alpha \in \mathbb{R}. \tag{3.2}$$

Using the Maclaurin series for the sin function, uniformity in rank requires

$$\begin{aligned} W(u) + W(\partial/\partial t) &= W(v), \\ W(v) + W(\partial/\partial t) &= W(u) + 2 = W(\alpha) + W(u) = W(\alpha) + 3W(u) = \cdots . \end{aligned}$$

This forces us to set $W(u) = 0$. Then, $W(\alpha) = 2$. By allowing the parameter α to scale, (3.2) becomes scaling invariant under the symmetry

$$(x, t, u, v, \alpha) \rightarrow (\lambda^{-1}x, \lambda^{-1}t, \lambda^0 u, \lambda^1 v, \lambda^2 \alpha),$$

corresponding to $W(\partial/\partial x) = W(\partial/\partial t) = 1, W(u) = 0, W(v) = 1, W(\alpha) = 2$. The first and second equations in (3.2) are uniform of ranks 1 and 2, respectively.

As in (3.2), the weight of an argument of a transcendental function is always 0.

Definition 3.9. System (2.1) is called *multi-uniform* in rank if it admits more than one dilation symmetry (not the result of adding parameters with weights).

Example 3.10. Uniformity in rank for the SWW equations (2.5) requires, after some algebra, that

$$\begin{aligned} &W(\partial/\partial t) = W(\Omega),\ W(\partial/\partial y) = W(\partial/\partial x) = 1,\ W(u) = W(v) = W(\Omega) - 1, \\ &W(\theta) = 2W(\Omega) - W(h) - 2, \end{aligned}$$

with $W(h)$ and $W(\Omega)$ free. The SWW system is thus multi-uniform. The symmetry

$$(x, y, t, u, v, \theta, h, \Omega) \rightarrow (\lambda^{-1}x, \lambda^{-1}y, \lambda^{-2}t, \lambda u, \lambda v, \lambda\theta, \lambda h, \lambda^2\Omega), \tag{3.3}$$

which is most useful for our computations later on, corresponds to $W(\partial/\partial x) = W(\partial/\partial y) = 1, W(\partial/\partial t) = 2, W(u) = W(v) = 1, W(\theta) = 1, W(h) = 1$, and $W(\Omega) = 2$. A second symmetry,

$$(x, y, t, u, v, \theta, h, \Omega) \rightarrow (\lambda^{-1}x, \lambda^{-1}y, \lambda^{-2}t, \lambda u, \lambda v, \lambda^2\theta, \lambda^0 h, \lambda^2\Omega), \tag{3.4}$$

matches $W(\partial/\partial x) = W(\partial/\partial y) = 1, W(\partial/\partial t) = 2, W(u) = W(v) = 1, W(\theta) = 2$, $W(h) = 0, W(\Omega) = 2$.

4. Conserved Densities and Fluxes of Nonlinear PDEs

Definition 4.1. A scalar differential function $\rho(\mathbf{u}^{(n)})$ is a conserved *density* if there exists a vector differential function $\mathbf{J}(\mathbf{u}^{(m)})$, called the associated *flux*, such that

$$\mathrm{D}_t\,\rho + \mathrm{Div}\,\mathbf{J} = 0 \tag{4.1}$$

is satisfied on solutions of (2.1).

Equation (4.1) is called a local[3] *conservation law*[4] [33], and Div is called the total divergence[5]. Clearly, $\mathrm{Div}\,\mathbf{J} = (\mathrm{D}_x, \mathrm{D}_y, \mathrm{D}_z) \cdot (J_1, J_2, J_3) = \mathrm{D}_x J_1 + \mathrm{D}_y J_2 + \mathrm{D}_z J_3$. In the case of one spacial variable (x), (4.1) reduces to

$$\mathrm{D}_t\,\rho + \mathrm{D}_x J = 0, \tag{4.2}$$

where both density ρ and flux J are scalar differential functions.

The flux $\mathbf{J}$ in (4.1) is not uniquely defined. In 3D, the flux can only be determined up to a curl. Indeed, if $(\rho, \mathbf{J})$ is a valid density-flux pair, so is $(\rho, \mathbf{J} + \nabla\times\mathbf{K})$ for any arbitrary vector differential function $\mathbf{K} = (K_1, K_2, K_3)$. Recall that $\nabla \times \mathbf{K} = (\mathrm{D}_y K_3 - \mathrm{D}_z K_2, \mathrm{D}_z K_1 - \mathrm{D}_x K_3, \mathrm{D}_x K_2 - \mathrm{D}_y K_1)$. In 2D, the flux is only determined up to a divergence-free vector $\mathbf{K} = (K_1, K_2) = (\mathrm{D}_y\theta), -\mathrm{D}_x\theta)$, where θ is an arbitrary scalar differential function. In (4.2) the flux is only determined up to an arbitrary constant.

In the 1D case,

$$\mathrm{D}_t\rho(u^{(n)}) = \frac{\partial\rho}{\partial t} + \sum_{k=0}^{n} \frac{\partial\rho}{\partial u_{kx}} \mathrm{D}_x^k u_t. \tag{4.3}$$

where $u^{(n)}$ is the highest-order term present in ρ. Upon replacement of u_t, u_{tx}, *etc.* from $u_t = G$, one gets

$$\mathrm{D}_t\rho = \frac{\partial\rho}{\partial t} + \rho(u)'[G],$$

where $\rho(u)'[G]$ is the Fréchet derivative of ρ in the direction of G. Similarly,

$$\mathrm{D}_x J(u^{(m)}) = \frac{\partial J}{\partial x} + \sum_{k=0}^{m} \frac{\partial J}{\partial u_{kx}} u_{(k+1)x}. \tag{4.4}$$

Generalization of (4.3) and (4.4) to multiple dependent variables is straightforward.

Example 4.2. Taking $\mathbf{u} = (u, v)$,

$$\begin{aligned}
\mathrm{D}_t\rho(u^{(n_1)}, v^{(n_2)}) &= \frac{\partial\rho}{\partial t} + \sum_{k=0}^{n_1} \frac{\partial\rho}{\partial u_{kx}} \mathrm{D}_x^k u_t + \sum_{k=0}^{n_2} \frac{\partial\rho}{\partial v_{kx}} \mathrm{D}_x^k v_t, \\
\mathrm{D}_x J(u^{(m_1)}, v^{(m_2)}) &= \frac{\partial J}{\partial x} + \sum_{k=0}^{m_1} \frac{\partial J}{\partial u_{kx}} u_{(k+1)x} + \sum_{k=0}^{m_2} \frac{\partial J}{\partial v_{kx}} v_{(k+1)x}.
\end{aligned}$$

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[3] We only compute densities and fluxes free of integral terms.

[4] In electromagnetism, this is the continuity equation relating charge density ρ to current $\mathbf{J}$.

[5] Gradient, curl, and divergence are in rectangular coordinates.

We will ignore densities and fluxes that explicitly depend on $\mathbf{x}$ and t. If $\mathbf{G}$ is polynomial then most, but not all, densities and fluxes are also polynomial.

Example 4.3. The first four density-flux pairs for the cKdV equations (2.2) are

$$\begin{aligned}
&\rho^{(1)} = u, \qquad J^{(1)} = -3\beta u^2 + 3v^2 - \beta u_{2x} \ (\text{any}\ \beta),\\
&\rho^{(2)} = u^2 - 2v^2, \quad J^{(2)} = -4\beta u^3 + \beta u_x^2 - 2\beta u u_{2x} + 2v_x^2 - 4vv_{2x} \ (\text{any}\ \beta),\\
&\rho^{(3)} = uv, \qquad J^{(3)} = 3u^2 v + 2u^3 - u_x v_x + u_{2x} v + u v_{2x} \ (\beta = -1),\\
&\rho^{(4)} = (1+\beta)u^3 - 3uv^2 - \tfrac{1}{2}(1+\beta){u_x}^2 + 3{v_x}^2,\\
&J^{(4)} = -\tfrac{9}{2}\beta(1+\beta)u^4 + 9\beta u^2 v^2 - \tfrac{9}{2}v^4 + 6\beta(1+\beta)u u_x^2 - 3\beta(1+\beta)u^2 u_{2x}\\
&\qquad + 3\beta v^2 u_{2x} - \tfrac{1}{2}\beta(1+\beta)u_{2x}^2 + \beta(1+\beta)u_x u_{3x} - 6\beta v u_x v_x + 12 u v_x^2\\
&\qquad - 6uvv_{2x} - 3v_{2x}^2 + 6v_x v_{3x} \quad (\beta \neq -1).
\end{aligned} \tag{4.5}$$

The above densities are uniform in ranks $2, 4$ and 6. Both $\rho^{(2)}$ and $\rho^{(3)}$ are of rank 4. The corresponding fluxes are also uniform in rank with ranks $4, 6,$ and 8. In [17], a few densities of rank ≥ 8 are listed, which only exist when $\beta = \frac{1}{2}$.

In general, if in (4.2) $\operatorname{rank}\rho = R$ then $\operatorname{rank} J = R + W(\partial/\partial t) - 1$. All the terms in (4.1) are also uniform in rank. This comes as no surprise since (4.1) vanishes on solutions of (2.1), hence it "inherits" the dilation symmetry of (2.1).

Example 4.4. The first few densities [3, 15] for the sG equation (3.2) are

$$\begin{aligned}
&\rho^{(1)} = 2\alpha\cos u + v^2 + {u_x}^2, \quad J^{(1)} = -2u_x v,\\
&\rho^{(2)} = 2u_x v, \qquad J^{(2)} = 2\alpha\cos u - v^2 - {u_x}^2,\\
&\rho^{(3)} = 6\alpha v u_x \cos u + v^3 u_x + v {u_x}^3 - 8 v_x u_{2x},\\
&\rho^{(4)} = 2\alpha^2\cos^2 u - 2\alpha^2 \sin^2 u + 4\alpha v^2 \cos u + 20\alpha {u_x}^2 \cos u + v^4\\
&\qquad + 6v^2 {u_x}^2 + {u_x}^4 - 16{v_x}^2 - 16u_{2x}^2.
\end{aligned} \tag{4.6}$$

$J^{(3)}$ and $J^{(4)}$ are not shown due to length. Again, all densities and fluxes are uniform in rank (before α is equated to 1).

Example 4.5. The first few conserved densities and fluxes for (2.5) are

$$\begin{aligned}
&\rho^{(1)} = h, \quad \mathbf{J}^{(1)} = \begin{pmatrix} uh \\ vh \end{pmatrix}, \qquad \rho^{(2)} = h\theta, \quad \mathbf{J}^{(2)} = \begin{pmatrix} uh\theta \\ vh\theta \end{pmatrix},\\
&\rho^{(3)} = h\theta^2, \quad \mathbf{J}^{(3)} = \begin{pmatrix} uh\theta^2 \\ vh\theta^2 \end{pmatrix},\\
&\rho^{(4)} = (u^2+v^2)h + h^2\theta, \qquad \mathbf{J}^{(4)} = \begin{pmatrix} u^3 h + uv^2 h + 2uh^2\theta \\ v^3 h + u^2 v h + 2vh^2\theta \end{pmatrix},\\
&\rho^{(5)} = v_x\theta - u_y\theta + 2\Omega\theta,\\
&\mathbf{J}^{(5)} = \tfrac{1}{6}\begin{pmatrix} 12\Omega u\theta - 4uu_y\theta + 6uv_x\theta + 2vv_y\theta + u^2\theta_y + v^2\theta_y - h\theta\theta_y + h_y\theta^2 \\ 12\Omega v\theta + 4vv_x\theta - 6vu_y\theta - 2uu_x\theta - u^2\theta_x - v^2\theta_x + h\theta\theta_x - h_x\theta^2 \end{pmatrix}.
\end{aligned} \tag{4.7}$$

All densities and fluxes are multi-uniform in rank, which will substantially simplify the computation of the densities. Under either of the two scaling symmetries, (3.3) or (3.4), $\operatorname{rank}(\mathbf{J}) = \operatorname{rank}(\rho) + 1$. With the exception of $\rho^{(2)}$ and $\mathbf{J}^{(2)}$, the ranks of the densities under (3.3) and (3.4) differ by one. The same holds for the fluxes.

5. Tools from the Calculus of Variations

In this section we introduce the variational derivative (Euler operator), the higher Euler operators (also called Lie-Euler operators) from the calculus of variations, and the homotopy operator from homological algebra. These tools will be applied to the computation of densities and fluxes in Section 7.

5.1. Continuous Variational Derivative (Euler Operator)

Definition 5.1. A scalar differential function f is a *divergence* if and only if there exists a vector differential function $\mathbf{F}$ such that $f = \mathrm{Div}\,\mathbf{F}$. In 1D, we say that a differential function f is *exact*[6] if and only if there exists a scalar differential function F such that $f = \mathrm{D}_x F$. Obviously, $F = \mathrm{D}_x^{-1}(f) = \int f\,dx$ is then the primitive (or integral) of f.

