ENERGY PRESERVATION (DISSIPATION) IN NUMERICAL ODEs and PDEs

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Abstract

This note considers energy-preservation properties of Runge-Kutta and other one-step methods for ordinary and partial differential equations.

Average vector field method, Hamiltonian ODEs, time integration, discrete gradients, Runge-Kutta mehtods.

1 Introduction

Consider the ordinary differential equation (ODE)

$$\dot{y} = f(y), \quad y(0) = y_0 \in \mathbf{R}^n,$$

we have seen the the following definition of first integral (or invariant) of the ODE:

Definition 1.1. *A function $\mathcal{I} : \mathbf{R}^m \to \mathbf{R}$ is a first integral (or invariant) of the ODE if and only if*

$$\nabla \mathcal{I}(y)^T f(y) = 0, \quad \forall y. \tag{1}$$

This implies that $\mathcal{I}$ is constant along solutions of the differential equations i.e.

$$\frac{d\, I(y(t))}{dt} = \nabla\, I(y(t))^T f(y(t)) = 0, \quad \forall t > 0.$$

We distinguish between linear, quadratic and polynomial invariants of degree higher than 2. Linear invariants are of the type

$$I(y) = d^T y, \quad d \in \mathbf{R}^n.$$

Quadratic invariants are of the type

$$Q(y) = y^T C y, \quad C = C^T.$$

An example of a polynomial invariant of degree higher than 2 is the determinant of a matrix valued solution of a matricial ODE of the type

$$\dot{y} = A(y)y, \quad y(0) = I, \quad \text{trace}(A) = 0, \quad \det(y) = 1,$$

and A $n \times n$, $n \geq 3$.

We have seen that all Runge-Kutta methods preserve all linear invariants, and that a special class of Runge-Kutta methods preserve all quadratic invariants. We will next show that no (consistent) Runge-Kutta method can preserve all polynomial invariants of degree greater than or equal to 3. To this aim we will provide a counter example.

For the counter example we need two preliminary lemmas.

Lemma 1.2. *If $\dot{y} = By$, $y(0) = y_0$ with B an $m \times m$ matrix not depending on y and on t, $y_0 \in \mathbf{R}^m$, then using a Runge-Kutta method on this system of equations gives $y_{n+1} = R(hB)y_n$ where $R(z)$ is a rational function (the stability function of the Runge-Kutta method.*[1]*)*

Proof. Consider simply the scalar ode $\dot{u} = \lambda u$, $u(0) = u_0$, applying the Runge-Kutta method gives

$$u_{n+1} = u_n + h\sum_{i=1}^{s} b_i K_i$$
$$K_i = \lambda\big(u_n + h\sum_{j=1}^{s} a_{i,j}K_j\big), \quad i = 1, \ldots, s.$$

Consider the vector

$$\vec{K}^T := [K_1, \ldots, K_s].$$

The stages solve the linear algebraic equation

$$(I - h\lambda A)\vec{K} = \lambda u_n \mathbf{1}$$

with $\mathbf{1}$ the vector in $\mathbf{R}^s$ with components equal to 1. Then

$$u_{n+1} = u_n + hb^T\vec{K}$$

and

$$u_{n+1} = u_n\left(1 + h\lambda b^T(I - h\lambda A)^{-1}\mathbf{1}\right).$$

The expression in the parenthesis is the determinant of the rank one perturbation of the identity

$$I + h\lambda(I - h\lambda A)^{-1}\mathbf{1}b^T$$

which, since

$$I + h\lambda(I - h\lambda A)^{-1}\mathbf{1}b^T = (I - h\lambda A)^{-1}(I - h\lambda A + \lambda h\mathbf{1}b^T),$$

[1] See note in lecture 2, section 5.

can be written as a quotient of determinants so

$$u_{n+1} = u_n \frac{\det(I - h\lambda A + h\lambda \mathbf{1} b^T)}{\det(I - h\lambda A)}.$$

Which shows that $u_{n+1} = R(h\lambda)u_n$ with R a rational function (a quotient of two polynomials). The generalization to linear systems of ODEs involves the use of Kroneker tensor products of the matrix B and the Runge-Kutta matrix A and some extra linear algebra. □

Lemma 1.3. *$R(z)$ is an analytic function s.t. $R(0) = 1$ and $R'(0) = 1$ and satisfying*

$$R(z)^2 R(-2z) \equiv 1$$

if and only if

$$R(z) = e^z$$

.

Proof. By taking logarithms we have

$$\psi(z) := \log(R(z)) = \sum_{k=0}^{\infty} \psi_k \, z^k,$$

so $R(z) = e^{\psi(z)}$. By the properties of logarithms we have

$$\log(R(z)^2 R(-2z)) = 2\log(R(z)) + \log(R(-2z)) = 2\psi(z) + \psi(-2z) = 0.$$

So expanding the series and collecting terms we get

$$2\psi(z) + \psi(-2z) = \sum_{k=0}^{\infty} \psi_k \, z^k (2 - 2^k) = 0,$$

since $(2 - 2^k) \neq 0$ for $k \geq 2$, ψ_k must be zero for $k \geq 2$. Also since $R(0) = 1 = e^{\psi(0)}$ $\psi_0 = 0$ and

$$\psi(z) = \psi_1 \, z,$$

finally $R'(0) = \psi_1 e^{\psi_1 z}\big|_{z=0} = 1$ gives $\psi_1 = 1$ so

$$R(z) = e^z.$$

□

Remark: As from Lemma 1.2 the stability function of a Runge-Kutta method is a rational function, no Runge-Kutta method can have the exponential function as a stability function.

