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Discrete Variational Derivative Method

A Structure-Preserving Numerical Method for Partial Differential Equations

Daisuke Furihata and Takayasu Matsuo

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A Structure-Preserving Numerical Method for Partial Differential Equations

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Preface

This book describes a numerical method, called the "discrete variational derivative method," which is for designing numerical schemes for certain partial differential equations (PDEs, for short). The targets include, for example, (i) the Korteweg–de Vries equation:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(\frac{1}{2}u^2 + \frac{\partial^2 u}{\partial x^2}\right)$$

which describes shallow water waves, (ii) the nonlinear Schrödinger equation:

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2} - \gamma|u|^{p-1}u, \qquad \gamma \in \mathbb{R},\ p = 3, 4, \ldots$$

for modeling optical waves, (iii) the Cahn–Hilliard equation:

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

which is a model of certain phase separation phenomena, and (iv) the Newell–Whitehead equation:

$$\frac{\partial u}{\partial t}(t, x, y) = \mu u - |u|^2 u + \left(\frac{\partial}{\partial x} - \frac{\mathrm{i}}{2k_c}\frac{\partial^2}{\partial y^2}\right)^2 u, \qquad \mu, k_c \in \mathbb{R}$$

which simulates two-dimensional Bénard convection flow. Reflecting these physical backgrounds, the PDEs have one striking feature in common; associated with the PDEs there are scalar functions, often referred to as "energies," that strictly remain constant or monotonically decrease as time evolves. In fact, under appropriate conditions (i) the Korteweg–de Vries equation has the energy conservation property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{1}{6}u^3 - \frac{1}{2}(u_x)^2\right)\mathrm{d}x = 0,$$

and (ii) the nonlinear Schrödinger equation has the property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\left(-\frac{1}{2}|u_x|^2 + \frac{1}{p}|u|^p\right)\mathrm{d}x = 0.$$

Similarly, (iii) the Cahn–Hilliard equation has the energy dissipation property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\int\left(\frac{p}{2}u^2 + \frac{r}{4}u^4 - \frac{q}{2}(u_x)^2\right)\mathrm{d}x \le 0,$$

and (iv) the Newell–Whitehead equation has the property:

$$\frac{\mathrm{d}}{\mathrm{d}t}\iint\left(\frac{\mu}{2}|u|^2-\frac{1}{4}|u|^4+\left|u_x-\frac{\mathrm{i}}{2k_c}u_{yy}\right|^2\right)\mathrm{d}x\mathrm{d}y\le 0.$$

In this book those PDEs are said to be "conservative" or "dissipative" PDEs, respectively. (Note that this definition of "dissipative" is slightly different from the definition in dynamical systems theory, where dissipative property is defined with absorbing sets.)

In the numerical computation of such conservative or dissipative PDEs, it is often preferable to employ some special numerical schemes that retain the conservation/dissipation properties in a discrete sense; they are called "conservative" or "dissipative" schemes throughout this book. The reason for this preference is that, from the numerical point of view, the properties often lead us to stabler computation; and for practitioners such as physicists and engineers the motivation is that the properties themselves may be quite important since they reflect important physical aspects of the modeled phenomena. Thus, since around the 1970s, much effort has been devoted to the development of conservative and dissipative schemes for various PDEs. In the early phase of these researches, studies had been carried out for each individual PDE; it was only during and after 1990s that more unified approaches that can be applied to a certain large class of PDEs had been found. The main topic of this book, the discrete variational derivative method, is one of such newer developments.

Here we have to mention the case of *ordinary* differential equations (ODEs), for which the history of research in the above context dates back to several decades ago, and consequently the corresponding literature is far richer than that of PDEs. For ODEs several unified approaches have been established, not only for conservative and dissipative ODEs, but for many classes of ODEs with various geometric structures. They include, for example, the symplectic method for Hamiltonian systems, the Lie group method for constrained mechanical systems, methods that preserve first-integrals, and methods for ODEs on manifolds, among many others. Nowadays the methods are regarded to form a big group called "structure-preserving methods for ODEs," or "geometric numerical integration methods," and more and more efforts are being devoted to this area at an ever-increasing rate. An excellent textbook for both beginners and experts is also available, which surveys the history and the whole picture of structure-preserving methods for ODEs [83].

Compared to this maturity, the research in the PDE context seems to be still at its beginning stage. Few classes for which structure-preserving integration is possible have been identified so far, and accordingly, "structure-preserving method for PDEs" is not a popular expression yet. There is no question, however, about the increasing importance of PDEs themselves, both in mathematical and practical senses. We thus strongly believe that in the next decade structure-preserving methods for PDEs will draw more and more

interest, especially as the methods for ODEs come close to maximum maturity. In accordance with this belief, this book is written as the first one that is entirely dedicated to a structure-preserving method for PDEs.

This book is intended for both experts and non-experts. For both readers an introductory Chapter 1 is prepared, where all central ideas and essential examples are summarized. We believe that just glancing at this chapter will suffice to enable the reader to understand the essence of the discrete variational derivative method. The subsequent chapters, 2 to 4, are devoted to full description of the method: in Chapter 2 the PDEs which the method covers are classified; in Chapter 3 the procedure of the method is described in detail; in Chapter 4 the application examples are shown. Practitioners may, after reading Chapter 1, jump to Chapter 4 and see how the method is applied to typical problems. Chapters 5 to 7, including appendices, are for especially interested readers; there some advanced topics and technical details are summarized, which are too complicated to be included in the main sections.

We hope to thank all those who have helped this project. In particular, Kazuo Murota and Masaaki Sugihara for encouraging us to write this book, and continuously giving the authors many valuable comments. Masatake Mori, for guiding the authors to the rich world of numerical analysis. Our sincere thanks also go to Tetsuya Ishiwata, Toshiyuki Koto, Taketomo Mitsui, Yoshihisa Morita, Masaharu Nagayama, Shinji Odanaka, Takayoshi Ogawa, Masami Okada, Hisashi Okamoto, Norikazu Saito, Takashi Sakajo, and Takashi Suzuki, for valuable information related to the contents of this book. We also thank our colleagues Chris Budd, Jialin Hong, Takanori Ide, Brynjulf Owren, Reinout Quispel, Takaharu Yaguchi, among others, for fruitful discussions and valuable suggestions. We are also grateful to some of our students for drawing graphs, in particular Masayuki Hayashi, Satoshi Koide, Yohei Kubo, Yuto Miyatake, Yuki Sawada, Yuuki Sekino, Ken Takeya, Genta Tanaka, Eitaro Torii, Kenta Ueda, and Norio Yamaguchi. Leon LiMing, our editor at CRC Press, was so patient about our delayed manuscript, and very helpful during the whole project period. Finally, we acknowledge that this book was partially supported by the Global COE "The Research and Training Center for New Development in Mathematics."

We hope that this book be a help for all readers facing their problems and looking for "good" numerical solvers.

Osaka and Tokyo, December 2010

The Authors

Chapter 1

Introduction and Summary

The key ideas of the discrete variational derivative method are summarized with some illustrative examples. This chapter is a self-contained summary of this book. After reading this introductory chapter, readers are suggested to proceed to one of the subsequent chapters according to their points of interest.

1.1 An Introductory Example: Spinodal Decomposition

Let us have a look at an illustrative example, the "spinodal decomposition." This is a chemi-physical phenomenon which occurs when two liquids with different specific gravities are mixed. For example, when we put some oil and water in a glass and shake it well, the two ingredients first intermingle with each other, and then they are gradually separated. Figure 1.1[1] is a schematic view of that process, where, for example, the ingredient A is water and B is oil. Figure 1.2 shows an experimental result with polymer mixtures.

Mathematically, the phenomenon is modeled by the Cahn–Hilliard equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(pu + ru^3 + q\frac{\partial^2 u}{\partial x^2}\right),\ x \in (0, L),\ t > 0,\ p < 0,\ q < 0,\ r > 0. \quad (1.1)$$

The solution $u(x, t)$ describes the ratio of one component (oil, for example) to the other (water). Here we limit ourselves to the one-dimensional case, for simplicity of argument. We impose the boundary conditions below on the problem:

$$\frac{\partial u}{\partial x} = \frac{\partial^3 u}{\partial x^3} = 0, \quad x = 0, L. \quad (1.2)$$

[1]Reprinted figure with permission from H. Tanaka and T. Nishi, Direct determination of the probability distribution function of concentration in polymer mixtures undergoing phase separation, *Phys. Rev. Lett.*, 59, 692-695(1987). Copyright (1987) by the American Physical Society.

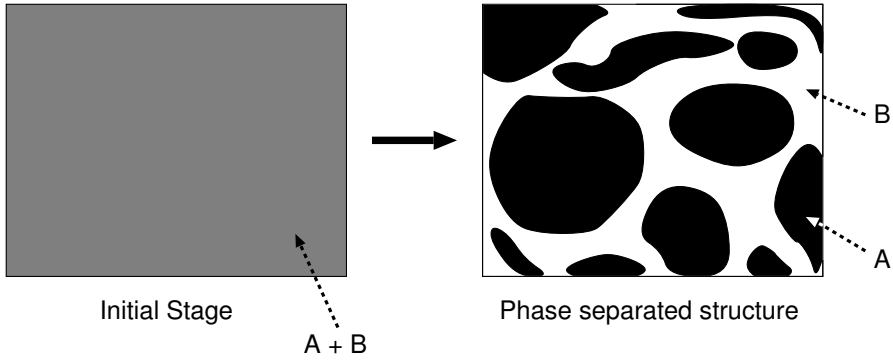

FIGURE 1.1: Schematic view of the spinodal decomposition.

