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# Preserving energy resp. dissipation in numerical PDEs using the "Average Vector Field" method

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ABSTRACT

We give a systematic method for discretizing Hamiltonian partial differential equations (PDEs) with constant symplectic structure, while preserving their energy exactly. The same method, applied to PDEs with constant dissipative structure, also preserves the correct monotonic decrease of energy. The method is illustrated by many examples. In the Hamiltonian case these include: the sine–Gordon, Korteweg–de Vries, nonlinear Schrödinger, (linear) time-dependent Schrödinger, and Maxwell equations. In the dissipative case the examples are: the Allen–Cahn, Cahn–Hilliard, Ginzburg–Landau, and heat equations.



## 1. Introduction

"The opening line of *Anna Karenina*, 'All happy families resemble one another, but each unhappy family is unhappy in its own way', is a useful metaphor for the relationship between computational ordinary differential equations (ODEs) and computational partial differential equations (PDEs). ODEs are a happy family – perhaps they do not resemble each other, but, at the very least, we can treat them by a relatively small compendium of computational techniques. . .PDEs are a huge and motley collection of problems, each unhappy in its own way" (Quote from Iserles' book [15]).

Whereas there is much truth in the above quote, in this paper we set out to convince the reader that, as far as conservation or dissipation of energy is concerned, many PDEs form part of one big happy family (cf. also [17]) that, after a very straightforward and uniform semi-discretization, may actually be solved by a single unique geometric integration method – the so-called average vector field method – while preserving the correct conservation, respectively, dissipation of energy. The concept of 'energy' has far-reaching importance throughout the physical sciences [10]. Therefore a single procedure, as presented here, that correctly conserves, resp. dissipates, energy for linear as well as nonlinear, low-order as well as high-order, PDEs would seem to be worthwhile.

Energy-preserving schemes have a long history, going back to Courant, Friedrichs, and Lewy's cunning derivation [6] of a discrete energy conservation law for the five-point finite difference approximation of the wave equation which they used to

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prove the scheme's convergence. The conservation law structure of many PDEs is considered fundamental to their derivation, their behaviour, and their discretization. Li and Vu-Quoc [18] give a historical survey of energy-preserving methods for PDEs and their applications, especially to nonlinear stability. What is relevant to us here is that many of these methods (e.g. [4,8,9,11,19–21,30,35]) have an ad hoc character and are not completely systematic either in their derivation or in their applicability; in contrast, the method discussed here (Eq. (16) below) is completely systematic, applies to a huge class of conservation and dissipative PDEs, and depends functionally only on the PDE itself, not its energy. In some cases it reduces to previously studied methods, for example, it reproduces one of Li and Vu-Quoc's schemes [18] for the nonlinear wave equation. Even in these cases, however, it sheds considerable light on the actual structure of the scheme and the origin of its conservative properties. See also the discussion comparing different constructions of energy-preserving integrators in [7].

We consider evolutionary PDEs with independent variables $(x,t) \in \mathbb{R}^{\mathbb{d}} \times \mathbb{R}$, functions $u$ belonging to a Hilbert space $\mathcal{B}$ with values[1] $u(x,t) \in \mathbb{R}^{\mathbb{m}}$, and PDEs of the form

$$\dot{u} = \mathcal{D}\frac{\delta \mathcal{H}}{\delta u}, \tag{1}$$

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

$$\mathcal{H}[u] = \int_\Omega H(x; u^{(n)})\, dx, \tag{2}$$

where $\Omega$ is a subset of $\mathbb{R}^{\mathbb{d}} \times \mathbb{R}$, 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

$$\frac{d}{d\epsilon}\mathcal{H}[u + \epsilon v]|_{\epsilon=0} = \left\langle \frac{\delta \mathcal{H}}{\delta u}, v \right\rangle \tag{3}$$

for all $u, v \in \mathcal{B}$ (cf. [28]), where $\langle , \rangle >$ is the inner product in $\mathcal{B}$. For example, if $d = m = 1$, $\mathcal{B} = L^2(\Omega)$, and

$$\mathcal{H}[u] = \int_\Omega H(x; u, u_x, u_{xx}, \dots)\, dx, \tag{4}$$

then

$$\frac{\delta \mathcal{H}}{\delta u} = \frac{\partial H}{\partial u} - \partial_x\left(\frac{\partial H}{\partial u_x}\right) + \partial_x^2\left(\frac{\partial H}{\partial u_{xx}}\right) - \cdots, \tag{5}$$

when the boundary terms are zero.

Similarly, for general $d$ and $m$, we obtain

$$\frac{\delta \mathcal{H}}{\delta u_l} = \frac{\partial H}{\partial u_l} - \sum_{k=1}^{d}\frac{\partial}{\partial x_k}\left(\frac{\partial H}{\partial u_{l,k}}\right) + \dots, \quad l = 1, \dots, m. \tag{6}$$

We consider Hamiltonian systems of the form (1), where $\mathcal{D}$ is a constant skew symmetric operator (cf. [28]) and $\mathcal{H}$ the energy (Hamiltonian). In this case, we prefer to designate the differential operator in (1) 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.

$$\int_\Omega u\mathcal{S}u\, dx = 0, \quad \forall u \in \mathcal{B}. \tag{7}$$

The system (1) 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 (1) where $\mathcal{D}$ is skew-adjoint, we also consider PDEs of type (1) where $\mathcal{D}$ is a constant negative (semi) definite operator with respect to the $L^2$ inner product, i.e.

$$\int_\Omega u\mathcal{D}u\, dx \leqslant 0, \quad \forall u \in \mathcal{B}. \tag{8}$$

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 (1), i.e.

$$\dot{u} = \mathcal{N}\frac{\delta \mathcal{H}}{\delta u} \tag{9}$$

has $\mathcal{H}$ as a Lyapunov function, i.e. $\dot{\mathcal{H}} = \int_\Omega \frac{\delta \mathcal{H}}{\delta u}\mathcal{N}\frac{\delta \mathcal{H}}{\delta u}\, dx \leqslant 0$. We will refer to systems (1) with a skew-adjoint $\mathcal{S}$ and an energy $\mathcal{H}$ as conservative and to systems (1) with a negative (semi) definite operator $\mathcal{N}$ and a Lyapunov function $\mathcal{H}$ as dissipative. Note that the operator $\mathcal{N}$ need *not* be self-adjoint. (In Example 10, the Ginzburg–Landau equation, $\mathcal{N} = \partial_x + \epsilon\partial_x^2$ is not self-adjoint.)

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