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Constructing invariant-preserving numerical schemes based on Poisson and Nambu brackets

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Abstract

A novel procedure for designing invariant-preserving numerical schemes for Poisson and Nambu systems is proposed. Such systems include important physical problems such as the Korteweg–de Vries equation and the shallow water equations, where often some physical invariants control the dynamics of the solutions. By the new procedure, numerical schemes that preserve one or two such invariants can be constructed. The key is a clever discretization of the brackets. Numerical results for the shallow water equations using a fully discretized extension of the legendary Arakawa–Lamb scheme confirm the validity of our procedure.

Keywords structure-preserving methods, Poisson brackets, Nambu brackets

Research Activity Group Scientific Computation and Numerical Analysis

1. Introduction

Suppose we need to solve some partial differential equations. Such equations often have physical backgrounds, and accordingly come with striking features such as energy preservation or the symplecticness of the flow map. In such a circumstance, specialized methods that well respect the feature are generally preferable than general methods in terms of the solution quality and the stability over long time interval. See, for example, [1], and the references therein.

Among them, one prominent successful example is the so-called Arakawa–Lamb (AL) scheme for the shallow water equations [2]. It is a semi-discretization of the equations (in space) which preserves two important invariants: the energy and enstrophy. These two are so important such that by preserving them it is possible to prevent the supurious cascade of energies between wavenumbers. Although the AL scheme runs well even if we simply discretize time by, say, for example, some explicit Runge–Kutta methods, mathematically it destroys the celebrated two invariants, and the existence of full discretization keeping them has remained open so far.

It had also remained open if there exists a sophisticated way of re-inventing the AL scheme, which was originally found by a brute-force way, but in 2005, Salmon [3] pointed out that AL type schemes can be derived based on the Poisson and Nambu bracket forms of the shallow water equations. This was epoch-making in that it introduced the concept of *discretized brackets*, which opened a door to new structure-preserving methods that can be used to wider range of problems. Still in his and related works only the discretization of space direction was discussed, and time discretization was left untouched.

Based on this background, this report is to fill the final missing part—we propose a concept of *time-discretized brackets*, and by combining this with Salmon's space-discretizations, we finally have a complete procedure of devising full discrete invariant-preserving schemes for Poisson and Nambu systems.

This letter is organized as follows. In Section 2, we consider a construction of invariant-preserving numerical schemes based on Poisson brackets. There, we introduce the new concept of time-discretized Poisson brackets. In this regime, we can aim at one invariant, the energy function of the system. Then in Section 3, following the strategy in [3], we consider its Nambu bracket extension, which enables us to preserve two invariants simultaneously. Until this point, to simplify the discussion, we take a vorticity equation as our working example. In Section 4, we consider the shallow water equations and present some numerical results for a fully-discretized scheme that is derived from the discretized Nambu bracket form. We confirm by numerical experiment that the two invariants are in fact well preserved.

2. Based on Poisson brackets

Let us illustrate our procedure by taking the following two-dimensional vorticity equation as our working example (for this equation, see, for example, [4]). For a stream function $\psi(t,\boldsymbol{x})$ and a vorticity field $\zeta(t,\boldsymbol{x}) = \Delta\psi$ ($\boldsymbol{x} \in \mathbb{R}^2$), it reads

$$\frac{\partial \zeta}{\partial t} = J(\zeta,\psi) = \zeta_x\psi_y - \zeta_y\psi_x.$$

For simplicity we consider the simplest spatial domain $\Omega = [0,L]\times[0,L]$ with the periodic boundary conditions imposed. The vorticity equation has the following two important invariants; the energy (Hamiltonian)

$$H = \frac{1}{2}\int_{\Omega} |\nabla\psi|^2 \mathrm{d}\boldsymbol{x} = \mathrm{const.},$$

and the enstrophy

$$Z = \frac{1}{2}\int_\Omega \zeta^2 \mathrm{d}\boldsymbol{x} = \text{const.}$$

In the rest of this section, we consider the preservation of the energy H. To see this, we first introduce a Poisson system representation of the equation.

Definition 1 *For functionals $F(\zeta)$, $G(\zeta)$, the Poisson bracket for the vorticity equation is given by*

$$\{F, G\}(\zeta) := \int_\Omega \zeta J(F_\zeta, G_\zeta)\mathrm{d}\boldsymbol{x},$$

where $F_\zeta = \frac{\delta F}{\delta \zeta}$ is the variational derivative.

