Tools from the Calculus of Variations and Differential Geometry to Investigate Conservation Laws of Nonlinear PDEs and DDEs

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Nonlinear Waves Seminar – Dept. Appl. Math.
University of Colorado–Boulder
Tuesday, January 28, 2020, 4:00p.m.

Acknowledgements

Bernard Deconinck (Univ. of Washington, Seattle)

Ünal Göktaş (Wolfram Research, Inc.)

Mark Hickman (Univ. of Canterbury, New Zealand)

Douglas Poole (Chadron State College, Nebraska)

Several undergraduate and graduate students

Research supported in part by NSF
under Grant No. CCF-0830783

This presentation was made in `TeXpower`

Outline

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  - Tools from topology, the calculus of variations, and differential geometry
  - Calculus-based formulas for the continuous Euler and homotopy operators (multi-variate)
  - Symbolic integration by parts and inversion of the total divergence operator
  - Application: symbolic computation of conservation laws of nonlinear PDEs in multiple space dimensions

- **Part II: Discrete Case**
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  - Tools from the Discrete Calculus of Variations
  - Analogy: Continuous and discrete formulas
  - Calculus-based formulas for the discrete Euler and homotopy operators
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  - Application: symbolic computation of conservation laws of nonlinear DDEs
- **Conclusions and Future Work**

Motivation, Problem Statement, Examples

Conservation laws of nonlinear PDEs

- System of evolution equations of order M

$$\mathbf{u}_t = \mathbf{F}(\mathbf{u}^{(M)}(\mathbf{x}))$$

with $\mathbf{u} = (u, v, w, \ldots)$ and $\mathbf{x} = (x, y, z)$.

- Conservation law in (1+1)-dimensions

$$\boxed{\mathrm{D}_t \rho + \mathrm{D}_x J \doteq 0}$$

where $\doteq$ means evaluated on the PDE.

Conserved density ρ and flux J.

• Example 1: **Short pulse equation (SPE)**

$$u_{xt} = u + (u^3)_{xx} = u + 6uu_x^2 + 3u^2 u_{xx}$$

for $u(x,t)$ is completely integrable.

First non-polynomial conservation law:

$$\mathrm{D}_t \left(\sqrt{1+6u_x^2}\right) + \mathrm{D}_x \left(-3u^2\sqrt{1+6u_x^2}\right) \doteq 0$$

$$\mathrm{D}_t \left(\sqrt{1+6u_x^2}\right) = \frac{6u_x u_{xt}}{\sqrt{1+6u_x^2}}$$

$$\doteq \frac{6u_x(u + 6uu_x^2 + 3u^2 u_{xx})}{\sqrt{1+6u_x^2}}$$

Let

$$f = -\frac{6u_x(u + 6uu_x^2 + 3u^2u_{xx})}{\sqrt{1+6u_x^2}}$$

Question: Can the expression be integrated?

If yes, find $F = \int f \, dx$ (so, $f = D_x F$)

Result (by hand): $F = -3u^2\sqrt{1+6u_x^2}$

Mathematica cannot compute this integral!

Can the integration capabilities of CAS be improved for expressions with arbitrary functions?

- Example 2: **sine-Gordon equation**

$$u_{tt} - u_{xx} = \sin u$$

or, equivalently,

$$u_t = v, \qquad v_t = u_{xx} + \sin u$$

First conservation laws:

$$\mathrm{D}_t\Big(2\cos u + v^2 + u_x^2\Big) + \mathrm{D}_x\Big(-2vu_x\Big) \doteq 0$$

$$\mathrm{D}_t\Big(2vu_x\Big) + \mathrm{D}_x\Big(2\cos u - v^2 - u_x^2\Big) \doteq 0$$

$$\mathrm{D}_t\Big(24vu_x\cos u + 4v^3u_x + 4vu_x^3 - 32v_xu_{2x}\Big)$$

$$+\mathrm{D}_x\Big(6\cos^2 u - 6\sin^2 u + 12v^2\cos u$$

$$+4u_x^2\cos u - 6v^2u_x^2 - v^4 - u_x^4 + 16v_x^2 + 16v_{xx}^2\Big) \doteq 0$$

Let

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

Question: Can the expression be integrated?

If yes, find $F = \int f \, dx$ (so, $f = D_x F$)

Result (by hand): $F = 4\, v_x^2 + u_x^2 \cos u - 3\, v^2 \cos u$

Mathematica cannot compute this integral!

- Conservation law in (2+1)-dimensions

$$\boxed{\mathrm{D}_t \rho + \nabla \cdot \mathbf{J} = \mathrm{D}_t \rho + \mathrm{D}_x J_1 + \mathrm{D}_y J_2 \doteq 0}$$

Conserved density ρ and flux $\mathbf{J} = (J_1, J_2)$.

- Conservation law in (3+1)-dimensions

$$\boxed{\mathrm{D}_t \rho + \nabla \cdot \mathbf{J} = \mathrm{D}_t \rho + \mathrm{D}_x J_1 + \mathrm{D}_y J_2 + \mathrm{D}_z J_3 \doteq 0}$$

Conserved density ρ and flux $\mathbf{J} = (J_1, J_2, J_3)$.

- Example 3: **Zakharov-Kuznetsov Equation**

$$u_t + \alpha u u_x + \beta(u_{xx} + u_{yy})_x = 0$$

(models ion-sound solitons in a low pressure uniform magnetized plasma).

Conservation laws:

$$\mathrm{D}_t\Big(u\Big) + \mathrm{D}_x\Big(\tfrac{\alpha}{2}u^2 + \beta u_{xx}\Big) + \mathrm{D}_y\Big(\beta u_{xy}\Big) \doteq 0$$

$$\mathrm{D}_t\Big(u^2\Big) + \mathrm{D}_x\Big(\tfrac{2\alpha}{3}u^3 - \beta(u_x^2 - u_y^2) + 2\beta u(u_{xx} + u_{yy})\Big)$$
$$+ \mathrm{D}_y\Big(-2\beta u_x u_y\Big) \doteq 0$$

$$
\begin{aligned}
&\mathrm{D}_t\Big(u^3 - \tfrac{3\beta}{\alpha}(u_x^2 + u_y^2)\Big) + \mathrm{D}_x\Big(3u^2(\tfrac{\alpha}{4}u^2 + \beta u_{xx}) \\
&- 6\beta u(u_x^2 + u_y^2) + \tfrac{3\beta^2}{\alpha}(u_{xx}^2 - u_{yy}^2) \\
&- \tfrac{6\beta^2}{\alpha}(u_x(u_{xxx} + u_{xyy}) + u_y(u_{xxy} + u_{yyy}))\Big) \\
&+ \mathrm{D}_y\Big(3\beta u^2 u_{xy} + \tfrac{6\beta^2}{\alpha}u_{xy}(u_{xx} + u_{yy})\Big) \doteq 0
\end{aligned}
$$

Mathematica has no function to compute Div^{-1}

Can this be done without integration by parts?

Can the computation be reduced to a single integral in one variable?

- Example 4: **Undo a Divergence**

For $u(x,y)$ and $v(x,y)$

$$f = u_x v_y - u_{2x} v_y - u_y v_x + u_{xy} v_x$$

Question: Is there an $\mathbf{F}$ so that $f = \mathrm{Div}\,\mathbf{F}$?

If yes, find $\mathbf{F}$.

Result (by hand): $\mathbf{F} = (u v_y - u_x v_y, -u v_x + u_x v_x)$

Mathematica has no function to compute Div^{-1}

Can the computation be reduced to a single integration?

Demonstration with Mathematica

Notation – Computations on the Jet Space

- Independent variables: t (time), $\mathbf{x} = (x, y, z)$

- Dependent variables $\mathbf{u} = (u^{(1)}, u^{(2)}, \ldots, u^{(j)}, \ldots, u^{(N)})$

  In examples: $\mathbf{u} = (u, v, w, \theta, h, \ldots)$

- Partial derivatives $u_{kx} = \frac{\partial^k u}{\partial x^k}$, $u_{kx\,ly} = \frac{\partial^{k+l} u}{\partial x^k y^l}$, etc.

