Structure-Preserving Exponential Integrators

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Acknowledgements

Structure-preserving algorithms for conservative systems
perturbed by linear damping

Joint work with

- Constance Schober, Professor UCF
- Laura Norena, UCF student, currently with Valencia College
- Dwayne Floyd, UCF student, currently with DOD
- Ashish Bhatt, UCF Ph.D. student

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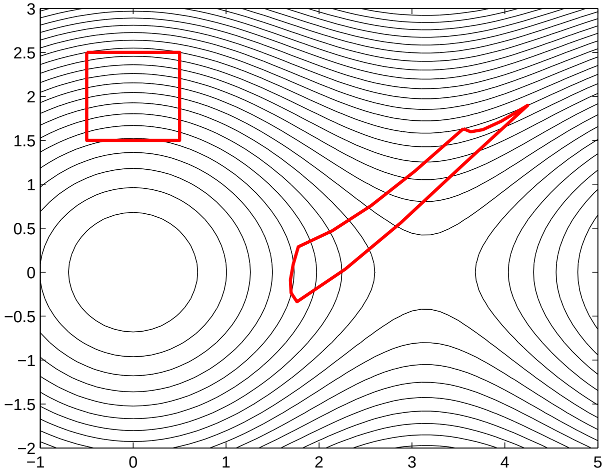
- NTNU Department of Mathematical Sciences for office space, facilities, and a stimulating research environment

Background: Phase space area

Example: Phase portrait for the pendulum problem, $\ddot{q} + \sin(q) = 0$



Background: Simple conservative systems

Models from Newtons 2nd law: $\ddot{q} + \nabla_q V(q) = 0$

- The energy $H = \frac{1}{2}\dot{q}^2 + V(q)$ is an invariant.

$$\frac{d}{dt}H = \frac{d}{dt}\left(\frac{1}{2}\dot{q}^2 + V(q)\right) = \dot{q}\left(\ddot{q} + \nabla_q V(q)\right) = 0$$

- The symplectic form $\omega = dq \wedge d\dot{q}$ is invariant.
  The variational equation $d\ddot{q} + V_{qq}(q)dq = 0$ implies

$$0 = dq \wedge d\ddot{q} + dq \wedge V_{qq}(q)dq = \frac{d}{dt}(dq \wedge d\dot{q})$$

  because V_{qq} symmetric implies $dq \wedge V_{qq}(q)dq = 0$.
  $\frac{d}{dt}\omega = 0$ corresponds to conservation of phase space area.

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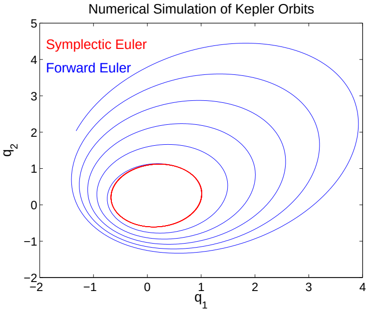
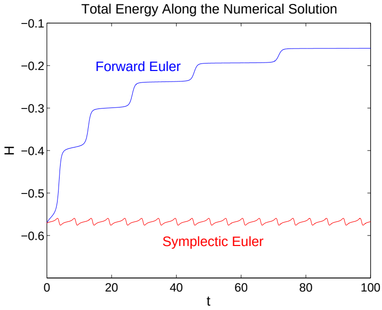
Background: Numerical solutions of conservative systems