Example 5.2. Consider

$$f = 3\,u_x\,v^2\,\sin u - u_x^3\,\sin u - 6\,v\,v_x\,\cos u + 2\,u_x\,u_{2x}\,\cos u + 8\,v_x v_{2x}, \tag{5.1}$$

which we encountered [3] while computing conservation laws for (3.2). The function f is exact. Indeed, upon integration by parts (by hand), one gets

$$F = 4\,v_x^2 + u_x^2\,\cos u - 3\,v^2\,\cos u. \tag{5.2}$$

Currently, CAS like *Mathematica*, *Maple*[7] and *Reduce* fail this integration!

Example 5.3. Consider

$$f = u_x v_y - u_{2x} v_y - u_y v_x + u_{xy} v_x. \tag{5.3}$$

It is easy to verify that $f = \mathrm{Div}\,\mathbf{F}$ with

$$\mathbf{F} = (u v_y - u_x v_y, -u v_x + u_x v_x). \tag{5.4}$$

As far as we know, the leading CAS currently lack tools to compute $\mathbf{F}$.
Three questions arise:

(i) Under what conditions for f does a closed form for $\mathbf{F}$ exist?

(ii) If f is a divergence, what is it the divergence of?

(iii) Without integration by parts, can one design an algorithm to compute $\mathbf{F}$?

To answer these questions we use the following tools from the calculus of variations: the variational derivative (Euler operator), its generalizations (higher Euler operators or Lie-Euler operators), and the homotopy operator.

Definition 5.4. The *variational derivative* (Euler operator), $\mathcal{L}^{(\mathbf{0})}_{\mathbf{u}(\mathbf{x})}$, is defined [33, p. 246] by

$$\mathcal{L}^{(\mathbf{0})}_{\mathbf{u}(\mathbf{x})} = \sum_J (-\mathrm{D})_J \frac{\partial}{\partial \mathbf{u}_J}, \tag{5.5}$$

where the sum is over all the unordered multi-indices J [33, p. 95].

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[6] We do not use *integrable* to avoid confusion with complete integrability from soliton theory.

[7] Versions 9.5 and higher of *Maple* can integrate such expressions as a result of our interactions with the developers.

For example, in the 2D case the multi-indices corresponding to second-order derivatives can be identified with $\{2x, 2y, 2z, xy, xz, yz\}$. Obviously, $(-D)_{2x} = (-\mathrm{D}_x)^2 = \mathrm{D}_x^2$, $(-D)_{xy} = (-\mathrm{D}_x)(-\mathrm{D}_y) = \mathrm{D}_x\mathrm{D}_y$, *etc.*. For notational details see [33, p. 95, p. 108, p. 246].

With applications in mind, we give explicit formulas for the variational derivatives in 1D, 2D, and 3D.

Example 5.5. For scalar component u they are

$$\mathcal{L}^{(0)}_{u(x)} = \sum_{k=0}^{\infty}(-\mathrm{D}_x)^k \frac{\partial}{\partial u_{kx}} = \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial}{\partial u_{2x}} - \mathrm{D}_x^3 \frac{\partial}{\partial u_{3x}} + \cdots, \quad (5.6)$$

$$\begin{aligned}\mathcal{L}^{(0,0)}_{u(x,y)} &= \sum_{k_x=0}^{\infty}\sum_{k_y=0}^{\infty}(-\mathrm{D}_x)^{k_x}(-\mathrm{D}_y)^{k_y}\frac{\partial}{\partial u_{k_x x\, k_y y}} = \frac{\partial}{\partial u} - \mathrm{D}_x\frac{\partial}{\partial u_x} - \mathrm{D}_y\frac{\partial}{\partial u_y} \\ &\quad + \mathrm{D}_x^2\frac{\partial}{\partial u_{2x}} + \mathrm{D}_x\mathrm{D}_y\frac{\partial}{\partial u_{xy}} + \mathrm{D}_y^2\frac{\partial}{\partial u_{2y}} - \mathrm{D}_x^3\frac{\partial}{\partial u_{3x}} - \cdots, \qquad (5.7)\end{aligned}$$

and

$$\begin{aligned}\mathcal{L}^{(0,0,0)}_{u(x,y,z)} &= \sum_{k_x=0}^{\infty}\sum_{k_y=0}^{\infty}\sum_{k_z=0}^{\infty}(-\mathrm{D}_x)^{k_x}(-\mathrm{D}_y)^{k_y}(-\mathrm{D}_z)^{k_z}\frac{\partial}{\partial \mathbf{u}_{k_x x\, k_y y\, k_z z}} \\ &= \frac{\partial}{\partial u} - \mathrm{D}_x\frac{\partial}{\partial u_x} - \mathrm{D}_y\frac{\partial}{\partial u_y} - \mathrm{D}_z\frac{\partial}{\partial u_z} + \mathrm{D}_x^2\frac{\partial}{\partial u_{2x}} + \mathrm{D}_y^2\frac{\partial}{\partial u_{2y}} + \mathrm{D}_z^2\frac{\partial}{\partial u_{2z}} \\ &\quad + \mathrm{D}_x\mathrm{D}_y\frac{\partial}{\partial u_{xy}} + \mathrm{D}_x\mathrm{D}_z\frac{\partial}{\partial u_{xz}} + \mathrm{D}_y\mathrm{D}_z\frac{\partial}{\partial u_{yz}} - \mathrm{D}_x^3\frac{\partial}{\partial u_{3x}} - \cdots. \qquad (5.8)\end{aligned}$$

Note that $\mathbf{u}_{k_x x\, k_y y}$ stands for $\mathbf{u}_{xx\cdots x\, yy\cdots y}$ where x is repeated k_x times and y is repeated k_y times. Similar formulas hold for components v, w, *etc.*. The first question is then answered by the following theorem [33, p. 248].

Theorem 5.6. *A necessary and sufficient condition for a function f to be a divergence, i.e. there exists a $\mathbf{F}$ so that $f = \mathrm{Div}\,\mathbf{F}$, is that $\mathcal{L}^{(0)}_{\mathbf{u}(\mathbf{x})}(f) \equiv 0$. In other words, the Euler operator annihilates divergences, just as the divergence annihilates curls, and the curl annihilates gradients.*

If, for example, $\mathbf{u} = (u, v)$ then both $\mathcal{L}^{(0)}_{u(\mathbf{x})}(f)$ and $\mathcal{L}^{(0)}_{v(\mathbf{x})}(f)$ must vanish identically. For the 1D case, the theorem says that a differential function f is exact, i.e. there exists a F so that $f = D_x F$, if and only if $\mathcal{L}^{(0)}_{\mathbf{u}(x)}(f) \equiv 0$.

Example 5.7. To test the exactness of f in (5.1) which involves just one independent variable x, we apply the zeroth Euler operator (5.5) to f for each component of $\mathbf{u} = (u, v)$ separately. For component u (of order 2), one computes

$$\begin{aligned}
\mathcal{L}^{(0)}_{u(x)}(f) &= \frac{\partial f}{\partial u} - \mathrm{D}_x \frac{\partial f}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial f}{\partial u_{2x}} \\
&= 3u_x\, v^2 \cos u - u_x^3 \cos u + 6v\, v_x \sin u - 2u_x\, u_{2x} \sin u \\
&\quad -\mathrm{D}_x[3v^2 \sin u - 3u_x^2 \sin u + 2u_{2x} \cos u] + \mathrm{D}_x^2[2u_x \cos u] \\
&= 3u_x\, v^2 \cos u - u_x^3 \cos u + 6v\, v_x \sin u - 2u_x\, u_{2x} \sin u \\
&\quad -[3u_x v^2 \cos u + 6v\, v_x \sin u - 3u_x^3 \cos u - 6u\, u_{2x} \sin u \\
&\quad -2u_x\, u_{2x} \sin u + 2u_{3x} \cos u] \\
&\quad +[-2u_{3x} \cos u - 6u_x\, u_{2x} \sin u + 2u_{3x} \cos u] \\
&\equiv 0.
\end{aligned}$$

Similarly, for component v (also of order 2) one readily verifies that $\mathcal{L}^{(0)}_{v(x)}(f) \equiv 0$.

Example 5.8. As an example in 2D, one can readily verify that $f = u_x v_y - u_{2x} v_y - u_y v_x + u_{xy} v_x$ from (5.3) is a divergence. Applying (5.7) to f for each component of $\mathbf{u} = (u, v)$ gives $\mathcal{L}^{(0,0)}_{u(x,y)}(f) \equiv 0$ and $\mathcal{L}^{(0,0)}_{v(x,y)}(f) \equiv 0$.

5.2. Continuous Higher Euler Operators

To compute $\mathbf{F} = \mathrm{Div}^{-1}(f)$ or, in the 1D case $F = \mathrm{D}_x^{-1}(f) = \int f\, dx$, we need higher-order versions of the variational derivative, called *higher Euler operators* [28, 33] or *Lie-Euler operators* [9]. The general formulas are given in [33, p. 367]. With applications in mind, we restrict ourselves to the 1D, 2D, and 3D cases.

Definition 5.9. The *higher Euler operators* in 1D (with variable x) are

$$\mathcal{L}^{(i)}_{\mathbf{u}(x)} = \sum_{k=i}^{\infty} \binom{k}{i} (-\mathrm{D}_x)^{k-i} \frac{\partial}{\partial \mathbf{u}_{kx}}, \tag{5.9}$$

where $\binom{k}{i}$ is the binomial coefficient.

Note that the higher Euler operator for $i = 0$ matches the variational derivative in (5.6).

Example 5.10. The explicit formulas for the first three higher Euler operators (for component u and variable x) are

$$\begin{aligned}
\mathcal{L}^{(1)}_{u(x)} &= \frac{\partial}{\partial u_x} - 2\mathrm{D}_x \frac{\partial}{\partial u_{2x}} + 3\mathrm{D}_x^2 \frac{\partial}{\partial u_{3x}} - 4\mathrm{D}_x^3 \frac{\partial}{\partial u_{4x}} + \cdots, \\
\mathcal{L}^{(2)}_{u(x)} &= \frac{\partial}{\partial u_{2x}} - 3\mathrm{D}_x \frac{\partial}{\partial u_{3x}} + 6\mathrm{D}_x^2 \frac{\partial}{\partial u_{4x}} - 10\mathrm{D}_x^3 \frac{\partial}{\partial u_{5x}} + \cdots, \\
\mathcal{L}^{(3)}_{u(x)} &= \frac{\partial}{\partial u_{3x}} - 4\mathrm{D}_x \frac{\partial}{\partial u_{4x}} + 10\mathrm{D}_x^2 \frac{\partial}{\partial u_{5x}} - 20\mathrm{D}_x^3 \frac{\partial}{\partial u_{6x}} + \cdots.
\end{aligned}$$

Definition 5.11. The *higher Euler operators* in 2D (with variables x, y) are

$$\mathcal{L}^{(i_x,i_y)}_{\mathbf{u}(x,y)} = \sum_{k_x=i_x}^{\infty} \sum_{k_y=i_y}^{\infty} \binom{k_x}{i_x} \binom{k_y}{i_y} (-\mathrm{D}_x)^{k_x-i_x} (-\mathrm{D}_y)^{k_y-i_y} \frac{\partial}{\partial \mathbf{u}_{k_x x\, k_y y}}. \tag{5.10}$$

Note that the higher Euler operator for $i_x = i_y = 0$ matches the variational derivative in (5.7).

Example 5.12. The first higher Euler operators (for component u and variables x and y) are

$$\mathcal{L}_{u(x,y)}^{(1,0)} = \frac{\partial}{\partial u_x} - 2\mathrm{D}_x \frac{\partial}{\partial u_{2x}} - \mathrm{D}_y \frac{\partial}{\partial u_{xy}} + 3\mathrm{D}_x^2 \frac{\partial}{\partial u_{3x}} + 2\mathrm{D}_x\mathrm{D}_y \frac{\partial}{\partial u_{2xy}} - \cdots ,$$

$$\mathcal{L}_{u(x,y)}^{(0,1)} = \frac{\partial}{\partial u_y} - 2\mathrm{D}_y \frac{\partial}{\partial u_{2y}} - \mathrm{D}_x \frac{\partial}{\partial u_{yx}} + 3\mathrm{D}_y^2 \frac{\partial}{\partial u_{3y}} + 2\mathrm{D}_x\mathrm{D}_y \frac{\partial}{\partial u_{x2y}} - \cdots ,$$

$$\mathcal{L}_{u(x,y)}^{(1,1)} = \frac{\partial}{\partial u_{xy}} - 2\mathrm{D}_x \frac{\partial}{\partial u_{2xy}} - 2\mathrm{D}_y \frac{\partial}{\partial u_{x2y}} + 3\mathrm{D}_x^2 \frac{\partial}{\partial u_{3xy}} + 4\mathrm{D}_x\mathrm{D}_y \frac{\partial}{\partial u_{2x2y}} + \cdots ,$$

$$\mathcal{L}_{u(x,y)}^{(2,1)} = \frac{\partial}{\partial u_{2xy}} - 3\mathrm{D}_x \frac{\partial}{\partial u_{3xy}} - 2\mathrm{D}_y \frac{\partial}{\partial u_{2x2y}} + 6\mathrm{D}_x^2 \frac{\partial}{\partial u_{4xy}} + \mathrm{D}_y^2 \frac{\partial}{\partial u_{2x3y}} - \cdots .$$

Definition 5.13. The *higher Euler operators* in 3D (with variables x, y, z) are

$$\mathcal{L}_{\mathbf{u}(x,y,z)}^{(i_x,i_y,i_z)} = \sum_{k_x=i_x}^{\infty} \sum_{k_y=i_y}^{\infty} \sum_{k_z=i_z}^{\infty} \binom{k_x}{i_x}\binom{k_y}{i_y}\binom{k_z}{i_z} (-\mathrm{D}_x)^{k_x-i_x}(-\mathrm{D}_y)^{k_y-i_y}(-\mathrm{D}_z)^{k_z-i_z} \frac{\partial}{\partial \mathbf{u}_{k_x x\, k_y y\, k_z z}}. \tag{5.11}$$

The higher Euler operator for $i_x = i_y = i_z = 0$ matches the variational derivative given in (5.8). The higher Euler operators are useful in their own right as the following theorem [28] indicates.