  Examples: $u_{xxxxx} = u_{5x} = \frac{\partial^5 u}{\partial x^5}$

  $$u_{xx\,yyyy} = u_{2x\,4y} = \frac{\partial^6 u}{\partial x^2 y^4}$$

- *Differential functions*

  Example: $f = uvv_x + x^2 u_x^3 v_x + u_x v_{xx}$

- *Total derivatives*: $\mathrm{D}_t,\ \mathrm{D}_x, \mathrm{D}_y, \ldots$

Example: Let $f = uvv_x + x^2u_x^3v_x + u_xv_{xx}$ Then

$$\begin{aligned}
\mathrm{D}_x f &= \frac{\partial f}{\partial x} + u_x \frac{\partial f}{\partial u} + u_{xx} \frac{\partial f}{\partial u_x} \\
&\quad + v_x \frac{\partial f}{\partial v} + v_{xx} \frac{\partial f}{\partial v_x} + v_{xxx} \frac{\partial f}{\partial v_{xx}} \\
&= 2xu_x^3v_x + u_x(vv_x) + u_{xx}(3x^2u_x^2v_x + v_{xx}) \\
&\quad + v_x(uv_x) + v_{xx}(uv + x^2u_x^3) + v_{xxx}(u_x) \\
&= 2xu_x^3v_x + vu_xv_x + 3x^2u_x^2v_xu_{xx} + u_{xx}v_{xx} \\
&\quad + uv_x^2 + uvv_{xx} + x^2u_x^3v_{xx} + u_xv_{xxx}
\end{aligned}$$

Tool from the Calculus of Variations

Euler Operator (Variational Derivative)

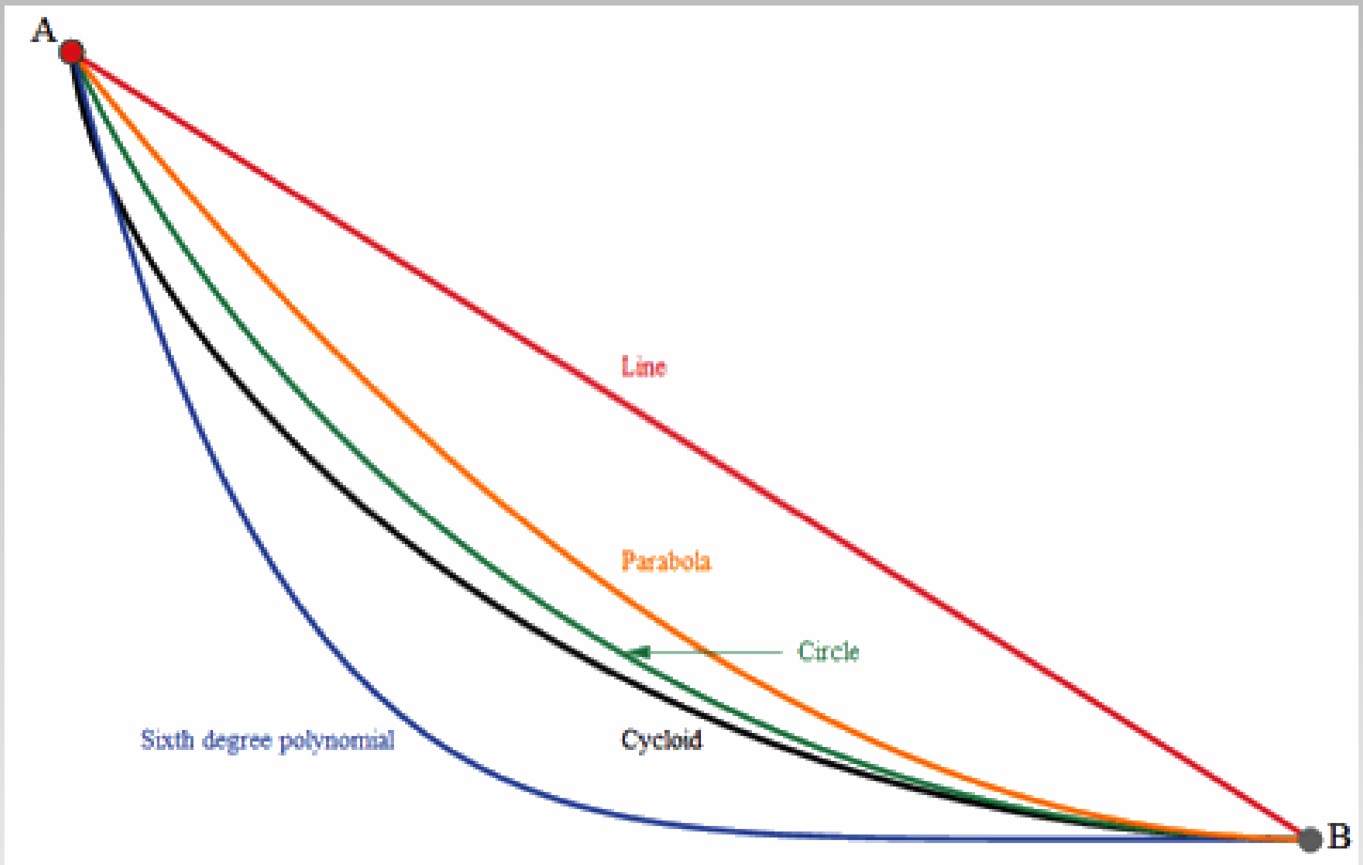
Find $y(x)$ that extremizes, e.g., the functional

$$J(y) = \int_a^b L(x, y(x), y'(x), y''(x))\, dx$$

where $y(a) = y_A$, $y(b) = y_B$, i.e., $y(x)$ passes through $A(a, y_A)$ and $B(b, y_B)$.

Let $y^\star$ be the extremizing function

Brachistochrone Problem



Functional (time to be minimized):

$$J(y) = \int_a^b \frac{\sqrt{1 + y'^2}}{\sqrt{2gy}}\, dx$$

Solution: Consider a family of functions $y(x) = y^\star(x) + \epsilon h(x)$ with $h(a) = h(b) = h'(a) = h'(b) = 0$.

So,

$$J(y^\star + \epsilon h) = \int_a^b L(x, y^\star + \epsilon h, y^{\star\prime} + \epsilon h', y^{\star\prime\prime} + \epsilon h'')\, dx$$

View this as a function of ϵ and compute

$$\begin{aligned} \left.\frac{dJ}{d\epsilon}\right|_{\epsilon=0} &= J'(0) \\ &= \int_a^b \Big(L_y(x, y^\star, y^{\star\prime}, y^{\star\prime\prime})h + L_{y'}(x, y^\star, y^{\star\prime}, y^{\star\prime\prime})h' \\ &\quad + L_{y''}(x, y^\star, y^{\star\prime}, y^{\star\prime\prime})h'' \Big)\, dx \end{aligned}$$

Integrate by parts and use boundary conditions

$$\begin{aligned} J'(0) &= \int_a^b L_y h \, dx + (L_{y'} h)|_a^b - \int_a^b h \frac{d}{dx}(L_{y'}) \, dx \\ &\quad +(L_{y''} h')|_a^b - (h \frac{d}{dx}(L_{y''}))|_a^b + \int_a^b h \frac{d^2}{dx^2}(L_{y''}) \, dx \\ &= \int_a^b \left(L_y - \frac{d}{dx}(L_{y'}) + \frac{d^2}{dx^2}(L_{y''}) \right) h \, dx \end{aligned}$$

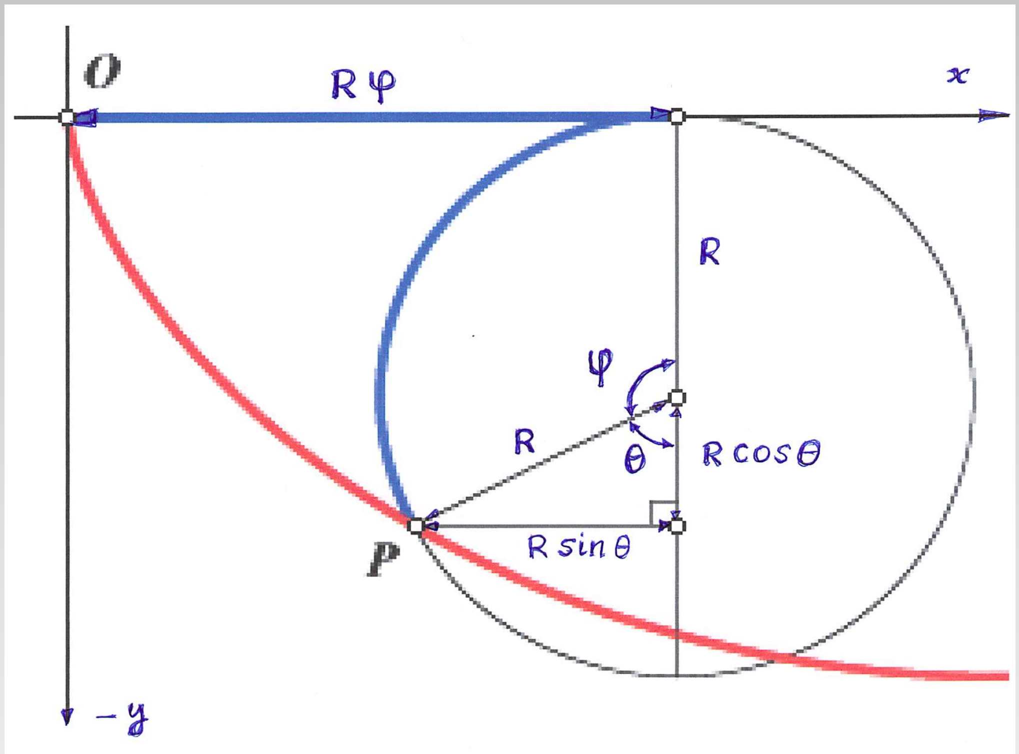
Use the fundamental lemma of the calculus of variations:

$$J'(0) = 0 \longrightarrow L_y - \frac{d}{dx}(L_{y'}) + \frac{d^2}{dx^2}(L_{y''}) = 0$$

Solve Euler-Lagrange equation to get $y^\star(x)$.