It is skew-symmetric: $\{F, G\}(\zeta) = -\{G, F\}(\zeta)$. The vorticity equation can be rewritten with this as follows.

Lemma 2

$$\zeta_t = J(\zeta, \psi) = \{\zeta(\boldsymbol{x}), H\}(\zeta).$$

Proof Noting $\int_\Omega fJ(g, h)\mathrm{d}\boldsymbol{x} = \int_\Omega gJ(h, f)\mathrm{d}\boldsymbol{x}$, $H_\zeta = -\psi$, and $\delta(\zeta(\boldsymbol{x}))/\delta\zeta(\boldsymbol{x}') = \delta(\boldsymbol{x}' - \boldsymbol{x})$ (see [4]), we see

$$\begin{aligned}\{\zeta(\boldsymbol{x}), H\}(\zeta) &= \int_\Omega \zeta(\boldsymbol{x}')J(\zeta(\boldsymbol{x})_\zeta, H_\zeta)\mathrm{d}\boldsymbol{x}' \\ &= \int_\Omega \delta(\boldsymbol{x}' - \boldsymbol{x})J(H_\zeta, \zeta)\mathrm{d}\boldsymbol{x}' \\ &= J(\zeta, \psi).\end{aligned}$$

(QED)

Poisson systems have a strong feature that the evolution of arbitrary functionals can be described with the brackets. This immediately gives rise to the desired preservation property.

Lemma 3 *If ζ is a solution of $\zeta_t = \{\zeta(\boldsymbol{x}), H\}(\zeta)$, for any functional $F(\zeta)$,*

$$\frac{\mathrm{d}}{\mathrm{d}t}F(\zeta(t)) = \{F, H\}(\zeta).$$

Proof $\dfrac{\mathrm{d}}{\mathrm{d}t}F(\zeta(t)) = \displaystyle\int_\Omega F_\zeta \zeta_t \mathrm{d}\boldsymbol{x} = \int_\Omega F_\zeta J(H_\zeta, \zeta)\mathrm{d}\boldsymbol{x} = \{F, H\}(\zeta)$. **(QED)**

Theorem 4 (Energy preservation)

$$H(\zeta(t)) = \text{const.}$$

Proof From the skew-symmetry of the Poisson bracket, we see $\dfrac{\mathrm{d}}{\mathrm{d}t}H(\zeta(t)) = \{H, H\}(\zeta) = 0$. **(QED)**

What we are going to do is to discretize time t without destroying the above structure. We start by defining a time-discretized Poisson bracket.

Definition 5 *For functionals $F(\zeta)$, $G(\zeta)$, let $\frac{\delta F}{\delta(\tilde{\zeta}, \zeta)}$, $\frac{\delta G}{\delta(\tilde{\zeta}, \zeta)}$ be some discrete variational derivatives (see, for example, [1]). We then define*

$$\{F, G\}_{\mathrm{d}}(\tilde{\zeta}, \zeta) := \int_\Omega \left(\frac{\tilde{\zeta} + \zeta}{2}\right) J\left(\frac{\delta F}{\delta(\tilde{\zeta}, \zeta)}, \frac{\delta G}{\delta(\tilde{\zeta}, \zeta)}\right)\mathrm{d}\boldsymbol{x}.$$

Note that, this time the bracket takes two variables $\tilde{\zeta}, \zeta$, but is again skew-symmetric in the sense that $\{F, G\}_{\mathrm{d}}(\tilde{\zeta}, \zeta) = -\{G, F\}_{\mathrm{d}}(\tilde{\zeta}, \zeta)$. Also notice that the definition depends on the choice of discrete variational derivatives, which is generally not unique; we here do not put it in the notation to avoid cumbersomeness.

We then define a scheme with it. Note that the "definition" is formally done by the time-discretized bracket, which (after some calculation) results in the concrete form with the Jacobian.

Definition 6 *For $m = 0, 1, 2, \ldots$,*

$$\begin{aligned}&\frac{\zeta^{(m+1)}(\boldsymbol{x}) - \zeta^{(m)}(\boldsymbol{x})}{\Delta t} \\ &\quad := \{\zeta(\boldsymbol{x}), H\}_{\mathrm{d}}(\zeta^{(m+1)}, \zeta^{(m)}) \\ &\quad = J\left(\frac{\zeta^{(m+1)} + \zeta^{(m)}}{2}, \frac{\psi^{(m+1)} + \psi^{(m)}}{2}\right)(\boldsymbol{x}).\end{aligned}$$

Then the next claims successfully follow obeying the continuous case.