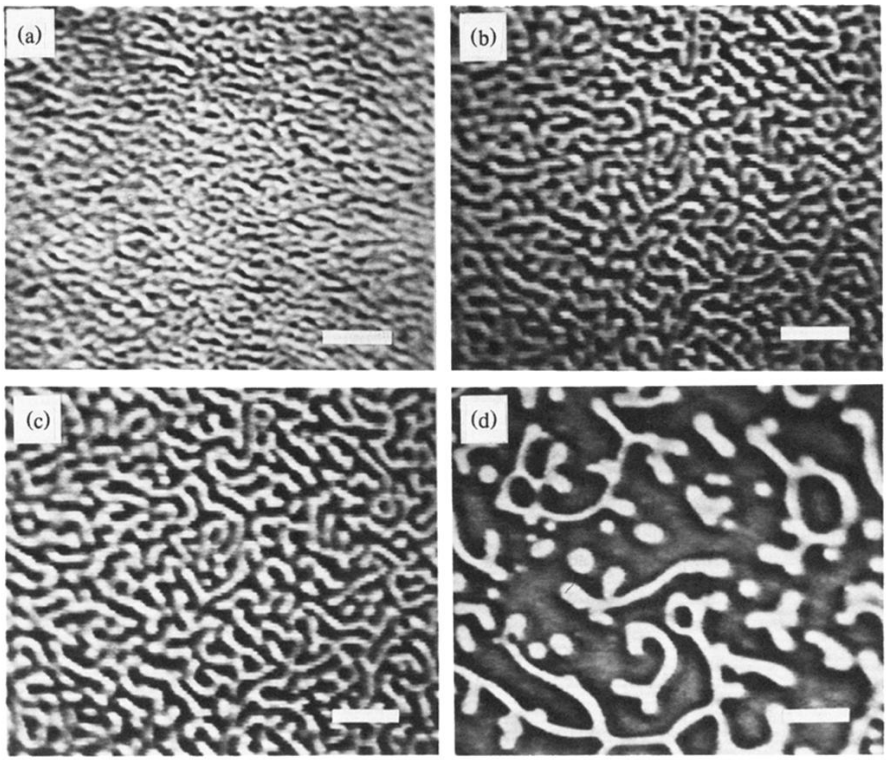

FIGURE 1.2: Temporal change of phase-separated structure of mixtures of polystyrene and polyvinyl methyl ether [163]. Bar corresponds to 20 μm. (a)–(d) structures at 480, 720, 1200, and 2400 s after quench, respectively.

It is not easy to integrate the Cahn–Hilliard equation numerically [70]. The right hand side of (1.1) includes a diffusion term pu_{xx} whose coefficient is *negative* (recall $p < 0$). This means that in the numerical integration we have to solve a diffusion equation in the *negative* time direction, which is obviously numerically unstable. In order to illustrate this, let us try an explicit Euler scheme as the simplest example. Let the spatial discretization width be $\Delta x = L/N$, where N is the number of the spatial grid points, and denote the time mesh width by $\Delta t > 0$. We denote the approximate solution by ${U_k}^{(m)} \simeq u(k\Delta x, m\Delta t)$ $(k = 0, 1, \ldots, N,\ m = 0, 1, 2, \ldots)$. We also write $\boldsymbol{U}^{(m)} = \left(U_0^{(m)}, \ldots, U_N^{(m)}\right)^\top$. Then the Euler scheme reads as follows.

Scheme 1.1 (Standard Euler scheme for Cahn–Hilliard equation) *Given an initial data* $\boldsymbol{U}^{(0)}$*, the approximate solutions* $\boldsymbol{U}^{(m)}$ *are calculated by, for* $m = 0, 1, 2, \ldots$*,*

$$\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = \delta_k^{\langle 2\rangle}\left(p\,{U_k}^{(m)} + r\,({U_k}^{(m)})^3 + q\,\delta_k^{\langle 2\rangle}{U_k}^{(m)}\right), \qquad k = 0, \ldots, N, \tag{1.3}$$

with the discrete boundary condition corresponding to (1.2)*:*

$$\delta_k^{\langle 1\rangle}{U_k}^{(m)} = \delta_k^{\langle 3\rangle}{U_k}^{(m)} = 0, \quad k = 0, N. \tag{1.4}$$

The symbols $\delta_k^{\langle p\rangle}$ $(p = 1, 2, 3)$ mean the standard second-order central difference operators for $\partial^p/\partial x^p$, which are explicitly written as

$$\delta_k^{\langle 1\rangle} f_k = \frac{f_{k+1} - f_{k-1}}{2\Delta x}, \tag{1.5}$$

$$\delta_k^{\langle 2\rangle} f_k = \frac{f_{k+1} - 2f_k + f_{k-1}}{(\Delta x)^2}, \tag{1.6}$$

$$\delta_k^{\langle 3\rangle} f_k = \frac{f_{k+2} - 2f_{k+1} + 2f_{k-1} - f_{k-2}}{2(\Delta x)^3}. \tag{1.7}$$

Figure 1.3 shows the result obtained by the scheme. In the example, the parameters are $p = -1.0$, $q = -0.001$, $r = 1.0$, and $L = 1$, $N = 50$ (thus $\Delta x = 1/50$). Two time mesh sizes: $\Delta t = 1/1200$ and $1/12000$ are tested. In both graphs, the staggered line lying around $u = 0$ line is the initial pattern:

$$u_0(x) = 0.1\sin(2\pi x) + 0.01\cos(4\pi x) + 0.06\sin(4\pi x) + 0.02\cos(10\pi x). \tag{1.8}$$

The numerical solution with $\Delta t = 1/1200$ (top graph) rapidly blows up, exhibiting strong oscillation in only four or five steps. This hardly improves even when we refine the time mesh; the numerical solution with $\Delta t = 1/12000$ (bottom graph) also blows up in only six or seven steps.

Facing this difficulty, we have two options: one is to use some reliable ODE solver which allows adaptive integration, after suitably discretizing the space

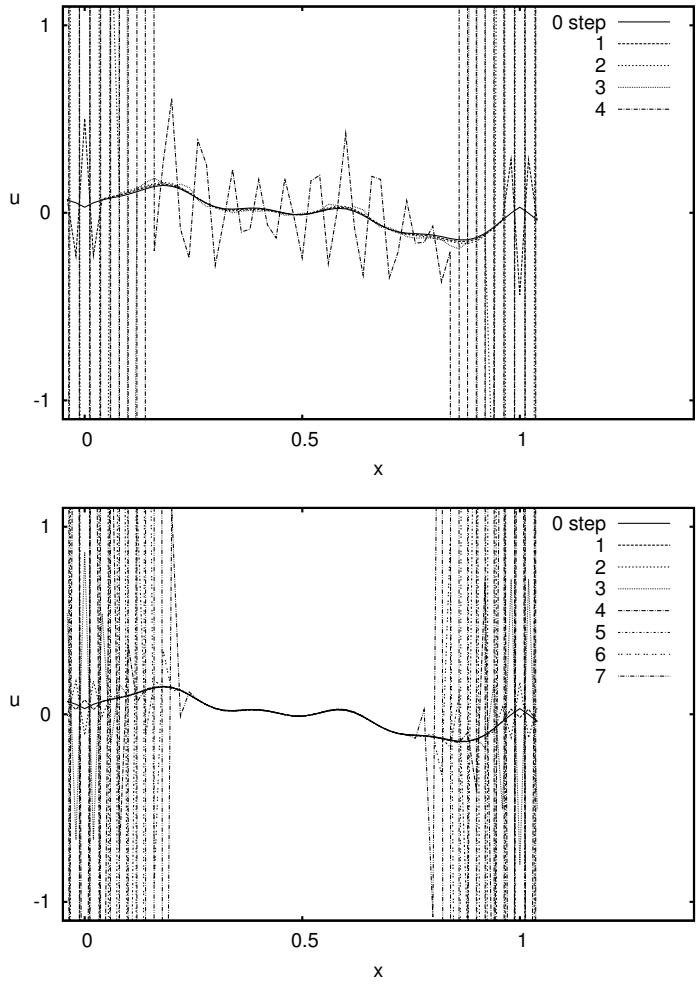

FIGURE 1.3: Numerical solutions of the Cahn–Hilliard equation by the explicit Euler scheme: (top) $\Delta t = 1/1200$; (bottom)$\Delta t = 1/12000$.

variable. This might work, though it may need considerable computation time because the package should be forced to choose very small time mesh size. The other option—which *is* the basic concept throughout this book—is to use some special scheme designed for stable integration of the equation.