Example 1.4. *[8] We consider the following simple ODE*

$$\begin{aligned} \dot{x} &= x \\ \dot{y} &= y \\ \dot{z} &= -2z \end{aligned}$$

with initial value $x(0) = x_0$, $y(0) = y_0$, $z(0) = z_0$. *We observe that*

$$x(t)y(t)z(t) = e^t x_0 e^t y_0 e^{-2t} z_0 = x_0 y_0 z_0$$

is a cubic invariant of the flow. The equation can be written in the form

$$\dot{\mathbf{x}} = B\,\mathbf{x}, \quad \mathbf{x}(0) = \mathbf{x}_0,$$

where B *is the diagonal matrix with diagonal entries* $1, 1, -2$. *Applying a consistent Runge-Kutta method to this problem amounts to compute*

$$\mathbf{x}_1 = R(hB)\mathbf{x}_0,$$

where $R(z)$ *is the stability function of the Runge-Kutta method,* $R(0) = 1$ *and* $R'(0) = 1$ *(because of consistency), and* $R(z)$ *is a rational function. In particular multiplying together the components of* $\mathbf{x}_1$ *we obtain*

$$x_1 y_1 z_1 = R(h)^2 R(-2h) x_0 y_0 z_0.$$

The invariant is preserved by the Runge-Kutta method if and only if

$$R(h)^2 R(-2h) = 1, \quad \forall h.$$

Now since from the Lemma 1.3 this can happen only if $R(z) = e^z$, *and since no Runge-Kutta method has* e^z *as stability function, the preservation of this cubic invariant cannot be achieved with Runge-Kutta methods.*

2 Discrete Gradients

We consider a general ODE problem with an invariant I. It is always possible to write the ODE in the following form

$$\dot{y} = f(y) = S(y)\nabla I(y), \quad y(0) = y_0, \tag{2}$$

where $S(y)$ is a skew-symmetric matrix. A choice for $S(y)$, under the assumption that $\nabla I(y)$ does not vanish, is

$$S(y) = \frac{1}{\|\nabla I\|_2}(f(y)\nabla I(y)^T - \nabla I(y) f(y)^T),$$

[14], see the same reference for a discussion on the boundedness of $S(y)$ defined above around non degenerate fixed points of $\nabla I(y)$.

For problems reformulated in the form (2) it is is always possible to build an energy-preserving method by approximating ∇I by a so called discrete gradient.

Definition 2.1. *(Gonzalez 96, [9]).*
If I is differentiable then $\bar{\nabla} I : \mathbf{R}^n \times \mathbf{R}^n \to \mathbf{R}^n$ is a discrete gradient if I is continuous and

$$\begin{cases} \bar{\nabla} I(u,v)^T (v-u) &= I(v) - I(u) \\ \bar{\nabla} I(u,u) &= \nabla I(u) \end{cases}$$

Example 2.2. *Examples of discrete gradients*

1. $$\bar{\nabla} I(u,v) = \int_0^1 \nabla I\left((1-\xi)u + \xi v\right) d\xi$$
   is the average vector field discrete gradient;

2. $$\bar{\nabla} I(u,v) = \nabla I(\frac{u+v}{2}) + \frac{I(v) - I(u) - \nabla I(\frac{u+v}{2}^T (v-u)}{\|v-u\|^2}(v-u),$$
   this discrete gradient is due to Gonzalez.

Theorem 2.3. *A numerical integrator having the format*

$$y_{n+1} = y_n + h\bar{S}(y_n, y_{n+1})\bar{\nabla} I(y_n, y_{n+1}),$$

where $\bar{S}(y_n, y_{n+1}) \approx S(y)$ is a skew-symmetric matrix and $\bar{\nabla} I(y_n, y_{n+1}) \approx \nabla I$ in a neighborhood of y_n, is an energy-preserving integrator.

Proof. Using the definition of discrete gradient and the skew-symmetry of $\bar{S}(y_n, y_{n+1})$ we get

$$I(y_{n+1}) - I(y_n) = \bar{\nabla} I(y_n, y_{n+1})^T (y_{n+1} - y_n) = h\bar{\nabla} I(y_n, y_{n+1})^T \bar{S}(y_n, y_{n+1})\bar{\nabla} I(y_n, y_{n+1}) = 0.$$

□

Example 2.4. *The method*

$$y_{n+1} = y_n + hS(\frac{y_n + y_{n+1}}{2}) \int_0^1 \nabla I\left((1-\xi)u + \xi v\right) d\xi,$$

fits the framework of the previous theorem and is an energy preserving method. By using Taylor expansion it is possible to show that this method has order 2.

3 Preservation of the energy of Hamiltonian systems in the form $\dot{y} = J^{-1}\nabla H(y)$.

Consider the ODE $\dot{y} = f(y)$, $y(0) = y_0$, we call the integration method

$$\frac{y_{n+1} - y_n}{\Delta t} = \int_0^1 f((1-\xi)y_n + \xi y_{n+1})\, d\xi, \tag{3}$$

"Avegrage Vector Field method", [19].

Consider Hamiltonian systems

$$\dot{y} = f(y) = J^{-1}\nabla H(y), \quad y(0) = y_0. \tag{4}$$

Theorem 3.1. *Let y_n be the solution of the average vector field (AVF) method (18) applied to equation (4). Then the energy H is preserved exactly :*

$$H(y_{n+1}) = H(y_n).$$

Proof H is preserved since

$$\dot{H} = (\nabla H)^T J^{-1} \nabla H = 0. \tag{5}$$

It is possible to prove that this method has order 2 by usual Taylor expansion.