Theorem 5.14. *A necessary and sufficient condition for a function f to be a r^{th} order derivative, i.e. $\exists F$ so that $f = D_x^r F$, is that $\mathcal{L}_{\mathbf{u}(x)}^{(i)}(f) \equiv 0$ for $i = 0, 1, \ldots, r-1$.*

5.3. Continuous Homotopy Operator

We now discuss the homotopy operator which will allow us to reduce the computation of $\mathbf{F} = \mathrm{Div}^{-1}(f)$ (or in the 1D case, $F = \mathrm{D}_x^{-1}(f) = \int f\, dx$) to a single integral with respect to an auxiliary variable denoted by λ (not to be confused with λ in Section 3). Hence, the homotopy operator circumvents integration by parts and reduces the inversion of the total divergence operator, Div, to a problem of single-variable calculus.

As mentioned in Section 5.1, Div^{-1} is only defined up to a divergence-free term (a curl term). For example in 3D, Div^{-1} is represented by an equivalence class $\mathrm{Div}^{-1}(f) = \mathbf{F} + \nabla \times \mathbf{K}$ where $\mathbf{K}$ is an arbitrary vector differential function. The homotopy operator selects a particular choice of $\mathbf{K}$.

The homotopy operator is given in explicit form, which makes it easier to implement in CAS. To keep matters transparent, we present the formulas of the homotopy operator in 1D, 2D, and 3D.

Definition 5.15. The *homotopy operator* in 1D (with variable x) [33, p. 372] is

$$\mathcal{H}_{\mathbf{u}(x)}(f) = \int_0^1 \sum_{j=1}^{N} I_{u_j}(f)[\lambda \mathbf{u}] \, \frac{d\lambda}{\lambda}, \tag{5.12}$$

where u_j is jth component of $\mathbf{u}$ and the integrand $I_{u_j}(f)$ is given by

$$I_{u_j}(f) = \sum_{i=0}^{\infty} \mathrm{D}_x^i \left(u_j \, \mathcal{L}_{u_j(x)}^{(i+1)}(f) \right). \tag{5.13}$$

The integrand involves the 1D higher Euler operators in (5.9).

In (5.12), N is the number of dependent variables and $I_{u_j}(f)[\lambda \mathbf{u}]$ means that in $I_{u_j}(f)$ one replaces $\mathbf{u}(x) \to \lambda \mathbf{u}(x)$, $\mathbf{u}_x(x) \to \lambda \mathbf{u}_x(x)$, *etc.*.

Given an exact function f, the question how to compute $F = \mathrm{D}_x^{-1}(f) = \int f \, dx$ is then answered by the following theorem [33, p. 372].

Theorem 5.16. *For an exact function f, one has $F = \mathcal{H}_{\mathbf{u}(x)}(f)$.*

Thus, in the 1D case, applying the homotopy operator (5.12) allows one to bypass integration by parts. As an experiment, one can start from a function $\tilde{F}$, compute $f = \mathrm{D}_x \tilde{F}$, subsequently compute $F = \mathcal{H}_{\mathbf{u}(x)}(f)$, and finally verify that $F - \tilde{F}$ is a constant. Using (5.1), we show how the homotopy operator (5.12) is applied.

Example 5.17. For a system with $N = 2$ components, $\mathbf{u} = (u_1, u_2) = (u, v)$, the homotopy operator formulas are

$$\mathcal{H}_{\mathbf{u}(x)}(f) = \int_0^1 \left(I_u(f)[\lambda \mathbf{u}] + I_v(f)[\lambda \mathbf{u}] \right) \frac{d\lambda}{\lambda}, \tag{5.14}$$

with

$$I_u(f) = \sum_{i=0}^{\infty} \mathrm{D}_x^i \left(u \, \mathcal{L}_{u(x)}^{(i+1)}(f) \right) \quad \text{and} \quad I_v(f) = \sum_{i=0}^{\infty} \mathrm{D}_x^i \left(v \, \mathcal{L}_{v(x)}^{(i+1)}(f) \right). \tag{5.15}$$

These sums have only finitely many non-zero terms. For example, the sum in $I_u(f)$ terminates at $p-1$ where p is the order of u. Take, for example, $f = 3\, u_x \, v^2 \, \sin u - u_x^3 \, \sin u - 6\, v \, v_x \, \cos u + 2\, u_x \, u_{2x} \, \cos u + 8\, v_x v_{2x}$. First, we compute

$$\begin{aligned} I_u(f) &= u \mathcal{L}_{u(x)}^{(1)}(f) + \mathrm{D}_x \left(u \mathcal{L}_{u(x)}^{(2)}(f) \right) \\ &= u \frac{\partial f}{\partial u_x} - 2u \mathrm{D}_x \left(\frac{\partial f}{\partial u_{2x}} \right) + \mathrm{D}_x \left(u \frac{\partial f}{\partial u_{2x}} \right) \\ &= 3uv^2 \sin u - u u_x^2 \sin u + 2 u_x^2 \cos u. \end{aligned}$$

Next,

$$\begin{aligned} I_v(f) &= v \mathcal{L}_{v(x)}^{(1)}(f) + \mathrm{D}_x \left(v \mathcal{L}_{v(x)}^{(2)}(f) \right) \\ &= v \frac{\partial f}{\partial v_x} - 2v \mathrm{D}_x \left(\frac{\partial f}{\partial v_{2x}} \right) + \mathrm{D}_x \left(v \frac{\partial f}{\partial v_{2x}} \right) \\ &= -6v^2 \cos u + 8 v_x^2. \end{aligned}$$

Formula (5.14) gives an integral with respect to λ :

$$\begin{aligned} F = \mathcal{H}_{\mathbf{u}(x)}(f) &= \int_0^1 (I_u(f)[\lambda \mathbf{u}] + I_v(f)[\lambda \mathbf{u}]) \, \frac{d\lambda}{\lambda} \\ &= \int_0^1 \left(3\lambda^2 uv^2 \sin(\lambda u) - \lambda^2 u u_x^2 \sin(\lambda u) + 2\lambda u_x^2 \cos(\lambda u) - 6\lambda v^2 \cos(\lambda u) + 8\lambda v_x^2\right) d\lambda \\ &= 4v_x^2 + u_x^2 \cos u - 3v^2 \cos u. \end{aligned}$$

which agrees with (5.2), previously computed by hand.
We now turn to inverting the Div operator using the homotopy operator.

Definition 5.18. We define the *homotopy operator* in 2D (with variables x, y) through its two components $(\mathcal{H}^{(x)}_{\mathbf{u}(x,y)}(f), \mathcal{H}^{(y)}_{\mathbf{u}(x,y)}(f))$. The x-component of the operator is given by

$$\mathcal{H}^{(x)}_{\mathbf{u}(x,y)}(f) = \int_0^1 \sum_{j=1}^{N} I^{(x)}_{u_j}(f)[\lambda \mathbf{u}] \, \frac{d\lambda}{\lambda}, \tag{5.16}$$

with

$$I^{(x)}_{u_j}(f) = \sum_{i_x=0}^{\infty} \sum_{i_y=0}^{\infty} \left(\frac{1+i_x}{1+i_x+i_y} \right) \mathrm{D}_x^{i_x} \mathrm{D}_y^{i_y} \left(u_j \, \mathcal{L}^{(1+i_x, i_y)}_{u_j(x,y)}(f) \right). \tag{5.17}$$

Analogously, the y-component is given by

$$\mathcal{H}^{(y)}_{\mathbf{u}(x,y)}(f) = \int_0^1 \sum_{j=1}^{N} I^{(y)}_{u_j}(f)[\lambda \mathbf{u}] \, \frac{d\lambda}{\lambda}, \tag{5.18}$$

with

$$I^{(y)}_{u_j}(f) = \sum_{i_x=0}^{\infty} \sum_{i_y=0}^{\infty} \left(\frac{1+i_y}{1+i_x+i_y} \right) \mathrm{D}_x^{i_x} \mathrm{D}_y^{i_y} \left(u_j \, \mathcal{L}^{(i_x, 1+i_y)}_{u_j(x,y)}(f) \right). \tag{5.19}$$

Integrands (5.17) and (5.19) involve the 2D higher Euler operators in (5.10).

After verification that f is a divergence, the question how to compute $\mathbf{F} = (F_1, F_2) = \mathrm{Div}^{-1}(f)$ is then answered by the following theorem.

Theorem 5.19. *If F is a divergence, then*

$$\mathbf{F} = (F_1, F_2) = \mathrm{Div}^{-1}(f) = (\mathcal{H}^{(x)}_{\mathbf{u}(x,y)}(f), \mathcal{H}^{(y)}_{\mathbf{u}(x,y)}(f)).$$

The superscript (x) in $\mathcal{H}^{(x)}(f)$ reminds us that we are computing the x-component of $\mathbf{F}$. As a test, one can start from any vector $\tilde{\mathbf{F}}$ and compute $f = \mathrm{Div}\, \tilde{\mathbf{F}}$. Next, compute $\mathbf{F} = (F_1, F_2) = (\mathcal{H}^{(x)}_{\mathbf{u}(x,y)}(f), \mathcal{H}^{(y)}_{\mathbf{u}(x,y)}(f))$ and, finally, verify that $\mathbf{K} = \tilde{\mathbf{F}} - \mathbf{F}$ is divergence free.

Example 5.20. Using (5.3), we show how the application of the 2D homotopy operator leads to (5.4), up to a divergence free vector. Consider $f = u_x v_y - u_{2x} v_y - u_y v_x + u_{xy} v_x$, which is easily verified to be a divergence. In order to compute $\mathrm{Div}^{-1}(f)$, we use (5.17) to get

$$\begin{aligned} I_u^{(x)}(f) &= u\mathcal{L}_{u(x,y)}^{(1,0)}(f) + \mathrm{D}_x\left(u\mathcal{L}_{u(x,y)}^{(2,0)}(f)\right) + \frac{1}{2}\mathrm{D}_y\left(u\mathcal{L}_{u(x,y)}^{(1,1)}(f)\right) \\ &= u\left(\frac{\partial f}{\partial u_x} - 2\mathrm{D}_x\frac{\partial f}{\partial u_{2x}} - \mathrm{D}_y\frac{\partial f}{\partial u_{xy}}\right) + \mathrm{D}_x\left(u\frac{\partial f}{\partial u_{2x}}\right) + \frac{1}{2}\mathrm{D}_y\left(u\frac{\partial f}{\partial u_{xy}}\right) \\ &= uv_y + \frac{1}{2}u_y v_x - u_x v_y + \frac{1}{2}uv_{xy}. \end{aligned}$$

Similarly, for the v component of $\mathbf{u} = (u, v)$ one gets

$$I_v^{(x)}(f) = v\mathcal{L}_{v(x,y)}^{(1,0)}(f) = v\frac{\partial f}{\partial v_x} = -u_y v + u_{xy} v.$$

Hence, using (5.16),

$$\begin{aligned} F_1 &= \mathcal{H}_{\mathbf{u}(x,y)}^{(x)}(f) = \int_0^1 \left(I_u^{(x)}(f)[\lambda\mathbf{u}] + I_v^{(x)}(f)[\lambda\mathbf{u}]\right)\frac{d\lambda}{\lambda} \\ &= \int_0^1 \lambda\left(uv_y + \frac{1}{2}u_y v_x - u_x v_y + \frac{1}{2}uv_{xy} - u_y v + u_{xy} v\right)d\lambda \\ &= \frac{1}{2}uv_y + \frac{1}{4}u_y v_x - \frac{1}{2}u_x v_y + \frac{1}{4}uv_{xy} - \frac{1}{2}u_y v + \frac{1}{2}u_{xy} v. \end{aligned}$$

Without showing the details, using (5.18) and (5.19) one computes

$$\begin{aligned} F_2 &= \mathcal{H}_{\mathbf{u}(x,y)}^{(y)}(f) = \int_0^1 \left(I_u^{(y)}(f)[\lambda\mathbf{u}] + I_v^{(y)}(f)[\lambda\mathbf{u}]\right)\frac{d\lambda}{\lambda} \\ &= \int_0^1 \left(\lambda\left(-uv_x - \frac{1}{2}uv_{2x} + \frac{1}{2}u_x v_x\right) + \lambda\left(u_x v - u_{2x} v\right)\right)d\lambda \\ &= -\frac{1}{2}uv_x - \frac{1}{4}uv_{2x} + \frac{1}{4}u_x v_x + \frac{1}{2}u_x v - \frac{1}{2}u_{2x} v. \end{aligned}$$

One can readily verify that the resulting vector

$$\mathbf{F} = \begin{pmatrix} F_1 \\ F_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}uv_y + \frac{1}{4}u_y v_x - \frac{1}{2}u_x v_y + \frac{1}{4}uv_{xy} - \frac{1}{2}u_y v + \frac{1}{2}u_{xy} v \\ -\frac{1}{2}uv_x - \frac{1}{4}uv_{2x} + \frac{1}{4}u_x v_x + \frac{1}{2}u_x v - \frac{1}{2}u_{2x} v \end{pmatrix}$$

differs from $\tilde{\mathbf{F}} = (uv_y - u_x v_y, -uv_x + u_x v_x)$ by a the divergence-free vector

$$\mathbf{K} = \tilde{\mathbf{F}} - \mathbf{F} = \begin{pmatrix} K_1 \\ K_2 \end{pmatrix} = \begin{pmatrix} \frac{1}{2}uv_y - \frac{1}{4}u_y v_x - \frac{1}{2}u_x v_y - \frac{1}{4}uv_{xy} = \frac{1}{2}u_y v - \frac{1}{2}u_{xy} v \\ -\frac{1}{2}uv_x + \frac{1}{4}uv_{2x} + \frac{3}{4}u_x v_x - \frac{1}{2}u_x v + \frac{1}{2}u_{2x} v \end{pmatrix}.$$

As mentioned in Section 5.1, $\mathbf{K}$ can be written as $(\mathrm{D}_y\theta, -\mathrm{D}_x\theta)$, with $\theta = \frac{1}{2}uv - \frac{1}{4}uv_x - \frac{1}{2}u_x v$.

