Welcome!

MiniSymposium on Algorithms and Software to Compute Conservation Laws of Nonlinear PDEs Speakers: Hereman, Bluman, Nivala, Wolf

Symbolic Computation of Conservation Laws of Nonlinear PDEs in Multi-dimensions

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Collaborators:

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Outline

- Conservation Laws of PDEs in multi-dimensions
- Example: shallow water wave equations (Dellar)
- Algorithmic Methods for conservation laws
- Computer Demonstration
- Tools:
 - Euler operators (testing exactness)
 - Calculus-based formulas for homotopy operator
 - * symbolic integration by parts
 - * inversion of the total divergence operator
- Application: shallow water wave equations
- Conclusions: future work, software and publications

Notations – 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 $u_{kx}=rac{\partial^k u}{\partial x^k}, \ u_{kx\,ly}=rac{\partial^{k+l} u}{\partial x^k y^l},$ etc.
- Differential functions

Example:
$$f = uvv_x + x^2u_x^3v_x + u_xv_{xx}$$
 for $u(x)$, $v(x)$

• Total derivative (with respect to x)

$$D_{x} = \frac{\partial}{\partial x} + \sum_{k=0}^{M_{x}^{(1)}} u_{(k+1)x} \frac{\partial}{\partial u_{kx}} + \sum_{k=0}^{M_{x}^{(2)}} v_{(k+1)x} \frac{\partial}{\partial v_{kx}}$$

 $M_x^{(1)}$ is the order of f in u (with respect to x), etc.

Conservation Laws

• Conservation law in (1+1) dimensions

$$\boxed{\mathbf{D}_t \rho + \mathbf{D}_x J = 0} \quad \text{(on PDE)}$$

conserved density ρ and flux J

• Example: Korteweg-de Vries (KdV) equation $u_t + uu_x + u_{3x} = 0$

Sample conservation law

$$D_t \left(u^3 - 3u_x^2 \right) +$$

$$D_x \left(\frac{3}{4} u^4 - 6u u_x^2 + 3u^2 u_{2x} + 3u_{2x}^2 - 6u_x u_{3x} \right) = 0$$

- Key property: Dilation invariance
- Example: KdV equation and its density-flux pairs are invariant under the scaling symmetry

$$(x,t,u) \rightarrow (\frac{x}{\lambda}, \frac{t}{\lambda^3}, \lambda^2 u),$$

 λ is arbitrary parameter.

Some density-flux pairs for the KdV equation:

$$\rho^{(1)} = u J^{(1)} = \frac{u^2}{2} + u_{2x}$$

$$\rho^{(2)} = u^2 \qquad J^{(2)} = \frac{2u^3}{3} + 2uu_{2x} - u_x^2$$

$$\rho^{(3)} = u^3 - 3u_x^2$$

$$J^{(3)} = \frac{3}{4}u^4 - 6uu_x^2 + 3u^2u_{2x} + 3u_{2x}^2 - 6u_xu_{3x}$$

:

$$\rho^{(6)} = u^6 - 60 u^3 u_x^2 - 30 u_x^4 + 108 u^2 u_{2x}^2 + \frac{720}{7} u_{2x}^3 - \frac{648}{7} u u_{3x}^2 + \frac{216}{7} u_{4x}^2$$

:

• Conservation law in (3+1) dimensions

$$\boxed{\mathbf{D}_t \rho + \nabla \cdot \mathbf{J} = \mathbf{D}_t \rho + \mathbf{D}_x J_1 + \mathbf{D}_y J_2 + \mathbf{D}_z J_3 = 0} \text{ (on PDE)}$$

conserved density ho and flux ${f J}=(J_1,J_2,J_3)$

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

$$\mathbf{u}_{t} + (\mathbf{u} \cdot \nabla)\mathbf{u} + 2\mathbf{\Omega} \times \mathbf{u} + \nabla(\theta h) - \frac{1}{2}h\nabla\theta = \mathbf{0}$$
$$\theta_{t} + \mathbf{u} \cdot (\nabla\theta) = 0$$
$$h_{t} + \nabla \cdot (\mathbf{u}h) = 0$$

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

In components:

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

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

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

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

SWW equations are invariant under

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

where W(h) = a and $W(\Omega) = b$ $(a, b \in \mathbb{Q})$.

