# Energy Preserving Numerical Integration Methods

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# Outline of the talk

Energy-preserving integrators for ODEs

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Energy-preserving integrators for ODEs

Energy-preserving integrators for PDEs

# PART I

Energy-preserving integrators for Ordinary Differential Equations

Consider a Poisson ODE:

$$\frac{dx}{dt} = S(x)\nabla H(x).$$

Here $S(x)$ is a skew matrix, and $\nabla H$ is the gradient of the Hamiltonian energy function.

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### Definition (Skew matrix)

$S(x)$ is skew if

$$(a \cdot S(x)b) = -(b \cdot S(x)a) \quad \forall a, b$$

# ENERGY-PRESERVING DISCRETE GRADIENT METHOD

## Definition (Discrete gradient)

A discrete gradient $\overline{\nabla} H(x_n, x_{n+1})$ is defined by

(i) $(x_{n+1} - x_n) \cdot \overline{\nabla} H(x_n, x_{n+1}) \equiv H(x_{n+1}) - H(x_n)$

and

(ii) $\lim_{x_{n+1} \to x_n} \overline{\nabla} H(x_n, x_{n+1}) = \nabla H(x_n)$

## Theorem

*Let* $\overline{\nabla} H$ *be a discrete gradient. Then the discretization*

$$\frac{x_{n+1} - x_n}{\Delta t} = S(x_n)\overline{\nabla} H(x_n, x_{n+1})$$

*is energy-preserving.*

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*is energy-preserving.*

## Proof.

$$\begin{aligned} H(x_{n+1}) - H(x_n) &= \overline{\nabla} H(x_n, x_{n+1}) \cdot (x_{n+1} - x_n) \\ &= \Delta t \overline{\nabla} H(x_n, x_{n+1}) \cdot S(x_n) \overline{\nabla} H(x_n, x_{n+1}) \\ &= 0 \end{aligned}$$

□

# TWO EXAMPLES OF DISCRETE GRADIENTS

Remember $(x_{n+1} - x_n) \cdot \overline{\nabla} H(x_n, x_{n+1}) \equiv H(x_{n+1}) - H(x_n)$

**Example 1.** (Itoh-Abe discrete gradient):

$$\overline{\nabla} H := \begin{pmatrix} \frac{H(x_{n+1}, y_n) - H(x_n, y_n)}{x_{n+1} - x_n} \\ \frac{H(x_{n+1}, y_{n+1}) - H(x_{n+1}, y_n)}{y_{n+1} - y_n} \end{pmatrix}.$$

(This can be generalised to any dimension)

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(This can be generalised to any dimension)

**Example 2.** ("Average" discrete gradient):

$$\overline{\nabla} H \quad := \int_0^1 \nabla H(\xi x_{n+1} + (1 - \xi) x_n)\, d\xi$$

## Proof.

$$
\begin{aligned}
(x_{n+1} - x_n) \cdot \overline{\nabla} H &= \int_0^1 (x_{n+1} - x_n) \nabla H(\xi x_{n+1} + (1-\xi) x_n)\, d\xi \\
&= \int_0^1 \frac{d}{d\xi} H(\xi x_{n+1} + (1-\xi) x_n)\, d\xi \\
&= H(\xi x_{n+1} + (1-\xi) x_n) \Big|_{\xi=0}^{\xi=1} \\
&= H(x_{n+1}) - H(x_n)
\end{aligned}
$$

□

So

$$\frac{x_{n+1} - x_n}{\Delta t} = S(x) \int_0^1 \nabla H(\xi x_{n+1} + (1-\xi)x_n)\, d\xi$$

is an energy preserving integrator for the ODE

$$\frac{dx}{dt} = S(x)\nabla H(x)$$

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But note that $S\nabla H$ is the vector field! We get:

## Theorem (The "average vector field method")

*The numerical integration method*

$$\frac{x_{n+1} - x_n}{\Delta t} = \int_0^1 f(\xi x_{n+1} + (1-\xi) x_n)\, d\xi$$

