Continuous and Discrete Homotopy Operators:

A Theoretical Approach Made Concrete and Applicable

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Outline

Part I: Continuous Case

- Calculus-based formulas for the continuous homotopy operator (in multi-dimensions)
- 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

- Simple formula for the homotopy operator
- Symbolic summation by parts and inversion of the forward difference operator
- Analogy: continuous and discrete formulas
- Application: symbolic computation of conservation laws of nonlinear DDEs
- Demonstration of ConservationLawsMD.m
- Demonstration of DDEDensityFlux.m
- Conclusions

Motivation of the Research

Conservation Laws for Nonlinear PDEs

ullet 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

$$D_t \rho + D_x J = 0$$

evaluated on the PDE.

Conserved density ρ and flux J.

Conservation law in (2+1)-dimensions

$$D_t \rho + \nabla \cdot \mathbf{J} = D_t \rho + D_x J_1 + D_y J_2 = 0$$

evaluated on the PDE.

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

Conservation law in (3+1)-dimensions

$$D_t \rho + \nabla \cdot \mathbf{J} = D_t \rho + D_x J_1 + D_y J_2 + D_z J_3 = 0$$

evaluated on the PDE.

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

Notation – Computations on the Jet Space

- Independent variables $\mathbf{x} = (x, y, z)$
- Dependent variables $\mathbf{u}=(u^{(1)},u^{(2)},\dots,u^{(j)},\dots,u^{(N)})$ In examples: $\mathbf{u}=(u,v,\theta,h,\dots)$
- Partial derivatives $u_{kx}=\frac{\partial^k u}{\partial x^k},\ u_{kx\,ly}=\frac{\partial^{k+l} u}{\partial x^k y^l},\ \text{etc.}$ 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: $f = uvv_x + x^2u_x^3v_x + u_xv_{xx}$

• Total derivatives: D_t , D_x , D_y , . . .

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

$$D_x f = \frac{\partial f}{\partial x} + u_x \frac{\partial f}{\partial u} + u_{xx} \frac{\partial f}{\partial u_x}$$

$$+ v_x \frac{\partial f}{\partial v} + v_{xx} \frac{\partial f}{\partial v_x} + v_{xxx} \frac{\partial f}{\partial v_{xx}}$$

$$= 2xu_x^3 v_x + u_x (vv_x) + u_{xx} (3x^2 u_x^2 v_x + v_{xx})$$

$$+ v_x (uv_x) + v_{xx} (uv + x^2 u_x^3) + v_{xxx} (u_x)$$

$$= 2xu_x^3 v_x + vu_x v_x + 3x^2 u_x^2 v_x u_{xx} + u_{xx} v_{xx}$$

$$+ uv_x^2 + uvv_{xx} + x^2 u_x^3 v_{xx} + u_x v_{xxx}$$

An Example in (2+1) Dimensions

- Example: Shallow water wave (SWW) equations
 - [P. Dellar, Phys. Fluids 15 (2003) 292-297]

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} + 2\mathbf{\Omega} \times \mathbf{u} + \nabla(\theta h) - \frac{1}{2}h\nabla\theta = \mathbf{0}$$
$$\theta_t + \mathbf{u} \cdot (\nabla\theta) = 0$$
$$h_t + \nabla \cdot (\mathbf{u}h) = 0$$

with constant Ω

In components:

$$u_t + uu_x + vu_y - 2\Omega v + \frac{1}{2}h\theta_x + \theta h_x = 0$$

$$v_t + uv_x + vv_y + 2\Omega u + \frac{1}{2}h\theta_y + \theta h_y = 0$$

$$\theta_t + u\theta_x + v\theta_y = 0$$

$$h_t + hu_x + uh_x + hv_y + vh_y = 0$$

where $\mathbf{u}(x,y,t), \theta(x,y,t)$ and h(x,y,t).