• First few densities-flux pairs of SWW system:

$$\rho^{(1)} = h \qquad \mathbf{J}^{(1)} = \begin{pmatrix} uh \\ vh \end{pmatrix}$$

$$\rho^{(2)} = h\theta \qquad \mathbf{J}^{(2)} = \begin{pmatrix} uh\theta \\ vh\theta \end{pmatrix}$$

$$\rho^{(3)} = h\theta^2 \qquad \mathbf{J}^{(3)} = \begin{pmatrix} uh\theta^2 \\ vh\theta^2 \end{pmatrix}$$

$$\rho^{(4)} = (u^2 + v^2)h + h^2\theta \qquad \mathbf{J}^{(4)} = \begin{pmatrix} u^3h + uv^2h + 2uh^2\theta \\ v^3h + u^2vh + 2vh^2\theta \end{pmatrix}$$

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

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

Computer Demonstration

Algorithmic Methods for Conservation Laws

- Use Noether's Theorem (Lagrangian formulation).
- Direct methods (Anderson, Bluman, Anco, Wolf, etc.) based on solving ODEs (or PDEs).
- Strategy (linear algebra and variational calculus).
 - Density is linear combination of scaling invariant terms with undetermined coefficients.
 - Use variational derivative (Euler operator) to compute the undetermined coefficients.
 - Use the homotopy operator to compute the flux (invert D_x or Div) (Deconinck and Nivala).
 - Work with linearly independent pieces in finite dimensional spaces.

Review of Vector Calculus

- The curl annihilates gradients!
- The divergence annihilates curls!
- The Euler operator annihilates divergences!

Formula for Euler operator (variational derivative)

in 1D:

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

$$= \frac{\partial}{\partial u^{(j)}} - D_x \frac{\partial}{\partial u_x^{(j)}} + D_x^2 \frac{\partial}{\partial u_{2x}^{(j)}} - D_x^3 \frac{\partial}{\partial u_{3x}^{(j)}} + \cdots$$

Formula for Euler operator in 2D:

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

$$= \frac{\partial}{\partial u^{(j)}} - D_x \frac{\partial}{\partial u_x^{(j)}} - D_y \frac{\partial}{\partial u_y^{(j)}}$$

$$+ D_x^2 \frac{\partial}{\partial u_{2x}^{(j)}} + D_x D_y \frac{\partial}{\partial u_{xy}^{(j)}} + D_y^2 \frac{\partial}{\partial u_{2y}^{(j)}} - D_x^3 \frac{\partial}{\partial u_{3x}^{(j)}} \cdots$$

Inverting D_x and Div

Problem Statement

• In 1D:

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

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

• Find $F = \int f \ dx$ Thus, $f = D_x F$.

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- Find $F = \int f \ dx$ Thus, $f = D_x F$.
- Result (by hand):

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

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Mathematica cannot compute this integral!

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

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

• Find $\mathbf{F} = \mathrm{Div}^{-1} f$ Thus, $f = \mathrm{Div} \mathbf{F}$.

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

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Can this be done without integration by parts?

Can this be reduced to single integral in one variable?

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Mathematica cannot do this!

Can this be done without integration by parts?

Can this be reduced to single integral in one variable?

Yes! With the Homotopy operator.