*preserves the energy $H(x)$ exactly for any Hamiltonian ODE with constant symplectic structure, i.e. for*

$$\frac{dx}{dt} = f(x)$$

*with*

$$f(x) = S\nabla H(x)$$

## Example (DOUBLE WELL POTENTIAL)

$$\begin{aligned} \frac{dx}{dt} &= y \\ \frac{dy}{dt} &= 2x(1-x^2) \end{aligned}$$

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AVF integrator

$$\frac{1}{\Delta t}\begin{pmatrix} x_{n+1}-x_n \\ y_{n+1}-y_n \end{pmatrix} = \begin{pmatrix} \frac{1}{2}(y_{n+1}+y_n) \\ x_{n+1}+x_n-\frac{1}{2}(x_n^3+x_n^2x_{n+1}+x_nx_{n+1}^2+x_{n+1}^3) \end{pmatrix}$$

# PART II

Energy-preserving integrators for Partial Differential Equations

# Hamiltonian PDEs

## Definition

The PDE

$$\frac{\partial u}{\partial t} = f\left(u, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \dots\right)$$

is Hamiltonian if it is of the form

$$f\left(u, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \dots\right) = \hat{\mathcal{S}}\,\frac{\delta \mathcal{H}}{\delta u}$$

where $\hat{\mathcal{S}}$ is a constant skew operator, and $\dfrac{\delta \mathcal{H}}{\delta u}$ is the variational derivative of $\mathcal{H}$.

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where $\hat{\mathcal{S}}$ is a constant skew operator, and $\frac{\delta \mathcal{H}}{\delta u}$ is the variational derivative of $\mathcal{H}$.

(Note: $f, u$, and $x$ can also be taken to be vectors. Although $u$ is usually real, it may also be complex).

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## Definition (Variational derivative)

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$$\mathcal{H}(u) := \int H\left(u, \frac{\partial u}{\partial x}, \frac{\partial^2 u}{\partial x^2}, \ldots\right) dx$$

then

$$\frac{\delta \mathcal{H}}{\delta u} := \frac{\partial H}{\partial u} - \frac{\partial}{\partial x}\left(\frac{\partial H}{\partial u_x}\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\partial H}{\partial u_{xx}}\right) - \cdots$$

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## Definition (skew operator)

$\hat{S}$ is skew if $\langle a.\hat{S}b\rangle = -\langle b.\hat{S}a\rangle, \ \forall a, b$ where $\langle a.c\rangle := \int a(x)b(x)dx$

## Example (1. sine-Gordon equation (a))

$$\frac{\partial^2 \varphi}{\partial t^2} = \frac{\partial^2 \varphi}{\partial x^2} + \alpha \sin \varphi$$

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Continuous:

$$\begin{aligned}\mathcal{H} &= \int\left[\frac{1}{2}\pi^2 + \frac{1}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 + \alpha(1-\cos(\varphi))\right]dx \\ \hat{\mathcal{S}} &= \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}.\end{aligned}$$

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Semi-discrete $\left(\frac{\partial\varphi}{\partial x} \to \frac{\varphi_n - \varphi_{n-1}}{\Delta x}\right)$

$$\begin{aligned}H &= \Delta x\sum_n\left[\frac{1}{2}\pi_n^2 + \frac{1}{2(\Delta x)^2}(\varphi_n - \varphi_{n-1})^2 + \alpha\left(1-\cos(\varphi_n)\right)\right] \\ S &= \begin{pmatrix} 0 & id \\ -id & 0 \end{pmatrix}, \nabla \text{ denotes standard gradient}\end{aligned}$$

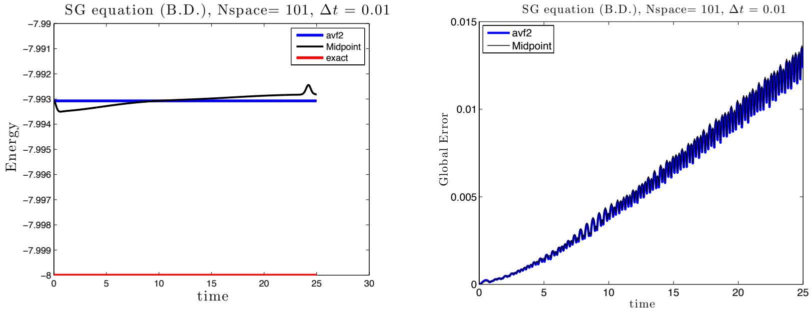


Figure: sine-Gordon equation, Backward Differences for spatial discretizations : Energy (left) and global error (right) vs time, for AVF and implicit midpoint integrators.