Corollary 3.2. *Given $b_1, \ldots, b_s$ and $c_1, \ldots, c_s$ defining a quadrature formula of polynomial order $m-1$. Consider an ODE of the type (4) where H is a polynomial of degree m. Then the s-stages Runge-Kutta method*

$$y_{n+1} = y_n + h \sum_{i=1}^{s} b_i \, f(y_n + (y_{n+1} - y_n)c_i)$$

preserves H and has order $\min(m, 2)$.

Proof. For polynomial Hamiltonians of degree m, $f = J^{-1}\nabla H$ has polynomial components of degree at most $m-1$ and

$$h \sum_{i=1}^{s} b_i \, f(y_n + (y_{n+1} - y_n)c_i) = \int_0^1 f((1-\xi)y_n + \xi y_{n+1}) \, d\xi.$$

So the given quadrature formula coincides with the exact integral, and the given method coincides with the AVF method. □

4 Hamiltonian PDEs and preservation of energy

This part is taken from [6]. We consider evolutionary PDEs with independent variables $(x,t) \in \mathbb{R}^d \times \mathbb{R}$, functions u belonging to a Banach space $\mathcal{B}$ with values[2] $u(x,t) \in \mathbb{R}^m$, and PDEs of the form

$$\dot{u} = \mathcal{D}\frac{\delta \mathcal{H}}{\delta u}, \tag{6}$$

[2]Although it is generally real-valued, the function u may also be complex-valued, for example, the nonlinear Schrödinger equation.

where $\mathcal{D}$ is a constant linear differential operator, the dot denotes $\frac{\partial}{\partial t}$, and

$$\mathcal{H}[u] = \int_\Omega H(x; u^{(n)})\, dx \tag{7}$$

where Ω is a subset of $\mathbb{R}^d \times \mathbb{R}$, and $dx = dx_1 dx_2 \dots dx_d$. $\frac{\delta \mathcal{H}}{\delta u}$ is the variational derivative of $\mathcal{H}$ in the sense that

$$\frac{d}{d\epsilon}\mathcal{H}[u + \epsilon v]\big|_{\epsilon=0} = \int_\Omega \frac{\delta \mathcal{H}}{\delta u} v\, dx, \tag{8}$$

for all $u, v \in \mathcal{B}$ (cf. [18]). For example, if $d = m = 1$,

$$\mathcal{H}[u] = \int_\Omega H(x; u, u_x, u_{xx}, \dots)\, dx, \tag{9}$$

then

$$\frac{\delta \mathcal{H}}{\delta u} = \frac{\partial H}{\partial u} - \partial_x \left(\frac{\partial H}{\partial u_x}\right) + \partial_x^2 \left(\frac{\partial H}{\partial u_{xx}}\right) - \cdots, \tag{10}$$

when the boundary terms are zero.

Similarly, for general d and m, we obtain

$$\frac{\delta \mathcal{H}}{\delta u_l} = \frac{\partial H}{\partial u_l} - \sum_{k=1}^{d} \frac{\partial}{\partial x_k}\left(\frac{\partial H}{\partial u_{l,k}}\right) + \dots, \quad l = 1, \dots, m. \tag{11}$$

We consider Hamiltonian systems of the form (6), where $\mathcal{D}$ is a constant skew symmetric operator (cf. [18]) and $\mathcal{H}$ the energy (Hamiltonian). In this case, we prefer to designate the differential operator in (6) with $\mathcal{S}$ instead of $\mathcal{D}$. The PDE preserves the energy because $\mathcal{S}$ is skew-adjoint with respect to the L_2 inner product, i.e.

$$\int_\Omega u \mathcal{S} u\, dx = 0, \quad \forall u \in \mathcal{B}. \tag{12}$$

The system (6) has $\mathcal{I} : \mathcal{B} \to \mathbb{R}$ as an integral if $\dot{\mathcal{I}} = \int_\Omega \frac{\delta \mathcal{I}}{\delta u} \mathcal{S} \frac{\delta \mathcal{H}}{\delta u}\, dx = 0$.
Integrals $\mathcal{C}$ with $\mathcal{D}\frac{\delta \mathcal{C}}{\delta u} = 0$ are called Casimirs.

Besides PDEs of type (6) where $\mathcal{D}$ is skew-adjoint, we also consider PDEs of type (6) where $\mathcal{D}$ is a constant negative (semi)definite operator with respect to the L_2 inner product, i.e.

$$\int_\Omega u \mathcal{D} u\, dx \le 0, \quad \forall u \in \mathcal{B}. \tag{13}$$

In this case, we prefer to designate the differential operator $\mathcal{D}$ with $\mathcal{N}$ and the function $\mathcal{H}$ is a Lyapunov function, since then the system (6), i.e.

$$\dot{u} = \mathcal{N}\frac{\delta \mathcal{H}}{\delta u}, \tag{14}$$

has $\mathcal{H}$ as a Lyapunov function, i.e. $\dot{\mathcal{H}} = \int_\Omega \frac{\delta \mathcal{H}}{\delta u} \mathcal{N} \frac{\delta \mathcal{H}}{\delta u}\, dx \le 0$. We will refer to systems (6) with a skew-adjoint $\mathcal{S}$ and an energy $\mathcal{H}$ as conservative and to systems (6) with a negative (semi)definite operator $\mathcal{N}$ and a Lyapunov function $\mathcal{H}$ as dissipative.