To seek such a special scheme, let us cast a spotlight on a quantity, the "free energy" or "local energy" of the problem:

$$G(u, u_x) = \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(u_x)^2. \tag{1.9}$$

We call its spatial integration:

$$J(u) = \int_0^L G(u, u_x)\mathrm{d}x \tag{1.10}$$

the "global energy." Note that J is a functional of u, but at the same time it can be regarded as a function of t. The equation (1.1) can then be written as

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2}\left(\frac{\delta G}{\delta u}\right), \tag{1.11}$$

where $\delta G/\delta u$ is the (first) variational derivative of $G(u, u_x)$ obtained from the following variation calculation.

$$\begin{aligned}
&\int_0^L (G(u+\delta u, u_x+\delta u_x) - G(u, u_x))\mathrm{d}x \\
&= \int_0^L \left(\frac{\partial G}{\partial u}\delta u + \frac{\partial G}{\partial u_x}\delta u_x\right)\mathrm{d}x + O(\delta u^2) \\
&= \int_0^L \left(\frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}\right)\delta u\,\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\delta u\right]_0^L + O(\delta u^2) \\
&= \int_0^L \frac{\delta G}{\delta u}\delta u\,\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\delta u\right]_0^L + O(\delta u^2).
\end{aligned} \tag{1.12}$$

The last equality defines $\delta G/\delta u$. The form (1.11) states that the evolution of the solution is roughly a "gradient-flow"; it evolves in such a direction that the global energy is decreased:

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}J(u) &= \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_0^L \\
&= -\int_0^L \left(\frac{\partial}{\partial x}\frac{\delta G}{\delta u}\right)^2 \mathrm{d}x + \left[\left(\frac{\delta G}{\delta u}\right)\frac{\partial}{\partial x}\left(\frac{\delta G}{\delta u}\right)\right]_0^L \\
&\le 0.
\end{aligned} \tag{1.13}$$

Note that $(\partial/\partial x)u = 0$ and $(\partial/\partial x)^3 u = 0$ mean $\partial G/\partial u_x = 0$ and $(\partial/\partial x)\delta G/\delta u = 0$, and thus the boundary terms vanish thanks to the boundary condition (1.2).

From the dissipation property, the next important proposition immediately follows.

PROPOSITION 1.1* L^∞*-boundedness of solution
As to the solution of (1.1) *under the boundary condition* (1.2)*, we have this a priori estimate*:

$$\|u\|_\infty < \infty, \quad t > 0, \tag{1.14}$$

where $\|\cdot\|_p$ $(p = 1, 2, \ldots, \infty)$ *is the standard* L^p *norm.*

PROOF Recalling $p, q < 0, r > 0$, we have the trivial identity:

$$\frac{p}{2}u^2 + \frac{r}{4}u^4 \geq -pu^2 - \frac{9p^2}{4r}.$$

Then by the energy dissipation property (1.13) we know for any $t > 0$,

$$\begin{aligned} J(u(x,0)) &\geq J(u(x,t)) \\ &= \int_0^L \left\{ \frac{1}{2}pu^2 + \frac{1}{4}ru^4 - \frac{1}{2}q(u_x)^2 \right\} \mathrm{d}x \\ &\geq \int_0^L \left\{ -pu^2 - \frac{9p^2}{4r} - \frac{1}{2}q(u_x)^2 \right\} \mathrm{d}x \\ &= -p\|u\|_2^2 - \frac{9p^2 L}{4r} - \frac{q}{2}\|u_x\|_2^2. \end{aligned} \tag{1.15}$$

Thus we have

$$J(u(x,0)) + \frac{9p^2 L}{4r} \geq -p\|u\|_2^2 - \frac{q}{2}\|u_x\|_2^2.$$

Again recalling $p, q < 0, r > 0$, we see that

$$\|u\|_2, \|u_x\|_2 < \infty. \tag{1.16}$$

Then with the aid of the Sobolev type inequality (see, for example, John [94]):

$$\|u\|_\infty^2 \leq c\left(\|u\|_2^2 + \|u_x\|_2^2\right),$$

which holds for every function $u(\cdot, t) \in H^1(0, L)$, we obtain $\|u\|_\infty < \infty$. □

In other words,

[Key observation 1]
The dissipation property prevents the solution's blow-up.

This observation encourages us to seek a scheme which retains the dissipation property, because it may also prevent the blow-up of the approximate solution. We here present such a scheme. (At the time being, we do not discuss how it is constructed. It will be covered in Chapter 4.)

Scheme 1.2 (Dissipative scheme for Cahn–Hilliard equation) *Given an initial data* $\boldsymbol{U}^{(0)}$*, the approximate solutions* $\boldsymbol{U}^{(m)}$ *are calculated by, for* $m = 0, 1, 2, \ldots,$

$$\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = \delta_k^{\langle 2 \rangle} \left\{ p \left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2} \right) + q \delta_k^{\langle 2 \rangle} \left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2} \right) + r \left(\frac{({U_k}^{(m+1)})^3 + ({U_k}^{(m+1)})^2 {U_k}^{(m)} + {U_k}^{(m+1)} ({U_k}^{(m)})^2 + ({U_k}^{(m)})^3}{4} \right) \right\}, \quad k = 0, \ldots, N, \tag{1.17}$$

with the discrete boundary condition (1.4)*.*

Scheme 1.2 has the desired discrete dissipation property.

PROPOSITION 1.2 Dissipation property of Scheme 1.2
Let us define a "discrete local energy" $G_{\mathrm{d}} : \mathbb{R}^{N+1} \to \mathbb{R}^{N+1}$ *by*

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) \stackrel{\mathrm{d}}{\equiv} \frac{p}{2} ({U_k}^{(m)})^2 + \frac{r}{4} ({U_k}^{(m)})^2 - \frac{q}{2} \left(\frac{\left(\delta_k^+ {U_k}^{(m)} \right)^2 + \left(\delta_k^- {U_k}^{(m)} \right)^2}{2} \right), \tag{1.18}$$

where $G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})$ *denotes the k-th element (the detail of this expression will be explained soon in Section 1.3). We also define the discrete global energy accordingly by*

$$J_{\mathrm{d}}(\boldsymbol{U}^{(m)}) \stackrel{\mathrm{d}}{\equiv} \sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) \Delta x, \tag{1.19}$$

where

$$\sum_{k=0}^{N}{}'' f_k \stackrel{\mathrm{d}}{\equiv} \frac{1}{2} f_0 + f_1 + \cdots + f_{N-1} + \frac{1}{2} f_N \tag{1.20}$$

is the trapezoidal rule. Then the solution by Scheme 1.2 satisfies the following inequality.

$$J_{\mathrm{d}}(\boldsymbol{U}^{(m+1)}) \leq J_{\mathrm{d}}(\boldsymbol{U}^{(m)}), \quad m = 0, 1, 2, \ldots. \tag{1.21}$$

REMARK 1.1 Throughout this book, we basically adopt the trapezoidal rule as our main summation rule. Other rules, for example, the rectangle rule, can be also adopted. For example, when the periodic boundary condition is applied, the trapezoidal rule naturally coincides with the rectangle rule, and the latter is more convenient. Another example is the case where the use of the rectangle rule substantially simplifies the treatment of discrete boundary condition. This will be illustrated in Section 3.2.3.2. □

The proof of the proposition is left to Chapter 3 (generic theory) or Chapter 4 (the specific Cahn–Hilliard case). With this dissipation property, and a *discrete* Sobolev type inequality, we can prove that numerical solution *never* blows up (we leave the detail of this discussion to Chapter 4.)

For the moment we only show some numerical results. Figure 1.4 shows the result by Scheme 1.2 with a coarse time mesh $\Delta t = 1/1000$ (other parameters are the same as in the explicit Euler case). The calculation proceeds quite stably, and a physically correct pattern (a phase separation) is obtained. Figure 1.5 shows the evolution of the energy. The discrete energy is properly dissipated. For comparison, we present in Figure 1.6 the result obtained by the explicit scheme. There the energy is not dissipative at all; it even blows up. This fact agrees with the failure of the numerical computation.

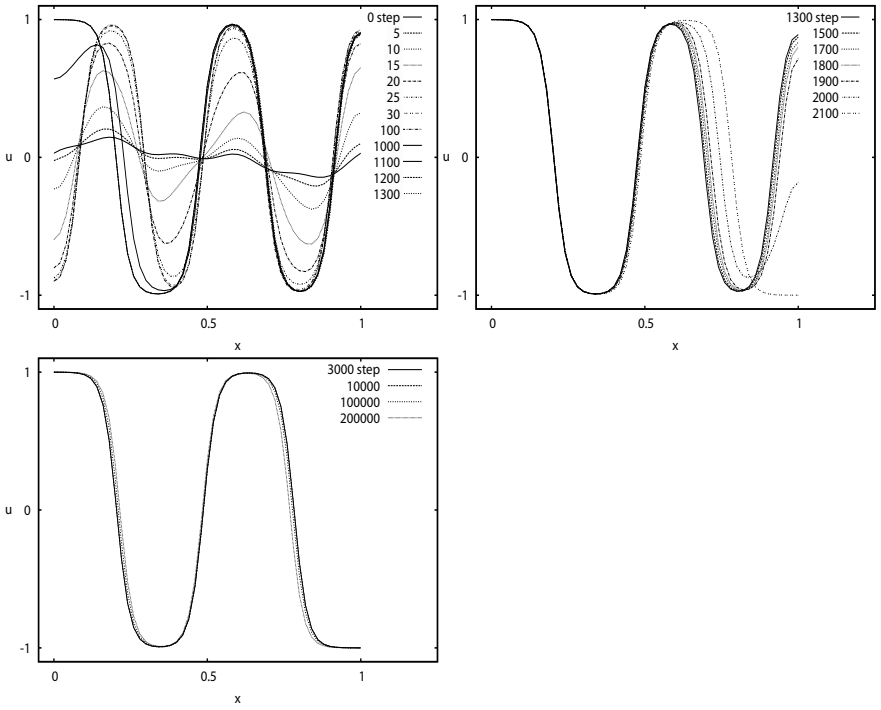

FIGURE 1.4: Numerical solutions of the Cahn–Hilliard equation by Scheme 1.2 ($\Delta t = 1/1000$): (top-left) steps 0 to 1300 (top-right) 1300 to 2100 (bottom) 3000 to 200,000.