Lemma 7 *If $\{\zeta^{(m)}\}$ is a solution of the scheme, for any functional $F(\zeta)$, for $m = 0, 1, 2, \ldots$,*

$$\frac{F(\zeta^{(m+1)}) - F(\zeta^{(m)})}{\Delta t} = \{F, H\}_{\mathrm{d}}(\zeta^{(m+1)}, \zeta^{(m)}).$$

Proof Exactly as the continuous case, we see

$$\begin{aligned}&\frac{F(\zeta^{(m+1)}) - F(\zeta^{(m)})}{\Delta t} \\ &\quad = \int_\Omega \frac{\delta F}{\delta(\zeta^{(m+1)}, \zeta^{(m)})}\left(\frac{\zeta^{(m+1)} - \zeta^{(m)}}{\Delta t}\right)\mathrm{d}\boldsymbol{x} \\ &\quad = \{F, H\}_{\mathrm{d}}(\zeta^{(m+1)}, \zeta^{(m)}).\end{aligned}$$

(QED)

Theorem 8 (Discrete energy preservation)

$$H(\zeta^{(m)}) = \text{const.} \qquad (m = 0, 1, 2, \ldots).$$

Proof Similarly to the continuous case, from the skew-symmetry of the time-discretized Poisson bracket,

$$\frac{H(\zeta^{(m+1)}) - H(\zeta^{(m)})}{\Delta t} = \{H, H\}_{\mathrm{d}}(\zeta^{(m+1)}, \zeta^{(m)}) = 0.$$

(QED)

In this way, we can naturally *inherit* the energy-preservation from the continuous case. In this formulation, the enstrophy Z appears as a Casimir of the Poisson system. In order to preserve the enstrophy Z as well, we need to elevate it to a Hamiltonian, which can be actually done as follows.

3. Based on Nambu brackets

Such a trick can be (sometime) done by introducing Nambu brackets [5].

Definition 9 *For functionals $F(\zeta)$, $G(\zeta)$, $K(\zeta)$, the Nambu bracket for the vorticity equation is given by*

$$\{F, G, K\}(\zeta) := \int_\Omega J(F_\zeta, G_\zeta)K_\zeta \mathrm{d}\boldsymbol{x}.$$

It is skew-symmetric in the sense that $\{F, G, K\}(\zeta) = -\{G, F, K\}(\zeta) = -\{F, K, G\}(\zeta) = -\{K, G, F\}(\zeta)$. We omit the proofs of the next two lemmas, which are quite similar to the Poisson case.

Lemma 10 *With the energy $H(\zeta)$ and the enstrophy*

$Z(\zeta)$ of the vorticity equation, we have

$$\zeta_t = \{\zeta(\boldsymbol{x}), H, Z\}(\zeta).$$

Lemma 11 *For any functional $F(\zeta)$, we have*

$$\frac{\mathrm{d}}{\mathrm{d}t}F(\zeta(t)) = \{F, H, Z\}(\zeta).$$

Then the preservation of H and Z is immediate.

Theorem 12 (**Energy and enstrophy preservation**)

$$H(\zeta(t)) = \text{const.}, \quad Z(\zeta(t)) = \text{const.}$$

Proof Again from the skew-symmetry, $\frac{\mathrm{d}}{\mathrm{d}t}H(\zeta(t)) = \{H, H, Z\}(\zeta) = 0$, $\frac{\mathrm{d}}{\mathrm{d}t}Z(\zeta(t)) = \{Z, H, Z\}(\zeta) = 0$.

(QED)

Then, again, we do exactly the same thing as in the Poisson case, but this time under the Nambu regime. We start by introducing a time-discretized Nambu bracket.

Definition 13 *For functionals $F(\zeta)$, $G(\zeta)$, $K(\zeta)$,*

$$\{F, G, K\}_{\mathrm{d}}(\tilde{\zeta}, \zeta) := \int_\Omega J\left(\frac{\delta F}{\delta(\tilde{\zeta}, \zeta)}, \frac{\delta G}{\delta(\tilde{\zeta}, \zeta)}\right)\frac{\delta K}{\delta(\tilde{\zeta}, \zeta)}\mathrm{d}\boldsymbol{x}.$$

It is also skew-symmetric similarly to the continuous case.