The generalization of the homotopy operator to 3D is straightforward.

Definition 5.21. The *homotopy operator* in 3D (with variables x, y, z) is $(\mathcal{H}^{(x)}_{\mathbf{u}(x,y,z)}(f), \mathcal{H}^{(y)}_{\mathbf{u}(x,y,z)}(f), \mathcal{H}^{(z)}_{\mathbf{u}(x,y,z)}(f))$. By analogy with (5.16),

$$\mathcal{H}^{(x)}_{\mathbf{u}(x,y,z)}(f) = \int_0^1 \sum_{j=1}^{N} I^{(x)}_{u_j}(f)[\lambda \mathbf{u}] \, \frac{d\lambda}{\lambda},$$

with,

$$I^{(x)}_{u_j}(f) = \sum_{i_x=0}^{\infty} \sum_{i_y=0}^{\infty} \sum_{i_z=0}^{\infty} \left(\frac{1+i_x}{1+i_x+i_y+i_z} \right) \mathrm{D}_x^{i_x} \mathrm{D}_y^{i_y} \mathrm{D}_z^{i_z} \left(u_j \, \mathcal{L}^{(1+i_x, i_y, i_x)}_{u_j(x,y,z)}(f) \right).$$

The y and z-operators are defined analogously. The integrands $I^{(x)}_{u_j}(f)$ involve the 3D higher Euler operators in (5.11).

By analogy with the 2D case the following theorem holds.

Theorem 5.22. *Given a divergence f one has*

$$\mathbf{F} = \mathrm{Div}^{-1}(f) = (\mathcal{H}^{(x)}_{\mathbf{u}(x,y,z)}(f), \mathcal{H}^{(y)}_{\mathbf{u}(x,y,z)}(f), \mathcal{H}^{(z)}_{\mathbf{u}(x,y,z)}(f)).$$

6. Removing Divergences and Divergence-equivalent Terms

We present an algorithm to remove divergences and divergence-equivalent which simplifies the computation of densities.

Definition 6.1. Two scalar differential functions, $f^{(1)}$ and $f^{(2)}$, are *divergence-equivalent* if and only if they differ by the divergence of some vector $\mathbf{V}$, i.e. $f^{(1)} \sim f^{(2)}$ if and only if $f^{(1)} - f^{(2)} = \mathrm{Div}\, \mathbf{V}$. Obviously, if a scalar expression is divergence-equivalent to zero, then it is a divergence.

Example 6.2. Functions $f^{(1)} = u u_{2x}$ and $f^{(2)} = -u_x^2$ are divergence-equivalent because $f^{(1)} - f^{(2)} = u u_{2x} + u_x^2 = \mathrm{D}_x(u u_x)$. Using (5.6), note that $\mathcal{L}^{(0)}_{u(x)}(u u_{2x}) = 2u_{2x}$ and $\mathcal{L}^{(0)}_{u(x)}(-u_x^2) = 2u_{2x}$ are equal. Also, $f = u_{4x} = \mathrm{D}_x(u_{3x})$ is a divergence and, as expected, $\mathcal{L}^{(0)}_{u(x)}(u_{4x}) = 0$.

Example 6.3. In the 2D case, $f^{(1)} = (u_x - u_{2x}) v_y$ and $f^{(2)} = (u_y - u_{xy}) v_x$ are divergence-equivalent since $f^{(1)} - f^{(2)} = u_x v_y - u_{2x} v_y - u_y v_x + u_{xy} v_x = \mathrm{Div}\,(u v_y - u_x v_y, -u v_x + u_x v_x)$. Using (5.7), note that $\mathcal{L}^{(0)}_{\mathbf{u}(x,y)}(f^{(1)}) = \mathcal{L}^{(0)}_{\mathbf{u}(x,y)}(f^{(2)}) = (-v_{xy} - v_{xxy}, -u_{xy} + u_{xxy})$.

Divergences and divergence-equivalent terms can be removed with the following algorithm.

Algorithm 6.4. REMOVE-DIVERGENCES-AND-DIVERGENCE-EQUIVALENT-TERMS

```
/* GIVEN IS LIST R OF MONOMIAL DIFFERENTIAL FUNCTIONS */
/* INITIALIZE TWO NEW LISTS S, B */
S ← ∅
B ← ∅
/* FIND FIRST MEMBER OF S */
for each term t_i ∈ R
        do v_i ← L^(0)_u(x)(t_i)
                if v_i ≠ 0
                        then S ← {t_i}
                             B ← {v_i}
                             break
                        else discard t_i and v_i
/* FIND REMAINING MEMBERS OF S */
for each term t_j ∈ R \ {t_1, t_2, ··· , t_i}
        do v_j ← L^(0)_u(x)(t_j)
                if v_j ≠ 0
                        then if v_j ∉ Span(B)
                                then S ← S ∪ {t_j}
                                     B ← B ∪ {v_j}
                                else discard t_j and v_j
return S
/* LIST S IS FREE OF DIVERGENCES AND DIVERGENCE-EQUIVALENT
   TERMS */
```

Example 6.5. Let $\mathcal{R}=\{u^3, u^2v, uv^2, v^3, u_x^2, u_xv_x, v_x^2, uu_{2x}, u_{2x}v, uv_{2x}, vv_{2x}, u_{4x}, v_{4x}\}$. We remove divergences and divergence-equivalent terms in $\mathcal{R}$ by using the above algorithm. Since $\mathbf{v}_1 = \mathcal{L}^{(0)}_{\mathbf{u(x)}}(u^3) = (3u^2, 0) \neq (0,0)$ we have $\mathcal{S} = \{t_1\} = \{u^3\}$ and $\mathcal{B} = \{\mathbf{v}_1\} = \{(3u^2, 0)\}$. The first for loop is halted and the second for loop starts. Next, $\mathbf{v}_2 = \mathcal{L}^{(0)}_{\mathbf{u(x)}}(u^2v) = (2uv, u^2) \neq (0,0)$. We verify that $\mathbf{v}_1$ and $\mathbf{v}_2$ are independent and update the sets resulting in $\mathcal{S} = \{t_1, t_2\} = \{u^3, u^2v\}$ and $\mathcal{B}=\{\mathbf{v}_1, \mathbf{v}_2\}=\{(3u^2, 0), (2uv, u^2)\}$.

Proceeding in a similar fashion, since the first seven terms are indeed independent, we have $\mathcal{S}=\{t_1, t_2, \cdots, t_7\}$ and $\mathcal{B}=\{\mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_7\}=\{(3u^2, 0), (2uv, u^2), \cdots, (0, -2v_{2x})\}$. For $t_8 = uu_{2x}$ we compute $\mathbf{v}_8 = \mathcal{L}^{(0)}_{\mathbf{u(x)}}(uu_{2x}) = (2u_{2x}, 0)$ and verify that $\mathbf{v}_8 = -\mathbf{v}_5$. So, $\mathbf{v}_8 \in \mathrm{Span}(\mathcal{B})$ and t_8 and $\mathbf{v}_8$ are discarded (i.e. *not* added to the respective sets). For similar reasons, t_9, t_{10}, and t_{11} as well as $\mathbf{v}_9, \mathbf{v}_{10}$, and $\mathbf{v}_{11}$ are discarded. The terms $t_{12} = u_{4x}$ and $t_{13} = v_{4x}$ are discarded because $\mathbf{v}_{12} = \mathbf{v}_{13} = (0,0)$. So, $\mathcal{R}$ is replaced by $\mathcal{S}=\{u^3, u^2v, uv^2, v^3, u_x^2, u_xv_x, v_x^2\}$ which is free of divergences and divergence-equivalent terms.

7. Application: Conservation Laws of Nonlinear PDEs

As an application of the Euler and homotopy operators we show how to compute conserved densities and fluxes for the three PDEs introduced in Section 2. The first PDE illustrates the 1D case (one independent variable), but it involves two dependent variables $u(x)$ and $v(x)$. The second PDE (again in 1D) has a transcendental nonlinearity which complicates the computation of conserved densities and fluxes [15]. A third example illustrates the algorithm for a 2D case.

To compute conservation laws, $\mathrm{D}_t\,\rho + \mathrm{Div}\,\mathbf{J} = 0$, of polynomial systems of nonlinear PDEs, we use a direct approach. First, we build the candidate density ρ as a linear combination (with constant coefficients c_i) of terms which are uniform in rank (with respect to the scaling symmetry of the PDE). It is of paramount importance that the candidate density is free of divergences and divergence-equivalent terms. If such terms were present, their coefficients could not be determined because such terms can be moved into flux $\mathbf{J}$. We will use Algorithm 6.4 to construct a shortest density.

Second, we evaluate $\mathrm{D}_t\rho$ on solutions of the PDE, thus removing all time derivatives from the problem. The resulting expression (called E) must be a divergence (of the thus far unknown flux). Thus, we set $\mathcal{L}^{(0)}_{\mathbf{u(x)}}(E) \equiv 0$. Setting the coefficients of like terms to zero leads to a linear system for the undetermined coefficients c_i. In the most difficult case, such systems are parameterized by the constant parameters appearing in the given PDE. If so, a careful analysis of the eliminant (and solution branching) must be carried out. For each branch, the solution of the linear system is substituted into ρ and E.

Third, since $E = \mathrm{Div}\,\mathbf{J}$ we use the homotopy operator $\mathcal{H}_{\mathbf{u(x)}}$ to compute $\mathbf{J} = \mathrm{Div}^{-1}(E)$. The computations are done with our *Mathematica* packages [20]. Recall that $\mathbf{J}$ is only defined up a curl. Inversion of Div via the homotopy operator does not guarantee the shortest flux. Removing the curl term in $\mathbf{J}$ may lead to a shorter flux.

7.1. Conservation Laws for the Coupled KdV Equations

In (4.5) we gave the first four density-flux pairs. As an example, we will compute density $\rho^{(4)}$ and associated flux $J^{(4)}$.

Recall that the weights for the cKdV equations are $W(\partial/\partial x) = 1$ and $W(u) = W(v) = 2$. The parameter β has no weight. Hence, $\rho^{(4)}$ has rank 6. The algorithm has three steps:

Step 1: Construct the form of the density

Start from $\mathcal{V} = \{u, v\}$, i.e. the list of dependent variables with weight. Construct the set $\mathcal{M}$ which contains all monomials of selected rank 6 or less (without derivatives). Thus $\mathcal{M} = \{u^3, v^3, u^2v, uv^2, u^2, v^2, uv, u, v, 1\}$. Next, for each monomial in $\mathcal{M}$, introduce the correct number of x-derivatives so that each term has rank 6.