The Cahn–Hilliard example clearly shows the superiority of the specialized scheme. The scheme preserves a discrete counterpart of the energy dissipation

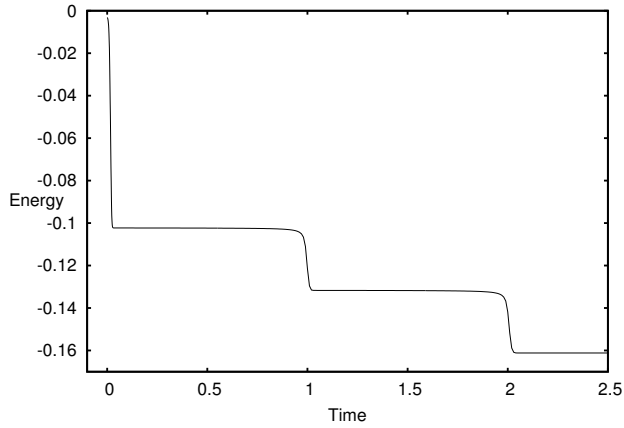

FIGURE 1.5: The evolution of the discrete energy in Scheme 1.2.

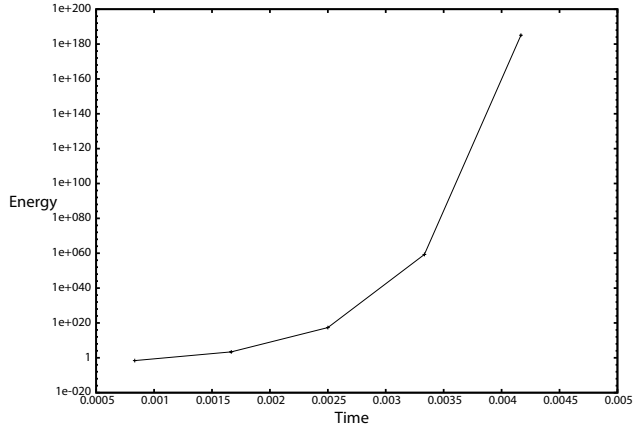

FIGURE 1.6: The evolution of the discrete energy in Scheme 1.1.

property, and the property is quite crucial for better numerical integration. The same thing often happens also in many conservative problems (i.e., problems with conservation laws). Next we will see how dissipative or conservative schemes, such as Scheme 1.2, can be constructed.

1.2 History

In this section, we briefly mention the related studies on the main subject of this book.

First attempts on dissipative/conservative schemes, or more generally on structure-preserving algorithms, focused on ordinary differential equations such as Hamiltonian systems. For example, in the beginning of the 1970's Greenspan [77] considered strictly conservative discretization of some mechanical systems. The method was then extended to general mechanical systems by Gonzalez [74] and McLachlan–Quispel–Robidoux [126, 127] decades later. A strong alternative to these works is the so-called symplectic method, which is a specialized numerical method for Hamiltonian systems. Though symplectic schemes are not strictly conservative, they are nearly conservative, and provide us very effective ways to integrate Hamiltonian systems. For the symplectic method, see Hairer–Lubich–Wanner [83], Sanz-Serna–Calvo [151] and Leimkuhler–Reich [104]. Related interesting studies on nearly conservative numerical schemes include: Faou–Hairer–Pham [52] and Hairer [81].

After these successes on Hamiltonian ODEs, many other classes of ODEs that have some intrinsic geometric structure have been identified, and structure-preserving algorithms for these ODEs have been extensively studied. These activities for ODEs are now also referred to as the "geometric numerical integration of ODEs," and form a big trend in numerical analysis. Interested readers may refer to Hairer–Lubich–Wanner [83] and Budd–Piggott [23].

In the PDE context, a number of studies on dissipative/conservative schemes have been carried out on individual dissipative or conservative PDEs, since around the 1970's. Below are quite limited examples. Strauss–Vazquez [155] presented a conservative finite difference scheme for the nonlinear Klein–Gordon equation. Hughes–Caughey–Liu [89] presented a conservative finite element scheme for the nonlinear elastodynamics problem. Delfour–Fortin–Payre [35] presented a conservative finite difference scheme for the nonlinear Schrödinger equation, then Akrivis–Dougalis–Karakashian [8] presented a finite element version of the scheme and proved the convergence of the finite element scheme. Sanz–Serna [150] considered the nonlinear Schrödinger equation as well. Taha–Ablowitz [159, 160] presented conservative finite difference schemes for the nonlinear Schrödinger equation and the Korteweg–de Vries equation. Du–Nicolaides [39] presented a dissipative finite element scheme for

the Cahn–Hilliard equation. Around the same time, in a completely different context from above, studies on soliton PDEs such as the KdV equation were done to find finite difference schemes that preserved discrete bilinear form or Wronskian form, corresponding to the original equations; see, for example, Hirota [85, 86]. They can be also regarded as structure-preserving methods.

Then during the 1990s, more general approaches that cover not only several individual PDEs but also a wide class of PDEs have been independently introduced by several groups. The discrete variational derivative method—the main subject of the present book—is one of such methods, proposed by Furihata–Mori [63, 64, 69, 65] around 1996 for PDEs with variational structure. The method has then been extended in various ways mainly by a Japanese group including Furihata, Matsuo, Ide, and Yaguchi [66, 67, 68, 90, 91, 116, 119, 120, 121, 122, 165, 166, 167], and succeeded in proving its effectiveness in various applications. At the same time, Gonzalez [75] proposed a conservative method for some general class of PDEs describing finite-deformation elastodynamics. There, the key is a special technique in time discretization devised for ODEs by Gonzalez [74]. Another excellent set of studies were given by McLachlan [129] and McLachlan–Robidoux [128], where a general method for designing conservative schemes for conservative PDEs based on their techniques on ODEs [126, 127] (and the related basic studies Quispel–Turner [145] and Quispel–Capel [144]) was developed (see also the recent related results: McLaren–Quispel [130], Quispel–McLaren [146], Celledoni *et al.* [26]). Jimenez [92] has also studied a systematic approach to obtain discrete conservation laws for certain finite difference schemes.

Aside from strictly conservative or dissipative methods, several interesting approaches for structure-preserving integration of PDEs have emerged as of the writing of the present book. For a very comprehensive review including these topics, see Budd–Piggot [23]. For Hamiltonian PDEs, a unique approach was proposed by Marsden–Patrick–Shkoller [112] (see also Marsden–West [113] for a good review), and it has been intensively studied by their group. Their method is based on the discretization of the variational principle. Its name "variational integrator" is quite close to the discrete variational derivative method, but these methods are quite different. For Hamiltonian PDEs, there is another interesting emerging method, the "multi-symplectic method," developed by Bridges–Reich [22]. In the method, Hamiltonian PDEs are transformed into a special "multi-symplectic form," and then integrated in such a way that the multi-symplecticity is conserved. This method can be regarded as a generalization of the symplectic method for ODEs (see also McLachlan [124]). For the recent literature in this context, see, for example, [27, 87, 88] and the references therein.

Finally we would like to note that in this short summary we could by no means cover all of the related studies. We recommend that interested readers refer to several key reviews, such as Hairer–Lubich–Wanner [83], Budd–Piggott [23], Leimkuhler–Reich [104], and Lubich [110], and consult their references as well.

1.3 Derivation of Dissipative or Conservative Schemes

In this section we demonstrate how numerical schemes that retain dissipation or conservation properties are constructed. To avoid exhaustive discussion involving cumbersome symbols, we here limit ourselves to some typical PDEs, possibly ignoring some details. More precise description will be found in Chapter 3 (generic theory) and Chapter 4 (application examples). We consider the following four cases: first-order real-valued PDEs, first-order complex-valued PDEs, systems of first-order PDEs, and second-order PDEs.

1.3.1 Procedure for First-Order Real-Valued PDEs

Suppose that $u(x,t)$ is a real-valued function, and the local energy function is given as a real-valued function $G(u,u_x)$. We define the associated global energy by

$$J(u) \overset{\mathrm{d}}{\equiv} \int_0^L G(u,u_x)\mathrm{d}x. \tag{1.22}$$

Let us consider a real-valued PDE:

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta u}, \quad x \in (0,L),\ t>0. \tag{1.23}$$

The equation (1.23) is dissipative in the sense that

$$\frac{\mathrm{d}}{\mathrm{d}t}J(u) = \int_0^L \frac{\delta G}{\delta u}\frac{\partial u}{\partial t}\mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\frac{\partial u}{\partial t}\right]_0^L = -\int_0^L \left(\frac{\delta G}{\delta u}\right)^2 \mathrm{d}x \le 0, \tag{1.24}$$

if boundary conditions are set so that the boundary term $[\,\cdot\,]_0^L$ vanishes. In fact it does, for example, under the Dirichlet boundary condition $u(0,t) = u(L,t) = 0$. Throughout this introductory chapter, we basically neglect boundary terms for simplicity.

