Structure-Preserving Discretizations for Hamiltonian PDE with Added Dissipation

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Multi-Symplectic PDE, Bridges (1997)

These equations can be written

\[ K z_t + L z_x = \nabla_{z} S(z) \]

- \( K \) and \( L \) are skew-symmetric matrices
- \( z = z(x, t) \) is the vector of state variables
- \( S \) is smooth

Examples include KdV, Boussinesq, Zakharov-Kuznetsov, nonlinear Schrödinger, nonlinear wave equations, etc.

Conservation laws are derived directly from the equation. An example is the multi-symplectic conservation law

\[ \partial_t \langle KU, V \rangle + \partial_x \langle LU, V \rangle = 0 \]

where \( U \) and \( V \) satisfy the variational equation.
These equations can be written

\[ \mathbf{K} \dot{z} + \mathbf{L} \frac{\partial z}{\partial x} = \nabla_z S(z) - \frac{a}{2} \mathbf{K} z - \frac{b}{2} \mathbf{L} z + F(x, t) \]

- \( a \) and \( b \) are positive real constants
- \( S \) is smooth and may depend on \( a \) and \( b \)
- \( F \) is a forcing term

Equation satisfies a conformal multi-symplectic conservation law

\[ \partial_t \langle \mathbf{K} U, V \rangle + \partial_x \langle \mathbf{L} U, V \rangle = -a \langle \mathbf{K} U, V \rangle - b \langle \mathbf{L} U, V \rangle. \]

Methods that preserve this property behave similarly to standard multi-symplectic methods for small \( a \) and \( b \).
General Conformal Conservation Laws

If

$$K \dot{z} + L z_x = \nabla_z S(z)$$

has a conservation law

$$\partial_t P + \partial_x Q = 0,$$

then

$$K \dot{z} + L z_x = \nabla_z S(z) - \frac{a}{2} K z - \frac{b}{2} L z$$

has a conformal conservation law if it satisfies

$$\partial_t P + \partial_x Q = -a P - b Q.$$
Examples of Conservation Laws for $Kz_t + Lz_x = \nabla_z S(z)$

Energy: inner product of the equation with $z_t$

$$\partial_t \left( S(z) + \frac{1}{2}(z^T_x L z) \right) + \partial_x \frac{1}{2}(z^T L z_t) = 0$$
Examples of Conservation Laws for

\[ \mathbf{K} \dot{z} + \mathbf{L} \ddot{z} = \nabla_z S(z) \]

- **Energy**: inner product of the equation with \( \dot{z}_t \)

\[
\partial_t \left( S(z) + \frac{1}{2} (\dot{z}_x^T \mathbf{L} \dot{z}) \right) + \partial_x \frac{1}{2} (z^T \mathbf{L} \dot{z}_t) = 0
\]

- **Momentum**: inner product of the equation with \( \ddot{z}_x \)

\[
\partial_x \left( S(z) + \frac{1}{2} (\ddot{z}_t^T \mathbf{K} \ddot{z}) \right) + \partial_t \frac{1}{2} (z^T \mathbf{K} \ddot{z}_x) = 0
\]
Examples of Conservation Laws for
\[ Kz_t + Lz_x = \nabla_z S(z) \]

- Energy: inner product of the equation with \( z_t \)
  \[ \partial_t \left( S(z) + \frac{1}{2} (z_x^T L z) \right) + \partial_x \frac{1}{2} (z^T L z_t) = 0 \]

- Momentum: inner product of the equation with \( z_x \)
  \[ \partial_x \left( S(z) + \frac{1}{2} (z_t^T K z) \right) + \partial_t \frac{1}{2} (z^T K z_x) = 0 \]

- Linear Symmetries: inner product with \( B z \)
  \[ \partial_t (z^T K B z) + \partial_x (z^T L B z) = 0 \]
Examples of Conformal Conservation Laws for

$$K z_t + L z_x = \nabla_z S(z) - \frac{a}{2} K z - \frac{b}{2} L z$$

- **Energy:** inner product of the equation with $z_t$

  $$\partial_t \left( S(z) + \frac{1}{2} (z^T L z) \right) + \partial_x \frac{1}{2} (z^T L z_t) = -\frac{b}{2} (z^T L z_t)$$