Numerical solutions:
One method is conservative the other is non-conservative

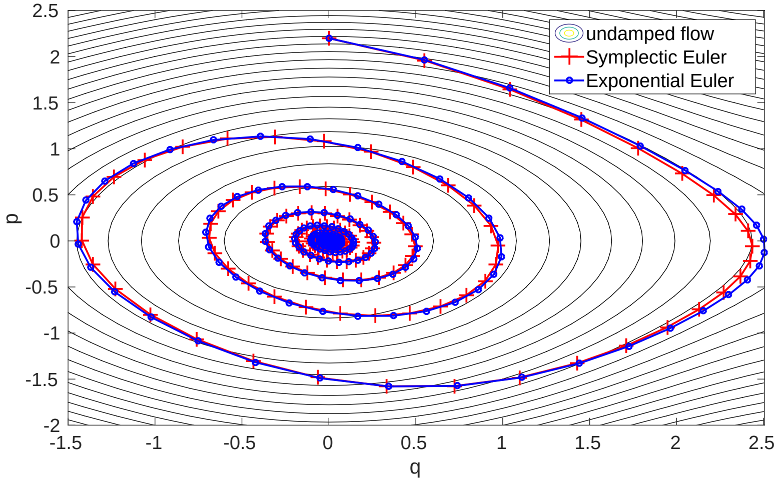




Background: Books on structure-preserving algorithms

- R.E. Mickens, *Nonstandard Finite Difference Models of Differential Equations*, 1993
- J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, 1994
- A. Stuart and A.R. Humphries, *Dynamical Systems and Numerical Analysis*, 1998
- E. Hairer, G. Wanner, and C. Lubich, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations*, 2002
- B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, 2005
- D. Furihata and T. Matsuo, *Discrete Variational Derivative Method: A Structure-Preserving Numerical Method for Partial Differential Equations*, 2010
- X. Wu, X. You, and B. Wang, *Structure-Preserving Algorithms for Oscillatory Differential Equations*, 2013

Trajectories for a damped pendulum problem, $\ddot{q} + \gamma\dot{q} + \sin(q) = 0$



Background: Conformal Symplectic Models and Methods

- McLachlan and Perlmutter (2001): conformal Hamiltonian systems; contraction of the symplectic form

$$\partial_t \omega = -2\gamma\omega \qquad \Longleftrightarrow \qquad \omega(t) = e^{-2\gamma t}\omega(0)$$

- McLachlan and Quispel (2001) and (2002): splitting methods that preserve conformal symplecticity; they satisfy

$$\omega^{n+1} = e^{-2\gamma h}\omega^n$$

where $h = t_{n+1} - t_n$ is the step size.

Splitting Methods for solving $\dot{y} = N(y) - \gamma y$

1. Solve $\dot{y} = N(y)$ with a conservative (symplectic) method
2. Solve $\dot{y} = -\gamma y$ exactly: $y(t) = y_0 e^{-\gamma t}$
3. Compose the flow maps to get a conformal symplectic scheme

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Example: Conformal Implicit Midpoint (CIMP)

Given

$$\dot{y} = N(y) - \gamma y$$

an implicit midpoint type discretization that preserves the conformal symplectic structure is

$$\frac{e^{\gamma_1 h} y^{n+1} - e^{-\gamma_2 h} y^n}{h} = N\left(\frac{e^{\gamma_1 h} y^{n+1} + e^{-\gamma_2 h} y^n}{2}\right)$$

with $\gamma_1 + \gamma_2 = \gamma$.

- $\gamma_1 = \gamma$ and $\gamma_2 = 0$ (first order) is discussed for Birkhoffian systems by Sun & Shang, *Phys. Lett. A* (2005), and Kong, Wu, & Mei, *J. Geom. Phys.* (2012)
- $\gamma_1 = \gamma_2 = \gamma/2$ (second order) was presented by Bhatt, Floyd, & M. *J. Sci. Comp.* (2015)

Example: Conformal Störmer-Verlet (CSV1)

Given the Hamiltonian system perturbed by Rayleigh damping

$$\dot{q} = \nabla_p T(p), \qquad \dot{p} = -\nabla_q V(q) - \gamma p$$

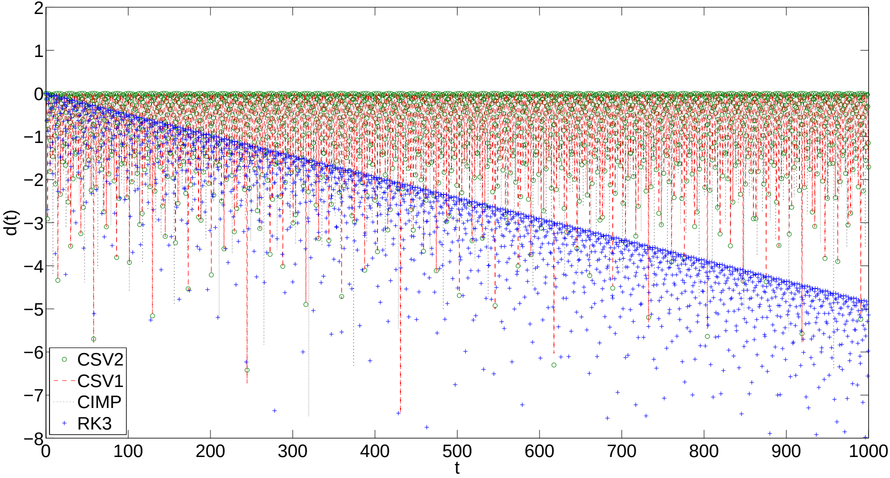
a Störmer-Verlet-like discretization that preserves the conformal symplectic structure is