Let us construct a dissipative scheme, i.e., a scheme that keeps a discrete version of the dissipation property, for the equation. Our strategy is based on the following important observation:

> [Key observation 2]
> *The dissipation property* (1.24) *immediately follows from the variational form* (1.23).

In fact, in the proof of the dissipation property (1.24), the concrete form of the energy G, and accordingly the concrete form of the PDE, are not relevant. The variational form itself *is* the key in the dissipation property. This observation leads us to a strategy summarized in Figure 1.7. The left half of the diagram summarizes the continuous PDE case, which reads (starting from the top)

[step 1] Define an energy G.

[step 2] Take its variation to obtain the variational derivative $\delta G/\delta u$.

[step 3] Define a PDE with the variational derivative. Then, as a consequence (the up-pointing arrow), the energy dissipation property follows.

Our idea here is to simulate this round trip structure, from the energy $G(u)$ to its dissipation property via variational derivative, in a discrete setting. In this way the method is "structure-preserving." The right half of the diagram reads

[step 1_{d}] Define a *discrete* energy (as an approximation of the continuous energy G).

[step 2_{d}] Take its *discrete* variation to obtain the *discrete* variational derivative.

[step 3_{d}] Define a scheme with the *discrete* variational derivative. Then, the *discrete* dissipation property should follow (again, denoted by the up-pointing arrow).

As opposed to this structure-preserving strategy, the usual way of constructing a scheme is to directly discretize the concrete form of the PDE (the bottom right-pointing arrow from PDE to finite difference scheme). In such an way, however, the beautiful round trip structure is highly likely to be destroyed, and thus generally the desired dissipation property is lost.

Let us actually follow the strategy to construct a dissipative scheme for the equation (1.23). To illustrate how the calculation goes exactly, we pick the linear diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{1.25}$$

as a concrete example, which is of the form (1.23) with $G(u, u_x) = (u_x)^2/2$.

[step 1_{d}] *Defining a discrete energy*

By simply replacing u in $G(u, u_x)$ with ${U_k}^{(m)}$, and u_x with some finite difference, we obtain a discrete energy $G_{\mathrm{d}}(\boldsymbol{U}^{(m)})$. The subscript "d", standing for "discrete", is added to distinguish this quantity from the continuous energy G. The discrete energy G_{d} is a real-valued $(N+1)$-dimensional vector function of $\boldsymbol{U}^{(m)}$; we denote its each elements by $G_{\mathrm{d},k}$ $(k = 0, \ldots, N)$. (See the example below.)

Note that there are several possibilities in approximating u_x, since there are many difference operators representing the same differentiation. For example, ${u_x}^2$ can be

$$(\delta_k^{\langle 1 \rangle} {U_k}^{(m)})^2,\ (\delta_k^{+} {U_k}^{(m)})^2,\ (\delta_k^{-} {U_k}^{(m)})^2,\ \text{or}\ \frac{(\delta_k^{+} {U_k}^{(m)})^2 + (\delta_k^{-} {U_k}^{(m)})^2}{2}, \tag{1.26}$$

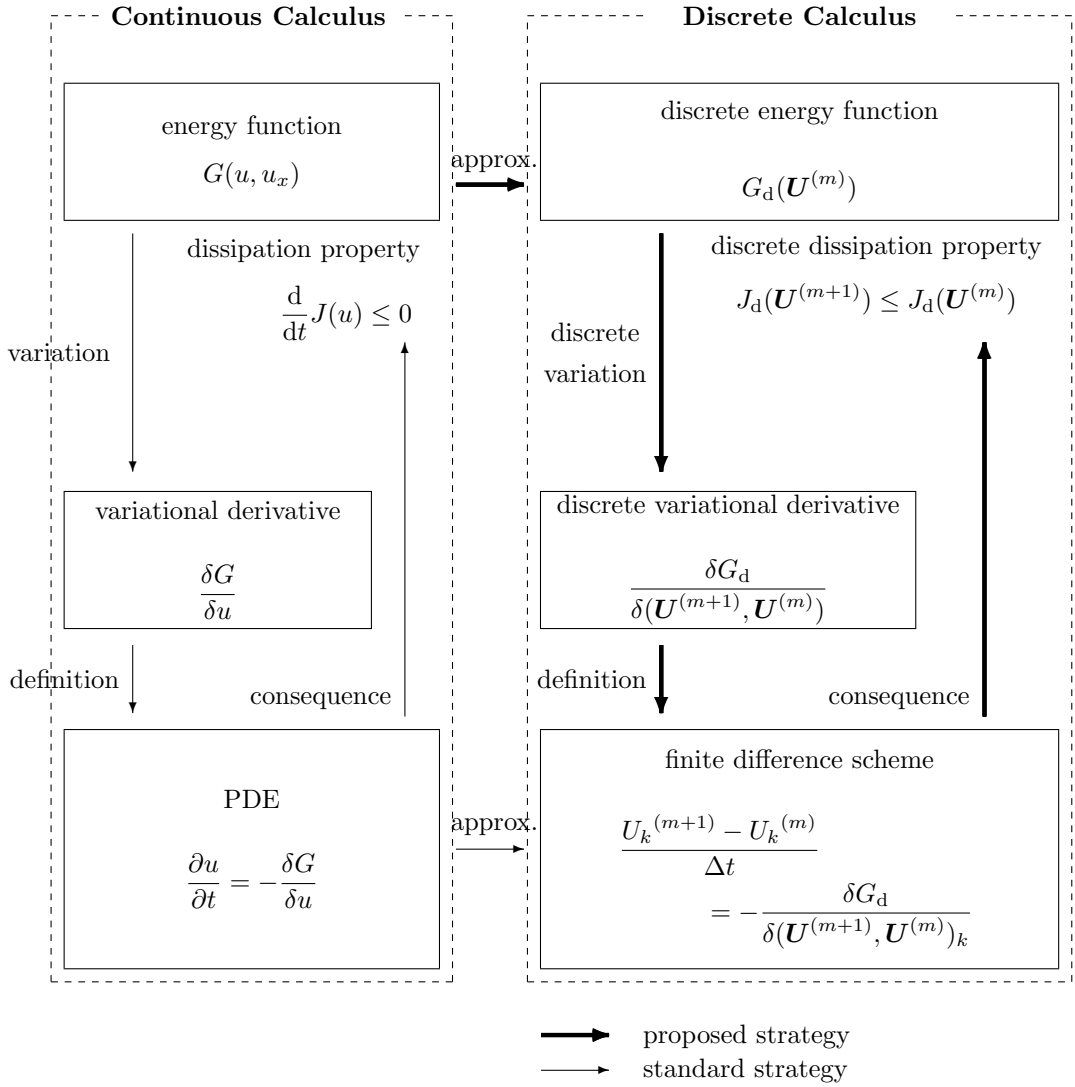

FIGURE 1.7: Standard strategy versus proposed strategy.

where

$$\delta_k^{\langle 1\rangle} f_k = \frac{f_{k+1} - f_{k-1}}{2\Delta x},\ \delta_k^+ f_k = \frac{f_{k+1} - f_k}{\Delta x},\ \delta_k^- f_k = \frac{f_k - f_{k-1}}{\Delta x} \tag{1.27}$$

are the standard difference operators for $\partial/\partial x$. We can choose *any* of them. Regardless of the choice, we will obtain a dissipative scheme. We must note, however, that *a different choice leads to a different scheme* (see Remark 1.2).

In the concrete example of (1.25), let us choose a symmetric approximation:

$$(u_x)^2 \simeq \frac{(\delta_k^+ {U_k}^{(m)})^2 + (\delta_k^- {U_k}^{(m)})^2}{2}. \tag{1.28}$$

Then the discrete local energy becomes

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) = \frac{1}{2}\left(\frac{(\delta_k^+ {U_k}^{(m)})^2 + (\delta_k^- {U_k}^{(m)})^2}{2}\right), \tag{1.29}$$

and the corresponding discrete global energy is

$$J_{\mathrm{d}}(\boldsymbol{U}^{(m)}) = {\sum_{k=0}^{N}}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\Delta x. \tag{1.30}$$

[step 2_{d}] *Taking the discrete variation*

Recall the continuous variation calculation (1.12), which is summarized as

$$\begin{aligned}&\int_0^L \{G(u+\delta u, u_x+\delta u_x) - G(u,u_x)\}\,\mathrm{d}x\\ &= \int_0^L \frac{\delta G}{\delta u}\delta u\,\mathrm{d}x + (\text{boundary term}) + O(\delta u^2).\end{aligned} \tag{1.31}$$

We hope to simulate this in a discrete setting. That is, we hope to find an identity:

$$\begin{aligned}&{\sum_{k=0}^{N}}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x =\\ &{\sum_{k=0}^{N}}'' \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}\left({U_k}^{(m+1)} - {U_k}^{(m)}\right)\Delta x + (\text{boundary term}).\end{aligned} \tag{1.32}$$

At this point, readers need not fully understand the discrete symbols; they will be introduced in Chapter 3. For now it is sufficient to just recognize the correspondences between the continuous and discrete symbols:

$$\begin{aligned}G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) &\Leftrightarrow G(u+\delta u, u_x+\delta u_x) - G(u,u_x),\\ \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} &\Leftrightarrow \frac{\delta G}{\delta u},\\ {U_k}^{(m+1)} - {U_k}^{(m)} &\Leftrightarrow \delta u.\end{aligned}$$

The abstract identity (1.32) demands that the difference of the energies,

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}),$$

should be decomposable into the discrete version of δu,

$$U_k{}^{(m+1)} - U_k{}^{(m)},$$

and a discrete quantity which corresponds to the variational derivative, called the "discrete variational derivative,"

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}.$$

Later in Chapter 3, it is shown that in fact for any given G_{d} this decomposition is possible.