For example,

$$\begin{aligned}\frac{\partial^2 u^2}{\partial x^2} &= 2u_x^2 + 2uu_{2x}, \;\; \frac{\partial^2 v^2}{\partial x^2} = 2v_x^2 + 2vv_{2x}, \;\; \frac{\partial^2 (uv)}{\partial x^2} = u_{2x}v + 2u_x v_x + uv_{2x},\\ \frac{\partial^4 u}{\partial x^4} &= u_{4x}, \;\; \frac{\partial^4 v}{\partial x^4} = v_{4x}, \;\; \frac{\partial^6 1}{\partial x^6} = 0. \end{aligned} \tag{7.1}$$

Ignore the highest-order terms (typically the last terms) in each of the right hand sides of (7.1). Augment $\mathcal{M}$ with the remaining terms, after stripping off numerical factors, to get $\mathcal{R} = \{u^3, u^2v, uv^2, v^3, u_x^2, u_xv_x, v_x^2, u_{2x}v\}$, where the 8 terms[8] are listed by increasing order

Use Algorithm 6.4 to replace $\mathcal{R}$ by $\mathcal{S} = \{u^3, u^2v, uv^2, v^3, u_x^2, u_xv_x, v_x^2\}$. Linearly combine the terms in $\mathcal{S}$ with constant coefficients to get the shortest candidate density:

$$\rho = c_1u^3 + c_2u^2v + c_3uv^2 + c_4v^3 + c_5u_x^2 + c_6u_xv_x + c_7v_x^2. \tag{7.2}$$

Step 2: Determine the constants c_i

Compute

$$\begin{aligned} E = \mathrm{D}_t\rho &= \frac{\partial \rho}{\partial t} + \rho'(\mathbf{u})[\mathbf{F}] = \frac{\partial \rho}{\partial u}u_t + \frac{\partial \rho}{\partial u_x}u_{tx} + \frac{\partial \rho}{\partial v}v_t + \frac{\partial \rho}{\partial v_x}v_{tx}\\ &= (3c_1u^2 + 2c_2uv + c_3v^2)u_t + (2c_5u_x + c_6v_x)u_{tx}\\ &\quad +(c_2u^2 + 2c_3uv + 3c_4v^2)v_t + (c_6u_x + 2c_7v_x)v_{tx}. \end{aligned}$$

Replace u_t, v_t, u_{tx} and v_{tx} from (2.2) to obtain

$$\begin{aligned} E = &(3c_1u^2 + 2c_2uv + c_3v^2)(6\beta uu_x - 6vv_x + \beta u_{3x})\\ &+(2c_5u_x + c_6v_x)(6\beta uu_x - 6vv_x + \beta u_{3x})_x\\ &-(c_2u^2 + 2c_3uv + 3c_4v^2)(3uv_x + v_{3x}) - (c_6u_x + 2c_7v_x)(3uv_x + v_{3x})_x. \end{aligned} \tag{7.3}$$

Since $E = \mathrm{D}_t\,\rho = -\mathrm{D}_xJ$, the expression E must be exact. Therefore, apply the variational derivative (5.6) and require that $\mathcal{L}^{(0)}_{u(x)}(E) \equiv 0$ and $\mathcal{L}^{(0)}_{v(x)}(E) \equiv 0$. Group like terms and set their coefficients equal to zero to obtain the following (parameterized) linear system for the unknown coefficients c_1 through c_7 :

$$\begin{aligned} &(3+4\beta)c_2 = 0, \quad 3c_1 + (1+\beta)c_3 = 0, \quad 4c_2 + 3c_4 = 0, \quad (1+\beta)c_3 - 6c_5 = 0,\\ &\beta(c_1 + 2c_5) = 0, \quad \beta c_2 - c_6 = 0, \quad (1+\beta)c_6 = 0, \quad c_4 + c_6 = 0,\\ &2(1+\beta)c_2 - 3(1+2\beta)c_6 = 0, \quad 2c_2 - (1+6\beta)c_6 = 0,\\ &\beta c_3 - 6c_5 - c_7 = 0, \quad c_3 + c_7 = 0. \end{aligned}$$

Investigate the eliminant of the system. In this example, there exists a solution for any $\beta \neq -1$. Set $c_1 = 1$ and obtain

$$c_1 = 1, \quad c_2 = c_4 = c_6 = 0, \quad c_3 = -\tfrac{3}{1+\beta}, \quad c_5 = -\tfrac{1}{2}, \quad c_7 = \tfrac{3}{1+\beta}. \tag{7.4}$$

---

[8]Note that keeping all terms in (7.1) would have resulted in the list $\mathcal{R}$ (with 13 terms) given in the example at the end of Section 6. As shown, the algorithm would reduce $\mathcal{R}$ to 7 terms.

Substitute the solution into (7.2) and multiply by $1+\beta$ to get

$$\rho = (1+\beta)u^3 - 3uv^2 - \tfrac{1}{2}(1+\beta){u_x}^2 + 3{v_x}^2, \tag{7.5}$$

which is $\rho^{(4)}$ in (4.5).

Step 3: Compute the flux J

Compute the flux corresponding to ρ in (7.5). Substitute (7.4) into (7.3), reverse the sign and multiply by $1+\beta$, to get

$$\begin{aligned} E \;=\; & 18\beta(1+\beta)u^3u_x - 18\beta u^2vv_x - 18\beta uu_xv^2 + 18v^3v_x - 6\beta(1+\beta)u_x^3 \\ & - 6\beta(1+\beta)uu_xu_{2x} + 3\beta(1+\beta)u^2u_{3x} - 3\beta v^2u_{3x} - 6v_xv_{4x} - \beta(1+\beta)u_xu_{4x} \\ & + 6uvu_{3x} + 6(\beta-2)u_xv_x^2 + 6(1+\beta)u_xvv_{2x} - 18uv_xv_{2x}. \end{aligned} \tag{7.6}$$

Apply (5.14) and (5.15) to (7.6) to obtain

$$\begin{aligned} J \;=\; & -\tfrac{9}{2}\beta(1+\beta)u^4 + 9\beta u^2v^2 - \tfrac{9}{2}v^4 + 6\beta(1+\beta)uu_x^2 - 3\beta(1+\beta)u^2u_{2x} \\ & + 3\beta v^2u_{2x} - \tfrac{1}{2}\beta(1+\beta)u_{2x}^2 + \beta(1+\beta)u_xu_{3x} - 6\beta vu_xv_x \\ & + 12uv_x^2 - 6uvv_{2x} - 3v_{2x}^2 + 6v_xv_{3x}, \end{aligned}$$

which is $J^{(4)}$ in (4.5).

If $\beta = \frac{1}{2}$, the cKdV equations (2.2) are completely integrable [1, 23] and admit conserved densities at every even rank.

7.2. Conservation Laws for the Sine-Gordon Equation

Recall that the weights for the sG equation (2.3) are $W(\frac{\partial}{\partial x}) = 1$, $W(u) = 0$, $W(v) = 1$, and $W(\alpha) = 2$. The first few (of infinitely many) densities and fluxes were given in (4.6). We show how to compute densities $\rho^{(1)}$ and $\rho^{(2)}$, both of rank 2, and their associated fluxes $J^{(1)}$ and $J^{(2)}$.

In contrast to the previous example, the candidate density will no longer have *constant* undetermined coefficients c_i but *functional* coefficients $h_i(u)$ which depend on the transcendental variable u with weight zero [3]. Avoiding having to solve PDEs, we only consider examples where *one* dependent variable has weight zero.

Step 1: Construct the form of the density

Augment the list of dependent variables with α (with non-zero weight) and replace u by u_x (since $W(u) = 0$). Hence, $\mathcal{V} = \{\alpha, u_x, v\}$. Next, compute $\mathcal{R} = \{\alpha, v^2, u_{2x}, u_xv, u_x^2\}$ and remove divergences and divergence-equivalent terms to get $\mathcal{S} = \{\alpha, v^2, u_x^2, u_xv\}$. The candidate density is

$$\rho = \alpha h_1(u) + h_2(u)v^2 + h_3(u){u_x}^2 + h_4(u)u_xv, \tag{7.7}$$

with undetermined functional coefficients $h_i(u)$.

Step 2: Determine the functions $h_i(u)$

Compute

$$\begin{aligned} E &= \mathrm{D}_t\rho = \frac{\partial \rho}{\partial t} + \rho'(\mathbf{u})[\mathbf{F}] = \frac{\partial \rho}{\partial u}u_t + \frac{\partial \rho}{\partial u_x}u_{tx} + \frac{\partial \rho}{\partial v}v_t \\ &= (\alpha h_1' + v^2 h_2' + u_x^2 h_3' + u_x v h_4')v + (2u_x h_3 + v h_4)v_x \\ &\quad +(2vh_2 + u_x h_4)(\alpha \sin(u) + u_{2x}). \end{aligned} \tag{7.8}$$

where h_i' means $\frac{dh_i}{du}$. Since $E = \mathrm{D}_t\,\rho = -\mathrm{D}_x J$, the expression E must be exact. Therefore, require that $\mathcal{L}^{(0)}_{u(x)}(E) \equiv 0$ and $\mathcal{L}^{(0)}_{v(x)}(E) \equiv 0$. Set the coefficients of like terms equal to zero to get a mixed linear system of algebraic and ODEs:

$$\begin{aligned} &h_2(u) - h_3(u) = 0,\ \ h_2'(u) = 0,\ \ h_3'(u) = 0,\ \ h_4'(u) = 0,\ \ h_2''(u) = 0, \\ &h_4''(u) = 0,\ \ 2h_2'(u) - h_3'(u) = 0,\ \ 2h_2''(u) - h_3''(u) = 0, \\ &h_1'(u) + 2h_2(u)\sin u = 0,\ \ h_1''(u) + 2h_2'(u)\sin u + 2h_2(u)\cos u = 0. \end{aligned}$$

Solve the system [3] and substitute the solution

$$h_1(u) = 2c_1\cos u + c_3, \quad h_2(u) = h_3(u) = c_1, \quad h_4(u) = c_2, \tag{7.9}$$

(with arbitrary constants c_i) into (7.7) to obtain

$$\rho = c_1(2\alpha\cos u + v^2 + {u_x}^2) + c_2 u_x v + c_3\alpha. \tag{7.10}$$

Step 3: Compute the flux J

Compute the flux corresponding to ρ in (7.10). Substitute (7.9) into (7.8), to get

$$E = c_1(2u_{2x}v + 2u_x v_x) + c_2(v v_x + u_x u_{2x} + \alpha u_x \sin u). \tag{7.11}$$

Since $E = \mathrm{D}_t\,\rho = -\mathrm{D}_x J$, one must integrate $f = -E$. Applying (5.15) yields $I_u(f) = -2c_1 u_x v - c_2(u_x^2 + \alpha u \sin u)$ and $I_v(f) = -2c_1 u_x v - c_2 v^2$. Use formula (5.14) to obtain

$$\begin{aligned} J &= \mathcal{H}_{\mathbf{u}(x)}(f) = \int_0^1 \left(I_u(f)[\lambda\mathbf{u}] + I_v(f)[\lambda\mathbf{u}]\right)\,\frac{d\lambda}{\lambda} \\ &= -\int_0^1 \left(4c_1\lambda u_x v + c_2(\lambda u_x^2 + \alpha u\sin(\lambda u) + \lambda v^2)\right)\,d\lambda \\ &= -c_1(2u_x v) - c_2\left(\frac{1}{2}v^2 + \frac{1}{2}u_x^2 - \alpha\cos u\right). \end{aligned} \tag{7.12}$$

Finally, split density (7.10) and flux (7.12) into independent pieces (for c_1 and c_2):

$$\begin{aligned} \rho^{(1)} &= 2\alpha\cos u + v^2 + {u_x}^2 \quad \text{and} \quad J^{(1)} = -2u_x v, \\ \rho^{(2)} &= u_x v \quad \text{and} \quad J^{(2)} = -\frac{1}{2}v^2 - \frac{1}{2}u_x^2 + \alpha\cos u. \end{aligned}$$

For E in (7.11), J in (7.12) can easily be computed by hand [3]. However, the computation of fluxes corresponding to densities of ranks ≥ 2 is cumbersome and requires integration with the homotopy operator.

7.3. Conservation Laws for the Shallow Water Wave Equations

In contrast to the previous two examples, (2.5) is not completely integrable as far as we know. One cannot expect to find a complete set of conserved densities and fluxes (of different ranks).

The first few densities and fluxes were given in (4.7). We show how to compute densities $\rho^{(1)}, \rho^{(3)}, \rho^{(4)}$, and $\rho^{(5)}$, which are of rank 3 under the following (choices for the) weights

$$W(\partial/\partial x)=W(\partial/\partial y)=1, W(u)=W(v)=1, W(\theta)=1, W(h)=1, W(\Omega)=2. \quad (7.13)$$

We will also compute the associated fluxes $J^{(1)}, J^{(3)}, J^{(4)}$, and $J^{(5)}$.

The fact that (2.5) is multi-uniform is advantageous. Indeed, one can use the invariance of (2.5) under one scale to construct the terms of ρ, and, subsequently, use additional scale(s) to split ρ into smaller densities. This "divide and conquer" strategy drastically reduces the complexity of the computations.

Step 1: Construct the form of the density

Start from $\mathcal{V} = \{u, v, \theta, h, \Omega\}$, i.e. the list of variables *and* parameters with weights. Use (7.13) to get $\mathcal{M} = \{\Omega u, \Omega v, \ldots, u^3, v^3, \ldots, u^2 v, uv^2, \ldots, u^2, v^2, \ldots, u, v, \theta, h\}$ which has 38 monomials of rank 3 or less (without derivatives).