Brachistochrone Problem

$$L_y - \frac{d}{dx}(L_{y'}) = 0 \longrightarrow 2yy'' + 1 + y'^2 = 0$$



Solution $y^\star$: Cycloid

$$x = R(\phi - \sin\phi) = R(\pi - \theta - \sin\theta)$$
$$y = R(1 - \cos\phi) = R(1 + \cos\theta)$$

Special case

If $L = G'$ for some function $G(x, y(x), y'(x), y''(x))$ then

$$\begin{aligned} J(y) &= \int_a^b G' \, dx = G(x, y(x), y'(x), y''(x))\Big|_a^b \\ &= G(b, y(b), y'(b), y''(b)) - G(a, y(a), y'(a), y''(a)) \end{aligned}$$

is **independent** of the path $y^{\star}(x)$. Therefore,

$$L_y - \frac{d}{dx}(L_{y'}) + \frac{d^2}{dx^2}(L_{y''}) \equiv 0$$

Define the Euler-Lagrange operator as

$$\mathcal{L} = \frac{\partial}{\partial y} - \mathrm{D}_x \frac{\partial}{\partial y'} + \mathrm{D}_x^2 \frac{\partial}{\partial y''} - \mathrm{D}_x^3 \frac{\partial}{\partial y'''} + \cdots$$

- Definition:

  A differential function f is a exact iff $f = \mathrm{Div}\,\mathbf{F}$.

  Special case (1D): $f = \mathrm{D}_x\, F$.

- Question: How can one test that $f = \mathrm{Div}\,\mathbf{F}\,$?

- Theorem (exactness test):

  $f = \mathrm{Div}\,\mathbf{F}$ iff $\mathcal{L}_{u^{(j)}(\mathbf{x})}\, f \equiv 0, \quad j = 1, 2, \ldots, N.$

  N is the number of dependent variables.

  The Euler operator annihilates divergences

- Comparison: curl annihilates gradients; divergence annihilates curls.

- Euler operator in 1D (variable $u(x)$):

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

- Euler operator in 2D (variable $u(x, y)$):

$$\mathcal{L}_{u(x,y)} = \sum_{k=0}^{M_x} \sum_{\ell=0}^{M_y} (-\mathrm{D}_x)^k (-\mathrm{D}_y)^\ell \frac{\partial}{\partial u_{kx\,\ell y}}$$
$$= \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u_x} - \mathrm{D}_y \frac{\partial}{\partial u_y}$$
$$+ \mathrm{D}_x^2 \frac{\partial}{\partial u_{xx}} + \mathrm{D}_x \mathrm{D}_y \frac{\partial}{\partial u_{xy}} + \mathrm{D}_y^2 \frac{\partial}{\partial u_{yy}} - \mathrm{D}_x^3 \frac{\partial}{\partial u_{xxx}} \cdots$$

Application: Testing Exactness

Example:

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

where $u(x)$ and $v(x)$

- f is exact
- After integration by parts (by hand):

$$F = \int f \, dx = 4\, v_x^2 + u_x^2 \, \cos u - 3\, v^2 \, \cos u$$

- Exactness test with Euler operator:

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

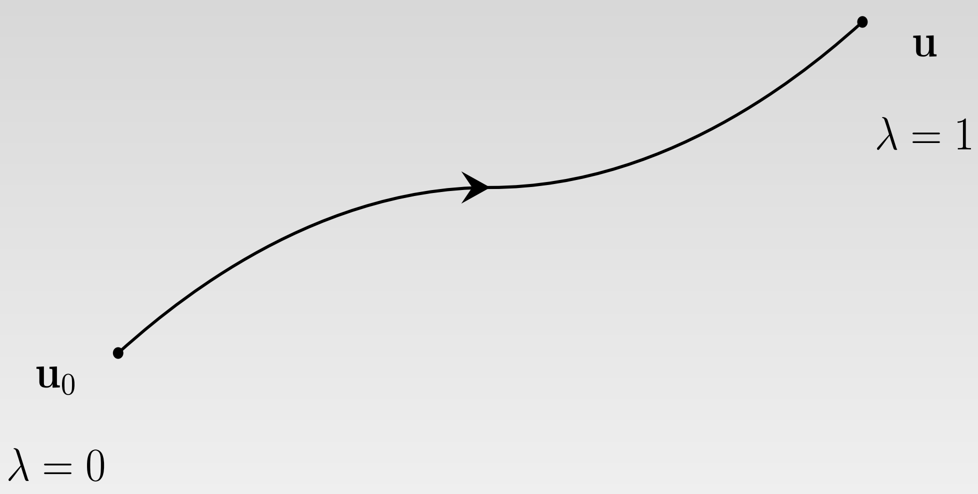
$$\mathcal{L}_{u(x)}\, f = \frac{\partial f}{\partial u} - \mathrm{D}_x \frac{\partial f}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial f}{\partial u_{xx}} \equiv 0$$

$$\mathcal{L}_{v(x)}\, f = \frac{\partial f}{\partial v} - \mathrm{D}_x \frac{\partial f}{\partial v_x} + \mathrm{D}_x^2 \frac{\partial f}{\partial v_{xx}} \equiv 0$$

Concept from (differential) Topology

Homotopic & Homotopy

Two continuous functions are called homotopic if one can be "continuously deformed" into the other. Such a deformation is called a homotopy between the two functions.



$$T(\mathbf{u}_0, \mathbf{u}) = \mathbf{u}_0 + \lambda(\mathbf{u} - \mathbf{u}_0) = (1 - \lambda)\mathbf{u}_0 + \lambda\mathbf{u}$$

Demonstration with Mathematica

Tool from Differential Geometry

- Question: How can one compute $\mathbf{F} = \mathrm{Div}^{-1} f$?
- Theorem (integration by parts):
  - In 1D: If f is exact then

$$\boxed{F = \mathrm{D}_x^{-1} f = \int f \, dx = \mathcal{H}_{\mathbf{u}(x)} f}$$

  - In 2D: If f is a divergence then

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

The homotopy operator inverts total derivatives and divergences!

- Homotopy operator in 1D (variable x):

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

with integrand

$$I_{u^{(j)}} f = \sum_{k=1}^{M_x^{(j)}} \left(\sum_{i=0}^{k-1} u_{ix}^{(j)} \, (-\mathcal{D}_x)^{k-(i+1)} \right) \frac{\partial f}{\partial u_{kx}^{(j)}}$$

$(I_{u^{(j)}} f)[\lambda \mathbf{u}]$ means that in $I_{u^{(j)}} f$ one replaces $\mathbf{u} \to \lambda \mathbf{u}$, $\mathbf{u}_x \to \lambda \mathbf{u}_x$, *etc.*

More general: $\mathbf{u} \to \lambda(\mathbf{u} - \mathbf{u}_0) + \mathbf{u}_0$

$\mathbf{u}_x \to \lambda(\mathbf{u}_x - \mathbf{u}_{x0}) + \mathbf{u}_{x0}$ etc.

- Homotopy operator in 2D (variables x and y):

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

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

where for dependent variable $u(x,y)$

$$\mathcal{I}^{(x)}_u f = \sum_{k=1}^{M_x} \sum_{\ell=0}^{M_y} \left(\sum_{i=0}^{k-1} \sum_{j=0}^{\ell} u_{ix\,jy} \frac{\binom{i+j}{i}\binom{k+\ell-i-j-1}{k-i-1}}{\binom{k+\ell}{k}} (-\mathrm{D}_x)^{k-i-1} (-\mathrm{D}_y)^{\ell-j} \right) \frac{\partial f}{\partial u_{kx\,\ell y}}$$

Peter Olver's First Book

Peter J. Olver

Applications of Lie Groups to Differential Equations

Second Edition

Springer-Verlag
New York Berlin Heidelberg London Paris
Tokyo Hong Kong Barcelona Budapest

Homotopy Story in Olver's Book

where

$$R_{jk} = \sum_{\alpha=1}^{q} \sum_{\# I \geq 0} D_I \left\{ Q_\alpha \left(\frac{\tilde{\imath}_j + 1}{\# I + 2} \mathsf{E}_\alpha^{I,j}(P_k) - \frac{\tilde{\imath}_k + 1}{\# I + 2} \mathsf{E}_\alpha^{I,k}(P_j) \right) \right\}.$$

The Lie derivative formula (5.133) takes the form

$$\operatorname{pr} \mathbf{v}_Q(P_k) = \sum_{j=1}^{p} D_j R_{jk} + A_k, \tag{5.136}$$

where A_k is given by (5.129) when $L = \operatorname{Div} P$, which, using (5.130), is

$$A_k = \sum_{\alpha, I} \sum_{l \subset I} \frac{\tilde{\imath}_k + 1}{\# I + 1} D_I[Q_\alpha \mathsf{E}_\alpha^{I,k \setminus l}(P_l)]. \tag{5.137}$$

(We leave to the reader the direct verification of (5.136).)