In the case of example (1.25), the identity (1.32) can be easily found as follows.

$$\begin{aligned}
&\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x \\
&= \frac{1}{2}\sum_{k=0}^{N}{}'' \left(\frac{(\delta_k^+ U_k{}^{(m+1)})^2 - (\delta_k^+ U_k{}^{(m)})^2}{2} + \frac{(\delta_k^- U_k{}^{(m+1)})^2 - (\delta_k^- U_k{}^{(m)})^2}{2}\right)\Delta x \\
&= \frac{1}{2}\sum_{k=0}^{N}{}'' \left\{\delta_k^+\left(\frac{U_k{}^{(m+1)} + U_k{}^{(m)}}{2}\right)\cdot \delta_k^+(U_k{}^{(m+1)} - U_k{}^{(m)})\right. \\
&\qquad \left. +\delta_k^-\left(\frac{U_k{}^{(m+1)} + U_k{}^{(m)}}{2}\right)\cdot \delta_k^-(U_k{}^{(m+1)} - U_k{}^{(m)})\right\}\Delta x \\
&= -\sum_{k=0}^{N}{}'' \left\{\delta_k^{\langle 2\rangle}\left(\frac{U_k{}^{(m+1)} + U_k{}^{(m)}}{2}\right)\right\}(U_k{}^{(m+1)} - U_k{}^{(m)})\Delta x \\
&\qquad\qquad + (\text{boundary term}). \qquad (1.33)
\end{aligned}$$

The symbol $\delta_k^{\langle 2\rangle}$ is the standard central difference operator for $\partial^2/\partial x^2$ defined by

$$\delta_k^{\langle 2\rangle} f_k = \frac{f_{k+1} - 2f_k + f_{k-1}}{(\Delta x)^2}.$$

In (1.33) a trivial identity $\delta_k^+\delta_k^- = \delta_k^-\delta_k^+ = \delta_k^{\langle 2\rangle}$ is used. The summation-by-parts formula:

$$\sum_{k=0}^{N}{}''(\delta_k^+ f_k)g_k\Delta x = -\sum_{k=0}^{N}{}'' f_k(\delta_k^- g_k)\Delta x + (\text{boundary term}) \qquad (1.34)$$

is used as well, which is a discrete analogue of the integration-by-parts formula. The precise form of the boundary term is omitted here in order to avoid complications. From (1.33), we find the concrete form of the discrete variational derivative in the case of (1.25) as

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k} = -\delta_k^{\langle 2\rangle}\left(\frac{{U_k}^{(m+1)}+{U_k}^{(m)}}{2}\right). \tag{1.35}$$

Note that this in fact approximates the continuous version: $\delta G/\delta u = -u_{xx}$. This supports the view that the above calculation is in fact *discrete* variation.

[step $\mathbf{3_d}$] *Defining a scheme*

Once the discrete variational derivative is found for a given discrete energy G_{d}, a scheme is defined with it in an abstract manner, analogously to the continuous one (1.23).

Scheme 1.3 (Dissipative scheme for (1.23)) *With given initial data* $\boldsymbol{U}^{(0)}$ *and appropriate boundary conditions, we compute* $\boldsymbol{U}^{(m)}$ *by, for* $m = 0, 1, 2, \ldots$,

$$\frac{{U_k}^{(m+1)}-{U_k}^{(m)}}{\Delta t} = -\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}, \qquad k = 0, \ldots, N. \tag{1.36}$$

This scheme keeps the desired dissipation property as follows. Observe that the proof proceeds exactly analogously to the continuous case (1.24); in particular, the concrete forms of the discrete energy function G_{d} and the discrete variational derivative $\delta G_{\mathrm{d}}/\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})$ are not relevant. Only the discrete variational structure matters.

PROPOSITION 1.3 Dissipation property of Scheme 1.3
Scheme 1.3 is dissipative in the sense that

$$J_{\mathrm{d}}(\boldsymbol{U}^{(m+1)}) \le J_{\mathrm{d}}(\boldsymbol{U}^{(m)}), \quad m = 0, 1, 2 \ldots. \tag{1.37}$$

PROOF By the identity (1.32), we obtain

$$\begin{aligned}
&J_{\mathrm{d}}(\boldsymbol{U}^{(m+1)}) - J_{\mathrm{d}}(\boldsymbol{U}^{(m)}) \\
&= \frac{1}{\Delta t}{\sum_{k=0}^{N}}''\left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x \\
&= {\sum_{k=0}^{N}}''\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\left(\frac{{U_k}^{(m+1)}-{U_k}^{(m)}}{\Delta t}\right)\Delta x + (\text{boundary term}) \\
&= -{\sum_{k=0}^{N}}''\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)},\boldsymbol{U}^{(m)})_k}\right)^2\Delta x \\
&\le 0.
\end{aligned} \tag{1.38}$$

In the second equality the boundary terms are assumed to vanish due to some appropriate boundary conditions. In the last equality the scheme in variational form (1.36) is used. □

In the case of the linear diffusion equation (1.25), Scheme 1.3 reads

$$\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = -\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} = \delta_k^{\langle 2\rangle}\left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}\right). \tag{1.39}$$

The concrete form of the discrete variational derivative has been obtained in (1.35). The dissipation property is guaranteed by Proposition 1.3, where the discrete energy function is given by (1.29).

Note that in this case the resulting scheme is just the standard Crank–Nicolson scheme. Although we can say the project has successfully completed in the sense that we obtained a stable scheme (the stability of this Crank–Nicolson scheme is widely known, while it is also possible to prove it directly by utilizing the discrete dissipation property), it is not so exciting in that the obtained scheme is a trivial one. In more generic nonlinear problems, however, resulting schemes are non-trivial, and that is exactly where the discrete variational derivative method is of considerable benefit.

REMARK 1.2 As noted **[step 1$_{\mathrm{d}}$]** (page 13), the definition of discrete energy function is not unique, and a different choice will generally leads us to a different scheme. For example, let us approximate

$$(u_x)^2 \simeq (\delta_k^{\langle 1\rangle} {U_k}^{(m)})^2, \tag{1.40}$$

instead of (1.28); that is, we start from the discrete energy function

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) = \frac{(\delta_k^{\langle 1\rangle} {U_k}^{(m)})^2}{2}. \tag{1.41}$$

Then the associated discrete variational derivative will be

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} = -(\delta_k^{\langle 1\rangle})^2\left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}\right), \tag{1.42}$$

which then leads us to a scheme:

$$\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} = -\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} = (\delta_k^{\langle 1\rangle})^2\left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}\right). \tag{1.43}$$

This is different from (1.39). Still, the scheme is "dissipative," in the sense that Proposition 1.3 holds for the $G_{\mathrm{d}}(\boldsymbol{U}^{(m)})$ defined in (1.41).

As this example illustrates, there is generally a degree of freedom in choosing a discrete energy function, and this is left to each user. Once it is fixed, however, by following the procedure of the discrete variational derivative method, we automatically obtain a scheme that preserves the desired dissipation (or in the conservative case, conservation) property *with respect to the specified discrete energy function.* The performance of the resulting scheme, such as stability and accuracy, often heavily depends on the choice. This issue will be discussed in detail in Section 3.2.3. □

Above procedure can be easily extended to more general real-valued dissipative or conservative PDEs of the following types.

[real-valued dissipative PDEs]

$$\frac{\partial u}{\partial t} = -(-1)^{s+1}\left(\frac{\partial}{\partial x}\right)^{2s}\frac{\delta G}{\delta u}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x \le 0, \tag{1.44}$$

where $s = 0, 1, 2, \ldots$. The linear diffusion equation belongs to this class with $s = 0$. The Cahn–Hilliard equation in the previous section is another example, where $s = 1$.

[real-valued conservative PDEs]

$$\frac{\partial u}{\partial t} = \left(\frac{\partial}{\partial x}\right)^{2s+1}\frac{\delta G}{\delta u}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x = 0, \tag{1.45}$$

where $s = 0, 1, 2 \ldots$. This class includes, for example, the Korteweg–de Vries equation.

More detailed description on these PDEs is given in Chapter 2, and the full procedures for them are described in Chapter 3. Concrete examples will be found in Chapter 4.