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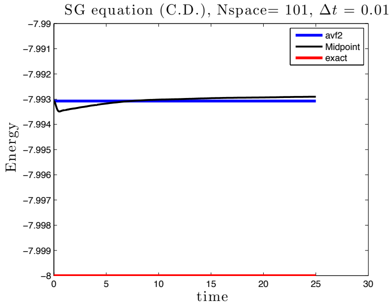
Semi-discrete $\left(\frac{\partial \varphi}{\partial x} \to \frac{\varphi_{n+1} - \varphi_{n-1}}{2\Delta x}\right)$

$$\begin{aligned} H &= \Delta x \sum_n \left[ \frac{1}{2}\pi_n^2 + \frac{1}{8(\Delta x)^2}(\varphi_n - \varphi_{n-1})^2 + \alpha\left(1-\cos(\varphi_n)\right) \right] \\ S &= \begin{pmatrix} 0 & id \\ -id & 0 \end{pmatrix}. \end{aligned}$$



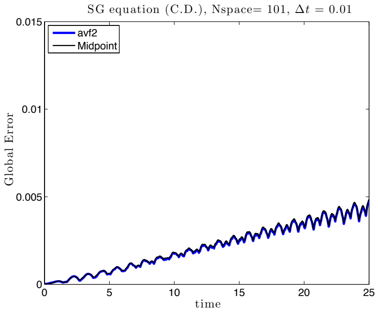




Figure: sine-Gordon equation, Central Differences for spatial discretizations : Energy (left) and global error (right) vs time, for AVF and implicit midpoint integrators.

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Semi-discrete: $(u^3 \to u_n^3)$

$$\begin{aligned} H &= \Delta x \sum_n \left[\frac{1}{2(\Delta x)^2}(u_n - u_{n-1})^2 - u_n^3\right] \\ S &= \frac{1}{2\Delta x}\begin{pmatrix} 0 & 1 & & \dots & & & -1 \\ -1 & 0 & 1 & 0 & & & \\ & -1 & 0 & 1 & & & \\ \vdots & & & & \ddots & & \\ & & & & & & \\ & & & & -1 & 0 & 1 \\ 1 & & & & & -1 & 0 \end{pmatrix} \end{aligned}$$

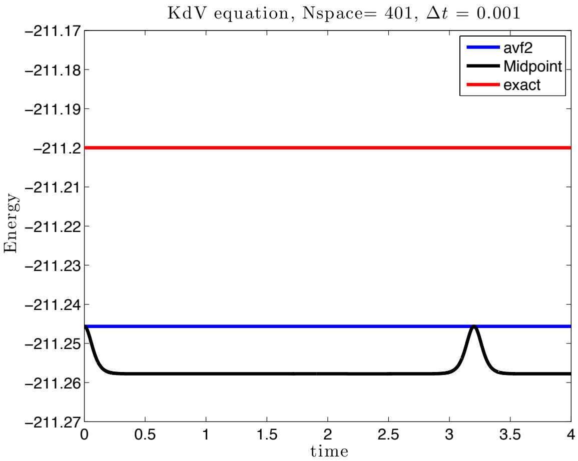


Figure: KdV equation: Exact energy, and energy vs time given by AVF and implicit midpoint methods, using discretization (a).

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Semi-discrete: $(u^3 \to u_n u_{n+1} u_{n+2})$ (for illustrative purposes only)

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Note: Large freedom in semi-discretisation $H$ without destroying energy preservation. But $S$ must be **skew**!

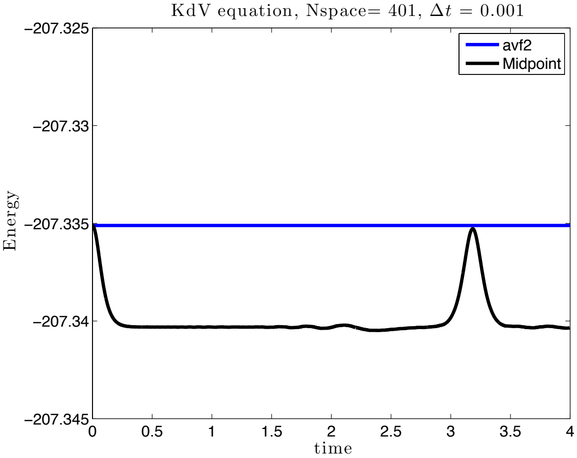


Figure: KdV equation: Energy vs time given by AVF and implicit midpoint methods, using discretization (b).