• First few densities-flux pairs of SWW system:

$$\rho_{(1)} = h$$

$$\mathbf{J}^{(1)} = h \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\rho_{(2)} = h \theta$$

$$\mathbf{J}^{(2)} = h \theta \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\rho_{(3)} = h \theta^{2}$$

$$\mathbf{J}^{(3)} = h \theta^{2} \begin{pmatrix} u \\ v \end{pmatrix}$$

$$\rho_{(4)} = h (u^{2} + v^{2} + h\theta)$$

$$\mathbf{J}^{(4)} = h \begin{pmatrix} u (u^{2} + v^{2} + 2h\theta) \\ v (v^{2} + u^{2} + 2h\theta) \end{pmatrix}$$

$$\rho_{(5)} = \theta (2\Omega + v_{x} - u_{y})$$

$$\mathbf{J}^{(5)} = \frac{1}{2} \theta \begin{pmatrix} 4\Omega u - 2uu_{y} + 2uv_{x} - h\theta_{y} \\ 4\Omega v + 2vv_{x} - 2vu_{y} + h\theta_{x} \end{pmatrix}$$

Generalizations:

$$D_t (f(\theta)h) + D_x (f(\theta)hu) + D_y (f(\theta)hv) = 0$$

$$D_t \left(g(\theta)(2\Omega + v_x - u_x) \right)$$

$$+ D_x \left(\frac{1}{2} g(\theta)(4\Omega u - 2uu_y + 2uv_x - h\theta_y) \right)$$

$$+ D_y \left(\frac{1}{2} g(\theta)(4\Omega v - 2u_y v + 2vv_x + h\theta_x) \right) = 0$$

for any functions $f(\theta)$ and $g(\theta)$

Conservation Laws for Nonlinear Differential-Difference Equations (DDEs)

System of DDEs

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

• Conservation law in (1+1) dimensions

$$D_t \rho_n + \Delta J_n = 0 \quad \text{(on DDE)}$$

conserved density ho_n and flux J_n

Example: Toda lattice

$$\dot{u}_n = v_{n-1} - v_n$$

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

First few densities-flux pairs for Toda lattice:

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

$$J_n^{(0)} = u_n$$

$$\rho_n^{(1)} = u_n$$

$$J_n^{(1)} = v_{n-1}$$

$$\rho_n^{(2)} = \frac{1}{2}u_n^2 + v_n$$

$$J_n^{(2)} = u_n v_{n-1}$$

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

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

PART I: CONTINUOUS CASE

Problem Statement

Continuous case in 1D:

Example: For u(x) and v(x)

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

Question: Can the expression be integrated?

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

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

Continuous case in 2D or 3D:

Example: 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 **F** so that $f = \text{Div } \mathbf{F}$?

If yes, find **F**.

Result (by hand): $\mathbf{F} = (uv_y - u_xv_y, -uv_x + u_xv_x)$

Can this be done without integration by parts?

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

Tools from the Calculus of Variations

Definition:

A differential function f is a exact iff $f = \text{Div } \mathbf{F}$. Special case (1D): $f = D_x F$.

- Question: How can one test that $f = \text{Div } \mathbf{F}$?
- Theorem (exactness test):

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

N is the number of dependent variables.

The Euler operator annihilates divergences

• Euler operator in 1D (variable u(x)):

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

$$= \frac{\partial}{\partial u} - D_x \frac{\partial}{\partial u_x} + D_x^2 \frac{\partial}{\partial u_{xx}} - D_x^3 \frac{\partial}{\partial u_{xxx}} + \cdots$$

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

$$\mathcal{L}_{u(x,y)} = \sum_{k=0}^{M_x} \sum_{\ell=0}^{M_y} (-D_x)^k (-D_y)^\ell \frac{\partial}{\partial u_{kx\ell y}}$$

$$= \frac{\partial}{\partial u} - D_x \frac{\partial}{\partial u_x} - D_y \frac{\partial}{\partial u_y}$$

$$+ D_x^2 \frac{\partial}{\partial u_{xx}} + D_x D_y \frac{\partial}{\partial u_{xy}} + D_y^2 \frac{\partial}{\partial u_{yy}} - D_x^3 \frac{\partial}{\partial u_{xxx}} \cdots$$

Application: Testing Exactness – Continous Case

Example:

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

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:

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

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

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

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

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

• In 2D: If f is a divergence then

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

The homotopy operator inverts total derivatives and divergences!