The proof of (5.133) is perhaps the most complex calculation of this book. (However, the present proof of the exactness of the D-complex is much easier than previous computational proofs!) We begin by analyzing the right-hand side using (5.132):

$$\mathsf{I}_Q(\mathsf{D}\omega) = \sum_{l=1}^{p} \mathsf{I}_Q[D_l(dx^l \wedge \omega)]$$

$$= \sum_{\alpha, I} \sum_{k,l=1}^{p} \frac{\tilde{\imath}_k + 1}{p - r + \# I} D_I \left\{ Q_\alpha \mathsf{E}_\alpha^{I,k} \left[\frac{\partial}{\partial x^k} \lrcorner D_l(dx^l \wedge \omega) \right] \right\}, \tag{5.138}$$

since $\mathsf{D}\omega$ is an $(r + 1)$-form. The principal constituent in (5.138) is the interior summation

$$\sum_{k,l=1}^{p} (\tilde{\imath}_k + 1) \mathsf{E}_\alpha^{I,k} \left[\frac{\partial}{\partial x^k} \lrcorner D_l(dx^l \wedge \omega) \right]$$

$$= \sum_{k,l=1}^{p} (\tilde{\imath}_k + 1) \mathsf{E}_\alpha^{I,k} \left[D_l \left(\frac{\partial}{\partial x^k} \lrcorner (dx^l \wedge \omega) \right) \right], \tag{5.139}$$

which we break into two pieces according to whether $k = l$ or $k \neq l$. If $k \neq l$, then by (5.130), $\mathsf{E}_\alpha^{I,k} \cdot D_l = \mathsf{E}_\alpha^{I \setminus l, k}$, where, by convention, this operator is 0 if l does not appear in I. Also, according to Exercise 1.37,

$$\frac{\partial}{\partial x^k} \lrcorner (dx^l \wedge \omega) = -dx^l \wedge \left(\frac{\partial}{\partial x^k} \lrcorner \omega \right), \qquad k \neq l.$$

We conclude that

$$\mathsf{E}_\alpha^{I,k} \left[\frac{\partial}{\partial x^k} \lrcorner D_l(dx^l \wedge \omega) \right] = -\mathsf{E}_\alpha^{I \setminus l, k} \left[dx^l \wedge \left(\frac{\partial}{\partial x^k} \lrcorner \omega \right) \right] \quad \text{whenever} \quad k \neq l. \tag{5.140}$$

Homotopy Formula in Olver's Book

But these two summations agree upon changing the multi-index summation variable from J to $I = (J, l)$, noting that $\tilde{\imath}_k = \tilde{\jmath}_k + \delta_l^k$, $\#I = \#J + 1$. This completes the proof of (5.133).

We now specialize (5.133) to the case of the scaling vector field $\mathrm{pr}\,\mathbf{v}_u$ introduced earlier in the proof of the exactness of the variational complex. Note that if $P[u] = P(x, u^{(n)})$ is any smooth differential function defined on a vertically star-shaped domain, then

$$\frac{d}{d\lambda} P[\lambda u] = \sum_{\alpha, J} u_J^\alpha \frac{\partial P}{\partial u_J^\alpha}[\lambda u] = \frac{1}{\lambda} \mathrm{pr}\,\mathbf{v}_u(P)[\lambda u],$$

where the notation means that we first apply $\mathrm{pr}\,\mathbf{v}_u$ to P and then evaluate at λu. Integrating, we find

$$P[u] - P[0] = \int_0^1 \mathrm{pr}\,\mathbf{v}_u(P)[\lambda u] \frac{d\lambda}{\lambda},$$

where $P[0] = P(x, 0)$ is a function of x alone. Since $\mathrm{pr}\,\mathbf{v}_u$ acts coefficient-wise on a total differential form $\omega(x, u^{(n)})$, we have the analogous formula

$$\omega[u] - \omega[0] = \int_0^1 \mathrm{pr}\,\mathbf{v}_u(\omega)[\lambda u] \frac{d\lambda}{\lambda}, \tag{5.144}$$

where $\omega[0] = \omega(x, 0)$ is an ordinary differential form on the base space X. If we now use (5.133) in the case $Q = u$, whereby

$$\mathrm{I}_u(\omega) = \sum_{\alpha=1}^{q} \sum_{I} \sum_{k=1}^{p} \frac{\tilde{\imath}_k + 1}{p - r + \#I + 1} D_I \left\{ u^\alpha \mathrm{E}_\alpha^{I,k} \left(\frac{\partial}{\partial x^k} \lrcorner\, \omega \right) \right\}, \tag{5.145}$$

we obtain the homotopy formula

$$\omega[u] - \omega[0] = \mathrm{DH}(\omega) + \mathrm{H}(\mathrm{D}\omega), \tag{5.146}$$

where the *total homotopy operator* is

$$\mathrm{H}(\omega) = \int_0^1 \mathrm{I}_u(\omega)[\lambda u] \frac{d\lambda}{\lambda}, \tag{5.147}$$

meaning that we first evaluate $\mathrm{I}_u(\omega)$ and then replace u by λu wherever it occurs. Except for the extra term $\omega[0]$ this would suffice to prove the exactness of the D-complex. However, $\omega[0]$ is an ordinary differential form on $\Omega = M \cap \{u = 0\}$, so provided Ω is also star-shaped we can use the ordinary Poincaré homotopy operator (1.69), with

$$\omega[0] - \omega_0 = dh(\omega[0]) + h(d\omega[0]), \tag{5.148}$$

where $\omega_0 = 0$ if $r > 0$, while $\omega_0 = f(0)$ if $\omega[0] = f(x)$ is a function, $r = 0$. For such forms, the total derivatives D_i and the partial derivatives $\partial/\partial x^i$ are the same, so we can replace the differential d by the total differential D. Combining (5.146) and (5.148), we obtain

$$\omega - \omega_0 = \mathrm{DH}^*(\omega) + \mathrm{H}^*(\mathrm{D}\omega), \tag{5.149}$$

Zoom into Homotopy Formula in Olver's Book

$$\mathsf{I}_u(\omega) = \sum_{\alpha=1}^{q} \sum_{I} \sum_{k=1}^{p} \frac{\tilde{i}_k + 1}{p - r + \#I + 1} D_I \left\{ u^\alpha \mathsf{E}_\alpha^{I,k} \left(\frac{\partial}{\partial x^k} \lrcorner\, \omega \right) \right\}, \quad (5.145)$$

we obtain the homotopy formula

$$\omega[u] - \omega[0] = \mathsf{DH}(\omega) + \mathsf{H}(\mathsf{D}\omega), \quad (5.146)$$

where the *total homotopy operator* is

$$\mathsf{H}(\omega) = \int_0^1 \mathsf{I}_u(\omega)[\lambda u] \frac{d\lambda}{\lambda}, \quad (5.147)$$

meaning that we first evaluate $\mathsf{I}_u(\omega)$ and then replace u by λu wherever it occurs. Except for the extra term $\omega[0]$ this would suffice to prove the exact-

Homotopy Operator

Recall: Euler's theorem for homogeneous functions

If $f(x_1, x_2, \ldots, x_n)$ is homogeneous of degree p, i.e.,

$$f(\lambda x_1, \lambda x_2, \ldots, \lambda x_n) = \lambda^p \, f(x_1, x_2, \ldots, x_n)$$

then, with g and $\mathcal{P}$ defined as follows

$$g \equiv \mathcal{P} f \equiv \sum_{i=1}^{n} x_i \, \frac{\partial f}{\partial x_i} = p \, f$$

Proof: Differentiate both sides with respect to λ:

$$\sum_{i=1}^{n} \frac{\partial f}{\partial(\lambda x_i)} \, \frac{\partial(\lambda x_i)}{\partial \lambda} = \sum_{i=1}^{n} x_i \, \frac{\partial f}{\partial(\lambda x_i)} = p \lambda^{p-1} \, f$$

and set $\lambda = 1$.

What is the inverse of $\mathcal{P}$?