Conservative PDEs (6) can be semi-discretised in "skew-gradient" form

$$\dot{u} = \overline{\mathcal{S}}\nabla\overline{\mathcal{H}}(u), \qquad \overline{\mathcal{S}}^T = -\overline{\mathcal{S}}, \tag{15}$$

when $\mathcal{D} = \mathcal{S}$ is skew-adjoint. $u \in \mathbb{R}^k$, and here, and in the following, we will always denote the discretisations with bars. $\overline{\mathcal{H}}$ is chosen in such a way that $\overline{\mathcal{H}}\Delta x$ is an approximation to $\mathcal{H}$.

Lemma 4.1. *Let*

$$\mathcal{H}[u] = \int_\Omega H(x; u^{(n)})dx, \tag{16}$$

and let $\overline{\mathcal{H}}\Delta x$ be any consistent (finite difference) approximation to $\mathcal{H}$ (where $\Delta x := \Delta x_1 \Delta x_2 \dots \Delta x_d$). Then the discrete analogue of the variational derivative $\dfrac{\delta\mathcal{H}}{\delta u}$ is given by $\nabla\overline{\mathcal{H}}$.

Proof. For the proof see [6]. □

It is worth noting that the above lemma also applies directly when the approximation to $\mathcal{H}$ is obtained by a spectral discretization, since such an approximation can be viewed as a finite difference approximation where the finite difference stencil has the same number of entries as the number of grid points on which it is defined.

The operator ∇ is the standard gradient, which replaces the variational derivative because we are now working in a finite (although large) number of dimensions (cf. e.g. (11)).

When dealing with (semi-)discrete systems we use the notation $u_{j,n}$ where the index j corresponds to increments in space and n to increments in time. That is, the point $u_{j,n}$ is the discrete equivalent of $u(a + j\Delta x, t_0 + n\Delta t)$ where $x \in [a, b]$ and where t_0 is the initial time. In most of the equations we present, one of the indices is held constant, in which case, for simplicity, we drop it from the notation. For example, we use u_j to refer to the values of u at different points in space and at a fixed time level.

Theorem 4.2. *Let $\overline{\mathcal{S}}$ (resp. $\overline{\mathcal{N}}$) be any consistent constant skew (resp. negative-definite) matrix approximation to $\mathcal{S}$ (resp. $\mathcal{N}$). Let $\overline{\mathcal{H}}\Delta x$ be any consistent (finite difference) approximation to $\mathcal{H}$. Finally, let*

$$f(u) := \overline{\mathcal{S}}\nabla\overline{\mathcal{H}}(u) \qquad (\textit{resp. } f(u) := \overline{\mathcal{N}}\nabla\overline{\mathcal{H}}(u)), \tag{17}$$

and let u_n be the solution of the average vector field (AVF) method

$$\frac{u_{n+1} - u_n}{\Delta t} = \int_0^1 f((1-\xi)u_n + \xi u_{n+1})\, d\xi, \tag{18}$$

applied to equation (17). Then the semidiscrete energy $\overline{\mathcal{H}}$ is preserved exactly (resp. dissipated monotonically):

$$\overline{\mathcal{H}}(u_{n+1}) = \overline{\mathcal{H}}(u_n) \qquad (\textit{resp } \overline{\mathcal{H}}(u_{n+1}) \le \overline{\mathcal{H}}(u_n)).$$

$\overline{\mathcal{H}}$ is preserved since

$$\dot{\overline{\mathcal{H}}} = \left(\nabla\overline{\mathcal{H}}\right)^T \overline{\mathcal{S}}\nabla\overline{\mathcal{H}} = 0. \tag{19}$$

Discretisations of this type can be given for pseudospectral, finite-element, Galerkin and finite-difference methods (cf. [16, 17]); for simplicity's sake, we will concentrate on finite-difference methods, though we include one example of a pseudospectral method for good measure.

The AVF method was recently [19] shown to preserve the energy $\overline{\mathcal{H}}$ exactly for any vector field f of the form $f(u) = \overline{\mathcal{S}}\nabla\overline{\mathcal{H}}(u)$, where $\overline{\mathcal{H}}$ is an arbitrary function, and $\overline{\mathcal{S}}$ is any **constant** skew matrix [3]. The AVF method is related to discrete gradient methods (cf. [14]).

If $\mathcal{D}$ is a constant negative-definite operator, then the dissipative PDE (6) can be discretized in the form

$$\dot{u} = \overline{\mathcal{N}}\nabla\overline{\mathcal{H}}(u), \tag{20}$$

where $\overline{\mathcal{N}}$ is a negative (semi)definite matrix and $\overline{\mathcal{H}}$ is a discretisation as above.