$$\begin{aligned} p^{n+1/2} &= e^{-\gamma h} p^n - \frac{h}{2} \nabla_q V(q^n), \\ q^{n+1} &= q^n + h \nabla_p T(p^{n+1/2}), \\ p^{n+1} &= e^{-\gamma h} \left[p^{n+1/2} - \frac{h}{2} \nabla_q V(q^{n+1}) \right] \end{aligned}$$

- Modin & Söderlind, *BIT Numer. Math.* (2011)
- Bhatt, Floyd, & M. *J. Sci. Comp.* (2015)

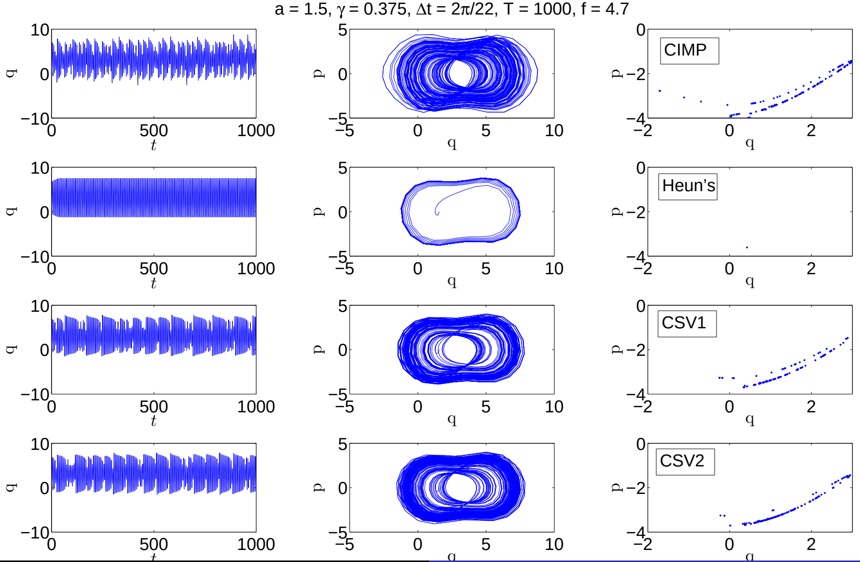
Numerical Dissipation Rates for a Damped Oscillator

$$\dot{q} = p, \quad \dot{p} = -\omega^2 q - 2\gamma p, \qquad d(t_n) = \ln(q_n) + \gamma t_n$$



Forced-Damped Chaotic Pendulum

$$\dot{q} = p, \qquad \dot{p} = -a^2 \sin(q) + f_d \sin(t) - 2\gamma p$$



Consider the IVP

$$\dot{y}(t) = N(y(t)) - \gamma(t)y(t), \quad y(0) = y_0$$

where $y \in \mathbb{R}^d$ with $d \in \mathbb{N}$, $\gamma : \mathbb{R} \to \mathbb{R}$, and $N : \mathbb{R}^d \to \mathbb{R}^d$

Definition of conformal invariant

$\mathcal{I} : \mathbb{R}^d \to \mathbb{R}$ is a *conformal invariant* for the IVP if $\frac{d}{dt}\mathcal{I} = -\gamma(t)\mathcal{I}$.

Note: $\mathcal{I}(y(t)) = e^{-\int_0^t \gamma(s)ds}\mathcal{I}(y_0) \implies \frac{d}{dt}\mathcal{I} = -\gamma(t)\mathcal{I}$.