$f = \mathcal{P}^{-1} g(x_1, x_2, \ldots, x_n) = \int_0^1 g(\lambda x_1, \lambda x_2, \ldots, \lambda x_n)\, \frac{d\lambda}{\lambda}$

Proof:

$$
\begin{aligned}
& \int_0^1 g(\lambda x_1, \lambda x_2, \ldots, \lambda x_n)\, \frac{d\lambda}{\lambda} \\
= \;& \int_0^1 p f(\lambda x_1, \lambda x_2, \ldots, \lambda x_n))\, \frac{d\lambda}{\lambda} \\
= \;& \int_0^1 p \lambda^p\, f(x_1, x_2, \ldots, x_n))\, \frac{d\lambda}{\lambda} \\
= \;& f \int_0^1 p \lambda^{p-1}\, d\lambda = f\, \lambda^p \big|_0^1 = f
\end{aligned}
$$

Sketch of Derivation and Proof

(in 1D with variable x, and for one component u)

Definition: Degree operator $\mathcal{M}$

$$\mathcal{M}f = \sum_{i=0}^{M} u_{ix} \frac{\partial f}{\partial u_{ix}} = u\frac{\partial f}{\partial u} + u_x \frac{\partial f}{\partial u_x} + u_{2x} \frac{\partial f}{\partial u_{2x}} + \cdots + u_{Mx} \frac{\partial f}{\partial u_{Mx}}$$

f is of order M in x

Example: $f[u] = u^p u_x^q u_{3x}^r$ (p, q, r non-negative integers)

$$g[u] \equiv \mathcal{M}f = \sum_{i=0}^{3} u_{ix} \frac{\partial f}{\partial u_{ix}} = (p + q + r)\, u^p u_x^q u_{3x}^r$$

Application of $\mathcal{M}$ computes the total *degree*

Theorem (inverse operator) $\mathcal{M}^{-1} g[u] = \int_0^1 g[\lambda u]\, \frac{d\lambda}{\lambda}$

Proof:

$$\frac{d}{d\lambda} g[\lambda u] = \sum_{i=0}^{M} \frac{\partial g[\lambda u]}{\partial \lambda u_{ix}} \frac{d\lambda u_{ix}}{d\lambda} = \frac{1}{\lambda} \sum_{i=0}^{M} u_{ix} \frac{\partial g[\lambda u]}{\partial u_{ix}} = \frac{1}{\lambda} \mathcal{M} g[\lambda u]$$

Integrate both sides with respect to λ

$$\begin{aligned} \int_0^1 \frac{d}{d\lambda} g[\lambda u]\, d\lambda &= g[\lambda u]\Big|_{\lambda=0}^{\lambda=1} = g[u] - g[0] \\ &= \int_0^1 \mathcal{M} g[\lambda u]\, \frac{d\lambda}{\lambda} = \mathcal{M} \int_0^1 g[\lambda u]\, \frac{d\lambda}{\lambda} \end{aligned}$$

Assuming $g[0] = 0$,

$$\mathcal{M}^{-1} g[u] = \int_0^1 g[\lambda u]\, \frac{d\lambda}{\lambda}$$

Example:

If $g[u] = (p+q+r)\, u^p u_x^q u_{3x}^r$, then

$$g[\lambda u] = (p+q+r)\lambda^{p+q+r}\, u^p u_x^q u_{3x}^r$$

Hence,

$$\begin{aligned} \mathcal{M}^{-1} g[u] &= \int_0^1 (p+q+r)\, \lambda^{p+q+r-1}\, u^p u_x^q u_{3x}^r \, d\lambda \\ &= u^p u_x^q u_{3x}^r \;\; \lambda^{p+q+r} \Big|_{\lambda=0}^{\lambda=1} = u^p u_x^q u_{3x}^r \end{aligned}$$

Note: Idea comes from converse part of Poincaré Lemma (closed forms are exact on contractable domains)

Theorem: If f is an exact differential function, then

$$F = \mathcal{D}_x^{-1} f = \int f \, dx = \mathcal{H}_{u(x)} f$$

Proof: Multiply

$$\mathcal{L}_{u(x)} \, f = \sum_{k=0}^{M} (-\mathcal{D}_x)^k \frac{\partial f}{\partial u_{kx}}$$

by u to restore the degree.

Split off $u \frac{\partial f}{\partial u}$. Integrate by parts.

Split off $u_x \frac{\partial f}{\partial u_x}$. Repeat the process.

Lastly, split off $u_{Mx} \frac{\partial f}{\partial u_{Mx}}$.

$$u\mathcal{L}_{u(x)}f = u\sum_{k=0}^{M}(-\mathcal{D}_x)^k\frac{\partial f}{\partial u_{kx}}$$

$$= \; u\frac{\partial f}{\partial u} - \mathcal{D}_x\left(u\sum_{k=1}^{M}(-\mathcal{D}_x)^{k-1}\frac{\partial f}{\partial u_{kx}}\right) + u_x\sum_{k=1}^{M}(-\mathcal{D}_x)^{k-1}\frac{\partial f}{\partial u_{kx}}$$

$$= \; u\frac{\partial f}{\partial u} + u_x\frac{\partial f}{\partial u_x} - \mathcal{D}_x\left(u\sum_{k=1}^{M}(-\mathcal{D}_x)^{k-1}\frac{\partial f}{\partial u_{kx}}\right.$$

$$\left. + u_x\sum_{k=2}^{M}(-\mathcal{D}_x)^{k-2}\frac{\partial f}{\partial u_{kx}}\right) + u_{2x}\sum_{k=2}^{M}(-\mathcal{D}_x)^{k-2}\frac{\partial f}{\partial u_{kx}}$$

$$= \; \ldots$$

$$
\begin{aligned}
&= u\frac{\partial f}{\partial u} + u_x\frac{\partial f}{\partial u_x} + \ldots + u_{Mx}\frac{\partial f}{\partial u_{Mx}} \\
&\quad -\mathcal{D}_x\left(u\sum_{k=1}^{M}(-\mathcal{D}_x)^{k-1}\frac{\partial f}{\partial u_{kx}} + u_x\sum_{k=2}^{M}(-\mathcal{D}_x)^{k-2}\frac{\partial f}{\partial u_{kx}}\right. \\
&\quad \left. + \ldots + u_{(M-1)x}\sum_{k=M}^{M}(-\mathcal{D}_x)^{k-M}\frac{\partial f}{\partial u_{kx}}\right) \\
&= \sum_{i=0}^{M} u_{ix}\frac{\partial f}{\partial u_{ix}} - \mathcal{D}_x\left(\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right) \\
&= \mathcal{M}f - \mathcal{D}_x\left(\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right) \\
&= 0
\end{aligned}
$$

$$\mathcal{M}f = \mathcal{D}_x \left(\sum_{i=0}^{M-1} u_{ix} \sum_{k=i+1}^{M} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right)$$

Apply $\mathcal{M}^{-1}$ and use $\mathcal{M}^{-1}\mathcal{D}_x = \mathcal{D}_x \mathcal{M}^{-1}$.

$$f = \mathcal{D}_x \left(\mathcal{M}^{-1} \sum_{i=0}^{M-1} u_{ix} \sum_{k=i+1}^{M} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right)$$

Apply $\mathcal{D}_x^{-1}$ and use the formula for $\mathcal{M}^{-1}$.

$$\begin{aligned} F &= \mathcal{D}_x^{-1} f = \int_0^1 \left(\sum_{i=0}^{M-1} u_{ix} \sum_{k=i+1}^{M} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right) [\lambda u] \, \frac{d\lambda}{\lambda} \\ &= \int_0^1 \left(\sum_{k=1}^{M} \left(\sum_{i=0}^{k-1} u_{ix} (-\mathcal{D}_x)^{k-(i+1)} \right) \frac{\partial f}{\partial u_{kx}} \right) [\lambda u] \, \frac{d\lambda}{\lambda} \\ &= \mathcal{H}_{u(x)} f \end{aligned}$$

Early Work by Kruskal and Collaborators

JOURNAL OF MATHEMATICAL PHYSICS VOLUME 11, NUMBER 3 MARCH 1970

Korteweg–deVries Equation and Generalizations. V. Uniqueness and Nonexistence of Polynomial Conservation Laws

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The conservation laws derived in an earlier paper for the Korteweg–deVries equation are proved to be the only ones of polynomial form. An algebraic operator formalism is developed to obtain explicit formulas for them.

Zoom into the formula for computation of fluxes

We apply $\mathcal{M}^{-1}$ and note that $\mathcal{M}^{-1}\mathcal{M}P = P$ because only constant terms are annihilated by $\mathcal{M}$, and P has none. Furthermore $\mathcal{M}^{-1}$ commutes with $\mathfrak{D}$: for, by (13), $\mathcal{M}(= \mathfrak{D}_0)$ does, so that

$$\mathcal{M}^{-1}(\mathcal{M}\mathfrak{D})\mathcal{M}^{-1} = \mathcal{M}^{-1}(\mathfrak{D}\mathcal{M})\mathcal{M}^{-1},$$

while $\mathcal{M}^{-1}\mathcal{M} = \mathcal{M}\mathcal{M}^{-1}$ is the identity operator except for constant terms, which, by (8), do not occur in derivatives and are annihilated by $\mathfrak{D}$. Thus we have

$$P = \mathfrak{D}\left(\mathcal{M}^{-1}\sum_j u_j \sum_{i=j+1}^{\infty} (-\mathfrak{D})^{i-j-1}\partial_i P\right). \qquad (22)$$

Note that the infinite summations are (formally) well defined since we could have worked with derivative index slices, in each instance of which the summations would obviously be finite. For the same reason, if P is a polynomial, so is the expression in brackets. ∎

Application of Homotopy Operator in 1D

Example:

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

Goal: Find

$$F = 4\, v_x^2 + u_x^2\, \cos u - 3\, v^2\, \cos u$$

Easy to verify: $f = \mathrm{D}_x F$

- Compute

$$\begin{aligned} I_u\, f &= u \frac{\partial f}{\partial u_x} + (u_x \mathrm{I} - u \mathrm{D}_x) \frac{\partial f}{\partial u_{xx}} \\ &= -u u_x^2 \sin u + 3u v^2 \sin u + 2u_x^2 \cos u \end{aligned}$$