- **Momentum:** inner product of the equation with $z_x$

  $$\partial_x \left( S(z) + \frac{1}{2} (z^T K z) \right) + \partial_t \frac{1}{2} (z^T K z_x) = -\frac{a}{2} (z^T K z_x)$$

- **Linear Symmetries:** inner product with $B z$

  $$\partial_t (z^T K B z) + \partial_x (z^T L B z) = -a (z^T K B z) - b (z^T L B z)$$
Suppose we have the following PDE and Conformal CL

\[ K \frac{\partial z}{\partial t} + L \frac{\partial z}{\partial x} = \nabla S(z) - \frac{a}{2} K z \]

\[ \partial_t P + \partial_x Q = -aP \]
Numerical Preservation

Suppose we have the following PDE and Conformal CL

\[ K \dot{z}_t + L \dot{z}_x = \nabla S(z) - \frac{a}{2} K z \]

\[ \partial_t P + \partial_x Q = -aP \]

Integrating with appropriate boundary conditions, yields

\[ \partial_t \hat{P} = -a \hat{P} \iff \hat{P}(t) = \exp(-at) \hat{P}(0) \text{ with } \hat{P} = \int P \, dx. \]
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A numerical method preserves this property if it satisfies

\[ \hat{P}^{i+1} = \exp(-a \Delta t) \hat{P}^i \quad \text{with} \quad \hat{P}^i = \sum_n P^{n,i} \Delta x. \]
Numerical Preservation

Suppose we have the following PDE and Conformal CL

\[
K \frac{dz}{dt} + L \frac{dz}{dx} = \nabla S(z) - \frac{a}{2} K z \quad \quad \partial_t P + \partial_x Q = -a P
\]

Integrating with appropriate boundary conditions, yields

\[
\partial_t \hat{P} = -a \hat{P} \iff \hat{P}(t) = \exp(-at) \hat{P}(0) \quad \text{with} \quad \hat{P} = \int P \, dx.
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A numerical method preserves this property if it satisfies

\[
\hat{P}_{i+1} = \exp(-a \Delta t) \hat{P}_i \quad \text{with} \quad \hat{P}_i = \sum_n P^{n,i} \Delta x.
\]

Note: \(\partial_t P < 0\) is typically considered preserved if \(P^{i+1} < P^i\)
Splitting Methods, McLachlan and Quispel (2002)

\[ z_t = F_H(z) + F_D(z) \]

- Solve \( z_t = f_H(z) \) with conservative method \( z^{i+1} = \Psi_{\Delta t}(z^i) \).
- Solve \( z_t = Dz \) exactly with flow map \( \Phi_t(z) = \exp(Dt)z \).
- Original system is solved by composing these flow maps.
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**Example**: Define non-standard difference/average operators

\[
D^a_t z = \frac{z^{i+1} - e^{-a\Delta t}z^i}{\Delta t} \quad \text{and} \quad A^a_t z = \frac{z^{i+1} + e^{-a\Delta t}z^i}{2}
\]

Implicit midpoint for \( z_t = F_H(z) \) is \( D^0_t z = F_H(A^0_t z) \).

Splitting method for \( z_t = F_H(z) + F_D(z) \) is \( D^{a/2}_t z = F_H(A^{a/2}_t z) \).
Structure-Preservation

A non-standard 1-step FD method preserves a conformal CL, if it has a discrete product rule and the corresponding CL is preserved by the conservative method upon which it is based.

Example: The conformal box scheme

\[ \mathbf{K} \left( D_t^{a/2} A_x^{b/2} z \right) + \mathbf{L} \left( D_x^{b/2} A_t^{a/2} z \right) = \nabla S \left( A_t^{a/2} A_x^{b/2} z \right) \]

satisfies

\[ D_t^a \left\langle A_x^{b/2} z, \mathbf{K} \mathbf{B} A_x^{b/2} z \right\rangle + D_x^b \left\langle A_t^{a/2} z, \mathbf{L} \mathbf{B} A_t^{a/2} z \right\rangle = 0. \]