Integration by Parts with Homotopy Operator

- Theorem (integration with homotopy operator):
 - 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

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

In 3D: If f is a divergence then

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

Simplified Formula for Homotopy Operator

• In 1D (with 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

$$I_{u^{(j)}} f = \sum_{i=0}^{M_x^{(j)}-1} \mathcal{D}_x^i \left(u^{(j)} \mathcal{L}_{u^{(j)}(x)}^{(i+1)} f \right)$$

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

N dependent variables, $(I_{u^{(j)}}f)[\lambda \mathbf{u}]$ means that in $I_{u^{(j)}}f$ one replaces $\mathbf{u}(x) \to \lambda \mathbf{u}(x), \ \mathbf{u}_x(x) \to \lambda \mathbf{u}_x(x), \dots$

In 2D (with variables x and y):

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

with integrand

$$\begin{split} \mathcal{I}_{u^{(j)}}^{(x)}f &= \sum_{i_{x}=0}^{M_{x}^{(j)}-1} \sum_{i_{y}=0}^{M_{y}^{(j)}} \left(\frac{1+i_{x}}{1+i_{x}+i_{y}}\right) \mathcal{D}_{x}^{i_{x}} \mathcal{D}_{y}^{i_{y}} \left(u^{(j)} \mathcal{L}_{u^{(j)}(x,y)}^{(1+i_{x},i_{y})} f\right) \\ &= \sum_{i_{x}=0}^{M_{x}^{(j)}-1} \sum_{i_{y}=0}^{M_{y}^{(j)}} \binom{i_{x}+i_{y}}{i_{x}} u_{i_{x}x\,i_{y}y} \sum_{k_{x}=i_{x}+1}^{M_{x}^{(j)}} \sum_{k_{y}=i_{y}}^{M_{y}^{(j)}} \frac{\binom{k_{x}+k_{y}-i_{x}-i_{y}-1}{k_{x}-i_{x}-1}}{\binom{k_{x}+k_{y}}{k_{x}}} \\ &\qquad \qquad (-\mathcal{D}_{x})^{k_{x}-i_{x}-1} \left(-\mathcal{D}_{y}\right)^{k_{y}-i_{y}} \frac{\partial f}{\partial u_{k_{x}x\,k_{y}y}^{(j)}} \end{split}$$

Analogous formulas for $\mathcal{H}_{\mathbf{u}(x,y)}^{(y)}f$ and $I_{u^{(j)}}^{(y)}f$

Application of Homotopy Operator in 1D

Example:

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

Compute

$$I_{u}f = u\frac{\partial f}{\partial u_{x}} + u_{x}\frac{\partial f}{\partial u_{2x}} - uD_{x}\frac{\partial f}{\partial u_{2x}}$$
$$= 3uv^{2}\sin u - uu_{x}^{2}\sin u + 2u_{x}^{2}\cos u$$

Similarly,

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

Finally,

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

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

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

Computation of Conservation Laws for SWW

Quick Recapitulation

• Conservation law in (2+1) dimensions

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

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

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

Algorithm

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

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

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

$$\rho = 2\Omega\theta - u_y\theta + v_x\theta$$

Step 3: Compute the flux J

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

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

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

$$+ 2\Omega u \theta_x + 2\Omega v \theta_y - u u_y \theta_x$$

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

Apply the 2D homotopy operator:

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

Compute

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

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,

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

After removing the curl term (by hand)

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

Needed: Algorithm to remove curl terms!

Conclusions and Future Work

- Usefulness of the homotopy operator: Integration by parts, D_x^{-1} , and Div^{-1} .
- To do: integration of non-exact expressions.

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

$$\int f dx = u v + \int u^2 u_{2x} dx.$$

 To do: integration of parametrized differential functions.

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Example: f = au_xv + buv_x

\int f dx = uv if a = b.
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- To do: various PDEs (other than those of evolution type).
- To do: full implementation in Mathematica.

Software packages in Mathematica

Codes are available via the Internet:

URL: http://www.mines.edu/fs_home/whereman/
and via anonymous FTP from mines.edu in directory:
pub/papers/math_cs_dept/software/

Publications

 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.

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