- Similarly,

$$I_v\, f = v\frac{\partial f}{\partial v_x} + (v_x \mathrm{I} - v \mathrm{D}_x)\frac{\partial f}{\partial v_{xx}}$$
$$= -6v^2 \cos u + 8v_x^2$$

- Finally,

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

Application of Homotopy Operator in 2D

- **Application 1: Undo a Divergence**

  Given: $f = u_x v_y - u_{xx} v_y - u_y v_x + u_{xy} v_x$

  By hand: $\tilde{\mathbf{F}} = (u v_y - u_x v_y, -u v_x + u_x v_x)$

  Easy to verify: $f = \mathrm{Div}\, \tilde{\mathbf{F}}$

- Compute $\mathrm{Div}^{-1} f$

$$
\begin{aligned}
I_u^{(x)} f \;&=\; u \frac{\partial f}{\partial u_x} + (u_x \mathrm{I} - u \mathrm{D}_x) \frac{\partial f}{\partial u_{xx}} \\
&\quad + \left(\tfrac{1}{2} u_y \mathrm{I} - \tfrac{1}{2} u \mathrm{D}_y \right) \frac{\partial f}{\partial u_{xy}} \\
&=\; u v_y + \tfrac{1}{2} u_y v_x - u_x v_y + \tfrac{1}{2} u v_{xy}
\end{aligned}
$$

- Similarly,

$$I_v^{(x)} f = v \frac{\partial f}{\partial v_x} = -u_y v + u_{xy} v$$

- Hence,

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

- Analogously,

$$F_2 = \mathcal{H}^{(y)}_{\mathbf{u}(x,y)} f = \int_0^1 \left(I_u^{(y)} f + I_v^{(y)} f \right) [\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$$
$$= \int_0^1 \left(\lambda \left(-u v_x - \tfrac{1}{2} u v_{xx} + \tfrac{1}{2} u_x v_x \right) + \lambda \left(u_x v - u_{xx} v \right) \right) d\lambda$$
$$= -\tfrac{1}{2} u v_x - \tfrac{1}{4} u v_{xx} + \tfrac{1}{4} u_x v_x + \tfrac{1}{2} u_x v - \tfrac{1}{2} u_{xx} v$$

- So,

$$\mathbf{F} = \frac{1}{4} \begin{pmatrix} 2 u v_y + u_y v_x - 2 u_x v_y + u v_{xy} - 2 u_y v + 2 u_{xy} v \\ -2 u v_x - u v_{xx} + u_x v_x + 2 u_x v - 2 u_{xx} v \end{pmatrix}$$

Let $\mathbf{K} = \tilde{\mathbf{F}} - \mathbf{F}$ then

$$\mathbf{K} = \frac{1}{4}\begin{pmatrix} 2uv_y - u_y v_x - 2u_x v_y - uv_{xy} + 2u_y v - 2u_{xy} v \\ -2uv_x + uv_{xx} + 3u_x v_x - 2u_x v + 2u_{xx} v \end{pmatrix}$$

then $\mathrm{Div}\,\mathbf{K} = 0$

- Also, $\mathbf{K} = (\mathrm{D}_y \phi, -\mathrm{D}_x \phi)$ with $\phi = \frac{1}{4}(2uv - uv_x - 2u_x v)$

  ($curl$ in 2D)

  After removing the curl term $\mathbf{K}$:

$$\tilde{\mathbf{F}} = \mathbf{F} + \mathbf{K} = (uv_y - u_x v_y, -uv_x + u_x v_x)$$

Avoid curl terms algorithmically!

Application 2: Zakharov-Kuznetsov Equation
Computation of Conservation Laws

$$\boxed{u_t + \alpha u u_x + \beta(u_{xx} + u_{yy})_x = 0}$$

- Step 1: Compute the dilation invariance

  ZK equation is invariant under scaling symmetry

$$(t, x, y, u) \to (\frac{t}{\lambda^3}, \frac{x}{\lambda}, \frac{y}{\lambda}, \lambda^2 u) = (\tilde{t}, \tilde{x}, \tilde{y}, \tilde{u})$$

  λ is an arbitrary parameter.

- Hence, the weights of the variables are

$$W(u) = 2, \;\; W(\mathrm{D}_t) = 3, \;\; W(\mathrm{D}_x) = 1, \;\; W(\mathrm{D}_y) = 1.$$

- A conservation law is invariant under the scaling symmetry of the PDE.

$$W(u) = 2, \;\; W(\mathrm{D}_t) = 3, \;\; W(\mathrm{D}_x) = 1, \;\; W(\mathrm{D}_y) = 1.$$

For example,

$$\mathrm{D}_t\Big(u^3 - \tfrac{3\beta}{\alpha}(u_x^2 + u_y^2)\Big) + \mathrm{D}_x\Big(3u^2(\tfrac{\alpha}{4}u^2 + \beta u_{xx}) - 6\beta u(u_x^2 + u_y^2)$$
$$+ \tfrac{3\beta^2}{\alpha}(u_{xx}^2 - u_{xy}^2) - \tfrac{6\beta^2}{\alpha}(u_x(u_{xxx} + u_{xyy}) + u_y(u_{xxy} + u_{yyy}))\Big)$$
$$+ \mathrm{D}_y\Big(3\beta u^2 u_{xy} + \tfrac{6\beta^2}{\alpha}u_{xy}(u_{xx} + u_{yy})\Big) \doteq 0$$

Rank (ρ) = 6, Rank (J) = 8.

Rank (conservation law) = 9.

Compute the density of selected **rank**, say, 6.

- Step 2: Construct the candidate density

For example, construct a density of rank 6.

Make a list of all terms with rank 6:

$$\{u^3, u_x^2, uu_{xx}, u_y^2, uu_{yy}, u_x u_y, uu_{xy}, u_{4x}, u_{3xy}, u_{2x2y}, u_{x3y}, u_{4y}\}$$

Remove divergences and divergence-equivalent terms.

Candidate density of rank 6:

$$\boxed{\rho = c_1 u^3 + c_2 u_x^2 + c_3 u_y^2 + c_4 u_x u_y}$$

- Step 3: Compute the undetermined coefficients

Compute

$$
\begin{aligned}
\mathrm{D}_t \rho &= \frac{\partial \rho}{\partial t} + \rho'(u)[u_t] \\
&= \frac{\partial \rho}{\partial t} + \sum_{k=0}^{M_x} \sum_{\ell=0}^{M_y} \frac{\partial \rho}{\partial u_{kx\,\ell y}} \mathrm{D}_x^k \, \mathrm{D}_y^\ell \, u_t \\
&= \Big(3c_1 u^2 \mathrm{I} + 2c_2 u_x \mathrm{D}_x + 2c_3 u_y \mathrm{D}_y + c_4 (u_y \mathrm{D}_x + u_x \mathrm{D}_y) \Big) u_t
\end{aligned}
$$

Substitute $u_t = -\Big(\alpha u u_x + \beta (u_{xx} + u_{yy})_x\Big).$

$$
\begin{aligned}
E \;=\; & -\mathrm{D}_t \rho \doteq 3c_1 u^2(\alpha u u_x + \beta(u_{xx} + u_{xy})_x) \\
& + 2c_2 u_x(\alpha u u_x + \beta(u_{xx} + u_{yy})_x)_x + 2c_3 u_y(\alpha u u_x \\
& + \beta(u_{xx} + u_{yy})_x)_y + c_4(u_y(\alpha u u_x + \beta(u_{xx} + u_{yy})_x)_x \\
& + u_x(\alpha u u_x + \beta(u_{xx} + u_{yy})_x)_y)
\end{aligned}
$$

Apply the Euler operator (variational derivative)

$$
\mathcal{L}_{u(x,y)} E = \sum_{k=0}^{M_x} \sum_{\ell=0}^{M_y} (-\mathrm{D}_x)^k (-\mathrm{D}_y)^\ell \frac{\partial E}{\partial u_{kx\,\ell y}}
$$

$$
\begin{aligned}
= & -2\Big((3c_1\beta + c_3\alpha)u_x u_{yy} + 2(3c_1\beta + c_3\alpha)u_y u_{xy} \\
& + 2c_4\alpha u_x u_{xy} + c_4\alpha u_y u_{xx} + 3(3c_1\beta + c_2\alpha)u_x u_{xx}\Big) \\
\equiv & \; 0
\end{aligned}
$$

Solve a parameterized linear system for the c_i:

$$3c_1\beta + c_3\alpha = 0, \quad c_4\alpha = 0, \quad 3c_1\beta + c_2\alpha = 0$$

Solution:

$$c_1 = 1, \quad c_2 = -\frac{3\beta}{\alpha}, \quad c_3 = -\frac{3\beta}{\alpha}, \quad c_4 = 0$$

Substitute the solution into the candidate density

$$\rho = c_1 u^3 + c_2 u_x^2 + c_3 u_y^2 + c_4 u_x u_y$$

Final density of rank 6:

$$\boxed{\rho = u^3 - \frac{3\beta}{\alpha}(u_x^2 + u_y^2)}$$

- Step 4: Compute the flux

Use the homotopy operator to invert Div:

$$\mathbf{J} = \mathrm{Div}^{-1} E = \left(\mathcal{H}^{(x)}_{u(x,y)} E,\ \mathcal{H}^{(y)}_{u(x,y)} E\right)$$

where
$$\mathcal{H}^{(x)}_{u(x,y)} E = \int_0^1 (I^{(x)}_u E)[\lambda u]\, \frac{d\lambda}{\lambda}$$

with
$$\mathcal{I}^{(x)}_u E \;=\; \sum_{k=1}^{M_x} \sum_{\ell=0}^{M_y} \Bigg(\sum_{i=0}^{k-1} \sum_{j=0}^{\ell} u_{ix\,jy} \frac{\binom{i+j}{i} \binom{k+\ell-i-j-1}{k-i-1}}{\binom{k+\ell}{k}}$$
$$(-\mathrm{D}_x)^{k-i-1} \, (-\mathrm{D}_y)^{\ell-j} \Bigg) \frac{\partial E}{\partial u_{kx\,\ell y}}$$

Similar formulas for $\mathcal{H}^{(y)}_{u(x,y)} E$ and $\mathcal{I}^{(y)}_u E$.

