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Abstract

An adaptive conservative or dissipative numerical method for nonlinear partial differential equations is established. The method not only inherits the welcome conservation or dissipation property of the equation but also uses suitable non-uniform grids at each time step. Our numerical experiments indicate that the method is useful especially for localized solutions such as solitary wave solutions.

keyword
Energy conservation/dissipation, Discrete gradient method, Discrete variational derivative method, Dynamic grid adaptation

1 Introduction

In this note, we show that by a simple idea we can establish an adaptive conservative or dissipative numerical method for partial differential equations (PDEs) of the form

$$\frac{\partial u}{\partial t} = \mathcal{D}\frac{\delta G}{\delta u}, \tag{1}$$

where $\mathcal{D}$ is a skew-symmetric or negative semi definite differential operator, and $\delta G/\delta u$ denotes the variational derivative. In a certain area of numerical analysis for differential equations, "structure-preserving" methods have been attracting much attention. They are methods preserving geometric properties of a differential equation (for example, see [6] for ODEs and [7] for PDEs). In this note we restrict our attention to PDEs of the form (1) which have the following property. If $\mathcal{D}$ is skew-symmetric, (1) has a conservation property

$$\frac{\mathrm{d}}{\mathrm{d}t}\int G(u,u_x)\mathrm{d}x = 0,$$

under appropriate boundary conditions. A typical example of this class is the KdV equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(-3u^2 - \frac{\partial^2 u}{\partial x^2}\right), \qquad 0 < x < L, \quad t > 0, \tag{2}$$

where $G(u,u_x) = -u^3 + u_x^2/2$. If $\mathcal{D}$ is negative semi definite, (1) has a dissipation property

$$\frac{\mathrm{d}}{\mathrm{d}t}\int G(u,u_x)\mathrm{d}x \leq 0,$$

again under appropriate boundary conditions.[1] A typical example of this class is the Cahn–Hilliard equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right), \qquad 0 < x < L, \quad t > 0, \tag{3}$$

where $G(u,u_x) = pu^2/2 + ru^4/4 - qu_x^2/2$.

In the last two decades, much effort has been devoted in order to construct several frameworks which derive conservative/dissipative schemes. For example, Furihata proposed the discrete variational derivative method (DVDM) [4] (see also Furihata–Matsuo [5], Celledoni et al. [3]) in finite difference context. It has then been applied to some fundamental PDEs to prove that the method is in fact effective.

However, there remained several issues to be settled so that the method could be truly useful for large, practical applications. The first issue was the adaptation to non-uniform grids—the original DVDM was constructed only on uniform grids since it required summation-by-parts formula regarding difference operators. Obviously such formulas are not easily expected on non-uniform grids. Fortunately, this issue has been successfully settled by some recent studies. Yaguchi–Matsuo–Sugihara found their way by using either the mapping method [12] or discrete differential forms [13]. Matsuo [8] gave another solution by extending the DVDM to Galerkin (finite element) context.

Another difficulty lain in the original DVDM was that it assumed *static* grids, and it was not clear at all if it could be incorporated with a *dynamic* grid technique. Such a technique is strongly hoped in some practical problems where a localized point (or area) moves as time passes (consider, for

[1] Hereafter $G(u,u_x)$ is often abbreviated as $G(u)$ when no confusions occur.

example, a moving solitary wave), in order to increase the overall efficiency. Unfortunately, however, it seems that no study has ever succeeded in such a challenge, not only in the context of the DVDM, but in more general context of the structure-preserving methods for PDEs. The reason for this is that such structure-preserving methods usually employ a very sophisticated time stepping for the desired structure-preservation, which generally seems to contradicts the concept of grid adaptation.

Motivated by this background, in this note we shall show that by a simple idea we can establish an adaptive conservative/dissipative method. This is done by combining the following two main techniques: the conservative/dissipative method on *static* non-uniform grids mentioned above, and the grid adaptation technique frequently used in the context of the wavelet based numerical methods [2, 9, 10, 11]. Here we would like to emphasize that a simple combination of them would destroy the desired conservation/dissipation properties from the reason above. The key is to introduce an additional optimization step, by which the destruction can be avoided. As far as the authors know, this is the first study where a systematic grid adaptation is realized in the context of structure-preserving methods.