Definition of numerical preservation

A numerical method *preserves* a conformal invariant if it satisfies

$$\mathcal{I}_{n+1} = e^{-\int_{t_n}^{t_{n+1}} \gamma(s)ds}\mathcal{I}_n$$

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Generalizations

Consider the IVP

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Examples of conformal invariants

- Pendulum: $\ddot{q} + 2\gamma\dot{q} + \sin q = 0$
  $\mathcal{I} = dq \wedge d\dot{q}$
- Oscillator: $\ddot{q} + 2\gamma\dot{q} + \kappa^2 q = 0$
  $\mathcal{I} = (\kappa^2 q^2 + \dot{q}^2)/2 + \gamma q\dot{q}$
- Rigid Body: $\dot{y} = B(y)\nabla H(y) - \gamma y$ with $y = [y_1, y_2, y_3]^T$
  $\mathcal{I} = y_1^2 + y_2^2 + y_3^2$ and $H(y) = \frac{1}{2}\left(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\right)$
- Klein-Gordon: $u_{tt} - u_{xx} + cu + 2\gamma u_t = 0$
  $\mathcal{I} = \int u_t u_x \ dx$
- Schrödinger: $\mathtt{i}\psi_t + \psi_{xx} + V'(|\psi|^2)\psi + \mathtt{i}\gamma\psi = 0$
  $\mathcal{I} = \int |\psi|^2 \ dx$
- Camassa Holm: $u_t - u_{xxt} + 3uu_x + \gamma(u - u_{xx}) = 2u_x u_{xx} + uu_{xxx}$
  $\mathcal{I} = \int (u^2 + u_x^2) \ dx$
- KdV: $u_t + uu_x + u_{xxx} + 2\gamma u = 0$
  $\mathcal{I} = \int u \ dx$

Exponential Runge-Kutta Methods

Runge-Kutta type methods for solving $\dot{y} = N(y) - \gamma y$

$$Y_i = \phi_i(h;\gamma_n)y_n + h\sum_{j=1}^{s} a_{ij}(h;\gamma_n)N(Y_j), \quad i = 1,\ldots,s,$$

$$y_{n+1} = \phi_0(h;\gamma_n)y_n + h\sum_{i=1}^{s} b_i(h;\gamma_n)N(Y_i).$$

The *coefficient functions*, ϕ_i, ϕ_0, a_{ij}, and b_i satisfy

$$\phi_i(h;0) = \phi_0(h;0) = 1, \qquad a_{ij}(h;0) = \alpha_{ij}, \qquad b_i(h;0) = \beta_i$$

for all $i, j = 1, 2, \ldots, s$.

Similar results hold for partitioned exponential RK methods.

Numerical structure preservation

Theorem

An ERK method is conformal symplectic and preserves conformal quadratic invariants if it has scalar coefficient functions which satisfy $\phi_0 = e^{-\int_{t_n}^{t_{n+1}} \gamma(s)ds}$ *and*

$$a_{ji} b_i \frac{\phi_0}{\phi_i} + a_{ij} b_j \frac{\phi_0}{\phi_j} - b_i b_j = 0 \qquad \forall i, j = 1, 2, \ldots, s.$$

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Example

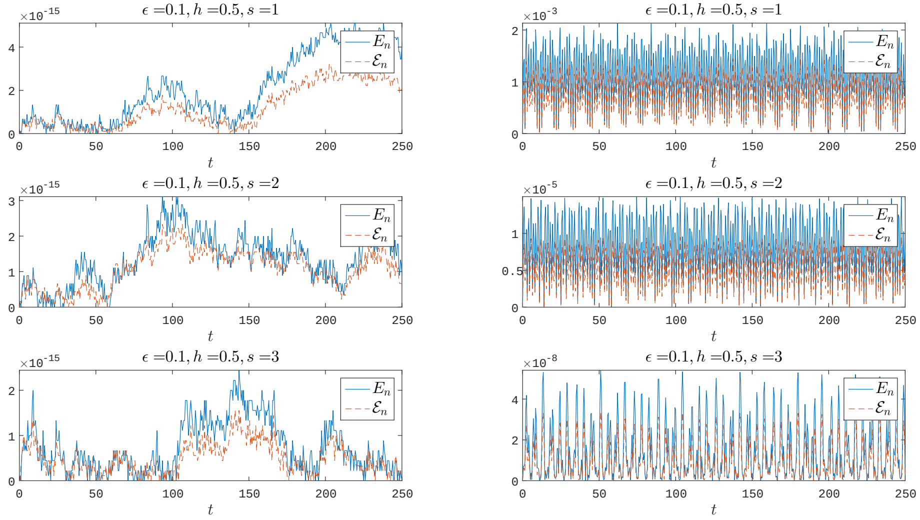
Setting $s = 1$, $a_{11} = 1/2$, $b_1 = e^{-\int_{t_{n+1/2}}^{t_{n+1}} \gamma(s)ds}$, $\phi_1 = e^{-\int_{t_n}^{t_{n+1/2}} \gamma(s)ds}$, gives an implicit midpoint type method