That is, $\overline{\mathcal{H}}$ is a Lyapunov-function for the semi-discretized system, since

$$\dot{\overline{\mathcal{H}}} = \left(\nabla\overline{\mathcal{H}}\right)^T \overline{\mathcal{N}}\nabla\overline{\mathcal{H}} \leq 0. \tag{21}$$

The AVF method (18) again preserves this structure, i.e. we have

$$\overline{\mathcal{H}}(u_{n+1}) \leq \overline{\mathcal{H}}(u_n), \tag{22}$$

and $\overline{\mathcal{H}}$ is a Lyapunov function for the discrete system. Taking the scalar product of (18) with $\int_0^1 \nabla\overline{\mathcal{H}}((1-\xi)u_n + \xi u_{n+1})\,d\xi$ on both sides of the equation yields

$$\frac{1}{\Delta t}\int_0^1 (u_{n+1} - u_n)\cdot\nabla\overline{\mathcal{H}}((1-\xi)u_n + \xi u_{n+1})\,d\xi \leq 0, \tag{23}$$

i.e.

$$\frac{1}{\Delta t}\int_0^1 \frac{d}{d\xi}\overline{\mathcal{H}}((1-\xi)u_n + \xi u_{n+1})\,d\xi \leq 0, \tag{24}$$

and therefore

$$\frac{1}{\Delta t}(\overline{\mathcal{H}}(u_{n+1}) - \overline{\mathcal{H}}(u_n)) \leq 0. \tag{25}$$

Our purpose is to show that the procedure described above, namely

1. Discretize the energy functional $\mathcal{H}$ using any (consistent) approximation $\overline{\mathcal{H}}\Delta x$
2. Discretize $\mathcal{D}$ by a constant skew-symmetric (resp. negative (semi)definite) matrix
3. Apply the AVF method

can be generally applied and leads, in a systematic way, to energy-preserving methods for conservative PDEs and energy-dissipating methods for dissipative PDEs. We shall demonstrate the procedure by going through several well-known nonlinear and linear PDEs step by step. In particular we give examples of how to discretise nonlinear conservative PDEs (in subsection 2.1), linear conservative PDEs (in subsection 2.2), nonlinear dissipative PDEs (in subsection 3.1), and linear dissipative PDEs (in subsection 3.2).

[3] The relationship of (18) to Runge-Kutta methods was explored in [5].

5 Conservative PDEs

Example 5.1. *Sine-Gordon equation:*
Continuous:

$$\frac{\partial^2\varphi}{\partial t^2} = \frac{\partial^2\varphi}{\partial x^2} - \alpha \sin\varphi. \tag{26}$$

The Sine-Gordon equation is of type (6) with

$$\mathcal{H} = \int \left[\frac{1}{2}\pi^2 + \frac{1}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 + \alpha\left(1-\cos\varphi\right)\right] dx, \tag{27}$$

where $u := \begin{pmatrix} \varphi \\ \pi \end{pmatrix}$ and

$$\mathcal{S} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{28}$$

(Note that it follows that $\pi = \frac{\partial\varphi}{\partial t}$.)

Boundary conditions: periodic, $u(-20,t) = u(20,t)$.

Semi-discrete: finite differences[4]

$$\overline{\mathcal{H}}_{fd} = \sum_j \left[\frac{1}{2}\pi_j^2 + \frac{1}{2(\Delta x)^2}(\varphi_{j+1}-\varphi_j)^2 + \alpha\left(1-\cos\varphi_j\right)\right]. \tag{29}$$

$$\overline{\mathcal{S}} = \begin{pmatrix} 0 & \mathrm{id} \\ -\mathrm{id} & 0 \end{pmatrix}. \tag{30}$$

The resulting system of ordinary differential equations is

$$\begin{bmatrix} \dot{\boldsymbol{\varphi}} \\ \dot{\boldsymbol{\pi}} \end{bmatrix} = \overline{\mathcal{S}}\nabla\overline{\mathcal{H}}_{fd} = \begin{bmatrix} \boldsymbol{\pi} \\ \frac{1}{\Delta x^2} L\boldsymbol{\varphi} - \alpha\sin\boldsymbol{\varphi} \end{bmatrix}, \tag{31}$$

where L is the circulant matrix

$$L = \begin{bmatrix} -2 & 1 & & 1 \\ 1 & \ddots & \ddots & \\ & \ddots & \ddots & 1 \\ 1 & & 1 & -2 \end{bmatrix}.$$

We have used the bold variables $\boldsymbol{\varphi}$ and $\boldsymbol{\pi}$ for the finite dimensional vectors $[\varphi_1, \varphi_2, \ldots, \varphi_N]^\top$, *et cetera*, which replace the functions π and φ in the (semi-) discrete case. Where necessary, we will write $\boldsymbol{\varphi}_n$, *et cetera* to denote the vector $\boldsymbol{\varphi}$ at time $t_0 + n\Delta t$.

[4]Summations of the form $\sum_j$ mean $\sum_{j=0}^{N-1}$ unless stated otherwise.

The integral in the AVF method can be calculated exactly to give[5]

$$\frac{1}{\Delta t}\begin{bmatrix} \boldsymbol{\varphi}_{n+1}-\boldsymbol{\varphi}_n \\ \boldsymbol{\pi}_{n+1}-\boldsymbol{\pi}_n \end{bmatrix} = \begin{bmatrix} (\boldsymbol{\pi}_{n+1}+\boldsymbol{\pi}_n)/2 \\ L(\boldsymbol{\varphi}_{n+1}+\boldsymbol{\varphi}_n)/2 - \alpha(\cos\boldsymbol{\varphi}_{n+1}-\cos\boldsymbol{\varphi}_n)/(\boldsymbol{\varphi}_{n+1}-\boldsymbol{\varphi}_n) \end{bmatrix}. \tag{32}$$