This note is organized as follows. In Section 2, the standard conservative/dissipative method on non-uniform grids is reviewed. As an example, we employ the Galerkin approach [8]. In Section 3, the standard dynamic grid adaptation technique is reviewed to show how to obtain appropriate grids at each time step. In Section 4, the adaptive conservative/dissipative algorithm and numerical experiments are shown. Discussions and conclusions are drawn in Section 5.

Throughout this note, numerical solutions are denoted by $u^{(n)} \simeq u(n\Delta t, \cdot)$ where Δt is the time mesh size, and the inner product is defined by $(f, g) = \int_0^L fg \mathrm{d}x$. Although the idea in the present paper should carry to two- or three-dimensional cases, we restrict ourselves to one-dimensional problems for the clarity of description.

2 Energy conservative/dissipative method on static non-uniform grids

In this section, we review the energy conservative/dissipative Galerkin method [8], with the examples for the KdV and Cahn–Hilliard equations.

Suppose that the interval $[0, L]$ is partitioned appropriately (not necessarily uniformly), and let $S_h \in H^1(0, L)$ (H^1 denotes the first order Sobolev space) be, for example, the piecewise linear function space over the grid. For the KdV equation (2), let us use the space $X_K = \{v \mid v \in S_h,\ v(0) = v(L)\}$ in order to consider the periodic boundary conditions. The KdV equation can be written as the variational (Hamiltonian) form

$$u_t = \partial_x \frac{\delta G}{\delta u}, \quad G(u, u_x) = u^3 - \frac{u_x^2}{2},$$

or equivalently, the following system

$$u_t = p_x, \quad p_1 = \frac{\delta G}{\delta u}.$$

The conservative scheme was defined as follows [8]. Find $u^{(n)}, p_1^{(n+\frac{1}{2})} \in X_K$ such that, for all $v_1, v_2 \in X_K$,

$$\left(\frac{u^{(n+1)} - u^{(n)}}{\Delta t}, v_1 \right) = \left((p_1^{(n+\frac{1}{2})})_x, v_1 \right), \tag{4}$$

$$\left(p_1^{(n+\frac{1}{2})}, v_2 \right) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(n+1)}, u^{(n)})}, v_2 \right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(n+1)}, u_x^{(n)})}, (v_2)_x \right) \tag{5}$$

hold, where

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(n+1)}, u^{(n)})} = (u^{(n+1)})^2 + u^{(n+1)} u^{(n)} + (u^{(n)})^2,$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(n+1)}, u_x^{(n)})} = -\frac{u_x^{(n+1)} + u_x^{(n)}}{2}$$

correspond to the partial derivatives $\partial G / \partial u$ and $\partial G / \partial u_x$. The numerical solution of this scheme has the following conservation property

$$\int_0^L G(u^{(n)}, u_x^{(n)}) \mathrm{d}x = \text{const}.$$

For the Cahn–Hilliard equation, let us set $X_C = S_h$. The Cahn–Hilliard equation can be rewritten as the variational form

$$u_t = \partial_x^2 \frac{\delta G}{\delta u}, \quad G(u, u_x) = \frac{p}{2} u^2 + \frac{r}{4} u^4 - \frac{q}{2} u_x^2,$$

or equivalently, the following system

$$u_t = p_{xx}, \quad p_1 = \frac{\delta G}{\delta u}.$$

The dissipative scheme was defined as follows [8]. Find $u^{(n)}, p_1^{(n+\frac{1}{2})} \in X_C$ such that, for all $v_1, v_2 \in X_C$,

$$\left(\frac{u^{(n+1)} - u^{(n)}}{\Delta t}, v_1 \right) = -\left((p_1^{(n+\frac{1}{2})})_x, (v_1)_x \right), \tag{6}$$

$$\left(p_1^{(n+\frac{1}{2})}, v_2 \right) = \left(\frac{\partial G_{\mathrm{d}}}{\partial(u^{(n+1)}, u^{(n)})}, v_2 \right) + \left(\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(n+1)}, u_x^{(n)})}, (v_2)_x \right) \tag{7}$$