$$w_1 y_{n+1} - w_0 y_n = hN\left(\frac{1}{2}(w_1 y_{n+1} + w_0 y_n)\right),$$

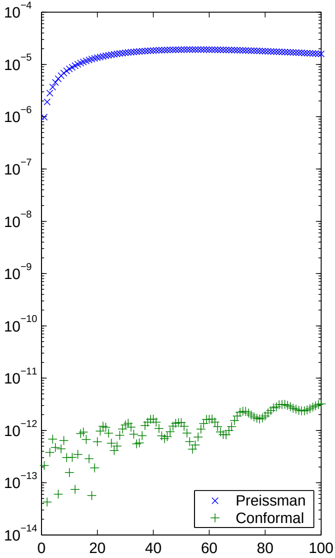
with $w_0 = \phi_1$ and $w_1 = 1/b_1$.

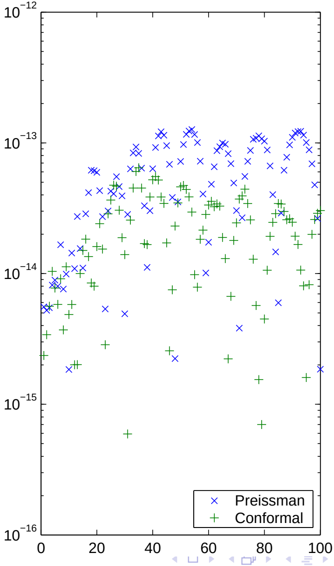
Periodically perturbed rigid body, $\gamma(t) = \epsilon \cos(2t)$

Conformal invariant error. Left: ERK; Right: Gauss-Legendre



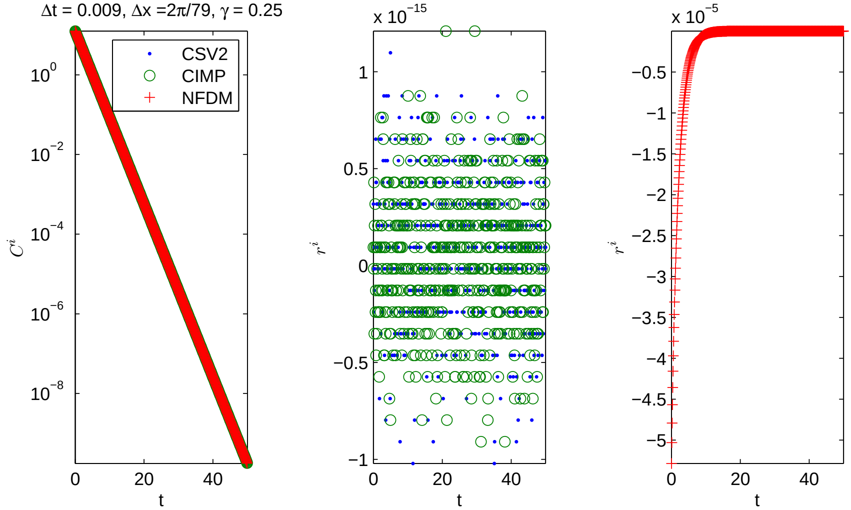
Preservation of Dissipation in Norm and Momentum for $i\psi_t + \psi_{xx} + 2|\psi|^2\psi + i0.005\psi = 0$





Preservation of Mass Dissipation for $u_t + uu_x = -2\gamma u$

$$\partial_t C = -2\gamma C \qquad \text{with} \qquad C = \int u dx$$



We have seen ODEs that satisfy properties of the form

$$\frac{d}{dt}\mathcal{I} = -\gamma\mathcal{I}.$$

There are PDEs that satisfy properties of the form

$$P_t + Q_x = -aP - bQ.$$

which is a direct result of

$$\partial_t \left(e^{(at+bx)} P \right) + \partial_x \left(e^{(at+bx)} Q \right) = 0.$$

Thus, we say a numerical method preserves this property if it satisfies a discrete version of the property.