Semi-discrete: spectral discretization

Instead of using finite differences for the discretization of the spatial derivative in (27), one may use a spectral discretization. This can be thought of as replacing φ with its Fourier series, truncated after N terms, where N is the number of spatial intervals, and differentiating the Fourier series. This can be calculated, using the discrete Fourier transform[6] (DFT), as $\mathcal{F}_N^{-1} d_N \mathcal{F}_N \boldsymbol{\varphi}$ where $\mathcal{F}_N$ is the matrix of DFT coefficients with entries given by $[\mathcal{F}_N]_{n,k} = \omega_N^{nk}$, $\omega_N = e^{\theta}$ and $\theta = i2\pi/l$ where $l = b-a$ is the extent of the spatial domain; that is $l/N = \Delta x$. Additionally, $[\mathcal{F}_N^{-1}]_{n,k} = \omega_N^{-nk}$ and d_N is a diagonal matrix whose (non-zero) entries are the wave-numbers $\theta_k = i2\pi k/l$, $k = 1, \ldots, N$, i.e., $[d_N]_{k,k} = \theta_k$. (For more details on properties of the DFT and its application to spectral methods see [2] and [21].)

$$\overline{\mathcal{H}}_{sp} = \sum_j \left[\frac{1}{2}\pi_j^2 + \frac{1}{2}\left[\mathcal{F}_N^{-1} d_N \mathcal{F}_N \boldsymbol{\varphi}\right]_j^2 + \alpha(1-\cos\varphi_j) \right], \tag{33}$$

$$\overline{\mathcal{S}} = \begin{pmatrix} 0 & \mathrm{id} \\ -\mathrm{id} & 0 \end{pmatrix}. \tag{34}$$

The resulting system of ODEs is then given by

$$\begin{bmatrix} \dot{\boldsymbol{\varphi}} \\ \dot{\boldsymbol{\pi}} \end{bmatrix} = \overline{\mathcal{S}}\nabla\overline{\mathcal{H}}_{sp} = \begin{bmatrix} \boldsymbol{\pi} \\ -(\mathcal{F}_N^{-1} D_N \mathcal{F}_N)^\top (\mathcal{F}_N^{-1} d_N \mathcal{F}_N \boldsymbol{\varphi}) - \alpha \sin\boldsymbol{\varphi} \end{bmatrix}, \tag{35}$$

where $[D_N]_{n,k} = \theta_k$. Again, the integral in the AVF method can be calculated exactly to give

$$\frac{\boldsymbol{\varphi}_{n+1}-\boldsymbol{\varphi}_n}{\Delta t} = (\boldsymbol{\pi}_{n+1}+\boldsymbol{\pi}_n)/2, \tag{36}$$

$$\frac{\boldsymbol{\pi}_{n+1}-\boldsymbol{\pi}_n}{\Delta t} = -(\mathcal{F}_N^{-1} D_N \mathcal{F}_N)^\top (\mathcal{F}_N^{-1} d_N \mathcal{F}_N)(\boldsymbol{\varphi}_{n+1}+\boldsymbol{\varphi}_n)/2 - \alpha(\cos\boldsymbol{\varphi}_{n+1}-\cos\boldsymbol{\varphi}_n)/(\boldsymbol{\varphi}_{n+1}-\boldsymbol{\varphi}_n). \tag{37}$$

Initial conditions and numerical data for both discretizations:

Spatial domain, number N of spatial intervals, and time-step size Δt used were [7]

$$x \in [-20, 20], \qquad N = 200, \qquad \Delta t = 0.01, \qquad \text{parameter: } \alpha = 1.$$

[5] For numerical computations, care must be taken to avoid problems when the difference $\boldsymbol{\varphi}_{n+1}-\boldsymbol{\varphi}_n$ in the denominator of (32) becomes small. We used the sum-to-product identity $\cos a - \cos b = -2\sin((a+b)/2)\sin((a-b)/2)$ to give a more numerically amenable expression.

[6] In practice, one uses the fast Fourier transform algorithm to calculate the DFTs in $\mathcal{O}(N \log N)$ operations.

[7] Here and below, if $x \in [a, b]$, then $\Delta x = \frac{b-a}{N}$, and $x_j = a + j\Delta x, j = 0, 1, \ldots, N$.

Figure 1: Sine-Gordon equation with finite differences semi-discretization: Energy error (left) and global error (right) vs time, for AVF and implicit midpoint integrators.

Initial conditions:

$$\left.\begin{array}{rcl} \varphi(x,0) &=& 0, \\ \pi(x,0) &=& \dfrac{8}{\cosh(2x)}. \end{array}\right\} \quad \begin{array}{l}\text{Right-moving}\\ \text{kink and left-}\\ \text{moving anti-kink}\\ \text{solution.}\end{array} \tag{38}$$

Numerical comparisons of the AVF method with the well known (symplectic) implicit midpoint integrator[8] are given in figure 1 for the finite differences discretization.

Example 5.2. *Korteweg-de Vries equation:*

Continuous:

$$\frac{\partial u}{\partial t} = -6u\frac{\partial u}{\partial x} - \frac{\partial^3 u}{\partial x^3}, \tag{39}$$

$$\mathcal{H} = \int \left[\frac{1}{2}\left(u_x\right)^2 - u^3\right] dx, \tag{40}$$

$$\mathcal{S} = \frac{\partial}{\partial x}. \tag{41}$$

Boundary conditions: periodic, $u(-20,t) = u(20,t)$.