hold, where

$$\frac{\partial G_{\mathrm{d}}}{\partial(u^{(n+1)}, u^{(n)})} = p\left(\frac{u^{(n+1)} + u^{(n)}}{2}\right) + r\left(\frac{(u^{(n+1)})^2 + (u^{(n)})^2}{2}\right)\left(\frac{u^{(n+1)} + u^{(n)}}{2}\right),$$

$$\frac{\partial G_{\mathrm{d}}}{\partial(u_x^{(n+1)}, u_x^{(n)})} = -q\left(\frac{u_x^{(n+1)} + u_x^{(n)}}{2}\right)$$

correspond to the partial derivatives $\partial G/\partial u$ and $\partial G/\partial u_x$. The numerical solution of this scheme has the following dissipation property

$$\int_0^L G(u^{(n+1)}, u_x^{(n+1)})\mathrm{d}x \leq \int_0^L G(u^{(n)}, u_x^{(n)})\mathrm{d}x.$$

In the subsequent sections, the energy conservative/dissipative integrators on static non-uniform grids are denoted by Φ_{NU}: $u^{(n+1)} = \Phi_{\mathrm{NU}}(u^{(n)})$.

3 Dynamic grid adaptation technique

In this section a standard dynamic grid adaptation technique which is known in the context of wavelet based numerical methods [9, 10, 11] is briefly reviewed. Below we explain this without getting involved in the concept of wavelets. Let $V^0 \subset V^1 \subset V^2 \subset \cdots$ which satisfy $\overline{\cup_{j=0}^{\infty} V^j} = L^2(0, L)$ be a sequence of finite dimensional function spaces, and $\{\phi_k^j(x)\}_k$ be the basis functions of V^j. The basis functions of W^j, the complement of V^j in V^{j+1}, i.e., $V^{j+1} = V^j \oplus W^j$, are denoted by $\{\psi_k^j(x)\}_k$.

The function $u^J \in V^J$ which approximates $u \in L^2$ can be expressed as

$$u^J(x) = \sum_{k \in \mathcal{K}(J)} c_k^J \phi_k^J(x), \tag{8}$$

where $\mathcal{K}(J)$ denotes the set of indices of the basis functions. If the basis function has the interpolation property: i.e., $\phi_k^j(x_i^j) = \delta_{i,k}$, $u(x_k^J)$ can be chosen as the coefficient c_k^J. Since $V^J = V^0 \oplus W^1 \oplus \cdots \oplus W^{J-1}$, the approximate function (8) can be also rewritten as

$$u^J(x) = \sum_{k \in \mathcal{K}(0)} c_k^0 \phi_k^0(x) + \sum_{j=0}^{J-1} \sum_{k \in \mathcal{K}_C(j)} d_k^j \psi_k^j(x), \tag{9}$$

where $\mathcal{K}_C(j)$ denotes the set of indices of the basis functions $\{\psi_k^j\}_k$. The second term can be further decomposed into a sum of two groups whose coefficients are above and below the threshold ϵ^j:

$$u^J(x) = \underbrace{\sum_{k \in \mathcal{K}(0)} c_k^0 \phi_k^0(x) + \sum_{j=0}^{J-1} \sum_{\substack{k \in \mathcal{K}_C(j) \\ |d_k^j| \geq \epsilon^j}} d_k^j \psi_k^j(x)}_{u_{\geq}^J(x)} + \underbrace{\sum_{j=0}^{J-1} \sum_{\substack{k \in \mathcal{K}_C(j) \\ |d_k^j| < \epsilon^j}} d_k^j \psi_k^j(x)}_{u_{<}^J(x)}. \tag{10}$$

When the threshold $\epsilon^j(\geq 0)$ is sufficiently small, $u^J_{\geq}(x)$ can be regarded as a rough approximation in V^J. We call this separation the static grid adaptation.