Examples

- Generalized Diffusionless Burgers-Fisher Equation

$$u_t + \beta u^\alpha u_x = \gamma u(1 - u^\alpha)$$

- Damped Linear KdV-Burgers Equation

$$u_t + u_{xxx} + \alpha u_{xx} + \beta u_x + \gamma u = 0$$

- Non-linear Schrödinger Type Equation

$$i\psi_t + \psi_{xx} + (\alpha + i\beta)\psi_x + (\delta + i\gamma)\psi + V'(|\psi|)\psi = 0$$

- Non-linear Wave Equation

$$u_{tt} + 2au_t - (\partial_x + 2b)\sigma'(u_x) + f'(u) = 0$$

- etc.

General PDEs and Conservation Laws

The PDEs can, in general, be stated

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

where $\mathbf{K}$ and $\mathbf{L}$ are skew-symmetric.

- Multi-Symplectic: $\partial_t \left(e^{(at+bx)}\omega\right) + \partial_x \left(e^{(at+bx)}\kappa\right) = 0$
- Linear Symmetries: inner product of equation with $\mathbf{B}z$

  $$\partial_t \left(e^{(at+bx)} z^T \mathbf{KB}z\right) + \partial_x \left(e^{(at+bx)} z^T \mathbf{LB}z\right) = 0$$
- Energy: iff $a = 0$

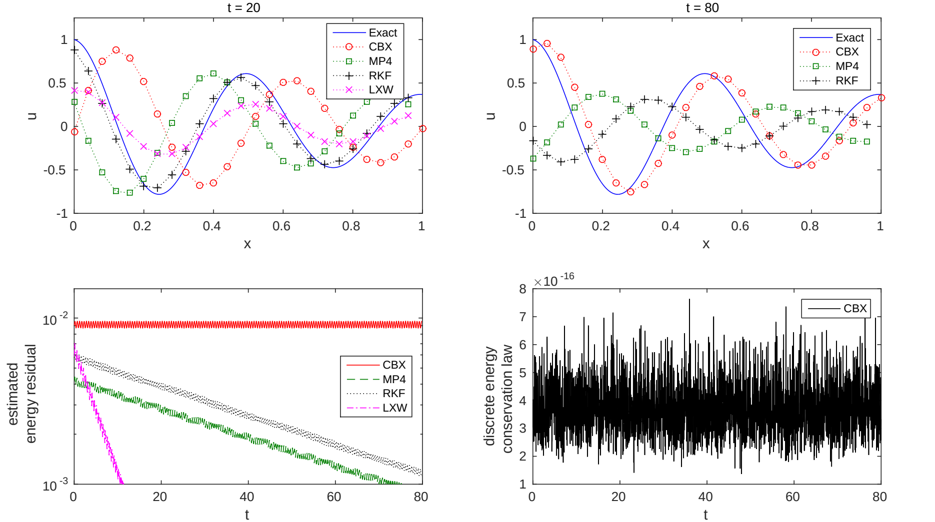
  $$\partial_t \left(e^{bx} \left(S(z) + \tfrac{1}{2}(z_x^T \mathbf{L}z)\right)\right) + \partial_x \tfrac{1}{2}(e^{bx} z^T \mathbf{L}z_t) = 0$$
- Momentum: iff $b = 0$

  $$\partial_x \left(e^{at} \left(S(z) + \tfrac{1}{2}(z_t^T \mathbf{K}z)\right)\right) + \partial_t \tfrac{1}{2}(e^{at} z^T \mathbf{K}z_x) = 0$$

To preserve, apply conformal methods in space and time.

$u = e^{-x}\cos(4\pi(x-t))$ as solution of $u_t + u_x + u = 0$

$\Delta t = 0.025,\ \Delta x = 0.04$



Conclusion and Future Work

Summary

- General approach for constructing high order (Runge-Kutta-like) structure-preserving algorithms.
- The methods are designed for conservative equations that are perturbed by linear non-conservative terms.
- Various properties (relating to energy, momentum, mass, symplecticity, etc.) may be preserved.
- Dissipation rates are exactly preserved for linear problems.

Future Work

- Backward error analysis.
- Usefulness for spatial discretizations of PDEs.
- Extensions to problems where γ is a matrix.
- Construction of exponential time-differencing methods.