• Homotopy Operator in 1D (variable x):

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

with integrand

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

 $(I_{u^{(j)}}f)[\lambda \mathbf{u}]$ 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):

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

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

where for dependent variable u(x,y)

$$\mathcal{I}_{u}^{(x)}f = \sum_{k=1}^{M_{x}} \sum_{\ell=0}^{M_{y}} \left(\sum_{i=0}^{k-1} \sum_{j=0}^{\ell} u_{ixjy} \frac{\binom{i+j}{i} \binom{k+\ell-i-j-1}{k-i-1}}{\binom{k+\ell}{k}} \right)$$
$$(-D_{x})^{k-i-1} \left(-D_{y} \right)^{\ell-j} \frac{\partial f}{\partial u_{kx\ell y}}$$

Application of Homotopy Operator in 1D

Example:

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

Compute

$$I_u f = u \frac{\partial f}{\partial u_x} + (u_x I - u D_x) \frac{\partial f}{\partial u_{xx}}$$
$$= -u u_x^2 \sin u + 3u v^2 \sin u + 2u_x^2 \cos u$$

Similarly,

$$I_{v} f = v \frac{\partial f}{\partial v_{x}} + (v_{x} I - v D_{x}) \frac{\partial f}{\partial v_{xx}}$$
$$= -6v^{2} \cos u + 8v_{x}^{2}$$

Finally,

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

$$= \int_0^1 \left(3\lambda^2 u v^2 \sin(\lambda u) - \lambda^2 u u_x^2 \sin(\lambda u) + 2\lambda u_x^2 \cos(\lambda u) - 6\lambda v^2 \cos(\lambda u) + 8\lambda v_x^2 \right) d\lambda$$

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

Application of Homotopy Operator in 2D

- Example: $f = u_x v_y u_{xx} v_y u_y v_x + u_{xy} v_x$
- By hand: $\tilde{\mathbf{F}} = (uv_y u_xv_y, -uv_x + u_xv_x)$
- Compute

$$I_{u}^{(x)}f = u\frac{\partial f}{\partial u_{x}} + (u_{x}I - uD_{x})\frac{\partial f}{\partial u_{xx}}$$
$$+ \left(\frac{1}{2}u_{y}I - \frac{1}{2}uD_{y}\right)\frac{\partial f}{\partial u_{xy}}$$
$$= uv_{y} + \frac{1}{2}u_{y}v_{x} - u_{x}v_{y} + \frac{1}{2}uv_{xy}$$

Similarly,

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

Hence,

$$F_{1} = \mathcal{H}_{\mathbf{u}(x,y)}^{(x)} f = \int_{0}^{1} \left(I_{u}^{(x)} f + I_{v}^{(x)} f \right) [\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} \lambda \left(uv_{y} + \frac{1}{2} u_{y} v_{x} - u_{x} v_{y} + \frac{1}{2} u v_{xy} - u_{y} v + u_{xy} v \right) d\lambda$$

$$= \frac{1}{2} uv_{y} + \frac{1}{4} u_{y} v_{x} - \frac{1}{2} u_{x} v_{y} + \frac{1}{4} u v_{xy} - \frac{1}{2} u_{y} v + \frac{1}{2} u_{xy} v$$

Analogously,

$$F_{2} = \mathcal{H}_{\mathbf{u}(x,y)}^{(y)} f = \int_{0}^{1} \left(I_{u}^{(y)} f + I_{v}^{(y)} f \right) [\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} \left(\lambda \left(-uv_{x} - \frac{1}{2}uv_{xx} + \frac{1}{2}u_{x}v_{x} \right) + \lambda \left(u_{x}v - u_{xx}v \right) \right) d\lambda$$

$$= -\frac{1}{2}uv_{x} - \frac{1}{4}uv_{xx} + \frac{1}{4}u_{x}v_{x} + \frac{1}{2}u_{x}v - \frac{1}{2}u_{xx}v$$

· So,

$$\mathbf{F} = \frac{1}{4} \begin{pmatrix} 2uv_y + u_yv_x - 2u_xv_y + uv_{xy} - 2u_yv + 2u_{xy}v \\ -2uv_x - uv_{xx} + u_xv_x + 2u_xv - 2u_{xx}v \end{pmatrix}$$