Remark 1. *In this note, We assume that V^j is the piecewise linear function space on uniform grids:*

$$\phi^j_k(x) = \begin{cases} \dfrac{x - x^j_{k-1}}{x^j_k - x^j_{k-1}}, & x \in [x^j_{k-1}, x^j_k], \\ \dfrac{x^j_{k+1} - x}{x^j_{k+1} - x^j_k}, & x \in [x^j_k, x^j_{k+1}], \\ 0, & \text{otherwise}, \end{cases}$$

for $k = 1, \dots, L2^j - 1$ where $x^j_k = k/2^j$ (special care for ϕ^j_0 and $\phi^j_{L2^j}$ is required to fit the boundary conditions). In this case, the basis functions of W^j are expressed as

$$\psi^j_k(x) = \begin{cases} \dfrac{x - x^{j+1}_{2k-2}}{x^{j+1}_{2k-1} - x^{j+1}_{2k-2}}, & x \in [x^{j+1}_{2k-2}, x^{j+1}_{2k-1}], \\ \dfrac{x^{j+1}_{2k} - x}{x^{j+1}_{2k} - x^{j+1}_{2k-1}}, & x \in [x^{j+1}_{2k-1}, x^{j+1}_{2k}], \\ 0, & \text{otherwise}. \end{cases}$$

Note that each basis function corresponds to a single grid, due to the interpolation property. In more general wavelet context, the basis function is usually constructed based on the so called scaling function, in particular, the autocorrelation function of the Daubechies scaling function (see [1, 10, 14], for example).

With these definitions, the standard dynamic grid adaptation algorithm can be described as the following two steps:

1. Integrate $u^{(n)}_{V^J_{(n)}}$ by a standard time discretization method to obtain $u^{(n+1)}_{V^J_{(n)}}$, where $V^J_{(n)}$ denotes the subspace of V^J, and $u^{(n)}_X \simeq u(n\Delta t, \cdot)$.
2. Do static grid adaptation and add its adjacent zone to update the space (grids) $V^J_{(n)}$ to $V^J_{(n+1)}$.

Here we say that the basis function ψ^s_i belongs to the adjacent zone of ψ^j_k, if the following relations are satisfied

$$|s - j| \leq M, \quad |x^s_i - x^j_k| \leq Ca_j, \tag{11}$$

where C defines the width of the adjacent zone, and M determines the extent of which coarser and finer scales are included into the adjacent zone.

4 Adaptive energy conservative/dissipative method and numerical experiments

4.1 Adaptive energy conservative/dissipative method

The dynamic grid adaptation reviewed in Section 3 loses the conservation/dissipation property, even if we utilize the conservative/dissipative method for the time stepping. In this subsection, an adaptive energy conservative/dissipative discretization technique is constructed. The algorithm involves the following three steps:

1. Compute $u^{(n+1)}_{V^J_{(n)}} = \Phi_{\mathrm{NU}}(u^{(n)}_{V^J_{(n)}})$ based on the standard energy conservative/dissipative method on the static non-uniform grids.

2. Determine the new space $V^J_{(n+1)}$ from $V^J_{(n)}$ based on the static grid adaptation technique and the concept of adjacent zone.

3. Solve the following minimization problem to obtain $u^{(n+1)}_{V^J_{(n+1)}}$.

$$\begin{aligned} &\min \quad \|u^{(n+1)}_{V^J_{(n+1)}} - u^{(n+1)}_{V^J_{(n)}}\|, \\ &\text{s.t.} \quad \int_0^L G(u^{(n+1)}_{V^J_{(n+1)}})\mathrm{d}x = \int_0^L G(u^{(n+1)}_{V^J_{(n)}})\mathrm{d}x. \end{aligned}$$

In the above algorithm, the minimization problem can be solved by the Lagrangian multiplier if the standard norm such as L^2 or H^1 norm is considered. The numerical solution obtained by the above algorithm has the following property.

Theorem 4.1. *For conservative PDEs, let Φ_{NU} be the conservative method. Then the numerical solution obtained by the above algorithm satisfies*

$$\int_0^L G(u^{(n+1)}_{V^J_{(n+1)}})\mathrm{d}x = \int_0^L G(u^{(n)}_{V^J_{(n)}})\mathrm{d}x.$$

Similarly, for dissipative PDEs, let Φ_{NU} be the dissipative method. Then the numerical solution obtained by the above algorithm satisfies

$$\int_0^L G(u^{(n+1)}_{V^J_{(n+1)}})\mathrm{d}x \le \int_0^L G(u^{(n)}_{V^J_{(n)}})\mathrm{d}x.$$

Proof.