Sum over spatial index with \( b = 0 \) and appropriate BCs gives

\[ \hat{P}^{i+1} = \exp(-a \Delta t) \hat{P}^i \quad \text{with} \quad \hat{P}^i = \sum_n \left\langle A_x^0 z, \mathbf{K} \mathbf{B} A_x^0 z \right\rangle \Delta x. \]
Nonlinear Schrödinger with Dissipation

\[ i\psi_t + \psi_{xx} + V'(|\psi|^2)\psi + i\frac{a}{2}\psi = 0 \]

Can be written \( Kz_t + Lz_x = \nabla_z S(z) - \frac{a}{2}Kz \) with

\[
J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} -J & 0 \\ 0 & 0 \end{bmatrix}, \quad L = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix},
\]

\( z = [v, w, p, q]^T \), \( S(z) = \frac{1}{2}(p^2 + q^2 + V(v^2 + w^2)) \)

The conformal probability conservation law

\[ \partial_t (w^2 + v^2) + 2\partial_x (vw_x - wv_x) = -a(w^2 + v^2) \]
Residual in Local Conformal Conservation Law

\[ a = 0.01, \quad h = 0.01, \]

MS–CC–CL–1: \( \Gamma = 0.010, \ |Ra_{\text{MAX}}| = 1.19904 \times 10^{-13} \)
Residual in Global Conformal Conservation

\[ \text{MS–CC–CL–1: } \Gamma = 0.010, \ |\text{Sum(Ra)}_{\text{MAX}}| = 5.75974 \times 10^{-14} \]
**Dissipative Semi-Linear Wave Equation**

\[ u_{tt} = u_{xx} - au_t - f'(u) \]

Can be written \( Kz_t + Lz_x = \nabla_z S(z) - \frac{a}{2} Kz \) with

\[
J = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad K = \begin{bmatrix} J & 0 \\ 0 & J \end{bmatrix}, \quad L = \begin{bmatrix} 0 & -I \\ I & 0 \end{bmatrix},
\]

\( z = [u, v, w, p]^T \), \( S(z) = \frac{1}{2} (a(uv + wp) + v^2 - w^2 + 2f(u)) \)

**momentum:**
\[
\partial_t (vu_x + pw_x) + \partial_x \left( f(u) + \frac{v^2}{2} - \frac{w^2}{2} - vu_t - pw_t \right) = -a(vu_x + pw_x)
\]

**angular momentum:** \( \partial_t (u \times u_t) + \partial_x (u_x \times u) = -a(u \times u_t) \)

**others:** \( \partial_t (vw + cu_p) + \frac{1}{2} \partial_x (v^2 + w^2 - c(u^2 + p^2)) = -a(vw + cu_p) \)
Solution Behavior for $u_{tt} = u_{xx} - au_t - cu$

$c = 1$, $a = 1/2$, $\Delta t = 0.0063$, $\Delta x = 0.042$
Residual in Conformal Momentum CL

\[ u_{tt} = u_{xx} - 0.005u_t - \sin(u) \text{ with } \Delta x = \Delta t = 0.4 \]
Residual in Global Conformal Momentum
Systems of Reaction Diffusion Equations

\[ u_t = u_{xx} - F(u, v), \quad v_t = v_{xx} - G(u, v) \]

For traveling waves set \( u(x, t) = \phi(\eta) \) and \( v(x, t) = \psi(\xi) \), where \( \eta = x - at \) and \( \xi = x - bt \).

\[-p\eta = -F(\phi, \psi) + ap, \quad \phi_{\eta} = p\]

\[-q\xi = -G(\phi, \psi) + bq, \quad \psi_{\xi} = q.\]

This is an elliptic boundary value problem with the form

\[ Kz_{\eta} + Lz_{\xi} = \nabla S(z) - \frac{a}{2}Kz - \frac{b}{2}Lz \]

with \( z = [\phi, p, \psi, q]^T \), \( S(z) = \frac{1}{2} \left( p^2 + q^2 + a\phi p + b\psi q \right) - H(\phi, \psi) \), provided \( F(\phi, \psi) = \partial_\phi H(\phi, \psi) \) and \( G(\phi, \psi) = \partial_\psi H(\phi, \psi) \).