Semi-discrete:

$$\overline{\mathcal{H}} = \sum_j \left[\frac{1}{2(\Delta x)^2}\left(u_{j+1} - u_j\right)^2 - u_j^3\right], \tag{42}$$

$$\overline{\mathcal{S}} = \frac{1}{2\Delta x}\begin{bmatrix} 0 & -1 & & & 1 \\ 1 & 0 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 0 & -1 \\ -1 & & & 1 & 0 \end{bmatrix}. \tag{43}$$

[8]Recall that the implicit midpoint integrator is given by $\frac{u_{n+1}-u_n}{\Delta t} = f\left(\frac{u_n+u_{n+1}}{2}\right)$.

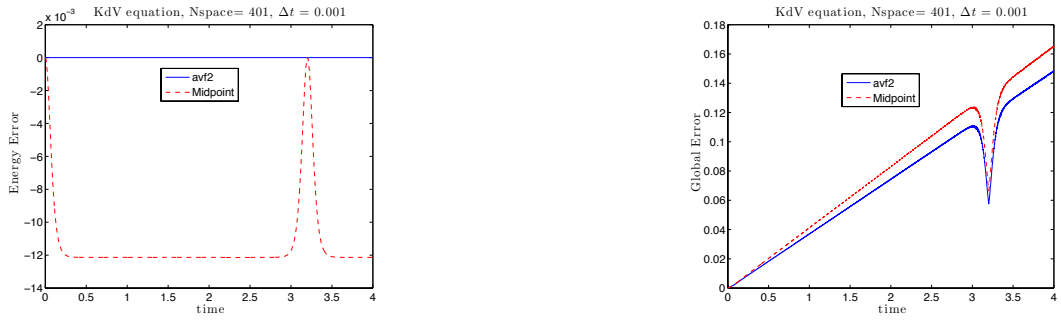

Figure 2: Korteweg-de Vries equation: Energy error (left) and global error (right) vs time, for AVF and implicit midpoint integrators.

Initial conditions and numerical data:

$$x \in [-20, 20], \qquad N = 400, \qquad \Delta t = 0.001.$$

6 Dissipative PDEs

Example 6.1. *Heat equation:*

Continuous:
The heat equation

$$\frac{\partial u}{\partial t} = u_{xx}, \tag{44}$$

is a dissipative PDE and can be written in the form (6), i.e.

$$\frac{\partial u}{\partial t} = \mathcal{N}_1 \frac{\delta \mathcal{H}_1}{\delta u}, \qquad \frac{\partial u}{\partial t} = \mathcal{N}_2 \frac{\delta \mathcal{H}_2}{\delta u}, \tag{45}$$

with the Lyapunov functions $\mathcal{H}_1(u) = \int_0^1 \frac{1}{2} u_x^2 \, dx$ and $\mathcal{H}_2(u) = \int_0^1 \frac{1}{2} u^2 \, dx$ and the operators $\mathcal{N}_1 = -1$ and $\mathcal{N}_2 = \partial_x^2$, respectively.

Boundary conditions: $u(0,t) = u(1,t) = 0$.

Semi-discrete:

$$\overline{\mathcal{H}}_1 = \frac{1}{2(\Delta x)^2} \left[u_1^2 + \sum_{j=2}^{N-1} (u_j - u_{j-1})^2 + u_{N-1}^2 \right] \tag{46}$$

and

$$\overline{\mathcal{H}}_2 = \sum_{j=1}^{N-1} \frac{1}{2} (u_j)^2, \tag{47}$$

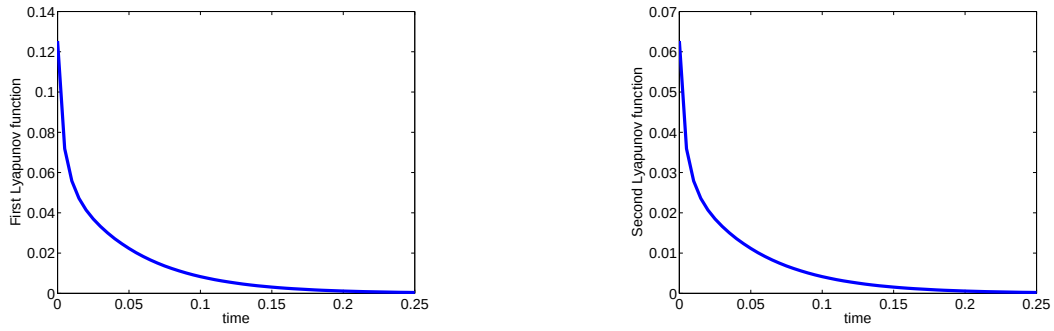

Figure 3: Heat equation: plots of Lyapunov functions $\overline{\mathcal{H}}_1\Delta x$ (left) and $\overline{\mathcal{H}}_2\Delta x$ (right) vs time, AVF integrator.

as well as

$$\overline{\mathcal{N}}_2 = \frac{1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix} \tag{48}$$

and the obvious discretisation of $\mathcal{N}_1$. With these choices, both discretisations yield identical semi-discrete equations of motion and therefore $\overline{\mathcal{H}}_1$ and $\overline{\mathcal{H}}_2$ are simultaneously Lyapunov functions of the semi-discrete system and therefore, the AVF integrator preserves both Lyapunov functions.

Initial conditions and numerical data:

$$x \in [0,1], \qquad N = 50, \qquad \Delta t = 0.0025. \tag{49}$$

Initial condition: $u(x,0) = x(1-x)$.

This system is numerically illustrated in Figure 3, where the monotonic decrease of the Lyapunov functions for the heat equation in (46) and (47) is shown.