The terms of rank 3 in $\mathcal{M}$ are left alone. To adjust the rank, differentiate each monomial of rank 2 in $\mathcal{M}$ with respect to x ignoring the highest-order term. For example, in $\frac{du^2}{dx} = 2uu_x$, the term can be ignored since it is a total derivative. The terms $u_x v$ and $-uv_x$ are divergence-equivalent since $\frac{d(uv)}{dx} = u_x v + uv_x$. Keep $u_x v$. Likewise, differentiate each monomial of rank 2 in $\mathcal{M}$ with respect to y and ignore the highest-order term.

Produce the remaining terms for rank 3 by differentiating the monomials of rank 1 in $\mathcal{M}$ with respect to x twice, or y twice, or once with respect to x and y. Again ignore the highest-order terms. Augment the set $\mathcal{M}$ with the derivative terms of rank 3 to get $\mathcal{R} = \{\Omega u, \Omega v, \cdots, uv^2, u_x v, u_x \theta, u_x h, \cdots, u_y v, u_y \theta, \cdots, \theta_y h\}$ which has 36 terms.

Instead of applying Algorithm 6.4 to $\mathcal{R}$, use the "divide and conquer" strategy to split $\mathcal{R}$ into sublists of terms of equal rank under the (general) weights

$$\begin{aligned} &W(\partial/\partial t) = W(\Omega),\ W(\partial/\partial y) = W(\partial/\partial x) = 1,\ W(u) = W(v) = W(\Omega) - 1, \\ &W(\theta) = 2W(\Omega) - W(h) - 2, \end{aligned} \quad (7.14)$$

where $W(\Omega)$ and $W(h)$ are arbitrary. Use (7.14), to compute the rank of each monomial in $\mathcal{R}$ and gather terms of like rank in separate lists.

For each rank R_i in Table 1, apply Algorithm 6.4 to each $\mathcal{R}_i$ to get the list $\mathcal{S}_i$. Coincidentally, in this example $\mathcal{R}_i = \mathcal{S}_i$ for all i. Linearly combine the monomials in each list $\mathcal{S}_i$ with coefficients to get the shortest candidate densities ρ_i. In Table 1, we list the 10 candidate densities and the final densities and fluxes with their ranks. These conservation laws were listed in (4.7).

i	Rank R_i	Candidate ρ_i	Final ρ_i	Final $\mathbf{J}_i$
1	$6W(\Omega)-3W(h)-6$	$c_1\theta^3$	0	0
2	$3W(h)$	c_1h^3	0	0
3	$5W(\Omega)-2W(h)-5$	$c_1u\theta^2+c_2v\theta^2$	0	0
4	$W(\Omega)+2W(h)-1$	$c_1uh^2+c_2vh^2$	0	0
5	$4W(\Omega)-W(h)-4$	$c_1u^2\theta+c_2uv\theta+c_3v^2\theta+c_4\theta^2h$	θ^2h	$\begin{pmatrix} uh\theta^2 \\ vh\theta^2 \end{pmatrix}$
6	$2W(\Omega)+W(h)-2$	$c_1u^2h+c_2uvh+c_3v^2h+c_4\theta h^2$	$u^2h+v^2h+\theta h^2$	$\mathbf{J}^{(4)}$
7	$3W(\Omega)-W(h)-2$	$c_1\Omega\theta+c_2u_y\theta+c_3v_y\theta+c_4u_x\theta$ $+c_5v_x\theta$	$2\Omega\theta-u_y\theta+v_x\theta$	$\mathbf{J}^{(5)}$
8	$W(\Omega)+W(h)$	$c_1\Omega h+c_2u_yh+c_3v_yh+c_4u_xh$ $+c_5v_xh$	Ωh	$\begin{pmatrix} \Omega uh \\ \Omega vh \end{pmatrix}$
9	$2W(\Omega)-1$	$c_1\Omega u+c_2\Omega v+c_3u_yv+c_4\theta_yh$ $+c_5u_xv+c_6\theta_xh$	0	0
10	$3W(\Omega)-3$	$c_1u^3+c_2u^2v+c_3uv^2+c_4v^3$ $+c_5u\theta h+c_6v\theta h$	0	0

TABLE 1. Candidate densities for the SWW equations.

Step 2: Determine the constants c_i

For each of the densities ρ_i in Table 1 compute $E_i = \mathrm{D}_t\rho_i$ and use (2.5) to remove all time derivatives. For example, proceeding with ρ_7,

$$
\begin{aligned}
E_7 \;&=\; {\rho_7}'(\mathbf{u})[\mathbf{F}] = \frac{\partial \rho_7}{\partial u_x}u_{tx} + \frac{\partial \rho_7}{\partial u_y}u_{ty} + \frac{\partial \rho_7}{\partial v_x}v_{tx} + \frac{\partial \rho_7}{\partial v_y}v_{ty} + \frac{\partial \rho_7}{\partial \theta}\theta_t \\
&=\; -c_4\theta(uu_x + vu_y - 2\Omega v + \tfrac{1}{2}h\theta_x + \theta h_x)_x \\
&\quad\; - c_2\theta(uu_x + vu_y - 2\Omega v + \tfrac{1}{2}h\theta_x + \theta h_x)_y \\
&\quad\; - c_5\theta(uv_x + vv_y + 2\Omega u + \tfrac{1}{2}h\theta_y + \theta h_y)_x \\
&\quad\; - c_3\theta(uv_x + vv_y + 2\Omega u + \tfrac{1}{2}h\theta_y + \theta h_y)_y \\
&\quad\; - (c_1\Omega + c_2u_y + c_3v_y + c_4u_x + c_5v_x)(u\theta_x + v\theta_y).
\end{aligned}
\tag{7.15}
$$

Require that $\mathcal{L}^{(0,0)}_{u(x,y)}(E_7) = \mathcal{L}^{(0,0)}_{v(x,y)}(E_7) = \mathcal{L}^{(0,0)}_{\theta(x,y)}(E_7) = \mathcal{L}^{(0,0)}_{h(x,y)}(E_7) \equiv 0$, where, for example, $\mathcal{L}^{(0,0)}_{u(x,y)}$ is given in (5.7). Gather like terms. Equate their coefficients to zero to obtain

$$
c_1 + 2c_2 = 0, \quad c_3 = c_4 = 0, \quad c_1 - 2c_5 = 0, \quad c_2 + c_5 = 0.
$$

Set $c_1 = 2$. Substitute the solution

$$c_1 = 2,\ c_2 = -1,\ c_3 = c_4 = 0,\ c_5 = 1. \tag{7.16}$$

into ρ_7 to obtain $\rho_7 = 2\Omega\theta - u_y\theta + v_x\theta$, which matches $\mathbf{J}^{(5)}$ in (4.7).

Proceed in a similar way with the remaining nine candidate densities to obtain the results given in the third column of Table 1.

Step 3: Compute the flux J

Compute the flux corresponding to all $\rho_i \neq 0$ in Table 1. For example, continuing with ρ_7, substitute (7.16) into (7.15) to get

$$\begin{aligned} E_7 \;=\; & -\theta(u_x v_x + u v_{2x} + v_x v_y + v v_{xy} + 2\Omega u_x + \tfrac{1}{2}\theta_x h_y - u_x u_y - u u_{xy} \\ & -u_y v_y - u_{2y} v + 2\Omega v_y - \tfrac{1}{2}\theta_y h_x) - (2\Omega u\theta_x + 2\Omega v\theta_y - u u_y \theta_x \\ & -u_y v\theta_y + u v_x\theta_x + v v_x \theta_y). \end{aligned}$$

Apply the 2D homotopy operator in (5.16)-(5.19) to $E_7 = -\mathrm{Div}\,\mathbf{J}_7$. So, compute

$$\begin{aligned} I_u^{(x)}(E_7) &= u\mathcal{L}_{u(x,y)}^{(1,0)}(E_7) + \mathrm{D}_x\left(u\mathcal{L}_{u(x,y)}^{(2,0)}(E_7)\right) + \frac{1}{2}\mathrm{D}_y\left(u\mathcal{L}_{u(x,y)}^{(1,1)}(E_7)\right) \\ &= u\left(\frac{\partial E_7}{\partial u_x} - 2\mathrm{D}_x\left(\frac{\partial E_7}{\partial u_{2x}}\right) - \mathrm{D}_y\left(\frac{\partial E_7}{\partial u_{xy}}\right)\right) + \mathrm{D}_x\left(u\frac{\partial E_7}{\partial u_{2x}}\right) + \frac{1}{2}\mathrm{D}_y\left(u\frac{\partial E_7}{\partial u_{xy}}\right) \\ &= -u v_x\theta - 2\Omega u\theta - \frac{1}{2}u^2\theta_y + u u_y\theta. \end{aligned}$$

Similarly, compute

$$\begin{aligned} I_v^{(x)}(E_7) &= -v v_y\theta - \frac{1}{2}v^2\theta_y - u v_x\theta, \\ I_\theta^{(x)}(E_7) &= -\frac{1}{2}\theta^2 h_y - 2\Omega u\theta + u u_y\theta - u v_x\theta, \\ I_h^{(x)}(E_7) &= \frac{1}{2}\theta\theta_y h. \end{aligned}$$

Next, compute

$$\begin{aligned} J_7^{(x)}(\mathbf{u}) &= -\mathcal{H}_{\mathbf{u}(x,y)}^{(x)}(E_7) \\ &= -\int_0^1 \left(I_u^{(x)}(E_7)[\lambda\mathbf{u}] + I_v^{(x)}(E_7)[\lambda\mathbf{u}] + I_\theta^{(x)}(E_7)[\lambda\mathbf{u}] + I_h^{(x)}(E_7)[\lambda\mathbf{u}]\right)\frac{d\lambda}{\lambda} \\ &= \int_0^1 \left(4\lambda\Omega u\theta + \lambda^2\left(3u v_x\theta + \frac{1}{2}u^2\theta_y - 2u u_y\theta + v v_y\theta + \frac{1}{2}v^2\theta_y \right.\right. \\ &\qquad \left.\left. + \frac{1}{2}\theta^2 h_y - \frac{1}{2}\theta\theta_y h\right)\right) d\lambda \\ &= 2\Omega u\theta - \frac{2}{3}u u_y\theta + u v_x\theta + \frac{1}{3}v v_y\theta + \frac{1}{6}u^2\theta_y + \frac{1}{6}v^2\theta_y - \frac{1}{6}h\theta\theta_y + \frac{1}{6}h_y\theta^2. \end{aligned}$$

Analogously, compute

$$\begin{aligned} J_7^{(y)}(\mathbf{u}) &= -\mathcal{H}^{(y)}_{\mathbf{u}(x,y)}(E_7) \\ &= 2\Omega v\theta + \frac{2}{3}vv_x\theta - vu_y\theta - \frac{1}{3}uu_x\theta - \frac{1}{6}u^2\theta_x - \frac{1}{6}v^2\theta_x + \frac{1}{6}h\theta\theta_x - \frac{1}{6}h_x\theta^2. \end{aligned}$$

Hence,

$$\mathbf{J}_7 = \frac{1}{6}\begin{pmatrix} 12\Omega u\theta - 4uu_y\theta + 6uv_x\theta + 2vv_y\theta + u^2\theta_y + v^2\theta_y - h\theta\theta_y + h_y\theta^2 \\ 12\Omega v\theta + 4vv_x\theta - 6vu_y\theta - 2uu_x\theta - u^2\theta_x - v^2\theta_x + h\theta\theta_x - h_x\theta^2 \end{pmatrix},$$

which matches $\mathbf{J}^{(5)}$ in (4.7).

Proceed in a similar way with the remaining nonzero densities to obtain the fluxes given in the last column of Table 1.

System (2.5) has conserved densities [14, p. 294] of the form

$$\rho = hf(\theta) \quad \text{and} \quad \rho = (v_x - u_y + 2\Omega)g(\theta),$$

for any functions f and g. Our algorithm can only find f and g of the form θ^k where $k \geq 0$ is integer. A comprehensive study of all conservation laws of (2.5) is beyond the scope of this chapter.

8. Examples of Nonlinear DDEs

We consider nonlinear systems of DDEs of the form

$$\dot{\mathbf{u}}_n = \mathbf{G}(..., \mathbf{u}_{n-1}, \mathbf{u}_n, \mathbf{u}_{n+1}, ...), \tag{8.1}$$

where $\mathbf{u}_n$ and $\mathbf{G}$ are vector-valued functions with N components. The integer n corresponds to discretization in space[9]; the dot denotes differentiation with respect to continuous time (t). For simplicity, we write $\mathbf{G}(\mathbf{u}_n)$, although $\mathbf{G}$ depends on $\mathbf{u}_n$ and a finite number of its forward and backward shifts. We assume that $\mathbf{G}$ is polynomial with constant coefficients. No restrictions are imposed on the forward or backward shifts or the degree of nonlinearity in $\mathbf{G}$. In the examples we denote the components of $\mathbf{u}_n$ by u_n, v_n, *etc.*. If present, parameters are denoted by lower-case Greek letters. We use the following two DDEs to illustrate the theorems and algorithms.

Example 8.1. The Kac-van Moerbeke (KvM) lattice [25],

$$\dot{u}_n = u_n(u_{n+1} - u_{n-1}), \tag{8.2}$$

arises in the study of Langmuir oscillations in plasmas, population dynamics, *etc.*.