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

$$\mathbf{K} = \frac{1}{4} \begin{pmatrix} 2uv_y - u_yv_x - 2u_xv_y - uv_{xy} + 2u_yv - 2u_{xy}v \\ -2uv_x + uv_{xx} + 3u_xv_x - 2u_xv + 2u_{xx}v \end{pmatrix}$$

then $Div \mathbf{K} = 0$

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

After removing the curl term **K**:

$$\tilde{\mathbf{F}} = \mathbf{F} + \mathbf{K} = (uv_y - u_xv_y, -uv_x + u_xv_x)$$

Avoid curl terms algorithmically!

Why does this work?

Sketch of Derivation and Proof

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

Definition: Degree operator \mathcal{M}

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

f is of order M in x

Example: $f = u^p u^q_x u^r_{3x}$ (p, q, r non-negative integers)

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

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

$$\int_0^1 \frac{d}{d\lambda} g[\lambda u] d\lambda = g[\lambda u] \Big|_{\lambda=0}^{\lambda=1} = g(u) - g(0)$$

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

Assuming g(0) = 0,

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

Example:

If
$$g(u)=(p+q+r)\,u^pu^q_xu^r_{3x}$$
, then
$$g[\lambda u]=(p+q+r)\lambda^{p+q+r}\,u^pu^q_xu^r_{3x}$$

Hence,

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

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 $u_{Mx} \frac{\partial f}{\partial u_{Mx}}$.

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

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

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

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

= ...



$$= u \frac{\partial f}{\partial u} + u_x \frac{\partial f}{\partial u_x} + \ldots + u_{Mx} \frac{\partial f}{\partial u_{Mx}}$$

$$-\mathcal{D}_x \left(u \sum_{k=1}^M (-\mathcal{D}_x)^{k-1} \frac{\partial f}{\partial u_{kx}} + u_x \sum_{k=2}^M (-\mathcal{D}_x)^{k-2} \frac{\partial f}{\partial u_{kx}} \right)$$

$$+\ldots + u_{(M-1)x} \sum_{k=M}^{M} (-\mathcal{D}_x)^{k-M} \frac{\partial f}{\partial u_{kx}}$$

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

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

$$= 0$$

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

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} .

$$F = \mathcal{D}_{x}^{-1} f = \int_{0}^{1} \left(\sum_{i=0}^{M-1} u_{ix} \sum_{k=i+1}^{M} (-\mathcal{D}_{x})^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right) [\lambda u] \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} \left(\sum_{k=1}^{M} \left(\sum_{i=0}^{K-1} u_{ix} (-\mathcal{D}_{x})^{k-(i+1)} \right) \frac{\partial f}{\partial u_{kx}} \right) [\lambda u] \frac{d\lambda}{\lambda}$$

$$= \mathcal{H}_{u(x)} f$$



Computation of Conservation Laws for SWW

Quick Recapitulation

Conservation law in (2+1) dimensions

$$D_t \rho + \nabla \cdot \mathbf{J} = D_t \rho + D_x J_1 + D_y J_2 = 0$$
 (on PDE)

conserved density ρ and flux ${\bf J}=(J_1,J_2)$

Example: Shallow water wave (SWW) equations

$$u_t + uu_x + vu_y - 2\Omega v + \frac{1}{2}h\theta_x + \theta h_x = 0$$

$$v_t + uv_x + vv_y + 2\Omega u + \frac{1}{2}h\theta_y + \theta h_y = 0$$

$$\theta_t + u\theta_x + v\theta_y = 0$$

$$h_t + hu_x + uh_x + hv_y + vh_y = 0$$

• Typical density-flux pair:

$$\rho_{(5)} = \theta (v_x - u_y + 2\Omega)$$

$$\mathbf{J}^{(5)} = \frac{1}{2} \theta \begin{pmatrix} 4\Omega u - 2uu_y + 2uv_x - h\theta_y \\ 4\Omega v + 2vv_x - 2vu_y + h\theta_x \end{pmatrix}$$

Algorithm for PDEs in (2+1)-dimensions

Step 1: Construct the form of the density

The SWW equations are invariant under the scaling symmetries

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

and

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

Construct a candidate density, for example,

$$\rho = c_1 \Omega \theta + c_2 u_y \theta + c_3 v_y \theta + c_4 u_x \theta + c_5 v_x \theta$$

which is scaling invariant under both symmetries.