## Example (5. NLS equation)

Continuous:

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ u^* \end{pmatrix} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}\begin{pmatrix} \frac{\delta \mathcal{H}}{\delta u} \\ \frac{\delta \mathcal{H}}{\delta u^*} \end{pmatrix}, \tag{1}$$

where $u^*$ denotes the complex conjugate of $u$.

$$\mathcal{H} = \int \left[ - \left| \frac{\partial u}{\partial x} \right|^2 + \frac{\gamma}{2} |u|^4 \right] dx, \tag{2}$$

$$\hat{\mathcal{S}} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}. \tag{3}$$

## Example (5. NLS equation)

Continuous:

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ u^* \end{pmatrix} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}\begin{pmatrix} \frac{\delta \mathcal{H}}{\delta u} \\ \frac{\delta \mathcal{H}}{\delta u^*} \end{pmatrix}, \tag{1}$$

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Semi-discrete:

$$H = \sum_j \left[ -\frac{1}{(\Delta x)^2} \left| u_{j+1} - u_j \right|^2 + \frac{\gamma}{2} |u_j|^4 \right], \tag{4}$$

$$S = i \begin{pmatrix} 0 & \mathrm{id} \\ -\mathrm{id} & 0 \end{pmatrix}. \tag{5}$$

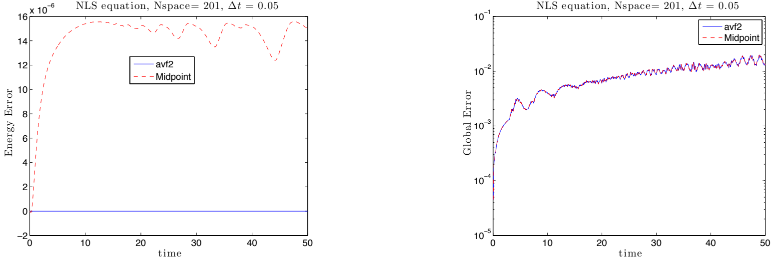


Figure: Nonlinear Schrödinger equation: Energy error (left) and global error (right) vs time, for AVF and implicit midpoint integrators.

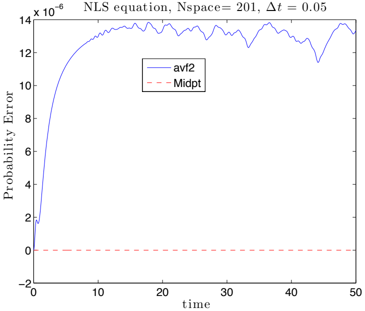


Figure: Nonlinear Schrödinger equation: Total probability error vs time, for AVF and implicit midpoint integrators.

## Example (6. Nonlinear Wave Equation)

$$\frac{\partial^2 \varphi}{\partial t^2} = (\partial_x^2 + \partial_y^2)\varphi - \varphi^3$$

Continuous:

$$\mathcal{H} = \int_{-1}^{1}\int_{-1}^{1} \left[\frac{1}{2}(\pi^2 + \varphi_x^2 + \varphi_y^2) + \frac{1}{4}\varphi^4\right] dx\, dy$$

$$\hat{\mathcal{S}} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

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Semi-discrete: We discretize the Hamiltonian in space with a tensor product Lagrange quadrature formula based on $p+1$ Gauss-Lobatto-Legendre (GLL) quadrature nodes in each space direction:

## Nonlinear Wave Equation II

$$\overline{\mathcal{H}} = \frac{1}{2}\sum_{j_1=0}^{p}\sum_{j_2=0}^{p} w_{j_1} w_{j_2}\left(\pi_{j_1,j_2}^2 + \left(\sum_{k=0}^{p} d_{j_1,k}\varphi_{k,j_2}\right)^2 + \left(\sum_{m=0}^{p} d_{j_2,m}\varphi_{j_1,m}\right)^2 + \frac{1}{2}\varphi_{j_1,j_2}^4\right)$$

where $d_{j_1,k} = \left.\frac{dl_k(x)}{dx}\right|_{x=x_{j_1}}$, and $l_k(x)$ is the $k$-th Lagrange basis function based on the GLL quadrature nodes $x_0,\ldots,x_p$, and with $w_0,\ldots,w_p$ the corresponding quadrature weights.