1.3.2 Procedure for First-Order Complex-Valued PDEs

Several complex-valued PDEs have variational structure, and the idea described above can be utilized. Suppose that $u(x,t)$ is a complex-valued function, and a real-valued function $G(u,u_x)$ is given as the local energy function. As before, the associated global energy is defined by

$$J(u) \stackrel{\mathrm{d}}{\equiv} \int_0^L G(u,u_x)\mathrm{d}x. \tag{1.46}$$

Let us consider first-order complex-valued PDEs of the form

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \quad x \in (0,L),\ t > 0, \tag{1.47}$$

where $\mathrm{i} = \sqrt{-1}$. The symbol $\delta G/\delta \overline{u}$ is the variational derivative of G with respect to $\overline{u}$, which is obtained as follows.

$$\begin{aligned}
&\int_0^L (G(u+\delta u, u_x+\delta u_x) - G(u,u_x))\mathrm{d}x \\
&= \int_0^L \left\{ \left(\frac{\partial G}{\partial u}\delta u + \frac{\partial G}{\partial u_x}\delta u_x \right) + \left(\frac{\partial G}{\partial \overline{u}}\delta \overline{u} + \frac{\partial G}{\partial \overline{u_x}}\delta \overline{u_x} \right) \right\} \mathrm{d}x + O(|\delta u|^2) \\
&= \int_0^L \left\{ \left(\frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x} \right) \delta u + \left(\frac{\partial G}{\partial \overline{u}} - \frac{\partial}{\partial x}\frac{\partial G}{\partial \overline{u_x}} \right) \delta \overline{u} \right\} \mathrm{d}x \\
&\quad + \left[\frac{\partial G}{\partial u_x}\delta u + \frac{\partial G}{\partial \overline{u_x}}\delta \overline{u} \right]_0^L + O(|\delta u|^2) \\
&= \int_0^L \left(\frac{\delta G}{\delta u}\delta u + \frac{\delta G}{\delta \overline{u}}\delta \overline{u} \right) \mathrm{d}x + \left[\frac{\partial G}{\partial u_x}\delta u + \frac{\partial G}{\partial \overline{u_x}}\delta \overline{u} \right]_0^L + O(|\delta u|^2). \qquad (1.48)
\end{aligned}$$

The quantities

$$\frac{\delta G}{\delta u} = \frac{\partial G}{\partial u} - \frac{\partial}{\partial x}\frac{\partial G}{\partial u_x}, \qquad \frac{\delta G}{\delta \overline{u}} = \frac{\partial G}{\partial \overline{u}} - \frac{\partial}{\partial x}\frac{\partial G}{\partial \overline{u_x}}$$

are complex variational derivatives. Note that they are in general complex conjugates of each other:

$$\overline{\frac{\delta G}{\delta u}} = \frac{\delta G}{\delta \overline{u}}.$$

(Strictly speaking, we need some assumption on G so that the conjugacy holds; this is left to the discussion in Chapter 3.) The PDE (1.47) is conservative in the sense that

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}J(u) &= \frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u,u_x)\mathrm{d}x \\
&= \int_0^L \left(\frac{\delta G}{\delta u}\frac{\partial u}{\partial t} + \frac{\delta G}{\delta \overline{u}}\frac{\partial \overline{u}}{\partial t} \right) \mathrm{d}x + (\text{boundary terms}) \\
&= \int_0^L \left(\mathrm{i}\left|\frac{\delta G}{\delta u}\right|^2 - \mathrm{i}\left|\frac{\delta G}{\delta u}\right|^2 \right) \mathrm{d}x \\
&= 0, \qquad (1.49)
\end{aligned}$$

provided some appropriate boundary conditions exist. For example, a linear conservative PDE

$$\mathrm{i}\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \qquad G(u,u_x) = |u_x|^2, \qquad (1.50)$$

belongs to this class.

Let us see how a conservative scheme is derived for (1.47). Again we follow the three steps.

[step 1_{d}] *Defining a discrete energy*

As in the real-valued case, we obtain a discrete energy $G_{\mathrm{d}}(\boldsymbol{U}^{(m)})$ by simply replacing u in $G(u, u_x)$ with ${U_k}^{(m)}$, and u_x with some finite difference. For the case of the linear PDE (1.50), we define a discrete local energy by, for example,

$$G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) = \frac{|\delta_k^+ {U_k}^{(m)}|^2 + |\delta_k^- {U_k}^{(m)}|^2}{2}. \tag{1.51}$$

This only differs from (1.29) in having $|\cdot|$ (absolute value) in place of $(\cdot)$. The associated discrete global energy is defined by

$$J_{\mathrm{d}}(\boldsymbol{U}^{(m)}) \overset{\mathrm{d}}{\equiv} {\sum_{k=0}^{N}}'' G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\Delta x. \tag{1.52}$$

[step 2_{d}] *Taking the discrete variation*

As in the real-valued case, we hope to simulate the variation calculation (1.48) which can be summarized as

$$\int_0^L \{G(u+\delta u, u_x+\delta u_x) - G(u,u_x)\}\,\mathrm{d}x = \int_0^L \left(\frac{\delta G}{\delta u}\delta u + \frac{\delta G}{\delta \overline{u}}\delta \overline{u}\right)\mathrm{d}x + (\text{boundary terms}), \tag{1.53}$$

in a discrete setting to find a discrete identity:

$$\begin{aligned}{\sum_{k=0}^{N}}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)})\right)\Delta x = \\ {\sum_{k=0}^{N}}'' \left\{ \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k}\left({U_k}^{(m+1)} - {U_k}^{(m)}\right) + \right. \\ \left. \frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}}, \boldsymbol{U}^{(m)})_k}\left(\overline{{U_k}^{(m+1)} - {U_k}^{(m)}}\right)\right\}\Delta x \\ + (\text{boundary terms}).\end{aligned} \tag{1.54}$$

In the above identity, there are new discrete symbols whose correspondences are

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \Leftrightarrow \frac{\delta G}{\delta u}, \tag{1.55a}$$

$$\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}})_k} \Leftrightarrow \frac{\delta G}{\delta \overline{u}}. \tag{1.55b}$$

They are called "complex discrete variational derivatives."

In the case of the linear PDE (1.50), we find an identity corresponding to (1.54) as follows.

$$
\begin{aligned}
&\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) \right) \Delta x \\
&= \sum_{k=0}^{N}{}'' \left(\frac{|\delta_k^+ {U_k}^{(m+1)}|^2 - |\delta_k^+ {U_k}^{(m)}|^2}{2} + \frac{|\delta_k^- {U_k}^{(m+1)}|^2 - |\delta_k^- {U_k}^{(m)}|^2}{2} \right) \Delta x \\
&= \frac{1}{2} \sum_{k=0}^{N}{}'' \left\{ \delta_k^+ \left(\overline{\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}} \right) \cdot \delta_k^+ \left({U_k}^{(m+1)} - {U_k}^{(m)} \right) + (\text{c.c.}) \right. \\
&\qquad \left. + \delta_k^- \left(\overline{\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}} \right) \cdot \delta_k^- \left({U_k}^{(m+1)} - {U_k}^{(m)} \right) + (\text{c.c.}) \right\} \Delta x \\
&= -\sum_{k=0}^{N}{}'' \left[\left\{ \delta_k^{\langle 2 \rangle} \left(\overline{\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}} \right) \right\} \left({U_k}^{(m+1)} - {U_k}^{(m)} \right) + (\text{c.c.}) \right] \Delta x \\
&\quad + (\text{boundary terms}).
\end{aligned}
\tag{1.56}
$$

The expression "(c.c.)" denotes the complex conjugate of the preceding term(s). In the above calculation, a trivial identity

$$
\frac{|a|^2 - |b|^2}{2} = \frac{1}{2} \left\{ \frac{a+b}{2} (\overline{a-b}) + (\text{c.c.}) \right\},
$$

and the summation-by-parts formula (1.34) are used. As a result we find the discrete versions of the complex variational derivatives:

$$
\frac{\delta G_{\mathrm{d}}}{\delta (\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} = -\delta_k^{\langle 2 \rangle} \left(\overline{\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2}} \right), \tag{1.57a}
$$

$$
\frac{\delta G_{\mathrm{d}}}{\delta (\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}})_k} = -\delta_k^{\langle 2 \rangle} \left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2} \right). \tag{1.57b}
$$

[step $\mathbf{3_d}$] *Defining a scheme*

With the discrete variational derivative, we define an abstract scheme analogously to (1.47).

Scheme 1.4 (Conservative scheme for (1.47)) *With given initial data* $\boldsymbol{U}^{(0)}$ *and appropriate boundary conditions, we compute* $\boldsymbol{U}^{(m)}$ *by, for* $m = 0, 1, 2, \ldots$,

$$
\mathrm{i} \left(\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} \right) = -\frac{\delta G_{\mathrm{d}}}{\delta (\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}})_k}, \qquad k = 0, \ldots, N. \tag{1.58}
$$

The scheme automatically becomes conservative as follows.

PROPOSITION 1.4 Conservation property of Scheme 1.4
Scheme 1.4 is conservative in the sense that

$$J_{\mathrm{d}}(\boldsymbol{U}^{(m)}) = J_{\mathrm{d}}(\boldsymbol{U}^{(0)}), \quad m = 1, 2, 3 \ldots . \tag{1.59}$$

PROOF By the identity (1.54), we obtain

$$\begin{aligned}
&J_{\mathrm{d}}(\boldsymbol{U}^{(m+1)}) - J_{\mathrm{d}}(\boldsymbol{U}^{(m)}) \\
&= \frac{1}{\Delta t}\sum_{k=0}^{N}{}'' \left(G_{\mathrm{d},k}(\boldsymbol{U}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{U}^{(m)}) \right) \Delta x \\
&= \sum_{k=0}^{N}{}'' \left\{ \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \left(\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} \right) + (\mathrm{c.c.}) \right\} \Delta x \\
&\quad + (\text{boundary terms}) \\
&= \sum_{k=0}^{N}{}'' \left\{ \mathrm{i} \left| \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{U}^{(m+1)}, \boldsymbol{U}^{(m)})_k} \right|^2 + (\mathrm{c.c.}) \right\} \Delta x \\
&= 0.
\end{aligned} \tag{1.60}$$

In the second equality the boundary terms are assumed to vanish with appropriate boundary conditions, and in the last equality (1.58) is used. □

In the case of the linear PDE (1.50), Scheme 1.4 reads

$$\mathrm{i}\left(\frac{{U_k}^{(m+1)} - {U_k}^{(m)}}{\Delta t} \right) = -\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{U}^{(m+1)}}, \overline{\boldsymbol{U}^{(m)}})_k} = \delta_k^{\langle 2 \rangle} \left(\frac{{U_k}^{(m+1)} + {U_k}^{(m)}}{2} \right),$$

where the concrete form of the complex discrete variational derivative has been obtained in (1.57b). Again this is just the standard Crank–Nicolson scheme. The conservation property is guaranteed by Proposition 1.4, where the discrete local energy is given by (1.51).