• Step 2: Determine the constants c_i

Compute $E = -D_t \rho$ and remove time derivatives

$$E = -\left(\frac{\partial \rho}{\partial u_x}u_{tx} + \frac{\partial \rho}{\partial u_y}u_{ty} + \frac{\partial \rho}{\partial v_x}v_{tx} + \frac{\partial \rho}{\partial v_y}v_{ty} + \frac{\partial \rho}{\partial \theta}\theta_t\right)$$

$$= c_4\theta(uu_x + vu_y - 2\Omega v + \frac{1}{2}h\theta_x + \theta h_x)_x$$

$$+ c_2\theta(uu_x + vu_y - 2\Omega v + \frac{1}{2}h\theta_x + \theta h_x)_y$$

$$+ c_5\theta(uv_x + vv_y + 2\Omega u + \frac{1}{2}h\theta_y + \theta h_y)_x$$

$$+ c_3\theta(uv_x + vv_y + 2\Omega u + \frac{1}{2}h\theta_y + \theta h_y)_y$$

$$+ (c_1\Omega + c_2u_y + c_3v_y + c_4u_x + c_5v_x)(u\theta_x + v\theta_y)$$

Require that

$$\mathcal{L}_{u(x,y)} E = \mathcal{L}_{v(x,y)} E = \mathcal{L}_{\theta(x,y)} E = \mathcal{L}_{h(x,y)} E \equiv 0.$$

• Solution: $c_1 = 2$, $c_2 = -1$, $c_3 = c_4 = 0$, $c_5 = 1$ gives

$$\rho = \theta \left(2\Omega - u_y + v_x \right)$$

Step 3: Compute the flux J

$$E = \theta(u_x v_x + u v_{xx} + v_x v_y + v v_{xy} + 2\Omega u_x$$

$$+ \frac{1}{2}\theta_x h_y - u_x u_y - u u_{xy} - u_y v_y - u_{yy} v$$

$$+ 2\Omega v_y - \frac{1}{2}\theta_y h_x) + 2\Omega u \theta_x + 2\Omega v \theta_y$$

$$- u u_y \theta_x - u_y v \theta_y + u v_x \theta_x + v v_x \theta_y$$

Apply the 2D homotopy operator:

$$\mathbf{J} = (J_1, J_2) = \operatorname{Div}^{-1} E = (\mathcal{H}_{\mathbf{u}(x,y)}^{(x)} E, \mathcal{H}_{\mathbf{u}(x,y)}^{(y)} E)$$

Compute

$$I_{u}^{(x)}E = u\frac{\partial E}{\partial u_{x}} + \left(\frac{1}{2}u_{y}I - \frac{1}{2}uD_{y}\right)\frac{\partial E}{\partial u_{xy}}$$
$$= uv_{x}\theta + 2\Omega u\theta + \frac{1}{2}u^{2}\theta_{y} - uu_{y}\theta$$

Similarly, compute

$$I_{v}^{(x)}E = vv_{y}\theta + \frac{1}{2}v^{2}\theta_{y} + uv_{x}\theta$$

$$I_{\theta}^{(x)}E = \frac{1}{2}\theta^{2}h_{y} + 2\Omega u\theta - uu_{y}\theta + uv_{x}\theta$$

$$I_{h}^{(x)}E = -\frac{1}{2}\theta\theta_{y}h$$

Next,

$$J_{1} = \mathcal{H}_{\mathbf{u}(x,y)}^{(x)} E$$

$$= \int_{0}^{1} \left(I_{u}^{(x)} E + I_{v}^{(x)} E + I_{\theta}^{(x)} E + I_{h}^{(x)} E \right) [\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} \left(4\lambda \Omega u \theta + \lambda^{2} \left(3uv_{x}\theta + \frac{1}{2}u^{2}\theta_{y} - 2uu_{y}\theta + vv_{y}\theta + \frac{1}{2}v^{2}\theta_{y} + \frac{1}{2}\theta^{2}h_{y} - \frac{1}{2}\theta\theta_{y}h \right) \right) d\lambda$$

$$= 2\Omega u \theta - \frac{2}{3}uu_{y}\theta + uv_{x}\theta + \frac{1}{3}vv_{y}\theta + \frac{1}{6}u^{2}\theta_{y} + \frac{1}{6}v^{2}\theta_{y} - \frac{1}{6}h\theta\theta_{y} + \frac{1}{6}h_{y}\theta^{2}$$