Definition 14 *With the energy $H(\zeta)$ and the enstrophy $Z(\zeta)$, we define*

$$\frac{\zeta^{(m+1)}(\boldsymbol{x}) - \zeta^{(m)}(\boldsymbol{x})}{\Delta t} := \{\zeta(\boldsymbol{x}), H, Z\}_{\mathrm{d}}(\zeta^{(m+1)}, \zeta^{(m)}).$$

Lemma 15 *For any functional $F(\zeta)$, for $m = 0, 1, 2, \ldots$,*

$$\frac{F(\zeta^{(m+1)}) - F(\zeta^{(m)})}{\Delta t} = \{F, H, Z\}_{\mathrm{d}}(\zeta^{(m+1)}, \zeta^{(m)}).$$

Theorem 16 (**Discrete energy/enstrophy preservation**)

$$H(\zeta^{(m)}) = \text{const.}, \ Z(\zeta^{(m)}) = \text{const.} \ (m = 0, 1, 2, \ldots).$$

Actually, by calculation we see this results in the same scheme as the Poisson case. Thus it turns out that the scheme defined in Def. 6 has already preserved Z as well. But this is just a coincidence; the vorticity equation actually has infinitely many invariants $Z_p := (1/(p+2)) \int_\Omega \zeta^{p+2}\mathrm{d}\boldsymbol{x}$ $(p = 0, 1, 2, \ldots)$, and in exactly the same way schemes preserving H and Z_p can be obtained, which are truly different for $p > 0$.

4. Some discussions

The following two points are worth mentioning. First, the above time discretization can be combined with Salmon's idea of the space-discretized brackets [3] to find a fully discretized scheme with H or H, Z preserved. The nontrivial point of the space discretization lies in the use of the Arakawa Jacobian, which is necessary to avoid the Leibniz rule of differentiations [6].

Second, one might feel that the above construction looks similar to the famous study on skew-gradient systems [7] and its infinite-dimensional extension [8]. Actually it is true in that all the studies (including this) deal with multilinear, skew systems, and draw out some invariants from there. Still the present authors feel the bracket-based approach deserves independent attention, since (i) it is more natural to consider it when the problem is given in bracket forms, and (ii) while the approach in [8] assumes skewness in the kernels themselves, the bracket approach does not, and thus is slightly different. Note also that in [7] it is clearly stated that the study itself had been motivated by the Nambu dynamics.

5. Generalizing the AL scheme

Now let us turn our attention to the shallow water equations:

$$u_t = -uu_x - vu_y - gh_x,$$
$$v_t = -uv_x - vv_y - gh_y,$$
$$h_t = -(hu)_x - (hv)_y,$$

where (u, v) are the speeds in x, y directions, h is the height of the water surface, and g is the gravitational acceleration constant.

This equations come with the two invariants; the energy

$$H = \frac{1}{2}\int_\Omega (hu^2 + hv^2 + gh^2)\mathrm{d}\boldsymbol{x} = \text{const.},$$

and the enstrophy

$$Z = \frac{1}{2}\int_\Omega \frac{(v_x - u_y)^2}{h}\mathrm{d}\boldsymbol{x} = \text{const.}$$

In the celebrated work [2], Arakawa and Lamb proposed a semi-discretization of the equations (in space) which successfully keeps the two invariants (in a discrete sense). Although this was done rather in a brute-force way, later Salmon [3] pointed out that a similar construction can be realized in more systematic way based on (space-discretized) Poisson and Nambu brackets. This gave a motivation to the present work with time-discretiszed brackets, and combining these two tools, we can obtain a fully discretized scheme that strictly retains two (discrete) invariants. As far as the present authors know, this is the first positive answer to the question if the AL scheme can be discretized in time without losing the invariants. Since the Nambu bracket and the resulting scheme are too complicated to show here in this case, we skip their concrete forms; interested readers may refer to Salmon [9] and Sugibuchi [10].

Instead we here only show some numerical evidences. We solved the problem on $\Omega = [0, 1]^2$, with $\Delta x = \Delta y = 1/15$, $\Delta t = 1/5000$, $g = 1$, and the initial conditions:

$$h(x, y, 0) = 1 + (1/2)\exp[-25(x - 1/2)^2 - 25(y - 1/2)^2],$$
$$u(x, y, 0) = -\sin(\pi x)\sin(2\pi y)/2\pi,$$
$$v(x, y, 0) = \sin(2\pi x)\sin(\pi y)/2\pi.$$

The scheme is fully-implicit, and we used MINPACK (Fortran) with the tolerance 10^{-10}. We compared the following three schemes.

- **DVDM**: a discrete variational derivative method based on a skew-gradient expression of the shallow water equations; this conserves H but not Z.