7 Conservation laws in partial differential equations

7.1 Conservation laws for partial differential equations

Given a PDE with solution $u = u(x,t)$, $x \in \Omega \subset \mathbf{R}$, $t \in [0,T]$, belonging to suitable function-space X, we say that we have a conservation law for the PDE if there exist two functions $E : \mathbf{R} \to \mathbf{R}$ and $F : \mathbf{R} \to \mathbf{R}$ such that

$$\frac{\partial E(u(x,t))}{\partial t} + \frac{\partial F(u(x,t))}{\partial x} = 0. \tag{50}$$

The function E is called local density and F is called local flux of the conserved quantity. Integrating the conservation law on the space domain we obtain

$$\frac{\partial}{\partial t}\int_\Omega E(u(x,t))\,dx + F(u(x,t))|_\Gamma = 0,$$

where Γ is the boundary of Ω.

Example 7.1. *Consider the inviscid Burgers equation*

$$u_t + \frac{\partial}{\partial x}(\frac{1}{2}u^2) = 0, \quad x \in [0,1], \quad t \geq 0,$$

with homogeneous Dirichlet boundary conditions. By taking $E(u(x,t)) = u(x,t)$ *and* $F(u(x,t)) = \frac{1}{2}u^2(x,t)$ *we can write the equation in the form (50). The conserved quantity is*

$$\frac{\partial}{\partial t}\int_0^1 u(x,t)\,dx = -\frac{1}{2}u^2\Big|_0^1 = 0.$$

8 Discrete gradient methods have an energy conservation law

This topic is discussed in [15].

References

[1] U. M. Ascher, R.I. McLachlan, *On symplectic and multisymplectic schemes for the KdV equation.* J. Sci. Comput. 25 (2005), no. 1-2, 83–104.

[2] W.L. Briggs and V.E. Henson, *The DFT: An Owner's Manual for the Discrete Fourier Transform*, SIAM, 1995.

[3] L. Brugnano, F. Iavernaro, and D. Trigiante, *Hamiltonian boundary value methods (energy preserving discrete line integral methods).* JNAIAM. J. Numer. Anal. Ind. Appl. Math., 5(1-2):17-37, 2010.

[4] T. J. Bridges and S. Reich, *Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity*, Phys. Lett. A 284 (2001), no. 4-5, 184–193.

[5] E. Celledoni, R.I. McLachlan, D.I. McLaren, B. Owren, G.R.W. Quispel, and W.M. Wright, *Energy-preserving Runge-Kutta methods*, M2AN, vol 43 (4), 645-649.

[6] E. Celledoni, F. Grimm, R.I. McLachlan, D.I. McLaren, D.R.J. O'Neale, B. Owren, G.R.W. Quispel, *Preserving energy resp. dissipation in numerical PDEs, using the "average vector field" method.* NTNU Reports nr. 7/2009. Submitted.

[7] M. Dahlby, B. Owren, T. Yaguchi, *Preserving multiple first integrals by discrete gradients.* Journal of Physics A: Mathematical and Theoretical. vol. 44 (30), 2011.

[8] K. Feng and Z. Shang, *Volume-preserving algorithms for source-free dynamical systems*, Numer. Math. 71 (1995) 451?463.

[9] O. Gonzalez, *Time integration and discrete Hamiltonian systems*, J. Nonlinear Science, vol 6:pp 449-467, 1996.

[10] E. Hairer, *Energy-preserving variant of collocation methods*, JNAIAM. J. Numer. Anal. Ind. Appl. Math., 5(1-2):73-84, 2010.

[11] E. Hairer, C. Lubich and G. Wanner, *Geometric Numerical Integration*, Springer, II edition.

[12] B. Leimkuhler and S. Reich, *Simulating Hamiltonian dynamics.* Cambridge Monographs on Applied and Computational Mathematics, 14. Cambridge University Press.

[13] T. Matsuo. *New conservative schemes with discrete variational derivatives for nonlinear wave equations*, J. Comput. Appl. Math., 203 (2007), pp. 32–56.

[14] R.I. McLachlan, G.R.W. Quispel, and N. Robidoux. *Geometric integration using discrete gradients*, Phil. Trans. Roy. Soc. A, 357 (1999), pp. 1021–1045.

[15] R I McLachlan and G R W Quispel, *Discrete gradient methods have an energy conservation law*, Disc. Cont. Dyn. S. A, 34(3) (2014), 1099-1104. doi:10.3934/dcds.2014.34.1099

[16] R.I. McLachlan and N. Robidoux. *Antisymmetry, pseudospectral methods, weighted residual discretizations, and energy conserving partial differential equations*, Preprint, 2000.

[17] R.I. McLachlan and N. Robidoux. *Antisymmetry, pseudospectral methods, and conservative PDEs*, in International Conference on Differential Equations, Vol. 1, 2 (Berlin, 1999), World Sci. Publ., River Edge, NJ, 2000, pp. 994–999. .

[18] P. Olver, *Applications of Lie Groups to Differential Equations, Second Edition*, Springer-Verlag, New York, 1993.

[19] G.R.W. Quispel and D.I. McLaren. *A new class of energy-preserving numerical integration methods*, J. Phys. A: Math. Theor., 41 (2008), 045206 (7pp).

[20] B.N. Ryland, *Multisymplectic integration* PhD thesis, Massey University, Palmerston North, New Zealand, available online http://muir.massey.ac.nz/handle/10179/809.

[21] L.N. Trefethen, *Spectral Methods in MATLAB*, SIAM, 2000.