Analogously,

$$J_2 = \mathcal{H}_{\mathbf{u}(x,y)}^{(y)} E$$

$$= 2\Omega v\theta + \frac{2}{3}vv_x\theta - vu_y\theta - \frac{1}{3}uu_x\theta - \frac{1}{6}u^2\theta_x - \frac{1}{6}v^2\theta_x$$

$$+ \frac{1}{6}h\theta\theta_x - \frac{1}{6}h_x\theta^2$$

Hence,

$$\mathbf{J} = \frac{1}{6} \left(\frac{12\Omega u\theta - 4uu_y\theta + 6uv_x\theta + 2vv_y\theta + (u^2 + v^2)\theta_y - h\theta\theta_y + h_y\theta^2}{12\Omega v\theta + 4vv_x\theta - 6vu_y\theta - 2uu_x\theta - (u^2 + v^2)\theta_x + h\theta\theta_x - h_x\theta^2} \right)$$

There are curl terms in J

Indeed, subtract **K** where $\text{Div } \mathbf{K} = 0$

Here

$$\mathbf{K} = \frac{1}{6} \left(\frac{-(2uu_y\theta + 2vv_y\theta + u^2\theta_y + v^2\theta_y + 2h\theta\theta_y + h_y\theta^2)}{2vv_x\theta + 2uu_x\theta + u^2\theta_x + v^2\theta_x + 2h\theta\theta_x + h_x\theta^2} \right)$$

Note that $\mathbf{K}=(\mathrm{D}_y\phi,-\mathrm{D}_x\phi)$ with $\phi=-(h\theta^2+u^2\theta+v^2\theta)$ (curl in 2D).

After removing the curl term K,

$$\tilde{\mathbf{J}}^{(5)} = \frac{1}{2} \theta \begin{pmatrix} 4\Omega u - 2uu_y + 2uv_x - h\theta_y \\ 4\Omega v + 2vv_x - 2vu_y + h\theta_x \end{pmatrix}$$

PART II: DISCRETE CASE

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

$$DF_n = F_{n+1} = F_{n|_{n \to n+1}}$$

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

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

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

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

• 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
$\mathcal{L}_{\mathbf{u}(x)} = \sum_{k=0}^{M} (-\mathbf{D}_x)^k \frac{\partial}{\partial \mathbf{u}_{kx}}$	$\mathcal{L}_{\mathbf{u}_n} = \sum_{k=0}^{M} D^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}}$ $= \frac{\partial}{\partial \mathbf{u}_n} \sum_{k=0}^{M} D^{-k}$

Analogy Continuous & Discrete Cases

Homotopy Operators & Integrands

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

Euler Operators Side by Side

Continuous Case (for component u)

$$\mathcal{L}_{u} = \frac{\partial}{\partial u} - D_{x} \frac{\partial}{\partial u_{x}} + D_{x}^{2} \frac{\partial}{\partial u_{2x}} - D_{x}^{3} \frac{\partial}{\partial u_{3x}} + \cdots$$

Discrete Case (for component u_n)

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

Homotopy Operators Side by Side

Continuous Case (for components u and v)

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

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

$$I_{v} f = \sum_{k=1}^{M^{(2)}} \left(\sum_{i=0}^{k-1} v_{ix} \left(-\mathcal{D}_{x} \right)^{k-(i+1)} \right) \frac{\partial f}{\partial v_{kx}}$$

Discrete Case (for components u_n and v_n)