Let $A = \alpha u u_x + \beta(u_{xxx} + u_{xyy})$ so that

$$E = 3u^2 A - \frac{6\beta}{\alpha} u_x A_x - \frac{6\beta}{\alpha} u_y A_y$$

Then,

$$\begin{aligned}
\mathbf{J} &= \left(\mathcal{H}^{(x)}_{u(x,y)} E, \, \mathcal{H}^{(y)}_{u(x,y)} E\right) \\
&= \Big(\tfrac{3\alpha}{4} u^4 + \beta u^2(3u_{xx} + 2u_{yy}) - 2\beta u(3u_x^2 + u_y^2) \\
&\qquad + \tfrac{3\beta^2}{4\alpha} u(u_{2x2y} + u_{4y}) - \tfrac{\beta^2}{\alpha} u_x(\tfrac{7}{2}u_{xyy} + 6u_{xxx}) \\
&\qquad - \tfrac{\beta^2}{\alpha} u_y(4u_{xxy} + \tfrac{3}{2}u_{yyy}) + \tfrac{\beta^2}{\alpha}(3u_{xx}^2 + \tfrac{5}{2}u_{xy}^2 + \tfrac{3}{4}u_{yy}^2) \\
&\qquad + \tfrac{5\beta^2}{4\alpha} u_{xx} u_{yy}, \quad \beta u^2 u_{xy} - 4\beta u u_x u_y \\
&\qquad - \tfrac{3\beta^2}{4\alpha} u(u_{x3y} + u_{3xy}) - \tfrac{\beta^2}{4\alpha} u_x(13u_{xxy} + 3u_{yyy}) \\
&\qquad - \tfrac{5\beta^2}{4\alpha} u_y(u_{xxx} + 3u_{xyy}) + \tfrac{9\beta^2}{4\alpha} u_{xy}(u_{xx} + u_{yy})\Big)
\end{aligned}$$

PART II: DISCRETE CASE
Motivation, Problem Statement, Example

Conservation Laws for Nonlinear DDEs

- System of DDEs

$$\dot{\mathbf{u}}_n = \mathbf{F}(\cdots, \mathbf{u}_{n-1}, \mathbf{u}_n, \mathbf{u}_{n+1}, \cdots)$$

with $\mathbf{u}_n = (u_n, v_n, w_n, \ldots)$

- Conservation law in $(1+1)$ dimensions

$$\boxed{\mathrm{D}_t \rho_n + \Delta J_n = \mathrm{D}_t \rho_n + J_{n+1} - J_n \doteq 0}$$

conserved density ρ_n and flux J_n

- Example: **Toda lattice**

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

- First few densities-flux pairs for Toda lattice:

$$\rho_n^{(0)} = \ln(v_n) \qquad J_n^{(0)} = u_n$$

$$\rho_n^{(1)} = u_n \qquad J_n^{(1)} = v_{n-1}$$

$$\rho_n^{(2)} = \frac{1}{2}u_n^2 + v_n \qquad J_n^{(2)} = u_n v_{n-1}$$

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

Mathematica has no function to compute Δ^{-1}

Problem Statement

Discrete case in 1D:

Example:

$$f_n = -u_n u_{n+1} v_n - v_n^2 + u_{n+1} u_{n+2} v_{n+1} + v_{n+1}^2 + u_{n+3} v_{n+2} - u_{n+1} v_n$$

Question: Can the expression be summed by parts?

If yes, find $F_n = \Delta^{-1} f_n$ (so, $f_n = \Delta F_n = F_{n+1} - F_n$)

Result (by hand):

$$F_n = v_n^2 + u_n u_{n+1} v_n + u_{n+1} v_n + u_{n+2} v_{n+1}$$

How can this be done algorithmically?

Can this be done as in the continuous case?

Tools from the Discrete Calculus of Variations

- Definitions:

D is the up-shift (forward or right-shift) operator

$$\mathrm{D}F_n = F_{n+1} = F_{n|_{n \to n+1}}$$

D^{-1} the down-shift (backward or left-shift) operator

$$\mathrm{D}^{-1}F_n = F_{n-1} = F_{n|_{n \to n-1}}$$

$\Delta = \mathrm{D} - \mathrm{I}$ is the forward difference operator

$$\Delta F_n = (\mathrm{D} - \mathrm{I})F_n = F_{n+1} - F_n$$

- Problem to be solved: Given f_n.

  Find $F_n = \Delta^{-1} f_n$ (so $f_n = \Delta F_n = F_{n+1} - F_n$)

Analogy Continuous & Discrete Cases

Euler Operators

Continuous Case	Discrete Case
$\mathcal{L}_{\mathbf{u}(x)} = \sum_{k=0}^{M} (-\mathrm{D}_x)^k \frac{\partial}{\partial \mathbf{u}_{k\,x}}$	$\mathcal{L}_{\mathbf{u}_n} = \sum_{k=0}^{M} \mathrm{D}^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}} = \frac{\partial}{\partial \mathbf{u}_n} \sum_{k=0}^{M} \mathrm{D}^{-k}$

Analogy Continuous & Discrete Cases

Homotopy Operators & Integrands

Continuous Case	Discrete Case
$\mathcal{H}_{\mathbf{u}(x)} f = \int_0^1 \sum_{j=1}^{N} (I_{u^{(j)}} f)[\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$	$\mathcal{H}_{\mathbf{u}_n} f_n = \int_0^1 \sum_{j=1}^{N} (I_{u_n^{(j)}} f_n)[\lambda \mathbf{u}_n] \frac{d\lambda}{\lambda}$
$I_{u^{(j)}} f = \sum_{k=1}^{M^{(j)}} \left(\sum_{i=0}^{k-1} u_{ix}^{(j)} \, (-\mathcal{D}_x)^{k-(i+1)} \right) \frac{\partial f}{\partial u_{kx}^{(j)}}$	$I_{u_n^{(j)}} f_n = \sum_{k=1}^{M^{(j)}} \left(\sum_{i=1}^{k} \mathcal{D}^{-i} \right) u_{n+k}^{(j)} \frac{\partial f_n}{\partial u_{n+k}^{(j)}}$

Euler Operators Side by Side

Continuous Case (for component u)

$$\mathcal{L}_u = \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial}{\partial u_{2x}} - \mathrm{D}_x^3 \frac{\partial}{\partial u_{3x}} + \cdots$$

Discrete Case (for component u_n)

$$\begin{aligned} \mathcal{L}_{u_n} &= \frac{\partial}{\partial u_n} + \mathrm{D}^{-1} \frac{\partial}{\partial u_{n+1}} + \mathrm{D}^{-2} \frac{\partial}{\partial u_{n+2}} + \mathrm{D}^{-3} \frac{\partial}{\partial u_{n+3}} + \cdots \\ &= \frac{\partial}{\partial u_n} (\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3} + \cdots) \end{aligned}$$

Homotopy Operators Side by Side

Continuous Case (for components u and v)

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

with

$$I_u\, f = \sum_{k=1}^{M^{(1)}} \left(\sum_{i=0}^{k-1} u_{ix} \, (-\mathcal{D}_x)^{k-(i+1)} \right) \frac{\partial f}{\partial u_{kx}}$$

and

$$I_v\, f = \sum_{k=1}^{M^{(2)}} \left(\sum_{i=0}^{k-1} v_{ix} \, (-\mathcal{D}_x)^{k-(i+1)} \right) \frac{\partial f}{\partial v_{kx}}$$

Discrete Case (for components u_n and v_n)

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

with

$$I_{u_n} f_n = \sum_{k=1}^{M^{(1)}} \left(\sum_{i=1}^{k} \mathrm{D}^{-i} \right) u_{n+k} \frac{\partial f_n}{\partial u_{n+k}}$$

and

$$I_{v_n} f_n = \sum_{k=1}^{M^{(2)}} \left(\sum_{i=1}^{k} \mathrm{D}^{-i} \right) v_{n+k} \frac{\partial f_n}{\partial v_{n+k}}$$