Example 8.2. The Toda lattice [35] in polynomial form [18],

$$\dot{u}_n = v_{n-1} - v_n, \quad \dot{v}_n = v_n(u_n - u_{n+1}), \tag{8.3}$$

models vibrations of masses in a lattice with an exponential interaction force.

---

[9]We only consider DDEs with one discrete variable.

9. Dilation Invariance and Uniformity in Rank for DDEs

The definitions for the discrete case are analogous to the continuous case. For brevity, we use the Toda lattice (8.3) to illustrate the definitions and concepts. (8.3) is dilation invariant under

$$(t, u_n, v_n) \rightarrow (\lambda^{-1} t, \lambda u_n, \lambda^2 v_n). \tag{9.1}$$

Definition 9.1. The *weight* W of a variable equals the exponent of the scaling parameter λ [18, 19].

Weights of dependent variables are non-negative and rational. We tacitly assume that weights are independent of n. For example, $W(u_{n-1}) = W(u_n) = W(u_{n+1})$, *etc.*.

Example 9.2. Since t is replaced by $\frac{t}{\lambda}$ we have $W(\frac{\mathrm{d}}{\mathrm{dt}}) = W(\mathrm{D}_t) = 1$. From (9.1) we have $W(u_n) = 1$ and $W(v_n) = 2$.

Definition 9.3. The *rank* of a monomial equals the total weight of the monomial. An expression is uniform in rank if all its monomial terms have equal rank.

Ranks must be positive natural or rational numbers.

Example 9.4. The three terms in the first equation in (8.3) have rank 2; all terms in the second equation have rank 3. Each equation is uniform in rank.

Conversely, requiring uniformity in rank in (8.3) yields $W(u_n) + 1 = W(v_n)$, and $W(v_n) + 1 = W(u_n) + W(v_n)$. Hence, $W(u_n) = 1$, $W(v_n) = 2$. So, the scaling symmetry can be computed with linear algebra.

Many integrable nonlinear DDEs are scaling invariant. If not, they can be made so by extending the set of dependent variables with parameters with weights.

10. Conserved Densities and Fluxes of Nonlinear DDEs

By analogy with D_x and D_x^{-1}, we define the following operators acting on monomials m_n in u_n, v_n, *etc.*.

Definition 10.1. D is the *up-shift operator* (also known as the forward- or right-shift operator) $\mathrm{D}\, m_n = m_{n+1}$. Its inverse, D^{-1}, is the *down-shift operator* (or backward- or left-shift operator), $\mathrm{D}^{-1}\, m_n = m_{n-1}$. The identity operator is denoted by I. Thus, $\mathrm{I}\, m_n = m_n$, and $\Delta = \mathrm{D} - \mathrm{I}$, is the *forward difference operator*. So, $\Delta\, m_n = (\mathrm{D} - \mathrm{I})\, m_n = m_{n+1} - m_n$.

Definition 10.2. A *conservation law* of (8.1),

$$\mathrm{D}_t\, \rho_n + \Delta\, J_n = 0, \tag{10.1}$$

which holds on solutions of (8.1), links a *conserved density* ρ_n to a *flux* J_n. Densities and fluxes depend on $\mathbf{u}_n$ as well as forward and backward shifts of $\mathbf{u}_n$.

To stress the analogy between one-dimensional PDEs and DDEs, we compare the defining equations in Table 2.

	Continuous Case (PDE)	Semi-discrete Case (DDE)
Evolution Equation	$\mathbf{u}_t = \mathbf{G}(\mathbf{u}, \mathbf{u}_x, \mathbf{u}_{2x}, \cdots)$	$\dot{\mathbf{u}}_n = \mathbf{G}(\cdots, \mathbf{u}_{n-1}, \mathbf{u}_n, \mathbf{u}_{n+1}, \cdots)$
Conservation Law	$\mathrm{D}_t \rho + \mathrm{D}_x J = 0$	$\dot{\rho}_n + \Delta J_n = 0$

TABLE 2. Defining equations for conservation laws of PDEs and DDEs.

Definition 10.3. Compositions of D and D^{-1} define an *equivalence relation* ($\equiv$) on monomials. All shifted monomials are equivalent.

Example 10.4. For example, $u_{n-1}v_{n+1} \equiv u_n v_{n+2} \equiv u_{n+1}v_{n+3} \equiv u_{n+2}v_{n+4}$. Factors in a monomial in u_n and its shifts are ordered by $u_{n+j} \prec u_{n+k}$ if $j < k$.

Definition 10.5. The *main representative* of an equivalence class is the monomial with u_n in the first position [18, 19].

Example 10.6. The main representative in $\{\cdots, u_{n-2}u_n, u_{n-1}u_{n+1},\, u_n u_{n+2}, \cdots\}$ is $u_n u_{n+2}$ (not $u_{n-2}u_n$).

For monomials involving u_n, v_n, w_n, *etc.* and their shifts, we lexicographically order the variables, that is $u_n \prec v_n \prec w_n$, *etc.*. Thus, for example, $u_n v_{n+2}$ and not $u_{n-2}v_n$ is the main representative of $\{\cdots, u_{n-2}v_n, u_{n-1}v_{n+1}, u_n v_{n+2}, u_{n+1}v_{n+3}, \cdots\}$.

Table 3 shows the KvM and Toda lattices with their scaling invariances, weights, and a few conserved densities. Note that the conservation law "inherits" the scaling symmetry of the DDE. Indeed, all ρ_n in Table 3 are uniform in rank.

	Kac-van Moerbeke Lattice	Toda Lattice
Lattice	$\dot{u}_n = u_n(u_{n+1} - u_{n-1})$	$\dot{u}_n = v_{n-1} - v_n,\ \dot{v}_n = v_n(u_n - u_{n+1})$
Scaling	$(t, u_n) \rightarrow (\lambda^{-1}t, \lambda u_n)$	$(t, u_n, v_n) \rightarrow (\lambda^{-1}t, \lambda u_n, \lambda^2 v_n)$
Weights	$W(\mathrm{D}_t) = 1$, $W(u_n) = 1$	$W(\mathrm{D}_t) = 1$, $W(u_n) = 1$, $W(v_n) = 2$
Densities	$\rho_n^{(1)} = u_n$ $\rho_n^{(2)} = \frac{1}{2}u_n^2 + u_n u_{n+1}$ $\rho_n^{(3)} = \frac{1}{3}u_n^3 + u_n u_{n+1}(u_n$ $+ u_{n+1} + u_{n+2})$	$\rho_n^{(1)} = u_n$ $\rho_n^{(2)} = \frac{1}{2}u_n^2 + v_n$ $\rho_n^{(3)} = \frac{1}{3}u_n^3 + u_n(v_{n-1} + v_n)$

TABLE 3. Examples of nonlinear DDEs with weights and densities.

11. Discrete Euler and Homotopy Operators

11.1. Discrete Variational Derivative (Euler Operator)

Given is a scalar function f_n in discrete variables $u_n, v_n, \ldots$ and their forward and backward shifts. The goal is to find the scalar function F_n so that $f_n = \Delta\, F_n = F_{n+1} - F_n$. We illustrate the computations with the following example:

$$f_n = -u_n u_{n+1} v_n - v_n^2 + u_{n+1} u_{n+2} v_{n+1} + v_{n+1}^2 + u_{n+3} v_{n+2} - u_{n+1} v_n. \quad (11.1)$$

By hand, one readily computes

$$F_n = v_n^2 + u_n\, u_{n+1}\, v_n + u_{n+1}\, v_n + u_{n+2}\, v_{n+1}. \quad (11.2)$$

Below we will address the questions:
(i) Under what conditions for f_n does F_n exist in closed form?
(ii) How can one compute $F_n = \Delta^{-1}(f_n)$?
(iii) Can one compute $F_n = \Delta^{-1}(f_n)$ in an analogous way as in the continuous case?

Expression f_n is called *exact* if it is a total difference, i.e. there exists a F_n so that $f_n = \Delta\, F_n$. With respect to the existence of F_n in closed form, the following exactness criterion is well-known and frequently used [4, 22].

Theorem 11.1. *A necessary and sufficient condition for a function f_n, with positive shifts, to be exact is that $\mathcal{L}^{(0)}_{\mathbf{u}_n}(f_n) \equiv 0$.*

$\mathcal{L}^{(0)}_{\mathbf{u}_n}$ is the *discrete variational derivative* (discrete Euler operator of order zero) [4] defined by

$$\mathcal{L}^{(0)}_{\mathbf{u}_n} = \sum_{k=0}^{\infty} \mathrm{D}^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}} = \frac{\partial}{\partial \mathbf{u}_n} (\sum_{k=0}^{\infty} \mathrm{D}^{-k}) = \frac{\partial}{\partial \mathbf{u}_n} (\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3} + \cdots). \quad (11.3)$$

A proof of the theorem is given in e.g. [22]. In practice, the series in (11.3) terminates at the highest shift in the expression the operator is applied to. To verify that an expression $E(u_{n-q}, \cdots, u_n, \cdots, u_{n+p})$ involving negative shifts is a total difference, one must first remove the negative shifts by replacing E_n by $\tilde{E}_n = \mathrm{D}^q E_n$.

Example 11.2. We return to (11.1), $f_n = -u_n\, u_{n+1}\, v_n - v_n^2 + u_{n+1}\, u_{n+2}\, v_{n+1} + v_{n+1}^2 + u_{n+3}\, v_{n+2} - u_{n+1}\, v_n$. We first test that f_n is exact (i.e., the total difference of some F_n to be computed later). We then apply the discrete zeroth Euler operator to f_n for each component of $\mathbf{u}_n = (u_n, v_n)$ separately. For component u_n (with maximum shift 3) one readily verifies that

$$\mathcal{L}^{(0)}_{u_n}(f_n) = \frac{\partial}{\partial u_n} \left(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3}\right)(f_n) \equiv 0.$$

Similarly, for component v_n (with maximum shift 2) one checks that $\mathcal{L}^{(0)}_{v_n}(f_n) \equiv 0$.

11.2. Discrete Higher Euler and Homotopy Operators

To compute F_n, we need higher-order versions of the discrete variational derivative. They are called *discrete higher Euler operators* or *discrete Lie-Euler operators*, $\mathcal{L}^{(i)}_{\mathbf{u}_n}$, in analogy with the continuous case [33].

In Table 4, we have put the continuous and discrete higher Euler operators side by side. Note that the discrete higher Euler operator for $i = 0$ is the discrete variational derivative.

Operator	Continuous Case	Discrete Case
Zeroth Euler	$\mathcal{L}^{(0)}_{\mathbf{u}(x)} = \sum_{k=0}^{\infty} (-\mathrm{D}_x)^k \frac{\partial}{\partial \mathbf{u}_{k\,x}}$	$\mathcal{L}^{(0)}_{\mathbf{u}_n} = \sum_{k=0}^{\infty} \mathrm{D}^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}} = \frac{\partial}{\partial \mathbf{u}_n} \sum_{k=0}^{\infty} \mathrm{D}^{-k}$
Higher Euler	$\mathcal{L}^{(i)}_{\mathbf{u}(x)} = \sum_{k=i}^{\infty} \binom{k}{i} (-\mathrm{D}_x)^{k-i} \frac{\partial}{\partial \mathbf{u}_{k\,x}}$	$\mathcal{L}^{(i)}_{\mathbf{u}_n} = \sum_{k=0}^{\infty} \binom{k}{i} \mathrm{D}^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}} = \frac{\partial}{\partial \mathbf{u}_n} \sum_{k=i}^{\infty} \binom{k}{i} \mathrm{D}^{-k}$
Homotopy	$\mathcal{H}_{\mathbf{u}(x)}(f) = \int_0^1 \sum_{j=1}^{N} I_{u_j}(f)[\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$	$\mathcal{H}_{\mathbf{u}_n}(f) = \int_0^1 \sum_{j=1}^{N} I_{u_{j,n}}(f)[\lambda \mathbf{u}_n] \frac{d\lambda}{\lambda}$
Integrand	$I_{u_j}(f) = \sum_{i=0}^{\infty} \mathrm{D}_x^i \left(u_j \mathcal{L}^{(i+1)}_{u_j(x)}(f) \right)$	$I_{u_{j,n}}(f) = \sum_{i=0}^{\infty} \Delta^i \left(u_{j,n} \mathcal{L}^{(i+1)}_{u_{j,n}}(f) \right)$

Table 4. Continuous and discrete Euler and homotopy operators in 1D side by side.

Example 11.3. The first three higher Euler operators for component u_n from Table 4 are

$$
\begin{aligned}
\mathcal{L}^{(1)}_{u_n} &= \frac{\partial}{\partial u_n} \left(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + \cdots \right), \\
\mathcal{L}^{(2)}_{u_n} &= \frac{\partial}{\partial u_n} \left(\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 6\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + \cdots \right), \\
\mathcal{L}^{(3)}_{u_n} &= \frac{\partial}{\partial u_n} \left(\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + 20\mathrm{D}^{-6} + \cdots \right).
\end{aligned}
$$

Similar formulae hold for $\mathcal{L}^{(i)}_{v_n}$.

The discrete higher Euler operators are useful in their own right as the following theorem indicates.