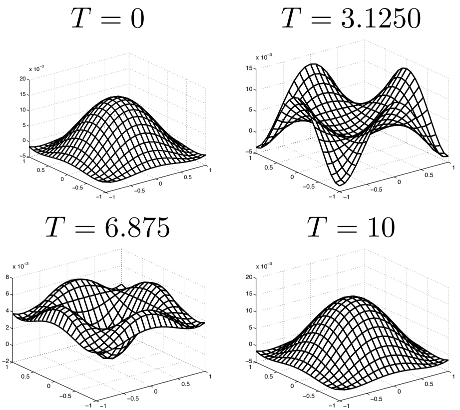


Figure: Snapshots of the solution of the 2D wave equation at different times. AVF method with step-size $\Delta t = 0.6250$. Space discretization with 6 Gauss Lobatto nodes in each space direction. Numerical solution interpolated on a equidistant grid of 21 nodes in each space direction.

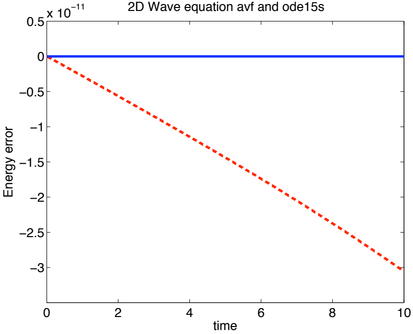


Figure: The 2D wave equation. MATLAB routine `ode15s` with absolute and relative tolerance $10^{-14}$ (dashed line), and AVF method with step size $\Delta t = 10/(2^5)$ (solid line). Energy error versus time. Time interval $[0, 10]$. Space discretization with 6 Gauss Lobatto nodes in each space direction.

# Leapfrog

# Exponential Integrator

# GENERALIZATIONS AND FURTHER REMARKS

- Instead of using finite differences for the (semi-)discretization of the spatial derivatives one may use e.g. a spectral discretization.

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- The method presented also applies to linear PDEs, e.g. the (Linear) Time-dependent Schrödinger equation, 3D Maxwell's equation.

# GENERALIZATIONS AND FURTHER REMARKS

- Instead of using finite differences for the (semi-)discretization of the spatial derivatives one may use e.g. a spectral discretization.

- The method presented also applies to linear PDEs, e.g. the (Linear) Time-dependent Schrödinger equation, 3D Maxwell's equation.

- The method presented can be generalised to

$$\frac{\partial u}{\partial t} = \hat{\mathcal{N}} \frac{\delta \mathcal{H}}{\delta u}$$

where $\hat{\mathcal{N}}$ is a constant negative (semi) definite operator, and where $\mathcal{H}$ is a Lyapunov function, i.e. $\frac{\partial \mathcal{H}}{\partial t} \leq 0$.
(e.g. Allen-Cahn eq, Cahn-Hilliard eq, Ginzburg-Landau eq.)

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- The Average Vector Field Method is a B-series method.

# Some references to our work

ODEs

1. McLachlan, Quispel & Robidoux, A unified approach to Hamiltonian systems, Poisson systems, gradient systems and systems with Lyapunov functions and/or first integrals, Phys. Rev. Lett. **81**(1998)2399–2103.
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3. Quispel & McLaren, A new class of energy-preserving numerical integration methods, J. Phys **A41**(2008)045206 (7pp).

PDEs

4. Celledoni, Grimm, McLachlan, McLaren, O'Neale & Quispel, Preserving energy resp. dissipation in numerical PDEs, using the 'Average Vector Field' method, Submitted for publication.

Of course there are also many important publications by Furihata, Matsuo, Yaguchi, and collaborators.