$$\int_0^L G(u^{(n+1)}_{V^J_{(n+1)}})\mathrm{d}x = \int_0^L G(u^{(n+1)}_{V^J_{(n)}})\mathrm{d}x = (\le) \int_0^L G(u^{(n)}_{V^J_{(n)}})\mathrm{d}x.$$

The first and second equalities follow from Steps 3 and 1 in the above algorithm, respectively. □

4.2 Numerical experiments

Let us check the algorithm numerically. All the computations were done in the computation environment: CPU Intel(R) Core(TM)2 Duo CPU (2.40 GHz), 4 GB memory, Linux OS. We used MATLAB (R2010a). Nonlinear equations and minimization problems were solved by "fsolve" and "fmincon" with tolerance 10^{-8}, respectively, instead of the standard Newton method and Lagrangian multiplier.

We apply the algorithm to the solitary wave solution of the KdV equation (2). The parameters were set to $x \in [0, 10]$ (the periodic boundary condition was considered), $\Delta t = 0.001$, $J = 7$, $\epsilon^j = 0$ $(j = 0, 1)$, 0.01 (otherwise), $M = 1$, $C = 1$ and $a_j = 1/2^j$. The initial value was set to $u(0, x) = \mathrm{sech}^2(\sqrt{2}(x - 4))$. Fig. 1 shows the evolution of the numerical solutions and the set of grids. The area where the grids are dense moved corresponding to the numerical solution. Next, we check the energy conservation. We compared the present algorithm with that without the minimization problem (the third step). We observed from Fig. 2 that the error of energy obtained by the algorithm without the minimization grew linearly, which indicates that this additional step is necessary for keeping the quality of the numerical solutions.