Theorem 11.4. *A necessary and sufficient condition for a function f_n to be a forward difference of order r, i.e. $\exists F_n$ so that $f_n = \Delta^r F_n$, is that $\mathcal{L}^{(i)}_{\mathbf{u}_n}(f_n) \equiv 0$ for $i = 0, 1, \ldots, r-1$.*

Also in Table 4, we put the formulae for the *discrete homotopy operator* $\mathcal{H}_{\mathbf{u}_n}$ and the continuous homotopy operator side by side. The integrand $I_{u_{j,n}}(f)$ of the homotopy operator involves the discrete higher Euler operators. As in the continuous case, N is the number of dependent variables $u_{j,n}$ and $I_{u_{j,n}}(f)[\lambda \mathbf{u}_n]$ means that after $I_{u_{j,n}}(f)$ is applied one replaces $\mathbf{u}_n$ by $\lambda \mathbf{u}_n$, $\mathbf{u}_{n+1}$ by $\lambda \mathbf{u}_{n+1}$, *etc.*. To compute F_n, one can use the following theorem [21, 24, 30].

Theorem 11.5. *Given an exact function f_n, one can compute $F_n = \Delta^{-1}(f_n)$ from $F_n = \mathcal{H}_{\mathbf{u}_n}(f_n)$.*

Thus, the homotopy operator reduces the inversion of Δ (and summation by parts) to a set of differentiations and shifts followed by a single integral with respect to an auxiliary parameter λ. We present a simplified version [21] of the homotopy operator given in [24, 30], where the problem is dealt with in greater generality and where the proofs are given in the context of discrete variational complexes.

Example 11.6. For a system with components, $(u_{1,n}, u_{2,n}) = (u_n, v_n)$, the discrete homotopy operator from Table 4 is

$$\mathcal{H}_{\mathbf{u}_n}(f) = \int_0^1 \left(I_{u_n}(f)[\lambda \mathbf{u}_n] + I_{v_n}(f)[\lambda \mathbf{u}_n] \right) \frac{d\lambda}{\lambda}, \tag{11.4}$$

with

$$I_{u_n}(f) = \sum_{i=0}^{\infty} \Delta^i \left(u_n \mathcal{L}^{(i+1)}_{u_n}(f) \right) \quad \text{and} \quad I_{v_n}(f) = \sum_{i=0}^{\infty} \Delta^i \left(v_n \mathcal{L}^{(i+1)}_{v_n}(f) \right). \tag{11.5}$$

Example 11.7. We return to (11.1). Using (11.5),

$$\begin{aligned} I_{u_n}(f_n) &= u_n \mathcal{L}^{(1)}_{u_n}(f_n) + \Delta\Big(u_n \mathcal{L}^{(2)}_{u_n}(f_n) \Big) + \Delta^2 \Big(u_n \mathcal{L}^{(3)}_{u_n}(f_n) \Big) \\ &= u_n \frac{\partial}{\partial u_n} \left(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} + 3\mathrm{D}^{-3} \right)(f_n) + \Delta\bigg(u_n \frac{\partial}{\partial u_n} \left(\mathrm{D}^{-2} + 3\mathrm{D}^{-3} \right)(f_n) \bigg) \\ &\quad + \Delta^2 \bigg(u_n \frac{\partial}{\partial u_n} \mathrm{D}^{-3}(f_n) \bigg) \\ &= 2u_n u_{n+1} v_n + u_{n+1} v_n + u_{n+2} v_{n+1}, \end{aligned}$$

and

$$\begin{aligned} I_{v_n}(f_n) &= v_n \mathcal{L}^{(1)}_{v_n}(f_n) + \Delta\Big(v_n \mathcal{L}^{(2)}_{v_n}(f_n) \Big) \\ &= v_n \frac{\partial}{\partial v_n} \left(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} \right)(f_n) + \Delta\bigg(v_n \frac{\partial}{\partial v_n} \mathrm{D}^{-2}(f_n) \bigg) \\ &= u_n u_{n+1} v_n + 2v_n^2 + u_{n+1} v_n + u_{n+2} v_{n+1}. \end{aligned}$$

The homotopy operator (11.4) thus leads to an integral with respect to λ :

$$
\begin{aligned}
F_n &= \int_0^1 \left(I_{u_n}(f_n)[\lambda \mathbf{u}_n] + I_{v_n}(f_n)[\lambda \mathbf{u}_n] \right) \frac{d\lambda}{\lambda} \\
&= \int_0^1 \left(2\lambda v_n^2 + 3\lambda^2 u_n u_{n+1} v_n + 2\lambda u_{n+1} v_n + 2\lambda u_{n+2} v_{n+1} \right) d\lambda \\
&= v_n^2 + u_n u_{n+1} v_n + u_{n+1} v_n + u_{n+2} v_{n+1},
\end{aligned}
$$

which agrees with (11.2), previously computed by hand.

12. Application: Conservation Laws of Nonlinear DDEs

In [16, 22], different algorithms are presented to compute fluxes of nonlinear DDEs. In this section we show how to compute fluxes with the discrete homotopy operator. For clarity, we compute a conservation law for (8.3) in Section 8. The computations are carried out with our *Mathematica* packages [20]. The completely integrable Toda lattice (8.3) has infinitely many conserved densities and fluxes. As an example, we compute density $\rho_n^{(3)}$ (of rank 3) and corresponding flux $J_n^{(3)}$ (of rank 4). In this example, $\mathbf{G} = (G_1, G_2) = (\, v_{n-1} - v_n,\, v_n(u_n - u_{n+1})\,)$. Assuming that the weights $W(u_n) = 1$ and $W(v_n) = 2$ are computed and the rank of the density is selected (say, $R{=}3$), our algorithm works as follows:

Step 1: Construct the form of the density

Start from $\mathcal{V} = \{u_n, v_n\}$, i.e. the list of dependent variables with weight. List all monomials in u_n and v_n of rank 3 or less: $\mathcal{M} = \{u_n^3, u_n^2, u_n v_n, u_n, v_n\}$.

Next, for each monomial in $\mathcal{M}$, introduce the correct number of t-derivatives so that each term has rank 3. Using (8.3), compute

$$
\begin{aligned}
&\frac{\mathrm{d}^0 u_n^3}{\mathrm{d}t^0} = u_n^3, \qquad \frac{\mathrm{d}^0 u_n v_n}{\mathrm{d}t^0} = u_n v_n, \\
&\frac{\mathrm{d}u_n^2}{\mathrm{d}t} = 2u_n \dot{u}_n = 2u_n v_{n-1} - 2u_n v_n, \qquad \frac{\mathrm{d}v_n}{\mathrm{d}t} = \dot{v}_n = u_n v_n - u_{n+1} v_n, \\
&\frac{\mathrm{d}^2 u_n}{\mathrm{d}t^2} = \frac{\mathrm{d}\dot{u}_n}{\mathrm{d}t} = \frac{\mathrm{d}(v_{n-1} - v_n)}{\mathrm{d}t} = u_{n-1} v_{n-1} - u_n v_{n-1} - u_n v_n + u_{n+1} v_n. \qquad (12.1)
\end{aligned}
$$

Augment $\mathcal{M}$ with the terms from the right hand sides of (12.1) to get $\mathcal{R} = \{u_n^3, u_n v_{n-1}, u_n v_n, u_{n-1} v_{n-1}, u_{n+1} v_n\}$.

Identify members belonging to the same equivalence classes and replace them by their main representatives. For example, $u_n v_{n-1} \equiv u_{n+1} v_n$, so the latter is replaced by $u_n v_{n-1}$. Hence, replace $\mathcal{R}$ by $\mathcal{S} = \{u_n^3, u_n v_{n-1}, u_n v_n\}$, which has the building blocks of the density. Linearly combine the monomials in $\mathcal{S}$ with coefficients c_i to get the candidate density:

$$
\rho_n = c_1\, u_n^3 + c_2\, u_n v_{n-1} + c_3\, u_n v_n. \qquad (12.2)
$$

Step 2: Determine the coefficients

Require that (10.1) holds. Compute $\mathrm{D}_t \rho_n$. Use (8.3) to remove $\dot{u}_n$ and $\dot{v}_n$ and their shifts. Thus,

$$\begin{aligned} E_n &= \mathrm{D}_t \rho_n = (3c_1 - c_2) u_n^2 v_{n-1} + (c_3 - 3c_1) u_n^2 v_n + (c_3 - c_2) v_{n-1} v_n \\ &\quad + c_2\, u_{n-1} u_n v_{n-1} + c_2 v_{n-1}^2 - c_3 u_n u_{n+1} v_n - c_3 v_n^2. \end{aligned} \tag{12.3}$$

To remove the negative shift $n-1$, compute $\tilde{E}_n = \mathrm{D} E_n$ Apply $\mathcal{L}_{u_n}^{(0)}$ to $\tilde{E}_n$, yielding

$$\begin{aligned} \mathcal{L}_{u_n}^{(0)}(\tilde{E}_n) &= \frac{\partial}{\partial u_n} (\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2})(\tilde{E}_n) \\ &= 2(3c_1 - c_2) u_n v_{n-1} + 2(c_3 - 3c_1) u_n v_n + (c_2 - c_3) u_{n-1} v_{n-1} \\ &\quad + (c_2 - c_3) u_{n+1} v_n. \end{aligned} \tag{12.4}$$

Next, apply $\mathcal{L}_{v_n}^{(0)}$ to $\tilde{E}_n$, yielding

$$\begin{aligned} \mathcal{L}_{v_n}^{(0)}(\tilde{E}_n) &= \frac{\partial}{\partial v_n} (\mathrm{I} + \mathrm{D}^{-1})(\tilde{E}_n) \\ &= (3c_1 - c_2) u_{n+1}^2 + (c_3 - c_2) v_{n+1} + (c_2 - c_3) u_n u_{n+1} \\ &\quad + 2(c_2 - c_3) v_n + (c_3 - 3c_1) u_n^2 + (c_3 - c_2) v_{n-1}. \end{aligned} \tag{12.5}$$

Both (12.4) and (12.5) must vanish identically. Solve the linear system

$$3c_1 - c_2 = 0, \quad c_3 - 3c_1 = 0, \quad c_2 - c_3 = 0.$$

Set $c_1 = \frac{1}{3}$ and substitute the solution $c_1 = \frac{1}{3}, c_2 = c_3 = 1$, into (12.2)

$$\rho_n = \frac{1}{3} u_n^3 + u_n (v_{n-1} + v_n). \tag{12.6}$$

Step 3: Compute the flux

In view of (10.1), one must compute $J_n = -\Delta^{-1}(E_n)$. Substitute $c_1 = \frac{1}{3}, c_2 = c_3 = 1$ into (12.3). Then, $\tilde{E}_n = \mathrm{D} E_n = u_n u_{n+1} v_n + v_n^2 - u_{n+1} u_{n+2} v_{n+1} - v_{n+1}^2$. Apply (11.5) to $-\tilde{E}_n$ to obtain

$$I_{u_n}(-\tilde{E}_n) = 2 u_n u_{n+1} v_n, \qquad I_{v_n}(-\tilde{E}_n) = u_n u_{n+1} v_n + 2 v_n^2.$$

Application of the homotopy operator (11.4) yields

$$\begin{aligned} \tilde{J}_n &= \int_0^1 \left(I_{u_n}(-\tilde{E}_n)[\lambda \mathbf{u}_n] + I_{v_n}(-\tilde{E}_n)[\lambda \mathbf{u}_n] \right) \frac{d\lambda}{\lambda} \\ &= \int_0^1 (3\lambda^2 u_n u_{n+1} v_n + 2\lambda v_n^2)\, d\lambda \\ &= u_n u_{n+1} v_n + v_n^2. \end{aligned}$$

After a backward shift, $J_n = \mathrm{D}^{-1}(\tilde{J}_n)$, we obtain J_n. With (12.6), the final result is then

$$\rho_n = \frac{1}{3}\, u_n^3 + u_n (v_{n-1} + v_n), \quad J_n = u_{n-1} u_n v_{n-1} + v_{n-1}^2.$$

The above density corresponds to $\rho_n^{(3)}$ in Table 3.

13. Conclusion

Based on the concept of scaling invariance and using tools of the calculus of variations, we presented algorithms to symbolically compute conserved densities and fluxes of nonlinear polynomial and transcendental systems of PDEs in multi-spacial dimensions and DDEs in one discrete variable.

The continuous homotopy operator is a powerful, algorithmic tool to compute fluxes explicitly. Indeed, the homotopy operator handles integration by parts in multi-variables which allows us to invert the total divergence operator. Likewise, the discrete homotopy operator handles summation by parts and inverts the forward difference operator. In both cases, the problem reduces to an explicit integral from 1D calculus.

Homotopy operators have a wide range of applications in the study of PDEs, DDEs, fully discretized lattices, and beyond. We extracted the Euler and homotopy operators from their abstract setting, introduced them into applied mathematics, thereby making them readily applicable to computational problems.

We purposely avoided differential forms and abstract concepts from differential geometry and homological algebra. Our down-to-earth approach might appeal to scientists who prefer not to juggle exterior products and Lie derivatives. Our calculus-based formulas for the Euler and homotopy operators can be readily implemented in major CAS.

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