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

with

$$I_{u_n} f_n = \sum_{i=0}^{M^{(1)}-1} u_{n+i} \frac{\partial}{\partial u_{n+i}} \sum_{k=i+1}^{M^{(1)}} D^{-(k-i)} f_n$$

and

$$I_{v_n} f_n = \sum_{i=0}^{M^{(2)}-1} v_{n+i} \frac{\partial}{\partial v_{n+i}} \sum_{k=i+1}^{M^{(2)}} D^{-(k-i)} f_n$$

Analogy of Definitions & Theorems

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

- 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

For example,

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

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

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

• Exactness test with Euler operator:

For component u_n (highest shift 3):

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

$$= -u_{n+1} v_n - u_{n-1} v_{n-1} + u_{n+1} v_n - v_{n-1}$$

$$+ u_{n-1} v_{n-1} + v_{n-1}$$

$$\equiv 0$$

Similarly,

$$\mathcal{L}_{v_n} f_n = \frac{\partial}{\partial v_n} \left(\mathbf{I} + \mathbf{D}^{-1} \right) f_n$$

$$= u_n u_{n+1} + 2v_n - u_n u_{n+1} - 2v_n$$

$$\equiv 0$$

Application of Discrete Homotopy Operator

Example:

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

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

Compute

$$I_{u_n} f_n = u_n \frac{\partial}{\partial u_n} (D^{-1} + D^{-2} + D^{-3}) f_n$$

$$+ u_{n+1} \frac{\partial}{\partial u_{n+1}} (D^{-1} + D^{-2}) f_n$$

$$+ u_{n+2} \frac{\partial}{\partial u_{n+2}} D^{-1} f_n$$

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

$$I_{v_n} f_n = v_n \frac{\partial}{\partial v_n} (D^{-1} + D^{-2}) f_n + v_{n+1} \frac{\partial}{\partial v_{n+1}} (D^{-1}) f_n$$
$$= u_n u_{n+1} v_n + 2v_n^2 + u_{n+1} v_n + u_{n+2} v_{n+1}$$

Finally,

$$F_{n} = \int_{0}^{1} (I_{u_{n}} f_{n} + I_{v_{n}} f_{n}) [\lambda \mathbf{u}_{n}] \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} (2\lambda v_{n}^{2} + 3\lambda^{2} u_{n} u_{n+1} v_{n} + 2\lambda u_{n+1} v_{n} + 2\lambda u_{n+2} v_{n+1}) d\lambda$$

$$= v_{n}^{2} + u_{n} u_{n+1} v_{n} + u_{n+1} v_{n} + u_{n+2} v_{n+1}$$

Application: Computation of Conservation Laws

System of DDEs

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

Conservation law

$$D_t \rho_n + \Delta J_n = 0$$
 (on DDE)

conserved density ρ_n and flux J_n

Example: Toda lattice

$$\dot{u}_n = v_{n-1} - v_n$$

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

Typical density-flux pair:

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

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 $E_n = D_t \rho_n$ and remove time derivatives

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

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

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

Step 3: Compute the flux J_n

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

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

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

Likewise,

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

Next, compute

$$\tilde{J}_{n} = -\int_{0}^{1} \left(I_{u_{n}} \tilde{E}_{n} + I_{v_{n}} \tilde{E}_{n} \right) \left[\lambda \mathbf{u}_{n} \right] \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} (3\lambda^{2} u_{n} u_{n+1} v_{n} + 2\lambda v_{n}^{2}) d\lambda$$

$$= u_{n} u_{n+1} v_{n} + v_{n}^{2}$$

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

$$J_n = u_{n-1}u_nv_{n-1} + v_{n-1}^2$$

Software Demonstration

Demonstrations of ConservationLawsMD.m

Demonstration of *DDEDensityFlux.m*

Software packages in Mathematica

Codes are available via the Internet:

URL: http://inside.mines.edu/~whereman/

Conclusions

- Continuous Euler and homotopy operators:
 - Testing exactness
 - ▶ Integration by parts: D_x^{-1} and Div^{-1}
 - Application: conservation laws of PDEs
- Discrete Euler and homotopy operators:
 - Testing exactness (summability)
 - ▶ Summation by parts: Δ^{-1}
 - Application: conservation laws of DDEs and lattices
- Useful analogy between the formulas.



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