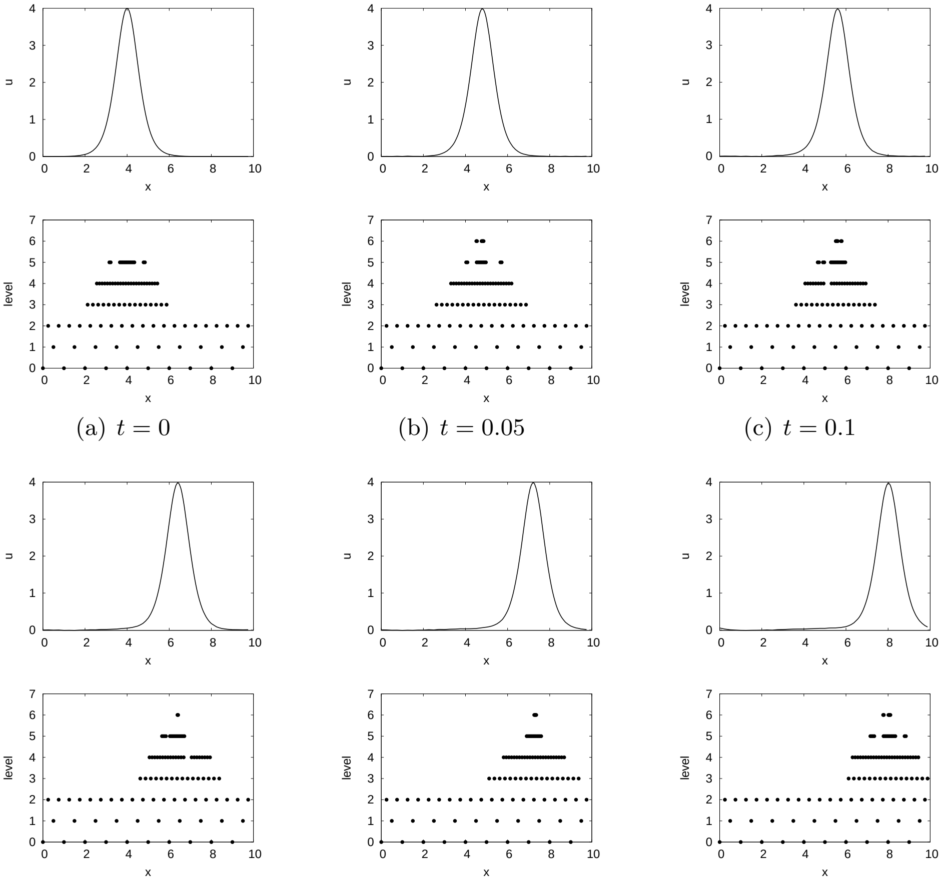
5 Discussions and Conclusions

In this note, we combined the energy conservative/dissipative numerical method on static non-uniform grids for PDEs with the grid adaptation technique. As far as the authors know, this is the first study where these two elements are combined. This combination was made possible by a simple idea that the destroyed conservation/dissipation property in the grid adaptation step can be recovered by the minimization problem newly introduced in the algorithm. The numerical experiments indicate that we can in fact obtain qualitatively good numerical solutions when the algorithm are applied to localized solutions.

The present paper remains, however, to propose the idea itself, and the actual efficiency of the method was set outside its scope. For example, we did not compare the computational cost of the proposed algorithm with any existing schemes. This is because we feel that this issue should be carefully discussed in view of various computational aspects such as below.

- In the present algorithm, we have to solve two different types of nonlinear equations, whose costs should strongly depend on the employed nonlinear solvers.

- Obviously the efficiency of the grid adaptation largely depends on to which extent the solution is localised, and thus the efficiency should



(a) $t = 0$

(b) $t = 0.05$

(c) $t = 0.1$

(d) $t = 0.15$

(e) $t = 0.2$

(f) $t = 0.25$

Figure 1: The evolution of numerical solutions and set of grids.

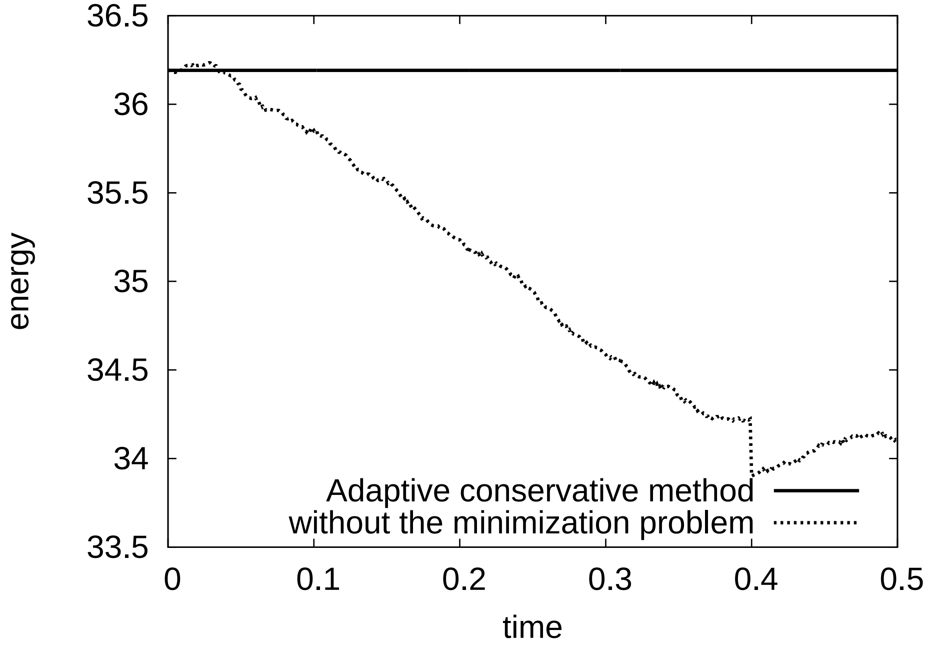


Figure 2: Evolution of the energy.

be discussed in view of this factor. In this respect, we feel that the algorithm is more useful in two or three dimensional problems where solutions can be quite sparse, and the efficiency should be investigated in such situations. In the present paper, we only focused on one-dimensional problems in order to illustrate the idea itself.

- The grid adaptation is done based on the expectation that the localized areas do not drastically change. Therefore, in order to hold the number of grids almost constant, we have to keep the time mesh size small enough. This, however, contradicts the philosophy of the standard conservative/dissipative method (in general, we expect qualitatively better numerical solutions using a relatively large time mesh size thanks to the structure-preserving properties), and the balance should be carefully adjusted.

The authors feel the third point is the most crucial. Some efficiency results considering these points will be reported elsewhere in the future.

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