In the subsequent chapters, we will deal with the following complex-valued PDEs.

[complex-valued dissipative PDEs]

$$\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u, u_x)\mathrm{d}x \leq 0. \tag{1.61}$$

This includes, for example, the complex Ginzburg–Landau equation and the Newell–Whitehead equation.

[complex-valued conservative PDEs]

$$\mathrm{i}\frac{\partial u}{\partial t} = -\frac{\delta G}{\delta \overline{u}}, \quad \frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(u, u_x)\mathrm{d}x = 0. \tag{1.62}$$

The linear PDE (1.50) and the nonlinear Schrödinger equation belong to this class.

1.3.3 Procedure for Systems of First-Order PDEs

The idea described in the previous sections can be also applied to the systems of PDEs. The following is an example.

Let us consider the Zakharov equations [72],

$$\mathrm{i}\frac{\partial E}{\partial t} + \frac{\partial^2 E}{\partial x^2} = nE, \quad \frac{\partial^2 n}{\partial t^2} - \frac{\partial^2 n}{\partial x^2} = \frac{\partial^2}{\partial x^2}|E|^2, \qquad x \in (0, L),\ t > 0, \tag{1.63}$$

where $E(x,t)$ is complex-valued, and $n(x,t)$ is real-valued. The equations can be written with variational derivatives as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} E \\ \overline{E} \\ n \\ v \end{pmatrix} = \begin{pmatrix} 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} \delta G/\delta E \\ \delta G/\delta \overline{E} \\ \delta G/\delta n \\ \delta G/\delta v \end{pmatrix}, \tag{1.64}$$

where $v(x,t)$ is a real-valued intermediate variable such that $v_t = n + |E|^2$, and $G(E, n, v)$ is the energy function defined by

$$G(E, n, v) \overset{\mathrm{d}}{\equiv} |E_x|^2 + n|E|^2 + \frac{1}{2}(n^2 + (v_x)^2). \tag{1.65}$$

The concrete forms of the variational derivatives are

$$\frac{\delta G}{\delta E} = -\overline{E}_{xx} + n\overline{E}, \tag{1.66a}$$

$$\frac{\delta G}{\delta \overline{E}} = \overline{\frac{\delta G}{\delta E}}, \tag{1.66b}$$

$$\frac{\delta G}{\delta n} = n + |E|^2, \tag{1.66c}$$

$$\frac{\delta G}{\delta v} = -v_{xx}. \tag{1.66d}$$

It is easy to see that

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\int_0^L G(E,n,v)\mathrm{d}x \\
&= \int_0^L \left(\frac{\delta G}{\delta E}\frac{\partial E}{\partial t} + (\text{c.c.}) + \frac{\delta G}{\delta n}\frac{\partial n}{\partial t} + \frac{\delta G}{\delta v}\frac{\partial v}{\partial t}\right)\mathrm{d}x + (\text{boundary terms}) \\
&= \int_0^L \left(-\mathrm{i}\left|\frac{\delta G}{\delta E}\right|^2 + (\text{c.c.}) - \frac{\delta G}{\delta n}\frac{\delta G}{\delta v} + \frac{\delta G}{\delta v}\frac{\delta G}{\delta n}\right)\mathrm{d}x \\
&= 0.
\end{aligned}$$

Thus the Zakharov equations conserve the energy

$$J(E,n,v) \overset{\mathrm{d}}{\equiv} \int_0^L G(E,n,v)\mathrm{d}x. \tag{1.67}$$

As in the single PDE cases, we can construct discrete versions of the above variational derivatives, $\delta G/\delta E$, $\delta G/\delta\overline{E}$, $\delta G/\delta n$, and $\delta G/\delta v$, by which a conservative scheme for the Zakharov equations can be defined. Let us denote numerical solutions by ${E_k}^{(m)}$, ${n_k}^{(m)}$, $v_k^{(m)}$. Then we follow the three steps again as follows.

[step $\mathbf{1_d}$] *Defining a discrete energy*

We define the discrete local energy by

$$\begin{aligned}
G_{\mathrm{d},k}(\boldsymbol{E}^{(m)},\boldsymbol{n}^{(m)},\boldsymbol{v}^{(m)}) = \\
&\frac{|\delta_k^+ {E_k}^{(m)}|^2 + |\delta_k^- {E_k}^{(m)}|^2}{2} + {n_k}^{(m)}|{E_k}^{(m)}|^2 \\
&+ \frac{1}{2}\left({n_k}^{(m)^2} + \frac{(\delta_k^+ v_k^{(m)})^2 + (\delta_k^- v_k^{(m)})^2}{2}\right).
\end{aligned} \tag{1.68}$$

We define the discrete global energy accordingly by

$$J_{\mathrm{d}}(\boldsymbol{E}^{(m)},\boldsymbol{n}^{(m)},\boldsymbol{v}^{(m)}) \overset{\mathrm{d}}{\equiv} \sum_{k=0}^{N}{}'' G_{\mathrm{d},k}(\boldsymbol{E}^{(m)},\boldsymbol{n}^{(m)},\boldsymbol{v}^{(m)})\Delta x. \tag{1.69}$$

[step $\mathbf{2_d}$] *Taking the discrete variation*

Taking discrete variation, we have

$$\begin{aligned}
&\sum_{k=0}^{N}{}'' \left\{ G_{\mathrm{d},k}(\boldsymbol{E}^{(m+1)}, \boldsymbol{n}^{(m+1)}, \boldsymbol{v}^{(m+1)}) - G_{\mathrm{d},k}(\boldsymbol{E}^{(m)}, \boldsymbol{n}^{(m)}, \boldsymbol{v}^{(m)}) \right\} \Delta x \\
&\quad = \sum_{k=0}^{N}{}'' \left\{ \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{E}^{(m+1)}, \boldsymbol{E}^{(m)})_k} (E_k{}^{(m+1)} - E_k{}^{(m)}) \right. \\
&\qquad + \frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{E}^{(m+1)}}, \overline{\boldsymbol{E}^{(m)}})_k} (\overline{E_k{}^{(m+1)} - E_k{}^{(m)}}) \\
&\qquad + \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{n}^{(m+1)}, \boldsymbol{n}^{(m)})_k} (n_k{}^{(m+1)} - n_k{}^{(m)}) \\
&\qquad \left. + \frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{v}^{(m+1)}, \boldsymbol{v}^{(m)})_k} (v_k^{(m+1)} - v_k^{(m)}) \right\} \Delta x, \qquad (1.70)
\end{aligned}$$

where

$$\begin{aligned}
\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{E}^{(m+1)}, \boldsymbol{E}^{(m)})_k} &= -\delta_k^{\langle 2 \rangle} \left(\overline{\frac{E_k{}^{(m+1)} + E_k{}^{(m)}}{2}} \right) \\
&\quad + \left(\overline{\frac{E_k{}^{(m)} + E_k{}^{(m)}}{2}} \right) \left(\frac{n_k{}^{(m+1)} + n_k{}^{(m)}}{2} \right), \qquad (1.71a)
\end{aligned}$$

$$\frac{\delta G_{\mathrm{d}}}{\delta(\overline{\boldsymbol{E}^{(m+1)}}, \overline{\boldsymbol{E}^{(m)}})_k} = \overline{\left(\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{E}^{(m+1)}, \boldsymbol{E}^{(m)})_k} \right)}, \qquad (1.71b)$$

$$\begin{aligned}
\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{n}^{(m+1)}, \boldsymbol{n}^{(m)})_k} &= \frac{n_k{}^{(m+1)} + n_k{}^{(m)}}{2} \\
&\quad + \frac{|E_k{}^{(m+1)}|^2 + |E_k{}^{(m)}|^2}{2}, \qquad (1.71c)
\end{aligned}$$

$$\frac{\delta G_{\mathrm{d}}}{\delta(\boldsymbol{v}^{(m+1)}, \boldsymbol{v}^{(m)})_k} = -\delta_k^{\langle 2 \rangle} \left(\frac{v_k^{(m+1)} + v_k^{(m)}}{2} \right). \qquad (1.71d)$$

They are obviously discrete analogues of (1.66a) through (1.66d).

[step 3_{d}] *Defining a scheme*

With the discrete variational derivatives, we define a numerical scheme.

Scheme 1.5 (Conservative scheme for the Zakharov equations) *With given initial data* $\boldsymbol{E}^{(0)}, \boldsymbol{n}^{(0)}, \boldsymbol{u}^{(0)}$ *and appropriate boundary conditions, we*