Analogy of Definitions & Theorems

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

- Definition: f_n is exact iff $f_n = \Delta\, F_n = F_{n+1} - F_n$
- Theorem (exactness test): $f_n = \Delta F_n$ iff $\mathcal{L}_{\mathbf{u}_n} f_n \equiv 0$
- Theorem (summation with homotopy operator):

  If f_n is exact then $F_n = \Delta^{-1} f_n = \mathcal{H}_{\mathbf{u}_n}(f_n)$

Testing Exactness – Discrete Case

$$f_n = -u_n u_{n+1} v_n - v_n^2 + u_{n+1} u_{n+2} v_{n+1} + v_{n+1}^2 + u_{n+3} v_{n+2} - u_{n+1} v_n$$

- f_n is exact
- After summation by parts (done by hand):

$$F_n = v_n^2 + u_n u_{n+1} v_n + u_{n+1} v_n + u_{n+2} v_{n+1}$$

Easy to verify: $f_n = \Delta\, F_n = F_{n+1} - F_n$

- Exactness test with Euler operator:

For component u_n (highest shift 3):

$$\begin{aligned}\mathcal{L}_{u_n} f_n &= \frac{\partial}{\partial u_n}\left(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3}\right) f_n \\ &= -u_{n+1}v_n - u_{n-1}v_{n-1} + u_{n+1}v_n - v_{n-1} \\ &\quad + u_{n-1}v_{n-1} + v_{n-1} \\ &\equiv 0\end{aligned}$$

Similarly,

$$\begin{aligned}\mathcal{L}_{v_n} f_n &= \frac{\partial}{\partial v_n}\left(\mathrm{I} + \mathrm{D}^{-1}\right) f_n \\ &= u_n u_{n+1} + 2v_n - u_n u_{n+1} - 2v_n \\ &\equiv 0\end{aligned}$$

Application of Discrete Homotopy Operator

$$f_n = -u_n u_{n+1} v_n - v_n^2 + u_{n+1} u_{n+2} v_{n+1} + v_{n+1}^2 + u_{n+3} v_{n+2} - u_{n+1} v_n$$

Here, $M^{(1)} = 3$ and $M^{(2)} = 2$.

Compute

$$\begin{aligned} I_{u_n} f_n &= (\mathrm{D}^{-1})\, u_{n+1} \frac{\partial f_n}{\partial u_{n+1}} \\ &\quad + (\mathrm{D}^{-1} + \mathrm{D}^{-2})\, u_{n+2} \frac{\partial f_n}{\partial u_{n+2}} \\ &\quad + (\mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3})\, u_{n+3} \frac{\partial f_n}{\partial u_{n+3}} \\ &= 2u_n u_{n+1} v_n + u_{n+1} v_n + u_{n+2} v_{n+1} \end{aligned}$$

$$
\begin{aligned}
I_{v_n}\, f_n &= (\mathrm{D}^{-1})\, v_{n+1}\, \frac{\partial f_n}{\partial v_{n+1}} \\
&\quad + (\mathrm{D}^{-1} + \mathrm{D}^{-2})\, v_{n+2}\, \frac{\partial f_n}{\partial v_{n+2}} \\
&= u_n u_{n+1} v_n + 2v_n^2 + u_{n+1} v_n + u_{n+2} v_{n+1}
\end{aligned}
$$

Finally,

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

Application: Computation of Conservation Laws

- Conservation law:

$$\boxed{\mathrm{D}_t \rho_n + \Delta\, J_n = \mathrm{D}_t \rho_n + J_{n+1} - J_n \doteq 0}$$

conserved density ρ_n and flux J_n

- Example: Toda lattice

$$\begin{aligned} \dot{u}_n &= v_{n-1} - v_n \\ \dot{v}_n &= v_n (u_n - u_{n+1}) \end{aligned}$$

- Typical density-flux pair:

$$\begin{aligned} \rho_n^{(3)} &= \tfrac{1}{3} u_n^3 + u_n (v_{n-1} + v_n) \\ J_n^{(3)} &= u_{n-1} u_n v_{n-1} + v_{n-1}^2 \end{aligned}$$

Computation Conservation Laws for Toda Lattice

Step 1: Construct the form of the density

The Toda lattice is invariant under scaling symmetry

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

Construct a candidate density, for example,

$$\rho_n = c_1 \, u_n^3 + c_2 \, u_n v_{n-1} + c_3 \, u_n v_n$$

which is scaling invariant under the symmetry

Step 2: Determine the constants c_i

Compute $E_n = \mathrm{D}_t \rho_n$ and evaluate on DDE

$$E_n \ = \ (3c_1 - c_2) u_n^2 v_{n-1} + (c_3 - 3c_1) u_n^2 v_n + (c_3 - c_2) v_{n-1} v_n \\ + c_2 u_{n-1} u_n v_{n-1} + c_2 v_{n-1}^2 - c_3 u_n u_{n+1} v_n - c_3 v_n^2$$

Compute $\tilde{E}_n = \mathrm{D} E_n$ to remove negative shift $n-1$

Require that $\mathcal{L}_{u_n} \tilde{E}_n = \mathcal{L}_{v_n} \tilde{E}_n \equiv 0$

Solution: $c_1 = \frac{1}{3}, c_2 = c_3 = 1$ gives

$$\boxed{\rho_n = \rho_n^{(3)} = \frac{1}{3}\, u_n^3 + u_n(v_{n-1} + v_n)}$$

Step 3: Compute the flux J_n

$$\tilde{E}_n = \mathrm{D} E_n = u_n u_{n+1} v_n + v_n^2 - u_{n+1} u_{n+2} v_{n+1} - v_{n+1}^2$$

Apply the homotopy operator

$$\tilde{J}_n = \mathrm{D} J_n = -\Delta^{-1}(\tilde{E}_n) = -\mathcal{H}_{\mathbf{u}_n}(\tilde{E}_n)$$

Compute

$$\begin{aligned} I_{u_n} \tilde{E}_n &= (\mathrm{D}^{-1})\, u_{n+1} \frac{\partial \tilde{E}_n}{\partial u_{n+1}} + (\mathrm{D}^{-1} + \mathrm{D}^{-2})\, u_{n+2} \frac{\partial \tilde{E}_n}{\partial u_{n+2}} \\ &= -2 u_n u_{n+1} v_n \end{aligned}$$

Likewise,

$$I_{v_n} \tilde{E}_n = (\mathrm{D}^{-1})\, v_{n+1} \frac{\partial \tilde{E}_n}{\partial v_{n+1}} = -(u_n u_{n+1} v_n + 2 v_n^2)$$

Next, compute

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

Finally, backward shift $J_n = \mathrm{D}^{-1}(\tilde{J}_n)$ given

$$\boxed{J_n = J_n^{(3)} = u_{n-1} u_n v_{n-1} + v_{n-1}^2}$$

Conclusions and Future Work

- The power of Euler and homotopy operators:
  - Testing exactness
  - Integration by parts: D_x^{-1} and Div^{-1}
- Integration of non-exact expressions

  Example: $f = u_x v + u v_x + u^2 u_{xx}$

  $\int f\, dx = uv + \int u^2 u_{xx}\, dx$
- Use other homotopy formulas (moving terms amongst the components of the flux; prevent curl terms)

- Homotopy operator approach pays off for computing irrational fluxes

  Example: short pulse equation (nonlinear optics)

$$u_{xt} = u + (u^3)_{xx} = u + 6uu_x^2 + 3u^2u_{xx}$$

  with non-polynomial conservation law

$$\mathrm{D}_t \left(\sqrt{1+6u_x^2}\right) - \mathrm{D}_x \left(3u^2\sqrt{1+6u_x^2}\right) \doteq 0$$

- Continue the implementation in *Mathematica*
- Software: http://inside.mines.edu/∼whereman

Thank You

Publications

1. D. Poole and W. Hereman, Symbolic computation of conservation laws for nonlinear partial differential equations in multiple space dimensions, J. Symb. Comp. **46**(12), 1355-1377 (2011).

2. W. Hereman, P. J. Adams, H. L. Eklund, M. S. Hickman, and B. M. Herbst, Direct Methods and Symbolic Software for Conservation Laws of Nonlinear Equations, In: Advances of Nonlinear Waves and Symbolic Computation, Ed.: Z. Yan, Nova Science Publishers, New York (2009), Chapter 2, pp. 19-79.

3. W. Hereman, M. Colagrosso, R. Sayers, A. Ringler, B. Deconinck, M. Nivala, and M. S. Hickman, Continuous and Discrete Homotopy Operators and the Computation of Conservation Laws. In: Differential Equations with Symbolic Computation, Eds.: D. Wang and Z. Zheng, Birkhäuser Verlag, Basel (2005), Chapter 15, pp. 249-285.

4. W. Hereman, B. Deconinck, and L. D. Poole, Continuous and discrete homotopy operators: A theoretical approach made concrete, Math. Comput. Simul. **74**(4-5), 352-360 (2007).

5. W. Hereman, Symbolic computation of conservation laws of nonlinear partial differential equations in multi-dimensions, Int. J. Quan. Chem. **106**(1), 278-299 (2006).