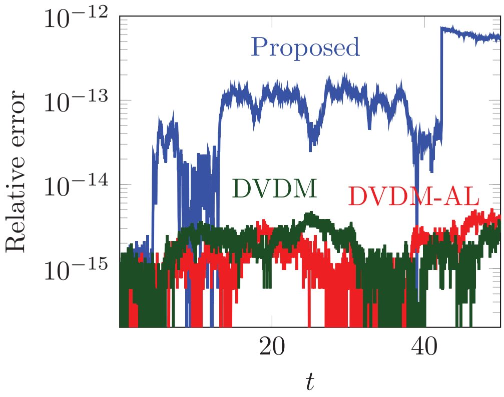

Fig. 1. Relative errors in the energy H.

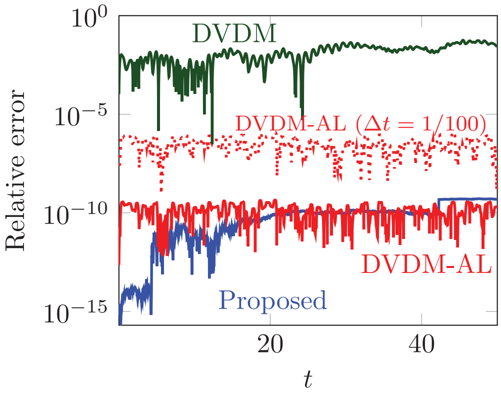

Fig. 2. Relative errors in the enstrophy Z.

- **DVDM with an Arakawa–Lamb modification (DVDM-AL)**: this is a modification of the above scheme, which coincides with the AL scheme as far as the time variable is left continuous. Thus it keeps the two invariant at this stage, and only the energy H is kept invariant after time discretization.
- **Proposed scheme based on the Nambu form (Proposed)**: it keeps the two invariants.

Under the prescribed setting, all the schemes basically work well (we skip the illustration of the solutions themselves). However, the accuracy of the invariants behaves different. Fig. 1 (and 2, respectively) shows the evolution of the energy H (the enstrophy Z). Since all the schemes theoretically preserve H, it is well preserved up to the tolerance of the nonlinear solver. On the other hand, the relative error of Z increases in the DVDM. Though Z seems to be preserved up to the prescribed tolerance in the DVDM-AL, it is actually confirmed that it is contaminated by the errors governed by Δt as indicated by the numerical result with larger time step $\Delta t = 1/100$ (dotted line in Fig. 2). Still it seems bounded in time, i.e. nearly conserved, which is mathematically interesting (we leave it to future works). Above all, we emphasize here that the invariant preservation up to the prescribed tolerance is achieved only in the proposed scheme. This confirms the validity of our approach.

Unfortunately, however, it should be also mentioned for fairness that our scheme instead suffers from severe restriction on the time-stepping. In a preliminary numerical test, we employed an adaptive step size control (the other settings are the same): it first tries the default width $\Delta t = 1/100$, but sometimes difficulties arise in solving the fully-implicit scheme, and at such moments we tentatively halve the step sizes until the scheme goes out from such a difficult region. Then, we observe that

- **DVDM**: the very small width $\Delta t = 1/(100 \times 2^9)$ is employed only for the first time step.
- **DVDM-AL**: it works for $\Delta t = 1/100$ at all t.
- **Proposed**: it often employs smaller widths (Fig. 3).

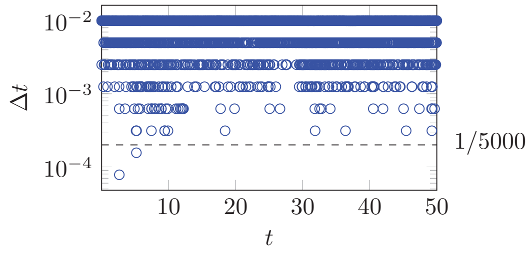

Fig. 3. Chosen time-step widths in the proposed scheme.

The tiny fixed time step is actually employed for the proposed scheme (see dashed line in Fig. 3). Moreover, even when we employ such a fine time step size, the nonlinear solver sometimes fails to achieve the prescribed tolerance in the proposed scheme, while the residuals are actually in order 10^{-15} in the other schemes.

We understand this restriction comes from the fact that we forced two invariants. In this way, imposing multiple invariants is not always advantageous in an overall view. Similar restriction was also found in [8]. But so far multiple preservation has not been popular, and we need some more tests before we conclude anything.

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